



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:11 PM UTC

PDB ID : 1KIU / pdb\_00001kiu  
Title : FimH adhesin Q133N mutant-FimC chaperone complex with methyl-alpha-D-mannose  
Authors : Hung, C.S.; Bouckaert, J.  
Deposited on : 2001-12-03  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

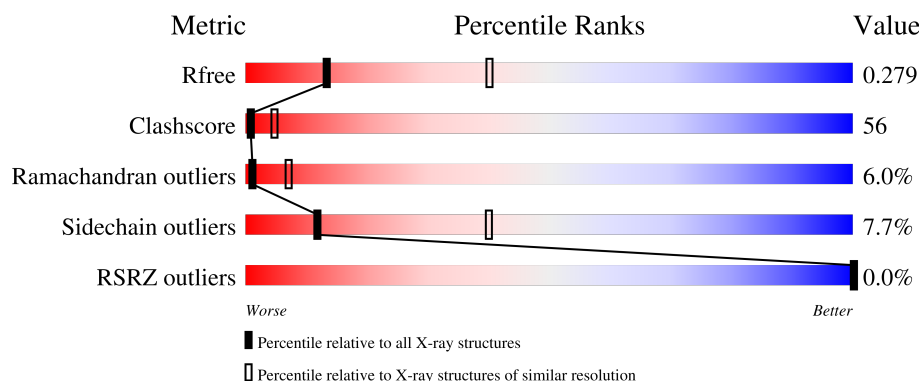
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



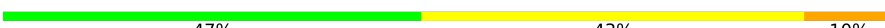
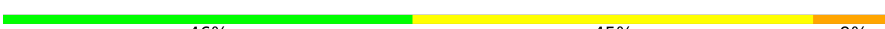
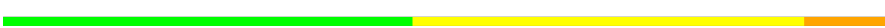
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2672 (3.00-3.00)                                      |
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |
| RSRZ outliers         | 180081                      | 2671 (3.00-3.00)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                       |
|-----|-------|--------|------------------------------------------------------------------------|
| 1   | A     | 205    | <div> <div>35%</div> <div>54%</div> <div>11%</div> <div>.</div> </div> |
| 1   | C     | 205    | <div> <div>33%</div> <div>56%</div> <div>10%</div> <div>.</div> </div> |
| 1   | E     | 205    | <div> <div>32%</div> <div>57%</div> <div>10%</div> <div>.</div> </div> |
| 1   | G     | 205    | <div> <div>35%</div> <div>54%</div> <div>11%</div> <div>.</div> </div> |
| 1   | I     | 205    | <div> <div>21%</div> <div>66%</div> <div>12%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                                |
|-----|-------|--------|-------------------------------------------------------------------------------------------------|
| 1   | K     | 205    |  22% 65% 12%  |
| 1   | M     | 205    |  23% 65% 12%  |
| 1   | O     | 205    |  22% 65% 12%  |
| 2   | B     | 279    |  47% 43% 10%  |
| 2   | D     | 279    |  46% 45% 9%   |
| 2   | F     | 279    |  46% 44% 10%  |
| 2   | H     | 279    |  46% 44% 9%   |
| 2   | J     | 279    |  30% 63% 6% • |
| 2   | L     | 279    |  29% 64% 6% • |
| 2   | N     | 279    |  30% 63% 6% • |
| 2   | P     | 279    |  30% 62% 6% • |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29657 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 CHAPERONE PROTEIN FimC.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | C     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | E     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | G     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | I     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | K     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | M     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | O     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| C     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| E     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| G     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| I     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| K     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| M     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| O     | 18      | VAL      | GLU    | conflict | UNP P31697 |

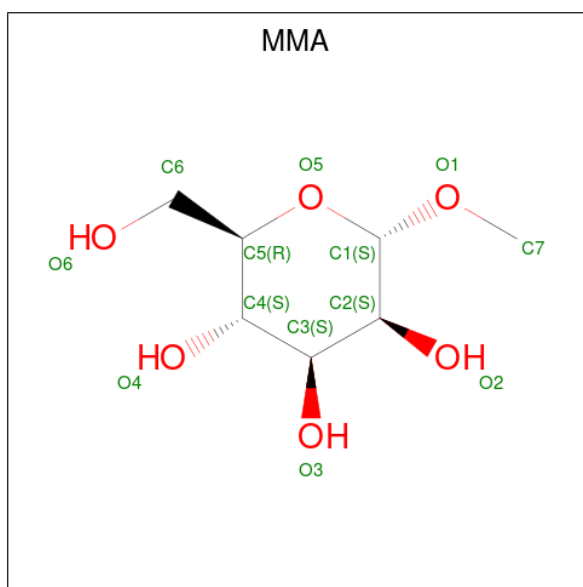
- Molecule 2 is a protein called FimH PROTEIN.

| Mol | Chain | Residues | Atoms         |           |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 2   | B     | 279      | Total<br>2051 | C<br>1296 | N<br>342 | O<br>409 | S<br>4 | 0       | 0       | 0     |
| 2   | D     | 279      | Total<br>2051 | C<br>1296 | N<br>342 | O<br>409 | S<br>4 | 0       | 0       | 0     |
| 2   | F     | 279      | Total<br>2051 | C<br>1296 | N<br>342 | O<br>409 | S<br>4 | 0       | 0       | 0     |
| 2   | H     | 279      | Total<br>2051 | C<br>1296 | N<br>342 | O<br>409 | S<br>4 | 0       | 0       | 0     |
| 2   | J     | 279      | Total<br>2051 | C<br>1296 | N<br>342 | O<br>409 | S<br>4 | 0       | 0       | 0     |
| 2   | L     | 279      | Total<br>2051 | C<br>1296 | N<br>342 | O<br>409 | S<br>4 | 0       | 0       | 0     |
| 2   | N     | 279      | Total<br>2051 | C<br>1296 | N<br>342 | O<br>409 | S<br>4 | 0       | 0       | 0     |
| 2   | P     | 279      | Total<br>2051 | C<br>1296 | N<br>342 | O<br>409 | S<br>4 | 0       | 0       | 0     |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | 133     | ASN      | GLN    | engineered mutation | UNP P08191 |
| D     | 133     | ASN      | GLN    | engineered mutation | UNP P08191 |
| F     | 133     | ASN      | GLN    | engineered mutation | UNP P08191 |
| H     | 133     | ASN      | GLN    | engineered mutation | UNP P08191 |
| J     | 133     | ASN      | GLN    | engineered mutation | UNP P08191 |
| L     | 133     | ASN      | GLN    | engineered mutation | UNP P08191 |
| N     | 133     | ASN      | GLN    | engineered mutation | UNP P08191 |
| P     | 133     | ASN      | GLN    | engineered mutation | UNP P08191 |

- Molecule 3 is methyl alpha-D-mannopyranoside (CCD ID: MMA) (formula: C<sub>7</sub>H<sub>14</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 7 | 6 |         |         |
| 3   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 7 | 6 |         |         |
| 3   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 7 | 6 |         |         |
| 3   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 7 | 6 |         |         |
| 3   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 7 | 6 |         |         |
| 3   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 7 | 6 |         |         |
| 3   | N     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 7 | 6 |         |         |
| 3   | P     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 7 | 6 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |
| 4   | B     | 58       | Total | O  | 0       | 0       |
|     |       |          | 58    | 58 |         |         |
| 4   | C     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 4   | D     | 54       | Total | O  | 0       | 0       |
|     |       |          | 54    | 54 |         |         |

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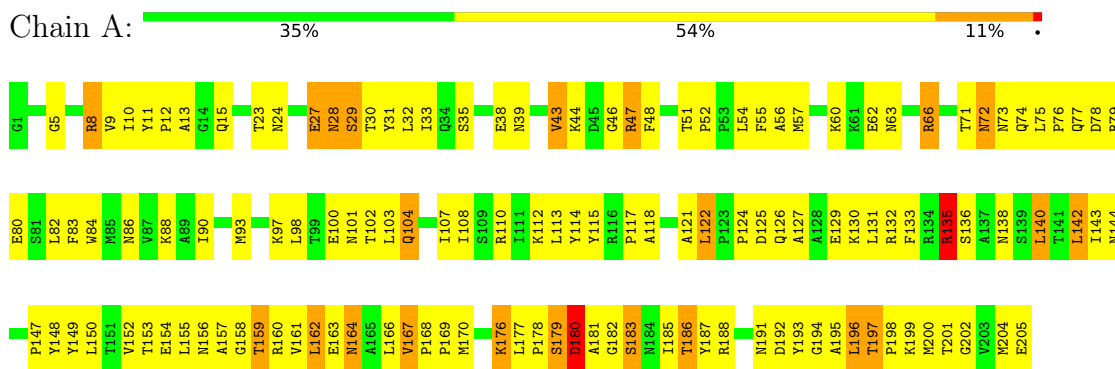
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | E     | 28       | Total<br>28 | O<br>28 | 0       | 0       |
| 4   | F     | 47       | Total<br>47 | O<br>47 | 0       | 0       |
| 4   | G     | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 4   | H     | 54       | Total<br>54 | O<br>54 | 0       | 0       |
| 4   | I     | 5        | Total<br>5  | O<br>5  | 0       | 0       |
| 4   | J     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 4   | K     | 8        | Total<br>8  | O<br>8  | 0       | 0       |
| 4   | L     | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 4   | M     | 5        | Total<br>5  | O<br>5  | 0       | 0       |
| 4   | N     | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 4   | O     | 7        | Total<br>7  | O<br>7  | 0       | 0       |
| 4   | P     | 14       | Total<br>14 | O<br>14 | 0       | 0       |

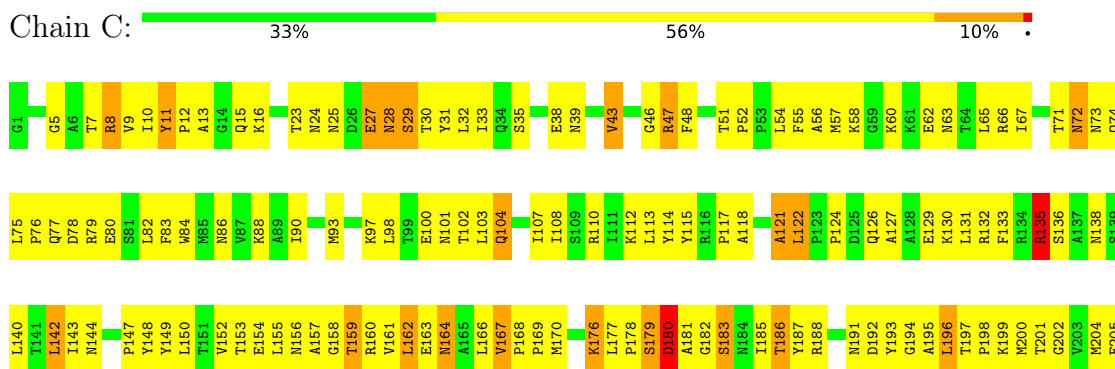
### 3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: CHAPERONE PROTEIN FimC



#### • Molecule 1: CHAPERONE PROTEIN FimC



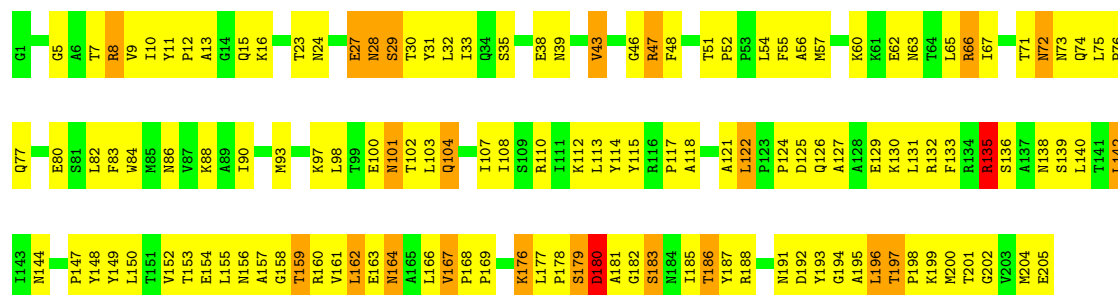
#### • Molecule 1: CHAPERONE PROTEIN FimC



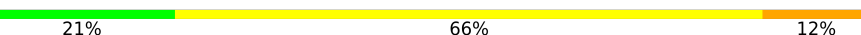


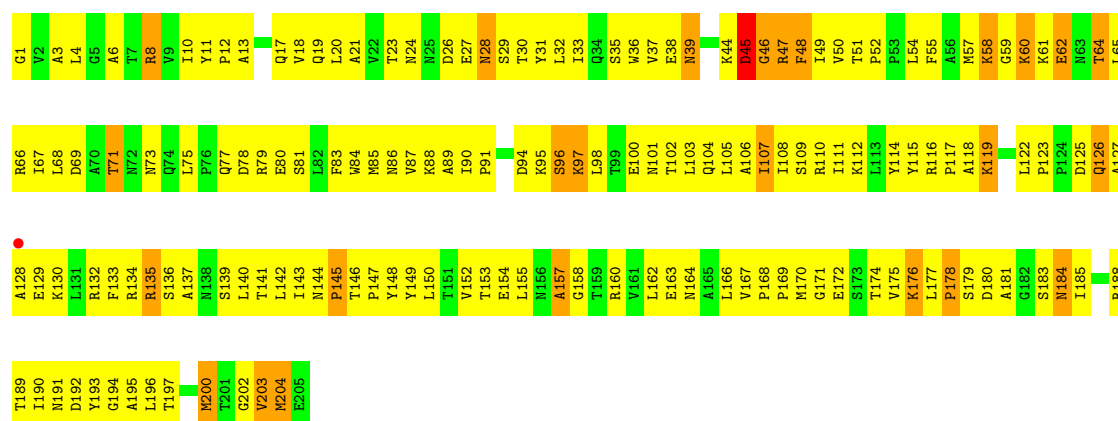
- Molecule 1: CHAPERONE PROTEIN FimC

Chain G: 

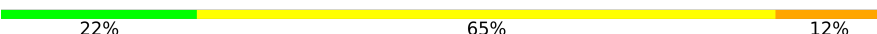


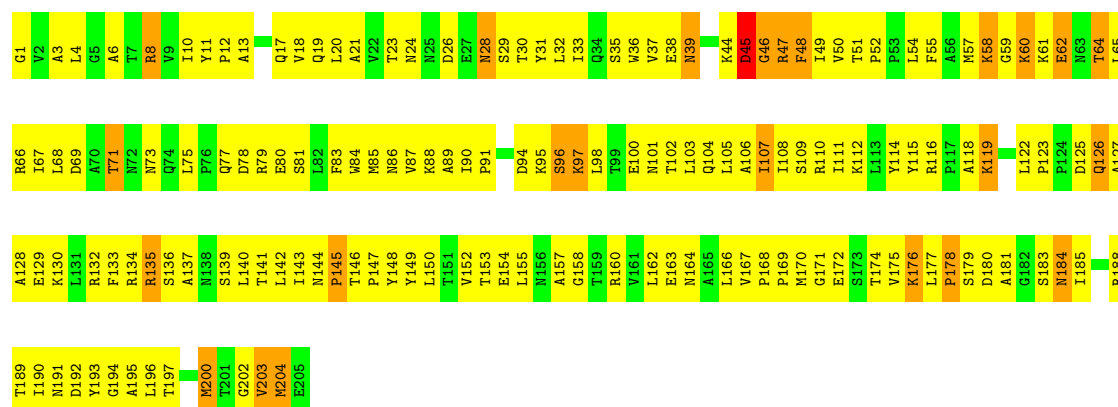
- Molecule 1: CHAPERONE PROTEIN FimC

Chain I: 

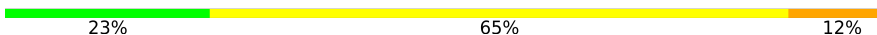


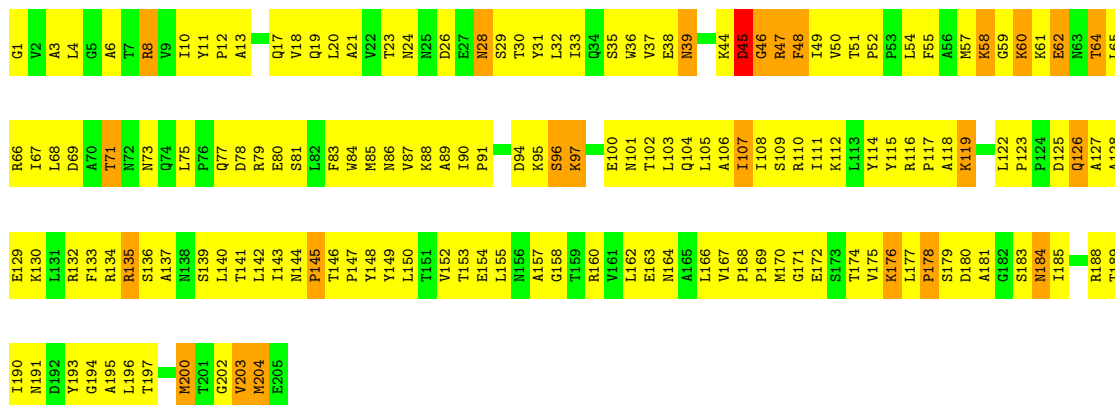
- Molecule 1: CHAPERONE PROTEIN FimC

Chain K: 



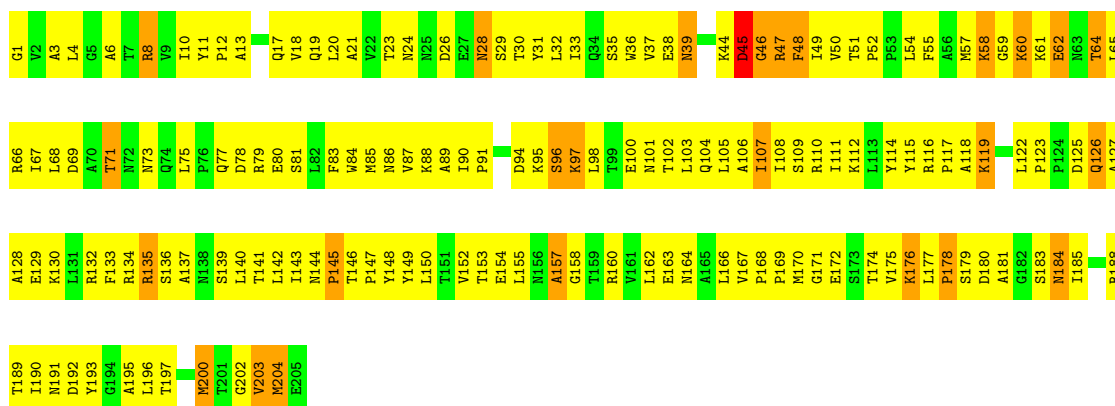
- Molecule 1: CHAPERONE PROTEIN FimC

Chain M: 



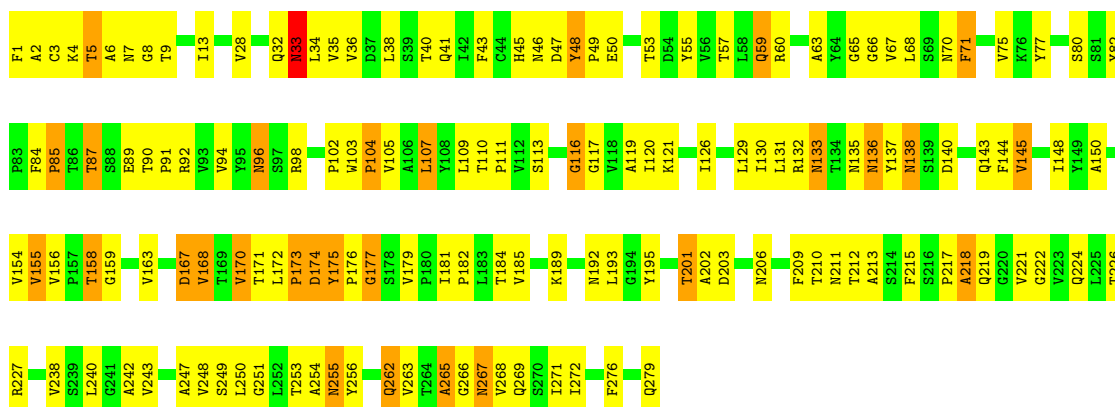
### • Molecule 1: CHAPERONE PROTEIN FimC

Chain O: 22% 65% 12%



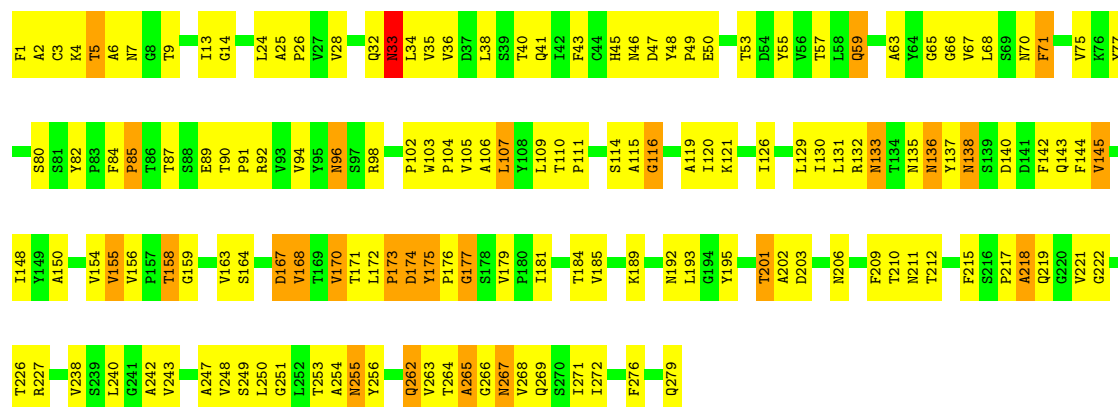
### • Molecule 2: FimH PROTEIN

Chain B: 47% 43% 10%



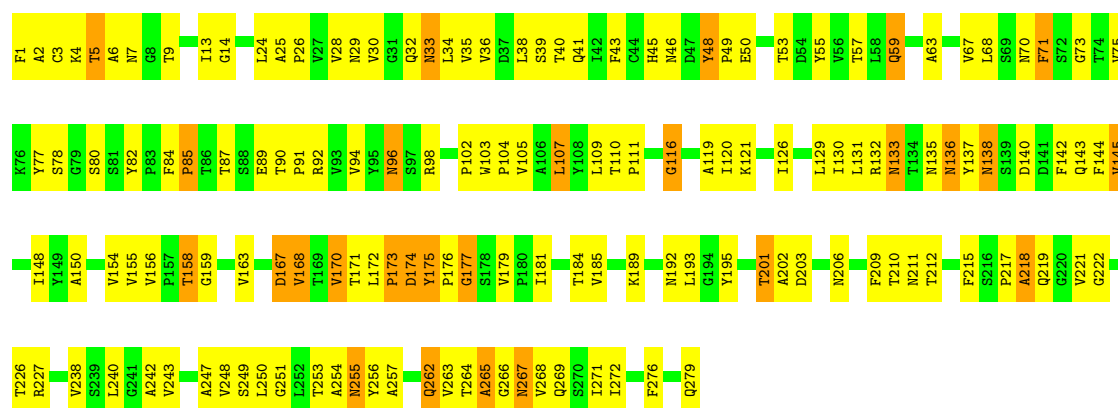
### • Molecule 2: FimH PROTEIN

Chain D: 46% 45% 9%



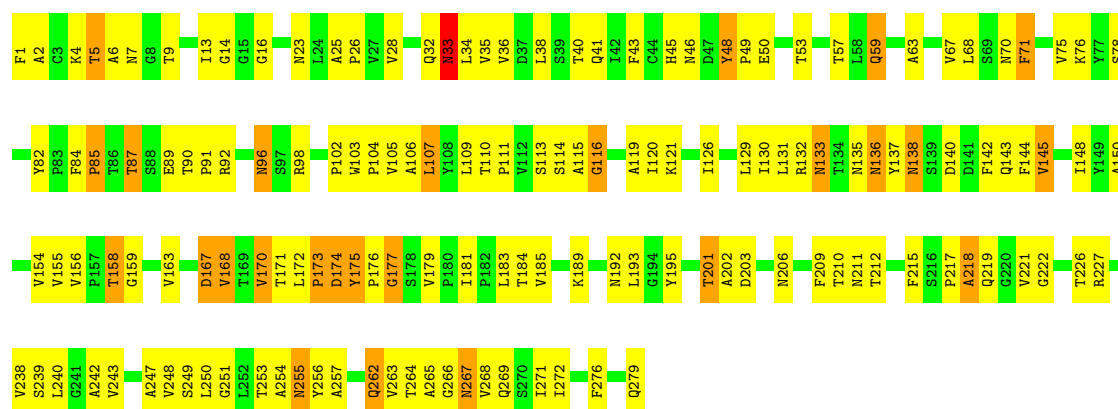
• Molecule 2: FimH PROTEIN

Chain F: 46% 44% 10%



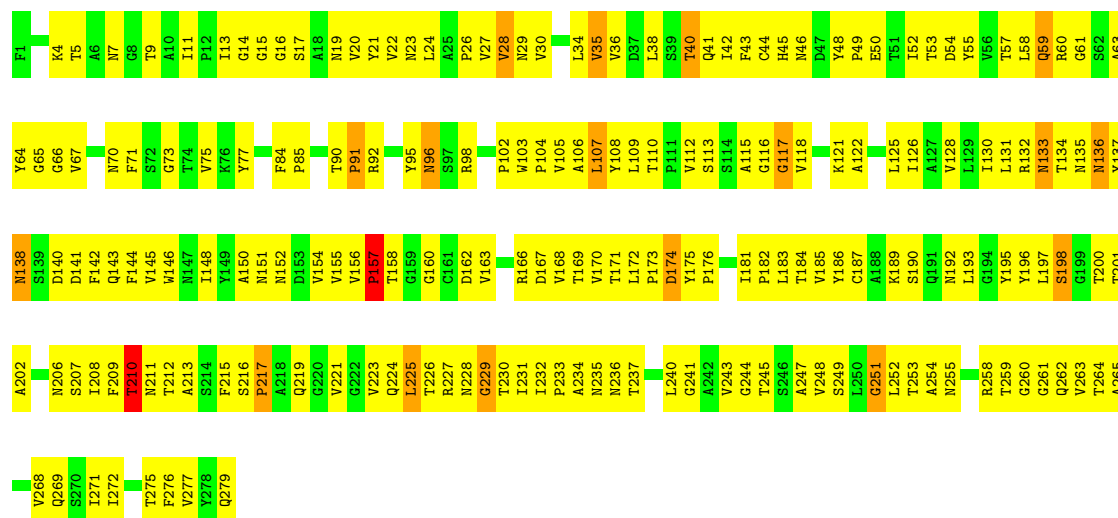
• Molecule 2: FimH PROTEIN

Chain H: 46% 44% 9%



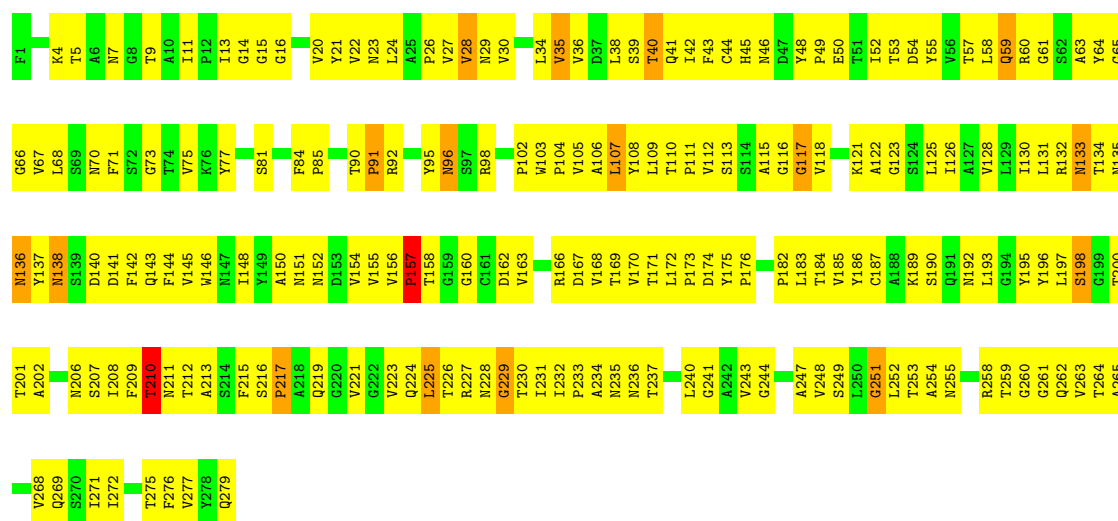
• Molecule 2: FimH PROTEIN

Chain J: 30% 63% 6%



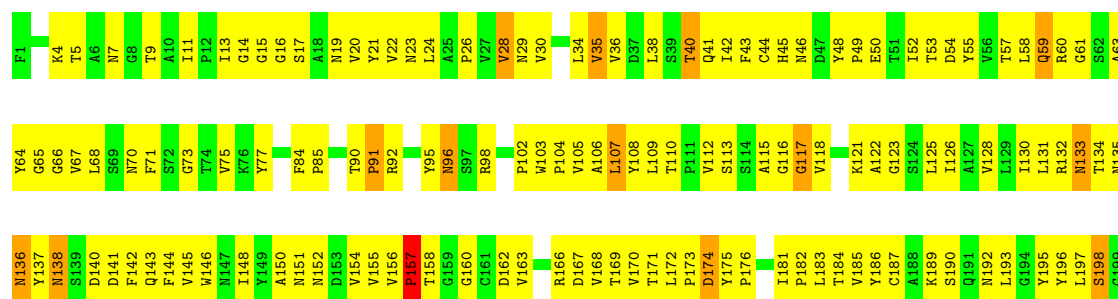
### • Molecule 2: FimH PROTEIN

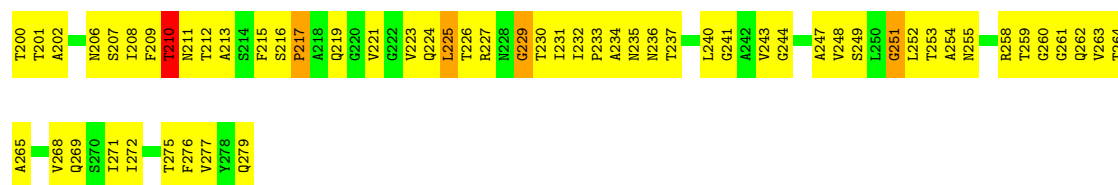
Chain L: 29% 64% 6% •



### • Molecule 2: FimH PROTEIN

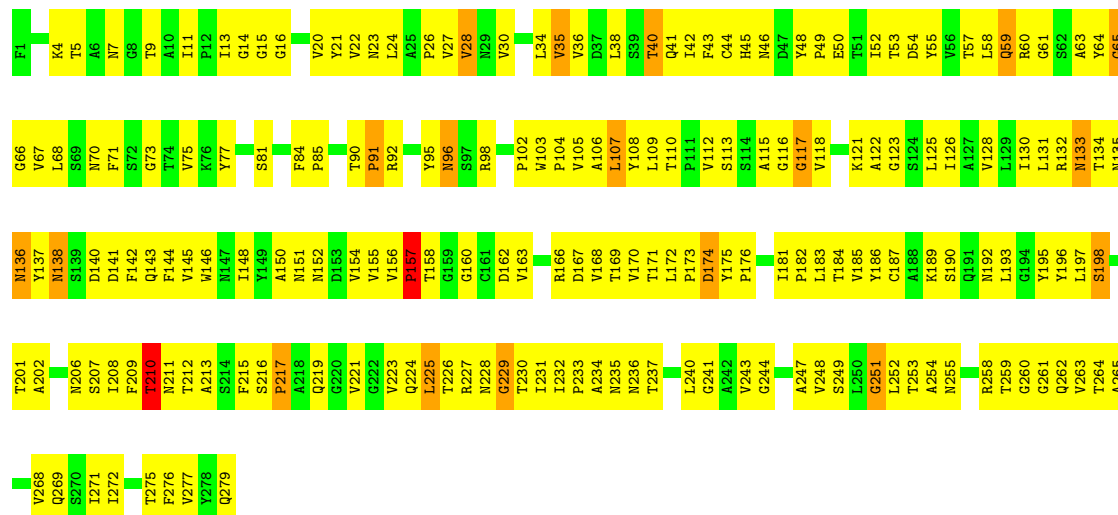
Chain N: 30% 63% 6% •





• Molecule 2: FimH PROTEIN

Chain P: 30% 62% 6% .



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 138.35Å 138.33Å 213.21Å<br>90.00° 89.98° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 45.00 – 3.00<br>45.00 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 89.1 (45.00-3.00)<br>89.2 (45.00-3.00)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | 0.09                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.31 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.236 , 0.278<br>0.236 , 0.279                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 7267 reflections (10.13%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 59.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.102                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 67.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | 0.457 for k,h,-l<br>0.457 for -k,-h,-l<br>0.447 for -h,-k,l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 29657                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 77.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

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     | 0.56         | 0/1625      | 1.10        | 10/2209 (0.5%)  |
| 1   | C     | 0.56         | 0/1625      | 1.10        | 12/2209 (0.5%)  |
| 1   | E     | 0.56         | 0/1625      | 1.10        | 13/2209 (0.6%)  |
| 1   | G     | 0.56         | 0/1625      | 1.10        | 13/2209 (0.6%)  |
| 1   | I     | 0.36         | 0/1625      | 0.82        | 2/2209 (0.1%)   |
| 1   | K     | 0.36         | 0/1625      | 0.82        | 1/2209 (0.0%)   |
| 1   | M     | 0.37         | 0/1625      | 0.82        | 1/2209 (0.0%)   |
| 1   | O     | 0.36         | 0/1625      | 0.82        | 2/2209 (0.1%)   |
| 2   | B     | 0.62         | 0/2096      | 1.09        | 9/2880 (0.3%)   |
| 2   | D     | 0.62         | 0/2096      | 1.09        | 9/2880 (0.3%)   |
| 2   | F     | 0.62         | 0/2096      | 1.09        | 9/2880 (0.3%)   |
| 2   | H     | 0.62         | 0/2096      | 1.09        | 10/2880 (0.3%)  |
| 2   | J     | 0.39         | 0/2096      | 0.87        | 2/2880 (0.1%)   |
| 2   | L     | 0.40         | 0/2096      | 0.87        | 2/2880 (0.1%)   |
| 2   | N     | 0.40         | 0/2096      | 0.87        | 2/2880 (0.1%)   |
| 2   | P     | 0.39         | 0/2096      | 0.87        | 2/2880 (0.1%)   |
| All | All   | 0.50         | 0/29768     | 0.98        | 99/40712 (0.2%) |

There are no bond length outliers.

All (99) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 157 | ALA  | N-CA-C | -9.89 | 102.49      | 112.97   |
| 1   | E     | 157 | ALA  | N-CA-C | -9.63 | 102.76      | 112.97   |
| 1   | C     | 157 | ALA  | N-CA-C | -9.58 | 102.81      | 112.97   |
| 1   | A     | 157 | ALA  | N-CA-C | -9.28 | 103.14      | 112.97   |
| 2   | D     | 103 | TRP  | CA-C-N | 8.22  | 130.12      | 119.84   |
| 2   | D     | 103 | TRP  | C-N-CA | 8.22  | 130.12      | 119.84   |
| 2   | H     | 103 | TRP  | CA-C-N | 8.19  | 130.08      | 119.84   |
| 2   | H     | 103 | TRP  | C-N-CA | 8.19  | 130.08      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | B     | 103 | TRP  | CA-C-N | 8.03 | 129.88      | 119.84   |
| 2   | B     | 103 | TRP  | C-N-CA | 8.03 | 129.88      | 119.84   |
| 2   | F     | 103 | TRP  | CA-C-N | 7.94 | 129.76      | 119.84   |
| 2   | F     | 103 | TRP  | C-N-CA | 7.94 | 129.76      | 119.84   |
| 1   | E     | 167 | VAL  | CA-C-N | 7.12 | 124.86      | 119.66   |
| 1   | E     | 167 | VAL  | C-N-CA | 7.12 | 124.86      | 119.66   |
| 1   | A     | 167 | VAL  | CA-C-N | 7.08 | 124.83      | 119.66   |
| 1   | A     | 167 | VAL  | C-N-CA | 7.08 | 124.83      | 119.66   |
| 2   | L     | 73  | GLY  | N-CA-C | 6.98 | 121.29      | 111.10   |
| 2   | N     | 73  | GLY  | N-CA-C | 6.95 | 121.25      | 111.10   |
| 2   | J     | 73  | GLY  | N-CA-C | 6.90 | 121.17      | 111.10   |
| 2   | P     | 73  | GLY  | N-CA-C | 6.86 | 121.12      | 111.10   |
| 1   | G     | 167 | VAL  | CA-C-N | 6.77 | 124.60      | 119.66   |
| 1   | G     | 167 | VAL  | C-N-CA | 6.77 | 124.60      | 119.66   |
| 1   | C     | 167 | VAL  | CA-C-N | 6.56 | 124.45      | 119.66   |
| 1   | C     | 167 | VAL  | C-N-CA | 6.56 | 124.45      | 119.66   |
| 2   | B     | 215 | PHE  | N-CA-C | 6.48 | 119.28      | 108.20   |
| 2   | D     | 215 | PHE  | N-CA-C | 6.47 | 119.26      | 108.20   |
| 2   | H     | 215 | PHE  | N-CA-C | 6.45 | 119.23      | 108.20   |
| 2   | F     | 215 | PHE  | N-CA-C | 6.43 | 119.20      | 108.20   |
| 2   | H     | 71  | PHE  | N-CA-C | 6.26 | 118.69      | 109.24   |
| 2   | D     | 33  | ASN  | N-CA-C | 6.17 | 119.46      | 109.40   |
| 2   | D     | 48  | TYR  | CA-C-N | 6.16 | 125.65      | 119.24   |
| 2   | D     | 48  | TYR  | C-N-CA | 6.16 | 125.65      | 119.24   |
| 1   | A     | 162 | LEU  | N-CA-C | 6.10 | 116.62      | 108.38   |
| 2   | H     | 48  | TYR  | CA-C-N | 6.10 | 125.59      | 119.24   |
| 2   | H     | 48  | TYR  | C-N-CA | 6.10 | 125.59      | 119.24   |
| 1   | C     | 162 | LEU  | N-CA-C | 6.09 | 116.60      | 108.38   |
| 2   | F     | 71  | PHE  | N-CA-C | 6.05 | 118.38      | 109.24   |
| 2   | D     | 71  | PHE  | N-CA-C | 6.02 | 118.33      | 109.24   |
| 1   | E     | 33  | ILE  | N-CA-C | 5.99 | 115.99      | 106.88   |
| 2   | F     | 33  | ASN  | N-CA-C | 5.99 | 119.16      | 109.40   |
| 2   | F     | 145 | VAL  | N-CA-C | 5.98 | 116.43      | 107.51   |
| 1   | G     | 162 | LEU  | N-CA-C | 5.96 | 116.43      | 108.38   |
| 2   | H     | 33  | ASN  | N-CA-C | 5.96 | 119.12      | 109.40   |
| 2   | B     | 71  | PHE  | N-CA-C | 5.90 | 118.16      | 109.24   |
| 2   | B     | 33  | ASN  | N-CA-C | 5.88 | 118.98      | 109.40   |
| 1   | E     | 162 | LEU  | N-CA-C | 5.85 | 116.28      | 108.38   |
| 2   | H     | 145 | VAL  | N-CA-C | 5.84 | 116.21      | 107.51   |
| 1   | G     | 33  | ILE  | N-CA-C | 5.65 | 115.47      | 106.88   |
| 1   | C     | 33  | ILE  | N-CA-C | 5.64 | 115.45      | 106.88   |
| 1   | A     | 33  | ILE  | N-CA-C | 5.64 | 115.45      | 106.88   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | D     | 47  | ASP  | N-CA-C | 5.64  | 118.62      | 111.69   |
| 2   | B     | 47  | ASP  | N-CA-C | 5.53  | 118.49      | 111.69   |
| 1   | A     | 135 | ARG  | N-CA-C | 5.48  | 118.45      | 110.17   |
| 2   | D     | 145 | VAL  | N-CA-C | 5.48  | 115.67      | 107.51   |
| 1   | I     | 97  | LYS  | N-CA-C | -5.45 | 105.89      | 112.54   |
| 1   | E     | 135 | ARG  | N-CA-C | 5.44  | 118.39      | 110.17   |
| 1   | C     | 135 | ARG  | N-CA-C | 5.44  | 118.38      | 110.17   |
| 1   | E     | 167 | VAL  | N-CA-C | 5.44  | 112.51      | 107.56   |
| 1   | G     | 135 | ARG  | N-CA-C | 5.42  | 118.36      | 110.17   |
| 2   | L     | 30  | VAL  | N-CA-C | 5.42  | 116.25      | 108.93   |
| 1   | A     | 166 | LEU  | CA-C-N | -5.42 | 118.92      | 122.60   |
| 1   | A     | 166 | LEU  | C-N-CA | -5.42 | 118.92      | 122.60   |
| 2   | J     | 30  | VAL  | N-CA-C | 5.42  | 116.24      | 108.93   |
| 1   | M     | 97  | LYS  | N-CA-C | -5.41 | 105.94      | 112.54   |
| 1   | O     | 97  | LYS  | N-CA-C | -5.39 | 105.96      | 112.54   |
| 1   | K     | 97  | LYS  | N-CA-C | -5.36 | 106.00      | 112.54   |
| 1   | A     | 197 | THR  | CA-C-N | 5.35  | 125.29      | 119.78   |
| 1   | A     | 197 | THR  | C-N-CA | 5.35  | 125.29      | 119.78   |
| 2   | B     | 48  | TYR  | CA-C-N | 5.35  | 125.42      | 119.32   |
| 2   | B     | 48  | TYR  | C-N-CA | 5.35  | 125.42      | 119.32   |
| 2   | H     | 16  | GLY  | N-CA-C | -5.34 | 103.46      | 110.29   |
| 1   | G     | 167 | VAL  | N-CA-C | 5.33  | 112.41      | 107.56   |
| 1   | C     | 11  | TYR  | CA-C-N | 5.33  | 126.50      | 119.84   |
| 1   | C     | 11  | TYR  | C-N-CA | 5.33  | 126.50      | 119.84   |
| 2   | N     | 30  | VAL  | N-CA-C | 5.31  | 116.10      | 108.93   |
| 1   | G     | 166 | LEU  | CA-C-N | -5.31 | 118.99      | 122.60   |
| 1   | G     | 166 | LEU  | C-N-CA | -5.31 | 118.99      | 122.60   |
| 2   | P     | 30  | VAL  | N-CA-C | 5.29  | 116.08      | 108.93   |
| 1   | C     | 166 | LEU  | CA-C-N | -5.29 | 119.00      | 122.60   |
| 1   | C     | 166 | LEU  | C-N-CA | -5.29 | 119.00      | 122.60   |
| 2   | B     | 145 | VAL  | N-CA-C | 5.24  | 115.32      | 107.51   |
| 1   | E     | 197 | THR  | CA-C-N | 5.23  | 125.17      | 119.78   |
| 1   | E     | 197 | THR  | C-N-CA | 5.23  | 125.17      | 119.78   |
| 1   | G     | 7   | THR  | N-CA-C | -5.22 | 105.78      | 113.61   |
| 2   | H     | 257 | ALA  | N-CA-C | -5.19 | 101.40      | 109.24   |
| 2   | F     | 257 | ALA  | N-CA-C | -5.17 | 101.43      | 109.24   |
| 2   | F     | 48  | TYR  | CA-C-N | 5.16  | 125.20      | 119.32   |
| 2   | F     | 48  | TYR  | C-N-CA | 5.16  | 125.20      | 119.32   |
| 1   | G     | 197 | THR  | CA-C-N | 5.14  | 125.07      | 119.78   |
| 1   | G     | 197 | THR  | C-N-CA | 5.14  | 125.07      | 119.78   |
| 1   | E     | 166 | LEU  | CA-C-N | -5.11 | 119.13      | 122.60   |
| 1   | E     | 166 | LEU  | C-N-CA | -5.11 | 119.13      | 122.60   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 167 | VAL  | N-CA-C | 5.07  | 112.17      | 107.56   |
| 1   | E     | 7   | THR  | N-CA-C | -5.07 | 106.00      | 113.61   |
| 1   | C     | 7   | THR  | N-CA-C | -5.04 | 106.04      | 113.61   |
| 1   | I     | 157 | ALA  | N-CA-C | -5.04 | 104.95      | 111.71   |
| 1   | E     | 101 | ASN  | N-CA-C | -5.04 | 101.10      | 109.46   |
| 1   | O     | 157 | ALA  | N-CA-C | -5.02 | 104.99      | 111.71   |
| 1   | G     | 101 | ASN  | N-CA-C | -5.02 | 101.13      | 109.46   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1596  | 0        | 1639     | 161     | 0            |
| 1   | C     | 1596  | 0        | 1639     | 169     | 0            |
| 1   | E     | 1596  | 0        | 1639     | 167     | 0            |
| 1   | G     | 1596  | 0        | 1639     | 158     | 0            |
| 1   | I     | 1596  | 0        | 1639     | 249     | 0            |
| 1   | K     | 1596  | 0        | 1639     | 253     | 0            |
| 1   | M     | 1596  | 0        | 1639     | 244     | 0            |
| 1   | O     | 1596  | 0        | 1639     | 250     | 0            |
| 2   | B     | 2051  | 0        | 2005     | 192     | 0            |
| 2   | D     | 2051  | 0        | 2005     | 183     | 0            |
| 2   | F     | 2051  | 0        | 2005     | 186     | 0            |
| 2   | H     | 2051  | 0        | 2005     | 192     | 0            |
| 2   | J     | 2051  | 0        | 2005     | 267     | 0            |
| 2   | L     | 2051  | 0        | 2005     | 272     | 0            |
| 2   | N     | 2051  | 0        | 2005     | 260     | 0            |
| 2   | P     | 2051  | 0        | 2005     | 270     | 0            |
| 3   | B     | 13    | 0        | 14       | 2       | 0            |
| 3   | D     | 13    | 0        | 14       | 0       | 0            |
| 3   | F     | 13    | 0        | 14       | 2       | 0            |
| 3   | H     | 13    | 0        | 14       | 3       | 0            |
| 3   | J     | 13    | 0        | 14       | 1       | 0            |
| 3   | L     | 13    | 0        | 14       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | N     | 13    | 0        | 14       | 1       | 0            |
| 3   | P     | 13    | 0        | 14       | 1       | 0            |
| 4   | A     | 19    | 0        | 0        | 4       | 0            |
| 4   | B     | 58    | 0        | 0        | 11      | 0            |
| 4   | C     | 20    | 0        | 0        | 9       | 0            |
| 4   | D     | 54    | 0        | 0        | 6       | 0            |
| 4   | E     | 28    | 0        | 0        | 9       | 0            |
| 4   | F     | 47    | 0        | 0        | 10      | 0            |
| 4   | G     | 20    | 0        | 0        | 3       | 0            |
| 4   | H     | 54    | 0        | 0        | 9       | 0            |
| 4   | I     | 5     | 0        | 0        | 2       | 0            |
| 4   | J     | 12    | 0        | 0        | 5       | 0            |
| 4   | K     | 8     | 0        | 0        | 2       | 0            |
| 4   | L     | 13    | 0        | 0        | 5       | 0            |
| 4   | M     | 5     | 0        | 0        | 0       | 0            |
| 4   | N     | 13    | 0        | 0        | 0       | 0            |
| 4   | O     | 7     | 0        | 0        | 2       | 0            |
| 4   | P     | 14    | 0        | 0        | 2       | 0            |
| All | All   | 29657 | 0        | 29264    | 3251    | 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 56.

All (3251) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 1:K:141:THR:HA  | 1:K:174:THR:CG2  | 1.33                     | 1.59              |
| 1:M:141:THR:HA  | 1:M:174:THR:CG2  | 1.32                     | 1.55              |
| 1:O:141:THR:HA  | 1:O:174:THR:CG2  | 1.33                     | 1.54              |
| 1:I:141:THR:HA  | 1:I:174:THR:CG2  | 1.33                     | 1.54              |
| 1:O:141:THR:HA  | 1:O:174:THR:HG21 | 1.26                     | 1.16              |
| 1:M:141:THR:CA  | 1:M:174:THR:HG22 | 1.76                     | 1.15              |
| 1:O:141:THR:CA  | 1:O:174:THR:HG22 | 1.76                     | 1.14              |
| 1:I:141:THR:CA  | 1:I:174:THR:HG22 | 1.76                     | 1.14              |
| 1:K:141:THR:CA  | 1:K:174:THR:HG22 | 1.76                     | 1.14              |
| 2:L:258:ARG:HD3 | 2:L:261:GLY:HA2  | 1.26                     | 1.14              |
| 1:K:141:THR:HA  | 1:K:174:THR:HG21 | 1.26                     | 1.13              |
| 1:I:141:THR:HA  | 1:I:174:THR:HG21 | 1.27                     | 1.12              |
| 1:I:141:THR:CA  | 1:I:174:THR:CG2  | 2.30                     | 1.10              |
| 1:M:141:THR:HA  | 1:M:174:THR:HG21 | 1.25                     | 1.10              |
| 1:M:141:THR:CA  | 1:M:174:THR:CG2  | 2.29                     | 1.10              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:141:THR:CA   | 1:K:174:THR:CG2  | 2.29                     | 1.10              |
| 1:O:141:THR:CA   | 1:O:174:THR:CG2  | 2.29                     | 1.10              |
| 2:P:258:ARG:HD3  | 2:P:261:GLY:HA2  | 1.27                     | 1.09              |
| 2:J:258:ARG:HD3  | 2:J:261:GLY:HA2  | 1.26                     | 1.08              |
| 2:N:258:ARG:HD3  | 2:N:261:GLY:HA2  | 1.26                     | 1.08              |
| 1:I:140:LEU:HG   | 1:I:177:LEU:HD22 | 1.37                     | 1.06              |
| 1:O:140:LEU:HG   | 1:O:177:LEU:HD22 | 1.38                     | 1.05              |
| 1:K:140:LEU:HG   | 1:K:177:LEU:HD22 | 1.37                     | 1.04              |
| 1:M:140:LEU:HG   | 1:M:177:LEU:HD22 | 1.38                     | 1.03              |
| 1:A:122:LEU:HD11 | 1:A:130:LYS:HE3  | 1.43                     | 1.00              |
| 1:G:122:LEU:HD11 | 1:G:130:LYS:HE3  | 1.41                     | 0.99              |
| 2:B:113:SER:HB3  | 2:P:81:SER:H     | 1.28                     | 0.99              |
| 2:J:210:THR:HG23 | 2:J:259:THR:HG21 | 1.45                     | 0.99              |
| 1:E:122:LEU:HD11 | 1:E:130:LYS:HE3  | 1.41                     | 0.98              |
| 2:L:210:THR:HG23 | 2:L:259:THR:HG21 | 1.44                     | 0.98              |
| 2:P:210:THR:HG23 | 2:P:259:THR:HG21 | 1.45                     | 0.98              |
| 1:E:160:ARG:HB2  | 1:E:180:ASP:HB2  | 1.46                     | 0.97              |
| 2:H:113:SER:HB3  | 2:L:81:SER:H     | 1.30                     | 0.97              |
| 1:C:122:LEU:HD11 | 1:C:130:LYS:HE3  | 1.43                     | 0.97              |
| 1:A:160:ARG:HB2  | 1:A:180:ASP:HB2  | 1.46                     | 0.96              |
| 2:H:173:PRO:HG3  | 2:H:179:VAL:HG13 | 1.48                     | 0.96              |
| 2:F:173:PRO:HG3  | 2:F:179:VAL:HG13 | 1.47                     | 0.95              |
| 2:B:173:PRO:HG3  | 2:B:179:VAL:HG13 | 1.48                     | 0.95              |
| 1:K:163:GLU:H    | 1:K:175:VAL:HG11 | 1.31                     | 0.95              |
| 1:O:97:LYS:HD2   | 2:P:170:VAL:HG21 | 1.49                     | 0.95              |
| 2:N:210:THR:HG23 | 2:N:259:THR:HG21 | 1.45                     | 0.95              |
| 1:G:160:ARG:HB2  | 1:G:180:ASP:HB2  | 1.46                     | 0.95              |
| 1:K:97:LYS:HD2   | 2:L:170:VAL:HG21 | 1.49                     | 0.95              |
| 2:D:173:PRO:HG3  | 2:D:179:VAL:HG13 | 1.47                     | 0.94              |
| 1:M:97:LYS:HD2   | 2:N:170:VAL:HG21 | 1.49                     | 0.94              |
| 1:I:163:GLU:H    | 1:I:175:VAL:HG11 | 1.31                     | 0.94              |
| 1:C:160:ARG:HB2  | 1:C:180:ASP:HB2  | 1.46                     | 0.94              |
| 1:I:141:THR:HA   | 1:I:174:THR:HG22 | 0.95                     | 0.94              |
| 2:D:211:ASN:HD21 | 2:D:269:GLN:H    | 1.14                     | 0.94              |
| 2:J:11:ILE:HG23  | 2:J:16:GLY:HA3   | 1.49                     | 0.94              |
| 1:I:97:LYS:HD2   | 2:J:170:VAL:HG21 | 1.49                     | 0.93              |
| 2:H:211:ASN:HD21 | 2:H:269:GLN:H    | 1.13                     | 0.93              |
| 1:K:141:THR:HA   | 1:K:174:THR:HG22 | 0.96                     | 0.93              |
| 1:O:163:GLU:H    | 1:O:175:VAL:HG11 | 1.30                     | 0.93              |
| 1:O:141:THR:HA   | 1:O:174:THR:HG22 | 0.96                     | 0.93              |
| 1:M:141:THR:HA   | 1:M:174:THR:HG22 | 0.96                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:163:GLU:H    | 1:M:175:VAL:HG11 | 1.31                     | 0.93              |
| 2:B:211:ASN:HD21 | 2:B:269:GLN:H    | 1.14                     | 0.92              |
| 2:P:11:ILE:HG23  | 2:P:16:GLY:HA3   | 1.49                     | 0.92              |
| 2:L:11:ILE:HG23  | 2:L:16:GLY:HA3   | 1.50                     | 0.91              |
| 2:N:11:ILE:HG23  | 2:N:16:GLY:HA3   | 1.49                     | 0.90              |
| 1:O:102:THR:HG22 | 2:P:170:VAL:HG22 | 1.54                     | 0.90              |
| 1:I:102:THR:HG22 | 2:J:170:VAL:HG22 | 1.53                     | 0.90              |
| 1:K:4:LEU:HD21   | 1:K:87:VAL:HG21  | 1.53                     | 0.89              |
| 2:F:211:ASN:HD21 | 2:F:269:GLN:H    | 1.14                     | 0.89              |
| 1:O:4:LEU:HD21   | 1:O:87:VAL:HG21  | 1.52                     | 0.89              |
| 1:M:102:THR:HG22 | 2:N:170:VAL:HG22 | 1.54                     | 0.89              |
| 1:I:4:LEU:HD21   | 1:I:87:VAL:HG21  | 1.53                     | 0.89              |
| 1:I:21:ALA:HA    | 1:I:64:THR:HA    | 1.55                     | 0.88              |
| 1:M:21:ALA:HA    | 1:M:64:THR:HA    | 1.55                     | 0.88              |
| 1:K:21:ALA:HA    | 1:K:64:THR:HA    | 1.54                     | 0.88              |
| 1:K:102:THR:HG22 | 2:L:170:VAL:HG22 | 1.54                     | 0.88              |
| 1:M:4:LEU:HD21   | 1:M:87:VAL:HG21  | 1.52                     | 0.87              |
| 1:O:21:ALA:HA    | 1:O:64:THR:HA    | 1.55                     | 0.86              |
| 2:B:67:VAL:HG21  | 2:B:126:ILE:HG23 | 1.57                     | 0.86              |
| 2:H:136:ASN:HD22 | 2:H:136:ASN:C    | 1.84                     | 0.86              |
| 2:F:254:ALA:C    | 2:F:255:ASN:HD22 | 1.84                     | 0.85              |
| 2:H:254:ALA:C    | 2:H:255:ASN:HD22 | 1.84                     | 0.85              |
| 2:B:254:ALA:C    | 2:B:255:ASN:HD22 | 1.85                     | 0.85              |
| 2:D:254:ALA:C    | 2:D:255:ASN:HD22 | 1.83                     | 0.85              |
| 2:F:136:ASN:HD22 | 2:F:136:ASN:C    | 1.83                     | 0.85              |
| 2:H:221:VAL:HG12 | 2:H:222:GLY:H    | 1.39                     | 0.85              |
| 2:F:67:VAL:HG21  | 2:F:126:ILE:HG23 | 1.58                     | 0.85              |
| 2:H:201:THR:HG21 | 2:H:206:ASN:HD22 | 1.42                     | 0.85              |
| 1:O:149:TYR:HB3  | 1:O:166:LEU:HD11 | 1.58                     | 0.85              |
| 2:P:60:ARG:HG2   | 2:P:61:GLY:H     | 1.40                     | 0.85              |
| 2:L:60:ARG:HG2   | 2:L:61:GLY:H     | 1.42                     | 0.84              |
| 2:B:136:ASN:C    | 2:B:136:ASN:HD22 | 1.83                     | 0.84              |
| 2:B:221:VAL:HG12 | 2:B:222:GLY:H    | 1.41                     | 0.84              |
| 1:K:149:TYR:HB3  | 1:K:166:LEU:HD11 | 1.57                     | 0.84              |
| 2:F:221:VAL:HG12 | 2:F:222:GLY:H    | 1.40                     | 0.84              |
| 2:N:60:ARG:HG2   | 2:N:61:GLY:H     | 1.40                     | 0.84              |
| 1:A:161:VAL:HG22 | 1:A:162:LEU:H    | 1.43                     | 0.84              |
| 2:J:227:ARG:HH11 | 2:J:232:ILE:HG12 | 1.43                     | 0.84              |
| 2:L:227:ARG:HH11 | 2:L:232:ILE:HG12 | 1.43                     | 0.83              |
| 1:I:149:TYR:HB3  | 1:I:166:LEU:HD11 | 1.58                     | 0.83              |
| 2:D:67:VAL:HG21  | 2:D:126:ILE:HG23 | 1.59                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:19:GLN:HG2   | 1:O:66:ARG:HG3   | 1.60                     | 0.83              |
| 1:C:112:LYS:HG3  | 4:C:209:HOH:O    | 1.77                     | 0.83              |
| 2:D:136:ASN:C    | 2:D:136:ASN:HD22 | 1.85                     | 0.83              |
| 2:J:28:VAL:O     | 2:J:157:PRO:HD2  | 1.79                     | 0.83              |
| 1:M:149:TYR:HB3  | 1:M:166:LEU:HD11 | 1.58                     | 0.83              |
| 2:D:138:ASN:C    | 2:D:138:ASN:HD22 | 1.85                     | 0.83              |
| 1:M:19:GLN:HG2   | 1:M:66:ARG:HG3   | 1.60                     | 0.83              |
| 2:P:213:ALA:HB2  | 2:P:269:GLN:HB2  | 1.60                     | 0.83              |
| 2:B:138:ASN:C    | 2:B:138:ASN:HD22 | 1.86                     | 0.82              |
| 2:J:60:ARG:HG2   | 2:J:61:GLY:H     | 1.42                     | 0.82              |
| 2:H:67:VAL:HG21  | 2:H:126:ILE:HG23 | 1.58                     | 0.82              |
| 2:J:213:ALA:HB2  | 2:J:269:GLN:HB2  | 1.60                     | 0.82              |
| 1:O:17:GLN:HB3   | 1:O:68:LEU:HD23  | 1.62                     | 0.82              |
| 2:D:201:THR:HG21 | 2:D:206:ASN:HD22 | 1.44                     | 0.82              |
| 2:D:221:VAL:HG12 | 2:D:222:GLY:H    | 1.41                     | 0.82              |
| 2:P:227:ARG:HH11 | 2:P:232:ILE:HG12 | 1.43                     | 0.82              |
| 2:H:138:ASN:C    | 2:H:138:ASN:HD22 | 1.87                     | 0.82              |
| 1:K:17:GLN:HB3   | 1:K:68:LEU:HD23  | 1.62                     | 0.82              |
| 1:E:161:VAL:HG22 | 1:E:162:LEU:H    | 1.44                     | 0.82              |
| 1:E:27:GLU:HG3   | 1:E:60:LYS:NZ    | 1.94                     | 0.82              |
| 1:I:17:GLN:HB3   | 1:I:68:LEU:HD23  | 1.62                     | 0.82              |
| 2:N:227:ARG:HH11 | 2:N:232:ILE:HG12 | 1.44                     | 0.82              |
| 2:P:28:VAL:O     | 2:P:157:PRO:HD2  | 1.80                     | 0.82              |
| 2:F:138:ASN:HD22 | 2:F:138:ASN:C    | 1.87                     | 0.81              |
| 1:G:27:GLU:HG3   | 1:G:60:LYS:NZ    | 1.95                     | 0.81              |
| 1:I:19:GLN:HG2   | 1:I:66:ARG:HG3   | 1.60                     | 0.81              |
| 2:L:213:ALA:HB2  | 2:L:269:GLN:HB2  | 1.61                     | 0.81              |
| 1:M:17:GLN:HB3   | 1:M:68:LEU:HD23  | 1.62                     | 0.81              |
| 1:C:161:VAL:HG22 | 1:C:162:LEU:H    | 1.43                     | 0.81              |
| 2:L:116:GLY:HA2  | 2:L:189:LYS:HG3  | 1.62                     | 0.81              |
| 1:C:27:GLU:HG3   | 1:C:60:LYS:NZ    | 1.96                     | 0.81              |
| 1:K:88:LYS:HG3   | 1:K:108:ILE:HG12 | 1.62                     | 0.81              |
| 2:N:28:VAL:O     | 2:N:157:PRO:HD2  | 1.80                     | 0.81              |
| 2:N:213:ALA:HB2  | 2:N:269:GLN:HB2  | 1.61                     | 0.81              |
| 1:I:88:LYS:HG3   | 1:I:108:ILE:HG12 | 1.62                     | 0.81              |
| 1:M:141:THR:CA   | 1:M:174:THR:HG21 | 2.04                     | 0.81              |
| 2:B:32:GLN:O     | 2:B:110:THR:HG23 | 1.81                     | 0.80              |
| 2:L:28:VAL:O     | 2:L:157:PRO:HD2  | 1.80                     | 0.80              |
| 2:F:201:THR:HG21 | 2:F:206:ASN:HD22 | 1.44                     | 0.80              |
| 1:A:27:GLU:HG3   | 1:A:60:LYS:HZ2   | 1.43                     | 0.80              |
| 2:B:201:THR:HG21 | 2:B:206:ASN:HD22 | 1.46                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:240:LEU:HD11 | 2:F:250:LEU:CD2  | 2.10                     | 0.80              |
| 2:B:59:GLN:HG2   | 2:B:132:ARG:HD2  | 1.64                     | 0.80              |
| 2:H:255:ASN:HD22 | 2:H:255:ASN:N    | 1.76                     | 0.80              |
| 1:K:19:GLN:HG2   | 1:K:66:ARG:HG3   | 1.61                     | 0.80              |
| 2:N:116:GLY:HA2  | 2:N:189:LYS:HG3  | 1.62                     | 0.80              |
| 2:P:264:THR:HG22 | 2:P:265:ALA:H    | 1.46                     | 0.80              |
| 1:A:27:GLU:HG3   | 1:A:60:LYS:NZ    | 1.95                     | 0.80              |
| 2:J:264:THR:HG22 | 2:J:265:ALA:H    | 1.47                     | 0.80              |
| 2:H:240:LEU:HD11 | 2:H:250:LEU:CD2  | 2.11                     | 0.80              |
| 1:M:88:LYS:HG3   | 1:M:108:ILE:HG12 | 1.62                     | 0.80              |
| 2:D:218:ALA:HB2  | 2:D:266:GLY:C    | 2.07                     | 0.80              |
| 2:N:227:ARG:HG3  | 2:N:230:THR:HB   | 1.64                     | 0.80              |
| 1:G:13:ALA:HB3   | 1:G:118:ALA:H    | 1.46                     | 0.79              |
| 1:G:161:VAL:HG22 | 1:G:162:LEU:H    | 1.45                     | 0.79              |
| 1:O:88:LYS:HG3   | 1:O:108:ILE:HG12 | 1.62                     | 0.79              |
| 2:F:120:ILE:HB   | 2:F:154:VAL:HB   | 1.64                     | 0.79              |
| 1:I:190:ILE:HD12 | 2:J:279:GLN:HG2  | 1.64                     | 0.79              |
| 2:J:116:GLY:HA2  | 2:J:189:LYS:HG3  | 1.62                     | 0.79              |
| 2:B:240:LEU:HD11 | 2:B:250:LEU:CD2  | 2.12                     | 0.79              |
| 2:H:120:ILE:HB   | 2:H:154:VAL:HB   | 1.64                     | 0.79              |
| 2:H:218:ALA:HB2  | 2:H:266:GLY:C    | 2.08                     | 0.79              |
| 2:F:218:ALA:HB2  | 2:F:266:GLY:C    | 2.07                     | 0.79              |
| 2:P:116:GLY:HA2  | 2:P:189:LYS:HG3  | 1.61                     | 0.79              |
| 2:B:255:ASN:HD22 | 2:B:255:ASN:N    | 1.75                     | 0.79              |
| 2:H:32:GLN:O     | 2:H:110:THR:HG23 | 1.82                     | 0.79              |
| 1:K:190:ILE:HD12 | 2:L:279:GLN:HG2  | 1.63                     | 0.79              |
| 1:E:13:ALA:HB3   | 1:E:118:ALA:H    | 1.47                     | 0.79              |
| 2:N:264:THR:HG22 | 2:N:265:ALA:H    | 1.46                     | 0.79              |
| 2:D:240:LEU:HD11 | 2:D:250:LEU:CD2  | 2.13                     | 0.79              |
| 2:D:32:GLN:O     | 2:D:110:THR:HG23 | 1.83                     | 0.79              |
| 2:L:227:ARG:HG3  | 2:L:230:THR:HB   | 1.64                     | 0.79              |
| 2:F:255:ASN:HD22 | 2:F:255:ASN:N    | 1.77                     | 0.79              |
| 1:G:132:ARG:HG2  | 4:G:215:HOH:O    | 1.83                     | 0.79              |
| 2:P:227:ARG:HG3  | 2:P:230:THR:HB   | 1.65                     | 0.79              |
| 2:H:59:GLN:HG2   | 2:H:132:ARG:HD2  | 1.66                     | 0.78              |
| 1:M:190:ILE:HD12 | 2:N:279:GLN:HG2  | 1.64                     | 0.78              |
| 1:G:176:LYS:H    | 1:G:176:LYS:HD2  | 1.48                     | 0.78              |
| 1:K:157:ALA:CB   | 1:K:181:ALA:HB1  | 2.13                     | 0.78              |
| 1:K:69:ASP:OD1   | 1:K:71:THR:HG22  | 1.84                     | 0.78              |
| 1:O:157:ALA:CB   | 1:O:181:ALA:HB1  | 2.14                     | 0.78              |
| 2:D:59:GLN:HG2   | 2:D:132:ARG:HD2  | 1.65                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:211:ASN:ND2  | 2:H:269:GLN:H    | 1.81                     | 0.78              |
| 1:M:157:ALA:CB   | 1:M:181:ALA:HB1  | 2.14                     | 0.78              |
| 1:A:176:LYS:HD2  | 1:A:176:LYS:H    | 1.48                     | 0.78              |
| 1:A:132:ARG:HG2  | 4:A:215:HOH:O    | 1.82                     | 0.78              |
| 1:K:141:THR:CA   | 1:K:174:THR:HG21 | 2.06                     | 0.78              |
| 1:M:69:ASP:OD1   | 1:M:71:THR:HG22  | 1.84                     | 0.78              |
| 1:O:69:ASP:OD1   | 1:O:71:THR:HG22  | 1.84                     | 0.78              |
| 1:C:13:ALA:HB3   | 1:C:118:ALA:H    | 1.48                     | 0.78              |
| 2:J:227:ARG:HG3  | 2:J:230:THR:HB   | 1.65                     | 0.78              |
| 1:C:136:SER:O    | 1:C:177:LEU:HD23 | 1.85                     | 0.77              |
| 2:F:32:GLN:O     | 2:F:110:THR:HG23 | 1.84                     | 0.77              |
| 2:F:59:GLN:HG2   | 2:F:132:ARG:HD2  | 1.67                     | 0.77              |
| 2:L:264:THR:HG22 | 2:L:265:ALA:H    | 1.46                     | 0.77              |
| 1:I:157:ALA:CB   | 1:I:181:ALA:HB1  | 2.14                     | 0.77              |
| 2:P:96:ASN:N     | 2:P:96:ASN:HD22  | 1.81                     | 0.77              |
| 2:P:226:THR:HG22 | 2:P:255:ASN:HD21 | 1.49                     | 0.77              |
| 2:B:218:ALA:HB2  | 2:B:266:GLY:C    | 2.08                     | 0.77              |
| 1:C:140:LEU:HD12 | 1:C:177:LEU:HD13 | 1.66                     | 0.77              |
| 1:E:132:ARG:HG2  | 4:E:210:HOH:O    | 1.83                     | 0.77              |
| 1:E:176:LYS:H    | 1:E:176:LYS:HD2  | 1.48                     | 0.77              |
| 2:L:96:ASN:HD22  | 2:L:96:ASN:N     | 1.82                     | 0.77              |
| 1:I:142:LEU:O    | 1:I:172:GLU:HB2  | 1.84                     | 0.77              |
| 2:J:96:ASN:HD22  | 2:J:96:ASN:N     | 1.81                     | 0.77              |
| 1:O:153:THR:HG21 | 1:O:196:LEU:HD22 | 1.67                     | 0.77              |
| 1:O:190:ILE:HD12 | 2:P:279:GLN:HG2  | 1.64                     | 0.77              |
| 1:G:140:LEU:HD12 | 1:G:177:LEU:HD13 | 1.67                     | 0.77              |
| 1:K:160:ARG:HD3  | 1:K:180:ASP:HB2  | 1.66                     | 0.77              |
| 2:N:226:THR:HG22 | 2:N:255:ASN:HD21 | 1.49                     | 0.77              |
| 2:B:120:ILE:HB   | 2:B:154:VAL:HB   | 1.65                     | 0.77              |
| 1:I:160:ARG:HD3  | 1:I:180:ASP:HB2  | 1.67                     | 0.77              |
| 2:F:211:ASN:ND2  | 2:F:269:GLN:H    | 1.83                     | 0.77              |
| 1:M:160:ARG:HD3  | 1:M:180:ASP:HB2  | 1.66                     | 0.77              |
| 1:A:13:ALA:HB3   | 1:A:118:ALA:H    | 1.49                     | 0.76              |
| 2:D:120:ILE:HB   | 2:D:154:VAL:HB   | 1.65                     | 0.76              |
| 2:B:211:ASN:ND2  | 2:B:269:GLN:H    | 1.83                     | 0.76              |
| 1:I:69:ASP:OD1   | 1:I:71:THR:HG22  | 1.84                     | 0.76              |
| 2:D:211:ASN:ND2  | 2:D:269:GLN:H    | 1.83                     | 0.76              |
| 1:O:142:LEU:O    | 1:O:172:GLU:HB2  | 1.85                     | 0.76              |
| 2:L:226:THR:HG22 | 2:L:255:ASN:HD21 | 1.49                     | 0.76              |
| 2:D:172:LEU:O    | 2:D:173:PRO:C    | 2.28                     | 0.76              |
| 1:G:16:LYS:HB3   | 4:G:210:HOH:O    | 1.86                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:141:THR:CA   | 1:I:174:THR:HG21 | 2.06                     | 0.76              |
| 1:E:140:LEU:HD12 | 1:E:177:LEU:HD13 | 1.67                     | 0.76              |
| 2:H:184:THR:HB   | 2:H:247:ALA:HB1  | 1.67                     | 0.76              |
| 1:M:153:THR:HG21 | 1:M:196:LEU:HD22 | 1.67                     | 0.76              |
| 1:I:8:ARG:HB3    | 1:I:8:ARG:HH11   | 1.50                     | 0.76              |
| 1:I:28:ASN:H     | 1:I:28:ASN:HD22  | 1.34                     | 0.76              |
| 1:K:142:LEU:O    | 1:K:172:GLU:HB2  | 1.85                     | 0.76              |
| 1:I:153:THR:HG21 | 1:I:196:LEU:HD22 | 1.67                     | 0.76              |
| 1:K:153:THR:HG21 | 1:K:196:LEU:HD22 | 1.67                     | 0.76              |
| 1:M:142:LEU:O    | 1:M:172:GLU:HB2  | 1.86                     | 0.76              |
| 1:G:136:SER:O    | 1:G:177:LEU:HD23 | 1.86                     | 0.75              |
| 2:J:213:ALA:HB1  | 4:J:610:HOH:O    | 1.85                     | 0.75              |
| 2:N:96:ASN:HD22  | 2:N:96:ASN:N     | 1.82                     | 0.75              |
| 1:O:28:ASN:HD22  | 1:O:28:ASN:H     | 1.34                     | 0.75              |
| 2:B:217:PRO:O    | 2:B:219:GLN:N    | 2.20                     | 0.75              |
| 1:C:176:LYS:H    | 1:C:176:LYS:HD2  | 1.50                     | 0.75              |
| 1:A:136:SER:O    | 1:A:177:LEU:HD23 | 1.86                     | 0.75              |
| 1:K:145:PRO:HA   | 1:K:170:MET:HA   | 1.68                     | 0.75              |
| 1:M:8:ARG:HB3    | 1:M:8:ARG:HH11   | 1.52                     | 0.75              |
| 1:I:145:PRO:HA   | 1:I:170:MET:HA   | 1.67                     | 0.75              |
| 1:O:160:ARG:HD3  | 1:O:180:ASP:HB2  | 1.67                     | 0.75              |
| 1:K:28:ASN:H     | 1:K:28:ASN:HD22  | 1.35                     | 0.75              |
| 1:A:140:LEU:HD12 | 1:A:177:LEU:HD13 | 1.69                     | 0.75              |
| 1:G:52:PRO:HG2   | 1:G:55:PHE:CD1   | 2.22                     | 0.75              |
| 2:J:226:THR:HG22 | 2:J:255:ASN:HD21 | 1.50                     | 0.75              |
| 2:B:120:ILE:HD13 | 2:B:126:ILE:HD12 | 1.68                     | 0.74              |
| 2:F:120:ILE:HD13 | 2:F:126:ILE:HD12 | 1.69                     | 0.74              |
| 2:H:120:ILE:HD13 | 2:H:126:ILE:HD12 | 1.69                     | 0.74              |
| 1:M:28:ASN:HD22  | 1:M:28:ASN:H     | 1.35                     | 0.74              |
| 2:N:172:LEU:N    | 2:N:173:PRO:HD2  | 2.01                     | 0.74              |
| 1:O:8:ARG:HB3    | 1:O:8:ARG:HH11   | 1.52                     | 0.74              |
| 1:O:71:THR:HG23  | 1:O:73:ASN:H     | 1.52                     | 0.74              |
| 1:C:194:GLY:O    | 2:D:158:THR:HG21 | 1.87                     | 0.74              |
| 1:A:52:PRO:HG2   | 1:A:55:PHE:CD1   | 2.22                     | 0.74              |
| 1:A:86:ASN:HD21  | 1:A:110:ARG:HE   | 1.35                     | 0.74              |
| 2:B:172:LEU:O    | 2:B:173:PRO:C    | 2.30                     | 0.74              |
| 1:E:86:ASN:HD21  | 1:E:110:ARG:HE   | 1.35                     | 0.74              |
| 1:I:71:THR:HG23  | 1:I:73:ASN:H     | 1.51                     | 0.74              |
| 1:K:8:ARG:HB3    | 1:K:8:ARG:HH11   | 1.51                     | 0.74              |
| 2:P:27:VAL:HG12  | 4:P:616:HOH:O    | 1.88                     | 0.74              |
| 2:L:172:LEU:N    | 2:L:173:PRO:HD2  | 2.02                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:184:THR:HB   | 2:B:247:ALA:HB1  | 1.69                     | 0.74              |
| 1:C:52:PRO:HG2   | 1:C:55:PHE:CD1   | 2.22                     | 0.74              |
| 2:D:255:ASN:HD22 | 2:D:255:ASN:N    | 1.77                     | 0.74              |
| 2:F:184:THR:HB   | 2:F:247:ALA:HB1  | 1.69                     | 0.74              |
| 2:D:184:THR:HB   | 2:D:247:ALA:HB1  | 1.69                     | 0.74              |
| 2:N:135:ASN:HD21 | 2:N:138:ASN:HD21 | 1.34                     | 0.74              |
| 2:N:171:THR:C    | 2:N:173:PRO:HD2  | 2.13                     | 0.74              |
| 2:J:172:LEU:N    | 2:J:173:PRO:HD2  | 2.02                     | 0.74              |
| 1:M:71:THR:HG23  | 1:M:73:ASN:H     | 1.52                     | 0.74              |
| 1:G:88:LYS:HB2   | 1:G:108:ILE:HG12 | 1.70                     | 0.74              |
| 1:M:145:PRO:HA   | 1:M:170:MET:HA   | 1.68                     | 0.74              |
| 2:D:217:PRO:O    | 2:D:219:GLN:N    | 2.21                     | 0.73              |
| 1:E:136:SER:O    | 1:E:177:LEU:HD23 | 1.85                     | 0.73              |
| 2:J:5:THR:HG22   | 2:J:9:THR:O      | 1.88                     | 0.73              |
| 1:I:102:THR:HA   | 2:J:170:VAL:HA   | 1.70                     | 0.73              |
| 1:K:71:THR:HG23  | 1:K:73:ASN:H     | 1.52                     | 0.73              |
| 2:N:226:THR:HG22 | 2:N:253:THR:HB   | 1.70                     | 0.73              |
| 1:A:129:GLU:HA   | 1:A:200:MET:HE1  | 1.70                     | 0.73              |
| 2:F:217:PRO:O    | 2:F:219:GLN:N    | 2.21                     | 0.73              |
| 1:K:157:ALA:HB3  | 1:K:181:ALA:HB1  | 1.70                     | 0.73              |
| 2:J:226:THR:HG22 | 2:J:253:THR:HB   | 1.69                     | 0.73              |
| 1:K:102:THR:HA   | 2:L:170:VAL:HA   | 1.71                     | 0.73              |
| 2:N:5:THR:HG22   | 2:N:9:THR:O      | 1.89                     | 0.73              |
| 2:P:226:THR:HG22 | 2:P:253:THR:HB   | 1.71                     | 0.73              |
| 1:A:88:LYS:HB2   | 1:A:108:ILE:HG12 | 1.69                     | 0.73              |
| 2:P:171:THR:C    | 2:P:173:PRO:HD2  | 2.13                     | 0.73              |
| 2:H:172:LEU:O    | 2:H:173:PRO:C    | 2.30                     | 0.73              |
| 2:J:227:ARG:NH1  | 2:J:232:ILE:HG12 | 2.03                     | 0.73              |
| 1:K:132:ARG:HG2  | 1:K:203:VAL:O    | 1.89                     | 0.73              |
| 2:L:224:GLN:HG2  | 2:L:231:ILE:HD13 | 1.70                     | 0.73              |
| 2:P:227:ARG:NH1  | 2:P:232:ILE:HG12 | 2.03                     | 0.73              |
| 1:E:129:GLU:HA   | 1:E:200:MET:HE1  | 1.71                     | 0.73              |
| 2:J:171:THR:C    | 2:J:173:PRO:HD2  | 2.14                     | 0.73              |
| 1:O:145:PRO:HA   | 1:O:170:MET:HA   | 1.68                     | 0.73              |
| 2:P:135:ASN:HD21 | 2:P:138:ASN:HD21 | 1.33                     | 0.73              |
| 2:H:217:PRO:O    | 2:H:219:GLN:N    | 2.22                     | 0.73              |
| 2:L:227:ARG:NH1  | 2:L:232:ILE:HG12 | 2.03                     | 0.73              |
| 1:M:157:ALA:HB3  | 1:M:181:ALA:HB1  | 1.71                     | 0.73              |
| 1:E:52:PRO:HG2   | 1:E:55:PHE:CD1   | 2.24                     | 0.73              |
| 2:L:5:THR:HG22   | 2:L:9:THR:O      | 1.89                     | 0.73              |
| 2:L:219:GLN:HE21 | 2:L:262:GLN:HG2  | 1.54                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:102:THR:HA   | 2:N:170:VAL:HA   | 1.71                     | 0.72              |
| 2:P:172:LEU:N    | 2:P:173:PRO:HD2  | 2.02                     | 0.72              |
| 1:E:194:GLY:O    | 2:F:158:THR:HG21 | 1.90                     | 0.72              |
| 2:N:224:GLN:HG2  | 2:N:231:ILE:HD13 | 1.71                     | 0.72              |
| 2:N:227:ARG:NH1  | 2:N:232:ILE:HG12 | 2.04                     | 0.72              |
| 1:E:88:LYS:HB2   | 1:E:108:ILE:HG12 | 1.72                     | 0.72              |
| 2:L:171:THR:C    | 2:L:173:PRO:HD2  | 2.13                     | 0.72              |
| 2:L:226:THR:HG22 | 2:L:253:THR:HB   | 1.70                     | 0.72              |
| 2:P:219:GLN:HE21 | 2:P:262:GLN:HG2  | 1.55                     | 0.72              |
| 2:P:5:THR:HG22   | 2:P:9:THR:O      | 1.89                     | 0.72              |
| 1:C:88:LYS:HB2   | 1:C:108:ILE:HG12 | 1.70                     | 0.72              |
| 2:J:190:SER:HB2  | 2:J:244:GLY:HA2  | 1.72                     | 0.72              |
| 2:J:219:GLN:HE21 | 2:J:262:GLN:HG2  | 1.54                     | 0.72              |
| 2:N:190:SER:HB2  | 2:N:244:GLY:HA2  | 1.72                     | 0.72              |
| 2:N:219:GLN:HE21 | 2:N:262:GLN:HG2  | 1.54                     | 0.72              |
| 1:O:102:THR:HA   | 2:P:170:VAL:HA   | 1.71                     | 0.72              |
| 2:P:224:GLN:HG2  | 2:P:231:ILE:HD13 | 1.72                     | 0.72              |
| 1:A:194:GLY:O    | 2:B:158:THR:HG21 | 1.90                     | 0.72              |
| 1:G:9:VAL:HA     | 4:G:208:HOH:O    | 1.89                     | 0.72              |
| 1:G:86:ASN:HD21  | 1:G:110:ARG:HE   | 1.38                     | 0.72              |
| 1:I:157:ALA:HB3  | 1:I:181:ALA:HB1  | 1.71                     | 0.72              |
| 2:L:135:ASN:HD21 | 2:L:138:ASN:HD21 | 1.33                     | 0.72              |
| 1:O:141:THR:CA   | 1:O:174:THR:HG21 | 2.05                     | 0.72              |
| 1:O:157:ALA:HB3  | 1:O:181:ALA:HB1  | 1.71                     | 0.72              |
| 2:D:120:ILE:HD13 | 2:D:126:ILE:HD12 | 1.71                     | 0.72              |
| 2:L:190:SER:HB2  | 2:L:244:GLY:HA2  | 1.71                     | 0.72              |
| 1:M:79:ARG:HA    | 1:M:147:PRO:HB2  | 1.72                     | 0.72              |
| 2:B:28:VAL:HG21  | 2:B:34:LEU:HD13  | 1.70                     | 0.72              |
| 2:J:224:GLN:HG2  | 2:J:231:ILE:HD13 | 1.71                     | 0.71              |
| 1:M:103:LEU:C    | 2:N:168:VAL:HG23 | 2.15                     | 0.71              |
| 1:M:132:ARG:HG2  | 1:M:203:VAL:O    | 1.89                     | 0.71              |
| 2:F:218:ALA:HB2  | 2:F:266:GLY:CA   | 2.20                     | 0.71              |
| 2:J:135:ASN:HD21 | 2:J:138:ASN:HD21 | 1.36                     | 0.71              |
| 1:C:9:VAL:HA     | 4:C:208:HOH:O    | 1.91                     | 0.71              |
| 1:O:103:LEU:C    | 2:P:168:VAL:HG23 | 2.15                     | 0.71              |
| 2:F:28:VAL:HG21  | 2:F:34:LEU:HD13  | 1.72                     | 0.71              |
| 2:H:59:GLN:HA    | 2:H:89:GLU:HG3   | 1.72                     | 0.71              |
| 1:C:129:GLU:HA   | 1:C:200:MET:HE1  | 1.72                     | 0.71              |
| 2:D:218:ALA:HB2  | 2:D:266:GLY:CA   | 2.20                     | 0.71              |
| 1:O:79:ARG:HA    | 1:O:147:PRO:HB2  | 1.72                     | 0.71              |
| 2:P:190:SER:HB2  | 2:P:244:GLY:HA2  | 1.72                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:132:ARG:HG2  | 1:I:203:VAL:O    | 1.90                     | 0.71              |
| 2:D:201:THR:HG21 | 2:D:206:ASN:HA   | 1.71                     | 0.71              |
| 1:M:97:LYS:HB3   | 1:M:102:THR:HG21 | 1.72                     | 0.71              |
| 1:O:132:ARG:HG2  | 1:O:203:VAL:O    | 1.89                     | 0.71              |
| 1:G:129:GLU:HA   | 1:G:200:MET:HE1  | 1.72                     | 0.71              |
| 2:H:218:ALA:HB2  | 2:H:266:GLY:CA   | 2.21                     | 0.71              |
| 2:F:201:THR:HG21 | 2:F:206:ASN:HA   | 1.73                     | 0.71              |
| 1:I:97:LYS:HB3   | 1:I:102:THR:HG21 | 1.72                     | 0.71              |
| 1:I:103:LEU:C    | 2:J:168:VAL:HG23 | 2.15                     | 0.71              |
| 2:F:172:LEU:O    | 2:F:173:PRO:C    | 2.32                     | 0.70              |
| 2:F:240:LEU:HD11 | 2:F:250:LEU:HD22 | 1.73                     | 0.70              |
| 1:K:97:LYS:HB3   | 1:K:102:THR:HG21 | 1.72                     | 0.70              |
| 1:K:103:LEU:C    | 2:L:168:VAL:HG23 | 2.16                     | 0.70              |
| 2:F:59:GLN:HA    | 2:F:89:GLU:HG3   | 1.71                     | 0.70              |
| 1:G:135:ARG:HH22 | 1:G:181:ALA:HB1  | 1.56                     | 0.70              |
| 1:K:79:ARG:HA    | 1:K:147:PRO:HB2  | 1.71                     | 0.70              |
| 1:O:145:PRO:O    | 1:O:170:MET:HG3  | 1.91                     | 0.70              |
| 1:O:97:LYS:HB3   | 1:O:102:THR:HG21 | 1.72                     | 0.70              |
| 2:P:38:LEU:C     | 2:P:40:THR:H     | 1.99                     | 0.70              |
| 1:I:107:ILE:H    | 1:I:107:ILE:HD12 | 1.56                     | 0.70              |
| 1:K:163:GLU:O    | 1:K:175:VAL:HG21 | 1.91                     | 0.70              |
| 2:H:28:VAL:HG21  | 2:H:34:LEU:HD13  | 1.72                     | 0.70              |
| 2:H:201:THR:HG21 | 2:H:206:ASN:HA   | 1.74                     | 0.70              |
| 2:L:166:ARG:HG2  | 2:L:182:PRO:HB2  | 1.74                     | 0.70              |
| 2:D:28:VAL:HG21  | 2:D:34:LEU:HD13  | 1.74                     | 0.70              |
| 2:P:162:ASP:HB3  | 2:P:186:TYR:CE1  | 2.27                     | 0.70              |
| 1:G:194:GLY:O    | 2:H:158:THR:HG21 | 1.91                     | 0.70              |
| 2:H:136:ASN:HD22 | 2:H:137:TYR:N    | 1.89                     | 0.70              |
| 1:G:32:LEU:HD22  | 1:G:54:LEU:HD11  | 1.73                     | 0.70              |
| 2:N:162:ASP:HB3  | 2:N:186:TYR:CE1  | 2.27                     | 0.70              |
| 1:O:107:ILE:HD12 | 1:O:107:ILE:H    | 1.57                     | 0.70              |
| 2:P:166:ARG:HG2  | 2:P:182:PRO:HB2  | 1.74                     | 0.70              |
| 1:I:163:GLU:O    | 1:I:175:VAL:HG21 | 1.92                     | 0.70              |
| 2:J:206:ASN:ND2  | 2:J:234:ALA:HB3  | 2.07                     | 0.70              |
| 1:M:107:ILE:H    | 1:M:107:ILE:HD12 | 1.57                     | 0.70              |
| 2:P:206:ASN:ND2  | 2:P:234:ALA:HB3  | 2.07                     | 0.70              |
| 1:C:185:ILE:HB   | 1:C:202:GLY:HA3  | 1.74                     | 0.70              |
| 2:D:59:GLN:HA    | 2:D:89:GLU:HG3   | 1.74                     | 0.70              |
| 2:L:182:PRO:O    | 2:L:183:LEU:HG   | 1.92                     | 0.70              |
| 1:O:102:THR:HB   | 2:P:168:VAL:CG2  | 2.22                     | 0.70              |
| 2:B:171:THR:C    | 2:B:173:PRO:HD2  | 2.17                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:218:ALA:HB2  | 2:B:266:GLY:CA   | 2.22                     | 0.69              |
| 2:B:263:VAL:HG23 | 4:B:529:HOH:O    | 1.92                     | 0.69              |
| 2:J:209:PHE:CE2  | 2:J:234:ALA:HB2  | 2.27                     | 0.69              |
| 1:A:193:TYR:O    | 2:B:158:THR:HG22 | 1.92                     | 0.69              |
| 2:B:201:THR:HG21 | 2:B:206:ASN:HA   | 1.74                     | 0.69              |
| 1:E:135:ARG:HH22 | 1:E:181:ALA:HB1  | 1.57                     | 0.69              |
| 1:E:188:ARG:HE   | 1:E:196:LEU:HD22 | 1.56                     | 0.69              |
| 1:I:157:ALA:O    | 1:I:184:ASN:HB3  | 1.92                     | 0.69              |
| 2:N:182:PRO:O    | 2:N:183:LEU:HG   | 1.92                     | 0.69              |
| 1:K:157:ALA:O    | 1:K:184:ASN:HB3  | 1.92                     | 0.69              |
| 1:M:145:PRO:O    | 1:M:170:MET:HG3  | 1.91                     | 0.69              |
| 2:N:38:LEU:C     | 2:N:40:THR:H     | 1.99                     | 0.69              |
| 2:B:59:GLN:HA    | 2:B:89:GLU:HG3   | 1.73                     | 0.69              |
| 2:B:172:LEU:N    | 2:B:173:PRO:HD2  | 2.07                     | 0.69              |
| 1:G:27:GLU:HG3   | 1:G:60:LYS:HZ2   | 1.56                     | 0.69              |
| 2:J:126:ILE:HB   | 2:J:148:ILE:HG22 | 1.74                     | 0.69              |
| 2:J:193:LEU:HB3  | 2:J:240:LEU:HD12 | 1.74                     | 0.69              |
| 1:I:102:THR:HB   | 2:J:168:VAL:CG2  | 2.22                     | 0.69              |
| 2:J:162:ASP:HB3  | 2:J:186:TYR:CE1  | 2.27                     | 0.69              |
| 2:J:166:ARG:HG2  | 2:J:182:PRO:HB2  | 1.74                     | 0.69              |
| 2:L:38:LEU:C     | 2:L:40:THR:H     | 2.00                     | 0.69              |
| 2:N:193:LEU:HB3  | 2:N:240:LEU:HD12 | 1.75                     | 0.69              |
| 2:N:209:PHE:CE2  | 2:N:234:ALA:HB2  | 2.27                     | 0.69              |
| 2:J:182:PRO:O    | 2:J:183:LEU:HG   | 1.92                     | 0.69              |
| 1:K:145:PRO:O    | 1:K:170:MET:HG3  | 1.92                     | 0.69              |
| 2:L:162:ASP:HB3  | 2:L:186:TYR:CE1  | 2.27                     | 0.69              |
| 2:L:206:ASN:ND2  | 2:L:234:ALA:HB3  | 2.07                     | 0.69              |
| 2:N:126:ILE:HB   | 2:N:148:ILE:HG22 | 1.74                     | 0.69              |
| 1:K:107:ILE:H    | 1:K:107:ILE:HD12 | 1.56                     | 0.69              |
| 2:L:126:ILE:HB   | 2:L:148:ILE:HG22 | 1.74                     | 0.69              |
| 2:L:209:PHE:CE2  | 2:L:234:ALA:HB2  | 2.27                     | 0.69              |
| 2:N:206:ASN:ND2  | 2:N:234:ALA:HB3  | 2.07                     | 0.69              |
| 1:O:157:ALA:O    | 1:O:184:ASN:HB3  | 1.92                     | 0.69              |
| 1:A:32:LEU:HD22  | 1:A:54:LEU:HD11  | 1.74                     | 0.69              |
| 1:I:79:ARG:HA    | 1:I:147:PRO:HB2  | 1.72                     | 0.69              |
| 1:I:91:PRO:HG3   | 1:I:105:LEU:O    | 1.93                     | 0.69              |
| 1:I:145:PRO:O    | 1:I:170:MET:HG3  | 1.91                     | 0.69              |
| 1:M:102:THR:HB   | 2:N:168:VAL:CG2  | 2.22                     | 0.69              |
| 1:M:157:ALA:O    | 1:M:184:ASN:HB3  | 1.93                     | 0.69              |
| 1:C:86:ASN:HD21  | 1:C:110:ARG:HE   | 1.39                     | 0.69              |
| 1:C:135:ARG:HH22 | 1:C:181:ALA:HB1  | 1.57                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:5:THR:HG23   | 2:F:7:ASN:H      | 1.57                     | 0.69              |
| 2:F:171:THR:C    | 2:F:173:PRO:HD2  | 2.18                     | 0.69              |
| 1:K:102:THR:HB   | 2:L:168:VAL:CG2  | 2.21                     | 0.69              |
| 2:L:193:LEU:HB3  | 2:L:240:LEU:HD12 | 1.75                     | 0.69              |
| 1:G:185:ILE:HB   | 1:G:202:GLY:HA3  | 1.75                     | 0.69              |
| 2:L:59:GLN:HG3   | 2:L:143:GLN:HE21 | 1.57                     | 0.69              |
| 2:N:166:ARG:HG2  | 2:N:182:PRO:HB2  | 1.75                     | 0.69              |
| 1:A:135:ARG:HH22 | 1:A:181:ALA:HB1  | 1.57                     | 0.68              |
| 1:C:135:ARG:NH1  | 1:C:177:LEU:HD21 | 2.08                     | 0.68              |
| 2:P:209:PHE:CE2  | 2:P:234:ALA:HB2  | 2.27                     | 0.68              |
| 2:H:172:LEU:N    | 2:H:173:PRO:HD2  | 2.08                     | 0.68              |
| 1:I:8:ARG:HB3    | 1:I:8:ARG:NH1    | 2.07                     | 0.68              |
| 2:J:38:LEU:C     | 2:J:40:THR:H     | 2.01                     | 0.68              |
| 1:C:32:LEU:HD22  | 1:C:54:LEU:HD11  | 1.75                     | 0.68              |
| 1:E:27:GLU:HG3   | 1:E:60:LYS:HZ3   | 1.57                     | 0.68              |
| 1:K:143:ILE:HG13 | 1:K:172:GLU:HB3  | 1.76                     | 0.68              |
| 2:L:71:PHE:HA    | 2:L:110:THR:O    | 1.93                     | 0.68              |
| 1:M:163:GLU:O    | 1:M:175:VAL:HG21 | 1.92                     | 0.68              |
| 1:O:8:ARG:HB3    | 1:O:8:ARG:NH1    | 2.08                     | 0.68              |
| 1:O:112:LYS:HZ1  | 1:O:166:LEU:HD22 | 1.59                     | 0.68              |
| 1:O:163:GLU:O    | 1:O:175:VAL:HG21 | 1.91                     | 0.68              |
| 2:P:126:ILE:HB   | 2:P:148:ILE:HG22 | 1.74                     | 0.68              |
| 2:P:59:GLN:HG3   | 2:P:143:GLN:HE21 | 1.58                     | 0.68              |
| 1:A:185:ILE:HB   | 1:A:202:GLY:HA3  | 1.75                     | 0.68              |
| 2:D:172:LEU:N    | 2:D:173:PRO:HD2  | 2.09                     | 0.68              |
| 2:J:59:GLN:HG3   | 2:J:143:GLN:HE21 | 1.58                     | 0.68              |
| 1:M:91:PRO:HG3   | 1:M:105:LEU:O    | 1.93                     | 0.68              |
| 2:N:20:VAL:HG21  | 2:N:42:ILE:HD11  | 1.76                     | 0.68              |
| 2:F:136:ASN:HD22 | 2:F:137:TYR:N    | 1.92                     | 0.68              |
| 2:F:263:VAL:HG23 | 4:F:546:HOH:O    | 1.93                     | 0.68              |
| 2:H:171:THR:C    | 2:H:173:PRO:HD2  | 2.19                     | 0.68              |
| 2:N:59:GLN:HG3   | 2:N:143:GLN:HE21 | 1.59                     | 0.68              |
| 2:P:182:PRO:O    | 2:P:183:LEU:HG   | 1.93                     | 0.68              |
| 2:D:171:THR:C    | 2:D:173:PRO:HD2  | 2.19                     | 0.68              |
| 2:D:38:LEU:C     | 2:D:40:THR:H     | 2.02                     | 0.68              |
| 1:K:8:ARG:HB3    | 1:K:8:ARG:NH1    | 2.08                     | 0.68              |
| 1:M:8:ARG:HB3    | 1:M:8:ARG:NH1    | 2.09                     | 0.68              |
| 1:O:91:PRO:HG3   | 1:O:105:LEU:O    | 1.93                     | 0.68              |
| 2:B:136:ASN:HD22 | 2:B:137:TYR:N    | 1.91                     | 0.68              |
| 1:C:188:ARG:NH1  | 1:C:199:LYS:N    | 2.42                     | 0.68              |
| 1:M:143:ILE:HG13 | 1:M:172:GLU:HB3  | 1.76                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:267:ASN:HD22 | 2:H:267:ASN:N    | 1.92                     | 0.67              |
| 1:A:126:GLN:HG2  | 1:A:126:GLN:O    | 1.93                     | 0.67              |
| 2:D:136:ASN:HD22 | 2:D:137:TYR:N    | 1.91                     | 0.67              |
| 1:E:185:ILE:HB   | 1:E:202:GLY:HA3  | 1.76                     | 0.67              |
| 1:G:188:ARG:HE   | 1:G:196:LEU:HD22 | 1.59                     | 0.67              |
| 1:I:77:GLN:HE21  | 1:I:77:GLN:HA    | 1.59                     | 0.67              |
| 1:G:193:TYR:O    | 2:H:158:THR:HG22 | 1.95                     | 0.67              |
| 1:C:97:LYS:HD3   | 1:C:100:GLU:CD   | 2.20                     | 0.67              |
| 1:A:188:ARG:HE   | 1:A:196:LEU:HD22 | 1.58                     | 0.67              |
| 1:C:193:TYR:O    | 2:D:158:THR:HG22 | 1.95                     | 0.67              |
| 2:H:240:LEU:HD11 | 2:H:250:LEU:HD22 | 1.74                     | 0.67              |
| 2:J:71:PHE:HA    | 2:J:110:THR:O    | 1.95                     | 0.67              |
| 1:E:188:ARG:NH1  | 1:E:199:LYS:N    | 2.42                     | 0.67              |
| 2:N:5:THR:HG23   | 2:N:7:ASN:H      | 1.60                     | 0.67              |
| 1:O:143:ILE:HG13 | 1:O:172:GLU:HB3  | 1.76                     | 0.67              |
| 1:C:188:ARG:HE   | 1:C:196:LEU:HD22 | 1.60                     | 0.67              |
| 1:E:32:LEU:HD22  | 1:E:54:LEU:HD11  | 1.75                     | 0.67              |
| 1:I:143:ILE:HG13 | 1:I:172:GLU:HB3  | 1.77                     | 0.67              |
| 2:J:210:THR:HG22 | 2:J:221:VAL:O    | 1.95                     | 0.67              |
| 1:K:91:PRO:HG3   | 1:K:105:LEU:O    | 1.94                     | 0.67              |
| 2:P:5:THR:HG23   | 2:P:7:ASN:H      | 1.60                     | 0.67              |
| 2:D:240:LEU:HD11 | 2:D:250:LEU:HD22 | 1.75                     | 0.67              |
| 2:N:210:THR:HG22 | 2:N:221:VAL:O    | 1.95                     | 0.67              |
| 2:B:67:VAL:CG2   | 2:B:126:ILE:HG23 | 2.25                     | 0.67              |
| 2:F:193:LEU:HD12 | 2:F:243:VAL:HG21 | 1.77                     | 0.67              |
| 1:G:188:ARG:NH1  | 1:G:199:LYS:N    | 2.42                     | 0.67              |
| 1:M:177:LEU:HD11 | 1:M:181:ALA:HB3  | 1.77                     | 0.67              |
| 1:A:97:LYS:HD3   | 1:A:100:GLU:CD   | 2.20                     | 0.67              |
| 1:E:97:LYS:HD3   | 1:E:100:GLU:CD   | 2.20                     | 0.67              |
| 2:N:71:PHE:HA    | 2:N:110:THR:O    | 1.94                     | 0.67              |
| 2:P:193:LEU:HB3  | 2:P:240:LEU:HD12 | 1.76                     | 0.67              |
| 1:G:154:GLU:OE1  | 1:G:188:ARG:HD3  | 1.95                     | 0.66              |
| 2:P:71:PHE:HA    | 2:P:110:THR:O    | 1.94                     | 0.66              |
| 2:P:210:THR:HG22 | 2:P:221:VAL:O    | 1.95                     | 0.66              |
| 2:F:67:VAL:CG2   | 2:F:126:ILE:HG23 | 2.26                     | 0.66              |
| 2:F:221:VAL:HG12 | 2:F:222:GLY:N    | 2.10                     | 0.66              |
| 1:K:3:ALA:HB1    | 2:L:160:GLY:O    | 1.96                     | 0.66              |
| 1:M:112:LYS:HZ1  | 1:M:166:LEU:HD22 | 1.61                     | 0.66              |
| 1:O:177:LEU:HD11 | 1:O:181:ALA:HB3  | 1.78                     | 0.66              |
| 2:P:117:GLY:O    | 2:P:155:VAL:HA   | 1.96                     | 0.66              |
| 1:A:135:ARG:NH1  | 1:A:177:LEU:HD21 | 2.10                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:188:ARG:NH1  | 1:A:199:LYS:N    | 2.43                     | 0.66              |
| 2:F:172:LEU:N    | 2:F:173:PRO:HD2  | 2.09                     | 0.66              |
| 1:G:135:ARG:NH1  | 1:G:177:LEU:HD21 | 2.11                     | 0.66              |
| 2:H:219:GLN:HB3  | 4:H:644:HOH:O    | 1.95                     | 0.66              |
| 2:L:117:GLY:O    | 2:L:155:VAL:HA   | 1.95                     | 0.66              |
| 1:M:77:GLN:HA    | 1:M:77:GLN:HE21  | 1.60                     | 0.66              |
| 1:M:176:LYS:O    | 1:M:178:PRO:HD3  | 1.96                     | 0.66              |
| 2:D:267:ASN:HD22 | 2:D:267:ASN:N    | 1.93                     | 0.66              |
| 1:E:193:TYR:O    | 2:F:158:THR:HG22 | 1.95                     | 0.66              |
| 1:C:154:GLU:OE1  | 1:C:188:ARG:HD3  | 1.95                     | 0.66              |
| 1:K:77:GLN:HA    | 1:K:77:GLN:HE21  | 1.61                     | 0.66              |
| 2:L:268:VAL:O    | 2:L:269:GLN:HG3  | 1.95                     | 0.66              |
| 2:B:193:LEU:HD12 | 2:B:243:VAL:HG21 | 1.78                     | 0.66              |
| 2:D:5:THR:HG23   | 2:D:7:ASN:H      | 1.59                     | 0.66              |
| 2:D:67:VAL:CG2   | 2:D:126:ILE:HG23 | 2.26                     | 0.66              |
| 2:H:38:LEU:C     | 2:H:40:THR:H     | 2.02                     | 0.66              |
| 2:J:117:GLY:O    | 2:J:155:VAL:HA   | 1.96                     | 0.66              |
| 2:L:20:VAL:HG21  | 2:L:42:ILE:HD11  | 1.77                     | 0.66              |
| 2:N:21:TYR:HB3   | 2:N:151:ASN:HD21 | 1.60                     | 0.66              |
| 2:P:21:TYR:HB3   | 2:P:151:ASN:HD21 | 1.60                     | 0.66              |
| 2:P:64:TYR:HB2   | 2:P:125:LEU:O    | 1.96                     | 0.66              |
| 2:B:221:VAL:HG12 | 2:B:222:GLY:N    | 2.11                     | 0.66              |
| 2:B:240:LEU:HD11 | 2:B:250:LEU:HD22 | 1.76                     | 0.66              |
| 2:B:5:THR:HG23   | 2:B:7:ASN:H      | 1.59                     | 0.66              |
| 2:J:183:LEU:O    | 2:J:249:SER:HA   | 1.96                     | 0.66              |
| 1:K:176:LYS:O    | 1:K:178:PRO:HD3  | 1.96                     | 0.66              |
| 2:P:20:VAL:HG21  | 2:P:42:ILE:HD11  | 1.77                     | 0.66              |
| 1:G:97:LYS:HD3   | 1:G:100:GLU:CD   | 2.21                     | 0.66              |
| 2:H:221:VAL:HG12 | 2:H:222:GLY:N    | 2.09                     | 0.66              |
| 1:O:176:LYS:O    | 1:O:178:PRO:HD3  | 1.96                     | 0.66              |
| 2:B:38:LEU:C     | 2:B:40:THR:H     | 2.04                     | 0.65              |
| 1:I:23:THR:OG1   | 1:I:62:GLU:HG2   | 1.96                     | 0.65              |
| 2:J:20:VAL:HG21  | 2:J:42:ILE:HD11  | 1.76                     | 0.65              |
| 2:J:268:VAL:O    | 2:J:269:GLN:HG3  | 1.96                     | 0.65              |
| 1:K:112:LYS:NZ   | 1:K:166:LEU:HD22 | 2.11                     | 0.65              |
| 2:N:117:GLY:O    | 2:N:155:VAL:HA   | 1.96                     | 0.65              |
| 2:P:206:ASN:HD21 | 2:P:234:ALA:HB3  | 1.61                     | 0.65              |
| 1:C:126:GLN:O    | 1:C:126:GLN:HG2  | 1.94                     | 0.65              |
| 1:E:199:LYS:O    | 1:E:200:MET:HG3  | 1.96                     | 0.65              |
| 2:F:38:LEU:C     | 2:F:40:THR:H     | 2.03                     | 0.65              |
| 2:N:268:VAL:O    | 2:N:269:GLN:HG3  | 1.96                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:206:ASN:HD21 | 2:J:234:ALA:HB3  | 1.61                     | 0.65              |
| 1:O:3:ALA:HB1    | 2:P:160:GLY:O    | 1.96                     | 0.65              |
| 2:H:5:THR:HG23   | 2:H:7:ASN:H      | 1.60                     | 0.65              |
| 1:I:112:LYS:NZ   | 1:I:166:LEU:HD22 | 2.12                     | 0.65              |
| 1:K:23:THR:OG1   | 1:K:62:GLU:HG2   | 1.96                     | 0.65              |
| 1:K:112:LYS:HZ1  | 1:K:166:LEU:HD22 | 1.61                     | 0.65              |
| 1:K:177:LEU:HD11 | 1:K:181:ALA:HB3  | 1.78                     | 0.65              |
| 2:L:21:TYR:HB3   | 2:L:151:ASN:HD21 | 1.60                     | 0.65              |
| 1:I:3:ALA:HB1    | 2:J:160:GLY:O    | 1.95                     | 0.65              |
| 1:M:193:TYR:CE2  | 2:N:155:VAL:HG21 | 2.32                     | 0.65              |
| 2:P:268:VAL:O    | 2:P:269:GLN:HG3  | 1.95                     | 0.65              |
| 1:A:199:LYS:O    | 1:A:200:MET:HG3  | 1.97                     | 0.65              |
| 1:E:135:ARG:NH1  | 1:E:177:LEU:HD21 | 2.10                     | 0.65              |
| 1:G:97:LYS:HD3   | 1:G:100:GLU:OE1  | 1.97                     | 0.65              |
| 2:J:21:TYR:HB3   | 2:J:151:ASN:HD21 | 1.61                     | 0.65              |
| 1:K:193:TYR:CE2  | 2:L:155:VAL:HG21 | 2.32                     | 0.65              |
| 1:O:79:ARG:HD3   | 1:O:169:PRO:HB2  | 1.78                     | 0.65              |
| 1:O:193:TYR:CE2  | 2:P:155:VAL:HG21 | 2.32                     | 0.65              |
| 2:D:221:VAL:HG12 | 2:D:222:GLY:N    | 2.11                     | 0.65              |
| 1:I:177:LEU:HD11 | 1:I:181:ALA:HB3  | 1.78                     | 0.65              |
| 1:K:79:ARG:HD3   | 1:K:169:PRO:HB2  | 1.78                     | 0.65              |
| 2:L:183:LEU:O    | 2:L:249:SER:HA   | 1.97                     | 0.65              |
| 1:M:3:ALA:HB1    | 2:N:160:GLY:O    | 1.96                     | 0.65              |
| 1:M:23:THR:OG1   | 1:M:62:GLU:HG2   | 1.97                     | 0.65              |
| 2:N:64:TYR:HB2   | 2:N:125:LEU:O    | 1.96                     | 0.65              |
| 2:L:64:TYR:HB2   | 2:L:125:LEU:O    | 1.96                     | 0.65              |
| 2:B:182:PRO:HG3  | 4:B:512:HOH:O    | 1.97                     | 0.65              |
| 2:B:267:ASN:N    | 2:B:267:ASN:HD22 | 1.92                     | 0.65              |
| 2:H:67:VAL:CG2   | 2:H:126:ILE:HG23 | 2.27                     | 0.65              |
| 2:L:163:VAL:HA   | 2:L:185:VAL:HG12 | 1.79                     | 0.65              |
| 1:M:79:ARG:HD3   | 1:M:169:PRO:HB2  | 1.78                     | 0.65              |
| 1:C:197:THR:HB   | 1:C:198:PRO:HD2  | 1.79                     | 0.65              |
| 1:O:23:THR:OG1   | 1:O:62:GLU:HG2   | 1.97                     | 0.65              |
| 2:J:5:THR:HG23   | 2:J:7:ASN:H      | 1.60                     | 0.64              |
| 2:J:163:VAL:HA   | 2:J:185:VAL:HG12 | 1.79                     | 0.64              |
| 1:K:97:LYS:HD2   | 2:L:170:VAL:CG2  | 2.26                     | 0.64              |
| 1:K:149:TYR:HB3  | 1:K:166:LEU:CD1  | 2.27                     | 0.64              |
| 2:L:27:VAL:HG12  | 4:L:505:HOH:O    | 1.97                     | 0.64              |
| 2:P:163:VAL:HA   | 2:P:185:VAL:HG12 | 1.79                     | 0.64              |
| 2:P:183:LEU:O    | 2:P:249:SER:HA   | 1.97                     | 0.64              |
| 1:A:155:LEU:O    | 1:A:162:LEU:HB2  | 1.97                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:199:LYS:O    | 1:G:200:MET:HG3  | 1.97                     | 0.64              |
| 2:D:163:VAL:HG22 | 2:D:185:VAL:HG12 | 1.80                     | 0.64              |
| 2:D:172:LEU:O    | 2:D:174:ASP:N    | 2.31                     | 0.64              |
| 1:E:101:ASN:HB3  | 2:F:171:THR:HG23 | 1.79                     | 0.64              |
| 1:G:155:LEU:O    | 1:G:162:LEU:HB2  | 1.97                     | 0.64              |
| 1:K:158:GLY:HA3  | 1:K:184:ASN:HD22 | 1.62                     | 0.64              |
| 2:L:210:THR:HG22 | 2:L:221:VAL:O    | 1.96                     | 0.64              |
| 1:O:144:ASN:HB3  | 1:O:167:VAL:HG12 | 1.79                     | 0.64              |
| 1:C:155:LEU:O    | 1:C:162:LEU:HB2  | 1.97                     | 0.64              |
| 1:G:126:GLN:HG2  | 1:G:126:GLN:O    | 1.97                     | 0.64              |
| 1:G:197:THR:HB   | 1:G:198:PRO:HD2  | 1.78                     | 0.64              |
| 2:J:59:GLN:HG2   | 2:J:132:ARG:HD2  | 1.79                     | 0.64              |
| 1:M:144:ASN:HB3  | 1:M:167:VAL:HG12 | 1.78                     | 0.64              |
| 1:M:188:ARG:HH21 | 1:M:196:LEU:CD1  | 2.11                     | 0.64              |
| 2:D:59:GLN:CG    | 2:D:132:ARG:HD2  | 2.28                     | 0.64              |
| 1:E:97:LYS:HD3   | 1:E:100:GLU:OE1  | 1.97                     | 0.64              |
| 1:I:193:TYR:CE2  | 2:J:155:VAL:HG21 | 2.32                     | 0.64              |
| 2:L:206:ASN:HD21 | 2:L:234:ALA:HB3  | 1.61                     | 0.64              |
| 1:O:135:ARG:NH2  | 1:O:177:LEU:HD21 | 2.12                     | 0.64              |
| 1:E:126:GLN:O    | 1:E:126:GLN:HG2  | 1.97                     | 0.64              |
| 1:I:97:LYS:HD2   | 2:J:170:VAL:CG2  | 2.26                     | 0.64              |
| 2:H:131:LEU:HD23 | 2:H:131:LEU:C    | 2.23                     | 0.64              |
| 1:I:176:LYS:O    | 1:I:178:PRO:HD3  | 1.96                     | 0.64              |
| 2:L:5:THR:HG23   | 2:L:7:ASN:H      | 1.61                     | 0.64              |
| 1:M:158:GLY:HA3  | 1:M:184:ASN:HD22 | 1.62                     | 0.64              |
| 2:N:59:GLN:HG2   | 2:N:132:ARG:HD2  | 1.79                     | 0.64              |
| 1:C:101:ASN:HB3  | 2:D:171:THR:HG23 | 1.80                     | 0.64              |
| 1:O:158:GLY:HA3  | 1:O:184:ASN:HD22 | 1.62                     | 0.64              |
| 1:A:197:THR:HB   | 1:A:198:PRO:HD2  | 1.78                     | 0.64              |
| 1:I:144:ASN:HB3  | 1:I:167:VAL:HG12 | 1.79                     | 0.64              |
| 1:O:77:GLN:HE21  | 1:O:77:GLN:HA    | 1.62                     | 0.64              |
| 1:A:154:GLU:OE1  | 1:A:188:ARG:HD3  | 1.97                     | 0.64              |
| 2:B:172:LEU:O    | 2:B:174:ASP:N    | 2.31                     | 0.64              |
| 1:E:138:ASN:O    | 1:E:177:LEU:N    | 2.31                     | 0.64              |
| 1:E:154:GLU:OE1  | 1:E:188:ARG:HD3  | 1.98                     | 0.64              |
| 2:F:170:VAL:C    | 2:F:172:LEU:H    | 2.06                     | 0.64              |
| 2:L:163:VAL:HG13 | 2:L:185:VAL:HG12 | 1.80                     | 0.64              |
| 2:N:163:VAL:HA   | 2:N:185:VAL:HG12 | 1.79                     | 0.64              |
| 2:N:183:LEU:O    | 2:N:249:SER:HA   | 1.97                     | 0.64              |
| 2:P:96:ASN:N     | 2:P:96:ASN:ND2   | 2.45                     | 0.64              |
| 1:C:27:GLU:HG3   | 1:C:60:LYS:HZ3   | 1.62                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:172:LEU:O    | 2:F:174:ASP:N    | 2.31                     | 0.63              |
| 1:G:138:ASN:O    | 1:G:177:LEU:N    | 2.30                     | 0.63              |
| 2:H:172:LEU:O    | 2:H:174:ASP:N    | 2.31                     | 0.63              |
| 2:J:64:TYR:HB2   | 2:J:125:LEU:O    | 1.97                     | 0.63              |
| 1:K:144:ASN:HB3  | 1:K:167:VAL:HG12 | 1.79                     | 0.63              |
| 2:L:59:GLN:HG2   | 2:L:132:ARG:HD2  | 1.79                     | 0.63              |
| 1:C:58:LYS:HG3   | 4:C:224:HOH:O    | 1.97                     | 0.63              |
| 2:D:131:LEU:HD23 | 2:D:131:LEU:C    | 2.23                     | 0.63              |
| 2:D:138:ASN:C    | 2:D:138:ASN:ND2  | 2.54                     | 0.63              |
| 1:E:155:LEU:O    | 1:E:162:LEU:HB2  | 1.97                     | 0.63              |
| 1:G:156:ASN:C    | 1:G:158:GLY:H    | 2.06                     | 0.63              |
| 1:I:158:GLY:HA3  | 1:I:184:ASN:HD22 | 1.63                     | 0.63              |
| 1:K:135:ARG:NH2  | 1:K:177:LEU:HD21 | 2.13                     | 0.63              |
| 1:M:97:LYS:HD2   | 2:N:170:VAL:CG2  | 2.26                     | 0.63              |
| 2:N:96:ASN:N     | 2:N:96:ASN:ND2   | 2.46                     | 0.63              |
| 1:O:126:GLN:HG3  | 4:O:207:HOH:O    | 1.97                     | 0.63              |
| 1:C:199:LYS:O    | 1:C:200:MET:HG3  | 1.97                     | 0.63              |
| 2:H:170:VAL:C    | 2:H:172:LEU:H    | 2.06                     | 0.63              |
| 1:M:112:LYS:NZ   | 1:M:166:LEU:HD22 | 2.12                     | 0.63              |
| 2:N:227:ARG:C    | 2:N:229:GLY:H    | 2.07                     | 0.63              |
| 2:P:20:VAL:HG12  | 2:P:22:VAL:HG13  | 1.81                     | 0.63              |
| 1:G:32:LEU:HB2   | 1:G:90:ILE:HB    | 1.81                     | 0.63              |
| 1:I:79:ARG:HD3   | 1:I:169:PRO:HB2  | 1.78                     | 0.63              |
| 1:I:149:TYR:HB3  | 1:I:166:LEU:CD1  | 2.27                     | 0.63              |
| 2:J:14:GLY:HA2   | 2:J:142:PHE:CE2  | 2.33                     | 0.63              |
| 1:M:135:ARG:NH2  | 1:M:177:LEU:HD21 | 2.13                     | 0.63              |
| 1:O:97:LYS:HD2   | 2:P:170:VAL:CG2  | 2.26                     | 0.63              |
| 1:C:97:LYS:HD3   | 1:C:100:GLU:OE1  | 1.97                     | 0.63              |
| 1:E:27:GLU:HG3   | 1:E:60:LYS:HZ2   | 1.63                     | 0.63              |
| 1:I:135:ARG:NH2  | 1:I:177:LEU:HD21 | 2.13                     | 0.63              |
| 2:J:227:ARG:C    | 2:J:229:GLY:H    | 2.07                     | 0.63              |
| 1:M:149:TYR:HB3  | 1:M:166:LEU:CD1  | 2.28                     | 0.63              |
| 2:N:163:VAL:HG13 | 2:N:185:VAL:HG12 | 1.80                     | 0.63              |
| 1:A:97:LYS:HD3   | 1:A:100:GLU:OE1  | 1.98                     | 0.63              |
| 1:A:122:LEU:HD11 | 1:A:130:LYS:CE   | 2.26                     | 0.63              |
| 1:C:156:ASN:C    | 1:C:158:GLY:H    | 2.07                     | 0.63              |
| 1:M:19:GLN:HA    | 1:M:65:LEU:O     | 1.98                     | 0.63              |
| 1:O:112:LYS:NZ   | 1:O:166:LEU:HD22 | 2.12                     | 0.63              |
| 1:A:101:ASN:HB3  | 2:B:171:THR:HG23 | 1.81                     | 0.63              |
| 1:A:138:ASN:O    | 1:A:177:LEU:N    | 2.31                     | 0.63              |
| 2:B:163:VAL:HG22 | 2:B:185:VAL:HG12 | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:197:THR:HB   | 1:E:198:PRO:HD2  | 1.79                     | 0.63              |
| 1:C:138:ASN:O    | 1:C:177:LEU:N    | 2.31                     | 0.63              |
| 2:D:193:LEU:HD12 | 2:D:243:VAL:HG21 | 1.81                     | 0.63              |
| 1:I:19:GLN:HA    | 1:I:65:LEU:O     | 1.98                     | 0.63              |
| 1:I:140:LEU:HD12 | 1:I:162:LEU:CD1  | 2.29                     | 0.63              |
| 1:K:19:GLN:HA    | 1:K:65:LEU:O     | 1.99                     | 0.63              |
| 2:N:206:ASN:HD21 | 2:N:234:ALA:HB3  | 1.61                     | 0.63              |
| 2:D:170:VAL:C    | 2:D:172:LEU:H    | 2.06                     | 0.63              |
| 2:F:267:ASN:HD22 | 2:F:267:ASN:N    | 1.94                     | 0.63              |
| 1:I:188:ARG:HH21 | 1:I:196:LEU:CD1  | 2.12                     | 0.63              |
| 2:P:133:ASN:OD1  | 2:P:142:PHE:HB2  | 1.99                     | 0.63              |
| 1:C:27:GLU:HG3   | 1:C:60:LYS:HZ2   | 1.61                     | 0.62              |
| 2:F:136:ASN:C    | 2:F:136:ASN:ND2  | 2.54                     | 0.62              |
| 2:L:20:VAL:HG12  | 2:L:22:VAL:HG13  | 1.81                     | 0.62              |
| 1:O:19:GLN:HA    | 1:O:65:LEU:O     | 1.98                     | 0.62              |
| 2:P:14:GLY:HA2   | 2:P:142:PHE:CE2  | 2.34                     | 0.62              |
| 2:H:163:VAL:HG22 | 2:H:185:VAL:HG12 | 1.79                     | 0.62              |
| 2:L:112:VAL:HA   | 4:L:509:HOH:O    | 1.99                     | 0.62              |
| 2:P:227:ARG:C    | 2:P:229:GLY:H    | 2.07                     | 0.62              |
| 2:B:131:LEU:C    | 2:B:131:LEU:HD23 | 2.24                     | 0.62              |
| 2:D:211:ASN:OD1  | 2:D:268:VAL:HA   | 2.00                     | 0.62              |
| 2:F:116:GLY:HA2  | 2:F:189:LYS:HE2  | 1.80                     | 0.62              |
| 2:P:59:GLN:HG2   | 2:P:132:ARG:HD2  | 1.79                     | 0.62              |
| 1:C:72:ASN:O     | 1:C:74:GLN:HG3   | 1.98                     | 0.62              |
| 1:I:107:ILE:HD12 | 1:I:107:ILE:N    | 2.14                     | 0.62              |
| 1:K:140:LEU:HD12 | 1:K:162:LEU:CD1  | 2.30                     | 0.62              |
| 1:M:185:ILE:HG21 | 1:M:202:GLY:HA3  | 1.82                     | 0.62              |
| 2:J:163:VAL:HG13 | 2:J:185:VAL:HG12 | 1.81                     | 0.62              |
| 1:K:185:ILE:HG21 | 1:K:202:GLY:HA3  | 1.82                     | 0.62              |
| 1:O:149:TYR:HB3  | 1:O:166:LEU:CD1  | 2.27                     | 0.62              |
| 2:B:67:VAL:HG21  | 2:B:126:ILE:CG2  | 2.30                     | 0.62              |
| 2:D:84:PHE:HA    | 2:D:85:PRO:C     | 2.25                     | 0.62              |
| 2:F:67:VAL:HG21  | 2:F:126:ILE:CG2  | 2.30                     | 0.62              |
| 2:P:163:VAL:HG13 | 2:P:185:VAL:HG12 | 1.81                     | 0.62              |
| 2:D:116:GLY:HA2  | 2:D:189:LYS:HE2  | 1.82                     | 0.62              |
| 1:E:72:ASN:O     | 1:E:74:GLN:HG3   | 1.98                     | 0.62              |
| 1:E:122:LEU:HD11 | 1:E:130:LYS:CE   | 2.25                     | 0.62              |
| 1:A:32:LEU:HB2   | 1:A:90:ILE:HB    | 1.82                     | 0.62              |
| 2:H:84:PHE:HA    | 2:H:85:PRO:C     | 2.24                     | 0.62              |
| 2:N:133:ASN:OD1  | 2:N:142:PHE:HB2  | 2.00                     | 0.62              |
| 2:H:185:VAL:HG11 | 2:H:276:PHE:CE2  | 2.35                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:188:ARG:HH21 | 1:K:196:LEU:CD1  | 2.13                     | 0.62              |
| 2:B:185:VAL:HG11 | 2:B:276:PHE:CE2  | 2.35                     | 0.62              |
| 2:B:170:VAL:C    | 2:B:172:LEU:H    | 2.07                     | 0.61              |
| 2:H:193:LEU:HD12 | 2:H:243:VAL:HG21 | 1.81                     | 0.61              |
| 2:L:14:GLY:HA2   | 2:L:142:PHE:CE2  | 2.35                     | 0.61              |
| 1:O:188:ARG:HH21 | 1:O:196:LEU:CD1  | 2.13                     | 0.61              |
| 2:B:59:GLN:CG    | 2:B:132:ARG:HD2  | 2.29                     | 0.61              |
| 1:G:101:ASN:HB3  | 2:H:171:THR:HG23 | 1.81                     | 0.61              |
| 2:H:59:GLN:CG    | 2:H:132:ARG:HD2  | 2.29                     | 0.61              |
| 2:H:136:ASN:C    | 2:H:136:ASN:ND2  | 2.54                     | 0.61              |
| 2:J:20:VAL:HG12  | 2:J:22:VAL:HG13  | 1.81                     | 0.61              |
| 1:O:185:ILE:HG21 | 1:O:202:GLY:HA3  | 1.82                     | 0.61              |
| 2:F:59:GLN:CG    | 2:F:132:ARG:HD2  | 2.29                     | 0.61              |
| 2:L:226:THR:CG2  | 2:L:255:ASN:HD21 | 2.13                     | 0.61              |
| 2:D:67:VAL:HG21  | 2:D:126:ILE:CG2  | 2.31                     | 0.61              |
| 2:F:163:VAL:HG22 | 2:F:185:VAL:HG12 | 1.81                     | 0.61              |
| 2:L:227:ARG:C    | 2:L:229:GLY:H    | 2.07                     | 0.61              |
| 1:O:107:ILE:HD12 | 1:O:107:ILE:N    | 2.15                     | 0.61              |
| 2:H:201:THR:CG2  | 2:H:206:ASN:HD22 | 2.13                     | 0.61              |
| 1:I:185:ILE:HG21 | 1:I:202:GLY:HA3  | 1.82                     | 0.61              |
| 2:J:133:ASN:OD1  | 2:J:142:PHE:HB2  | 2.00                     | 0.61              |
| 2:N:219:GLN:NE2  | 2:N:262:GLN:HG2  | 2.15                     | 0.61              |
| 1:E:32:LEU:HB2   | 1:E:90:ILE:HB    | 1.83                     | 0.61              |
| 2:F:84:PHE:HA    | 2:F:85:PRO:C     | 2.26                     | 0.61              |
| 1:K:107:ILE:HD12 | 1:K:107:ILE:N    | 2.15                     | 0.61              |
| 2:L:219:GLN:NE2  | 2:L:262:GLN:HG2  | 2.15                     | 0.61              |
| 1:M:140:LEU:HD12 | 1:M:162:LEU:CD1  | 2.30                     | 0.61              |
| 2:D:185:VAL:HG11 | 2:D:276:PHE:CE2  | 2.36                     | 0.61              |
| 2:N:226:THR:CG2  | 2:N:255:ASN:HD21 | 2.12                     | 0.61              |
| 1:A:72:ASN:O     | 1:A:74:GLN:HG3   | 2.00                     | 0.61              |
| 1:M:107:ILE:HD12 | 1:M:107:ILE:N    | 2.14                     | 0.61              |
| 2:N:59:GLN:CG    | 2:N:132:ARG:HD2  | 2.31                     | 0.61              |
| 1:O:140:LEU:HD12 | 1:O:162:LEU:CD1  | 2.30                     | 0.61              |
| 2:B:138:ASN:C    | 2:B:138:ASN:ND2  | 2.56                     | 0.61              |
| 1:C:32:LEU:HB2   | 1:C:90:ILE:HB    | 1.81                     | 0.61              |
| 1:G:122:LEU:HD11 | 1:G:130:LYS:CE   | 2.24                     | 0.61              |
| 1:K:162:LEU:HB3  | 1:K:175:VAL:HG11 | 1.82                     | 0.61              |
| 2:P:219:GLN:NE2  | 2:P:262:GLN:HG2  | 2.16                     | 0.61              |
| 1:A:9:VAL:HG22   | 4:A:209:HOH:O    | 2.01                     | 0.60              |
| 1:E:156:ASN:C    | 1:E:158:GLY:H    | 2.07                     | 0.60              |
| 1:G:188:ARG:HH12 | 1:G:199:LYS:N    | 1.99                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:27:GLU:HG2   | 4:I:206:HOH:O    | 2.00                     | 0.60              |
| 1:I:162:LEU:HB3  | 1:I:175:VAL:HG11 | 1.83                     | 0.60              |
| 2:N:212:THR:HG21 | 2:N:271:ILE:HD11 | 1.83                     | 0.60              |
| 1:A:156:ASN:C    | 1:A:158:GLY:H    | 2.08                     | 0.60              |
| 1:C:122:LEU:HD11 | 1:C:130:LYS:CE   | 2.26                     | 0.60              |
| 2:F:185:VAL:HG11 | 2:F:276:PHE:CE2  | 2.36                     | 0.60              |
| 2:J:59:GLN:CG    | 2:J:132:ARG:HD2  | 2.31                     | 0.60              |
| 2:J:226:THR:CG2  | 2:J:255:ASN:HD21 | 2.13                     | 0.60              |
| 2:L:133:ASN:OD1  | 2:L:142:PHE:HB2  | 2.01                     | 0.60              |
| 2:N:14:GLY:HA2   | 2:N:142:PHE:CE2  | 2.36                     | 0.60              |
| 1:O:130:LYS:HA   | 1:O:203:VAL:HG21 | 1.83                     | 0.60              |
| 1:O:162:LEU:HB3  | 1:O:175:VAL:HG11 | 1.82                     | 0.60              |
| 1:C:188:ARG:HH12 | 1:C:199:LYS:N    | 2.00                     | 0.60              |
| 1:G:72:ASN:O     | 1:G:74:GLN:HG3   | 2.00                     | 0.60              |
| 1:K:31:TYR:CB    | 1:K:89:ALA:HB1   | 2.32                     | 0.60              |
| 2:D:227:ARG:HA   | 2:D:251:GLY:O    | 2.01                     | 0.60              |
| 2:H:116:GLY:HA2  | 2:H:189:LYS:HE2  | 1.82                     | 0.60              |
| 2:H:138:ASN:ND2  | 2:H:140:ASP:H    | 2.00                     | 0.60              |
| 1:K:169:PRO:C    | 1:K:171:GLY:H    | 2.10                     | 0.60              |
| 2:N:20:VAL:HG12  | 2:N:22:VAL:HG13  | 1.81                     | 0.60              |
| 2:P:59:GLN:CG    | 2:P:132:ARG:HD2  | 2.31                     | 0.60              |
| 2:D:24:LEU:HA    | 4:D:648:HOH:O    | 2.02                     | 0.60              |
| 1:I:102:THR:HB   | 2:J:168:VAL:HG22 | 1.82                     | 0.60              |
| 2:J:212:THR:HG21 | 2:J:271:ILE:HD11 | 1.84                     | 0.60              |
| 2:B:184:THR:HG22 | 2:B:249:SER:HA   | 1.84                     | 0.60              |
| 1:E:188:ARG:HH12 | 1:E:199:LYS:N    | 1.99                     | 0.60              |
| 2:J:219:GLN:NE2  | 2:J:262:GLN:HG2  | 2.16                     | 0.60              |
| 1:K:28:ASN:H     | 1:K:28:ASN:ND2   | 2.00                     | 0.60              |
| 1:K:130:LYS:HA   | 1:K:203:VAL:HG21 | 1.82                     | 0.60              |
| 1:M:130:LYS:HA   | 1:M:203:VAL:HG21 | 1.82                     | 0.60              |
| 1:I:130:LYS:HA   | 1:I:203:VAL:HG21 | 1.82                     | 0.60              |
| 2:J:98:ARG:HG3   | 2:J:98:ARG:HH11  | 1.67                     | 0.60              |
| 2:L:52:ILE:HG23  | 2:L:137:TYR:HB2  | 1.84                     | 0.60              |
| 1:M:162:LEU:HB3  | 1:M:175:VAL:HG11 | 1.82                     | 0.60              |
| 1:O:102:THR:HB   | 2:P:168:VAL:HG22 | 1.83                     | 0.60              |
| 2:P:226:THR:CG2  | 2:P:255:ASN:HD21 | 2.13                     | 0.60              |
| 2:D:184:THR:HG22 | 2:D:249:SER:HA   | 1.84                     | 0.60              |
| 1:M:28:ASN:H     | 1:M:28:ASN:ND2   | 2.00                     | 0.60              |
| 2:B:49:PRO:HD2   | 2:B:98:ARG:CZ    | 2.32                     | 0.60              |
| 1:I:169:PRO:C    | 1:I:171:GLY:H    | 2.10                     | 0.60              |
| 1:K:79:ARG:HB3   | 1:K:170:MET:HE3  | 1.84                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:96:ASN:N     | 2:L:96:ASN:ND2   | 2.46                     | 0.60              |
| 2:L:212:THR:HG21 | 2:L:271:ILE:HD11 | 1.84                     | 0.60              |
| 2:P:212:THR:HG21 | 2:P:271:ILE:HD11 | 1.84                     | 0.60              |
| 1:A:188:ARG:HH12 | 1:A:199:LYS:N    | 1.99                     | 0.60              |
| 2:B:84:PHE:HA    | 2:B:85:PRO:C     | 2.27                     | 0.60              |
| 2:B:116:GLY:HA2  | 2:B:189:LYS:HE2  | 1.82                     | 0.60              |
| 1:K:101:ASN:HB2  | 2:L:172:LEU:HA   | 1.83                     | 0.60              |
| 1:K:160:ARG:HB3  | 1:K:181:ALA:HB2  | 1.84                     | 0.60              |
| 2:L:122:ALA:HA   | 2:L:150:ALA:O    | 2.02                     | 0.60              |
| 1:O:101:ASN:HB2  | 2:P:172:LEU:HA   | 1.83                     | 0.60              |
| 1:C:66:ARG:HG2   | 1:C:66:ARG:HH11  | 1.67                     | 0.59              |
| 1:O:31:TYR:CB    | 1:O:89:ALA:HB1   | 2.31                     | 0.59              |
| 1:I:31:TYR:CB    | 1:I:89:ALA:HB1   | 2.32                     | 0.59              |
| 1:K:88:LYS:HE3   | 1:K:90:ILE:HG12  | 1.84                     | 0.59              |
| 1:K:126:GLN:HA   | 1:K:129:GLU:CD   | 2.27                     | 0.59              |
| 1:O:126:GLN:HA   | 1:O:129:GLU:CD   | 2.27                     | 0.59              |
| 2:B:113:SER:HB3  | 2:P:81:SER:N     | 2.10                     | 0.59              |
| 1:E:66:ARG:HG2   | 1:E:66:ARG:HH11  | 1.68                     | 0.59              |
| 2:F:131:LEU:HD23 | 2:F:131:LEU:C    | 2.27                     | 0.59              |
| 2:F:179:VAL:O    | 2:F:253:THR:HG23 | 2.02                     | 0.59              |
| 2:H:211:ASN:OD1  | 2:H:268:VAL:HA   | 2.02                     | 0.59              |
| 2:H:227:ARG:HA   | 2:H:251:GLY:O    | 2.02                     | 0.59              |
| 1:K:102:THR:HB   | 2:L:168:VAL:HG22 | 1.82                     | 0.59              |
| 1:M:126:GLN:HA   | 1:M:129:GLU:CD   | 2.27                     | 0.59              |
| 2:N:15:GLY:HA2   | 2:N:144:PHE:CD1  | 2.37                     | 0.59              |
| 2:B:28:VAL:O     | 2:B:156:VAL:HA   | 2.03                     | 0.59              |
| 1:I:28:ASN:H     | 1:I:28:ASN:ND2   | 1.99                     | 0.59              |
| 1:I:126:GLN:HA   | 1:I:129:GLU:CD   | 2.27                     | 0.59              |
| 2:J:15:GLY:HA2   | 2:J:144:PHE:CD1  | 2.37                     | 0.59              |
| 2:J:46:ASN:CB    | 2:J:96:ASN:HA    | 2.32                     | 0.59              |
| 1:M:101:ASN:HB2  | 2:N:172:LEU:HA   | 1.82                     | 0.59              |
| 1:O:160:ARG:HB3  | 1:O:181:ALA:HB2  | 1.84                     | 0.59              |
| 2:P:207:SER:OG   | 2:P:233:PRO:HB3  | 2.03                     | 0.59              |
| 2:F:28:VAL:O     | 2:F:156:VAL:HA   | 2.03                     | 0.59              |
| 2:F:138:ASN:C    | 2:F:138:ASN:ND2  | 2.57                     | 0.59              |
| 1:I:26:ASP:O     | 1:I:60:LYS:HB3   | 2.02                     | 0.59              |
| 1:I:160:ARG:HB3  | 1:I:181:ALA:HB2  | 1.85                     | 0.59              |
| 1:C:24:ASN:O     | 1:C:60:LYS:HA    | 2.03                     | 0.59              |
| 1:E:24:ASN:O     | 1:E:60:LYS:HA    | 2.03                     | 0.59              |
| 1:E:102:THR:CA   | 2:F:171:THR:HG22 | 2.33                     | 0.59              |
| 2:J:46:ASN:HB2   | 2:J:96:ASN:HA    | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:15:GLY:HA2   | 2:L:144:PHE:CD1  | 2.38                     | 0.59              |
| 2:L:98:ARG:HH11  | 2:L:98:ARG:HG3   | 1.67                     | 0.59              |
| 1:M:102:THR:HB   | 2:N:168:VAL:HG22 | 1.83                     | 0.59              |
| 1:O:100:GLU:HG2  | 2:P:172:LEU:HD12 | 1.85                     | 0.59              |
| 1:A:155:LEU:HD12 | 1:A:187:TYR:HB3  | 1.85                     | 0.59              |
| 2:B:213:ALA:HB3  | 4:B:527:HOH:O    | 2.02                     | 0.59              |
| 2:B:255:ASN:N    | 2:B:255:ASN:ND2  | 2.47                     | 0.59              |
| 2:F:211:ASN:OD1  | 2:F:268:VAL:HA   | 2.02                     | 0.59              |
| 1:G:136:SER:C    | 1:G:138:ASN:H    | 2.10                     | 0.59              |
| 2:H:34:LEU:HB3   | 2:H:109:LEU:HB2  | 1.84                     | 0.59              |
| 2:H:63:ALA:HB3   | 2:H:68:LEU:HD13  | 1.85                     | 0.59              |
| 2:L:207:SER:OG   | 2:L:233:PRO:HB3  | 2.03                     | 0.59              |
| 1:O:88:LYS:HE3   | 1:O:90:ILE:HG12  | 1.83                     | 0.59              |
| 1:O:169:PRO:C    | 1:O:171:GLY:H    | 2.10                     | 0.59              |
| 2:F:49:PRO:HD2   | 2:F:98:ARG:CZ    | 2.33                     | 0.59              |
| 1:K:33:ILE:CG1   | 1:K:57:MET:HB2   | 2.33                     | 0.59              |
| 2:L:46:ASN:CB    | 2:L:96:ASN:HA    | 2.33                     | 0.59              |
| 2:L:59:GLN:CG    | 2:L:132:ARG:HD2  | 2.32                     | 0.59              |
| 1:M:31:TYR:CB    | 1:M:89:ALA:HB1   | 2.32                     | 0.59              |
| 2:P:46:ASN:CB    | 2:P:96:ASN:HA    | 2.32                     | 0.59              |
| 2:B:59:GLN:HG3   | 2:B:143:GLN:HE21 | 1.68                     | 0.59              |
| 2:B:227:ARG:HA   | 2:B:251:GLY:O    | 2.03                     | 0.59              |
| 1:C:135:ARG:NH2  | 1:C:181:ALA:HB1  | 2.18                     | 0.59              |
| 1:M:160:ARG:HB3  | 1:M:181:ALA:HB2  | 1.85                     | 0.59              |
| 2:P:15:GLY:HA2   | 2:P:144:PHE:CD1  | 2.38                     | 0.59              |
| 1:G:27:GLU:HG3   | 1:G:60:LYS:HZ3   | 1.67                     | 0.59              |
| 1:I:100:GLU:HG2  | 2:J:172:LEU:HD12 | 1.85                     | 0.59              |
| 1:I:101:ASN:HA   | 2:J:268:VAL:O    | 2.03                     | 0.59              |
| 1:I:101:ASN:HB2  | 2:J:172:LEU:HA   | 1.83                     | 0.59              |
| 2:J:122:ALA:HA   | 2:J:150:ALA:O    | 2.02                     | 0.59              |
| 2:L:43:PHE:CE2   | 2:L:102:PRO:HG3  | 2.37                     | 0.59              |
| 1:M:26:ASP:O     | 1:M:60:LYS:HB3   | 2.02                     | 0.59              |
| 2:N:207:SER:OG   | 2:N:233:PRO:HB3  | 2.03                     | 0.59              |
| 1:O:26:ASP:O     | 1:O:60:LYS:HB3   | 2.03                     | 0.59              |
| 1:O:158:GLY:HA3  | 1:O:184:ASN:ND2  | 2.18                     | 0.59              |
| 2:P:52:ILE:HG23  | 2:P:137:TYR:HB2  | 1.84                     | 0.59              |
| 2:D:28:VAL:O     | 2:D:156:VAL:HA   | 2.02                     | 0.58              |
| 1:G:135:ARG:NH2  | 1:G:181:ALA:HB1  | 2.17                     | 0.58              |
| 1:I:23:THR:HG22  | 1:I:24:ASN:N     | 2.18                     | 0.58              |
| 2:J:207:SER:OG   | 2:J:233:PRO:HB3  | 2.03                     | 0.58              |
| 2:L:46:ASN:HB2   | 2:L:96:ASN:HA    | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:169:PRO:C    | 1:M:171:GLY:H    | 2.10                     | 0.58              |
| 2:D:201:THR:CG2  | 2:D:206:ASN:HD22 | 2.15                     | 0.58              |
| 1:E:86:ASN:ND2   | 1:E:110:ARG:HE   | 2.01                     | 0.58              |
| 2:F:227:ARG:HA   | 2:F:251:GLY:O    | 2.03                     | 0.58              |
| 1:G:66:ARG:HG2   | 1:G:66:ARG:HH11  | 1.68                     | 0.58              |
| 1:I:33:ILE:CG1   | 1:I:57:MET:HB2   | 2.33                     | 0.58              |
| 1:I:143:ILE:HA   | 1:I:172:GLU:CB   | 2.33                     | 0.58              |
| 1:K:143:ILE:HA   | 1:K:172:GLU:CB   | 2.33                     | 0.58              |
| 2:L:226:THR:HA   | 2:L:230:THR:O    | 2.03                     | 0.58              |
| 1:M:158:GLY:CA   | 1:M:184:ASN:HD22 | 2.16                     | 0.58              |
| 1:O:28:ASN:H     | 1:O:28:ASN:ND2   | 1.99                     | 0.58              |
| 1:I:88:LYS:HE3   | 1:I:90:ILE:HG12  | 1.84                     | 0.58              |
| 1:K:158:GLY:HA3  | 1:K:184:ASN:ND2  | 2.18                     | 0.58              |
| 1:M:36:TRP:HH2   | 1:M:88:LYS:HE2   | 1.68                     | 0.58              |
| 1:O:23:THR:HG22  | 1:O:24:ASN:N     | 2.18                     | 0.58              |
| 1:O:101:ASN:HA   | 2:P:268:VAL:O    | 2.03                     | 0.58              |
| 1:O:104:GLN:N    | 2:P:168:VAL:HG23 | 2.19                     | 0.58              |
| 1:O:143:ILE:HA   | 1:O:172:GLU:CB   | 2.32                     | 0.58              |
| 2:F:255:ASN:N    | 2:F:255:ASN:ND2  | 2.49                     | 0.58              |
| 1:G:24:ASN:O     | 1:G:60:LYS:HA    | 2.03                     | 0.58              |
| 2:H:126:ILE:CG1  | 2:H:150:ALA:HB2  | 2.33                     | 0.58              |
| 2:L:227:ARG:HH12 | 2:L:232:ILE:HA   | 1.69                     | 0.58              |
| 1:M:143:ILE:HA   | 1:M:172:GLU:CB   | 2.34                     | 0.58              |
| 2:N:43:PHE:CE2   | 2:N:102:PRO:HG3  | 2.38                     | 0.58              |
| 2:P:43:PHE:CE2   | 2:P:102:PRO:HG3  | 2.37                     | 0.58              |
| 2:P:98:ARG:HH11  | 2:P:98:ARG:HG3   | 1.67                     | 0.58              |
| 1:A:86:ASN:ND2   | 1:A:110:ARG:HE   | 2.00                     | 0.58              |
| 1:C:155:LEU:HD12 | 1:C:187:TYR:HB3  | 1.85                     | 0.58              |
| 2:D:49:PRO:HD2   | 2:D:98:ARG:CZ    | 2.34                     | 0.58              |
| 2:F:24:LEU:HA    | 4:F:545:HOH:O    | 2.02                     | 0.58              |
| 1:K:158:GLY:CA   | 1:K:184:ASN:HD22 | 2.16                     | 0.58              |
| 1:M:101:ASN:HA   | 2:N:268:VAL:O    | 2.04                     | 0.58              |
| 1:A:102:THR:CA   | 2:B:171:THR:HG22 | 2.34                     | 0.58              |
| 1:G:86:ASN:ND2   | 1:G:110:ARG:HE   | 2.01                     | 0.58              |
| 2:H:28:VAL:O     | 2:H:156:VAL:HA   | 2.03                     | 0.58              |
| 1:I:36:TRP:HH2   | 1:I:88:LYS:HE2   | 1.69                     | 0.58              |
| 2:N:98:ARG:HH11  | 2:N:98:ARG:HG3   | 1.68                     | 0.58              |
| 2:N:122:ALA:HA   | 2:N:150:ALA:O    | 2.04                     | 0.58              |
| 1:A:24:ASN:O     | 1:A:60:LYS:HA    | 2.04                     | 0.58              |
| 2:B:8:GLY:HA3    | 4:B:514:HOH:O    | 2.03                     | 0.58              |
| 1:G:161:VAL:O    | 1:G:162:LEU:HG   | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:262:GLN:HA   | 2:H:262:GLN:NE2  | 2.19                     | 0.58              |
| 1:I:18:VAL:HB    | 1:I:67:ILE:HB    | 1.85                     | 0.58              |
| 2:J:27:VAL:HG12  | 4:J:607:HOH:O    | 2.02                     | 0.58              |
| 1:K:23:THR:HG22  | 1:K:24:ASN:N     | 2.19                     | 0.58              |
| 1:K:36:TRP:HH2   | 1:K:88:LYS:HE2   | 1.69                     | 0.58              |
| 1:M:23:THR:HG22  | 1:M:24:ASN:N     | 2.18                     | 0.58              |
| 1:M:97:LYS:HB3   | 1:M:102:THR:CG2  | 2.34                     | 0.58              |
| 1:O:79:ARG:HB3   | 1:O:170:MET:HE3  | 1.85                     | 0.58              |
| 2:B:43:PHE:HE2   | 2:B:102:PRO:HG3  | 1.68                     | 0.58              |
| 1:C:161:VAL:O    | 1:C:162:LEU:HG   | 2.04                     | 0.58              |
| 1:E:136:SER:C    | 1:E:138:ASN:H    | 2.11                     | 0.58              |
| 2:F:2:ALA:HB3    | 2:F:45:HIS:CE1   | 2.39                     | 0.58              |
| 1:G:102:THR:CA   | 2:H:171:THR:HG22 | 2.34                     | 0.58              |
| 2:H:43:PHE:HE2   | 2:H:102:PRO:HG3  | 1.68                     | 0.58              |
| 2:J:52:ILE:HG23  | 2:J:137:TYR:HB2  | 1.85                     | 0.58              |
| 1:K:24:ASN:ND2   | 1:K:59:GLY:O     | 2.37                     | 0.58              |
| 1:K:100:GLU:HG2  | 2:L:172:LEU:HD12 | 1.86                     | 0.58              |
| 2:P:251:GLY:O    | 2:P:252:LEU:HD23 | 2.03                     | 0.58              |
| 2:B:34:LEU:HB3   | 2:B:109:LEU:HB2  | 1.85                     | 0.58              |
| 2:F:262:GLN:HA   | 2:F:262:GLN:NE2  | 2.19                     | 0.58              |
| 2:H:59:GLN:HE21  | 2:H:143:GLN:NE2  | 2.02                     | 0.58              |
| 1:I:79:ARG:HB3   | 1:I:170:MET:HE3  | 1.86                     | 0.58              |
| 1:K:26:ASP:O     | 1:K:60:LYS:HB3   | 2.02                     | 0.58              |
| 1:M:158:GLY:HA3  | 1:M:184:ASN:ND2  | 2.19                     | 0.58              |
| 1:O:24:ASN:ND2   | 1:O:59:GLY:O     | 2.37                     | 0.58              |
| 1:O:193:TYR:CG   | 2:P:155:VAL:HG11 | 2.39                     | 0.58              |
| 2:P:46:ASN:HB2   | 2:P:96:ASN:HA    | 1.85                     | 0.58              |
| 2:B:126:ILE:CG1  | 2:B:150:ALA:HB2  | 2.34                     | 0.58              |
| 2:D:63:ALA:HB3   | 2:D:68:LEU:HD13  | 1.86                     | 0.58              |
| 1:E:155:LEU:HD12 | 1:E:187:TYR:HB3  | 1.85                     | 0.58              |
| 2:F:63:ALA:HB3   | 2:F:68:LEU:HD13  | 1.86                     | 0.58              |
| 2:F:126:ILE:CG1  | 2:F:150:ALA:HB2  | 2.34                     | 0.58              |
| 1:I:158:GLY:CA   | 1:I:184:ASN:HD22 | 2.17                     | 0.58              |
| 2:J:251:GLY:O    | 2:J:252:LEU:HD23 | 2.04                     | 0.58              |
| 1:O:18:VAL:HB    | 1:O:67:ILE:HB    | 1.85                     | 0.58              |
| 2:B:211:ASN:OD1  | 2:B:268:VAL:HA   | 2.03                     | 0.57              |
| 1:E:13:ALA:HB3   | 1:E:118:ALA:N    | 2.19                     | 0.57              |
| 1:E:28:ASN:O     | 1:E:29:SER:HB3   | 2.04                     | 0.57              |
| 2:H:49:PRO:HD2   | 2:H:98:ARG:CZ    | 2.33                     | 0.57              |
| 1:I:104:GLN:N    | 2:J:168:VAL:HG23 | 2.19                     | 0.57              |
| 1:I:158:GLY:HA3  | 1:I:184:ASN:ND2  | 2.19                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:44:CYS:HB2   | 2:J:95:TYR:CE2   | 2.38                     | 0.57              |
| 1:M:33:ILE:CG1   | 1:M:57:MET:HB2   | 2.33                     | 0.57              |
| 2:P:38:LEU:C     | 2:P:40:THR:N     | 2.61                     | 0.57              |
| 2:B:138:ASN:ND2  | 2:B:140:ASP:H    | 2.00                     | 0.57              |
| 1:C:28:ASN:O     | 1:C:29:SER:HB3   | 2.03                     | 0.57              |
| 1:C:102:THR:CA   | 2:D:171:THR:HG22 | 2.33                     | 0.57              |
| 1:E:135:ARG:NH2  | 1:E:181:ALA:HB1  | 2.18                     | 0.57              |
| 2:J:43:PHE:CE2   | 2:J:102:PRO:HG3  | 2.38                     | 0.57              |
| 2:J:226:THR:HA   | 2:J:230:THR:O    | 2.04                     | 0.57              |
| 2:N:46:ASN:CB    | 2:N:96:ASN:HA    | 2.32                     | 0.57              |
| 2:N:226:THR:HA   | 2:N:230:THR:O    | 2.04                     | 0.57              |
| 2:P:122:ALA:HA   | 2:P:150:ALA:O    | 2.03                     | 0.57              |
| 1:A:161:VAL:HG22 | 1:A:162:LEU:N    | 2.16                     | 0.57              |
| 1:K:97:LYS:HB3   | 1:K:102:THR:CG2  | 2.34                     | 0.57              |
| 1:O:158:GLY:CA   | 1:O:184:ASN:HD22 | 2.16                     | 0.57              |
| 2:P:75:VAL:HG23  | 2:P:107:LEU:HD12 | 1.85                     | 0.57              |
| 1:A:66:ARG:HG2   | 1:A:66:ARG:HH11  | 1.69                     | 0.57              |
| 1:C:8:ARG:HB3    | 1:C:8:ARG:NH1    | 2.19                     | 0.57              |
| 1:C:13:ALA:HB3   | 1:C:118:ALA:N    | 2.19                     | 0.57              |
| 1:C:86:ASN:ND2   | 1:C:110:ARG:HE   | 2.02                     | 0.57              |
| 1:C:161:VAL:HG22 | 1:C:162:LEU:N    | 2.16                     | 0.57              |
| 2:F:34:LEU:HB3   | 2:F:109:LEU:HB2  | 1.86                     | 0.57              |
| 2:F:201:THR:CG2  | 2:F:206:ASN:HD22 | 2.14                     | 0.57              |
| 1:M:104:GLN:N    | 2:N:168:VAL:HG23 | 2.19                     | 0.57              |
| 1:M:193:TYR:CG   | 2:N:155:VAL:HG11 | 2.40                     | 0.57              |
| 1:C:136:SER:C    | 1:C:138:ASN:H    | 2.11                     | 0.57              |
| 2:D:136:ASN:C    | 2:D:136:ASN:ND2  | 2.56                     | 0.57              |
| 1:G:155:LEU:HD12 | 1:G:187:TYR:HB3  | 1.86                     | 0.57              |
| 2:H:111:PRO:HB3  | 2:H:156:VAL:HG21 | 1.85                     | 0.57              |
| 2:J:175:TYR:CE1  | 2:J:263:VAL:HG21 | 2.40                     | 0.57              |
| 1:K:193:TYR:CG   | 2:L:155:VAL:HG11 | 2.39                     | 0.57              |
| 1:M:100:GLU:HG2  | 2:N:172:LEU:HD12 | 1.85                     | 0.57              |
| 2:N:44:CYS:HB2   | 2:N:95:TYR:CE2   | 2.39                     | 0.57              |
| 2:N:46:ASN:HB2   | 2:N:96:ASN:HA    | 1.86                     | 0.57              |
| 1:O:33:ILE:CG1   | 1:O:57:MET:HB2   | 2.34                     | 0.57              |
| 2:P:227:ARG:HH12 | 2:P:232:ILE:HA   | 1.70                     | 0.57              |
| 2:B:111:PRO:HB3  | 2:B:156:VAL:HG21 | 1.86                     | 0.57              |
| 2:B:179:VAL:O    | 2:B:253:THR:HG23 | 2.04                     | 0.57              |
| 2:F:92:ARG:HG3   | 2:F:92:ARG:HH11  | 1.68                     | 0.57              |
| 2:H:184:THR:HG22 | 2:H:249:SER:HA   | 1.86                     | 0.57              |
| 1:I:193:TYR:CG   | 2:J:155:VAL:HG11 | 2.39                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:44:CYS:HB2   | 2:L:95:TYR:CE2   | 2.39                     | 0.57              |
| 2:L:67:VAL:HG22  | 2:L:109:LEU:HD13 | 1.87                     | 0.57              |
| 1:M:18:VAL:HB    | 1:M:67:ILE:HB    | 1.85                     | 0.57              |
| 1:M:24:ASN:ND2   | 1:M:59:GLY:O     | 2.37                     | 0.57              |
| 2:P:44:CYS:HB2   | 2:P:95:TYR:CE2   | 2.39                     | 0.57              |
| 1:A:135:ARG:NH2  | 1:A:181:ALA:HB1  | 2.18                     | 0.57              |
| 1:A:159:THR:CG2  | 1:A:180:ASP:HB3  | 2.35                     | 0.57              |
| 1:C:140:LEU:HD12 | 1:C:177:LEU:CD1  | 2.35                     | 0.57              |
| 2:F:184:THR:HG22 | 2:F:249:SER:HA   | 1.86                     | 0.57              |
| 2:F:219:GLN:HG3  | 4:F:503:HOH:O    | 2.05                     | 0.57              |
| 1:G:163:GLU:OE1  | 1:G:163:GLU:HA   | 2.05                     | 0.57              |
| 1:I:24:ASN:ND2   | 1:I:59:GLY:O     | 2.37                     | 0.57              |
| 1:M:88:LYS:HE3   | 1:M:90:ILE:HG12  | 1.85                     | 0.57              |
| 1:O:97:LYS:HB3   | 1:O:102:THR:CG2  | 2.34                     | 0.57              |
| 1:E:161:VAL:O    | 1:E:162:LEU:HG   | 2.05                     | 0.57              |
| 1:E:179:SER:O    | 1:E:181:ALA:N    | 2.38                     | 0.57              |
| 1:G:159:THR:CG2  | 1:G:180:ASP:HB3  | 2.35                     | 0.57              |
| 1:M:79:ARG:HB3   | 1:M:170:MET:HE3  | 1.85                     | 0.57              |
| 2:N:227:ARG:HH12 | 2:N:232:ILE:HA   | 1.69                     | 0.57              |
| 1:O:176:LYS:HZ3  | 1:O:176:LYS:HB2  | 1.70                     | 0.57              |
| 1:C:179:SER:O    | 1:C:181:ALA:N    | 2.38                     | 0.57              |
| 2:H:76:LYS:HB3   | 4:H:617:HOH:O    | 2.04                     | 0.57              |
| 1:K:47:ARG:HH12  | 1:K:71:THR:HA    | 1.70                     | 0.57              |
| 1:K:101:ASN:HA   | 2:L:268:VAL:O    | 2.04                     | 0.57              |
| 1:A:147:PRO:HG2  | 1:A:148:TYR:CE1  | 2.40                     | 0.57              |
| 3:F:502:MMA:H2   | 4:F:531:HOH:O    | 2.04                     | 0.57              |
| 1:G:84:TRP:CZ3   | 1:G:112:LYS:HG2  | 2.40                     | 0.57              |
| 1:K:18:VAL:HB    | 1:K:67:ILE:HB    | 1.86                     | 0.57              |
| 1:K:105:LEU:CD1  | 2:L:183:LEU:HD11 | 2.35                     | 0.57              |
| 1:M:77:GLN:HA    | 1:M:77:GLN:NE2   | 2.20                     | 0.57              |
| 2:N:38:LEU:C     | 2:N:40:THR:N     | 2.61                     | 0.57              |
| 2:N:52:ILE:HG23  | 2:N:137:TYR:HB2  | 1.86                     | 0.57              |
| 1:A:71:THR:HG23  | 1:A:71:THR:O     | 2.05                     | 0.56              |
| 2:B:2:ALA:HB3    | 2:B:45:HIS:CE1   | 2.40                     | 0.56              |
| 2:D:138:ASN:ND2  | 2:D:140:ASP:H    | 2.02                     | 0.56              |
| 1:G:179:SER:O    | 1:G:181:ALA:N    | 2.38                     | 0.56              |
| 2:H:59:GLN:HG3   | 2:H:143:GLN:HE21 | 1.70                     | 0.56              |
| 1:M:47:ARG:HH12  | 1:M:71:THR:HA    | 1.70                     | 0.56              |
| 1:M:142:LEU:N    | 1:M:174:THR:HG22 | 2.20                     | 0.56              |
| 2:N:212:THR:HG21 | 2:N:271:ILE:CD1  | 2.35                     | 0.56              |
| 1:A:136:SER:C    | 1:A:138:ASN:H    | 2.10                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:179:SER:O    | 1:A:181:ALA:N    | 2.39                     | 0.56              |
| 2:B:201:THR:CG2  | 2:B:206:ASN:HD22 | 2.16                     | 0.56              |
| 2:D:59:GLN:HE21  | 2:D:143:GLN:NE2  | 2.03                     | 0.56              |
| 2:D:126:ILE:CG1  | 2:D:150:ALA:HB2  | 2.35                     | 0.56              |
| 2:F:130:ILE:HG12 | 2:F:145:VAL:HG22 | 1.87                     | 0.56              |
| 2:L:175:TYR:CE1  | 2:L:263:VAL:HG21 | 2.40                     | 0.56              |
| 2:N:251:GLY:O    | 2:N:252:LEU:HD23 | 2.04                     | 0.56              |
| 2:P:226:THR:HA   | 2:P:230:THR:O    | 2.04                     | 0.56              |
| 2:B:262:GLN:NE2  | 2:B:262:GLN:HA   | 2.19                     | 0.56              |
| 2:D:111:PRO:HB3  | 2:D:156:VAL:HG21 | 1.85                     | 0.56              |
| 1:E:71:THR:HG23  | 1:E:71:THR:O     | 2.05                     | 0.56              |
| 1:E:84:TRP:CZ3   | 1:E:112:LYS:HG2  | 2.40                     | 0.56              |
| 2:H:2:ALA:HB3    | 2:H:45:HIS:CE1   | 2.41                     | 0.56              |
| 1:I:114:TYR:CZ   | 1:I:149:TYR:HB2  | 2.40                     | 0.56              |
| 2:J:96:ASN:N     | 2:J:96:ASN:ND2   | 2.45                     | 0.56              |
| 2:J:227:ARG:HH12 | 2:J:232:ILE:HA   | 1.69                     | 0.56              |
| 1:K:104:GLN:N    | 2:L:168:VAL:HG23 | 2.19                     | 0.56              |
| 1:M:105:LEU:CD1  | 2:N:183:LEU:HD11 | 2.35                     | 0.56              |
| 1:M:129:GLU:HB3  | 1:M:200:MET:SD   | 2.45                     | 0.56              |
| 2:N:40:THR:HG22  | 2:N:40:THR:O     | 2.04                     | 0.56              |
| 2:N:67:VAL:HG22  | 2:N:109:LEU:HD13 | 1.86                     | 0.56              |
| 1:O:114:TYR:CZ   | 1:O:149:TYR:HB2  | 2.40                     | 0.56              |
| 1:A:28:ASN:O     | 1:A:29:SER:HB3   | 2.05                     | 0.56              |
| 1:C:163:GLU:OE1  | 1:C:163:GLU:HA   | 2.05                     | 0.56              |
| 1:I:47:ARG:HH12  | 1:I:71:THR:HA    | 1.70                     | 0.56              |
| 1:I:88:LYS:HE3   | 1:I:90:ILE:CG1   | 2.36                     | 0.56              |
| 1:I:97:LYS:HB3   | 1:I:102:THR:CG2  | 2.34                     | 0.56              |
| 2:L:53:THR:HG22  | 2:L:96:ASN:OD1   | 2.06                     | 0.56              |
| 2:L:251:GLY:O    | 2:L:252:LEU:HD23 | 2.05                     | 0.56              |
| 1:O:36:TRP:HH2   | 1:O:88:LYS:HE2   | 1.69                     | 0.56              |
| 2:P:210:THR:CG2  | 2:P:259:THR:HG21 | 2.29                     | 0.56              |
| 1:A:178:PRO:O    | 1:A:180:ASP:N    | 2.39                     | 0.56              |
| 1:C:73:ASN:HA    | 4:C:213:HOH:O    | 2.06                     | 0.56              |
| 1:C:178:PRO:O    | 1:C:180:ASP:N    | 2.39                     | 0.56              |
| 1:E:161:VAL:HG22 | 1:E:162:LEU:N    | 2.16                     | 0.56              |
| 2:F:138:ASN:ND2  | 2:F:140:ASP:H    | 2.03                     | 0.56              |
| 1:G:147:PRO:HG2  | 1:G:148:TYR:CE1  | 2.40                     | 0.56              |
| 1:K:88:LYS:HE3   | 1:K:90:ILE:CG1   | 2.36                     | 0.56              |
| 1:K:129:GLU:HB3  | 1:K:200:MET:SD   | 2.46                     | 0.56              |
| 1:O:24:ASN:O     | 1:O:60:LYS:HB2   | 2.06                     | 0.56              |
| 1:O:176:LYS:HB2  | 1:O:176:LYS:NZ   | 2.21                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:175:TYR:CE1  | 2:P:263:VAL:HG21 | 2.40                     | 0.56              |
| 2:F:59:GLN:HG3   | 2:F:143:GLN:HE21 | 1.70                     | 0.56              |
| 1:I:77:GLN:HA    | 1:I:77:GLN:NE2   | 2.20                     | 0.56              |
| 1:I:107:ILE:H    | 1:I:107:ILE:CD1  | 2.19                     | 0.56              |
| 2:J:75:VAL:HG23  | 2:J:107:LEU:HD12 | 1.86                     | 0.56              |
| 2:N:75:VAL:HG23  | 2:N:107:LEU:HD12 | 1.87                     | 0.56              |
| 2:P:67:VAL:HG22  | 2:P:109:LEU:HD13 | 1.88                     | 0.56              |
| 2:P:197:LEU:HD11 | 2:P:225:LEU:HD12 | 1.88                     | 0.56              |
| 1:C:159:THR:CG2  | 1:C:180:ASP:HB3  | 2.36                     | 0.56              |
| 2:D:34:LEU:HB3   | 2:D:109:LEU:HB2  | 1.86                     | 0.56              |
| 1:K:114:TYR:CZ   | 1:K:149:TYR:HB2  | 2.40                     | 0.56              |
| 1:O:88:LYS:HE3   | 1:O:90:ILE:CG1   | 2.35                     | 0.56              |
| 2:P:40:THR:O     | 2:P:40:THR:HG22  | 2.05                     | 0.56              |
| 1:C:147:PRO:HG2  | 1:C:148:TYR:CE1  | 2.41                     | 0.56              |
| 2:F:111:PRO:HB3  | 2:F:156:VAL:HG21 | 1.87                     | 0.56              |
| 2:L:135:ASN:HD21 | 2:L:138:ASN:ND2  | 2.02                     | 0.56              |
| 1:M:24:ASN:O     | 1:M:60:LYS:HB2   | 2.06                     | 0.56              |
| 1:O:35:SER:HB2   | 1:O:50:VAL:HG11  | 1.88                     | 0.56              |
| 1:O:129:GLU:HB3  | 1:O:200:MET:SD   | 2.45                     | 0.56              |
| 2:P:135:ASN:HD21 | 2:P:138:ASN:ND2  | 2.03                     | 0.56              |
| 1:A:161:VAL:O    | 1:A:162:LEU:HG   | 2.06                     | 0.56              |
| 1:A:176:LYS:HD2  | 1:A:176:LYS:N    | 2.20                     | 0.56              |
| 1:C:10:ILE:O     | 1:C:12:PRO:HD3   | 2.06                     | 0.56              |
| 1:C:71:THR:HG23  | 1:C:71:THR:O     | 2.06                     | 0.56              |
| 2:J:44:CYS:HB2   | 2:J:95:TYR:HE2   | 1.71                     | 0.56              |
| 1:K:176:LYS:HB2  | 1:K:176:LYS:NZ   | 2.21                     | 0.56              |
| 1:M:176:LYS:HB2  | 1:M:176:LYS:NZ   | 2.21                     | 0.56              |
| 1:O:47:ARG:HH12  | 1:O:71:THR:HA    | 1.71                     | 0.56              |
| 1:O:105:LEU:CD1  | 2:P:183:LEU:HD11 | 2.35                     | 0.56              |
| 1:O:107:ILE:H    | 1:O:107:ILE:CD1  | 2.19                     | 0.56              |
| 1:A:8:ARG:NH1    | 1:A:8:ARG:HB3    | 2.21                     | 0.56              |
| 1:A:13:ALA:HB3   | 1:A:118:ALA:N    | 2.20                     | 0.56              |
| 1:G:129:GLU:HA   | 1:G:200:MET:CE   | 2.36                     | 0.56              |
| 1:I:105:LEU:CD1  | 2:J:183:LEU:HD11 | 2.35                     | 0.56              |
| 1:I:112:LYS:HZ2  | 1:I:166:LEU:HD22 | 1.70                     | 0.56              |
| 2:J:126:ILE:HD13 | 4:J:614:HOH:O    | 2.04                     | 0.56              |
| 1:K:24:ASN:O     | 1:K:60:LYS:HB2   | 2.06                     | 0.56              |
| 1:K:52:PRO:HD2   | 1:K:65:LEU:HA    | 1.88                     | 0.56              |
| 1:M:107:ILE:H    | 1:M:107:ILE:CD1  | 2.18                     | 0.56              |
| 1:O:142:LEU:N    | 1:O:174:THR:HG22 | 2.21                     | 0.56              |
| 2:B:113:SER:CB   | 2:P:81:SER:H     | 2.11                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:159:THR:CG2  | 1:E:180:ASP:HB3  | 2.36                     | 0.55              |
| 2:F:43:PHE:HE2   | 2:F:102:PRO:HG3  | 1.70                     | 0.55              |
| 1:G:71:THR:O     | 1:G:71:THR:HG23  | 2.05                     | 0.55              |
| 2:J:196:TYR:HB3  | 2:J:237:THR:HA   | 1.88                     | 0.55              |
| 2:N:135:ASN:HD21 | 2:N:138:ASN:ND2  | 2.03                     | 0.55              |
| 2:N:197:LEU:HD11 | 2:N:225:LEU:HD12 | 1.88                     | 0.55              |
| 2:P:212:THR:HG21 | 2:P:271:ILE:CD1  | 2.36                     | 0.55              |
| 2:D:262:GLN:NE2  | 2:D:262:GLN:HA   | 2.20                     | 0.55              |
| 1:E:102:THR:HA   | 2:F:171:THR:HG22 | 1.88                     | 0.55              |
| 2:J:184:THR:HA   | 2:J:248:VAL:O    | 2.06                     | 0.55              |
| 1:K:103:LEU:HB3  | 2:L:169:THR:HB   | 1.89                     | 0.55              |
| 2:N:84:PHE:HA    | 2:N:85:PRO:C     | 2.31                     | 0.55              |
| 2:B:59:GLN:HG3   | 2:B:143:GLN:NE2  | 2.21                     | 0.55              |
| 2:D:179:VAL:O    | 2:D:253:THR:HG23 | 2.06                     | 0.55              |
| 1:E:8:ARG:HB3    | 1:E:8:ARG:NH1    | 2.22                     | 0.55              |
| 2:J:40:THR:O     | 2:J:40:THR:HG22  | 2.05                     | 0.55              |
| 2:J:84:PHE:HA    | 2:J:85:PRO:C     | 2.31                     | 0.55              |
| 1:K:142:LEU:N    | 1:K:174:THR:HG22 | 2.21                     | 0.55              |
| 2:L:212:THR:HG21 | 2:L:271:ILE:CD1  | 2.35                     | 0.55              |
| 2:N:175:TYR:CE1  | 2:N:263:VAL:HG21 | 2.41                     | 0.55              |
| 1:A:75:LEU:HB2   | 4:A:218:HOH:O    | 2.07                     | 0.55              |
| 1:G:8:ARG:HB3    | 1:G:8:ARG:NH1    | 2.21                     | 0.55              |
| 1:G:140:LEU:HD12 | 1:G:177:LEU:CD1  | 2.36                     | 0.55              |
| 1:G:178:PRO:O    | 1:G:180:ASP:N    | 2.39                     | 0.55              |
| 1:I:35:SER:HB2   | 1:I:50:VAL:HG11  | 1.89                     | 0.55              |
| 1:I:142:LEU:N    | 1:I:174:THR:HG22 | 2.21                     | 0.55              |
| 2:J:212:THR:HG21 | 2:J:271:ILE:CD1  | 2.35                     | 0.55              |
| 1:M:114:TYR:CZ   | 1:M:149:TYR:HB2  | 2.41                     | 0.55              |
| 1:C:176:LYS:HD2  | 1:C:176:LYS:N    | 2.21                     | 0.55              |
| 2:D:59:GLN:HG3   | 2:D:143:GLN:HE21 | 1.71                     | 0.55              |
| 1:E:163:GLU:HA   | 1:E:163:GLU:OE1  | 2.07                     | 0.55              |
| 1:E:178:PRO:O    | 1:E:180:ASP:N    | 2.39                     | 0.55              |
| 1:I:24:ASN:O     | 1:I:60:LYS:HB2   | 2.06                     | 0.55              |
| 1:I:52:PRO:HD2   | 1:I:65:LEU:HA    | 1.88                     | 0.55              |
| 1:I:176:LYS:HB2  | 1:I:176:LYS:NZ   | 2.22                     | 0.55              |
| 2:J:67:VAL:HG22  | 2:J:109:LEU:HD13 | 1.87                     | 0.55              |
| 1:K:30:THR:OG1   | 1:K:58:LYS:HE3   | 2.06                     | 0.55              |
| 1:K:107:ILE:H    | 1:K:107:ILE:CD1  | 2.19                     | 0.55              |
| 2:N:145:VAL:HG12 | 2:N:146:TRP:N    | 2.21                     | 0.55              |
| 2:N:184:THR:HA   | 2:N:248:VAL:O    | 2.07                     | 0.55              |
| 1:I:30:THR:OG1   | 1:I:58:LYS:HE3   | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:79:ARG:HA    | 1:I:147:PRO:CB   | 2.37                     | 0.55              |
| 1:I:129:GLU:HB3  | 1:I:200:MET:SD   | 2.46                     | 0.55              |
| 1:M:154:GLU:OE1  | 1:M:188:ARG:HD3  | 2.07                     | 0.55              |
| 1:O:107:ILE:HG21 | 2:P:163:VAL:HG11 | 1.89                     | 0.55              |
| 1:E:144:ASN:ND2  | 1:E:150:LEU:HG   | 2.22                     | 0.55              |
| 1:G:161:VAL:HG22 | 1:G:162:LEU:N    | 2.18                     | 0.55              |
| 1:I:103:LEU:HB3  | 2:J:169:THR:HB   | 1.88                     | 0.55              |
| 1:I:122:LEU:CD2  | 1:I:146:THR:HG22 | 2.36                     | 0.55              |
| 2:L:75:VAL:HG23  | 2:L:107:LEU:HD12 | 1.87                     | 0.55              |
| 1:M:188:ARG:HH21 | 1:M:196:LEU:HD12 | 1.71                     | 0.55              |
| 2:P:196:TYR:HB3  | 2:P:237:THR:HA   | 1.88                     | 0.55              |
| 2:D:2:ALA:HB3    | 2:D:45:HIS:CE1   | 2.41                     | 0.55              |
| 1:E:129:GLU:HA   | 1:E:200:MET:CE   | 2.37                     | 0.55              |
| 1:E:140:LEU:HD12 | 1:E:177:LEU:CD1  | 2.35                     | 0.55              |
| 2:L:40:THR:O     | 2:L:40:THR:HG22  | 2.05                     | 0.55              |
| 2:L:44:CYS:HB2   | 2:L:95:TYR:HE2   | 1.72                     | 0.55              |
| 1:A:140:LEU:HD12 | 1:A:177:LEU:CD1  | 2.36                     | 0.55              |
| 2:J:17:SER:HB2   | 2:L:262:GLN:OE1  | 2.07                     | 0.55              |
| 1:K:122:LEU:CD2  | 1:K:146:THR:HG22 | 2.37                     | 0.55              |
| 1:M:88:LYS:HE3   | 1:M:90:ILE:CG1   | 2.37                     | 0.55              |
| 1:O:6:ALA:HB3    | 1:O:20:LEU:CD2   | 2.37                     | 0.55              |
| 1:O:52:PRO:HD2   | 1:O:65:LEU:HA    | 1.87                     | 0.55              |
| 2:P:44:CYS:HB2   | 2:P:95:TYR:HE2   | 1.72                     | 0.55              |
| 2:L:172:LEU:O    | 2:L:172:LEU:HD23 | 2.07                     | 0.55              |
| 1:O:103:LEU:HB3  | 2:P:169:THR:HB   | 1.88                     | 0.55              |
| 2:D:43:PHE:HE2   | 2:D:102:PRO:HG3  | 1.72                     | 0.54              |
| 1:I:188:ARG:HH21 | 1:I:196:LEU:HD12 | 1.72                     | 0.54              |
| 1:K:107:ILE:HG21 | 2:L:163:VAL:HG11 | 1.89                     | 0.54              |
| 1:M:79:ARG:HA    | 1:M:147:PRO:CB   | 2.37                     | 0.54              |
| 1:O:46:GLY:HA2   | 4:O:206:HOH:O    | 2.07                     | 0.54              |
| 1:C:191:ASN:HD21 | 1:C:195:ALA:HB3  | 1.73                     | 0.54              |
| 1:E:82:LEU:O     | 4:E:213:HOH:O    | 2.18                     | 0.54              |
| 2:J:172:LEU:O    | 2:J:172:LEU:HD23 | 2.08                     | 0.54              |
| 1:O:77:GLN:HA    | 1:O:77:GLN:NE2   | 2.22                     | 0.54              |
| 1:O:188:ARG:HH21 | 1:O:196:LEU:HD12 | 1.72                     | 0.54              |
| 2:B:135:ASN:HD22 | 2:B:137:TYR:HB3  | 1.72                     | 0.54              |
| 1:C:84:TRP:CZ3   | 1:C:112:LYS:HG2  | 2.42                     | 0.54              |
| 2:D:53:THR:HB    | 2:D:136:ASN:OD1  | 2.07                     | 0.54              |
| 2:H:262:GLN:HA   | 2:H:262:GLN:HE21 | 1.73                     | 0.54              |
| 1:I:107:ILE:HG21 | 2:J:163:VAL:HG11 | 1.90                     | 0.54              |
| 2:J:53:THR:HG22  | 2:J:96:ASN:OD1   | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:145:VAL:HG12 | 2:L:146:TRP:N    | 2.22                     | 0.54              |
| 1:M:52:PRO:HD2   | 1:M:65:LEU:HA    | 1.88                     | 0.54              |
| 2:F:59:GLN:HE21  | 2:F:143:GLN:NE2  | 2.04                     | 0.54              |
| 2:J:197:LEU:HD11 | 2:J:225:LEU:HD12 | 1.89                     | 0.54              |
| 1:K:77:GLN:HA    | 1:K:77:GLN:NE2   | 2.21                     | 0.54              |
| 2:L:196:TYR:HB3  | 2:L:237:THR:HA   | 1.88                     | 0.54              |
| 1:M:122:LEU:CD2  | 1:M:146:THR:HG22 | 2.37                     | 0.54              |
| 2:P:22:VAL:HG12  | 2:P:41:GLN:HG3   | 1.90                     | 0.54              |
| 2:B:130:ILE:HG12 | 2:B:145:VAL:HG22 | 1.90                     | 0.54              |
| 1:G:28:ASN:O     | 1:G:29:SER:HB3   | 2.05                     | 0.54              |
| 2:H:138:ASN:C    | 2:H:138:ASN:ND2  | 2.56                     | 0.54              |
| 2:J:22:VAL:HG12  | 2:J:41:GLN:HG3   | 1.90                     | 0.54              |
| 1:K:157:ALA:HA   | 1:K:184:ASN:O    | 2.08                     | 0.54              |
| 1:M:35:SER:HB2   | 1:M:50:VAL:HG11  | 1.89                     | 0.54              |
| 2:N:53:THR:HG22  | 2:N:96:ASN:OD1   | 2.08                     | 0.54              |
| 1:O:30:THR:OG1   | 1:O:58:LYS:HE3   | 2.06                     | 0.54              |
| 1:A:133:PHE:O    | 1:A:205:GLU:HG2  | 2.08                     | 0.54              |
| 2:F:209:PHE:CD1  | 2:F:272:ILE:HD12 | 2.43                     | 0.54              |
| 2:H:6:ALA:HB2    | 2:H:41:GLN:HA    | 1.90                     | 0.54              |
| 1:O:142:LEU:H    | 1:O:174:THR:HG22 | 1.73                     | 0.54              |
| 2:P:172:LEU:HD23 | 2:P:172:LEU:O    | 2.07                     | 0.54              |
| 1:A:163:GLU:OE1  | 1:A:163:GLU:HA   | 2.06                     | 0.54              |
| 2:B:63:ALA:HB3   | 2:B:68:LEU:HD13  | 1.90                     | 0.54              |
| 1:G:71:THR:O     | 1:G:73:ASN:N     | 2.41                     | 0.54              |
| 2:J:195:TYR:O    | 2:J:237:THR:HA   | 2.08                     | 0.54              |
| 1:M:30:THR:OG1   | 1:M:58:LYS:HE3   | 2.06                     | 0.54              |
| 1:M:107:ILE:HG21 | 2:N:163:VAL:HG11 | 1.90                     | 0.54              |
| 1:M:142:LEU:H    | 1:M:174:THR:HG22 | 1.71                     | 0.54              |
| 2:P:42:ILE:HD13  | 2:P:146:TRP:CD2  | 2.43                     | 0.54              |
| 2:P:184:THR:HA   | 2:P:248:VAL:O    | 2.07                     | 0.54              |
| 1:A:71:THR:O     | 1:A:73:ASN:N     | 2.40                     | 0.54              |
| 2:F:53:THR:HB    | 2:F:136:ASN:OD1  | 2.08                     | 0.54              |
| 2:F:67:VAL:CG2   | 2:F:120:ILE:HD11 | 2.38                     | 0.54              |
| 1:I:122:LEU:HD23 | 1:I:146:THR:HG22 | 1.90                     | 0.54              |
| 1:K:35:SER:HB2   | 1:K:50:VAL:HG11  | 1.89                     | 0.54              |
| 1:K:188:ARG:HH21 | 1:K:196:LEU:HD12 | 1.72                     | 0.54              |
| 2:L:197:LEU:HD11 | 2:L:225:LEU:HD12 | 1.89                     | 0.54              |
| 2:N:196:TYR:HB3  | 2:N:237:THR:HA   | 1.88                     | 0.54              |
| 1:O:157:ALA:HA   | 1:O:184:ASN:O    | 2.08                     | 0.54              |
| 2:P:145:VAL:HG12 | 2:P:146:TRP:N    | 2.22                     | 0.54              |
| 2:B:43:PHE:CE2   | 2:B:102:PRO:HG3  | 2.43                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:71:THR:O     | 1:C:73:ASN:N     | 2.41                     | 0.54              |
| 2:D:92:ARG:HH11  | 2:D:92:ARG:HG3   | 1.72                     | 0.54              |
| 1:G:176:LYS:HD2  | 1:G:176:LYS:N    | 2.20                     | 0.54              |
| 1:K:133:PHE:HB2  | 1:K:204:MET:SD   | 2.48                     | 0.54              |
| 2:L:42:ILE:HD13  | 2:L:146:TRP:CD2  | 2.43                     | 0.54              |
| 1:M:6:ALA:HB3    | 1:M:20:LEU:CD2   | 2.38                     | 0.54              |
| 1:O:140:LEU:HD12 | 1:O:162:LEU:HD11 | 1.90                     | 0.54              |
| 2:P:71:PHE:HB3   | 2:P:110:THR:H    | 1.73                     | 0.54              |
| 2:B:50:GLU:CD    | 2:B:98:ARG:HH12  | 2.16                     | 0.54              |
| 1:C:132:ARG:HG2  | 4:C:212:HOH:O    | 2.07                     | 0.54              |
| 1:E:176:LYS:HD2  | 1:E:176:LYS:N    | 2.20                     | 0.54              |
| 2:H:38:LEU:C     | 2:H:40:THR:N     | 2.66                     | 0.54              |
| 2:H:113:SER:CB   | 2:L:81:SER:H     | 2.13                     | 0.54              |
| 2:H:135:ASN:HD22 | 2:H:137:TYR:HB3  | 1.72                     | 0.54              |
| 1:I:154:GLU:OE1  | 1:I:188:ARG:HD3  | 2.08                     | 0.54              |
| 2:J:197:LEU:O    | 2:J:198:SER:HB3  | 2.08                     | 0.54              |
| 1:M:103:LEU:HB3  | 2:N:169:THR:HB   | 1.88                     | 0.54              |
| 2:H:192:ASN:HA   | 2:H:242:ALA:HA   | 1.89                     | 0.53              |
| 2:L:184:THR:HA   | 2:L:248:VAL:O    | 2.07                     | 0.53              |
| 2:L:195:TYR:O    | 2:L:237:THR:HA   | 2.09                     | 0.53              |
| 1:M:176:LYS:HB2  | 1:M:176:LYS:HZ3  | 1.73                     | 0.53              |
| 2:N:42:ILE:HD13  | 2:N:146:TRP:CD2  | 2.43                     | 0.53              |
| 2:P:197:LEU:O    | 2:P:198:SER:HB3  | 2.09                     | 0.53              |
| 2:D:126:ILE:HB   | 2:D:148:ILE:HG22 | 1.91                     | 0.53              |
| 2:F:135:ASN:HD22 | 2:F:137:TYR:HB3  | 1.72                     | 0.53              |
| 2:H:5:THR:HG22   | 2:H:9:THR:H      | 1.74                     | 0.53              |
| 1:I:133:PHE:HB2  | 1:I:204:MET:SD   | 2.48                     | 0.53              |
| 1:I:140:LEU:HD12 | 1:I:162:LEU:HD11 | 1.89                     | 0.53              |
| 2:L:103:TRP:O    | 2:L:105:VAL:N    | 2.41                     | 0.53              |
| 2:N:22:VAL:HG12  | 2:N:41:GLN:HG3   | 1.90                     | 0.53              |
| 2:N:44:CYS:HB2   | 2:N:95:TYR:HE2   | 1.73                     | 0.53              |
| 1:O:1:GLY:HA3    | 2:P:162:ASP:OD1  | 2.08                     | 0.53              |
| 1:O:81:SER:O     | 1:O:83:PHE:HD1   | 1.91                     | 0.53              |
| 2:D:184:THR:HG22 | 2:D:249:SER:CA   | 2.38                     | 0.53              |
| 1:G:133:PHE:O    | 1:G:205:GLU:HG2  | 2.08                     | 0.53              |
| 2:H:48:TYR:H     | 3:H:603:MMA:H62  | 1.73                     | 0.53              |
| 1:I:6:ALA:HB3    | 1:I:20:LEU:CD2   | 2.38                     | 0.53              |
| 2:J:172:LEU:N    | 2:J:173:PRO:CD   | 2.72                     | 0.53              |
| 1:K:122:LEU:HD23 | 1:K:146:THR:HG22 | 1.91                     | 0.53              |
| 1:K:154:GLU:OE1  | 1:K:188:ARG:HD3  | 2.09                     | 0.53              |
| 2:L:22:VAL:HG12  | 2:L:41:GLN:HG3   | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:157:ALA:HA   | 1:M:184:ASN:O    | 2.08                     | 0.53              |
| 1:O:91:PRO:HD2   | 1:O:106:ALA:HB2  | 1.90                     | 0.53              |
| 1:O:136:SER:HB2  | 1:O:139:SER:HB2  | 1.90                     | 0.53              |
| 2:P:11:ILE:HG23  | 2:P:16:GLY:CA    | 2.32                     | 0.53              |
| 2:P:172:LEU:N    | 2:P:173:PRO:CD   | 2.71                     | 0.53              |
| 1:A:84:TRP:CZ3   | 1:A:112:LYS:HG2  | 2.43                     | 0.53              |
| 1:A:144:ASN:ND2  | 1:A:150:LEU:HG   | 2.24                     | 0.53              |
| 1:C:129:GLU:HA   | 1:C:200:MET:CE   | 2.38                     | 0.53              |
| 2:F:90:THR:HB    | 2:F:91:PRO:HD2   | 1.91                     | 0.53              |
| 1:G:102:THR:HA   | 2:H:171:THR:HG22 | 1.90                     | 0.53              |
| 2:H:43:PHE:CE2   | 2:H:102:PRO:HG3  | 2.44                     | 0.53              |
| 2:H:50:GLU:CD    | 2:H:98:ARG:HH12  | 2.16                     | 0.53              |
| 1:I:157:ALA:HA   | 1:I:184:ASN:O    | 2.08                     | 0.53              |
| 2:J:14:GLY:HA2   | 2:J:142:PHE:CD2  | 2.44                     | 0.53              |
| 1:K:6:ALA:HB3    | 1:K:20:LEU:CD2   | 2.38                     | 0.53              |
| 1:K:79:ARG:HA    | 1:K:147:PRO:CB   | 2.36                     | 0.53              |
| 1:M:91:PRO:HD2   | 1:M:106:ALA:HB2  | 1.91                     | 0.53              |
| 1:O:122:LEU:CD2  | 1:O:146:THR:HG22 | 2.38                     | 0.53              |
| 2:B:173:PRO:O    | 2:B:174:ASP:C    | 2.52                     | 0.53              |
| 2:B:184:THR:HG22 | 2:B:249:SER:CA   | 2.38                     | 0.53              |
| 2:D:6:ALA:HB2    | 2:D:41:GLN:HA    | 1.90                     | 0.53              |
| 2:D:50:GLU:CD    | 2:D:98:ARG:HH12  | 2.17                     | 0.53              |
| 1:E:71:THR:O     | 1:E:73:ASN:N     | 2.42                     | 0.53              |
| 1:I:95:LYS:HD2   | 1:I:95:LYS:N     | 2.23                     | 0.53              |
| 2:J:103:TRP:O    | 2:J:105:VAL:N    | 2.42                     | 0.53              |
| 1:K:142:LEU:H    | 1:K:174:THR:HG22 | 1.73                     | 0.53              |
| 2:L:197:LEU:O    | 2:L:198:SER:HB3  | 2.08                     | 0.53              |
| 1:M:1:GLY:HA3    | 2:N:162:ASP:OD1  | 2.09                     | 0.53              |
| 1:O:79:ARG:HA    | 1:O:147:PRO:CB   | 2.37                     | 0.53              |
| 1:O:122:LEU:HD23 | 1:O:146:THR:HG22 | 1.91                     | 0.53              |
| 1:O:135:ARG:HH21 | 1:O:177:LEU:HD21 | 1.73                     | 0.53              |
| 1:O:154:GLU:OE1  | 1:O:188:ARG:HD3  | 2.07                     | 0.53              |
| 2:P:197:LEU:CD1  | 2:P:225:LEU:HD12 | 2.38                     | 0.53              |
| 1:A:129:GLU:HA   | 1:A:200:MET:CE   | 2.37                     | 0.53              |
| 2:D:135:ASN:HD22 | 2:D:137:TYR:HB3  | 1.73                     | 0.53              |
| 1:E:133:PHE:O    | 1:E:205:GLU:HG2  | 2.08                     | 0.53              |
| 2:F:262:GLN:HA   | 2:F:262:GLN:HE21 | 1.73                     | 0.53              |
| 2:H:67:VAL:HG21  | 2:H:126:ILE:CG2  | 2.32                     | 0.53              |
| 2:J:145:VAL:HG12 | 2:J:146:TRP:N    | 2.23                     | 0.53              |
| 1:M:122:LEU:HD23 | 1:M:146:THR:HG22 | 1.90                     | 0.53              |
| 2:N:195:TYR:O    | 2:N:237:THR:HA   | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:206:ASN:HD22 | 2:N:206:ASN:C    | 2.16                     | 0.53              |
| 1:A:104:GLN:HG3  | 2:B:168:VAL:HB   | 1.91                     | 0.53              |
| 2:B:90:THR:HB    | 2:B:91:PRO:HD2   | 1.91                     | 0.53              |
| 2:D:130:ILE:HG12 | 2:D:145:VAL:HG22 | 1.90                     | 0.53              |
| 1:E:147:PRO:HG2  | 1:E:148:TYR:CE1  | 2.43                     | 0.53              |
| 2:H:255:ASN:N    | 2:H:255:ASN:ND2  | 2.48                     | 0.53              |
| 1:I:136:SER:HB2  | 1:I:139:SER:HB2  | 1.90                     | 0.53              |
| 2:J:21:TYR:HB3   | 2:J:151:ASN:ND2  | 2.24                     | 0.53              |
| 1:K:1:GLY:HA3    | 2:L:162:ASP:OD1  | 2.08                     | 0.53              |
| 2:L:84:PHE:HA    | 2:L:85:PRO:C     | 2.32                     | 0.53              |
| 2:L:148:ILE:N    | 2:L:148:ILE:HD12 | 2.23                     | 0.53              |
| 1:O:28:ASN:HD22  | 1:O:28:ASN:N     | 1.98                     | 0.53              |
| 2:P:21:TYR:HB3   | 2:P:151:ASN:ND2  | 2.24                     | 0.53              |
| 2:P:53:THR:HG22  | 2:P:96:ASN:OD1   | 2.08                     | 0.53              |
| 2:P:103:TRP:O    | 2:P:105:VAL:N    | 2.41                     | 0.53              |
| 2:F:173:PRO:O    | 2:F:174:ASP:C    | 2.51                     | 0.53              |
| 2:F:262:GLN:HB3  | 4:F:510:HOH:O    | 2.07                     | 0.53              |
| 1:I:91:PRO:HD3   | 4:I:207:HOH:O    | 2.07                     | 0.53              |
| 1:I:142:LEU:H    | 1:I:174:THR:HG22 | 1.73                     | 0.53              |
| 2:J:71:PHE:HB3   | 2:J:110:THR:H    | 1.73                     | 0.53              |
| 2:J:135:ASN:HD21 | 2:J:138:ASN:ND2  | 2.06                     | 0.53              |
| 2:J:155:VAL:O    | 2:J:157:PRO:HD3  | 2.08                     | 0.53              |
| 1:K:140:LEU:HD12 | 1:K:162:LEU:HD11 | 1.89                     | 0.53              |
| 1:M:81:SER:O     | 1:M:83:PHE:HD1   | 1.92                     | 0.53              |
| 2:N:172:LEU:O    | 2:N:172:LEU:HD23 | 2.08                     | 0.53              |
| 2:B:262:GLN:HA   | 2:B:262:GLN:HE21 | 1.73                     | 0.53              |
| 1:C:133:PHE:O    | 1:C:205:GLU:HG2  | 2.08                     | 0.53              |
| 2:D:192:ASN:HA   | 2:D:242:ALA:HA   | 1.90                     | 0.53              |
| 2:D:262:GLN:HB3  | 4:D:604:HOH:O    | 2.09                     | 0.53              |
| 2:H:262:GLN:HB3  | 4:H:607:HOH:O    | 2.08                     | 0.53              |
| 2:P:84:PHE:HA    | 2:P:85:PRO:C     | 2.33                     | 0.53              |
| 1:A:191:ASN:HD21 | 1:A:195:ALA:HB3  | 1.73                     | 0.53              |
| 2:B:174:ASP:O    | 2:B:176:PRO:CD   | 2.56                     | 0.53              |
| 2:B:210:THR:HG22 | 2:B:211:ASN:N    | 2.24                     | 0.53              |
| 1:C:104:GLN:HG3  | 2:D:168:VAL:HB   | 1.91                     | 0.53              |
| 2:D:173:PRO:O    | 2:D:174:ASP:C    | 2.52                     | 0.53              |
| 2:H:126:ILE:HG13 | 2:H:150:ALA:HB2  | 1.91                     | 0.53              |
| 1:I:135:ARG:HH21 | 1:I:177:LEU:HD21 | 1.74                     | 0.53              |
| 2:J:42:ILE:HD13  | 2:J:146:TRP:CD2  | 2.44                     | 0.53              |
| 1:K:81:SER:O     | 1:K:83:PHE:HD1   | 1.91                     | 0.53              |
| 2:L:197:LEU:CD1  | 2:L:225:LEU:HD12 | 2.39                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:136:SER:HB2  | 1:M:139:SER:HB2  | 1.90                     | 0.53              |
| 2:N:71:PHE:HB3   | 2:N:110:THR:H    | 1.74                     | 0.53              |
| 2:N:197:LEU:O    | 2:N:198:SER:HB3  | 2.08                     | 0.53              |
| 1:O:85:MET:HB2   | 1:O:111:ILE:CG1  | 2.39                     | 0.53              |
| 1:A:144:ASN:ND2  | 1:A:148:TYR:O    | 2.39                     | 0.52              |
| 2:B:53:THR:HB    | 2:B:136:ASN:OD1  | 2.09                     | 0.52              |
| 1:C:102:THR:HA   | 2:D:171:THR:HG22 | 1.90                     | 0.52              |
| 1:C:107:ILE:HD12 | 1:C:107:ILE:N    | 2.25                     | 0.52              |
| 2:F:6:ALA:HB2    | 2:F:41:GLN:HA    | 1.91                     | 0.52              |
| 2:F:192:ASN:HA   | 2:F:242:ALA:HA   | 1.90                     | 0.52              |
| 1:M:140:LEU:HD12 | 1:M:162:LEU:HD11 | 1.90                     | 0.52              |
| 2:N:17:SER:HB2   | 2:P:262:GLN:OE1  | 2.09                     | 0.52              |
| 1:O:79:ARG:HB2   | 1:O:169:PRO:HB3  | 1.91                     | 0.52              |
| 2:P:155:VAL:O    | 2:P:157:PRO:HD3  | 2.09                     | 0.52              |
| 1:A:129:GLU:CA   | 1:A:200:MET:HE1  | 2.38                     | 0.52              |
| 2:B:6:ALA:HB2    | 2:B:41:GLN:HA    | 1.90                     | 0.52              |
| 2:B:209:PHE:CD1  | 2:B:272:ILE:HD12 | 2.44                     | 0.52              |
| 2:H:67:VAL:CG2   | 2:H:120:ILE:HD11 | 2.39                     | 0.52              |
| 1:I:1:GLY:HA3    | 2:J:162:ASP:OD1  | 2.09                     | 0.52              |
| 1:I:28:ASN:HD22  | 1:I:28:ASN:N     | 1.98                     | 0.52              |
| 1:I:85:MET:HB2   | 1:I:111:ILE:CG1  | 2.39                     | 0.52              |
| 1:K:135:ARG:HH21 | 1:K:177:LEU:HD21 | 1.73                     | 0.52              |
| 1:K:190:ILE:CD1  | 2:L:279:GLN:HG2  | 2.37                     | 0.52              |
| 2:L:155:VAL:O    | 2:L:157:PRO:HD3  | 2.10                     | 0.52              |
| 2:P:195:TYR:O    | 2:P:237:THR:HA   | 2.08                     | 0.52              |
| 1:A:102:THR:HA   | 2:B:171:THR:HG22 | 1.90                     | 0.52              |
| 1:C:144:ASN:ND2  | 1:C:150:LEU:HG   | 2.25                     | 0.52              |
| 2:F:90:THR:HB    | 2:F:91:PRO:CD    | 2.38                     | 0.52              |
| 2:H:126:ILE:HB   | 2:H:148:ILE:HG22 | 1.91                     | 0.52              |
| 2:H:173:PRO:O    | 2:H:174:ASP:C    | 2.52                     | 0.52              |
| 1:I:80:GLU:HG3   | 1:I:147:PRO:O    | 2.10                     | 0.52              |
| 1:K:136:SER:HB2  | 1:K:139:SER:HB2  | 1.90                     | 0.52              |
| 1:M:141:THR:C    | 1:M:174:THR:HG22 | 2.33                     | 0.52              |
| 2:N:155:VAL:O    | 2:N:157:PRO:HD3  | 2.09                     | 0.52              |
| 1:O:95:LYS:HD2   | 1:O:95:LYS:N     | 2.24                     | 0.52              |
| 2:B:5:THR:HG22   | 2:B:9:THR:H      | 1.74                     | 0.52              |
| 2:D:174:ASP:O    | 2:D:176:PRO:CD   | 2.58                     | 0.52              |
| 1:E:104:GLN:HG3  | 2:F:168:VAL:HB   | 1.91                     | 0.52              |
| 1:E:129:GLU:CA   | 1:E:200:MET:HE1  | 2.38                     | 0.52              |
| 1:G:107:ILE:HD12 | 1:G:107:ILE:N    | 2.25                     | 0.52              |
| 1:K:91:PRO:HD2   | 1:K:106:ALA:HB2  | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:141:THR:C    | 1:K:174:THR:HG22 | 2.34                     | 0.52              |
| 1:K:176:LYS:HB2  | 1:K:176:LYS:HZ3  | 1.75                     | 0.52              |
| 1:M:85:MET:HB2   | 1:M:111:ILE:CG1  | 2.39                     | 0.52              |
| 1:M:95:LYS:N     | 1:M:95:LYS:HD2   | 2.24                     | 0.52              |
| 2:B:92:ARG:HH11  | 2:B:92:ARG:HG3   | 1.73                     | 0.52              |
| 2:D:184:THR:HA   | 2:D:248:VAL:O    | 2.10                     | 0.52              |
| 2:H:92:ARG:HH11  | 2:H:92:ARG:HG3   | 1.73                     | 0.52              |
| 2:H:179:VAL:O    | 2:H:253:THR:HG23 | 2.09                     | 0.52              |
| 2:J:55:TYR:HB3   | 2:J:92:ARG:HB2   | 1.92                     | 0.52              |
| 2:J:192:ASN:HA   | 2:J:241:GLY:O    | 2.10                     | 0.52              |
| 1:K:54:LEU:HD23  | 1:K:54:LEU:C     | 2.34                     | 0.52              |
| 2:L:14:GLY:HA2   | 2:L:142:PHE:CD2  | 2.45                     | 0.52              |
| 1:M:190:ILE:CD1  | 2:N:279:GLN:HG2  | 2.38                     | 0.52              |
| 2:N:207:SER:O    | 2:N:224:GLN:HG3  | 2.09                     | 0.52              |
| 1:O:133:PHE:HB2  | 1:O:204:MET:SD   | 2.49                     | 0.52              |
| 2:P:14:GLY:HA2   | 2:P:142:PHE:CD2  | 2.44                     | 0.52              |
| 2:D:255:ASN:N    | 2:D:255:ASN:ND2  | 2.50                     | 0.52              |
| 1:E:191:ASN:HD21 | 1:E:195:ALA:HB3  | 1.75                     | 0.52              |
| 2:F:59:GLN:HG3   | 2:F:143:GLN:NE2  | 2.25                     | 0.52              |
| 1:G:104:GLN:HG3  | 2:H:168:VAL:HB   | 1.92                     | 0.52              |
| 1:G:191:ASN:HD21 | 1:G:195:ALA:HB3  | 1.75                     | 0.52              |
| 1:I:13:ALA:HB3   | 1:I:118:ALA:CB   | 2.40                     | 0.52              |
| 1:I:38:GLU:HA    | 1:I:44:LYS:HA    | 1.91                     | 0.52              |
| 2:J:11:ILE:CG2   | 2:J:16:GLY:HA3   | 2.34                     | 0.52              |
| 2:J:59:GLN:HE21  | 2:J:143:GLN:NE2  | 2.07                     | 0.52              |
| 1:K:46:GLY:C     | 1:K:48:PHE:H     | 2.18                     | 0.52              |
| 1:O:128:ALA:HA   | 1:O:150:LEU:HD22 | 1.91                     | 0.52              |
| 1:O:190:ILE:CD1  | 2:P:279:GLN:HG2  | 2.38                     | 0.52              |
| 2:P:206:ASN:C    | 2:P:206:ASN:HD22 | 2.16                     | 0.52              |
| 1:A:47:ARG:NH1   | 1:A:47:ARG:HG3   | 2.25                     | 0.52              |
| 2:D:90:THR:HB    | 2:D:91:PRO:HD2   | 1.91                     | 0.52              |
| 2:F:43:PHE:CE2   | 2:F:102:PRO:HG3  | 2.44                     | 0.52              |
| 2:F:135:ASN:ND2  | 2:F:137:TYR:HB3  | 2.25                     | 0.52              |
| 1:G:39:ASN:CG    | 1:G:43:VAL:HG22  | 2.34                     | 0.52              |
| 2:H:130:ILE:HG12 | 2:H:145:VAL:HG22 | 1.90                     | 0.52              |
| 1:I:30:THR:OG1   | 1:I:58:LYS:HG2   | 2.10                     | 0.52              |
| 1:I:31:TYR:HB2   | 1:I:89:ALA:HB1   | 1.91                     | 0.52              |
| 1:K:147:PRO:HA   | 1:K:169:PRO:HB3  | 1.92                     | 0.52              |
| 2:L:53:THR:HG22  | 2:L:96:ASN:CB    | 2.39                     | 0.52              |
| 1:M:135:ARG:HH21 | 1:M:177:LEU:HD21 | 1.73                     | 0.52              |
| 2:N:103:TRP:O    | 2:N:105:VAL:N    | 2.43                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:197:LEU:CD1  | 2:N:225:LEU:HD12 | 2.39                     | 0.52              |
| 1:A:47:ARG:CB    | 1:A:83:PHE:HE2   | 2.23                     | 0.52              |
| 2:B:67:VAL:CG2   | 2:B:120:ILE:HD11 | 2.39                     | 0.52              |
| 2:B:67:VAL:HG23  | 2:B:120:ILE:HD11 | 1.92                     | 0.52              |
| 1:C:9:VAL:HG22   | 4:C:208:HOH:O    | 2.10                     | 0.52              |
| 1:C:158:GLY:HA2  | 4:C:221:HOH:O    | 2.09                     | 0.52              |
| 1:E:131:LEU:HD23 | 1:E:187:TYR:CE2  | 2.45                     | 0.52              |
| 2:F:50:GLU:CD    | 2:F:98:ARG:HH12  | 2.17                     | 0.52              |
| 2:J:11:ILE:HG23  | 2:J:16:GLY:CA    | 2.32                     | 0.52              |
| 1:O:141:THR:C    | 1:O:174:THR:HG22 | 2.34                     | 0.52              |
| 2:B:48:TYR:H     | 3:B:500:MMA:H62  | 1.74                     | 0.52              |
| 2:B:59:GLN:HE21  | 2:B:143:GLN:NE2  | 2.07                     | 0.52              |
| 1:E:203:VAL:HB   | 4:E:210:HOH:O    | 2.10                     | 0.52              |
| 2:H:184:THR:HA   | 2:H:248:VAL:O    | 2.10                     | 0.52              |
| 1:I:79:ARG:HB2   | 1:I:169:PRO:HB3  | 1.92                     | 0.52              |
| 2:J:210:THR:CG2  | 2:J:259:THR:HG21 | 2.30                     | 0.52              |
| 1:K:95:LYS:N     | 1:K:95:LYS:HD2   | 2.23                     | 0.52              |
| 2:L:71:PHE:HB3   | 2:L:110:THR:H    | 1.74                     | 0.52              |
| 2:L:206:ASN:HD22 | 2:L:206:ASN:C    | 2.17                     | 0.52              |
| 1:M:79:ARG:HB2   | 1:M:169:PRO:HB3  | 1.91                     | 0.52              |
| 2:N:48:TYR:CE1   | 3:N:506:MMA:H73  | 2.45                     | 0.52              |
| 2:N:130:ILE:HD12 | 2:N:130:ILE:N    | 2.25                     | 0.52              |
| 2:P:192:ASN:HA   | 2:P:241:GLY:O    | 2.10                     | 0.52              |
| 1:A:38:GLU:CD    | 1:A:110:ARG:NH2  | 2.68                     | 0.52              |
| 2:B:90:THR:HB    | 2:B:91:PRO:CD    | 2.39                     | 0.52              |
| 1:E:39:ASN:CG    | 1:E:43:VAL:HG22  | 2.35                     | 0.52              |
| 1:E:144:ASN:ND2  | 1:E:148:TYR:O    | 2.39                     | 0.52              |
| 2:F:38:LEU:C     | 2:F:40:THR:N     | 2.67                     | 0.52              |
| 1:G:13:ALA:HB3   | 1:G:118:ALA:N    | 2.18                     | 0.52              |
| 1:I:54:LEU:C     | 1:I:54:LEU:HD23  | 2.35                     | 0.52              |
| 2:J:130:ILE:HD12 | 2:J:130:ILE:N    | 2.24                     | 0.52              |
| 2:J:197:LEU:CD1  | 2:J:225:LEU:HD12 | 2.39                     | 0.52              |
| 2:J:213:ALA:C    | 2:J:215:PHE:H    | 2.18                     | 0.52              |
| 1:K:128:ALA:HA   | 1:K:150:LEU:HD22 | 1.91                     | 0.52              |
| 2:L:38:LEU:C     | 2:L:40:THR:N     | 2.62                     | 0.52              |
| 1:M:38:GLU:HA    | 1:M:44:LYS:HA    | 1.91                     | 0.52              |
| 1:O:13:ALA:HB3   | 1:O:118:ALA:CB   | 2.40                     | 0.52              |
| 1:O:163:GLU:HB3  | 1:O:175:VAL:HG13 | 1.92                     | 0.52              |
| 1:A:10:ILE:O     | 1:A:12:PRO:HD3   | 2.10                     | 0.51              |
| 1:A:12:PRO:HB2   | 1:A:15:GLN:HG2   | 1.92                     | 0.51              |
| 2:D:90:THR:HB    | 2:D:91:PRO:CD    | 2.39                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:209:PHE:CD1  | 2:D:272:ILE:HD12 | 2.45                     | 0.51              |
| 1:E:175:VAL:HG12 | 4:E:230:HOH:O    | 2.09                     | 0.51              |
| 1:E:188:ARG:HG2  | 1:E:188:ARG:HH11 | 1.76                     | 0.51              |
| 2:F:35:VAL:HA    | 2:F:107:LEU:O    | 2.10                     | 0.51              |
| 1:K:31:TYR:HB2   | 1:K:89:ALA:HB1   | 1.91                     | 0.51              |
| 2:N:268:VAL:HG12 | 2:N:269:GLN:N    | 2.25                     | 0.51              |
| 1:O:31:TYR:HB2   | 1:O:89:ALA:HB1   | 1.92                     | 0.51              |
| 1:O:46:GLY:C     | 1:O:48:PHE:H     | 2.17                     | 0.51              |
| 2:B:174:ASP:O    | 2:B:176:PRO:HD2  | 2.09                     | 0.51              |
| 2:B:192:ASN:HA   | 2:B:242:ALA:HA   | 1.91                     | 0.51              |
| 1:C:12:PRO:HB2   | 1:C:15:GLN:HG2   | 1.91                     | 0.51              |
| 2:D:43:PHE:CE2   | 2:D:102:PRO:HG3  | 2.46                     | 0.51              |
| 2:H:59:GLN:HG3   | 2:H:143:GLN:NE2  | 2.24                     | 0.51              |
| 2:H:135:ASN:ND2  | 2:H:137:TYR:HB3  | 2.25                     | 0.51              |
| 1:I:81:SER:O     | 1:I:83:PHE:HD1   | 1.92                     | 0.51              |
| 1:K:79:ARG:HB2   | 1:K:169:PRO:HB3  | 1.91                     | 0.51              |
| 1:M:46:GLY:C     | 1:M:48:PHE:H     | 2.18                     | 0.51              |
| 2:N:59:GLN:HE21  | 2:N:143:GLN:NE2  | 2.08                     | 0.51              |
| 1:O:80:GLU:HG3   | 1:O:147:PRO:O    | 2.10                     | 0.51              |
| 2:P:268:VAL:HG12 | 2:P:269:GLN:N    | 2.25                     | 0.51              |
| 1:A:39:ASN:CG    | 1:A:43:VAL:HG22  | 2.35                     | 0.51              |
| 1:A:114:TYR:CE1  | 1:A:149:TYR:HB2  | 2.46                     | 0.51              |
| 1:C:129:GLU:CA   | 1:C:200:MET:HE1  | 2.39                     | 0.51              |
| 2:D:262:GLN:HA   | 2:D:262:GLN:HE21 | 1.74                     | 0.51              |
| 1:G:10:ILE:O     | 1:G:12:PRO:HD3   | 2.10                     | 0.51              |
| 1:G:144:ASN:ND2  | 1:G:150:LEU:HG   | 2.24                     | 0.51              |
| 2:H:174:ASP:O    | 2:H:176:PRO:CD   | 2.58                     | 0.51              |
| 1:K:6:ALA:HB3    | 1:K:20:LEU:HD21  | 1.93                     | 0.51              |
| 2:L:210:THR:CG2  | 2:L:259:THR:HG21 | 2.29                     | 0.51              |
| 1:M:147:PRO:HA   | 1:M:169:PRO:HB3  | 1.93                     | 0.51              |
| 2:N:53:THR:HG22  | 2:N:96:ASN:CB    | 2.41                     | 0.51              |
| 2:N:148:ILE:HD12 | 2:N:148:ILE:N    | 2.26                     | 0.51              |
| 2:P:131:LEU:HD22 | 2:P:144:PHE:HB2  | 1.92                     | 0.51              |
| 2:D:38:LEU:C     | 2:D:40:THR:N     | 2.66                     | 0.51              |
| 1:G:12:PRO:HB2   | 1:G:15:GLN:HG2   | 1.93                     | 0.51              |
| 2:H:184:THR:HG22 | 2:H:249:SER:CA   | 2.40                     | 0.51              |
| 1:I:6:ALA:HB3    | 1:I:20:LEU:HD21  | 1.93                     | 0.51              |
| 1:I:46:GLY:C     | 1:I:48:PHE:H     | 2.18                     | 0.51              |
| 1:I:86:ASN:HA    | 1:I:109:SER:O    | 2.11                     | 0.51              |
| 1:I:91:PRO:HD2   | 1:I:106:ALA:HB2  | 1.91                     | 0.51              |
| 2:J:148:ILE:HD12 | 2:J:148:ILE:N    | 2.24                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:264:THR:HG22 | 2:J:265:ALA:N    | 2.21                     | 0.51              |
| 1:K:30:THR:OG1   | 1:K:58:LYS:HG2   | 2.11                     | 0.51              |
| 2:L:102:PRO:HB2  | 4:L:508:HOH:O    | 2.11                     | 0.51              |
| 2:L:172:LEU:N    | 2:L:173:PRO:CD   | 2.71                     | 0.51              |
| 1:M:30:THR:OG1   | 1:M:58:LYS:HG2   | 2.10                     | 0.51              |
| 2:P:53:THR:HG22  | 2:P:96:ASN:CB    | 2.40                     | 0.51              |
| 1:A:188:ARG:CZ   | 1:A:197:THR:O    | 2.59                     | 0.51              |
| 1:C:16:LYS:HB3   | 4:C:223:HOH:O    | 2.10                     | 0.51              |
| 1:C:39:ASN:CG    | 1:C:43:VAL:HG22  | 2.35                     | 0.51              |
| 1:C:188:ARG:CZ   | 1:C:197:THR:O    | 2.58                     | 0.51              |
| 2:F:174:ASP:O    | 2:F:176:PRO:CD   | 2.59                     | 0.51              |
| 2:H:113:SER:HB3  | 2:L:81:SER:N     | 2.12                     | 0.51              |
| 2:H:219:GLN:HA   | 4:H:631:HOH:O    | 2.09                     | 0.51              |
| 1:I:55:PHE:HE1   | 1:I:57:MET:HG3   | 1.76                     | 0.51              |
| 2:J:53:THR:HG22  | 2:J:96:ASN:CB    | 2.40                     | 0.51              |
| 1:K:85:MET:HB2   | 1:K:111:ILE:CG1  | 2.40                     | 0.51              |
| 2:L:213:ALA:C    | 2:L:215:PHE:H    | 2.18                     | 0.51              |
| 1:M:80:GLU:HG3   | 1:M:147:PRO:O    | 2.11                     | 0.51              |
| 2:N:172:LEU:N    | 2:N:173:PRO:CD   | 2.71                     | 0.51              |
| 2:N:213:ALA:C    | 2:N:215:PHE:H    | 2.18                     | 0.51              |
| 1:O:6:ALA:HB3    | 1:O:20:LEU:HD21  | 1.92                     | 0.51              |
| 1:O:54:LEU:HD23  | 1:O:54:LEU:C     | 2.35                     | 0.51              |
| 2:P:122:ALA:HB1  | 2:P:151:ASN:O    | 2.11                     | 0.51              |
| 2:P:130:ILE:N    | 2:P:130:ILE:HD12 | 2.24                     | 0.51              |
| 1:A:107:ILE:HD12 | 1:A:107:ILE:N    | 2.26                     | 0.51              |
| 2:B:35:VAL:HA    | 2:B:107:LEU:O    | 2.10                     | 0.51              |
| 1:C:156:ASN:OD1  | 1:C:161:VAL:HG23 | 2.10                     | 0.51              |
| 1:E:45:ASP:HB2   | 4:E:214:HOH:O    | 2.10                     | 0.51              |
| 2:F:184:THR:HG22 | 2:F:249:SER:CA   | 2.41                     | 0.51              |
| 1:G:156:ASN:OD1  | 1:G:161:VAL:HG23 | 2.10                     | 0.51              |
| 1:G:188:ARG:CZ   | 1:G:197:THR:O    | 2.58                     | 0.51              |
| 2:H:271:ILE:O    | 2:H:272:ILE:HD13 | 2.10                     | 0.51              |
| 1:I:128:ALA:HA   | 1:I:150:LEU:HD22 | 1.92                     | 0.51              |
| 2:J:207:SER:O    | 2:J:224:GLN:HG3  | 2.09                     | 0.51              |
| 1:K:38:GLU:HA    | 1:K:44:LYS:HA    | 1.91                     | 0.51              |
| 1:K:60:LYS:HD3   | 1:K:60:LYS:O     | 2.11                     | 0.51              |
| 2:L:130:ILE:HD12 | 2:L:130:ILE:N    | 2.26                     | 0.51              |
| 1:M:163:GLU:HB3  | 1:M:175:VAL:HG13 | 1.92                     | 0.51              |
| 2:N:224:GLN:CG   | 2:N:231:ILE:HD13 | 2.40                     | 0.51              |
| 1:C:47:ARG:CB    | 1:C:83:PHE:HE2   | 2.24                     | 0.51              |
| 1:C:97:LYS:HD3   | 1:C:100:GLU:OE2  | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:35:VAL:HA    | 2:D:107:LEU:O    | 2.10                     | 0.51              |
| 1:E:156:ASN:OD1  | 1:E:161:VAL:HG23 | 2.10                     | 0.51              |
| 2:F:173:PRO:HB2  | 2:F:177:GLY:HA3  | 1.92                     | 0.51              |
| 2:J:122:ALA:HB1  | 2:J:151:ASN:O    | 2.10                     | 0.51              |
| 1:K:104:GLN:HG3  | 2:L:168:VAL:HB   | 1.93                     | 0.51              |
| 2:L:192:ASN:HA   | 2:L:241:GLY:O    | 2.10                     | 0.51              |
| 1:M:153:THR:HG21 | 1:M:196:LEU:CD2  | 2.39                     | 0.51              |
| 1:A:47:ARG:HG3   | 1:A:47:ARG:HH11  | 1.76                     | 0.51              |
| 2:D:67:VAL:CG2   | 2:D:120:ILE:HD11 | 2.41                     | 0.51              |
| 1:E:97:LYS:HD3   | 1:E:100:GLU:OE2  | 2.11                     | 0.51              |
| 2:F:67:VAL:HG23  | 2:F:120:ILE:HD11 | 1.91                     | 0.51              |
| 2:F:184:THR:HA   | 2:F:248:VAL:O    | 2.10                     | 0.51              |
| 2:F:210:THR:HG22 | 2:F:211:ASN:N    | 2.25                     | 0.51              |
| 2:F:271:ILE:O    | 2:F:272:ILE:HD13 | 2.10                     | 0.51              |
| 2:J:163:VAL:HG13 | 2:J:185:VAL:CG1  | 2.41                     | 0.51              |
| 1:K:13:ALA:HB3   | 1:K:118:ALA:CB   | 2.40                     | 0.51              |
| 2:L:201:THR:HA   | 2:L:209:PHE:HA   | 1.93                     | 0.51              |
| 1:M:54:LEU:HD23  | 1:M:54:LEU:C     | 2.36                     | 0.51              |
| 2:N:14:GLY:HA2   | 2:N:142:PHE:CD2  | 2.46                     | 0.51              |
| 2:N:192:ASN:HA   | 2:N:241:GLY:O    | 2.10                     | 0.51              |
| 1:O:38:GLU:HA    | 1:O:44:LYS:HA    | 1.91                     | 0.51              |
| 1:O:153:THR:HG21 | 1:O:196:LEU:CD2  | 2.39                     | 0.51              |
| 2:P:55:TYR:HB3   | 2:P:92:ARG:HB2   | 1.92                     | 0.51              |
| 2:P:96:ASN:HD22  | 2:P:96:ASN:H     | 1.58                     | 0.51              |
| 2:F:29:ASN:HA    | 4:F:526:HOH:O    | 2.09                     | 0.51              |
| 1:G:47:ARG:HG3   | 1:G:47:ARG:NH1   | 2.26                     | 0.51              |
| 2:H:106:ALA:HB3  | 4:H:617:HOH:O    | 2.10                     | 0.51              |
| 2:H:131:LEU:HB3  | 2:H:144:PHE:HB2  | 1.93                     | 0.51              |
| 2:L:207:SER:O    | 2:L:224:GLN:HG3  | 2.11                     | 0.51              |
| 1:M:133:PHE:HB2  | 1:M:204:MET:SD   | 2.50                     | 0.51              |
| 2:N:193:LEU:HD12 | 2:N:243:VAL:HG21 | 1.93                     | 0.51              |
| 2:P:148:ILE:HD12 | 2:P:148:ILE:N    | 2.26                     | 0.51              |
| 1:A:44:LYS:HG3   | 4:A:212:HOH:O    | 2.11                     | 0.51              |
| 1:A:156:ASN:HD22 | 1:A:186:THR:HB   | 1.76                     | 0.51              |
| 2:B:46:ASN:O     | 2:B:98:ARG:HA    | 2.11                     | 0.51              |
| 2:B:57:THR:OG1   | 2:B:132:ARG:HB3  | 2.11                     | 0.51              |
| 2:B:173:PRO:HB2  | 2:B:177:GLY:HA3  | 1.92                     | 0.51              |
| 2:D:173:PRO:HB2  | 2:D:177:GLY:HA3  | 1.93                     | 0.51              |
| 2:F:126:ILE:HB   | 2:F:148:ILE:HG22 | 1.92                     | 0.51              |
| 2:H:23:ASN:HB3   | 4:H:620:HOH:O    | 2.09                     | 0.51              |
| 2:H:90:THR:HB    | 2:H:91:PRO:CD    | 2.40                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:17:GLN:HA    | 1:I:67:ILE:O     | 2.11                     | 0.51              |
| 2:J:268:VAL:HG12 | 2:J:269:GLN:N    | 2.25                     | 0.51              |
| 1:K:110:ARG:HD3  | 2:L:277:VAL:HG13 | 1.93                     | 0.51              |
| 2:L:34:LEU:HG    | 2:L:34:LEU:O     | 2.11                     | 0.51              |
| 2:L:224:GLN:NE2  | 4:L:511:HOH:O    | 2.43                     | 0.51              |
| 1:M:13:ALA:HB3   | 1:M:118:ALA:CB   | 2.40                     | 0.51              |
| 1:M:20:LEU:HD12  | 1:M:21:ALA:N     | 2.26                     | 0.51              |
| 1:M:31:TYR:HB2   | 1:M:89:ALA:HB1   | 1.92                     | 0.51              |
| 1:M:33:ILE:HG13  | 1:M:57:MET:HB2   | 1.93                     | 0.51              |
| 2:N:58:LEU:HD12  | 2:N:130:ILE:O    | 2.11                     | 0.51              |
| 2:N:163:VAL:HG13 | 2:N:185:VAL:CG1  | 2.40                     | 0.51              |
| 1:O:20:LEU:HD12  | 1:O:21:ALA:N     | 2.26                     | 0.51              |
| 1:O:30:THR:OG1   | 1:O:58:LYS:HG2   | 2.11                     | 0.51              |
| 2:P:11:ILE:CG2   | 2:P:16:GLY:HA3   | 2.33                     | 0.51              |
| 1:A:188:ARG:HG2  | 1:A:188:ARG:HH11 | 1.76                     | 0.50              |
| 2:D:57:THR:OG1   | 2:D:132:ARG:HB3  | 2.12                     | 0.50              |
| 1:E:188:ARG:CZ   | 1:E:197:THR:O    | 2.59                     | 0.50              |
| 2:F:5:THR:HG22   | 2:F:9:THR:H      | 1.76                     | 0.50              |
| 1:G:47:ARG:CB    | 1:G:83:PHE:HE2   | 2.24                     | 0.50              |
| 2:H:90:THR:HB    | 2:H:91:PRO:HD2   | 1.93                     | 0.50              |
| 2:H:135:ASN:ND2  | 2:H:138:ASN:H    | 2.09                     | 0.50              |
| 2:J:206:ASN:C    | 2:J:206:ASN:HD22 | 2.17                     | 0.50              |
| 1:K:95:LYS:O     | 1:K:96:SER:HB2   | 2.11                     | 0.50              |
| 1:M:28:ASN:ND2   | 1:M:28:ASN:N     | 2.58                     | 0.50              |
| 1:M:95:LYS:O     | 1:M:96:SER:HB2   | 2.12                     | 0.50              |
| 1:M:128:ALA:HA   | 1:M:150:LEU:HD22 | 1.92                     | 0.50              |
| 1:O:33:ILE:HG13  | 1:O:57:MET:HB2   | 1.94                     | 0.50              |
| 2:H:46:ASN:O     | 2:H:98:ARG:HA    | 2.11                     | 0.50              |
| 2:H:209:PHE:CD1  | 2:H:272:ILE:HD12 | 2.46                     | 0.50              |
| 1:I:163:GLU:HB3  | 1:I:175:VAL:HG13 | 1.92                     | 0.50              |
| 1:I:190:ILE:CD1  | 2:J:279:GLN:HG2  | 2.37                     | 0.50              |
| 1:K:55:PHE:HE1   | 1:K:57:MET:HG3   | 1.76                     | 0.50              |
| 1:K:80:GLU:HG3   | 1:K:147:PRO:O    | 2.12                     | 0.50              |
| 1:K:163:GLU:HB3  | 1:K:175:VAL:HG13 | 1.92                     | 0.50              |
| 2:L:163:VAL:HG13 | 2:L:185:VAL:CG1  | 2.40                     | 0.50              |
| 2:L:193:LEU:HD12 | 2:L:243:VAL:HG21 | 1.93                     | 0.50              |
| 1:M:17:GLN:HA    | 1:M:67:ILE:O     | 2.11                     | 0.50              |
| 2:N:268:VAL:HG12 | 2:N:269:GLN:H    | 1.77                     | 0.50              |
| 2:P:34:LEU:O     | 2:P:34:LEU:HG    | 2.12                     | 0.50              |
| 2:P:207:SER:O    | 2:P:224:GLN:HG3  | 2.10                     | 0.50              |
| 1:A:47:ARG:NH1   | 1:A:71:THR:HB    | 2.26                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:97:LYS:HD3   | 1:A:100:GLU:OE2  | 2.11                     | 0.50              |
| 2:B:174:ASP:O    | 2:B:176:PRO:N    | 2.44                     | 0.50              |
| 1:C:144:ASN:ND2  | 1:C:148:TYR:O    | 2.39                     | 0.50              |
| 1:C:159:THR:HB   | 1:C:180:ASP:C    | 2.37                     | 0.50              |
| 2:D:227:ARG:HG3  | 2:D:227:ARG:O    | 2.11                     | 0.50              |
| 1:E:114:TYR:CE1  | 1:E:149:TYR:HB2  | 2.47                     | 0.50              |
| 1:I:20:LEU:HD12  | 1:I:21:ALA:N     | 2.26                     | 0.50              |
| 1:I:95:LYS:O     | 1:I:96:SER:HB2   | 2.11                     | 0.50              |
| 1:K:33:ILE:HG13  | 1:K:57:MET:HB2   | 1.93                     | 0.50              |
| 1:M:6:ALA:HB3    | 1:M:20:LEU:HD21  | 1.93                     | 0.50              |
| 1:M:60:LYS:O     | 1:M:60:LYS:HD3   | 2.12                     | 0.50              |
| 1:M:75:LEU:HB2   | 1:M:115:TYR:CE2  | 2.47                     | 0.50              |
| 2:N:103:TRP:CE2  | 2:N:131:LEU:HD12 | 2.46                     | 0.50              |
| 2:B:224:GLN:NE2  | 4:B:507:HOH:O    | 2.38                     | 0.50              |
| 1:G:129:GLU:CA   | 1:G:200:MET:HE1  | 2.38                     | 0.50              |
| 1:G:159:THR:HB   | 1:G:180:ASP:C    | 2.37                     | 0.50              |
| 2:H:67:VAL:HG23  | 2:H:120:ILE:HD11 | 1.91                     | 0.50              |
| 2:H:174:ASP:O    | 2:H:176:PRO:N    | 2.45                     | 0.50              |
| 1:I:33:ILE:HG13  | 1:I:57:MET:HB2   | 1.94                     | 0.50              |
| 1:I:55:PHE:CE1   | 1:I:57:MET:HG3   | 2.47                     | 0.50              |
| 1:I:176:LYS:HB2  | 1:I:176:LYS:HZ3  | 1.77                     | 0.50              |
| 2:J:201:THR:HA   | 2:J:209:PHE:HA   | 1.94                     | 0.50              |
| 2:L:96:ASN:HD22  | 2:L:96:ASN:H     | 1.60                     | 0.50              |
| 2:N:34:LEU:HG    | 2:N:34:LEU:O     | 2.11                     | 0.50              |
| 1:O:17:GLN:HA    | 1:O:67:ILE:O     | 2.11                     | 0.50              |
| 2:P:59:GLN:HE21  | 2:P:143:GLN:NE2  | 2.09                     | 0.50              |
| 2:B:184:THR:HA   | 2:B:248:VAL:O    | 2.11                     | 0.50              |
| 1:C:131:LEU:HD23 | 1:C:187:TYR:CE2  | 2.46                     | 0.50              |
| 1:G:114:TYR:CE1  | 1:G:149:TYR:HB2  | 2.45                     | 0.50              |
| 2:H:192:ASN:OD1  | 2:H:242:ALA:HB2  | 2.12                     | 0.50              |
| 1:K:20:LEU:HD12  | 1:K:21:ALA:N     | 2.26                     | 0.50              |
| 1:K:31:TYR:O     | 1:K:33:ILE:N     | 2.44                     | 0.50              |
| 1:K:55:PHE:CE1   | 1:K:57:MET:HG3   | 2.47                     | 0.50              |
| 2:L:122:ALA:HB1  | 2:L:151:ASN:O    | 2.12                     | 0.50              |
| 2:L:268:VAL:HG12 | 2:L:269:GLN:N    | 2.25                     | 0.50              |
| 2:N:115:ALA:HB3  | 2:N:156:VAL:HG11 | 1.94                     | 0.50              |
| 2:N:210:THR:CG2  | 2:N:259:THR:HG21 | 2.30                     | 0.50              |
| 1:O:75:LEU:HB2   | 1:O:115:TYR:CE2  | 2.47                     | 0.50              |
| 2:P:213:ALA:C    | 2:P:215:PHE:H    | 2.19                     | 0.50              |
| 2:B:135:ASN:ND2  | 2:B:137:TYR:HB3  | 2.25                     | 0.50              |
| 2:D:219:GLN:HA   | 4:D:625:HOH:O    | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:59:GLN:HE21  | 2:H:143:GLN:HE22 | 1.59                     | 0.50              |
| 1:K:75:LEU:HB2   | 1:K:115:TYR:CE2  | 2.47                     | 0.50              |
| 2:L:224:GLN:CG   | 2:L:231:ILE:HD13 | 2.40                     | 0.50              |
| 2:N:21:TYR:CB    | 2:N:151:ASN:HD21 | 2.24                     | 0.50              |
| 2:N:122:ALA:HB1  | 2:N:151:ASN:O    | 2.11                     | 0.50              |
| 1:A:102:THR:O    | 2:B:269:GLN:HA   | 2.11                     | 0.50              |
| 1:C:154:GLU:CD   | 1:C:188:ARG:HD3  | 2.37                     | 0.50              |
| 1:C:188:ARG:HH12 | 1:C:198:PRO:HA   | 1.76                     | 0.50              |
| 1:E:47:ARG:NH1   | 1:E:71:THR:HB    | 2.27                     | 0.50              |
| 2:H:53:THR:HB    | 2:H:136:ASN:OD1  | 2.12                     | 0.50              |
| 1:I:31:TYR:O     | 1:I:33:ILE:N     | 2.44                     | 0.50              |
| 2:J:115:ALA:HB3  | 2:J:156:VAL:HG11 | 1.94                     | 0.50              |
| 2:J:131:LEU:HD22 | 2:J:144:PHE:HB2  | 1.92                     | 0.50              |
| 2:J:211:ASN:CG   | 2:J:268:VAL:HG13 | 2.37                     | 0.50              |
| 2:L:11:ILE:CG2   | 2:L:16:GLY:HA3   | 2.34                     | 0.50              |
| 1:M:86:ASN:HA    | 1:M:109:SER:O    | 2.12                     | 0.50              |
| 2:N:55:TYR:HB3   | 2:N:92:ARG:HB2   | 1.93                     | 0.50              |
| 2:N:96:ASN:HD22  | 2:N:96:ASN:H     | 1.59                     | 0.50              |
| 2:N:201:THR:HA   | 2:N:209:PHE:HA   | 1.94                     | 0.50              |
| 1:O:86:ASN:HA    | 1:O:109:SER:O    | 2.11                     | 0.50              |
| 2:B:136:ASN:C    | 2:B:136:ASN:ND2  | 2.54                     | 0.50              |
| 1:E:10:ILE:O     | 1:E:12:PRO:HD3   | 2.12                     | 0.50              |
| 1:E:12:PRO:HB2   | 1:E:15:GLN:HG2   | 1.94                     | 0.50              |
| 1:E:38:GLU:CD    | 1:E:110:ARG:NH2  | 2.68                     | 0.50              |
| 2:H:181:ILE:HD11 | 2:H:254:ALA:HB2  | 1.94                     | 0.50              |
| 2:J:268:VAL:HG12 | 2:J:269:GLN:H    | 1.77                     | 0.50              |
| 2:L:48:TYR:CE1   | 3:L:504:MMA:H73  | 2.47                     | 0.50              |
| 2:L:55:TYR:HB3   | 2:L:92:ARG:HB2   | 1.92                     | 0.50              |
| 2:L:59:GLN:HE21  | 2:L:143:GLN:NE2  | 2.09                     | 0.50              |
| 1:M:177:LEU:C    | 1:M:179:SER:H    | 2.20                     | 0.50              |
| 2:N:21:TYR:HB3   | 2:N:151:ASN:ND2  | 2.24                     | 0.50              |
| 2:P:5:THR:HG22   | 2:P:9:THR:N      | 2.27                     | 0.50              |
| 2:P:21:TYR:CB    | 2:P:151:ASN:HD21 | 2.24                     | 0.50              |
| 2:P:201:THR:HA   | 2:P:209:PHE:HA   | 1.93                     | 0.50              |
| 2:P:211:ASN:CG   | 2:P:268:VAL:HG13 | 2.37                     | 0.50              |
| 1:C:47:ARG:HG3   | 1:C:47:ARG:HH11  | 1.77                     | 0.50              |
| 1:E:47:ARG:CB    | 1:E:83:PHE:HE2   | 2.24                     | 0.50              |
| 1:E:57:MET:HE3   | 1:E:63:ASN:OD1   | 2.12                     | 0.50              |
| 2:F:174:ASP:O    | 2:F:176:PRO:HD2  | 2.12                     | 0.50              |
| 1:G:77:GLN:NE2   | 1:G:77:GLN:HA    | 2.27                     | 0.50              |
| 1:G:102:THR:O    | 2:H:269:GLN:HA   | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:60:LYS:O     | 1:I:60:LYS:HD3   | 2.12                     | 0.50              |
| 2:J:34:LEU:HG    | 2:J:34:LEU:O     | 2.12                     | 0.50              |
| 2:L:131:LEU:HD22 | 2:L:144:PHE:HB2  | 1.93                     | 0.50              |
| 2:L:211:ASN:CG   | 2:L:268:VAL:HG13 | 2.37                     | 0.50              |
| 1:M:36:TRP:CH2   | 1:M:88:LYS:HE2   | 2.46                     | 0.50              |
| 1:O:60:LYS:O     | 1:O:60:LYS:HD3   | 2.12                     | 0.50              |
| 2:P:163:VAL:HG13 | 2:P:185:VAL:CG1  | 2.41                     | 0.50              |
| 1:A:9:VAL:HG12   | 1:A:113:LEU:HD13 | 1.94                     | 0.49              |
| 2:B:126:ILE:HB   | 2:B:148:ILE:HG22 | 1.94                     | 0.49              |
| 2:B:192:ASN:OD1  | 2:B:242:ALA:HB2  | 2.11                     | 0.49              |
| 1:C:121:ALA:HB3  | 4:C:216:HOH:O    | 2.12                     | 0.49              |
| 2:D:5:THR:HG22   | 2:D:9:THR:H      | 1.77                     | 0.49              |
| 2:D:210:THR:HG22 | 2:D:211:ASN:N    | 2.26                     | 0.49              |
| 2:F:181:ILE:HD11 | 2:F:254:ALA:HB2  | 1.93                     | 0.49              |
| 1:G:131:LEU:HD23 | 1:G:187:TYR:CE2  | 2.47                     | 0.49              |
| 1:I:143:ILE:HA   | 1:I:172:GLU:HB2  | 1.94                     | 0.49              |
| 1:I:147:PRO:HA   | 1:I:169:PRO:HB3  | 1.93                     | 0.49              |
| 2:J:5:THR:HG22   | 2:J:9:THR:N      | 2.27                     | 0.49              |
| 1:K:28:ASN:ND2   | 1:K:28:ASN:N     | 2.58                     | 0.49              |
| 2:P:58:LEU:HD12  | 2:P:130:ILE:O    | 2.12                     | 0.49              |
| 1:C:88:LYS:CB    | 1:C:108:ILE:HG12 | 2.42                     | 0.49              |
| 2:D:174:ASP:O    | 2:D:176:PRO:HD2  | 2.11                     | 0.49              |
| 1:E:159:THR:HB   | 1:E:180:ASP:C    | 2.37                     | 0.49              |
| 2:F:192:ASN:OD1  | 2:F:242:ALA:HB2  | 2.12                     | 0.49              |
| 2:F:227:ARG:HG3  | 2:F:227:ARG:O    | 2.12                     | 0.49              |
| 1:G:38:GLU:CD    | 1:G:110:ARG:NH2  | 2.70                     | 0.49              |
| 2:H:227:ARG:HG3  | 2:H:227:ARG:O    | 2.12                     | 0.49              |
| 1:K:86:ASN:HA    | 1:K:109:SER:O    | 2.11                     | 0.49              |
| 1:K:101:ASN:HB2  | 2:L:171:THR:O    | 2.12                     | 0.49              |
| 1:O:55:PHE:HE1   | 1:O:57:MET:HG3   | 1.76                     | 0.49              |
| 1:O:147:PRO:HA   | 1:O:169:PRO:HB3  | 1.93                     | 0.49              |
| 1:A:159:THR:HB   | 1:A:180:ASP:C    | 2.37                     | 0.49              |
| 2:B:28:VAL:HG12  | 2:B:111:PRO:HG2  | 1.94                     | 0.49              |
| 1:C:47:ARG:HG3   | 1:C:47:ARG:NH1   | 2.27                     | 0.49              |
| 2:D:59:GLN:HG3   | 2:D:143:GLN:NE2  | 2.26                     | 0.49              |
| 1:G:144:ASN:ND2  | 1:G:148:TYR:O    | 2.39                     | 0.49              |
| 1:I:104:GLN:HG3  | 2:J:168:VAL:HB   | 1.94                     | 0.49              |
| 1:O:31:TYR:O     | 1:O:33:ILE:N     | 2.45                     | 0.49              |
| 1:O:80:GLU:CD    | 1:O:148:TYR:HA   | 2.37                     | 0.49              |
| 1:O:95:LYS:O     | 1:O:96:SER:HB2   | 2.12                     | 0.49              |
| 1:O:110:ARG:HD3  | 2:P:277:VAL:HG13 | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:174:ASP:O    | 2:D:176:PRO:N    | 2.45                     | 0.49              |
| 2:F:46:ASN:O     | 2:F:98:ARG:HA    | 2.13                     | 0.49              |
| 2:F:172:LEU:HD23 | 2:F:172:LEU:C    | 2.38                     | 0.49              |
| 1:I:177:LEU:C    | 1:I:179:SER:H    | 2.20                     | 0.49              |
| 2:J:245:THR:HB   | 4:J:616:HOH:O    | 2.12                     | 0.49              |
| 2:L:271:ILE:HG13 | 2:L:271:ILE:O    | 2.13                     | 0.49              |
| 1:M:104:GLN:HG3  | 2:N:168:VAL:HB   | 1.94                     | 0.49              |
| 2:N:126:ILE:N    | 2:N:148:ILE:O    | 2.45                     | 0.49              |
| 2:P:264:THR:HG22 | 2:P:265:ALA:N    | 2.20                     | 0.49              |
| 2:P:268:VAL:HG12 | 2:P:269:GLN:H    | 1.77                     | 0.49              |
| 1:A:88:LYS:CB    | 1:A:108:ILE:HG12 | 2.41                     | 0.49              |
| 1:C:188:ARG:HG2  | 1:C:188:ARG:HH11 | 1.78                     | 0.49              |
| 2:D:126:ILE:HG13 | 2:D:150:ALA:HB2  | 1.94                     | 0.49              |
| 2:F:5:THR:HG23   | 2:F:7:ASN:N      | 2.26                     | 0.49              |
| 2:F:131:LEU:HB3  | 2:F:144:PHE:HB2  | 1.94                     | 0.49              |
| 1:G:80:GLU:HA    | 1:G:115:TYR:O    | 2.13                     | 0.49              |
| 1:G:156:ASN:HD22 | 1:G:186:THR:HB   | 1.78                     | 0.49              |
| 2:H:173:PRO:HB2  | 2:H:177:GLY:HA3  | 1.93                     | 0.49              |
| 1:I:75:LEU:HB2   | 1:I:115:TYR:CE2  | 2.47                     | 0.49              |
| 2:J:126:ILE:N    | 2:J:148:ILE:O    | 2.45                     | 0.49              |
| 2:L:268:VAL:HG12 | 2:L:269:GLN:H    | 1.77                     | 0.49              |
| 1:O:143:ILE:HA   | 1:O:172:GLU:HB2  | 1.94                     | 0.49              |
| 2:B:92:ARG:NH1   | 4:B:558:HOH:O    | 2.45                     | 0.49              |
| 2:B:135:ASN:ND2  | 2:B:138:ASN:H    | 2.11                     | 0.49              |
| 1:C:38:GLU:CD    | 1:C:110:ARG:NH2  | 2.70                     | 0.49              |
| 1:G:47:ARG:HG3   | 1:G:47:ARG:HH11  | 1.77                     | 0.49              |
| 1:I:20:LEU:HD12  | 1:I:21:ALA:H     | 1.78                     | 0.49              |
| 2:J:166:ARG:CG   | 2:J:182:PRO:HB2  | 2.43                     | 0.49              |
| 1:K:17:GLN:HA    | 1:K:67:ILE:O     | 2.11                     | 0.49              |
| 2:L:103:TRP:CE2  | 2:L:131:LEU:HD12 | 2.48                     | 0.49              |
| 1:M:31:TYR:O     | 1:M:33:ILE:N     | 2.45                     | 0.49              |
| 1:M:55:PHE:HE1   | 1:M:57:MET:HG3   | 1.76                     | 0.49              |
| 1:O:189:THR:O    | 1:O:197:THR:HG23 | 2.13                     | 0.49              |
| 1:A:156:ASN:OD1  | 1:A:161:VAL:HG23 | 2.12                     | 0.49              |
| 2:B:174:ASP:C    | 2:B:176:PRO:HD2  | 2.38                     | 0.49              |
| 1:C:46:GLY:O     | 1:C:47:ARG:C     | 2.56                     | 0.49              |
| 1:C:47:ARG:NH1   | 1:C:71:THR:HB    | 2.27                     | 0.49              |
| 2:D:271:ILE:O    | 2:D:272:ILE:HD13 | 2.13                     | 0.49              |
| 1:I:101:ASN:HB2  | 2:J:171:THR:O    | 2.13                     | 0.49              |
| 2:J:103:TRP:CE2  | 2:J:131:LEU:HD12 | 2.47                     | 0.49              |
| 1:K:153:THR:HG21 | 1:K:196:LEU:CD2  | 2.39                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:177:LEU:C    | 1:K:179:SER:H    | 2.20                     | 0.49              |
| 2:N:271:ILE:O    | 2:N:271:ILE:HG13 | 2.13                     | 0.49              |
| 1:O:55:PHE:CE1   | 1:O:57:MET:HG3   | 2.47                     | 0.49              |
| 2:F:126:ILE:HG13 | 2:F:150:ALA:HB2  | 1.93                     | 0.49              |
| 2:F:167:ASP:O    | 2:F:168:VAL:C    | 2.56                     | 0.49              |
| 1:G:188:ARG:HG2  | 1:G:188:ARG:HH11 | 1.78                     | 0.49              |
| 1:I:158:GLY:N    | 1:I:184:ASN:HD22 | 2.11                     | 0.49              |
| 2:J:211:ASN:HD21 | 2:J:213:ALA:HB3  | 1.77                     | 0.49              |
| 1:K:119:LYS:HE3  | 4:K:213:HOH:O    | 2.11                     | 0.49              |
| 1:K:158:GLY:N    | 1:K:184:ASN:HD22 | 2.11                     | 0.49              |
| 2:L:126:ILE:N    | 2:L:148:ILE:O    | 2.45                     | 0.49              |
| 2:N:211:ASN:CG   | 2:N:268:VAL:HG13 | 2.37                     | 0.49              |
| 1:O:36:TRP:CH2   | 1:O:88:LYS:HE2   | 2.47                     | 0.49              |
| 1:O:177:LEU:C    | 1:O:179:SER:H    | 2.20                     | 0.49              |
| 2:P:103:TRP:CE2  | 2:P:131:LEU:HD12 | 2.47                     | 0.49              |
| 2:B:75:VAL:O     | 2:B:75:VAL:HG13  | 2.12                     | 0.49              |
| 2:B:126:ILE:HG13 | 2:B:150:ALA:HB2  | 1.93                     | 0.49              |
| 2:D:135:ASN:ND2  | 2:D:137:TYR:HB3  | 2.26                     | 0.49              |
| 2:F:185:VAL:O    | 2:F:243:VAL:HG11 | 2.13                     | 0.49              |
| 1:G:39:ASN:ND2   | 1:G:43:VAL:HG22  | 2.28                     | 0.49              |
| 1:G:47:ARG:NH1   | 1:G:71:THR:HB    | 2.28                     | 0.49              |
| 1:G:97:LYS:HD3   | 1:G:100:GLU:OE2  | 2.13                     | 0.49              |
| 2:H:170:VAL:HG12 | 2:H:172:LEU:HB2  | 1.94                     | 0.49              |
| 2:H:210:THR:HG22 | 2:H:211:ASN:N    | 2.27                     | 0.49              |
| 2:L:166:ARG:CG   | 2:L:182:PRO:HB2  | 2.42                     | 0.49              |
| 2:N:11:ILE:HG23  | 2:N:16:GLY:CA    | 2.32                     | 0.49              |
| 2:N:131:LEU:HD22 | 2:N:144:PHE:HB2  | 1.94                     | 0.49              |
| 1:A:77:GLN:NE2   | 1:A:77:GLN:HA    | 2.28                     | 0.49              |
| 1:A:188:ARG:HH12 | 1:A:198:PRO:HA   | 1.77                     | 0.49              |
| 2:F:70:ASN:ND2   | 2:F:119:ALA:HA   | 2.28                     | 0.49              |
| 2:H:35:VAL:HA    | 2:H:107:LEU:O    | 2.12                     | 0.49              |
| 1:I:110:ARG:HD3  | 2:J:277:VAL:HG13 | 1.93                     | 0.49              |
| 1:I:189:THR:O    | 1:I:197:THR:HG23 | 2.13                     | 0.49              |
| 1:K:36:TRP:CH2   | 1:K:88:LYS:HE2   | 2.47                     | 0.49              |
| 1:K:80:GLU:CD    | 1:K:148:TYR:HA   | 2.38                     | 0.49              |
| 1:M:20:LEU:HD12  | 1:M:21:ALA:H     | 1.78                     | 0.49              |
| 1:M:110:ARG:HD3  | 2:N:277:VAL:HG13 | 1.93                     | 0.49              |
| 2:N:5:THR:HG22   | 2:N:9:THR:N      | 2.27                     | 0.49              |
| 1:O:20:LEU:HD12  | 1:O:21:ALA:H     | 1.78                     | 0.49              |
| 2:D:46:ASN:O     | 2:D:98:ARG:HA    | 2.13                     | 0.48              |
| 1:E:188:ARG:HH12 | 1:E:198:PRO:HA   | 1.77                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:188:ARG:HH12 | 1:G:198:PRO:HA   | 1.77                     | 0.48              |
| 2:H:174:ASP:O    | 2:H:176:PRO:HD2  | 2.13                     | 0.48              |
| 1:I:80:GLU:CD    | 1:I:148:TYR:HA   | 2.38                     | 0.48              |
| 1:K:20:LEU:HD12  | 1:K:21:ALA:H     | 1.78                     | 0.48              |
| 2:L:5:THR:HG22   | 2:L:9:THR:N      | 2.28                     | 0.48              |
| 1:O:101:ASN:HB2  | 2:P:171:THR:O    | 2.14                     | 0.48              |
| 1:O:104:GLN:HG3  | 2:P:168:VAL:HB   | 1.94                     | 0.48              |
| 2:D:167:ASP:O    | 2:D:168:VAL:C    | 2.55                     | 0.48              |
| 2:F:28:VAL:HG12  | 2:F:111:PRO:HG2  | 1.95                     | 0.48              |
| 2:H:28:VAL:HG12  | 2:H:111:PRO:HG2  | 1.95                     | 0.48              |
| 2:H:211:ASN:HD21 | 2:H:269:GLN:N    | 1.95                     | 0.48              |
| 2:J:46:ASN:HD22  | 2:J:49:PRO:HA    | 1.78                     | 0.48              |
| 2:J:58:LEU:HD12  | 2:J:130:ILE:O    | 2.13                     | 0.48              |
| 1:K:189:THR:O    | 1:K:197:THR:HG23 | 2.13                     | 0.48              |
| 2:N:117:GLY:HA2  | 2:N:156:VAL:H    | 1.78                     | 0.48              |
| 2:P:46:ASN:HD22  | 2:P:49:PRO:HA    | 1.78                     | 0.48              |
| 1:A:131:LEU:HD23 | 1:A:187:TYR:CE2  | 2.48                     | 0.48              |
| 2:B:181:ILE:HD11 | 2:B:254:ALA:HB2  | 1.93                     | 0.48              |
| 1:C:114:TYR:CE1  | 1:C:149:TYR:HB2  | 2.48                     | 0.48              |
| 1:E:102:THR:OG1  | 2:F:269:GLN:HG2  | 2.13                     | 0.48              |
| 1:E:156:ASN:HD22 | 1:E:186:THR:HB   | 1.79                     | 0.48              |
| 2:F:201:THR:HG23 | 2:F:202:ALA:N    | 2.29                     | 0.48              |
| 2:H:239:SER:HB3  | 4:H:640:HOH:O    | 2.13                     | 0.48              |
| 1:I:36:TRP:CH2   | 1:I:88:LYS:HE2   | 2.47                     | 0.48              |
| 2:J:112:VAL:O    | 2:J:113:SER:C    | 2.57                     | 0.48              |
| 2:J:271:ILE:O    | 2:J:271:ILE:HG13 | 2.13                     | 0.48              |
| 2:L:172:LEU:HD23 | 2:L:172:LEU:C    | 2.38                     | 0.48              |
| 2:L:264:THR:HG22 | 2:L:265:ALA:N    | 2.21                     | 0.48              |
| 1:M:55:PHE:CE1   | 1:M:57:MET:HG3   | 2.47                     | 0.48              |
| 2:P:271:ILE:O    | 2:P:271:ILE:HG13 | 2.13                     | 0.48              |
| 1:A:11:TYR:HB2   | 1:A:113:LEU:HD11 | 1.96                     | 0.48              |
| 2:D:28:VAL:HG12  | 2:D:111:PRO:HG2  | 1.95                     | 0.48              |
| 1:E:9:VAL:HA     | 4:E:209:HOH:O    | 2.13                     | 0.48              |
| 1:E:47:ARG:NH1   | 1:E:47:ARG:HG3   | 2.27                     | 0.48              |
| 1:E:124:PRO:HD3  | 1:E:148:TYR:OH   | 2.13                     | 0.48              |
| 1:G:114:TYR:CE1  | 1:G:149:TYR:CB   | 2.96                     | 0.48              |
| 1:G:154:GLU:CD   | 1:G:188:ARG:HD3  | 2.38                     | 0.48              |
| 2:J:21:TYR:CB    | 2:J:151:ASN:HD21 | 2.25                     | 0.48              |
| 2:J:172:LEU:HD23 | 2:J:172:LEU:C    | 2.38                     | 0.48              |
| 1:K:133:PHE:CE1  | 1:K:202:GLY:HA3  | 2.48                     | 0.48              |
| 2:L:21:TYR:CB    | 2:L:151:ASN:HD21 | 2.24                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:80:GLU:CD    | 1:M:148:TYR:HA   | 2.38                     | 0.48              |
| 1:M:132:ARG:HB2  | 1:M:143:ILE:HG23 | 1.95                     | 0.48              |
| 2:N:57:THR:HG22  | 2:N:91:PRO:O     | 2.13                     | 0.48              |
| 2:P:115:ALA:HB3  | 2:P:156:VAL:HG11 | 1.94                     | 0.48              |
| 2:P:201:THR:HG21 | 2:P:206:ASN:ND2  | 2.29                     | 0.48              |
| 1:A:39:ASN:ND2   | 1:A:43:VAL:HG22  | 2.29                     | 0.48              |
| 1:C:102:THR:O    | 2:D:269:GLN:HA   | 2.12                     | 0.48              |
| 1:E:102:THR:O    | 2:F:269:GLN:HA   | 2.12                     | 0.48              |
| 2:F:57:THR:OG1   | 2:F:132:ARG:HB3  | 2.14                     | 0.48              |
| 2:F:174:ASP:O    | 2:F:176:PRO:N    | 2.47                     | 0.48              |
| 2:F:218:ALA:HA   | 2:F:265:ALA:O    | 2.14                     | 0.48              |
| 2:H:57:THR:OG1   | 2:H:132:ARG:HB3  | 2.13                     | 0.48              |
| 2:J:211:ASN:HD21 | 2:J:213:ALA:CB   | 2.27                     | 0.48              |
| 2:L:21:TYR:HB3   | 2:L:151:ASN:ND2  | 2.25                     | 0.48              |
| 2:P:122:ALA:HB2  | 2:P:152:ASN:O    | 2.13                     | 0.48              |
| 2:P:193:LEU:HD12 | 2:P:243:VAL:HG21 | 1.94                     | 0.48              |
| 2:P:224:GLN:CG   | 2:P:231:ILE:HD13 | 2.41                     | 0.48              |
| 1:A:102:THR:OG1  | 2:B:269:GLN:HG2  | 2.14                     | 0.48              |
| 1:A:135:ARG:NH1  | 1:A:135:ARG:HB2  | 2.29                     | 0.48              |
| 2:D:67:VAL:HG23  | 2:D:120:ILE:HD11 | 1.94                     | 0.48              |
| 2:D:82:TYR:OH    | 2:D:91:PRO:HD2   | 2.14                     | 0.48              |
| 1:E:107:ILE:N    | 1:E:107:ILE:HD12 | 2.28                     | 0.48              |
| 2:F:175:TYR:O    | 2:F:256:TYR:CD1  | 2.67                     | 0.48              |
| 1:G:204:MET:N    | 1:G:204:MET:SD   | 2.87                     | 0.48              |
| 2:H:5:THR:HG23   | 2:H:7:ASN:N      | 2.27                     | 0.48              |
| 2:H:174:ASP:C    | 2:H:176:PRO:HD2  | 2.39                     | 0.48              |
| 2:H:185:VAL:O    | 2:H:243:VAL:HG11 | 2.14                     | 0.48              |
| 1:I:153:THR:HG21 | 1:I:196:LEU:CD2  | 2.39                     | 0.48              |
| 2:J:193:LEU:HD12 | 2:J:243:VAL:HG21 | 1.95                     | 0.48              |
| 1:K:143:ILE:HA   | 1:K:172:GLU:HB2  | 1.94                     | 0.48              |
| 1:M:189:THR:O    | 1:M:197:THR:HG23 | 2.13                     | 0.48              |
| 1:A:31:TYR:O     | 1:A:56:ALA:HA    | 2.14                     | 0.48              |
| 1:A:46:GLY:O     | 1:A:47:ARG:C     | 2.57                     | 0.48              |
| 2:B:38:LEU:C     | 2:B:40:THR:N     | 2.68                     | 0.48              |
| 2:B:167:ASP:O    | 2:B:168:VAL:C    | 2.56                     | 0.48              |
| 2:B:185:VAL:O    | 2:B:243:VAL:HG11 | 2.13                     | 0.48              |
| 1:C:77:GLN:HA    | 1:C:77:GLN:NE2   | 2.29                     | 0.48              |
| 1:C:135:ARG:NH1  | 1:C:135:ARG:HB2  | 2.28                     | 0.48              |
| 1:E:11:TYR:HB2   | 1:E:113:LEU:HD11 | 1.95                     | 0.48              |
| 1:M:101:ASN:HB2  | 2:N:171:THR:O    | 2.13                     | 0.48              |
| 1:M:158:GLY:N    | 1:M:184:ASN:HD22 | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:38:LEU:HD12  | 2:N:38:LEU:N     | 2.29                     | 0.48              |
| 1:O:79:ARG:HB2   | 1:O:169:PRO:CB   | 2.44                     | 0.48              |
| 2:B:262:GLN:HG3  | 2:B:262:GLN:O    | 2.14                     | 0.48              |
| 2:N:112:VAL:O    | 2:N:113:SER:C    | 2.57                     | 0.48              |
| 2:P:211:ASN:HD21 | 2:P:213:ALA:HB3  | 1.78                     | 0.48              |
| 1:A:154:GLU:CD   | 1:A:188:ARG:HD3  | 2.38                     | 0.48              |
| 1:C:127:ALA:C    | 1:C:129:GLU:H    | 2.22                     | 0.48              |
| 1:E:39:ASN:ND2   | 1:E:43:VAL:HG22  | 2.29                     | 0.48              |
| 1:E:77:GLN:HA    | 1:E:77:GLN:NE2   | 2.29                     | 0.48              |
| 1:E:135:ARG:NH1  | 1:E:135:ARG:HB2  | 2.28                     | 0.48              |
| 2:F:92:ARG:HG3   | 2:F:92:ARG:NH1   | 2.27                     | 0.48              |
| 2:F:170:VAL:C    | 2:F:172:LEU:N    | 2.72                     | 0.48              |
| 2:H:172:LEU:HD23 | 2:H:172:LEU:C    | 2.39                     | 0.48              |
| 1:I:188:ARG:NH2  | 1:I:196:LEU:HB2  | 2.29                     | 0.48              |
| 2:J:19:ASN:OD1   | 2:L:262:GLN:NE2  | 2.47                     | 0.48              |
| 1:K:79:ARG:HB2   | 1:K:169:PRO:CB   | 2.44                     | 0.48              |
| 1:K:191:ASN:HD21 | 1:K:195:ALA:HB3  | 1.79                     | 0.48              |
| 1:M:79:ARG:HB2   | 1:M:169:PRO:CB   | 2.44                     | 0.48              |
| 2:N:46:ASN:HD22  | 2:N:49:PRO:HA    | 1.79                     | 0.48              |
| 2:N:172:LEU:HD23 | 2:N:172:LEU:C    | 2.39                     | 0.48              |
| 2:N:264:THR:HG22 | 2:N:265:ALA:N    | 2.21                     | 0.48              |
| 2:P:48:TYR:CE1   | 3:P:607:MMA:H73  | 2.49                     | 0.48              |
| 2:B:82:TYR:OH    | 2:B:91:PRO:HD2   | 2.14                     | 0.48              |
| 2:B:170:VAL:HG12 | 2:B:172:LEU:HB2  | 1.95                     | 0.48              |
| 1:C:11:TYR:HB2   | 1:C:113:LEU:HD11 | 1.96                     | 0.48              |
| 1:C:156:ASN:HD22 | 1:C:186:THR:HB   | 1.79                     | 0.48              |
| 2:D:174:ASP:C    | 2:D:176:PRO:HD2  | 2.39                     | 0.48              |
| 2:D:175:TYR:O    | 2:D:256:TYR:CD2  | 2.66                     | 0.48              |
| 2:D:192:ASN:OD1  | 2:D:242:ALA:HB2  | 2.13                     | 0.48              |
| 1:E:46:GLY:O     | 1:E:47:ARG:C     | 2.56                     | 0.48              |
| 2:F:116:GLY:HA2  | 2:F:189:LYS:CE   | 2.42                     | 0.48              |
| 1:I:103:LEU:H    | 2:J:168:VAL:HG22 | 1.79                     | 0.48              |
| 2:L:262:GLN:O    | 2:L:262:GLN:HG3  | 2.14                     | 0.48              |
| 1:M:91:PRO:HB2   | 1:M:104:GLN:HE21 | 1.78                     | 0.48              |
| 1:M:133:PHE:CE1  | 1:M:202:GLY:HA3  | 2.49                     | 0.48              |
| 1:M:143:ILE:HA   | 1:M:172:GLU:HB2  | 1.95                     | 0.48              |
| 2:N:201:THR:HG21 | 2:N:206:ASN:ND2  | 2.29                     | 0.48              |
| 2:P:57:THR:HG22  | 2:P:91:PRO:O     | 2.13                     | 0.48              |
| 2:P:112:VAL:O    | 2:P:113:SER:C    | 2.57                     | 0.48              |
| 1:A:38:GLU:CD    | 1:A:110:ARG:HH22 | 2.21                     | 0.47              |
| 2:B:172:LEU:HD23 | 2:B:172:LEU:C    | 2.39                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:80:GLU:HA    | 1:C:115:TYR:O    | 2.14                     | 0.47              |
| 2:D:185:VAL:O    | 2:D:243:VAL:HG11 | 2.14                     | 0.47              |
| 1:E:31:TYR:O     | 1:E:56:ALA:HA    | 2.14                     | 0.47              |
| 2:F:170:VAL:HG12 | 2:F:172:LEU:HB2  | 1.94                     | 0.47              |
| 2:F:174:ASP:C    | 2:F:176:PRO:HD2  | 2.39                     | 0.47              |
| 2:J:38:LEU:C     | 2:J:40:THR:N     | 2.62                     | 0.47              |
| 2:J:48:TYR:CE1   | 3:J:605:MMA:H73  | 2.49                     | 0.47              |
| 1:K:102:THR:HB   | 2:L:168:VAL:HG21 | 1.95                     | 0.47              |
| 2:N:226:THR:CG2  | 2:N:253:THR:HB   | 2.42                     | 0.47              |
| 1:O:133:PHE:CE1  | 1:O:202:GLY:HA3  | 2.48                     | 0.47              |
| 1:A:127:ALA:C    | 1:A:129:GLU:H    | 2.22                     | 0.47              |
| 1:A:142:LEU:CD2  | 1:A:142:LEU:N    | 2.77                     | 0.47              |
| 2:D:170:VAL:C    | 2:D:172:LEU:N    | 2.72                     | 0.47              |
| 2:D:172:LEU:C    | 2:D:172:LEU:HD23 | 2.38                     | 0.47              |
| 1:G:31:TYR:O     | 1:G:56:ALA:HA    | 2.13                     | 0.47              |
| 2:H:218:ALA:HA   | 2:H:265:ALA:O    | 2.14                     | 0.47              |
| 2:J:201:THR:HG21 | 2:J:206:ASN:ND2  | 2.29                     | 0.47              |
| 2:L:11:ILE:HG23  | 2:L:16:GLY:CA    | 2.32                     | 0.47              |
| 2:L:115:ALA:HB3  | 2:L:156:VAL:HG11 | 1.94                     | 0.47              |
| 2:L:211:ASN:HD21 | 2:L:213:ALA:HB3  | 1.79                     | 0.47              |
| 1:O:132:ARG:HB2  | 1:O:143:ILE:HG23 | 1.96                     | 0.47              |
| 1:O:158:GLY:N    | 1:O:184:ASN:HD22 | 2.11                     | 0.47              |
| 2:P:262:GLN:HG3  | 2:P:262:GLN:O    | 2.14                     | 0.47              |
| 2:B:70:ASN:ND2   | 2:B:119:ALA:HA   | 2.29                     | 0.47              |
| 1:C:31:TYR:O     | 1:C:56:ALA:HA    | 2.14                     | 0.47              |
| 1:E:38:GLU:CD    | 1:E:110:ARG:HH22 | 2.22                     | 0.47              |
| 1:E:47:ARG:HG3   | 1:E:47:ARG:HH11  | 1.78                     | 0.47              |
| 2:F:135:ASN:ND2  | 2:F:138:ASN:H    | 2.12                     | 0.47              |
| 2:J:38:LEU:HD12  | 2:J:38:LEU:N     | 2.28                     | 0.47              |
| 2:J:216:SER:N    | 2:J:217:PRO:CD   | 2.77                     | 0.47              |
| 1:K:103:LEU:H    | 2:L:168:VAL:HG22 | 1.80                     | 0.47              |
| 1:O:103:LEU:H    | 2:P:168:VAL:HG22 | 1.79                     | 0.47              |
| 2:P:41:GLN:HA    | 2:P:41:GLN:NE2   | 2.29                     | 0.47              |
| 1:C:39:ASN:ND2   | 1:C:43:VAL:HG22  | 2.30                     | 0.47              |
| 2:D:75:VAL:HG13  | 2:D:75:VAL:O     | 2.15                     | 0.47              |
| 2:D:170:VAL:HG12 | 2:D:172:LEU:HB2  | 1.96                     | 0.47              |
| 2:D:181:ILE:HD11 | 2:D:254:ALA:HB2  | 1.95                     | 0.47              |
| 1:E:127:ALA:C    | 1:E:129:GLU:H    | 2.23                     | 0.47              |
| 1:E:188:ARG:NE   | 1:E:196:LEU:HD22 | 2.28                     | 0.47              |
| 2:H:70:ASN:ND2   | 2:H:119:ALA:HA   | 2.29                     | 0.47              |
| 1:I:52:PRO:HG2   | 1:I:55:PHE:CE2   | 2.50                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:79:ARG:HB2   | 1:I:169:PRO:CB   | 2.44                     | 0.47              |
| 2:J:224:GLN:CG   | 2:J:231:ILE:HD13 | 2.41                     | 0.47              |
| 2:N:211:ASN:HD21 | 2:N:213:ALA:HB3  | 1.79                     | 0.47              |
| 2:P:117:GLY:HA2  | 2:P:156:VAL:H    | 1.79                     | 0.47              |
| 2:P:172:LEU:HD23 | 2:P:172:LEU:C    | 2.38                     | 0.47              |
| 2:P:211:ASN:HD21 | 2:P:213:ALA:CB   | 2.28                     | 0.47              |
| 1:A:86:ASN:HD21  | 1:A:110:ARG:NE   | 2.09                     | 0.47              |
| 2:B:227:ARG:O    | 2:B:227:ARG:HG3  | 2.14                     | 0.47              |
| 1:G:135:ARG:NH1  | 1:G:135:ARG:HB2  | 2.29                     | 0.47              |
| 2:J:208:ILE:HA   | 2:J:223:VAL:O    | 2.15                     | 0.47              |
| 2:L:58:LEU:HD12  | 2:L:130:ILE:O    | 2.14                     | 0.47              |
| 1:M:24:ASN:HB2   | 1:M:57:MET:HE2   | 1.96                     | 0.47              |
| 2:N:122:ALA:HB2  | 2:N:152:ASN:O    | 2.13                     | 0.47              |
| 2:P:126:ILE:N    | 2:P:148:ILE:O    | 2.45                     | 0.47              |
| 2:P:216:SER:N    | 2:P:217:PRO:CD   | 2.78                     | 0.47              |
| 1:A:112:LYS:HE3  | 2:B:279:GLN:O    | 2.15                     | 0.47              |
| 1:A:114:TYR:CE1  | 1:A:149:TYR:CB   | 2.98                     | 0.47              |
| 1:C:133:PHE:HD2  | 1:C:140:LEU:HD21 | 1.80                     | 0.47              |
| 2:D:5:THR:HG23   | 2:D:7:ASN:N      | 2.28                     | 0.47              |
| 2:D:116:GLY:HA2  | 2:D:189:LYS:CE   | 2.44                     | 0.47              |
| 2:D:131:LEU:HB3  | 2:D:144:PHE:HB2  | 1.95                     | 0.47              |
| 2:D:218:ALA:HA   | 2:D:265:ALA:O    | 2.14                     | 0.47              |
| 1:I:193:TYR:CD2  | 2:J:155:VAL:HG21 | 2.50                     | 0.47              |
| 1:K:132:ARG:HB2  | 1:K:143:ILE:HG23 | 1.96                     | 0.47              |
| 2:L:117:GLY:HA2  | 2:L:156:VAL:H    | 1.79                     | 0.47              |
| 2:N:202:ALA:N    | 2:N:208:ILE:O    | 2.48                     | 0.47              |
| 1:O:91:PRO:HB2   | 1:O:104:GLN:HE21 | 1.79                     | 0.47              |
| 2:P:234:ALA:O    | 2:P:235:ASN:HB2  | 2.15                     | 0.47              |
| 2:P:268:VAL:C    | 2:P:269:GLN:HG3  | 2.38                     | 0.47              |
| 1:A:9:VAL:HG12   | 1:A:113:LEU:CD1  | 2.45                     | 0.47              |
| 1:A:80:GLU:HA    | 1:A:115:TYR:O    | 2.15                     | 0.47              |
| 1:A:132:ARG:HD2  | 1:A:205:GLU:HB3  | 1.96                     | 0.47              |
| 1:A:188:ARG:NE   | 1:A:196:LEU:HD22 | 2.29                     | 0.47              |
| 2:B:120:ILE:HG23 | 2:B:126:ILE:HD11 | 1.97                     | 0.47              |
| 2:B:271:ILE:O    | 2:B:272:ILE:HD13 | 2.15                     | 0.47              |
| 1:C:57:MET:HE3   | 1:C:63:ASN:OD1   | 2.15                     | 0.47              |
| 1:E:80:GLU:HA    | 1:E:115:TYR:O    | 2.15                     | 0.47              |
| 1:E:82:LEU:HD12  | 1:E:83:PHE:N     | 2.29                     | 0.47              |
| 1:E:86:ASN:HD21  | 1:E:110:ARG:NE   | 2.10                     | 0.47              |
| 1:E:114:TYR:CE1  | 1:E:149:TYR:CB   | 2.98                     | 0.47              |
| 1:G:11:TYR:HB2   | 1:G:113:LEU:HD11 | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:102:THR:OG1  | 2:H:269:GLN:HG2  | 2.14                     | 0.47              |
| 1:G:112:LYS:HE3  | 2:H:279:GLN:O    | 2.14                     | 0.47              |
| 2:H:167:ASP:O    | 2:H:168:VAL:C    | 2.57                     | 0.47              |
| 1:I:86:ASN:HD21  | 1:I:110:ARG:HG3  | 1.80                     | 0.47              |
| 1:I:91:PRO:HB2   | 1:I:104:GLN:HE21 | 1.79                     | 0.47              |
| 1:I:132:ARG:HB2  | 1:I:143:ILE:HG23 | 1.95                     | 0.47              |
| 1:I:149:TYR:CB   | 1:I:166:LEU:HD11 | 2.39                     | 0.47              |
| 2:J:26:PRO:HA    | 2:J:154:VAL:HA   | 1.97                     | 0.47              |
| 2:J:34:LEU:O     | 2:J:34:LEU:CG    | 2.63                     | 0.47              |
| 2:J:122:ALA:HB2  | 2:J:152:ASN:O    | 2.14                     | 0.47              |
| 2:J:138:ASN:HD21 | 2:J:140:ASP:HB2  | 1.80                     | 0.47              |
| 2:J:268:VAL:C    | 2:J:269:GLN:HG3  | 2.39                     | 0.47              |
| 2:L:61:GLY:HA2   | 2:L:128:VAL:O    | 2.15                     | 0.47              |
| 2:L:201:THR:HG21 | 2:L:206:ASN:ND2  | 2.29                     | 0.47              |
| 2:L:202:ALA:N    | 2:L:208:ILE:O    | 2.47                     | 0.47              |
| 2:L:225:LEU:HA   | 2:L:253:THR:O    | 2.15                     | 0.47              |
| 1:M:102:THR:HB   | 2:N:168:VAL:HG21 | 1.95                     | 0.47              |
| 1:M:103:LEU:H    | 2:N:168:VAL:CG2  | 2.28                     | 0.47              |
| 1:M:191:ASN:HD21 | 1:M:195:ALA:HB3  | 1.78                     | 0.47              |
| 2:N:50:GLU:OE1   | 2:N:98:ARG:NH2   | 2.48                     | 0.47              |
| 2:N:90:THR:HB    | 2:N:91:PRO:HD2   | 1.96                     | 0.47              |
| 2:N:166:ARG:CG   | 2:N:182:PRO:HB2  | 2.43                     | 0.47              |
| 2:N:208:ILE:HA   | 2:N:223:VAL:O    | 2.15                     | 0.47              |
| 1:O:160:ARG:CD   | 1:O:180:ASP:HB2  | 2.41                     | 0.47              |
| 1:O:188:ARG:NH2  | 1:O:196:LEU:HB2  | 2.29                     | 0.47              |
| 2:P:26:PRO:HA    | 2:P:154:VAL:HA   | 1.97                     | 0.47              |
| 2:P:208:ILE:HA   | 2:P:223:VAL:O    | 2.14                     | 0.47              |
| 1:A:133:PHE:HD2  | 1:A:140:LEU:HD21 | 1.80                     | 0.47              |
| 1:C:142:LEU:CD2  | 1:C:142:LEU:N    | 2.78                     | 0.47              |
| 2:D:106:ALA:HB3  | 4:D:626:HOH:O    | 2.15                     | 0.47              |
| 2:D:135:ASN:ND2  | 2:D:138:ASN:H    | 2.12                     | 0.47              |
| 1:G:127:ALA:C    | 1:G:129:GLU:H    | 2.23                     | 0.47              |
| 2:L:116:GLY:HA2  | 2:L:189:LYS:CG   | 2.41                     | 0.47              |
| 2:L:208:ILE:HA   | 2:L:223:VAL:O    | 2.15                     | 0.47              |
| 2:N:26:PRO:HA    | 2:N:154:VAL:HA   | 1.97                     | 0.47              |
| 2:P:50:GLU:OE1   | 2:P:98:ARG:NH2   | 2.48                     | 0.47              |
| 2:P:202:ALA:N    | 2:P:208:ILE:O    | 2.48                     | 0.47              |
| 2:P:225:LEU:HA   | 2:P:253:THR:O    | 2.14                     | 0.47              |
| 2:B:131:LEU:HB3  | 2:B:144:PHE:HB2  | 1.96                     | 0.47              |
| 2:B:175:TYR:O    | 2:B:256:TYR:CD1  | 2.68                     | 0.47              |
| 2:D:92:ARG:HG3   | 2:D:92:ARG:NH1   | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:132:ARG:HD2  | 1:E:205:GLU:HB3  | 1.97                     | 0.47              |
| 1:G:38:GLU:CD    | 1:G:110:ARG:HH22 | 2.22                     | 0.47              |
| 1:I:123:PRO:C    | 1:I:125:ASP:H    | 2.23                     | 0.47              |
| 1:I:133:PHE:CE1  | 1:I:202:GLY:HA3  | 2.49                     | 0.47              |
| 2:J:117:GLY:HA2  | 2:J:156:VAL:H    | 1.80                     | 0.47              |
| 1:K:24:ASN:HB2   | 1:K:57:MET:HE2   | 1.97                     | 0.47              |
| 2:L:46:ASN:HD22  | 2:L:49:PRO:HA    | 1.80                     | 0.47              |
| 1:M:105:LEU:HA   | 2:N:272:ILE:O    | 2.15                     | 0.47              |
| 1:M:160:ARG:CD   | 1:M:180:ASP:HB2  | 2.40                     | 0.47              |
| 1:M:188:ARG:NH2  | 1:M:196:LEU:HB2  | 2.29                     | 0.47              |
| 2:N:216:SER:N    | 2:N:217:PRO:CD   | 2.78                     | 0.47              |
| 2:B:209:PHE:CG   | 2:B:272:ILE:HD11 | 2.50                     | 0.47              |
| 1:E:107:ILE:HG12 | 2:F:163:VAL:HG11 | 1.97                     | 0.47              |
| 1:G:46:GLY:O     | 1:G:47:ARG:C     | 2.56                     | 0.47              |
| 1:I:191:ASN:HD21 | 1:I:195:ALA:HB3  | 1.80                     | 0.47              |
| 2:J:138:ASN:C    | 2:J:138:ASN:HD22 | 2.23                     | 0.47              |
| 1:K:188:ARG:NH2  | 1:K:196:LEU:HB2  | 2.29                     | 0.47              |
| 2:N:258:ARG:HE   | 2:N:263:VAL:CG2  | 2.28                     | 0.47              |
| 2:N:268:VAL:C    | 2:N:269:GLN:HG3  | 2.39                     | 0.47              |
| 1:O:103:LEU:H    | 2:P:168:VAL:CG2  | 2.28                     | 0.47              |
| 1:O:193:TYR:CD2  | 2:P:155:VAL:HG21 | 2.49                     | 0.47              |
| 1:C:132:ARG:HD2  | 1:C:205:GLU:HB3  | 1.96                     | 0.46              |
| 2:F:209:PHE:CG   | 2:F:272:ILE:HD11 | 2.50                     | 0.46              |
| 2:L:26:PRO:HA    | 2:L:154:VAL:HA   | 1.97                     | 0.46              |
| 2:L:50:GLU:OE1   | 2:L:98:ARG:NH2   | 2.48                     | 0.46              |
| 2:L:148:ILE:N    | 2:L:148:ILE:CD1  | 2.78                     | 0.46              |
| 2:L:216:SER:N    | 2:L:217:PRO:CD   | 2.78                     | 0.46              |
| 1:M:103:LEU:H    | 2:N:168:VAL:HG22 | 1.79                     | 0.46              |
| 2:B:116:GLY:HA2  | 2:B:189:LYS:CE   | 2.44                     | 0.46              |
| 2:D:70:ASN:ND2   | 2:D:119:ALA:HA   | 2.30                     | 0.46              |
| 1:E:154:GLU:CD   | 1:E:188:ARG:HD3  | 2.40                     | 0.46              |
| 2:F:120:ILE:HG23 | 2:F:126:ILE:HD11 | 1.96                     | 0.46              |
| 2:F:211:ASN:HD21 | 2:F:269:GLN:N    | 1.97                     | 0.46              |
| 1:G:86:ASN:HD21  | 1:G:110:ARG:HH21 | 1.62                     | 0.46              |
| 1:M:193:TYR:CD2  | 2:N:155:VAL:HG21 | 2.50                     | 0.46              |
| 2:N:34:LEU:O     | 2:N:34:LEU:CG    | 2.62                     | 0.46              |
| 1:O:105:LEU:HA   | 2:P:272:ILE:O    | 2.16                     | 0.46              |
| 1:C:204:MET:SD   | 1:C:204:MET:N    | 2.89                     | 0.46              |
| 2:D:201:THR:HG23 | 2:D:203:ASP:H    | 1.81                     | 0.46              |
| 2:H:175:TYR:O    | 2:H:256:TYR:CD2  | 2.69                     | 0.46              |
| 2:J:225:LEU:HA   | 2:J:253:THR:O    | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:38:LEU:N     | 2:L:38:LEU:HD12  | 2.30                     | 0.46              |
| 2:L:122:ALA:HB2  | 2:L:152:ASN:O    | 2.15                     | 0.46              |
| 2:L:138:ASN:HD21 | 2:L:140:ASP:HB2  | 1.80                     | 0.46              |
| 2:L:234:ALA:O    | 2:L:235:ASN:HB2  | 2.15                     | 0.46              |
| 2:N:262:GLN:HG3  | 2:N:262:GLN:O    | 2.15                     | 0.46              |
| 1:O:24:ASN:HB2   | 1:O:57:MET:HE2   | 1.96                     | 0.46              |
| 2:P:136:ASN:HD22 | 2:P:136:ASN:H    | 1.64                     | 0.46              |
| 1:E:9:VAL:HG12   | 1:E:113:LEU:HD13 | 1.97                     | 0.46              |
| 2:F:221:VAL:CG1  | 2:F:222:GLY:H    | 2.20                     | 0.46              |
| 1:G:185:ILE:O    | 1:G:201:THR:HA   | 2.16                     | 0.46              |
| 2:H:57:THR:HG22  | 2:H:92:ARG:HA    | 1.98                     | 0.46              |
| 2:H:59:GLN:NE2   | 2:H:143:GLN:HE22 | 2.12                     | 0.46              |
| 2:L:57:THR:HG22  | 2:L:91:PRO:O     | 2.16                     | 0.46              |
| 2:L:211:ASN:HD21 | 2:L:213:ALA:CB   | 2.29                     | 0.46              |
| 2:P:226:THR:CG2  | 2:P:253:THR:HB   | 2.43                     | 0.46              |
| 2:P:258:ARG:HE   | 2:P:263:VAL:CG2  | 2.28                     | 0.46              |
| 1:A:78:ASP:OD2   | 1:A:79:ARG:NH2   | 2.46                     | 0.46              |
| 1:A:107:ILE:HG12 | 2:B:163:VAL:HG11 | 1.96                     | 0.46              |
| 2:B:218:ALA:HA   | 2:B:265:ALA:O    | 2.15                     | 0.46              |
| 1:C:154:GLU:OE1  | 1:C:188:ARG:CD   | 2.63                     | 0.46              |
| 2:D:25:ALA:HA    | 2:D:26:PRO:HD3   | 1.82                     | 0.46              |
| 2:D:59:GLN:HE21  | 2:D:143:GLN:HE22 | 1.63                     | 0.46              |
| 2:F:78:SER:N     | 4:F:547:HOH:O    | 2.49                     | 0.46              |
| 2:F:262:GLN:HG3  | 2:F:262:GLN:O    | 2.15                     | 0.46              |
| 1:G:9:VAL:HG12   | 1:G:113:LEU:HD13 | 1.96                     | 0.46              |
| 1:K:44:LYS:C     | 1:K:45:ASP:CG    | 2.84                     | 0.46              |
| 1:K:86:ASN:HD21  | 1:K:110:ARG:HG3  | 1.81                     | 0.46              |
| 2:L:268:VAL:C    | 2:L:269:GLN:HG3  | 2.39                     | 0.46              |
| 1:M:28:ASN:HD22  | 1:M:28:ASN:N     | 1.99                     | 0.46              |
| 2:N:225:LEU:HA   | 2:N:253:THR:O    | 2.15                     | 0.46              |
| 2:P:138:ASN:HD21 | 2:P:140:ASP:HB2  | 1.80                     | 0.46              |
| 2:B:170:VAL:C    | 2:B:172:LEU:N    | 2.73                     | 0.46              |
| 1:C:38:GLU:CD    | 1:C:110:ARG:HH22 | 2.23                     | 0.46              |
| 1:C:78:ASP:OD2   | 1:C:79:ARG:NH2   | 2.47                     | 0.46              |
| 2:D:59:GLN:NE2   | 2:D:143:GLN:HE22 | 2.14                     | 0.46              |
| 1:E:156:ASN:C    | 1:E:158:GLY:N    | 2.73                     | 0.46              |
| 2:F:48:TYR:H     | 3:F:502:MMA:H62  | 1.80                     | 0.46              |
| 2:J:90:THR:HB    | 2:J:91:PRO:HD2   | 1.97                     | 0.46              |
| 2:J:258:ARG:HE   | 2:J:263:VAL:CG2  | 2.29                     | 0.46              |
| 1:K:52:PRO:HG2   | 1:K:55:PHE:CE2   | 2.50                     | 0.46              |
| 2:N:138:ASN:HD21 | 2:N:140:ASP:HB2  | 1.79                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:211:ASN:HD21 | 2:N:213:ALA:CB   | 2.29                     | 0.46              |
| 1:O:52:PRO:HG2   | 1:O:55:PHE:CE2   | 2.50                     | 0.46              |
| 1:O:162:LEU:HB3  | 1:O:175:VAL:CG1  | 2.44                     | 0.46              |
| 1:C:9:VAL:HG12   | 1:C:113:LEU:HD13 | 1.98                     | 0.46              |
| 1:C:185:ILE:O    | 1:C:201:THR:HA   | 2.16                     | 0.46              |
| 1:G:132:ARG:HD2  | 1:G:205:GLU:HB3  | 1.98                     | 0.46              |
| 2:H:185:VAL:O    | 2:H:247:ALA:HA   | 2.16                     | 0.46              |
| 1:I:52:PRO:HG2   | 1:I:55:PHE:HE2   | 1.81                     | 0.46              |
| 1:I:105:LEU:HA   | 2:J:272:ILE:O    | 2.16                     | 0.46              |
| 2:J:50:GLU:OE1   | 2:J:98:ARG:NH2   | 2.48                     | 0.46              |
| 1:K:91:PRO:HB2   | 1:K:104:GLN:HE21 | 1.80                     | 0.46              |
| 1:K:193:TYR:CD2  | 2:L:155:VAL:HG11 | 2.51                     | 0.46              |
| 2:L:112:VAL:O    | 2:L:113:SER:C    | 2.58                     | 0.46              |
| 2:L:227:ARG:C    | 2:L:229:GLY:N    | 2.74                     | 0.46              |
| 1:M:52:PRO:HG2   | 1:M:55:PHE:CE2   | 2.50                     | 0.46              |
| 1:M:110:ARG:N    | 2:N:276:PHE:O    | 2.49                     | 0.46              |
| 2:N:19:ASN:OD1   | 2:P:262:GLN:NE2  | 2.49                     | 0.46              |
| 2:N:116:GLY:HA2  | 2:N:189:LYS:CG   | 2.41                     | 0.46              |
| 2:P:166:ARG:CG   | 2:P:182:PRO:HB2  | 2.42                     | 0.46              |
| 1:C:112:LYS:HE3  | 2:D:279:GLN:O    | 2.14                     | 0.46              |
| 1:E:185:ILE:O    | 1:E:201:THR:HA   | 2.16                     | 0.46              |
| 1:G:88:LYS:CB    | 1:G:108:ILE:HG12 | 2.43                     | 0.46              |
| 1:K:28:ASN:HD22  | 1:K:28:ASN:N     | 1.99                     | 0.46              |
| 1:K:39:ASN:O     | 1:K:84:TRP:HD1   | 1.99                     | 0.46              |
| 2:L:41:GLN:NE2   | 2:L:41:GLN:HA    | 2.31                     | 0.46              |
| 1:M:108:ILE:HD12 | 2:N:275:THR:OG1  | 2.16                     | 0.46              |
| 2:N:60:ARG:HG2   | 2:N:61:GLY:N     | 2.21                     | 0.46              |
| 2:N:138:ASN:HD22 | 2:N:138:ASN:C    | 2.24                     | 0.46              |
| 2:P:206:ASN:HD21 | 2:P:234:ALA:CB   | 2.28                     | 0.46              |
| 1:A:204:MET:N    | 1:A:204:MET:SD   | 2.89                     | 0.46              |
| 2:D:57:THR:HG22  | 2:D:92:ARG:HA    | 1.98                     | 0.46              |
| 2:D:209:PHE:CG   | 2:D:272:ILE:HD11 | 2.50                     | 0.46              |
| 2:D:262:GLN:O    | 2:D:262:GLN:HG3  | 2.16                     | 0.46              |
| 2:H:211:ASN:ND2  | 2:H:269:GLN:N    | 2.59                     | 0.46              |
| 1:I:102:THR:HB   | 2:J:168:VAL:HG21 | 1.95                     | 0.46              |
| 1:I:162:LEU:HB3  | 1:I:175:VAL:CG1  | 2.45                     | 0.46              |
| 2:J:226:THR:CG2  | 2:J:253:THR:HB   | 2.42                     | 0.46              |
| 1:K:100:GLU:CG   | 2:L:172:LEU:HD12 | 2.46                     | 0.46              |
| 1:K:193:TYR:CD2  | 2:L:155:VAL:HG21 | 2.50                     | 0.46              |
| 2:N:41:GLN:NE2   | 2:N:41:GLN:HA    | 2.30                     | 0.46              |
| 1:E:112:LYS:HE3  | 2:F:279:GLN:O    | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:135:ARG:HB2  | 1:E:135:ARG:HH11 | 1.81                     | 0.46              |
| 1:G:142:LEU:N    | 1:G:142:LEU:CD2  | 2.79                     | 0.46              |
| 2:J:202:ALA:N    | 2:J:208:ILE:O    | 2.48                     | 0.46              |
| 2:L:34:LEU:O     | 2:L:34:LEU:CG    | 2.62                     | 0.46              |
| 2:L:138:ASN:C    | 2:L:138:ASN:HD22 | 2.24                     | 0.46              |
| 1:M:44:LYS:C     | 1:M:45:ASP:CG    | 2.84                     | 0.46              |
| 1:M:100:GLU:CG   | 2:N:172:LEU:HD12 | 2.46                     | 0.46              |
| 1:M:132:ARG:CG   | 1:M:203:VAL:O    | 2.63                     | 0.46              |
| 2:N:158:THR:HG23 | 2:N:158:THR:O    | 2.16                     | 0.46              |
| 1:O:52:PRO:HG2   | 1:O:55:PHE:HE2   | 1.81                     | 0.46              |
| 2:P:158:THR:HG23 | 2:P:158:THR:O    | 2.16                     | 0.46              |
| 2:P:227:ARG:C    | 2:P:229:GLY:N    | 2.73                     | 0.46              |
| 1:C:135:ARG:HB2  | 1:C:135:ARG:HH11 | 1.81                     | 0.45              |
| 1:C:153:THR:HA   | 1:C:164:ASN:OD1  | 2.16                     | 0.45              |
| 2:D:120:ILE:HG23 | 2:D:126:ILE:HD11 | 1.98                     | 0.45              |
| 2:D:201:THR:HG23 | 2:D:202:ALA:N    | 2.31                     | 0.45              |
| 2:D:211:ASN:HD22 | 2:D:212:THR:N    | 2.14                     | 0.45              |
| 1:G:135:ARG:HB2  | 1:G:135:ARG:HH11 | 1.82                     | 0.45              |
| 2:H:49:PRO:HG3   | 2:H:98:ARG:HG3   | 1.98                     | 0.45              |
| 1:I:88:LYS:CG    | 1:I:108:ILE:HG12 | 2.42                     | 0.45              |
| 1:I:141:THR:C    | 1:I:174:THR:HG22 | 2.34                     | 0.45              |
| 2:L:258:ARG:HE   | 2:L:263:VAL:CG2  | 2.28                     | 0.45              |
| 2:N:234:ALA:O    | 2:N:235:ASN:HB2  | 2.15                     | 0.45              |
| 1:O:191:ASN:HD21 | 1:O:195:ALA:HB3  | 1.79                     | 0.45              |
| 2:P:41:GLN:HA    | 2:P:41:GLN:HE21  | 1.81                     | 0.45              |
| 2:P:90:THR:HB    | 2:P:91:PRO:HD2   | 1.98                     | 0.45              |
| 2:P:138:ASN:C    | 2:P:138:ASN:HD22 | 2.23                     | 0.45              |
| 2:B:5:THR:HG23   | 2:B:7:ASN:N      | 2.27                     | 0.45              |
| 2:B:185:VAL:O    | 2:B:247:ALA:HA   | 2.16                     | 0.45              |
| 2:B:195:TYR:CE1  | 2:B:238:VAL:HB   | 2.51                     | 0.45              |
| 1:C:102:THR:OG1  | 2:D:269:GLN:HG2  | 2.16                     | 0.45              |
| 1:C:114:TYR:CE1  | 1:C:149:TYR:CB   | 2.99                     | 0.45              |
| 2:D:211:ASN:ND2  | 2:D:269:GLN:N    | 2.60                     | 0.45              |
| 1:I:103:LEU:H    | 2:J:168:VAL:CG2  | 2.28                     | 0.45              |
| 1:I:169:PRO:O    | 1:I:171:GLY:N    | 2.48                     | 0.45              |
| 2:J:41:GLN:HA    | 2:J:41:GLN:NE2   | 2.31                     | 0.45              |
| 1:K:103:LEU:H    | 2:L:168:VAL:CG2  | 2.28                     | 0.45              |
| 2:L:106:ALA:CB   | 2:L:108:TYR:HE1  | 2.29                     | 0.45              |
| 2:L:226:THR:CG2  | 2:L:253:THR:HB   | 2.42                     | 0.45              |
| 1:M:123:PRO:C    | 1:M:125:ASP:H    | 2.24                     | 0.45              |
| 2:N:90:THR:HB    | 2:N:91:PRO:CD    | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:13:ALA:CB    | 1:O:118:ALA:H    | 2.29                     | 0.45              |
| 1:O:110:ARG:N    | 2:P:276:PHE:O    | 2.50                     | 0.45              |
| 2:P:38:LEU:HD12  | 2:P:38:LEU:N     | 2.30                     | 0.45              |
| 1:C:46:GLY:O     | 1:C:48:PHE:N     | 2.50                     | 0.45              |
| 2:F:57:THR:HG22  | 2:F:92:ARG:HA    | 1.98                     | 0.45              |
| 2:F:82:TYR:OH    | 2:F:91:PRO:HD2   | 2.17                     | 0.45              |
| 2:F:201:THR:HG23 | 2:F:203:ASP:H    | 1.80                     | 0.45              |
| 1:G:57:MET:HE3   | 1:G:63:ASN:OD1   | 2.16                     | 0.45              |
| 1:G:77:GLN:HE21  | 1:G:117:PRO:HB3  | 1.80                     | 0.45              |
| 1:G:160:ARG:HH11 | 1:G:160:ARG:HG3  | 1.81                     | 0.45              |
| 2:H:82:TYR:OH    | 2:H:91:PRO:HD2   | 2.16                     | 0.45              |
| 1:I:24:ASN:HB2   | 1:I:57:MET:HE2   | 1.97                     | 0.45              |
| 2:J:148:ILE:N    | 2:J:148:ILE:CD1  | 2.79                     | 0.45              |
| 1:K:105:LEU:HA   | 2:L:272:ILE:O    | 2.16                     | 0.45              |
| 1:K:132:ARG:CG   | 1:K:203:VAL:O    | 2.62                     | 0.45              |
| 1:M:52:PRO:HG2   | 1:M:55:PHE:HE2   | 1.81                     | 0.45              |
| 2:N:71:PHE:CA    | 2:N:110:THR:O    | 2.64                     | 0.45              |
| 2:N:113:SER:O    | 2:N:115:ALA:N    | 2.48                     | 0.45              |
| 1:O:39:ASN:O     | 1:O:84:TRP:HD1   | 1.99                     | 0.45              |
| 1:O:102:THR:HB   | 2:P:168:VAL:HG21 | 1.95                     | 0.45              |
| 1:A:135:ARG:HB2  | 1:A:135:ARG:HH11 | 1.82                     | 0.45              |
| 1:A:156:ASN:C    | 1:A:158:GLY:N    | 2.74                     | 0.45              |
| 2:D:185:VAL:O    | 2:D:247:ALA:HA   | 2.16                     | 0.45              |
| 1:E:133:PHE:HD2  | 1:E:140:LEU:HD21 | 1.80                     | 0.45              |
| 2:H:170:VAL:C    | 2:H:172:LEU:N    | 2.72                     | 0.45              |
| 1:I:110:ARG:N    | 2:J:276:PHE:O    | 2.50                     | 0.45              |
| 1:I:144:ASN:HB3  | 1:I:167:VAL:CG1  | 2.47                     | 0.45              |
| 1:I:188:ARG:NH2  | 1:I:196:LEU:CB   | 2.80                     | 0.45              |
| 2:J:262:GLN:HG3  | 2:J:262:GLN:O    | 2.15                     | 0.45              |
| 1:K:37:VAL:HG22  | 1:K:85:MET:HG2   | 1.99                     | 0.45              |
| 1:M:162:LEU:HB3  | 1:M:175:VAL:CG1  | 2.45                     | 0.45              |
| 1:O:144:ASN:HB3  | 1:O:167:VAL:CG1  | 2.46                     | 0.45              |
| 1:O:193:TYR:CD2  | 2:P:155:VAL:HG11 | 2.51                     | 0.45              |
| 2:P:71:PHE:CA    | 2:P:110:THR:O    | 2.63                     | 0.45              |
| 1:E:204:MET:N    | 1:E:204:MET:SD   | 2.89                     | 0.45              |
| 1:I:4:LEU:C      | 1:I:6:ALA:N      | 2.72                     | 0.45              |
| 1:I:193:TYR:CD2  | 2:J:155:VAL:HG11 | 2.51                     | 0.45              |
| 2:J:57:THR:HG22  | 2:J:91:PRO:O     | 2.16                     | 0.45              |
| 2:J:90:THR:HB    | 2:J:91:PRO:CD    | 2.47                     | 0.45              |
| 1:K:110:ARG:N    | 2:L:276:PHE:O    | 2.49                     | 0.45              |
| 2:L:23:ASN:O     | 2:L:24:LEU:HD23  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:136:ASN:H    | 2:L:136:ASN:HD22 | 1.64                     | 0.45              |
| 1:M:86:ASN:HD21  | 1:M:110:ARG:HG3  | 1.81                     | 0.45              |
| 1:A:124:PRO:HD3  | 1:A:148:TYR:OH   | 2.16                     | 0.45              |
| 1:A:154:GLU:OE1  | 1:A:188:ARG:CD   | 2.65                     | 0.45              |
| 2:B:57:THR:HG22  | 2:B:92:ARG:HA    | 1.99                     | 0.45              |
| 2:B:92:ARG:HG3   | 2:B:92:ARG:NH1   | 2.31                     | 0.45              |
| 1:C:135:ARG:HH12 | 1:C:177:LEU:HD21 | 1.81                     | 0.45              |
| 1:E:142:LEU:N    | 1:E:142:LEU:CD2  | 2.79                     | 0.45              |
| 2:F:25:ALA:HA    | 2:F:26:PRO:HD3   | 1.82                     | 0.45              |
| 2:F:71:PHE:CE2   | 2:F:111:PRO:HG3  | 2.52                     | 0.45              |
| 2:F:75:VAL:HG13  | 2:F:75:VAL:O     | 2.15                     | 0.45              |
| 1:G:46:GLY:O     | 1:G:48:PHE:N     | 2.50                     | 0.45              |
| 2:J:61:GLY:HA2   | 2:J:128:VAL:O    | 2.16                     | 0.45              |
| 2:J:63:ALA:C     | 2:J:64:TYR:CD1   | 2.95                     | 0.45              |
| 1:M:140:LEU:O    | 1:M:142:LEU:HG   | 2.17                     | 0.45              |
| 1:M:188:ARG:NH2  | 1:M:196:LEU:CB   | 2.79                     | 0.45              |
| 1:M:193:TYR:CD2  | 2:N:155:VAL:HG11 | 2.51                     | 0.45              |
| 2:N:61:GLY:HA2   | 2:N:128:VAL:O    | 2.16                     | 0.45              |
| 2:N:66:GLY:O     | 2:N:70:ASN:HB2   | 2.17                     | 0.45              |
| 2:N:144:PHE:HD1  | 2:N:144:PHE:H    | 1.64                     | 0.45              |
| 2:N:190:SER:CB   | 2:N:244:GLY:HA2  | 2.45                     | 0.45              |
| 1:O:123:PRO:C    | 1:O:125:ASP:H    | 2.25                     | 0.45              |
| 2:P:34:LEU:O     | 2:P:34:LEU:CG    | 2.63                     | 0.45              |
| 1:C:167:VAL:HA   | 1:C:168:PRO:HD2  | 1.79                     | 0.45              |
| 2:D:185:VAL:HG23 | 2:D:243:VAL:HG11 | 1.99                     | 0.45              |
| 2:F:211:ASN:HD22 | 2:F:212:THR:N    | 2.15                     | 0.45              |
| 1:I:39:ASN:O     | 1:I:84:TRP:HD1   | 2.00                     | 0.45              |
| 1:I:44:LYS:C     | 1:I:45:ASP:CG    | 2.85                     | 0.45              |
| 2:J:136:ASN:HD22 | 2:J:136:ASN:H    | 1.65                     | 0.45              |
| 2:J:209:PHE:HE2  | 2:J:234:ALA:HB2  | 1.78                     | 0.45              |
| 2:J:227:ARG:C    | 2:J:229:GLY:N    | 2.74                     | 0.45              |
| 2:J:234:ALA:O    | 2:J:235:ASN:HB2  | 2.16                     | 0.45              |
| 1:K:135:ARG:CB   | 1:K:140:LEU:HD23 | 2.47                     | 0.45              |
| 1:K:169:PRO:C    | 1:K:171:GLY:N    | 2.75                     | 0.45              |
| 2:L:39:SER:HB2   | 4:L:508:HOH:O    | 2.15                     | 0.45              |
| 2:L:196:TYR:HB3  | 2:L:237:THR:CA   | 2.47                     | 0.45              |
| 1:M:11:TYR:CD1   | 1:M:18:VAL:HG21  | 2.52                     | 0.45              |
| 1:M:13:ALA:CB    | 1:M:118:ALA:H    | 2.30                     | 0.45              |
| 2:N:11:ILE:CG2   | 2:N:16:GLY:HA3   | 2.33                     | 0.45              |
| 2:N:106:ALA:CB   | 2:N:108:TYR:HE1  | 2.29                     | 0.45              |
| 1:O:86:ASN:HD21  | 1:O:110:ARG:HG3  | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:169:PRO:C    | 1:O:171:GLY:N    | 2.75                     | 0.45              |
| 2:P:196:TYR:HB3  | 2:P:237:THR:CA   | 2.46                     | 0.45              |
| 1:A:160:ARG:HH11 | 1:A:160:ARG:HG3  | 1.82                     | 0.45              |
| 2:B:263:VAL:N    | 4:B:550:HOH:O    | 2.49                     | 0.45              |
| 2:D:164:SER:HA   | 4:D:611:HOH:O    | 2.17                     | 0.45              |
| 2:F:59:GLN:NE2   | 2:F:143:GLN:HE22 | 2.14                     | 0.45              |
| 1:I:13:ALA:CB    | 1:I:118:ALA:H    | 2.30                     | 0.45              |
| 2:J:23:ASN:O     | 2:J:24:LEU:HD23  | 2.15                     | 0.45              |
| 2:J:233:PRO:HG2  | 2:J:236:ASN:HB2  | 1.99                     | 0.45              |
| 2:L:90:THR:HB    | 2:L:91:PRO:HD2   | 1.97                     | 0.45              |
| 1:M:10:ILE:HD13  | 1:M:114:TYR:HB2  | 1.99                     | 0.45              |
| 1:M:49:ILE:HD12  | 1:M:49:ILE:N     | 2.32                     | 0.45              |
| 1:O:11:TYR:CD1   | 1:O:18:VAL:HG21  | 2.52                     | 0.45              |
| 1:O:116:ARG:HD3  | 1:O:148:TYR:HE2  | 1.82                     | 0.45              |
| 2:P:209:PHE:HE2  | 2:P:234:ALA:HB2  | 1.79                     | 0.45              |
| 1:A:57:MET:HE3   | 1:A:63:ASN:OD1   | 2.17                     | 0.45              |
| 1:C:205:GLU:OXT  | 1:C:205:GLU:HG3  | 2.16                     | 0.45              |
| 2:F:59:GLN:HE21  | 2:F:143:GLN:HE22 | 1.63                     | 0.45              |
| 1:I:116:ARG:HD3  | 1:I:148:TYR:HE2  | 1.82                     | 0.45              |
| 2:J:66:GLY:O     | 2:J:70:ASN:HB2   | 2.17                     | 0.45              |
| 2:J:106:ALA:CB   | 2:J:108:TYR:HE1  | 2.29                     | 0.45              |
| 1:K:152:VAL:O    | 1:K:164:ASN:HB3  | 2.17                     | 0.45              |
| 1:K:160:ARG:CD   | 1:K:180:ASP:HB2  | 2.40                     | 0.45              |
| 2:L:41:GLN:HA    | 2:L:41:GLN:HE21  | 1.82                     | 0.45              |
| 1:M:39:ASN:O     | 1:M:84:TRP:HD1   | 1.99                     | 0.45              |
| 2:N:209:PHE:HE2  | 2:N:234:ALA:HB2  | 1.77                     | 0.45              |
| 2:P:144:PHE:H    | 2:P:144:PHE:HD1  | 1.64                     | 0.45              |
| 2:B:5:THR:CG2    | 2:B:7:ASN:HB2    | 2.47                     | 0.45              |
| 1:E:160:ARG:HG3  | 1:E:160:ARG:HH11 | 1.82                     | 0.45              |
| 2:F:201:THR:CB   | 2:F:206:ASN:HD22 | 2.30                     | 0.45              |
| 1:I:160:ARG:CD   | 1:I:180:ASP:HB2  | 2.40                     | 0.45              |
| 2:J:158:THR:O    | 2:J:158:THR:HG23 | 2.17                     | 0.45              |
| 1:K:140:LEU:O    | 1:K:142:LEU:HG   | 2.17                     | 0.45              |
| 1:K:177:LEU:O    | 1:K:179:SER:N    | 2.50                     | 0.45              |
| 2:L:66:GLY:O     | 2:L:70:ASN:HB2   | 2.17                     | 0.45              |
| 2:L:90:THR:HB    | 2:L:91:PRO:CD    | 2.47                     | 0.45              |
| 2:N:196:TYR:HB3  | 2:N:237:THR:CA   | 2.46                     | 0.45              |
| 1:O:108:ILE:HD12 | 2:P:275:THR:OG1  | 2.17                     | 0.45              |
| 2:P:63:ALA:C     | 2:P:64:TYR:CD1   | 2.95                     | 0.45              |
| 2:B:6:ALA:HB3    | 4:B:553:HOH:O    | 2.16                     | 0.44              |
| 2:B:185:VAL:HG23 | 2:B:243:VAL:HG11 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:211:ASN:HD22 | 2:B:212:THR:N    | 2.15                     | 0.44              |
| 1:E:153:THR:HA   | 1:E:164:ASN:OD1  | 2.17                     | 0.44              |
| 2:F:201:THR:CG2  | 2:F:202:ALA:N    | 2.80                     | 0.44              |
| 1:G:133:PHE:HD2  | 1:G:140:LEU:HD21 | 1.81                     | 0.44              |
| 2:H:105:VAL:HG11 | 2:H:129:LEU:HD13 | 1.99                     | 0.44              |
| 2:H:201:THR:HG23 | 2:H:203:ASP:H    | 1.82                     | 0.44              |
| 2:J:144:PHE:H    | 2:J:144:PHE:HD1  | 1.64                     | 0.44              |
| 2:J:196:TYR:HB3  | 2:J:237:THR:CA   | 2.46                     | 0.44              |
| 1:K:81:SER:O     | 1:K:83:PHE:CD1   | 2.70                     | 0.44              |
| 2:L:158:THR:HG23 | 2:L:158:THR:O    | 2.15                     | 0.44              |
| 1:M:152:VAL:O    | 1:M:164:ASN:HB3  | 2.17                     | 0.44              |
| 2:P:118:VAL:HG12 | 2:P:121:LYS:HE2  | 1.99                     | 0.44              |
| 2:P:184:THR:HG22 | 2:P:249:SER:CA   | 2.47                     | 0.44              |
| 1:A:30:THR:HG22  | 1:A:31:TYR:N     | 2.32                     | 0.44              |
| 1:A:167:VAL:HA   | 1:A:168:PRO:HD2  | 1.79                     | 0.44              |
| 1:C:66:ARG:HG2   | 1:C:66:ARG:NH1   | 2.32                     | 0.44              |
| 2:D:71:PHE:CE2   | 2:D:111:PRO:HG3  | 2.52                     | 0.44              |
| 1:E:205:GLU:HG3  | 1:E:205:GLU:OXT  | 2.17                     | 0.44              |
| 1:G:66:ARG:HG2   | 1:G:66:ARG:NH1   | 2.32                     | 0.44              |
| 1:G:205:GLU:HG3  | 1:G:205:GLU:OXT  | 2.17                     | 0.44              |
| 2:H:92:ARG:HG3   | 2:H:92:ARG:NH1   | 2.31                     | 0.44              |
| 2:H:120:ILE:HG23 | 2:H:126:ILE:HD11 | 1.98                     | 0.44              |
| 2:J:41:GLN:HA    | 2:J:41:GLN:HE21  | 1.83                     | 0.44              |
| 1:K:13:ALA:CB    | 1:K:118:ALA:H    | 2.30                     | 0.44              |
| 1:K:52:PRO:HG2   | 1:K:55:PHE:HE2   | 1.81                     | 0.44              |
| 2:L:63:ALA:C     | 2:L:64:TYR:CD1   | 2.95                     | 0.44              |
| 2:L:144:PHE:HD1  | 2:L:144:PHE:H    | 1.64                     | 0.44              |
| 1:A:9:VAL:CG1    | 1:A:113:LEU:HD13 | 2.47                     | 0.44              |
| 2:B:201:THR:HG23 | 2:B:203:ASP:H    | 1.82                     | 0.44              |
| 1:C:129:GLU:HG3  | 1:C:130:LYS:N    | 2.33                     | 0.44              |
| 1:C:142:LEU:HD12 | 1:C:152:VAL:HG21 | 1.99                     | 0.44              |
| 2:D:1:PHE:CG     | 2:D:133:ASN:ND2  | 2.86                     | 0.44              |
| 1:E:58:LYS:HG3   | 4:E:222:HOH:O    | 2.17                     | 0.44              |
| 2:H:116:GLY:HA2  | 2:H:189:LYS:CE   | 2.45                     | 0.44              |
| 2:H:211:ASN:HD22 | 2:H:212:THR:N    | 2.16                     | 0.44              |
| 2:J:15:GLY:HA2   | 2:J:144:PHE:CG   | 2.53                     | 0.44              |
| 1:K:116:ARG:HD3  | 1:K:148:TYR:HE2  | 1.83                     | 0.44              |
| 1:K:162:LEU:HB3  | 1:K:175:VAL:CG1  | 2.45                     | 0.44              |
| 1:M:110:ARG:HB3  | 2:N:277:VAL:HA   | 1.98                     | 0.44              |
| 1:M:169:PRO:C    | 1:M:171:GLY:N    | 2.75                     | 0.44              |
| 1:M:177:LEU:O    | 1:M:179:SER:N    | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:88:LYS:CG    | 1:O:108:ILE:HG12 | 2.42                     | 0.44              |
| 2:P:61:GLY:HA2   | 2:P:128:VAL:O    | 2.17                     | 0.44              |
| 1:A:39:ASN:OD1   | 1:A:43:VAL:HG22  | 2.18                     | 0.44              |
| 2:F:218:ALA:HB2  | 2:F:266:GLY:HA3  | 1.99                     | 0.44              |
| 1:G:75:LEU:HD22  | 1:G:76:PRO:HD2   | 1.99                     | 0.44              |
| 2:H:87:THR:HG21  | 2:L:68:LEU:CD1   | 2.48                     | 0.44              |
| 2:H:201:THR:CB   | 2:H:206:ASN:HD22 | 2.31                     | 0.44              |
| 2:H:209:PHE:CG   | 2:H:272:ILE:HD11 | 2.52                     | 0.44              |
| 1:I:108:ILE:HD12 | 2:J:275:THR:OG1  | 2.17                     | 0.44              |
| 2:J:181:ILE:HA   | 2:J:182:PRO:HD3  | 1.81                     | 0.44              |
| 2:J:184:THR:HG22 | 2:J:249:SER:CA   | 2.47                     | 0.44              |
| 1:K:4:LEU:HD11   | 1:K:87:VAL:HG23  | 2.00                     | 0.44              |
| 1:M:51:THR:O     | 1:M:66:ARG:N     | 2.50                     | 0.44              |
| 1:M:52:PRO:HG2   | 1:M:65:LEU:HD23  | 2.00                     | 0.44              |
| 2:N:136:ASN:H    | 2:N:136:ASN:HD22 | 1.65                     | 0.44              |
| 2:N:184:THR:HG22 | 2:N:249:SER:CA   | 2.47                     | 0.44              |
| 1:O:10:ILE:HD13  | 1:O:114:TYR:HB2  | 1.99                     | 0.44              |
| 1:O:100:GLU:CG   | 2:P:172:LEU:HD12 | 2.45                     | 0.44              |
| 2:P:23:ASN:O     | 2:P:24:LEU:HD23  | 2.17                     | 0.44              |
| 2:D:5:THR:CG2    | 2:D:7:ASN:HB2    | 2.48                     | 0.44              |
| 2:D:49:PRO:HG3   | 2:D:98:ARG:HG3   | 2.00                     | 0.44              |
| 2:H:221:VAL:CG1  | 2:H:222:GLY:H    | 2.19                     | 0.44              |
| 1:I:135:ARG:CB   | 1:I:140:LEU:HD23 | 2.47                     | 0.44              |
| 1:I:177:LEU:O    | 1:I:179:SER:N    | 2.50                     | 0.44              |
| 2:J:190:SER:CB   | 2:J:244:GLY:HA2  | 2.45                     | 0.44              |
| 1:K:4:LEU:C      | 1:K:6:ALA:N      | 2.74                     | 0.44              |
| 1:K:49:ILE:N     | 1:K:49:ILE:HD12  | 2.33                     | 0.44              |
| 1:K:52:PRO:HG2   | 1:K:65:LEU:HD23  | 2.00                     | 0.44              |
| 1:K:110:ARG:HB3  | 2:L:277:VAL:HA   | 1.99                     | 0.44              |
| 2:L:209:PHE:HE2  | 2:L:234:ALA:HB2  | 1.78                     | 0.44              |
| 1:M:116:ARG:HD3  | 1:M:148:TYR:HE2  | 1.81                     | 0.44              |
| 1:M:149:TYR:CD2  | 1:M:168:PRO:HA   | 2.53                     | 0.44              |
| 2:N:41:GLN:HA    | 2:N:41:GLN:HE21  | 1.82                     | 0.44              |
| 2:P:233:PRO:HG2  | 2:P:236:ASN:HB2  | 1.99                     | 0.44              |
| 1:A:205:GLU:HG3  | 1:A:205:GLU:OXT  | 2.17                     | 0.44              |
| 2:B:33:ASN:ND2   | 2:B:110:THR:OG1  | 2.51                     | 0.44              |
| 2:F:5:THR:CG2    | 2:F:7:ASN:HB2    | 2.48                     | 0.44              |
| 2:F:49:PRO:HG3   | 2:F:98:ARG:HG3   | 2.00                     | 0.44              |
| 2:H:82:TYR:CD1   | 2:H:82:TYR:N     | 2.86                     | 0.44              |
| 2:H:185:VAL:HG23 | 2:H:243:VAL:HG11 | 1.99                     | 0.44              |
| 1:I:78:ASP:OD1   | 1:I:79:ARG:N     | 2.51                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:80:GLU:OE2   | 1:K:116:ARG:NE   | 2.47                     | 0.44              |
| 2:L:184:THR:HG22 | 2:L:249:SER:CA   | 2.48                     | 0.44              |
| 2:N:59:GLN:HG3   | 2:N:143:GLN:NE2  | 2.31                     | 0.44              |
| 2:N:63:ALA:C     | 2:N:64:TYR:CD1   | 2.96                     | 0.44              |
| 2:N:148:ILE:N    | 2:N:148:ILE:CD1  | 2.80                     | 0.44              |
| 1:O:31:TYR:HB3   | 1:O:89:ALA:HB1   | 1.98                     | 0.44              |
| 1:O:44:LYS:C     | 1:O:45:ASP:CG    | 2.84                     | 0.44              |
| 1:O:81:SER:O     | 1:O:83:PHE:CD1   | 2.70                     | 0.44              |
| 1:O:135:ARG:CB   | 1:O:140:LEU:HD23 | 2.47                     | 0.44              |
| 2:P:55:TYR:OH    | 2:P:136:ASN:HB3  | 2.18                     | 0.44              |
| 1:A:8:ARG:HH22   | 2:B:279:GLN:C    | 2.25                     | 0.44              |
| 1:A:27:GLU:HG3   | 1:A:60:LYS:HZ3   | 1.79                     | 0.44              |
| 1:A:153:THR:HA   | 1:A:164:ASN:OD1  | 2.18                     | 0.44              |
| 1:A:185:ILE:O    | 1:A:201:THR:HA   | 2.17                     | 0.44              |
| 2:B:70:ASN:C     | 2:B:71:PHE:CD1   | 2.96                     | 0.44              |
| 2:B:71:PHE:CE2   | 2:B:111:PRO:HG3  | 2.53                     | 0.44              |
| 2:B:148:ILE:HD12 | 2:B:148:ILE:N    | 2.32                     | 0.44              |
| 2:D:70:ASN:C     | 2:D:71:PHE:CD1   | 2.96                     | 0.44              |
| 1:E:140:LEU:HB2  | 1:E:177:LEU:HD13 | 2.00                     | 0.44              |
| 1:G:77:GLN:HA    | 1:G:77:GLN:HE21  | 1.82                     | 0.44              |
| 2:H:5:THR:CG2    | 2:H:7:ASN:HB2    | 2.48                     | 0.44              |
| 2:H:262:GLN:HG3  | 2:H:262:GLN:O    | 2.18                     | 0.44              |
| 1:I:49:ILE:HD12  | 1:I:49:ILE:N     | 2.33                     | 0.44              |
| 2:J:118:VAL:HG12 | 2:J:121:LYS:HE2  | 2.00                     | 0.44              |
| 1:K:11:TYR:CD1   | 1:K:18:VAL:HG21  | 2.52                     | 0.44              |
| 1:K:123:PRO:C    | 1:K:125:ASP:H    | 2.25                     | 0.44              |
| 2:L:233:PRO:HG2  | 2:L:236:ASN:HB2  | 1.99                     | 0.44              |
| 2:N:118:VAL:HG12 | 2:N:121:LYS:HE2  | 2.00                     | 0.44              |
| 1:O:49:ILE:HD12  | 1:O:49:ILE:N     | 2.33                     | 0.44              |
| 2:P:148:ILE:N    | 2:P:148:ILE:CD1  | 2.81                     | 0.44              |
| 1:A:77:GLN:HE21  | 1:A:117:PRO:HB3  | 1.83                     | 0.44              |
| 2:D:96:ASN:C     | 2:D:96:ASN:HD22  | 2.25                     | 0.44              |
| 1:E:16:LYS:HB3   | 4:E:223:HOH:O    | 2.18                     | 0.44              |
| 2:H:70:ASN:C     | 2:H:71:PHE:CD1   | 2.96                     | 0.44              |
| 2:H:135:ASN:HD21 | 2:H:138:ASN:H    | 1.65                     | 0.44              |
| 1:I:110:ARG:HB3  | 2:J:277:VAL:HA   | 1.99                     | 0.44              |
| 1:I:140:LEU:O    | 1:I:142:LEU:HG   | 2.17                     | 0.44              |
| 1:K:188:ARG:NH2  | 1:K:196:LEU:CB   | 2.80                     | 0.44              |
| 2:L:168:VAL:HG13 | 2:L:168:VAL:O    | 2.18                     | 0.44              |
| 1:M:67:ILE:HD11  | 1:M:85:MET:SD    | 2.58                     | 0.44              |
| 2:N:168:VAL:HG13 | 2:N:168:VAL:O    | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:177:LEU:O    | 1:O:179:SER:N    | 2.50                     | 0.44              |
| 2:P:106:ALA:CB   | 2:P:108:TYR:HE1  | 2.30                     | 0.44              |
| 2:B:218:ALA:HB2  | 2:B:266:GLY:HA3  | 1.99                     | 0.44              |
| 1:C:160:ARG:HH11 | 1:C:160:ARG:HG3  | 1.82                     | 0.44              |
| 1:E:142:LEU:HD12 | 1:E:152:VAL:HG21 | 2.00                     | 0.44              |
| 2:F:70:ASN:C     | 2:F:71:PHE:CD1   | 2.96                     | 0.44              |
| 2:F:185:VAL:O    | 2:F:247:ALA:HA   | 2.18                     | 0.44              |
| 2:F:185:VAL:HG23 | 2:F:243:VAL:HG11 | 2.00                     | 0.44              |
| 2:F:201:THR:HB   | 4:F:529:HOH:O    | 2.17                     | 0.44              |
| 2:H:71:PHE:CE2   | 2:H:111:PRO:HG3  | 2.53                     | 0.44              |
| 1:I:4:LEU:HD11   | 1:I:87:VAL:HG23  | 2.00                     | 0.44              |
| 1:I:11:TYR:CD1   | 1:I:18:VAL:HG21  | 2.52                     | 0.44              |
| 1:I:17:GLN:HB3   | 1:I:68:LEU:CD2   | 2.41                     | 0.44              |
| 1:I:51:THR:O     | 1:I:66:ARG:N     | 2.50                     | 0.44              |
| 1:I:52:PRO:HG2   | 1:I:65:LEU:HD23  | 2.00                     | 0.44              |
| 1:I:81:SER:O     | 1:I:83:PHE:CD1   | 2.70                     | 0.44              |
| 1:K:149:TYR:CB   | 1:K:166:LEU:HD11 | 2.39                     | 0.44              |
| 1:M:80:GLU:OE2   | 1:M:116:ARG:NE   | 2.47                     | 0.44              |
| 1:M:127:ALA:HA   | 1:M:146:THR:HG21 | 2.00                     | 0.44              |
| 2:P:66:GLY:O     | 2:P:70:ASN:HB2   | 2.17                     | 0.44              |
| 2:P:75:VAL:HB    | 2:P:84:PHE:HB2   | 2.00                     | 0.44              |
| 2:B:49:PRO:HG3   | 2:B:98:ARG:HG3   | 2.00                     | 0.43              |
| 2:D:201:THR:HB   | 4:D:633:HOH:O    | 2.18                     | 0.43              |
| 1:G:5:GLY:O      | 2:H:159:GLY:HA2  | 2.18                     | 0.43              |
| 1:I:85:MET:HB2   | 1:I:111:ILE:HG13 | 2.00                     | 0.43              |
| 2:J:116:GLY:HA2  | 2:J:189:LYS:CG   | 2.40                     | 0.43              |
| 2:J:184:THR:HG22 | 2:J:249:SER:HA   | 1.99                     | 0.43              |
| 2:J:206:ASN:HD21 | 2:J:234:ALA:CB   | 2.28                     | 0.43              |
| 1:K:127:ALA:HA   | 1:K:146:THR:HG21 | 2.00                     | 0.43              |
| 2:L:118:VAL:HG12 | 2:L:121:LYS:HE2  | 2.00                     | 0.43              |
| 2:N:233:PRO:HG2  | 2:N:236:ASN:HB2  | 1.98                     | 0.43              |
| 1:O:28:ASN:ND2   | 1:O:28:ASN:N     | 2.57                     | 0.43              |
| 1:O:152:VAL:O    | 1:O:164:ASN:HB3  | 2.18                     | 0.43              |
| 1:A:77:GLN:HA    | 1:A:77:GLN:HE21  | 1.82                     | 0.43              |
| 1:A:142:LEU:HD12 | 1:A:152:VAL:HG21 | 2.00                     | 0.43              |
| 2:B:87:THR:HG21  | 2:P:68:LEU:CD1   | 2.47                     | 0.43              |
| 2:B:89:GLU:N     | 4:B:528:HOH:O    | 2.35                     | 0.43              |
| 2:B:171:THR:C    | 2:B:173:PRO:CD   | 2.89                     | 0.43              |
| 1:E:75:LEU:HD22  | 1:E:76:PRO:HD2   | 2.00                     | 0.43              |
| 1:I:149:TYR:CD2  | 1:I:168:PRO:HA   | 2.53                     | 0.43              |
| 2:N:192:ASN:HB2  | 2:N:279:GLN:NE2  | 2.34                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:163:GLU:N    | 1:O:175:VAL:HG11 | 2.14                     | 0.43              |
| 1:O:188:ARG:NH2  | 1:O:196:LEU:CB   | 2.80                     | 0.43              |
| 2:P:190:SER:CB   | 2:P:244:GLY:HA2  | 2.45                     | 0.43              |
| 1:C:82:LEU:HD12  | 1:C:83:PHE:N     | 2.33                     | 0.43              |
| 1:C:185:ILE:CB   | 1:C:202:GLY:HA3  | 2.47                     | 0.43              |
| 2:F:96:ASN:C     | 2:F:96:ASN:HD22  | 2.25                     | 0.43              |
| 2:F:105:VAL:HG11 | 2:F:129:LEU:HD13 | 2.00                     | 0.43              |
| 2:H:25:ALA:HA    | 2:H:26:PRO:HD3   | 1.83                     | 0.43              |
| 2:H:201:THR:HG23 | 2:H:202:ALA:N    | 2.32                     | 0.43              |
| 2:J:258:ARG:HG2  | 2:J:263:VAL:HG23 | 2.01                     | 0.43              |
| 1:K:108:ILE:HD12 | 2:L:275:THR:OG1  | 2.18                     | 0.43              |
| 1:K:128:ALA:CA   | 1:K:150:LEU:HD22 | 2.48                     | 0.43              |
| 1:M:135:ARG:CB   | 1:M:140:LEU:HD23 | 2.48                     | 0.43              |
| 2:N:55:TYR:OH    | 2:N:136:ASN:HB3  | 2.18                     | 0.43              |
| 1:O:51:THR:O     | 1:O:66:ARG:N     | 2.50                     | 0.43              |
| 2:P:184:THR:HG22 | 2:P:249:SER:HA   | 1.99                     | 0.43              |
| 2:B:96:ASN:C     | 2:B:96:ASN:HD22  | 2.26                     | 0.43              |
| 1:C:185:ILE:HB   | 1:C:202:GLY:CA   | 2.44                     | 0.43              |
| 1:E:77:GLN:HE21  | 1:E:117:PRO:HB3  | 1.83                     | 0.43              |
| 1:E:135:ARG:HH12 | 1:E:177:LEU:HD21 | 1.83                     | 0.43              |
| 1:E:185:ILE:HB   | 1:E:202:GLY:CA   | 2.47                     | 0.43              |
| 1:G:185:ILE:HB   | 1:G:202:GLY:CA   | 2.46                     | 0.43              |
| 1:I:10:ILE:HD13  | 1:I:114:TYR:HB2  | 1.99                     | 0.43              |
| 1:I:20:LEU:O     | 1:I:65:LEU:N     | 2.51                     | 0.43              |
| 1:I:24:ASN:HD22  | 1:I:60:LYS:HA    | 1.83                     | 0.43              |
| 1:I:100:GLU:CG   | 2:J:172:LEU:HD12 | 2.46                     | 0.43              |
| 1:K:51:THR:O     | 1:K:66:ARG:N     | 2.50                     | 0.43              |
| 1:M:8:ARG:NH1    | 1:M:8:ARG:CB     | 2.81                     | 0.43              |
| 1:M:85:MET:HB2   | 1:M:111:ILE:HG13 | 2.00                     | 0.43              |
| 1:M:128:ALA:CA   | 1:M:150:LEU:HD22 | 2.48                     | 0.43              |
| 2:N:206:ASN:HD21 | 2:N:234:ALA:CB   | 2.29                     | 0.43              |
| 2:N:258:ARG:HG2  | 2:N:263:VAL:HG23 | 2.01                     | 0.43              |
| 1:O:52:PRO:HG2   | 1:O:65:LEU:HD23  | 2.01                     | 0.43              |
| 1:O:110:ARG:HB3  | 2:P:277:VAL:HA   | 1.99                     | 0.43              |
| 2:P:258:ARG:HG2  | 2:P:263:VAL:HG23 | 2.01                     | 0.43              |
| 1:A:28:ASN:N     | 1:A:28:ASN:ND2   | 2.65                     | 0.43              |
| 1:A:75:LEU:HD22  | 1:A:76:PRO:HD2   | 1.99                     | 0.43              |
| 1:A:82:LEU:HD12  | 1:A:83:PHE:N     | 2.34                     | 0.43              |
| 1:C:30:THR:HG22  | 1:C:31:TYR:N     | 2.33                     | 0.43              |
| 2:D:226:THR:HG23 | 2:D:253:THR:HB   | 2.01                     | 0.43              |
| 1:E:30:THR:HG22  | 1:E:31:TYR:N     | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:46:GLY:O     | 1:E:48:PHE:N     | 2.51                     | 0.43              |
| 2:F:1:PHE:CG     | 2:F:133:ASN:ND2  | 2.87                     | 0.43              |
| 2:F:82:TYR:CD1   | 2:F:82:TYR:N     | 2.86                     | 0.43              |
| 1:I:128:ALA:CA   | 1:I:150:LEU:HD22 | 2.48                     | 0.43              |
| 1:K:28:ASN:ND2   | 1:K:28:ASN:O     | 2.51                     | 0.43              |
| 1:K:149:TYR:HD2  | 1:K:166:LEU:HG   | 1.83                     | 0.43              |
| 2:L:103:TRP:CH2  | 2:L:131:LEU:HB2  | 2.54                     | 0.43              |
| 2:L:258:ARG:HG2  | 2:L:263:VAL:HG23 | 2.00                     | 0.43              |
| 1:M:20:LEU:O     | 1:M:65:LEU:N     | 2.51                     | 0.43              |
| 1:M:81:SER:O     | 1:M:83:PHE:CD1   | 2.71                     | 0.43              |
| 2:N:184:THR:HG22 | 2:N:249:SER:HA   | 1.99                     | 0.43              |
| 2:P:60:ARG:HG2   | 2:P:61:GLY:N     | 2.21                     | 0.43              |
| 2:B:1:PHE:CG     | 2:B:133:ASN:ND2  | 2.87                     | 0.43              |
| 2:B:82:TYR:N     | 2:B:82:TYR:CD1   | 2.87                     | 0.43              |
| 2:B:135:ASN:HD21 | 2:B:138:ASN:H    | 1.67                     | 0.43              |
| 2:B:175:TYR:CD1  | 2:B:175:TYR:C    | 2.95                     | 0.43              |
| 2:D:82:TYR:N     | 2:D:82:TYR:CD1   | 2.86                     | 0.43              |
| 1:E:88:LYS:CB    | 1:E:108:ILE:HG12 | 2.44                     | 0.43              |
| 2:F:195:TYR:CE1  | 2:F:238:VAL:HB   | 2.53                     | 0.43              |
| 2:F:221:VAL:HG11 | 2:F:256:TYR:HD2  | 1.83                     | 0.43              |
| 1:G:82:LEU:HD12  | 1:G:83:PHE:N     | 2.33                     | 0.43              |
| 1:G:154:GLU:OE1  | 1:G:188:ARG:CD   | 2.65                     | 0.43              |
| 2:H:226:THR:HG23 | 2:H:253:THR:HB   | 2.01                     | 0.43              |
| 2:J:211:ASN:ND2  | 2:J:269:GLN:H    | 2.17                     | 0.43              |
| 1:K:88:LYS:CG    | 1:K:108:ILE:HG12 | 2.42                     | 0.43              |
| 2:L:15:GLY:HA2   | 2:L:144:PHE:CG   | 2.53                     | 0.43              |
| 2:L:59:GLN:HG3   | 2:L:143:GLN:NE2  | 2.29                     | 0.43              |
| 2:L:206:ASN:HD21 | 2:L:234:ALA:CB   | 2.28                     | 0.43              |
| 1:M:4:LEU:C      | 1:M:6:ALA:N      | 2.73                     | 0.43              |
| 1:M:28:ASN:ND2   | 1:M:28:ASN:O     | 2.52                     | 0.43              |
| 1:O:149:TYR:CD2  | 1:O:168:PRO:HA   | 2.54                     | 0.43              |
| 2:P:90:THR:HB    | 2:P:91:PRO:CD    | 2.48                     | 0.43              |
| 1:C:8:ARG:HH22   | 2:D:279:GLN:C    | 2.26                     | 0.43              |
| 1:C:82:LEU:C     | 1:C:83:PHE:CD1   | 2.97                     | 0.43              |
| 2:D:105:VAL:HG11 | 2:D:129:LEU:HD13 | 2.00                     | 0.43              |
| 1:E:66:ARG:HG2   | 1:E:66:ARG:NH1   | 2.33                     | 0.43              |
| 2:F:116:GLY:HA2  | 2:F:189:LYS:NZ   | 2.33                     | 0.43              |
| 2:F:267:ASN:N    | 2:F:267:ASN:ND2  | 2.65                     | 0.43              |
| 1:G:86:ASN:HD21  | 1:G:110:ARG:NE   | 2.10                     | 0.43              |
| 1:G:129:GLU:HG3  | 1:G:130:LYS:N    | 2.32                     | 0.43              |
| 1:G:153:THR:HA   | 1:G:164:ASN:OD1  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:31:TYR:HB3   | 1:I:89:ALA:HB1   | 1.99                     | 0.43              |
| 1:I:37:VAL:HG22  | 1:I:85:MET:HG2   | 2.00                     | 0.43              |
| 1:K:135:ARG:HB3  | 1:K:140:LEU:HD23 | 2.00                     | 0.43              |
| 1:M:126:GLN:HE21 | 1:M:126:GLN:HB2  | 1.53                     | 0.43              |
| 1:M:135:ARG:HD3  | 1:M:136:SER:O    | 2.18                     | 0.43              |
| 2:N:23:ASN:O     | 2:N:24:LEU:HD23  | 2.18                     | 0.43              |
| 2:N:211:ASN:ND2  | 2:N:269:GLN:H    | 2.17                     | 0.43              |
| 1:O:132:ARG:CG   | 1:O:203:VAL:O    | 2.63                     | 0.43              |
| 1:O:140:LEU:O    | 1:O:142:LEU:HG   | 2.18                     | 0.43              |
| 1:O:169:PRO:O    | 1:O:171:GLY:N    | 2.48                     | 0.43              |
| 1:A:129:GLU:HG3  | 1:A:130:LYS:N    | 2.33                     | 0.43              |
| 2:B:34:LEU:HD12  | 2:B:34:LEU:HA    | 1.90                     | 0.43              |
| 2:B:60:ARG:HD3   | 4:B:545:HOH:O    | 2.18                     | 0.43              |
| 2:B:65:GLY:O     | 2:B:66:GLY:C     | 2.61                     | 0.43              |
| 2:D:126:ILE:HD11 | 2:D:150:ALA:HB2  | 2.01                     | 0.43              |
| 1:E:28:ASN:N     | 1:E:28:ASN:HD22  | 2.16                     | 0.43              |
| 1:E:129:GLU:HG3  | 1:E:130:LYS:N    | 2.32                     | 0.43              |
| 2:F:226:THR:HG23 | 2:F:253:THR:HB   | 2.01                     | 0.43              |
| 2:H:218:ALA:HB2  | 2:H:266:GLY:HA3  | 1.99                     | 0.43              |
| 1:I:108:ILE:HG22 | 1:I:109:SER:N    | 2.34                     | 0.43              |
| 1:I:135:ARG:HD3  | 1:I:136:SER:O    | 2.18                     | 0.43              |
| 1:K:10:ILE:O     | 1:K:12:PRO:HD3   | 2.19                     | 0.43              |
| 1:K:78:ASP:OD1   | 1:K:79:ARG:N     | 2.52                     | 0.43              |
| 1:K:185:ILE:CG2  | 1:K:202:GLY:HA3  | 2.48                     | 0.43              |
| 1:M:135:ARG:HB3  | 1:M:140:LEU:HD23 | 2.00                     | 0.43              |
| 1:O:24:ASN:HB3   | 1:O:60:LYS:HA    | 2.00                     | 0.43              |
| 2:P:168:VAL:O    | 2:P:168:VAL:HG13 | 2.18                     | 0.43              |
| 1:A:140:LEU:HB2  | 1:A:177:LEU:HD13 | 2.01                     | 0.43              |
| 2:B:48:TYR:HE2   | 3:B:500:MMA:H73  | 1.83                     | 0.43              |
| 1:C:188:ARG:NE   | 1:C:196:LEU:HD22 | 2.31                     | 0.43              |
| 2:D:195:TYR:CE1  | 2:D:238:VAL:HB   | 2.53                     | 0.43              |
| 1:G:67:ILE:N     | 1:G:67:ILE:HD12  | 2.34                     | 0.43              |
| 2:H:78:SER:N     | 4:H:636:HOH:O    | 2.52                     | 0.43              |
| 2:H:175:TYR:CD1  | 2:H:175:TYR:C    | 2.96                     | 0.43              |
| 1:I:135:ARG:HB3  | 1:I:140:LEU:HD23 | 2.00                     | 0.43              |
| 1:I:152:VAL:O    | 1:I:164:ASN:HB3  | 2.18                     | 0.43              |
| 2:J:55:TYR:OH    | 2:J:136:ASN:HB3  | 2.19                     | 0.43              |
| 2:J:75:VAL:HB    | 2:J:84:PHE:HB2   | 2.00                     | 0.43              |
| 2:J:168:VAL:O    | 2:J:168:VAL:HG13 | 2.18                     | 0.43              |
| 1:K:85:MET:HB2   | 1:K:111:ILE:HG13 | 2.01                     | 0.43              |
| 2:L:43:PHE:HE2   | 2:L:102:PRO:HG3  | 1.82                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:55:TYR:OH    | 2:L:136:ASN:HB3  | 2.19                     | 0.43              |
| 1:M:4:LEU:HD11   | 1:M:87:VAL:HG23  | 2.00                     | 0.43              |
| 1:M:134:ARG:CZ   | 1:M:141:THR:HG21 | 2.49                     | 0.43              |
| 1:O:37:VAL:HG22  | 1:O:85:MET:HG2   | 2.00                     | 0.43              |
| 1:O:135:ARG:HB3  | 1:O:140:LEU:HD23 | 2.00                     | 0.43              |
| 2:D:65:GLY:O     | 2:D:66:GLY:C     | 2.62                     | 0.43              |
| 2:F:148:ILE:HD12 | 2:F:148:ILE:N    | 2.33                     | 0.43              |
| 3:H:603:MMA:H2   | 4:H:645:HOH:O    | 2.19                     | 0.43              |
| 2:J:43:PHE:HE2   | 2:J:102:PRO:HG3  | 1.83                     | 0.43              |
| 2:J:49:PRO:HD2   | 2:J:98:ARG:CZ    | 2.49                     | 0.43              |
| 2:L:24:LEU:O     | 2:L:152:ASN:ND2  | 2.52                     | 0.43              |
| 2:L:35:VAL:HA    | 2:L:107:LEU:O    | 2.19                     | 0.43              |
| 1:M:24:ASN:HB3   | 1:M:60:LYS:HA    | 2.01                     | 0.43              |
| 1:M:48:PHE:HD1   | 1:M:48:PHE:HA    | 1.72                     | 0.43              |
| 1:M:116:ARG:HA   | 1:M:117:PRO:HD3  | 1.87                     | 0.43              |
| 2:N:15:GLY:HA2   | 2:N:144:PHE:CG   | 2.53                     | 0.43              |
| 1:O:149:TYR:HD2  | 1:O:166:LEU:HG   | 1.83                     | 0.43              |
| 2:P:15:GLY:HA2   | 2:P:144:PHE:CG   | 2.53                     | 0.43              |
| 2:P:116:GLY:HA2  | 2:P:189:LYS:CG   | 2.40                     | 0.43              |
| 2:B:201:THR:CB   | 2:B:206:ASN:HD22 | 2.32                     | 0.42              |
| 2:D:201:THR:CG2  | 2:D:202:ALA:N    | 2.81                     | 0.42              |
| 1:E:8:ARG:HH22   | 2:F:279:GLN:C    | 2.26                     | 0.42              |
| 1:E:9:VAL:HG22   | 4:E:209:HOH:O    | 2.19                     | 0.42              |
| 1:E:82:LEU:C     | 1:E:83:PHE:HD1   | 2.27                     | 0.42              |
| 1:G:8:ARG:HH22   | 2:H:279:GLN:C    | 2.27                     | 0.42              |
| 1:G:103:LEU:HD11 | 2:H:272:ILE:HG12 | 2.01                     | 0.42              |
| 1:G:188:ARG:NE   | 1:G:196:LEU:HD22 | 2.31                     | 0.42              |
| 2:H:1:PHE:CG     | 2:H:133:ASN:ND2  | 2.87                     | 0.42              |
| 1:I:163:GLU:HB3  | 1:I:175:VAL:CG1  | 2.49                     | 0.42              |
| 2:J:49:PRO:HG2   | 2:J:50:GLU:CD    | 2.44                     | 0.42              |
| 2:J:71:PHE:CA    | 2:J:110:THR:O    | 2.64                     | 0.42              |
| 1:K:31:TYR:HB3   | 1:K:89:ALA:HB1   | 1.99                     | 0.42              |
| 1:K:135:ARG:HD3  | 1:K:136:SER:O    | 2.18                     | 0.42              |
| 1:M:108:ILE:HG22 | 1:M:109:SER:N    | 2.34                     | 0.42              |
| 1:O:126:GLN:HE21 | 1:O:126:GLN:HB2  | 1.53                     | 0.42              |
| 1:O:135:ARG:HA   | 1:O:140:LEU:HA   | 2.01                     | 0.42              |
| 1:O:149:TYR:CD2  | 1:O:166:LEU:HG   | 2.54                     | 0.42              |
| 1:A:28:ASN:N     | 1:A:28:ASN:HD22  | 2.16                     | 0.42              |
| 2:B:59:GLN:NE2   | 2:B:143:GLN:HE22 | 2.17                     | 0.42              |
| 2:B:116:GLY:HA2  | 2:B:189:LYS:NZ   | 2.34                     | 0.42              |
| 1:C:75:LEU:HD22  | 1:C:76:PRO:HD2   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:86:ASN:HD21  | 1:C:110:ARG:HH21 | 1.66                     | 0.42              |
| 1:E:77:GLN:HA    | 1:E:77:GLN:HE21  | 1.84                     | 0.42              |
| 1:G:9:VAL:HG12   | 1:G:113:LEU:CD1  | 2.48                     | 0.42              |
| 2:H:75:VAL:O     | 2:H:75:VAL:HG13  | 2.19                     | 0.42              |
| 1:I:149:TYR:HD2  | 1:I:166:LEU:HG   | 1.84                     | 0.42              |
| 2:J:200:THR:O    | 2:J:200:THR:HG22 | 2.19                     | 0.42              |
| 1:K:4:LEU:O      | 2:L:160:GLY:N    | 2.47                     | 0.42              |
| 1:K:67:ILE:HD11  | 1:K:85:MET:SD    | 2.60                     | 0.42              |
| 1:K:149:TYR:CD2  | 1:K:168:PRO:HA   | 2.54                     | 0.42              |
| 2:N:200:THR:O    | 2:N:200:THR:HG22 | 2.19                     | 0.42              |
| 1:O:4:LEU:HD11   | 1:O:87:VAL:HG23  | 2.00                     | 0.42              |
| 1:O:24:ASN:HD22  | 1:O:60:LYS:HA    | 1.83                     | 0.42              |
| 1:O:127:ALA:HA   | 1:O:146:THR:HG21 | 2.01                     | 0.42              |
| 1:O:128:ALA:CA   | 1:O:150:LEU:HD22 | 2.48                     | 0.42              |
| 1:O:134:ARG:CZ   | 1:O:141:THR:HG21 | 2.49                     | 0.42              |
| 1:O:135:ARG:HD3  | 1:O:136:SER:O    | 2.19                     | 0.42              |
| 2:P:211:ASN:ND2  | 2:P:269:GLN:H    | 2.17                     | 0.42              |
| 1:A:86:ASN:HD21  | 1:A:110:ARG:HH21 | 1.68                     | 0.42              |
| 1:E:9:VAL:HG12   | 1:E:113:LEU:CD1  | 2.48                     | 0.42              |
| 1:G:30:THR:HG22  | 1:G:31:TYR:N     | 2.32                     | 0.42              |
| 1:I:28:ASN:ND2   | 1:I:28:ASN:O     | 2.52                     | 0.42              |
| 1:I:194:GLY:HA3  | 2:J:158:THR:CG2  | 2.49                     | 0.42              |
| 2:J:36:VAL:O     | 2:J:36:VAL:HG12  | 2.20                     | 0.42              |
| 2:J:134:THR:HG22 | 2:J:141:ASP:HA   | 2.01                     | 0.42              |
| 2:J:173:PRO:O    | 2:J:174:ASP:O    | 2.38                     | 0.42              |
| 1:K:20:LEU:O     | 1:K:65:LEU:N     | 2.52                     | 0.42              |
| 1:K:33:ILE:HG13  | 1:K:55:PHE:CE1   | 2.54                     | 0.42              |
| 1:K:108:ILE:HG22 | 1:K:109:SER:N    | 2.34                     | 0.42              |
| 1:K:135:ARG:NH2  | 1:K:177:LEU:CD2  | 2.82                     | 0.42              |
| 2:L:166:ARG:HG2  | 2:L:182:PRO:CB   | 2.47                     | 0.42              |
| 2:P:181:ILE:HA   | 2:P:182:PRO:HD3  | 1.81                     | 0.42              |
| 2:P:211:ASN:HD22 | 2:P:211:ASN:C    | 2.27                     | 0.42              |
| 1:A:5:GLY:O      | 2:B:159:GLY:HA2  | 2.19                     | 0.42              |
| 1:A:82:LEU:C     | 1:A:83:PHE:CD1   | 2.98                     | 0.42              |
| 1:A:135:ARG:HH12 | 1:A:177:LEU:HD21 | 1.83                     | 0.42              |
| 1:A:188:ARG:NH1  | 1:A:188:ARG:HG2  | 2.33                     | 0.42              |
| 2:B:211:ASN:HD21 | 2:B:269:GLN:N    | 1.96                     | 0.42              |
| 1:C:28:ASN:N     | 1:C:28:ASN:ND2   | 2.66                     | 0.42              |
| 1:C:51:THR:HA    | 1:C:52:PRO:C     | 2.44                     | 0.42              |
| 1:C:107:ILE:HG12 | 2:D:163:VAL:HG11 | 1.99                     | 0.42              |
| 1:E:39:ASN:OD1   | 1:E:43:VAL:HG22  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:194:GLY:C    | 2:F:158:THR:HG21 | 2.45                     | 0.42              |
| 1:G:167:VAL:HA   | 1:G:168:PRO:HD2  | 1.79                     | 0.42              |
| 1:I:24:ASN:HB3   | 1:I:60:LYS:HA    | 2.00                     | 0.42              |
| 2:J:15:GLY:HA2   | 2:J:144:PHE:CE1  | 2.55                     | 0.42              |
| 2:J:192:ASN:HB2  | 2:J:279:GLN:NE2  | 2.34                     | 0.42              |
| 1:K:10:ILE:HD13  | 1:K:114:TYR:HB2  | 1.99                     | 0.42              |
| 2:L:71:PHE:CA    | 2:L:110:THR:O    | 2.63                     | 0.42              |
| 2:L:113:SER:O    | 2:L:115:ALA:N    | 2.47                     | 0.42              |
| 2:L:184:THR:HG22 | 2:L:249:SER:HA   | 2.00                     | 0.42              |
| 1:M:78:ASP:OD1   | 1:M:79:ARG:N     | 2.53                     | 0.42              |
| 2:N:75:VAL:HB    | 2:N:84:PHE:HB2   | 2.00                     | 0.42              |
| 2:N:192:ASN:HB2  | 2:N:279:GLN:HE21 | 1.84                     | 0.42              |
| 2:N:258:ARG:NE   | 2:N:263:VAL:HG23 | 2.35                     | 0.42              |
| 1:O:8:ARG:NH1    | 1:O:8:ARG:CB     | 2.81                     | 0.42              |
| 1:O:20:LEU:O     | 1:O:65:LEU:N     | 2.53                     | 0.42              |
| 1:O:78:ASP:OD1   | 1:O:79:ARG:N     | 2.51                     | 0.42              |
| 1:O:108:ILE:HG22 | 1:O:109:SER:N    | 2.35                     | 0.42              |
| 2:P:49:PRO:HD2   | 2:P:98:ARG:CZ    | 2.50                     | 0.42              |
| 1:A:185:ILE:HB   | 1:A:202:GLY:CA   | 2.46                     | 0.42              |
| 2:B:117:GLY:O    | 2:B:155:VAL:HG22 | 2.19                     | 0.42              |
| 1:C:28:ASN:N     | 1:C:28:ASN:HD22  | 2.17                     | 0.42              |
| 2:F:201:THR:CB   | 2:F:206:ASN:ND2  | 2.82                     | 0.42              |
| 2:F:240:LEU:HD23 | 2:F:240:LEU:HA   | 1.86                     | 0.42              |
| 1:G:107:ILE:HG12 | 2:H:163:VAL:HG11 | 2.01                     | 0.42              |
| 1:K:17:GLN:HB3   | 1:K:68:LEU:CD2   | 2.41                     | 0.42              |
| 1:K:134:ARG:CZ   | 1:K:141:THR:HG21 | 2.49                     | 0.42              |
| 2:L:13:ILE:HG22  | 2:L:14:GLY:N     | 2.34                     | 0.42              |
| 2:L:196:TYR:HD1  | 2:L:197:LEU:O    | 2.02                     | 0.42              |
| 1:M:118:ALA:O    | 1:M:119:LYS:HB2  | 2.20                     | 0.42              |
| 1:O:21:ALA:HB1   | 1:O:62:GLU:CD    | 2.45                     | 0.42              |
| 1:O:23:THR:CG2   | 1:O:24:ASN:N     | 2.82                     | 0.42              |
| 1:A:46:GLY:O     | 1:A:48:PHE:N     | 2.53                     | 0.42              |
| 1:C:39:ASN:OD1   | 1:C:43:VAL:HG22  | 2.19                     | 0.42              |
| 2:D:33:ASN:ND2   | 2:D:110:THR:OG1  | 2.52                     | 0.42              |
| 2:F:34:LEU:HD12  | 2:F:34:LEU:HA    | 1.91                     | 0.42              |
| 2:F:185:VAL:O    | 2:F:243:VAL:CG1  | 2.68                     | 0.42              |
| 2:H:183:LEU:HD22 | 2:H:250:LEU:CD1  | 2.49                     | 0.42              |
| 1:I:149:TYR:CD2  | 1:I:166:LEU:HG   | 2.55                     | 0.42              |
| 2:L:52:ILE:HG23  | 2:L:137:TYR:CB   | 2.49                     | 0.42              |
| 2:L:134:THR:HG22 | 2:L:141:ASP:HA   | 2.02                     | 0.42              |
| 2:N:211:ASN:C    | 2:N:211:ASN:HD22 | 2.27                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:28:ASN:ND2   | 1:O:28:ASN:O     | 2.53                     | 0.42              |
| 1:O:143:ILE:HA   | 1:O:172:GLU:HB3  | 2.00                     | 0.42              |
| 2:P:24:LEU:O     | 2:P:152:ASN:ND2  | 2.53                     | 0.42              |
| 2:P:35:VAL:HA    | 2:P:107:LEU:O    | 2.19                     | 0.42              |
| 2:P:41:GLN:HE21  | 2:P:41:GLN:CA    | 2.33                     | 0.42              |
| 1:A:82:LEU:C     | 1:A:83:PHE:HD1   | 2.27                     | 0.42              |
| 2:B:185:VAL:O    | 2:B:243:VAL:CG1  | 2.68                     | 0.42              |
| 1:C:77:GLN:HE21  | 1:C:117:PRO:HB3  | 1.84                     | 0.42              |
| 1:C:107:ILE:N    | 1:C:107:ILE:CD1  | 2.83                     | 0.42              |
| 2:D:55:TYR:CD1   | 2:D:94:VAL:HG12  | 2.55                     | 0.42              |
| 2:D:201:THR:CB   | 2:D:206:ASN:HD22 | 2.31                     | 0.42              |
| 1:G:39:ASN:OD1   | 1:G:43:VAL:HG22  | 2.19                     | 0.42              |
| 1:G:65:LEU:HD23  | 1:G:65:LEU:HA    | 1.75                     | 0.42              |
| 1:G:148:TYR:C    | 1:G:169:PRO:HG3  | 2.45                     | 0.42              |
| 2:H:201:THR:CB   | 2:H:206:ASN:ND2  | 2.83                     | 0.42              |
| 1:I:23:THR:CG2   | 1:I:24:ASN:N     | 2.83                     | 0.42              |
| 1:I:127:ALA:HA   | 1:I:146:THR:HG21 | 2.00                     | 0.42              |
| 1:K:23:THR:HB    | 4:K:212:HOH:O    | 2.19                     | 0.42              |
| 1:K:24:ASN:HD22  | 1:K:60:LYS:HA    | 1.84                     | 0.42              |
| 1:K:114:TYR:OH   | 1:K:149:TYR:HB2  | 2.20                     | 0.42              |
| 1:K:194:GLY:HA3  | 2:L:158:THR:CG2  | 2.50                     | 0.42              |
| 1:M:103:LEU:HD22 | 2:N:254:ALA:HB2  | 2.02                     | 0.42              |
| 1:M:194:GLY:HA3  | 2:N:158:THR:CG2  | 2.49                     | 0.42              |
| 2:N:45:HIS:CD2   | 2:N:98:ARG:O     | 2.73                     | 0.42              |
| 1:O:84:TRP:CE3   | 1:O:110:ARG:HG2  | 2.55                     | 0.42              |
| 1:O:85:MET:HB2   | 1:O:111:ILE:HG13 | 2.01                     | 0.42              |
| 1:O:98:LEU:O     | 1:O:98:LEU:HD22  | 2.19                     | 0.42              |
| 2:P:175:TYR:N    | 2:P:176:PRO:HD2  | 2.35                     | 0.42              |
| 1:A:51:THR:HA    | 1:A:52:PRO:C     | 2.45                     | 0.42              |
| 1:A:148:TYR:C    | 1:A:169:PRO:HG3  | 2.44                     | 0.42              |
| 2:B:201:THR:HG23 | 2:B:202:ALA:N    | 2.35                     | 0.42              |
| 1:C:140:LEU:HB2  | 1:C:177:LEU:HD13 | 2.02                     | 0.42              |
| 2:D:116:GLY:HA2  | 2:D:189:LYS:NZ   | 2.35                     | 0.42              |
| 2:D:131:LEU:C    | 2:D:131:LEU:CD2  | 2.93                     | 0.42              |
| 2:D:175:TYR:CD1  | 2:D:175:TYR:C    | 2.97                     | 0.42              |
| 2:F:173:PRO:CG   | 2:F:179:VAL:HG13 | 2.34                     | 0.42              |
| 2:F:209:PHE:CG   | 2:F:272:ILE:CD1  | 3.03                     | 0.42              |
| 2:H:96:ASN:H     | 2:H:96:ASN:HD22  | 1.68                     | 0.42              |
| 2:H:148:ILE:HD12 | 2:H:148:ILE:N    | 2.35                     | 0.42              |
| 1:I:28:ASN:ND2   | 1:I:28:ASN:N     | 2.57                     | 0.42              |
| 1:I:48:PHE:HD1   | 1:I:48:PHE:HA    | 1.72                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:132:ARG:CG   | 1:I:203:VAL:O    | 2.63                     | 0.42              |
| 2:J:59:GLN:HG3   | 2:J:143:GLN:NE2  | 2.31                     | 0.42              |
| 2:J:75:VAL:O     | 2:J:75:VAL:HG13  | 2.20                     | 0.42              |
| 2:J:98:ARG:HH11  | 2:J:98:ARG:CG    | 2.32                     | 0.42              |
| 2:J:136:ASN:HD22 | 2:J:136:ASN:N    | 2.18                     | 0.42              |
| 1:K:24:ASN:HB3   | 1:K:60:LYS:HA    | 2.01                     | 0.42              |
| 2:L:192:ASN:HB2  | 2:L:279:GLN:NE2  | 2.35                     | 0.42              |
| 2:L:211:ASN:C    | 2:L:211:ASN:HD22 | 2.27                     | 0.42              |
| 2:L:258:ARG:NE   | 2:L:263:VAL:HG23 | 2.35                     | 0.42              |
| 1:M:135:ARG:HA   | 1:M:140:LEU:HA   | 2.02                     | 0.42              |
| 1:M:169:PRO:O    | 1:M:171:GLY:N    | 2.49                     | 0.42              |
| 2:N:49:PRO:HD2   | 2:N:98:ARG:CZ    | 2.50                     | 0.42              |
| 2:N:185:VAL:HG11 | 2:N:276:PHE:CZ   | 2.55                     | 0.42              |
| 2:N:211:ASN:ND2  | 2:N:213:ALA:H    | 2.18                     | 0.42              |
| 1:O:4:LEU:C      | 1:O:6:ALA:N      | 2.73                     | 0.42              |
| 1:A:142:LEU:N    | 1:A:142:LEU:HD23 | 2.34                     | 0.42              |
| 2:B:226:THR:HG23 | 2:B:253:THR:HB   | 2.02                     | 0.42              |
| 1:C:124:PRO:HD3  | 1:C:148:TYR:OH   | 2.19                     | 0.42              |
| 1:C:148:TYR:CD1  | 1:C:148:TYR:N    | 2.88                     | 0.42              |
| 1:C:161:VAL:O    | 1:C:162:LEU:CG   | 2.68                     | 0.42              |
| 1:E:182:GLY:O    | 1:E:183:SER:HB2  | 2.20                     | 0.42              |
| 1:E:188:ARG:NH1  | 1:E:188:ARG:HG2  | 2.34                     | 0.42              |
| 1:G:28:ASN:N     | 1:G:28:ASN:ND2   | 2.66                     | 0.42              |
| 1:G:148:TYR:N    | 1:G:148:TYR:CD1  | 2.87                     | 0.42              |
| 2:H:48:TYR:HE2   | 3:H:603:MMA:H73  | 1.85                     | 0.42              |
| 1:I:134:ARG:CZ   | 1:I:141:THR:HG21 | 2.50                     | 0.42              |
| 2:J:35:VAL:HA    | 2:J:107:LEU:O    | 2.20                     | 0.42              |
| 1:K:149:TYR:CD2  | 1:K:166:LEU:HG   | 2.54                     | 0.42              |
| 2:L:75:VAL:HG13  | 2:L:75:VAL:O     | 2.18                     | 0.42              |
| 2:L:131:LEU:HD23 | 2:L:131:LEU:C    | 2.45                     | 0.42              |
| 1:M:24:ASN:HD22  | 1:M:60:LYS:HA    | 1.83                     | 0.42              |
| 1:M:149:TYR:CB   | 1:M:166:LEU:HD11 | 2.39                     | 0.42              |
| 2:N:35:VAL:HA    | 2:N:107:LEU:O    | 2.20                     | 0.42              |
| 1:O:4:LEU:O      | 2:P:160:GLY:N    | 2.50                     | 0.42              |
| 1:O:67:ILE:HD11  | 1:O:85:MET:SD    | 2.59                     | 0.42              |
| 2:P:36:VAL:O     | 2:P:36:VAL:HG12  | 2.19                     | 0.42              |
| 2:P:55:TYR:CG    | 2:P:92:ARG:HD2   | 2.55                     | 0.42              |
| 2:P:192:ASN:HB2  | 2:P:279:GLN:NE2  | 2.35                     | 0.42              |
| 1:A:148:TYR:CD1  | 1:A:148:TYR:N    | 2.87                     | 0.42              |
| 1:A:194:GLY:C    | 2:B:158:THR:HG21 | 2.45                     | 0.42              |
| 2:B:5:THR:HG22   | 2:B:9:THR:N      | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:201:THR:CB   | 2:B:206:ASN:ND2  | 2.83                     | 0.42              |
| 1:C:9:VAL:HG12   | 1:C:113:LEU:CD1  | 2.49                     | 0.42              |
| 1:C:103:LEU:HD11 | 2:D:272:ILE:HG12 | 2.02                     | 0.42              |
| 1:C:148:TYR:C    | 1:C:169:PRO:HG3  | 2.45                     | 0.42              |
| 2:D:201:THR:CB   | 2:D:206:ASN:ND2  | 2.83                     | 0.42              |
| 2:D:218:ALA:HB1  | 2:D:264:THR:O    | 2.20                     | 0.42              |
| 1:E:103:LEU:HD11 | 2:F:272:ILE:HG12 | 2.01                     | 0.42              |
| 2:F:96:ASN:HD22  | 2:F:96:ASN:H     | 1.68                     | 0.42              |
| 2:F:218:ALA:HB1  | 2:F:264:THR:O    | 2.19                     | 0.42              |
| 1:G:28:ASN:N     | 1:G:28:ASN:HD22  | 2.17                     | 0.42              |
| 1:I:84:TRP:CE3   | 1:I:110:ARG:HG2  | 2.55                     | 0.42              |
| 1:K:103:LEU:HD22 | 2:L:254:ALA:HB2  | 2.02                     | 0.42              |
| 2:L:75:VAL:HB    | 2:L:84:PHE:HB2   | 2.01                     | 0.42              |
| 1:M:31:TYR:HB3   | 1:M:89:ALA:HB1   | 1.99                     | 0.42              |
| 1:M:84:TRP:CE3   | 1:M:110:ARG:HG2  | 2.55                     | 0.42              |
| 2:N:121:LYS:HD2  | 2:N:121:LYS:N    | 2.35                     | 0.42              |
| 1:O:103:LEU:HD22 | 2:P:254:ALA:HB2  | 2.01                     | 0.42              |
| 2:P:258:ARG:NE   | 2:P:263:VAL:HG23 | 2.35                     | 0.42              |
| 1:A:103:LEU:HD11 | 2:B:272:ILE:HG12 | 2.02                     | 0.41              |
| 1:C:79:ARG:CZ    | 1:C:170:MET:HE3  | 2.50                     | 0.41              |
| 1:E:28:ASN:N     | 1:E:28:ASN:ND2   | 2.66                     | 0.41              |
| 1:I:103:LEU:HD22 | 2:J:254:ALA:HB2  | 2.02                     | 0.41              |
| 1:I:169:PRO:C    | 1:I:171:GLY:N    | 2.75                     | 0.41              |
| 2:L:36:VAL:O     | 2:L:36:VAL:HG12  | 2.19                     | 0.41              |
| 2:L:77:TYR:HD1   | 2:L:105:VAL:HG22 | 1.84                     | 0.41              |
| 2:L:211:ASN:ND2  | 2:L:269:GLN:H    | 2.18                     | 0.41              |
| 1:M:21:ALA:HB1   | 1:M:62:GLU:CD    | 2.45                     | 0.41              |
| 1:M:149:TYR:HD2  | 1:M:166:LEU:HG   | 1.85                     | 0.41              |
| 2:N:24:LEU:O     | 2:N:26:PRO:HD3   | 2.20                     | 0.41              |
| 2:N:24:LEU:O     | 2:N:152:ASN:ND2  | 2.53                     | 0.41              |
| 2:N:49:PRO:HG2   | 2:N:50:GLU:CD    | 2.45                     | 0.41              |
| 2:N:196:TYR:HD1  | 2:N:197:LEU:O    | 2.03                     | 0.41              |
| 1:O:104:GLN:O    | 2:P:271:ILE:HA   | 2.20                     | 0.41              |
| 1:O:185:ILE:CG2  | 1:O:202:GLY:HA3  | 2.48                     | 0.41              |
| 2:P:185:VAL:HG11 | 2:P:276:PHE:CZ   | 2.55                     | 0.41              |
| 2:B:59:GLN:HE21  | 2:B:143:GLN:HE22 | 1.67                     | 0.41              |
| 2:B:209:PHE:CG   | 2:B:272:ILE:CD1  | 3.02                     | 0.41              |
| 2:B:221:VAL:CG1  | 2:B:222:GLY:H    | 2.22                     | 0.41              |
| 1:C:5:GLY:O      | 2:D:159:GLY:HA2  | 2.20                     | 0.41              |
| 1:C:67:ILE:HD12  | 1:C:67:ILE:N     | 2.35                     | 0.41              |
| 1:C:82:LEU:C     | 1:C:83:PHE:HD1   | 2.27                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:142:LEU:HD23 | 1:C:142:LEU:H    | 1.85                     | 0.41              |
| 1:E:67:ILE:N     | 1:E:67:ILE:HD12  | 2.35                     | 0.41              |
| 1:E:144:ASN:CG   | 1:E:150:LEU:HG   | 2.45                     | 0.41              |
| 1:E:168:PRO:HA   | 1:E:169:PRO:HD3  | 1.96                     | 0.41              |
| 2:F:73:GLY:HA2   | 4:F:513:HOH:O    | 2.20                     | 0.41              |
| 2:F:126:ILE:HD11 | 2:F:150:ALA:HB2  | 2.02                     | 0.41              |
| 1:G:51:THR:HA    | 1:G:52:PRO:C     | 2.44                     | 0.41              |
| 1:G:124:PRO:HD3  | 1:G:148:TYR:OH   | 2.20                     | 0.41              |
| 1:G:140:LEU:HB2  | 1:G:177:LEU:HD13 | 2.02                     | 0.41              |
| 2:H:171:THR:C    | 2:H:173:PRO:CD   | 2.91                     | 0.41              |
| 2:H:195:TYR:CE1  | 2:H:238:VAL:HB   | 2.55                     | 0.41              |
| 2:J:55:TYR:CG    | 2:J:92:ARG:HD2   | 2.55                     | 0.41              |
| 2:J:196:TYR:HD1  | 2:J:197:LEU:O    | 2.03                     | 0.41              |
| 2:J:269:GLN:NE2  | 4:J:610:HOH:O    | 2.51                     | 0.41              |
| 1:K:21:ALA:HB1   | 1:K:62:GLU:CD    | 2.45                     | 0.41              |
| 1:K:57:MET:HE3   | 1:K:61:LYS:O     | 2.20                     | 0.41              |
| 1:K:143:ILE:HA   | 1:K:172:GLU:HB3  | 2.01                     | 0.41              |
| 1:K:163:GLU:HB3  | 1:K:175:VAL:CG1  | 2.50                     | 0.41              |
| 1:K:163:GLU:N    | 1:K:175:VAL:HG11 | 2.15                     | 0.41              |
| 2:L:15:GLY:HA2   | 2:L:144:PHE:CE1  | 2.56                     | 0.41              |
| 2:L:49:PRO:HG2   | 2:L:50:GLU:CD    | 2.45                     | 0.41              |
| 2:L:192:ASN:HB2  | 2:L:279:GLN:HE21 | 1.85                     | 0.41              |
| 1:M:37:VAL:HG22  | 1:M:85:MET:HG2   | 2.00                     | 0.41              |
| 2:N:41:GLN:HE21  | 2:N:41:GLN:CA    | 2.34                     | 0.41              |
| 2:N:196:TYR:C    | 2:N:197:LEU:HD23 | 2.45                     | 0.41              |
| 1:O:163:GLU:HB3  | 1:O:175:VAL:CG1  | 2.50                     | 0.41              |
| 2:P:211:ASN:ND2  | 2:P:213:ALA:H    | 2.18                     | 0.41              |
| 1:A:182:GLY:O    | 1:A:183:SER:HB2  | 2.20                     | 0.41              |
| 2:B:55:TYR:CD1   | 2:B:94:VAL:HG12  | 2.56                     | 0.41              |
| 2:D:5:THR:N      | 2:D:9:THR:O      | 2.48                     | 0.41              |
| 2:D:14:GLY:HA2   | 2:D:142:PHE:CD1  | 2.56                     | 0.41              |
| 2:D:262:GLN:O    | 2:D:263:VAL:C    | 2.64                     | 0.41              |
| 1:E:162:LEU:HD21 | 1:E:178:PRO:HD2  | 2.02                     | 0.41              |
| 2:F:55:TYR:CD1   | 2:F:94:VAL:HG12  | 2.55                     | 0.41              |
| 1:G:77:GLN:HE21  | 1:G:77:GLN:CA    | 2.34                     | 0.41              |
| 2:H:14:GLY:HA2   | 2:H:142:PHE:CD1  | 2.55                     | 0.41              |
| 1:I:4:LEU:HB3    | 1:I:6:ALA:O      | 2.20                     | 0.41              |
| 2:J:96:ASN:HD22  | 2:J:96:ASN:H     | 1.59                     | 0.41              |
| 2:J:113:SER:O    | 2:J:115:ALA:N    | 2.47                     | 0.41              |
| 2:J:192:ASN:HB2  | 2:J:279:GLN:HE21 | 1.85                     | 0.41              |
| 2:L:121:LYS:HD2  | 2:L:121:LYS:N    | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:185:VAL:HG11 | 2:L:276:PHE:CZ   | 2.54                     | 0.41              |
| 2:N:15:GLY:HA2   | 2:N:144:PHE:CE1  | 2.56                     | 0.41              |
| 2:P:13:ILE:HG22  | 2:P:14:GLY:N     | 2.34                     | 0.41              |
| 2:P:45:HIS:CD2   | 2:P:98:ARG:O     | 2.73                     | 0.41              |
| 2:P:121:LYS:N    | 2:P:121:LYS:HD2  | 2.35                     | 0.41              |
| 2:P:136:ASN:HD22 | 2:P:136:ASN:N    | 2.17                     | 0.41              |
| 2:P:166:ARG:HG2  | 2:P:182:PRO:CB   | 2.47                     | 0.41              |
| 2:P:196:TYR:HD1  | 2:P:197:LEU:O    | 2.02                     | 0.41              |
| 1:A:159:THR:HB   | 1:A:160:ARG:H    | 1.63                     | 0.41              |
| 2:B:105:VAL:HG11 | 2:B:129:LEU:HD13 | 2.02                     | 0.41              |
| 1:C:65:LEU:HD23  | 1:C:65:LEU:HA    | 1.76                     | 0.41              |
| 1:C:142:LEU:N    | 1:C:142:LEU:HD23 | 2.35                     | 0.41              |
| 1:C:144:ASN:CG   | 1:C:150:LEU:HG   | 2.46                     | 0.41              |
| 1:C:162:LEU:HD21 | 1:C:178:PRO:HD2  | 2.02                     | 0.41              |
| 1:C:193:TYR:CG   | 2:D:155:VAL:HG11 | 2.56                     | 0.41              |
| 1:E:51:THR:HA    | 1:E:52:PRO:C     | 2.45                     | 0.41              |
| 1:E:82:LEU:C     | 1:E:83:PHE:CD1   | 2.98                     | 0.41              |
| 1:G:9:VAL:CG1    | 1:G:113:LEU:HD13 | 2.50                     | 0.41              |
| 1:G:182:GLY:O    | 1:G:183:SER:HB2  | 2.20                     | 0.41              |
| 1:I:10:ILE:O     | 1:I:12:PRO:HD3   | 2.20                     | 0.41              |
| 1:I:135:ARG:HA   | 1:I:140:LEU:HA   | 2.02                     | 0.41              |
| 2:J:52:ILE:HG23  | 2:J:137:TYR:CB   | 2.50                     | 0.41              |
| 2:J:185:VAL:HG11 | 2:J:276:PHE:CZ   | 2.56                     | 0.41              |
| 1:K:10:ILE:HG13  | 1:K:192:ASP:CG   | 2.46                     | 0.41              |
| 2:L:211:ASN:ND2  | 2:L:213:ALA:H    | 2.19                     | 0.41              |
| 1:M:4:LEU:HB3    | 1:M:6:ALA:O      | 2.21                     | 0.41              |
| 2:N:13:ILE:HG22  | 2:N:14:GLY:N     | 2.35                     | 0.41              |
| 1:O:24:ASN:HD21  | 1:O:26:ASP:HB2   | 1.86                     | 0.41              |
| 2:P:52:ILE:HG23  | 2:P:137:TYR:CB   | 2.49                     | 0.41              |
| 2:P:227:ARG:O    | 2:P:229:GLY:N    | 2.53                     | 0.41              |
| 2:D:96:ASN:HD22  | 2:D:96:ASN:H     | 1.69                     | 0.41              |
| 2:D:114:SER:O    | 2:D:115:ALA:C    | 2.63                     | 0.41              |
| 2:F:226:THR:CG2  | 2:F:253:THR:HB   | 2.50                     | 0.41              |
| 1:G:82:LEU:C     | 1:G:83:PHE:CD1   | 2.98                     | 0.41              |
| 1:G:82:LEU:C     | 1:G:83:PHE:HD1   | 2.29                     | 0.41              |
| 2:H:218:ALA:HB1  | 2:H:264:THR:O    | 2.20                     | 0.41              |
| 2:H:262:GLN:O    | 2:H:263:VAL:C    | 2.63                     | 0.41              |
| 1:I:67:ILE:HD11  | 1:I:85:MET:SD    | 2.60                     | 0.41              |
| 1:I:116:ARG:HA   | 1:I:117:PRO:HD3  | 1.87                     | 0.41              |
| 2:J:196:TYR:C    | 2:J:197:LEU:HD23 | 2.45                     | 0.41              |
| 2:J:228:ASN:O    | 2:J:228:ASN:ND2  | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:258:ARG:NE   | 2:J:263:VAL:HG23 | 2.35                     | 0.41              |
| 1:K:8:ARG:NH1    | 1:K:8:ARG:CB     | 2.81                     | 0.41              |
| 1:K:23:THR:CG2   | 1:K:24:ASN:N     | 2.83                     | 0.41              |
| 1:K:104:GLN:O    | 2:L:271:ILE:HA   | 2.20                     | 0.41              |
| 2:L:200:THR:O    | 2:L:200:THR:HG22 | 2.19                     | 0.41              |
| 1:M:33:ILE:HG13  | 1:M:55:PHE:CE1   | 2.55                     | 0.41              |
| 1:M:49:ILE:HB    | 1:M:68:LEU:HB2   | 2.02                     | 0.41              |
| 1:O:48:PHE:HD1   | 1:O:48:PHE:HA    | 1.72                     | 0.41              |
| 2:P:123:GLY:N    | 2:P:150:ALA:O    | 2.53                     | 0.41              |
| 2:P:162:ASP:N    | 2:P:186:TYR:O    | 2.54                     | 0.41              |
| 1:A:142:LEU:HD23 | 1:A:142:LEU:H    | 1.84                     | 0.41              |
| 2:B:3:CYS:HA     | 2:B:43:PHE:O     | 2.20                     | 0.41              |
| 2:D:209:PHE:CG   | 2:D:272:ILE:CD1  | 3.04                     | 0.41              |
| 1:E:25:ASN:O     | 1:E:60:LYS:NZ    | 2.54                     | 0.41              |
| 1:G:142:LEU:HD12 | 1:G:152:VAL:HG21 | 2.02                     | 0.41              |
| 2:H:185:VAL:O    | 2:H:243:VAL:CG1  | 2.69                     | 0.41              |
| 1:I:10:ILE:HG13  | 1:I:192:ASP:CG   | 2.46                     | 0.41              |
| 1:I:21:ALA:HB1   | 1:I:62:GLU:CD    | 2.45                     | 0.41              |
| 1:I:33:ILE:HG13  | 1:I:55:PHE:CE1   | 2.55                     | 0.41              |
| 2:J:75:VAL:HG23  | 2:J:107:LEU:CD1  | 2.50                     | 0.41              |
| 2:J:136:ASN:ND2  | 2:J:136:ASN:C    | 2.78                     | 0.41              |
| 1:M:149:TYR:CD2  | 1:M:166:LEU:HG   | 2.55                     | 0.41              |
| 2:N:162:ASP:N    | 2:N:186:TYR:O    | 2.54                     | 0.41              |
| 2:P:15:GLY:HA2   | 2:P:144:PHE:CE1  | 2.55                     | 0.41              |
| 2:P:43:PHE:HE2   | 2:P:102:PRO:HG3  | 1.82                     | 0.41              |
| 2:P:173:PRO:O    | 2:P:174:ASP:O    | 2.38                     | 0.41              |
| 2:B:201:THR:HG21 | 2:B:206:ASN:ND2  | 2.25                     | 0.41              |
| 2:B:255:ASN:HB3  | 4:B:511:HOH:O    | 2.20                     | 0.41              |
| 1:C:8:ARG:HB3    | 1:C:8:ARG:CZ     | 2.50                     | 0.41              |
| 2:D:221:VAL:HG11 | 2:D:256:TYR:HD1  | 1.85                     | 0.41              |
| 1:G:107:ILE:N    | 1:G:107:ILE:CD1  | 2.84                     | 0.41              |
| 1:G:194:GLY:C    | 2:H:158:THR:HG21 | 2.45                     | 0.41              |
| 1:G:199:LYS:C    | 1:G:200:MET:HG3  | 2.45                     | 0.41              |
| 1:I:57:MET:HE3   | 1:I:61:LYS:O     | 2.20                     | 0.41              |
| 1:I:101:ASN:HB2  | 2:J:171:THR:C    | 2.46                     | 0.41              |
| 2:J:162:ASP:N    | 2:J:186:TYR:O    | 2.54                     | 0.41              |
| 2:J:175:TYR:N    | 2:J:176:PRO:HD2  | 2.35                     | 0.41              |
| 2:J:211:ASN:ND2  | 2:J:213:ALA:H    | 2.19                     | 0.41              |
| 1:M:23:THR:CG2   | 1:M:24:ASN:N     | 2.82                     | 0.41              |
| 1:M:101:ASN:O    | 2:N:171:THR:N    | 2.54                     | 0.41              |
| 1:M:143:ILE:HA   | 1:M:172:GLU:HB3  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:144:ASN:HB3  | 1:M:167:VAL:CG1  | 2.46                     | 0.41              |
| 1:M:163:GLU:HB3  | 1:M:175:VAL:CG1  | 2.49                     | 0.41              |
| 2:N:75:VAL:O     | 2:N:75:VAL:HG13  | 2.19                     | 0.41              |
| 2:N:77:TYR:HD1   | 2:N:105:VAL:HG22 | 1.85                     | 0.41              |
| 1:O:10:ILE:O     | 1:O:12:PRO:HD3   | 2.21                     | 0.41              |
| 1:O:33:ILE:HG13  | 1:O:55:PHE:CE1   | 2.55                     | 0.41              |
| 1:O:57:MET:HE3   | 1:O:61:LYS:O     | 2.21                     | 0.41              |
| 1:A:144:ASN:CG   | 1:A:150:LEU:HG   | 2.45                     | 0.41              |
| 1:A:168:PRO:HA   | 1:A:169:PRO:HD3  | 1.96                     | 0.41              |
| 2:D:148:ILE:N    | 2:D:148:ILE:HD12 | 2.36                     | 0.41              |
| 1:E:148:TYR:CD1  | 1:E:148:TYR:N    | 2.89                     | 0.41              |
| 1:G:161:VAL:O    | 1:G:162:LEU:CG   | 2.66                     | 0.41              |
| 2:H:5:THR:N      | 2:H:9:THR:O      | 2.48                     | 0.41              |
| 1:I:24:ASN:HD21  | 1:I:26:ASP:HB2   | 1.85                     | 0.41              |
| 1:I:114:TYR:OH   | 1:I:149:TYR:HB2  | 2.20                     | 0.41              |
| 2:J:13:ILE:HG22  | 2:J:14:GLY:N     | 2.35                     | 0.41              |
| 2:J:258:ARG:CD   | 2:J:261:GLY:HA2  | 2.20                     | 0.41              |
| 1:K:135:ARG:HA   | 1:K:140:LEU:HA   | 2.02                     | 0.41              |
| 2:L:21:TYR:O     | 2:L:151:ASN:ND2  | 2.54                     | 0.41              |
| 2:L:175:TYR:N    | 2:L:176:PRO:HD2  | 2.35                     | 0.41              |
| 1:M:10:ILE:O     | 1:M:12:PRO:HD3   | 2.20                     | 0.41              |
| 1:M:104:GLN:O    | 2:N:271:ILE:HA   | 2.21                     | 0.41              |
| 2:N:43:PHE:HE2   | 2:N:102:PRO:HG3  | 1.82                     | 0.41              |
| 2:N:55:TYR:CG    | 2:N:92:ARG:HD2   | 2.56                     | 0.41              |
| 2:N:134:THR:HG22 | 2:N:141:ASP:HA   | 2.02                     | 0.41              |
| 2:N:166:ARG:HG2  | 2:N:182:PRO:CB   | 2.48                     | 0.41              |
| 2:N:173:PRO:O    | 2:N:174:ASP:O    | 2.38                     | 0.41              |
| 1:O:153:THR:OG1  | 1:O:154:GLU:HG3  | 2.21                     | 0.41              |
| 2:P:228:ASN:ND2  | 2:P:228:ASN:O    | 2.54                     | 0.41              |
| 1:A:162:LEU:HD21 | 1:A:178:PRO:HD2  | 2.03                     | 0.41              |
| 2:B:33:ASN:HD22  | 2:B:33:ASN:HA    | 1.55                     | 0.41              |
| 2:B:77:TYR:N     | 2:B:80:SER:O     | 2.54                     | 0.41              |
| 2:B:226:THR:CG2  | 2:B:253:THR:HB   | 2.51                     | 0.41              |
| 1:C:25:ASN:O     | 1:C:60:LYS:NZ    | 2.54                     | 0.41              |
| 1:C:43:VAL:O     | 1:C:43:VAL:HG23  | 2.21                     | 0.41              |
| 1:C:182:GLY:O    | 1:C:183:SER:HB2  | 2.21                     | 0.41              |
| 1:C:188:ARG:NH1  | 1:C:188:ARG:HG2  | 2.36                     | 0.41              |
| 1:C:194:GLY:C    | 2:D:158:THR:HG21 | 2.45                     | 0.41              |
| 2:D:3:CYS:HA     | 2:D:43:PHE:O     | 2.20                     | 0.41              |
| 1:E:9:VAL:CG1    | 1:E:113:LEU:HD13 | 2.50                     | 0.41              |
| 1:E:11:TYR:HA    | 1:E:12:PRO:HD3   | 1.83                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:125:ASP:OD1  | 1:E:125:ASP:N    | 2.53                     | 0.41              |
| 1:E:148:TYR:C    | 1:E:169:PRO:HG3  | 2.46                     | 0.41              |
| 1:E:158:GLY:CA   | 1:E:184:ASN:O    | 2.69                     | 0.41              |
| 1:E:159:THR:HB   | 1:E:160:ARG:H    | 1.63                     | 0.41              |
| 1:E:199:LYS:C    | 1:E:200:MET:HG3  | 2.45                     | 0.41              |
| 2:F:179:VAL:O    | 2:F:253:THR:CG2  | 2.69                     | 0.41              |
| 1:G:8:ARG:HB3    | 1:G:8:ARG:CZ     | 2.50                     | 0.41              |
| 1:G:125:ASP:OD1  | 1:G:125:ASP:N    | 2.54                     | 0.41              |
| 1:G:138:ASN:OD1  | 1:G:139:SER:N    | 2.51                     | 0.41              |
| 2:H:5:THR:HG22   | 2:H:9:THR:N      | 2.35                     | 0.41              |
| 2:H:50:GLU:CD    | 2:H:50:GLU:H     | 2.29                     | 0.41              |
| 2:H:114:SER:O    | 2:H:115:ALA:C    | 2.64                     | 0.41              |
| 1:I:8:ARG:NH1    | 1:I:8:ARG:CB     | 2.80                     | 0.41              |
| 1:I:98:LEU:O     | 1:I:98:LEU:HD22  | 2.20                     | 0.41              |
| 1:I:105:LEU:HD11 | 2:J:183:LEU:HD11 | 2.03                     | 0.41              |
| 1:I:135:ARG:NH2  | 1:I:177:LEU:CD2  | 2.83                     | 0.41              |
| 1:I:143:ILE:HA   | 1:I:172:GLU:HB3  | 2.01                     | 0.41              |
| 1:I:185:ILE:CG2  | 1:I:202:GLY:HA3  | 2.49                     | 0.41              |
| 2:J:21:TYR:O     | 2:J:151:ASN:ND2  | 2.54                     | 0.41              |
| 2:J:29:ASN:OD1   | 2:J:157:PRO:HB2  | 2.21                     | 0.41              |
| 2:J:67:VAL:HA    | 2:J:71:PHE:HD1   | 1.86                     | 0.41              |
| 2:J:103:TRP:CH2  | 2:J:131:LEU:HB2  | 2.56                     | 0.41              |
| 1:K:48:PHE:HD1   | 1:K:48:PHE:HA    | 1.73                     | 0.41              |
| 1:K:84:TRP:CE3   | 1:K:110:ARG:HG2  | 2.55                     | 0.41              |
| 1:K:169:PRO:O    | 1:K:171:GLY:N    | 2.48                     | 0.41              |
| 2:L:110:THR:HA   | 2:L:111:PRO:HD3  | 1.95                     | 0.41              |
| 2:L:162:ASP:N    | 2:L:186:TYR:O    | 2.54                     | 0.41              |
| 2:L:196:TYR:C    | 2:L:197:LEU:HD23 | 2.45                     | 0.41              |
| 2:N:21:TYR:O     | 2:N:151:ASN:ND2  | 2.54                     | 0.41              |
| 2:N:60:ARG:HB3   | 2:N:130:ILE:HD13 | 2.02                     | 0.41              |
| 2:N:123:GLY:N    | 2:N:150:ALA:O    | 2.52                     | 0.41              |
| 1:O:4:LEU:HB3    | 1:O:6:ALA:O      | 2.21                     | 0.41              |
| 2:P:144:PHE:CD1  | 2:P:144:PHE:N    | 2.89                     | 0.41              |
| 2:P:192:ASN:HB2  | 2:P:279:GLN:HE21 | 1.85                     | 0.41              |
| 2:P:196:TYR:C    | 2:P:197:LEU:HD23 | 2.46                     | 0.41              |
| 2:P:209:PHE:CZ   | 2:P:234:ALA:HB2  | 2.55                     | 0.41              |
| 2:P:248:VAL:HG13 | 4:P:614:HOH:O    | 2.21                     | 0.41              |
| 1:A:169:PRO:O    | 1:A:170:MET:C    | 2.64                     | 0.41              |
| 1:A:199:LYS:C    | 1:A:200:MET:HG3  | 2.46                     | 0.41              |
| 2:D:50:GLU:CD    | 2:D:50:GLU:H     | 2.29                     | 0.41              |
| 1:E:5:GLY:O      | 2:F:159:GLY:HA2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:65:LEU:HA    | 1:E:65:LEU:HD23  | 1.72                     | 0.41              |
| 1:E:185:ILE:CB   | 1:E:202:GLY:HA3  | 2.48                     | 0.41              |
| 2:F:30:VAL:C     | 2:F:32:GLN:H     | 2.29                     | 0.41              |
| 2:F:77:TYR:N     | 2:F:80:SER:O     | 2.54                     | 0.41              |
| 1:G:162:LEU:HD21 | 1:G:178:PRO:HD2  | 2.03                     | 0.41              |
| 1:I:104:GLN:O    | 2:J:271:ILE:HA   | 2.21                     | 0.41              |
| 2:J:45:HIS:CD2   | 2:J:98:ARG:O     | 2.73                     | 0.41              |
| 1:K:24:ASN:HD21  | 1:K:26:ASP:HB2   | 1.86                     | 0.41              |
| 1:M:107:ILE:N    | 1:M:107:ILE:CD1  | 2.81                     | 0.41              |
| 2:N:138:ASN:ND2  | 2:N:140:ASP:HB2  | 2.36                     | 0.41              |
| 2:N:144:PHE:CD1  | 2:N:144:PHE:N    | 2.89                     | 0.41              |
| 2:N:175:TYR:N    | 2:N:176:PRO:HD2  | 2.36                     | 0.41              |
| 2:N:209:PHE:CZ   | 2:N:234:ALA:HB2  | 2.55                     | 0.41              |
| 1:O:17:GLN:HB3   | 1:O:68:LEU:CD2   | 2.41                     | 0.41              |
| 1:O:105:LEU:HD11 | 2:P:183:LEU:HD11 | 2.03                     | 0.41              |
| 1:O:135:ARG:NH2  | 1:O:177:LEU:CD2  | 2.82                     | 0.41              |
| 2:P:60:ARG:HB3   | 2:P:130:ILE:HD13 | 2.02                     | 0.41              |
| 2:P:75:VAL:O     | 2:P:75:VAL:HG13  | 2.21                     | 0.41              |
| 2:P:134:THR:HG22 | 2:P:141:ASP:HA   | 2.02                     | 0.41              |
| 2:P:223:VAL:HA   | 2:P:255:ASN:O    | 2.21                     | 0.41              |
| 2:B:96:ASN:HD22  | 2:B:96:ASN:H     | 1.70                     | 0.40              |
| 2:D:171:THR:C    | 2:D:173:PRO:CD   | 2.91                     | 0.40              |
| 2:D:211:ASN:HD21 | 2:D:269:GLN:N    | 1.96                     | 0.40              |
| 2:H:33:ASN:ND2   | 2:H:110:THR:OG1  | 2.53                     | 0.40              |
| 2:H:96:ASN:HD22  | 2:H:96:ASN:C     | 2.27                     | 0.40              |
| 2:H:131:LEU:C    | 2:H:131:LEU:CD2  | 2.93                     | 0.40              |
| 2:H:183:LEU:HD22 | 2:H:250:LEU:HD11 | 2.03                     | 0.40              |
| 1:I:101:ASN:O    | 2:J:171:THR:N    | 2.54                     | 0.40              |
| 1:K:4:LEU:HB3    | 1:K:6:ALA:O      | 2.21                     | 0.40              |
| 1:K:11:TYR:HB3   | 1:K:115:TYR:HA   | 2.03                     | 0.40              |
| 1:K:101:ASN:HB2  | 2:L:171:THR:C    | 2.46                     | 0.40              |
| 1:K:101:ASN:O    | 2:L:171:THR:N    | 2.54                     | 0.40              |
| 2:L:45:HIS:CD2   | 2:L:98:ARG:O     | 2.74                     | 0.40              |
| 2:L:60:ARG:HG2   | 2:L:61:GLY:N     | 2.22                     | 0.40              |
| 2:L:67:VAL:HA    | 2:L:71:PHE:HD1   | 1.85                     | 0.40              |
| 2:L:228:ASN:O    | 2:L:228:ASN:ND2  | 2.54                     | 0.40              |
| 1:M:57:MET:HE3   | 1:M:61:LYS:O     | 2.21                     | 0.40              |
| 2:N:36:VAL:O     | 2:N:36:VAL:HG12  | 2.20                     | 0.40              |
| 2:N:136:ASN:HD22 | 2:N:136:ASN:N    | 2.18                     | 0.40              |
| 2:P:67:VAL:HA    | 2:P:71:PHE:HD1   | 1.87                     | 0.40              |
| 2:P:77:TYR:HD1   | 2:P:105:VAL:HG22 | 1.86                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:125:ASP:OD1  | 1:A:125:ASP:N    | 2.53                     | 0.40              |
| 1:A:185:ILE:CB   | 1:A:202:GLY:HA3  | 2.49                     | 0.40              |
| 2:B:174:ASP:O    | 2:B:175:TYR:C    | 2.65                     | 0.40              |
| 1:C:9:VAL:CG1    | 1:C:113:LEU:HD13 | 2.51                     | 0.40              |
| 1:C:71:THR:OG1   | 1:C:74:GLN:HB2   | 2.22                     | 0.40              |
| 2:F:39:SER:HB3   | 4:F:512:HOH:O    | 2.21                     | 0.40              |
| 2:F:175:TYR:CD1  | 2:F:175:TYR:C    | 2.97                     | 0.40              |
| 1:G:144:ASN:CG   | 1:G:150:LEU:HG   | 2.47                     | 0.40              |
| 1:G:188:ARG:NH1  | 1:G:188:ARG:HG2  | 2.35                     | 0.40              |
| 2:H:135:ASN:OD1  | 2:H:138:ASN:ND2  | 2.55                     | 0.40              |
| 2:H:201:THR:CG2  | 2:H:202:ALA:N    | 2.82                     | 0.40              |
| 1:I:11:TYR:HB3   | 1:I:115:TYR:HA   | 2.03                     | 0.40              |
| 2:J:209:PHE:CZ   | 2:J:234:ALA:HB2  | 2.55                     | 0.40              |
| 1:K:98:LEU:O     | 1:K:98:LEU:HD22  | 2.20                     | 0.40              |
| 1:K:114:TYR:CE2  | 1:K:149:TYR:HB2  | 2.56                     | 0.40              |
| 1:K:145:PRO:HG2  | 1:K:146:THR:H    | 1.86                     | 0.40              |
| 2:L:49:PRO:HD2   | 2:L:98:ARG:CZ    | 2.50                     | 0.40              |
| 2:L:136:ASN:HD22 | 2:L:136:ASN:N    | 2.18                     | 0.40              |
| 1:M:21:ALA:HA    | 1:M:64:THR:CA    | 2.40                     | 0.40              |
| 1:M:77:GLN:HE21  | 1:M:77:GLN:CA    | 2.26                     | 0.40              |
| 2:N:181:ILE:HA   | 2:N:182:PRO:HD3  | 1.81                     | 0.40              |
| 1:O:101:ASN:HB2  | 2:P:171:THR:C    | 2.46                     | 0.40              |
| 1:O:116:ARG:HA   | 1:O:117:PRO:HD3  | 1.88                     | 0.40              |
| 1:O:145:PRO:HG2  | 1:O:146:THR:H    | 1.85                     | 0.40              |
| 2:P:35:VAL:HG22  | 2:P:108:TYR:CD2  | 2.56                     | 0.40              |
| 2:P:49:PRO:HG2   | 2:P:50:GLU:CD    | 2.46                     | 0.40              |
| 2:D:77:TYR:N     | 2:D:80:SER:O     | 2.54                     | 0.40              |
| 2:D:135:ASN:OD1  | 2:D:138:ASN:ND2  | 2.54                     | 0.40              |
| 1:E:86:ASN:HD21  | 1:E:110:ARG:HH21 | 1.70                     | 0.40              |
| 2:F:3:CYS:HA     | 2:F:43:PHE:O     | 2.21                     | 0.40              |
| 2:H:116:GLY:HA2  | 2:H:189:LYS:NZ   | 2.36                     | 0.40              |
| 2:H:209:PHE:CG   | 2:H:272:ILE:CD1  | 3.04                     | 0.40              |
| 1:I:118:ALA:O    | 1:I:119:LYS:HB2  | 2.21                     | 0.40              |
| 2:J:24:LEU:O     | 2:J:26:PRO:HD3   | 2.21                     | 0.40              |
| 2:J:138:ASN:ND2  | 2:J:140:ASP:HB2  | 2.37                     | 0.40              |
| 1:K:189:THR:O    | 1:K:197:THR:N    | 2.54                     | 0.40              |
| 2:L:24:LEU:O     | 2:L:26:PRO:HD3   | 2.21                     | 0.40              |
| 1:M:24:ASN:HD21  | 1:M:26:ASP:HB2   | 1.85                     | 0.40              |
| 2:N:75:VAL:HG23  | 2:N:107:LEU:CD1  | 2.51                     | 0.40              |
| 2:N:103:TRP:CH2  | 2:N:131:LEU:HB2  | 2.56                     | 0.40              |
| 1:O:10:ILE:HG13  | 1:O:192:ASP:CG   | 2.46                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:O:118:ALA:O   | 1:O:119:LYS:HB2  | 2.21                     | 0.40              |
| 2:P:64:TYR:O    | 2:P:65:GLY:C     | 2.65                     | 0.40              |
| 2:P:98:ARG:HH11 | 2:P:98:ARG:CG    | 2.33                     | 0.40              |
| 2:B:131:LEU:C   | 2:B:131:LEU:CD2  | 2.94                     | 0.40              |
| 1:C:86:ASN:HD21 | 1:C:110:ARG:NE   | 2.12                     | 0.40              |
| 1:E:43:VAL:O    | 1:E:43:VAL:HG23  | 2.21                     | 0.40              |
| 1:E:161:VAL:O   | 1:E:162:LEU:CG   | 2.68                     | 0.40              |
| 2:F:14:GLY:HA2  | 2:F:142:PHE:CD1  | 2.56                     | 0.40              |
| 1:I:13:ALA:HB3  | 1:I:118:ALA:HB3  | 2.04                     | 0.40              |
| 2:J:19:ASN:CG   | 2:L:219:GLN:HE22 | 2.30                     | 0.40              |
| 2:J:60:ARG:HB3  | 2:J:130:ILE:HD13 | 2.03                     | 0.40              |
| 2:J:77:TYR:HD1  | 2:J:105:VAL:HG22 | 1.86                     | 0.40              |
| 2:J:227:ARG:O   | 2:J:229:GLY:N    | 2.53                     | 0.40              |
| 1:K:144:ASN:HB3 | 1:K:167:VAL:CG1  | 2.47                     | 0.40              |
| 2:L:55:TYR:CG   | 2:L:92:ARG:HD2   | 2.57                     | 0.40              |
| 2:L:75:VAL:HG23 | 2:L:107:LEU:CD1  | 2.51                     | 0.40              |
| 2:L:123:GLY:N   | 2:L:150:ALA:O    | 2.54                     | 0.40              |
| 2:L:144:PHE:CD1 | 2:L:144:PHE:N    | 2.89                     | 0.40              |
| 1:M:135:ARG:NH2 | 1:M:177:LEU:CD2  | 2.82                     | 0.40              |
| 1:O:8:ARG:HG3   | 1:O:192:ASP:O    | 2.22                     | 0.40              |
| 1:O:49:ILE:HB   | 1:O:68:LEU:HB2   | 2.03                     | 0.40              |
| 2:P:24:LEU:O    | 2:P:26:PRO:HD3   | 2.21                     | 0.40              |
| 2:P:42:ILE:HG21 | 2:P:146:TRP:CZ2  | 2.57                     | 0.40              |
| 2:P:103:TRP:CH2 | 2:P:131:LEU:HB2  | 2.56                     | 0.40              |
| 2:P:113:SER:O   | 2:P:115:ALA:N    | 2.47                     | 0.40              |
| 1:A:133:PHE:HD2 | 1:A:140:LEU:CD2  | 2.35                     | 0.40              |
| 2:H:172:LEU:N   | 2:H:173:PRO:CD   | 2.83                     | 0.40              |
| 2:J:166:ARG:HG2 | 2:J:182:PRO:CB   | 2.47                     | 0.40              |
| 1:K:13:ALA:HB3  | 1:K:118:ALA:HB3  | 2.04                     | 0.40              |
| 1:K:193:TYR:HB3 | 2:L:155:VAL:HG11 | 2.03                     | 0.40              |
| 2:L:29:ASN:OD1  | 2:L:157:PRO:HB2  | 2.21                     | 0.40              |
| 2:L:41:GLN:HE21 | 2:L:41:GLN:CA    | 2.34                     | 0.40              |
| 2:L:60:ARG:HB3  | 2:L:130:ILE:HD13 | 2.04                     | 0.40              |
| 1:M:35:SER:CB   | 1:M:50:VAL:HG11  | 2.52                     | 0.40              |
| 2:N:29:ASN:OD1  | 2:N:157:PRO:HB2  | 2.20                     | 0.40              |
| 2:N:68:LEU:HG   | 2:N:68:LEU:O     | 2.22                     | 0.40              |
| 2:N:223:VAL:HA  | 2:N:255:ASN:O    | 2.21                     | 0.40              |
| 2:P:136:ASN:ND2 | 2:P:136:ASN:C    | 2.79                     | 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 203/205 (99%)   | 164 (81%)  | 27 (13%)  | 12 (6%)  | 1           | 7  |
| 1   | C     | 203/205 (99%)   | 163 (80%)  | 28 (14%)  | 12 (6%)  | 1           | 7  |
| 1   | E     | 203/205 (99%)   | 163 (80%)  | 29 (14%)  | 11 (5%)  | 1           | 9  |
| 1   | G     | 203/205 (99%)   | 164 (81%)  | 28 (14%)  | 11 (5%)  | 1           | 9  |
| 1   | I     | 203/205 (99%)   | 138 (68%)  | 47 (23%)  | 18 (9%)  | 0           | 3  |
| 1   | K     | 203/205 (99%)   | 138 (68%)  | 47 (23%)  | 18 (9%)  | 0           | 3  |
| 1   | M     | 203/205 (99%)   | 138 (68%)  | 47 (23%)  | 18 (9%)  | 0           | 3  |
| 1   | O     | 203/205 (99%)   | 138 (68%)  | 47 (23%)  | 18 (9%)  | 0           | 3  |
| 2   | B     | 277/279 (99%)   | 248 (90%)  | 18 (6%)   | 11 (4%)  | 2           | 14 |
| 2   | D     | 277/279 (99%)   | 248 (90%)  | 18 (6%)   | 11 (4%)  | 2           | 14 |
| 2   | F     | 277/279 (99%)   | 248 (90%)  | 18 (6%)   | 11 (4%)  | 2           | 14 |
| 2   | H     | 277/279 (99%)   | 249 (90%)  | 18 (6%)   | 10 (4%)  | 2           | 16 |
| 2   | J     | 277/279 (99%)   | 203 (73%)  | 57 (21%)  | 17 (6%)  | 1           | 7  |
| 2   | L     | 277/279 (99%)   | 204 (74%)  | 56 (20%)  | 17 (6%)  | 1           | 7  |
| 2   | N     | 277/279 (99%)   | 204 (74%)  | 56 (20%)  | 17 (6%)  | 1           | 7  |
| 2   | P     | 277/279 (99%)   | 203 (73%)  | 57 (21%)  | 17 (6%)  | 1           | 7  |
| All | All   | 3840/3872 (99%) | 3013 (78%) | 598 (16%) | 229 (6%) | 1           | 7  |

All (229) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | SER  |
| 1   | A     | 72  | ASN  |
| 1   | A     | 159 | THR  |
| 1   | A     | 179 | SER  |
| 1   | A     | 180 | ASP  |
| 1   | A     | 183 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 168 | VAL  |
| 2   | B     | 175 | TYR  |
| 2   | B     | 218 | ALA  |
| 1   | C     | 29  | SER  |
| 1   | C     | 72  | ASN  |
| 1   | C     | 159 | THR  |
| 1   | C     | 179 | SER  |
| 1   | C     | 180 | ASP  |
| 1   | C     | 183 | SER  |
| 2   | D     | 168 | VAL  |
| 2   | D     | 173 | PRO  |
| 2   | D     | 175 | TYR  |
| 2   | D     | 218 | ALA  |
| 1   | E     | 29  | SER  |
| 1   | E     | 72  | ASN  |
| 1   | E     | 159 | THR  |
| 1   | E     | 179 | SER  |
| 1   | E     | 180 | ASP  |
| 1   | E     | 183 | SER  |
| 2   | F     | 168 | VAL  |
| 2   | F     | 173 | PRO  |
| 2   | F     | 175 | TYR  |
| 2   | F     | 218 | ALA  |
| 1   | G     | 29  | SER  |
| 1   | G     | 72  | ASN  |
| 1   | G     | 159 | THR  |
| 1   | G     | 179 | SER  |
| 1   | G     | 180 | ASP  |
| 1   | G     | 183 | SER  |
| 2   | H     | 168 | VAL  |
| 2   | H     | 173 | PRO  |
| 2   | H     | 175 | TYR  |
| 2   | H     | 218 | ALA  |
| 1   | I     | 45  | ASP  |
| 1   | I     | 96  | SER  |
| 1   | I     | 119 | LYS  |
| 2   | J     | 174 | ASP  |
| 2   | J     | 210 | THR  |
| 1   | K     | 45  | ASP  |
| 1   | K     | 96  | SER  |
| 1   | K     | 119 | LYS  |
| 2   | L     | 174 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 210 | THR  |
| 1   | M     | 96  | SER  |
| 1   | M     | 119 | LYS  |
| 2   | N     | 174 | ASP  |
| 2   | N     | 210 | THR  |
| 2   | N     | 225 | LEU  |
| 1   | O     | 96  | SER  |
| 1   | O     | 119 | LYS  |
| 2   | P     | 174 | ASP  |
| 2   | P     | 210 | THR  |
| 2   | P     | 225 | LEU  |
| 2   | B     | 116 | GLY  |
| 2   | B     | 167 | ASP  |
| 2   | B     | 173 | PRO  |
| 2   | B     | 177 | GLY  |
| 2   | B     | 262 | GLN  |
| 1   | C     | 47  | ARG  |
| 2   | D     | 116 | GLY  |
| 2   | D     | 167 | ASP  |
| 2   | D     | 177 | GLY  |
| 2   | D     | 262 | GLN  |
| 1   | E     | 192 | ASP  |
| 2   | F     | 116 | GLY  |
| 2   | F     | 167 | ASP  |
| 2   | F     | 177 | GLY  |
| 2   | F     | 262 | GLN  |
| 1   | G     | 47  | ARG  |
| 2   | H     | 116 | GLY  |
| 2   | H     | 167 | ASP  |
| 2   | H     | 177 | GLY  |
| 2   | H     | 262 | GLN  |
| 1   | I     | 64  | THR  |
| 1   | I     | 94  | ASP  |
| 1   | I     | 137 | ALA  |
| 1   | I     | 203 | VAL  |
| 2   | J     | 40  | THR  |
| 2   | J     | 91  | PRO  |
| 2   | J     | 167 | ASP  |
| 2   | J     | 198 | SER  |
| 2   | J     | 217 | PRO  |
| 2   | J     | 225 | LEU  |
| 2   | J     | 247 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 251 | GLY  |
| 1   | K     | 64  | THR  |
| 1   | K     | 94  | ASP  |
| 1   | K     | 137 | ALA  |
| 1   | K     | 203 | VAL  |
| 2   | L     | 40  | THR  |
| 2   | L     | 91  | PRO  |
| 2   | L     | 167 | ASP  |
| 2   | L     | 217 | PRO  |
| 2   | L     | 225 | LEU  |
| 2   | L     | 247 | ALA  |
| 2   | L     | 251 | GLY  |
| 1   | M     | 45  | ASP  |
| 1   | M     | 64  | THR  |
| 1   | M     | 94  | ASP  |
| 1   | M     | 137 | ALA  |
| 1   | M     | 203 | VAL  |
| 2   | N     | 40  | THR  |
| 2   | N     | 91  | PRO  |
| 2   | N     | 167 | ASP  |
| 2   | N     | 198 | SER  |
| 2   | N     | 217 | PRO  |
| 2   | N     | 247 | ALA  |
| 2   | N     | 251 | GLY  |
| 1   | O     | 45  | ASP  |
| 1   | O     | 64  | THR  |
| 1   | O     | 94  | ASP  |
| 1   | O     | 137 | ALA  |
| 1   | O     | 203 | VAL  |
| 2   | P     | 40  | THR  |
| 2   | P     | 91  | PRO  |
| 2   | P     | 167 | ASP  |
| 2   | P     | 217 | PRO  |
| 2   | P     | 247 | ALA  |
| 2   | P     | 251 | GLY  |
| 1   | A     | 27  | GLU  |
| 1   | A     | 47  | ARG  |
| 1   | A     | 192 | ASP  |
| 2   | B     | 174 | ASP  |
| 1   | C     | 27  | GLU  |
| 1   | C     | 192 | ASP  |
| 2   | D     | 174 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 27  | GLU  |
| 1   | E     | 47  | ARG  |
| 2   | F     | 174 | ASP  |
| 1   | G     | 27  | GLU  |
| 1   | G     | 192 | ASP  |
| 2   | H     | 174 | ASP  |
| 1   | I     | 71  | THR  |
| 1   | I     | 155 | LEU  |
| 1   | I     | 183 | SER  |
| 1   | I     | 184 | ASN  |
| 1   | I     | 204 | MET  |
| 2   | J     | 104 | PRO  |
| 2   | J     | 117 | GLY  |
| 2   | J     | 229 | GLY  |
| 2   | J     | 260 | GLY  |
| 1   | K     | 71  | THR  |
| 1   | K     | 155 | LEU  |
| 1   | K     | 183 | SER  |
| 1   | K     | 184 | ASN  |
| 1   | K     | 204 | MET  |
| 2   | L     | 104 | PRO  |
| 2   | L     | 117 | GLY  |
| 2   | L     | 198 | SER  |
| 2   | L     | 229 | GLY  |
| 2   | L     | 260 | GLY  |
| 1   | M     | 71  | THR  |
| 1   | M     | 155 | LEU  |
| 1   | M     | 183 | SER  |
| 1   | M     | 184 | ASN  |
| 1   | M     | 204 | MET  |
| 2   | N     | 104 | PRO  |
| 2   | N     | 117 | GLY  |
| 2   | N     | 229 | GLY  |
| 2   | N     | 260 | GLY  |
| 1   | O     | 71  | THR  |
| 1   | O     | 155 | LEU  |
| 1   | O     | 183 | SER  |
| 1   | O     | 184 | ASN  |
| 1   | O     | 204 | MET  |
| 2   | P     | 104 | PRO  |
| 2   | P     | 117 | GLY  |
| 2   | P     | 198 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 229 | GLY  |
| 2   | P     | 260 | GLY  |
| 1   | A     | 121 | ALA  |
| 1   | A     | 164 | ASN  |
| 1   | C     | 121 | ALA  |
| 1   | E     | 121 | ALA  |
| 1   | G     | 121 | ALA  |
| 1   | I     | 32  | LEU  |
| 1   | I     | 46  | GLY  |
| 1   | I     | 178 | PRO  |
| 1   | I     | 200 | MET  |
| 2   | J     | 65  | GLY  |
| 1   | K     | 32  | LEU  |
| 1   | K     | 46  | GLY  |
| 1   | K     | 178 | PRO  |
| 1   | K     | 200 | MET  |
| 2   | L     | 65  | GLY  |
| 1   | M     | 32  | LEU  |
| 1   | M     | 46  | GLY  |
| 1   | M     | 178 | PRO  |
| 1   | M     | 200 | MET  |
| 2   | N     | 65  | GLY  |
| 1   | O     | 46  | GLY  |
| 1   | O     | 178 | PRO  |
| 1   | O     | 200 | MET  |
| 2   | P     | 65  | GLY  |
| 2   | B     | 265 | ALA  |
| 1   | C     | 164 | ASN  |
| 2   | D     | 265 | ALA  |
| 1   | E     | 164 | ASN  |
| 2   | F     | 265 | ALA  |
| 1   | G     | 164 | ASN  |
| 1   | I     | 29  | SER  |
| 1   | I     | 145 | PRO  |
| 1   | K     | 29  | SER  |
| 1   | K     | 145 | PRO  |
| 1   | M     | 29  | SER  |
| 1   | M     | 145 | PRO  |
| 1   | O     | 29  | SER  |
| 1   | O     | 32  | LEU  |
| 1   | O     | 145 | PRO  |
| 2   | F     | 104 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 35  | VAL  |
| 2   | L     | 35  | VAL  |
| 2   | N     | 35  | VAL  |
| 2   | P     | 35  | VAL  |
| 2   | B     | 104 | PRO  |
| 2   | D     | 104 | PRO  |
| 2   | H     | 104 | PRO  |
| 2   | J     | 157 | PRO  |
| 2   | L     | 157 | PRO  |
| 2   | N     | 157 | PRO  |
| 2   | P     | 157 | PRO  |
| 1   | C     | 143 | ILE  |
| 1   | A     | 143 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 176/176 (100%) | 158 (90%) | 18 (10%) | 7           | 29 |
| 1   | C     | 176/176 (100%) | 160 (91%) | 16 (9%)  | 9           | 33 |
| 1   | E     | 176/176 (100%) | 159 (90%) | 17 (10%) | 8           | 30 |
| 1   | G     | 176/176 (100%) | 159 (90%) | 17 (10%) | 8           | 30 |
| 1   | I     | 176/176 (100%) | 163 (93%) | 13 (7%)  | 13          | 42 |
| 1   | K     | 176/176 (100%) | 163 (93%) | 13 (7%)  | 13          | 42 |
| 1   | M     | 176/176 (100%) | 163 (93%) | 13 (7%)  | 13          | 42 |
| 1   | O     | 176/176 (100%) | 163 (93%) | 13 (7%)  | 13          | 42 |
| 2   | B     | 226/226 (100%) | 205 (91%) | 21 (9%)  | 8           | 32 |
| 2   | D     | 226/226 (100%) | 206 (91%) | 20 (9%)  | 9           | 35 |
| 2   | F     | 226/226 (100%) | 206 (91%) | 20 (9%)  | 9           | 35 |
| 2   | H     | 226/226 (100%) | 206 (91%) | 20 (9%)  | 9           | 35 |
| 2   | J     | 226/226 (100%) | 214 (95%) | 12 (5%)  | 20          | 54 |
| 2   | L     | 226/226 (100%) | 214 (95%) | 12 (5%)  | 20          | 54 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 2   | N     | 226/226 (100%)   | 214 (95%)  | 12 (5%)  | 20          | 54 |
| 2   | P     | 226/226 (100%)   | 214 (95%)  | 12 (5%)  | 20          | 54 |
| All | All   | 3216/3216 (100%) | 2967 (92%) | 249 (8%) | 12          | 40 |

All (249) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | ARG  |
| 1   | A     | 23  | THR  |
| 1   | A     | 28  | ASN  |
| 1   | A     | 35  | SER  |
| 1   | A     | 43  | VAL  |
| 1   | A     | 62  | GLU  |
| 1   | A     | 66  | ARG  |
| 1   | A     | 93  | MET  |
| 1   | A     | 98  | LEU  |
| 1   | A     | 104 | GLN  |
| 1   | A     | 122 | LEU  |
| 1   | A     | 135 | ARG  |
| 1   | A     | 140 | LEU  |
| 1   | A     | 142 | LEU  |
| 1   | A     | 176 | LYS  |
| 1   | A     | 180 | ASP  |
| 1   | A     | 186 | THR  |
| 1   | A     | 196 | LEU  |
| 2   | B     | 4   | LYS  |
| 2   | B     | 5   | THR  |
| 2   | B     | 13  | ILE  |
| 2   | B     | 33  | ASN  |
| 2   | B     | 36  | VAL  |
| 2   | B     | 59  | GLN  |
| 2   | B     | 85  | PRO  |
| 2   | B     | 87  | THR  |
| 2   | B     | 96  | ASN  |
| 2   | B     | 104 | PRO  |
| 2   | B     | 107 | LEU  |
| 2   | B     | 121 | LYS  |
| 2   | B     | 133 | ASN  |
| 2   | B     | 136 | ASN  |
| 2   | B     | 138 | ASN  |
| 2   | B     | 155 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 158 | THR  |
| 2   | B     | 170 | VAL  |
| 2   | B     | 201 | THR  |
| 2   | B     | 255 | ASN  |
| 2   | B     | 267 | ASN  |
| 1   | C     | 8   | ARG  |
| 1   | C     | 23  | THR  |
| 1   | C     | 28  | ASN  |
| 1   | C     | 35  | SER  |
| 1   | C     | 43  | VAL  |
| 1   | C     | 62  | GLU  |
| 1   | C     | 93  | MET  |
| 1   | C     | 98  | LEU  |
| 1   | C     | 104 | GLN  |
| 1   | C     | 122 | LEU  |
| 1   | C     | 135 | ARG  |
| 1   | C     | 142 | LEU  |
| 1   | C     | 176 | LYS  |
| 1   | C     | 180 | ASP  |
| 1   | C     | 186 | THR  |
| 1   | C     | 196 | LEU  |
| 2   | D     | 4   | LYS  |
| 2   | D     | 5   | THR  |
| 2   | D     | 13  | ILE  |
| 2   | D     | 33  | ASN  |
| 2   | D     | 36  | VAL  |
| 2   | D     | 59  | GLN  |
| 2   | D     | 85  | PRO  |
| 2   | D     | 87  | THR  |
| 2   | D     | 96  | ASN  |
| 2   | D     | 107 | LEU  |
| 2   | D     | 121 | LYS  |
| 2   | D     | 133 | ASN  |
| 2   | D     | 136 | ASN  |
| 2   | D     | 138 | ASN  |
| 2   | D     | 155 | VAL  |
| 2   | D     | 158 | THR  |
| 2   | D     | 170 | VAL  |
| 2   | D     | 201 | THR  |
| 2   | D     | 255 | ASN  |
| 2   | D     | 267 | ASN  |
| 1   | E     | 8   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 23  | THR  |
| 1   | E     | 28  | ASN  |
| 1   | E     | 35  | SER  |
| 1   | E     | 43  | VAL  |
| 1   | E     | 62  | GLU  |
| 1   | E     | 93  | MET  |
| 1   | E     | 98  | LEU  |
| 1   | E     | 104 | GLN  |
| 1   | E     | 122 | LEU  |
| 1   | E     | 135 | ARG  |
| 1   | E     | 140 | LEU  |
| 1   | E     | 142 | LEU  |
| 1   | E     | 176 | LYS  |
| 1   | E     | 180 | ASP  |
| 1   | E     | 186 | THR  |
| 1   | E     | 196 | LEU  |
| 2   | F     | 4   | LYS  |
| 2   | F     | 5   | THR  |
| 2   | F     | 13  | ILE  |
| 2   | F     | 33  | ASN  |
| 2   | F     | 36  | VAL  |
| 2   | F     | 59  | GLN  |
| 2   | F     | 85  | PRO  |
| 2   | F     | 87  | THR  |
| 2   | F     | 96  | ASN  |
| 2   | F     | 107 | LEU  |
| 2   | F     | 121 | LYS  |
| 2   | F     | 133 | ASN  |
| 2   | F     | 136 | ASN  |
| 2   | F     | 138 | ASN  |
| 2   | F     | 155 | VAL  |
| 2   | F     | 158 | THR  |
| 2   | F     | 170 | VAL  |
| 2   | F     | 201 | THR  |
| 2   | F     | 255 | ASN  |
| 2   | F     | 267 | ASN  |
| 1   | G     | 8   | ARG  |
| 1   | G     | 23  | THR  |
| 1   | G     | 28  | ASN  |
| 1   | G     | 35  | SER  |
| 1   | G     | 43  | VAL  |
| 1   | G     | 62  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 66  | ARG  |
| 1   | G     | 93  | MET  |
| 1   | G     | 98  | LEU  |
| 1   | G     | 104 | GLN  |
| 1   | G     | 122 | LEU  |
| 1   | G     | 135 | ARG  |
| 1   | G     | 142 | LEU  |
| 1   | G     | 176 | LYS  |
| 1   | G     | 180 | ASP  |
| 1   | G     | 186 | THR  |
| 1   | G     | 196 | LEU  |
| 2   | H     | 4   | LYS  |
| 2   | H     | 5   | THR  |
| 2   | H     | 13  | ILE  |
| 2   | H     | 33  | ASN  |
| 2   | H     | 36  | VAL  |
| 2   | H     | 59  | GLN  |
| 2   | H     | 85  | PRO  |
| 2   | H     | 87  | THR  |
| 2   | H     | 96  | ASN  |
| 2   | H     | 107 | LEU  |
| 2   | H     | 121 | LYS  |
| 2   | H     | 133 | ASN  |
| 2   | H     | 136 | ASN  |
| 2   | H     | 138 | ASN  |
| 2   | H     | 155 | VAL  |
| 2   | H     | 158 | THR  |
| 2   | H     | 170 | VAL  |
| 2   | H     | 201 | THR  |
| 2   | H     | 255 | ASN  |
| 2   | H     | 267 | ASN  |
| 1   | I     | 8   | ARG  |
| 1   | I     | 28  | ASN  |
| 1   | I     | 39  | ASN  |
| 1   | I     | 45  | ASP  |
| 1   | I     | 47  | ARG  |
| 1   | I     | 48  | PHE  |
| 1   | I     | 58  | LYS  |
| 1   | I     | 60  | LYS  |
| 1   | I     | 62  | GLU  |
| 1   | I     | 107 | ILE  |
| 1   | I     | 126 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 135 | ARG  |
| 1   | I     | 176 | LYS  |
| 2   | J     | 4   | LYS  |
| 2   | J     | 28  | VAL  |
| 2   | J     | 54  | ASP  |
| 2   | J     | 59  | GLN  |
| 2   | J     | 96  | ASN  |
| 2   | J     | 107 | LEU  |
| 2   | J     | 133 | ASN  |
| 2   | J     | 136 | ASN  |
| 2   | J     | 138 | ASN  |
| 2   | J     | 157 | PRO  |
| 2   | J     | 187 | CYS  |
| 2   | J     | 210 | THR  |
| 1   | K     | 8   | ARG  |
| 1   | K     | 28  | ASN  |
| 1   | K     | 39  | ASN  |
| 1   | K     | 45  | ASP  |
| 1   | K     | 47  | ARG  |
| 1   | K     | 48  | PHE  |
| 1   | K     | 58  | LYS  |
| 1   | K     | 60  | LYS  |
| 1   | K     | 62  | GLU  |
| 1   | K     | 107 | ILE  |
| 1   | K     | 126 | GLN  |
| 1   | K     | 135 | ARG  |
| 1   | K     | 176 | LYS  |
| 2   | L     | 4   | LYS  |
| 2   | L     | 28  | VAL  |
| 2   | L     | 54  | ASP  |
| 2   | L     | 59  | GLN  |
| 2   | L     | 96  | ASN  |
| 2   | L     | 107 | LEU  |
| 2   | L     | 133 | ASN  |
| 2   | L     | 136 | ASN  |
| 2   | L     | 138 | ASN  |
| 2   | L     | 157 | PRO  |
| 2   | L     | 187 | CYS  |
| 2   | L     | 210 | THR  |
| 1   | M     | 8   | ARG  |
| 1   | M     | 28  | ASN  |
| 1   | M     | 39  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 45  | ASP  |
| 1   | M     | 47  | ARG  |
| 1   | M     | 48  | PHE  |
| 1   | M     | 58  | LYS  |
| 1   | M     | 60  | LYS  |
| 1   | M     | 62  | GLU  |
| 1   | M     | 107 | ILE  |
| 1   | M     | 126 | GLN  |
| 1   | M     | 135 | ARG  |
| 1   | M     | 176 | LYS  |
| 2   | N     | 4   | LYS  |
| 2   | N     | 28  | VAL  |
| 2   | N     | 54  | ASP  |
| 2   | N     | 59  | GLN  |
| 2   | N     | 96  | ASN  |
| 2   | N     | 107 | LEU  |
| 2   | N     | 133 | ASN  |
| 2   | N     | 136 | ASN  |
| 2   | N     | 138 | ASN  |
| 2   | N     | 157 | PRO  |
| 2   | N     | 187 | CYS  |
| 2   | N     | 210 | THR  |
| 1   | O     | 8   | ARG  |
| 1   | O     | 28  | ASN  |
| 1   | O     | 39  | ASN  |
| 1   | O     | 45  | ASP  |
| 1   | O     | 47  | ARG  |
| 1   | O     | 48  | PHE  |
| 1   | O     | 58  | LYS  |
| 1   | O     | 60  | LYS  |
| 1   | O     | 62  | GLU  |
| 1   | O     | 107 | ILE  |
| 1   | O     | 126 | GLN  |
| 1   | O     | 135 | ARG  |
| 1   | O     | 176 | LYS  |
| 2   | P     | 4   | LYS  |
| 2   | P     | 28  | VAL  |
| 2   | P     | 54  | ASP  |
| 2   | P     | 59  | GLN  |
| 2   | P     | 96  | ASN  |
| 2   | P     | 107 | LEU  |
| 2   | P     | 133 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 136 | ASN  |
| 2   | P     | 138 | ASN  |
| 2   | P     | 157 | PRO  |
| 2   | P     | 187 | CYS  |
| 2   | P     | 210 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (215) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 15  | GLN  |
| 1   | A     | 17  | GLN  |
| 1   | A     | 19  | GLN  |
| 1   | A     | 24  | ASN  |
| 1   | A     | 28  | ASN  |
| 1   | A     | 72  | ASN  |
| 1   | A     | 73  | ASN  |
| 1   | A     | 77  | GLN  |
| 1   | A     | 86  | ASN  |
| 1   | A     | 104 | GLN  |
| 2   | B     | 19  | ASN  |
| 2   | B     | 29  | ASN  |
| 2   | B     | 33  | ASN  |
| 2   | B     | 41  | GLN  |
| 2   | B     | 59  | GLN  |
| 2   | B     | 70  | ASN  |
| 2   | B     | 96  | ASN  |
| 2   | B     | 135 | ASN  |
| 2   | B     | 136 | ASN  |
| 2   | B     | 138 | ASN  |
| 2   | B     | 143 | GLN  |
| 2   | B     | 206 | ASN  |
| 2   | B     | 211 | ASN  |
| 2   | B     | 219 | GLN  |
| 2   | B     | 255 | ASN  |
| 2   | B     | 262 | GLN  |
| 2   | B     | 267 | ASN  |
| 2   | B     | 279 | GLN  |
| 1   | C     | 15  | GLN  |
| 1   | C     | 17  | GLN  |
| 1   | C     | 19  | GLN  |
| 1   | C     | 24  | ASN  |
| 1   | C     | 28  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 72  | ASN  |
| 1   | C     | 73  | ASN  |
| 1   | C     | 77  | GLN  |
| 1   | C     | 86  | ASN  |
| 1   | C     | 104 | GLN  |
| 2   | D     | 7   | ASN  |
| 2   | D     | 33  | ASN  |
| 2   | D     | 70  | ASN  |
| 2   | D     | 96  | ASN  |
| 2   | D     | 135 | ASN  |
| 2   | D     | 136 | ASN  |
| 2   | D     | 138 | ASN  |
| 2   | D     | 143 | GLN  |
| 2   | D     | 206 | ASN  |
| 2   | D     | 211 | ASN  |
| 2   | D     | 219 | GLN  |
| 2   | D     | 235 | ASN  |
| 2   | D     | 255 | ASN  |
| 2   | D     | 262 | GLN  |
| 2   | D     | 267 | ASN  |
| 2   | D     | 279 | GLN  |
| 1   | E     | 15  | GLN  |
| 1   | E     | 17  | GLN  |
| 1   | E     | 19  | GLN  |
| 1   | E     | 24  | ASN  |
| 1   | E     | 28  | ASN  |
| 1   | E     | 72  | ASN  |
| 1   | E     | 73  | ASN  |
| 1   | E     | 74  | GLN  |
| 1   | E     | 77  | GLN  |
| 1   | E     | 86  | ASN  |
| 1   | E     | 104 | GLN  |
| 2   | F     | 19  | ASN  |
| 2   | F     | 29  | ASN  |
| 2   | F     | 33  | ASN  |
| 2   | F     | 59  | GLN  |
| 2   | F     | 70  | ASN  |
| 2   | F     | 96  | ASN  |
| 2   | F     | 135 | ASN  |
| 2   | F     | 136 | ASN  |
| 2   | F     | 138 | ASN  |
| 2   | F     | 143 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 206 | ASN  |
| 2   | F     | 211 | ASN  |
| 2   | F     | 219 | GLN  |
| 2   | F     | 235 | ASN  |
| 2   | F     | 255 | ASN  |
| 2   | F     | 262 | GLN  |
| 2   | F     | 267 | ASN  |
| 2   | F     | 279 | GLN  |
| 1   | G     | 15  | GLN  |
| 1   | G     | 17  | GLN  |
| 1   | G     | 19  | GLN  |
| 1   | G     | 24  | ASN  |
| 1   | G     | 28  | ASN  |
| 1   | G     | 72  | ASN  |
| 1   | G     | 73  | ASN  |
| 1   | G     | 77  | GLN  |
| 1   | G     | 86  | ASN  |
| 1   | G     | 104 | GLN  |
| 2   | H     | 19  | ASN  |
| 2   | H     | 29  | ASN  |
| 2   | H     | 33  | ASN  |
| 2   | H     | 70  | ASN  |
| 2   | H     | 96  | ASN  |
| 2   | H     | 135 | ASN  |
| 2   | H     | 136 | ASN  |
| 2   | H     | 138 | ASN  |
| 2   | H     | 143 | GLN  |
| 2   | H     | 206 | ASN  |
| 2   | H     | 211 | ASN  |
| 2   | H     | 219 | GLN  |
| 2   | H     | 255 | ASN  |
| 2   | H     | 262 | GLN  |
| 2   | H     | 267 | ASN  |
| 2   | H     | 279 | GLN  |
| 1   | I     | 17  | GLN  |
| 1   | I     | 19  | GLN  |
| 1   | I     | 24  | ASN  |
| 1   | I     | 28  | ASN  |
| 1   | I     | 72  | ASN  |
| 1   | I     | 74  | GLN  |
| 1   | I     | 104 | GLN  |
| 1   | I     | 126 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 144 | ASN  |
| 1   | I     | 184 | ASN  |
| 2   | J     | 33  | ASN  |
| 2   | J     | 41  | GLN  |
| 2   | J     | 45  | HIS  |
| 2   | J     | 136 | ASN  |
| 2   | J     | 138 | ASN  |
| 2   | J     | 143 | GLN  |
| 2   | J     | 151 | ASN  |
| 2   | J     | 206 | ASN  |
| 2   | J     | 211 | ASN  |
| 2   | J     | 219 | GLN  |
| 2   | J     | 224 | GLN  |
| 2   | J     | 228 | ASN  |
| 2   | J     | 235 | ASN  |
| 2   | J     | 255 | ASN  |
| 2   | J     | 269 | GLN  |
| 2   | J     | 279 | GLN  |
| 1   | K     | 17  | GLN  |
| 1   | K     | 19  | GLN  |
| 1   | K     | 24  | ASN  |
| 1   | K     | 28  | ASN  |
| 1   | K     | 72  | ASN  |
| 1   | K     | 74  | GLN  |
| 1   | K     | 104 | GLN  |
| 1   | K     | 126 | GLN  |
| 1   | K     | 138 | ASN  |
| 1   | K     | 144 | ASN  |
| 1   | K     | 184 | ASN  |
| 2   | L     | 32  | GLN  |
| 2   | L     | 41  | GLN  |
| 2   | L     | 45  | HIS  |
| 2   | L     | 136 | ASN  |
| 2   | L     | 138 | ASN  |
| 2   | L     | 143 | GLN  |
| 2   | L     | 151 | ASN  |
| 2   | L     | 206 | ASN  |
| 2   | L     | 211 | ASN  |
| 2   | L     | 219 | GLN  |
| 2   | L     | 224 | GLN  |
| 2   | L     | 228 | ASN  |
| 2   | L     | 255 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 269 | GLN  |
| 2   | L     | 279 | GLN  |
| 1   | M     | 17  | GLN  |
| 1   | M     | 19  | GLN  |
| 1   | M     | 24  | ASN  |
| 1   | M     | 28  | ASN  |
| 1   | M     | 72  | ASN  |
| 1   | M     | 74  | GLN  |
| 1   | M     | 104 | GLN  |
| 1   | M     | 126 | GLN  |
| 1   | M     | 144 | ASN  |
| 1   | M     | 184 | ASN  |
| 2   | N     | 41  | GLN  |
| 2   | N     | 45  | HIS  |
| 2   | N     | 136 | ASN  |
| 2   | N     | 138 | ASN  |
| 2   | N     | 143 | GLN  |
| 2   | N     | 151 | ASN  |
| 2   | N     | 192 | ASN  |
| 2   | N     | 206 | ASN  |
| 2   | N     | 211 | ASN  |
| 2   | N     | 219 | GLN  |
| 2   | N     | 224 | GLN  |
| 2   | N     | 228 | ASN  |
| 2   | N     | 235 | ASN  |
| 2   | N     | 255 | ASN  |
| 2   | N     | 269 | GLN  |
| 2   | N     | 279 | GLN  |
| 1   | O     | 17  | GLN  |
| 1   | O     | 19  | GLN  |
| 1   | O     | 24  | ASN  |
| 1   | O     | 28  | ASN  |
| 1   | O     | 72  | ASN  |
| 1   | O     | 74  | GLN  |
| 1   | O     | 104 | GLN  |
| 1   | O     | 126 | GLN  |
| 1   | O     | 138 | ASN  |
| 1   | O     | 144 | ASN  |
| 1   | O     | 184 | ASN  |
| 2   | P     | 41  | GLN  |
| 2   | P     | 45  | HIS  |
| 2   | P     | 46  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 136 | ASN  |
| 2   | P     | 138 | ASN  |
| 2   | P     | 143 | GLN  |
| 2   | P     | 151 | ASN  |
| 2   | P     | 192 | ASN  |
| 2   | P     | 206 | ASN  |
| 2   | P     | 211 | ASN  |
| 2   | P     | 219 | GLN  |
| 2   | P     | 224 | GLN  |
| 2   | P     | 228 | ASN  |
| 2   | P     | 235 | ASN  |
| 2   | P     | 255 | ASN  |
| 2   | P     | 269 | GLN  |
| 2   | P     | 279 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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   | MMA  | B     | 500 | -    | 13,13,13     | 1.56 | 3 (23%)  | 18,18,18    | 0.94 | 0        |
| 3   | MMA  | P     | 607 | -    | 13,13,13     | 1.47 | 2 (15%)  | 18,18,18    | 0.87 | 0        |
| 3   | MMA  | L     | 504 | -    | 13,13,13     | 1.48 | 2 (15%)  | 18,18,18    | 0.85 | 0        |
| 3   | MMA  | F     | 502 | -    | 13,13,13     | 1.50 | 3 (23%)  | 18,18,18    | 0.91 | 0        |
| 3   | MMA  | N     | 506 | -    | 13,13,13     | 1.44 | 2 (15%)  | 18,18,18    | 0.86 | 0        |
| 3   | MMA  | D     | 601 | -    | 13,13,13     | 1.52 | 3 (23%)  | 18,18,18    | 0.91 | 0        |
| 3   | MMA  | H     | 603 | -    | 13,13,13     | 1.62 | 3 (23%)  | 18,18,18    | 0.89 | 0        |
| 3   | MMA  | J     | 605 | -    | 13,13,13     | 1.36 | 2 (15%)  | 18,18,18    | 0.93 | 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   | MMA  | B     | 500 | -    | -       | 2/4/24/24 | 0/1/1/1 |
| 3   | MMA  | P     | 607 | -    | -       | 4/4/24/24 | 0/1/1/1 |
| 3   | MMA  | L     | 504 | -    | -       | 1/4/24/24 | 0/1/1/1 |
| 3   | MMA  | F     | 502 | -    | -       | 2/4/24/24 | 0/1/1/1 |
| 3   | MMA  | N     | 506 | -    | -       | 3/4/24/24 | 0/1/1/1 |
| 3   | MMA  | D     | 601 | -    | -       | 2/4/24/24 | 0/1/1/1 |
| 3   | MMA  | H     | 603 | -    | -       | 2/4/24/24 | 0/1/1/1 |
| 3   | MMA  | J     | 605 | -    | -       | 4/4/24/24 | 0/1/1/1 |

All (20) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | B     | 500 | MMA  | O1-C1 | 4.00 | 1.47        | 1.40     |
| 3   | H     | 603 | MMA  | O1-C1 | 3.97 | 1.46        | 1.40     |
| 3   | D     | 601 | MMA  | O1-C1 | 3.69 | 1.46        | 1.40     |
| 3   | L     | 504 | MMA  | O1-C1 | 3.63 | 1.46        | 1.40     |
| 3   | F     | 502 | MMA  | O1-C1 | 3.51 | 1.46        | 1.40     |
| 3   | N     | 506 | MMA  | O1-C1 | 3.45 | 1.46        | 1.40     |
| 3   | P     | 607 | MMA  | O1-C1 | 3.39 | 1.45        | 1.40     |
| 3   | J     | 605 | MMA  | O1-C1 | 3.22 | 1.45        | 1.40     |
| 3   | H     | 603 | MMA  | O5-C1 | 3.09 | 1.49        | 1.41     |
| 3   | F     | 502 | MMA  | O5-C1 | 2.93 | 1.49        | 1.41     |
| 3   | D     | 601 | MMA  | O5-C1 | 2.86 | 1.49        | 1.41     |
| 3   | B     | 500 | MMA  | O5-C1 | 2.78 | 1.49        | 1.41     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | P     | 607 | MMA  | O5-C1 | 2.78 | 1.49        | 1.41     |
| 3   | N     | 506 | MMA  | O5-C1 | 2.67 | 1.48        | 1.41     |
| 3   | L     | 504 | MMA  | O5-C1 | 2.58 | 1.48        | 1.41     |
| 3   | H     | 603 | MMA  | C1-C2 | 2.43 | 1.59        | 1.52     |
| 3   | D     | 601 | MMA  | C1-C2 | 2.40 | 1.59        | 1.52     |
| 3   | J     | 605 | MMA  | O5-C1 | 2.37 | 1.47        | 1.41     |
| 3   | B     | 500 | MMA  | C1-C2 | 2.35 | 1.59        | 1.52     |
| 3   | F     | 502 | MMA  | C1-C2 | 2.30 | 1.59        | 1.52     |

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | D     | 601 | MMA  | C2-C1-O1-C7 |
| 3   | D     | 601 | MMA  | O5-C1-O1-C7 |
| 3   | F     | 502 | MMA  | C2-C1-O1-C7 |
| 3   | F     | 502 | MMA  | O5-C1-O1-C7 |
| 3   | B     | 500 | MMA  | O5-C1-O1-C7 |
| 3   | H     | 603 | MMA  | O5-C1-O1-C7 |
| 3   | B     | 500 | MMA  | C2-C1-O1-C7 |
| 3   | H     | 603 | MMA  | C2-C1-O1-C7 |
| 3   | J     | 605 | MMA  | O5-C5-C6-O6 |
| 3   | J     | 605 | MMA  | C4-C5-C6-O6 |
| 3   | P     | 607 | MMA  | O5-C1-O1-C7 |
| 3   | P     | 607 | MMA  | C2-C1-O1-C7 |
| 3   | P     | 607 | MMA  | O5-C5-C6-O6 |
| 3   | P     | 607 | MMA  | C4-C5-C6-O6 |
| 3   | J     | 605 | MMA  | O5-C1-O1-C7 |
| 3   | N     | 506 | MMA  | O5-C5-C6-O6 |
| 3   | N     | 506 | MMA  | C4-C5-C6-O6 |
| 3   | J     | 605 | MMA  | C2-C1-O1-C7 |
| 3   | L     | 504 | MMA  | O5-C1-O1-C7 |
| 3   | N     | 506 | MMA  | O5-C1-O1-C7 |

There are no ring outliers.

7 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | B     | 500 | MMA  | 2       | 0            |
| 3   | P     | 607 | MMA  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | L     | 504 | MMA  | 1       | 0            |
| 3   | F     | 502 | MMA  | 2       | 0            |
| 3   | N     | 506 | MMA  | 1       | 0            |
| 3   | H     | 603 | MMA  | 3       | 0            |
| 3   | J     | 605 | MMA  | 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 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2 |     |     | OWAB(Å²)          | Q<0.9 |
|-----|-------|------------------|--------|---------|-----|-----|-------------------|-------|
| 1   | A     | 205/205 (100%)   | -1.48  | 0       | 100 | 100 | 15, 44, 85, 105   | 0     |
| 1   | C     | 205/205 (100%)   | -1.50  | 0       | 100 | 100 | 12, 44, 86, 105   | 0     |
| 1   | E     | 205/205 (100%)   | -1.49  | 0       | 100 | 100 | 16, 43, 87, 103   | 0     |
| 1   | G     | 205/205 (100%)   | -1.51  | 0       | 100 | 100 | 12, 44, 85, 102   | 0     |
| 1   | I     | 205/205 (100%)   | -1.04  | 1 (0%)  | 87  | 72  | 20, 133, 152, 161 | 0     |
| 1   | K     | 205/205 (100%)   | -1.04  | 0       | 100 | 100 | 20, 133, 149, 161 | 0     |
| 1   | M     | 205/205 (100%)   | -1.03  | 0       | 100 | 100 | 20, 133, 149, 159 | 0     |
| 1   | O     | 205/205 (100%)   | -1.02  | 0       | 100 | 100 | 20, 133, 149, 162 | 0     |
| 2   | B     | 279/279 (100%)   | -1.52  | 0       | 100 | 100 | 11, 35, 66, 97    | 0     |
| 2   | D     | 279/279 (100%)   | -1.53  | 0       | 100 | 100 | 11, 35, 70, 97    | 0     |
| 2   | F     | 279/279 (100%)   | -1.53  | 0       | 100 | 100 | 11, 35, 66, 96    | 0     |
| 2   | H     | 279/279 (100%)   | -1.51  | 0       | 100 | 100 | 12, 33, 68, 97    | 0     |
| 2   | J     | 279/279 (100%)   | -1.14  | 0       | 100 | 100 | 52, 98, 154, 164  | 0     |
| 2   | L     | 279/279 (100%)   | -1.16  | 0       | 100 | 100 | 51, 97, 156, 163  | 0     |
| 2   | N     | 279/279 (100%)   | -1.13  | 0       | 100 | 100 | 53, 98, 154, 163  | 0     |
| 2   | P     | 279/279 (100%)   | -1.13  | 0       | 100 | 100 | 52, 100, 154, 160 | 0     |
| All | All   | 3872/3872 (100%) | -1.30  | 1 (0%)  | 100 | 100 | 11, 71, 148, 164  | 0     |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 128 | ALA  | 2.3  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | MMA  | B     | 500 | 13/13 | 0.99 | 0.05 | 36,56,63,64                | 0     |
| 3   | MMA  | D     | 601 | 13/13 | 0.99 | 0.05 | 39,65,67,68                | 0     |
| 3   | MMA  | F     | 502 | 13/13 | 0.99 | 0.04 | 34,54,58,58                | 0     |
| 3   | MMA  | H     | 603 | 13/13 | 0.99 | 0.05 | 32,55,58,59                | 0     |
| 3   | MMA  | J     | 605 | 13/13 | 0.99 | 0.05 | 116,117,120,121            | 0     |
| 3   | MMA  | L     | 504 | 13/13 | 0.99 | 0.04 | 102,108,111,112            | 0     |
| 3   | MMA  | N     | 506 | 13/13 | 0.99 | 0.05 | 93,96,98,100               | 0     |
| 3   | MMA  | P     | 607 | 13/13 | 0.99 | 0.04 | 112,115,117,117            | 0     |

### 6.5 Other polymers [i](#)

There are no such residues in this entry.