



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:51 PM UTC

PDB ID : 4Y7J / pdb\_00004y7j  
Title : Structure of an archaeal mechanosensitive channel in expanded state  
Authors : Li, J.; Liu, Z.  
Deposited on : 2015-02-15  
Resolution : 4.10 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  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

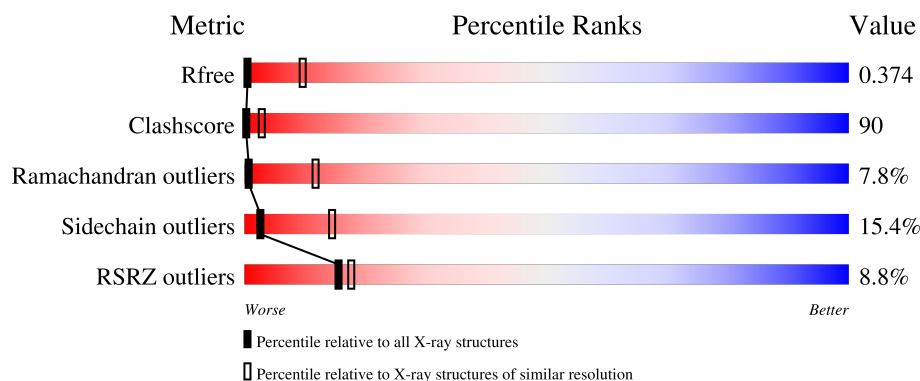
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1243 (4.40-3.80)                                      |
| Clashscore            | 190562                      | 1293 (4.40-3.80)                                      |
| Ramachandran outliers | 187476                      | 1206 (4.40-3.80)                                      |
| Sidechain outliers    | 187428                      | 1193 (4.40-3.80)                                      |
| RSRZ outliers         | 180081                      | 1240 (4.40-3.80)                                      |

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     | 277    | <div> <div>8%</div> <div>20% 47% 17% 13%</div> </div> |
| 1   | B     | 277    | <div> <div>6%</div> <div>16% 47% 18% 17%</div> </div> |
| 1   | C     | 277    | <div> <div>8%</div> <div>13% 49% 19% 16%</div> </div> |
| 1   | D     | 277    | <div> <div>6%</div> <div>17% 49% 17% 15%</div> </div> |
| 1   | E     | 277    | <div> <div>9%</div> <div>21% 45% 15% 17%</div> </div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | BNG  | B     | 301 | -         | -        | X       | -                |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8893 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 Large conductance mechanosensitive channel protein, Riboflavin synthase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 241      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1829  | 1207 | 281 | 329 | 12 |         |         |       |
| 1   | B     | 230      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1757  | 1151 | 275 | 320 | 11 |         |         |       |
| 1   | C     | 234      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1778  | 1171 | 282 | 313 | 12 |         |         |       |
| 1   | D     | 235      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 1789  | 1181 | 274 | 322 | 12 |         |         |       |
| 1   | E     | 231      | Total | C    | N   | O   | S  | 0       | 0       | 1     |
|     |       |          | 1719  | 1133 | 270 | 305 | 11 |         |         |       |

There are 100 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -19     | MET      | -      | expression tag | UNP Q8TNK0 |
| A     | -18     | GLY      | -      | expression tag | UNP Q8TNK0 |
| A     | -17     | SER      | -      | expression tag | UNP Q8TNK0 |
| A     | -16     | SER      | -      | expression tag | UNP Q8TNK0 |
| A     | -15     | HIS      | -      | expression tag | UNP Q8TNK0 |
| A     | -14     | HIS      | -      | expression tag | UNP Q8TNK0 |
| A     | -13     | HIS      | -      | expression tag | UNP Q8TNK0 |
| A     | -12     | HIS      | -      | expression tag | UNP Q8TNK0 |
| A     | -11     | HIS      | -      | expression tag | UNP Q8TNK0 |
| A     | -10     | HIS      | -      | expression tag | UNP Q8TNK0 |
| A     | -9      | SER      | -      | expression tag | UNP Q8TNK0 |
| A     | -8      | SER      | -      | expression tag | UNP Q8TNK0 |
| A     | -7      | GLY      | -      | expression tag | UNP Q8TNK0 |
| A     | -6      | LEU      | -      | expression tag | UNP Q8TNK0 |
| A     | -5      | VAL      | -      | expression tag | UNP Q8TNK0 |
| A     | -4      | PRO      | -      | expression tag | UNP Q8TNK0 |
| A     | -3      | ARG      | -      | expression tag | UNP Q8TNK0 |
| A     | -2      | GLY      | -      | expression tag | UNP Q8TNK0 |

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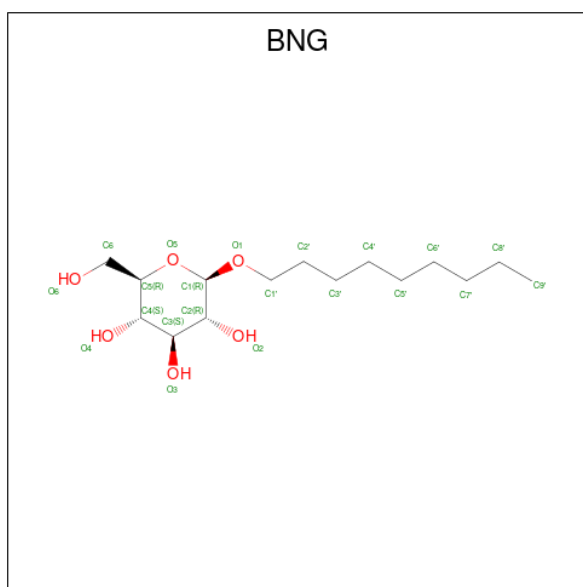
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -1      | SER      | -      | expression tag | UNP Q8TNK0 |
| A     | 0       | HIS      | -      | expression tag | UNP Q8TNK0 |
| B     | -19     | MET      | -      | expression tag | UNP Q8TNK0 |
| B     | -18     | GLY      | -      | expression tag | UNP Q8TNK0 |
| B     | -17     | SER      | -      | expression tag | UNP Q8TNK0 |
| B     | -16     | SER      | -      | expression tag | UNP Q8TNK0 |
| B     | -15     | HIS      | -      | expression tag | UNP Q8TNK0 |
| B     | -14     | HIS      | -      | expression tag | UNP Q8TNK0 |
| B     | -13     | HIS      | -      | expression tag | UNP Q8TNK0 |
| B     | -12     | HIS      | -      | expression tag | UNP Q8TNK0 |
| B     | -11     | HIS      | -      | expression tag | UNP Q8TNK0 |
| B     | -10     | HIS      | -      | expression tag | UNP Q8TNK0 |
| B     | -9      | SER      | -      | expression tag | UNP Q8TNK0 |
| B     | -8      | SER      | -      | expression tag | UNP Q8TNK0 |
| B     | -7      | GLY      | -      | expression tag | UNP Q8TNK0 |
| B     | -6      | LEU      | -      | expression tag | UNP Q8TNK0 |
| B     | -5      | VAL      | -      | expression tag | UNP Q8TNK0 |
| B     | -4      | PRO      | -      | expression tag | UNP Q8TNK0 |
| B     | -3      | ARG      | -      | expression tag | UNP Q8TNK0 |
| B     | -2      | GLY      | -      | expression tag | UNP Q8TNK0 |
| B     | -1      | SER      | -      | expression tag | UNP Q8TNK0 |
| B     | 0       | HIS      | -      | expression tag | UNP Q8TNK0 |
| C     | -19     | MET      | -      | expression tag | UNP Q8TNK0 |
| C     | -18     | GLY      | -      | expression tag | UNP Q8TNK0 |
| C     | -17     | SER      | -      | expression tag | UNP Q8TNK0 |
| C     | -16     | SER      | -      | expression tag | UNP Q8TNK0 |
| C     | -15     | HIS      | -      | expression tag | UNP Q8TNK0 |
| C     | -14     | HIS      | -      | expression tag | UNP Q8TNK0 |
| C     | -13     | HIS      | -      | expression tag | UNP Q8TNK0 |
| C     | -12     | HIS      | -      | expression tag | UNP Q8TNK0 |
| C     | -11     | HIS      | -      | expression tag | UNP Q8TNK0 |
| C     | -10     | HIS      | -      | expression tag | UNP Q8TNK0 |
| C     | -9      | SER      | -      | expression tag | UNP Q8TNK0 |
| C     | -8      | SER      | -      | expression tag | UNP Q8TNK0 |
| C     | -7      | GLY      | -      | expression tag | UNP Q8TNK0 |
| C     | -6      | LEU      | -      | expression tag | UNP Q8TNK0 |
| C     | -5      | VAL      | -      | expression tag | UNP Q8TNK0 |
| C     | -4      | PRO      | -      | expression tag | UNP Q8TNK0 |
| C     | -3      | ARG      | -      | expression tag | UNP Q8TNK0 |
| C     | -2      | GLY      | -      | expression tag | UNP Q8TNK0 |
| C     | -1      | SER      | -      | expression tag | UNP Q8TNK0 |
| C     | 0       | HIS      | -      | expression tag | UNP Q8TNK0 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | -19     | MET      | -      | expression tag | UNP Q8TNK0 |
| D     | -18     | GLY      | -      | expression tag | UNP Q8TNK0 |
| D     | -17     | SER      | -      | expression tag | UNP Q8TNK0 |
| D     | -16     | SER      | -      | expression tag | UNP Q8TNK0 |
| D     | -15     | HIS      | -      | expression tag | UNP Q8TNK0 |
| D     | -14     | HIS      | -      | expression tag | UNP Q8TNK0 |
| D     | -13     | HIS      | -      | expression tag | UNP Q8TNK0 |
| D     | -12     | HIS      | -      | expression tag | UNP Q8TNK0 |
| D     | -11     | HIS      | -      | expression tag | UNP Q8TNK0 |
| D     | -10     | HIS      | -      | expression tag | UNP Q8TNK0 |
| D     | -9      | SER      | -      | expression tag | UNP Q8TNK0 |
| D     | -8      | SER      | -      | expression tag | UNP Q8TNK0 |
| D     | -7      | GLY      | -      | expression tag | UNP Q8TNK0 |
| D     | -6      | LEU      | -      | expression tag | UNP Q8TNK0 |
| D     | -5      | VAL      | -      | expression tag | UNP Q8TNK0 |
| D     | -4      | PRO      | -      | expression tag | UNP Q8TNK0 |
| D     | -3      | ARG      | -      | expression tag | UNP Q8TNK0 |
| D     | -2      | GLY      | -      | expression tag | UNP Q8TNK0 |
| D     | -1      | SER      | -      | expression tag | UNP Q8TNK0 |
| D     | 0       | HIS      | -      | expression tag | UNP Q8TNK0 |
| E     | -19     | MET      | -      | expression tag | UNP Q8TNK0 |
| E     | -18     | GLY      | -      | expression tag | UNP Q8TNK0 |
| E     | -17     | SER      | -      | expression tag | UNP Q8TNK0 |
| E     | -16     | SER      | -      | expression tag | UNP Q8TNK0 |
| E     | -15     | HIS      | -      | expression tag | UNP Q8TNK0 |
| E     | -14     | HIS      | -      | expression tag | UNP Q8TNK0 |
| E     | -13     | HIS      | -      | expression tag | UNP Q8TNK0 |
| E     | -12     | HIS      | -      | expression tag | UNP Q8TNK0 |
| E     | -11     | HIS      | -      | expression tag | UNP Q8TNK0 |
| E     | -10     | HIS      | -      | expression tag | UNP Q8TNK0 |
| E     | -9      | SER      | -      | expression tag | UNP Q8TNK0 |
| E     | -8      | SER      | -      | expression tag | UNP Q8TNK0 |
| E     | -7      | GLY      | -      | expression tag | UNP Q8TNK0 |
| E     | -6      | LEU      | -      | expression tag | UNP Q8TNK0 |
| E     | -5      | VAL      | -      | expression tag | UNP Q8TNK0 |
| E     | -4      | PRO      | -      | expression tag | UNP Q8TNK0 |
| E     | -3      | ARG      | -      | expression tag | UNP Q8TNK0 |
| E     | -2      | GLY      | -      | expression tag | UNP Q8TNK0 |
| E     | -1      | SER      | -      | expression tag | UNP Q8TNK0 |
| E     | 0       | HIS      | -      | expression tag | UNP Q8TNK0 |

- Molecule 2 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: C<sub>15</sub>H<sub>30</sub>O<sub>6</sub>).

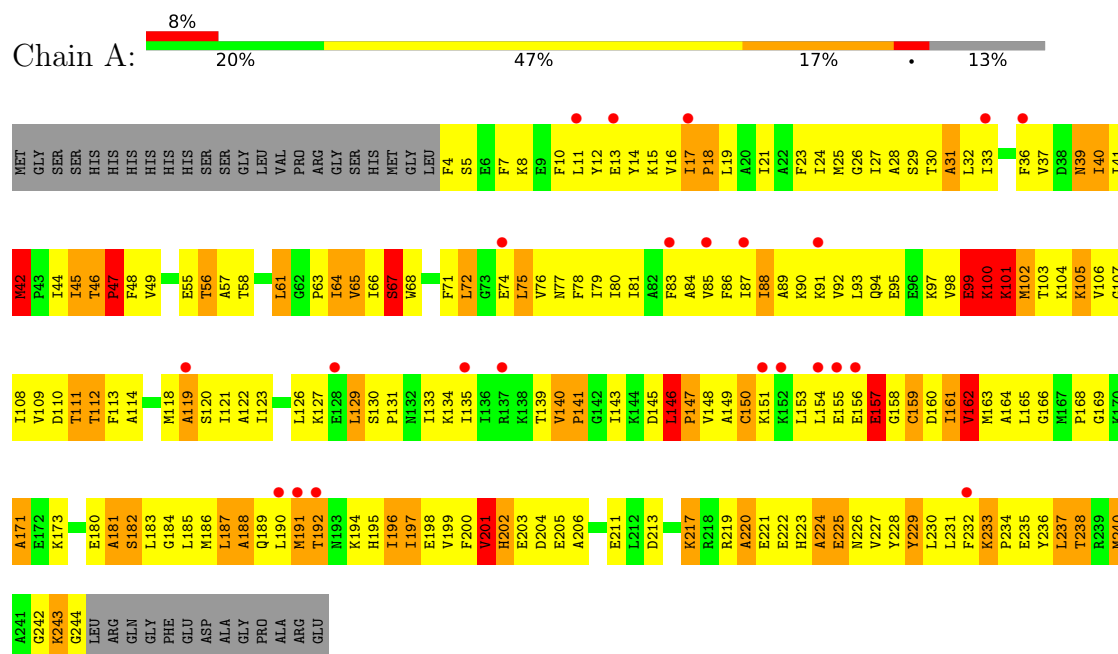


| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 2   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 21    | 15 | 6 |         |         |

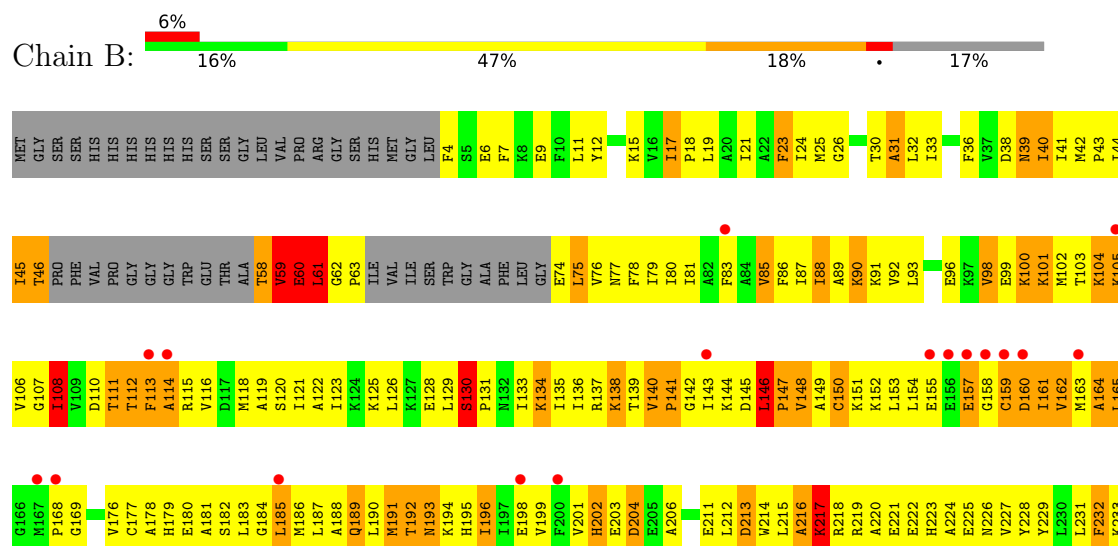
### 3 Residue-property plots

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.

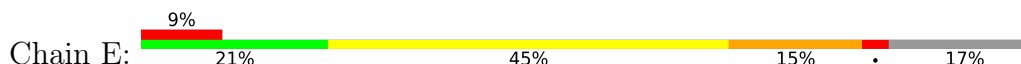
- Molecule 1: Large conductance mechanosensitive channel protein, Riboflavin synthase

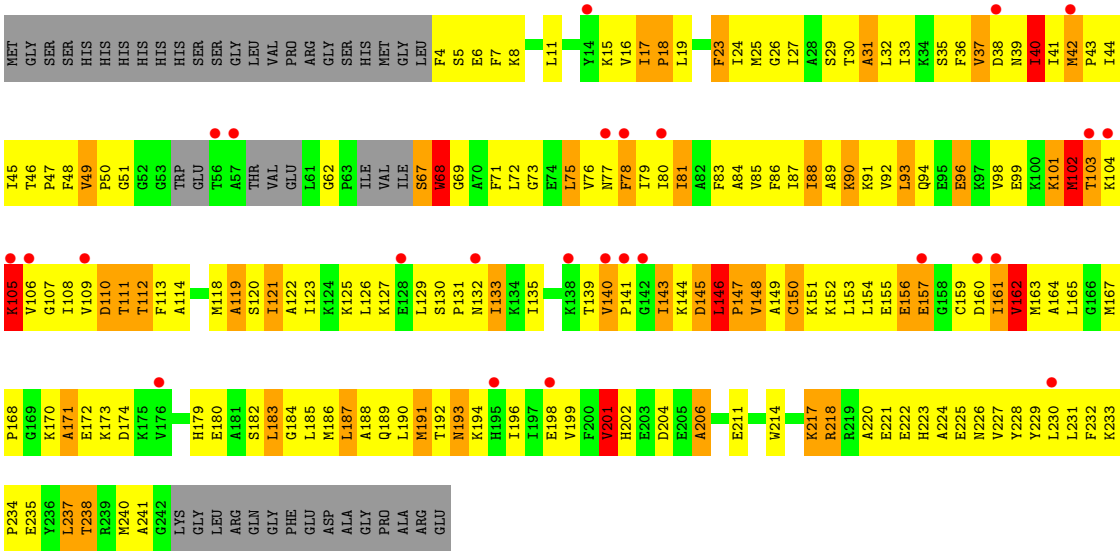


- Molecule 1: Large conductance mechanosensitive channel protein, Riboflavin synthase









## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 147.36Å 149.25Å 99.17Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 40.00 – 4.10<br>40.00 – 4.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.5 (40.00-4.10)<br>99.5 (40.00-4.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.11                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.67 (at 4.13Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0103                                             | Depositor        |
| R, $R_{free}$                                                           | 0.321 , 0.376<br>0.320 , 0.374                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 899 reflections (5.06%)                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 168.8                                                       | Xtriage          |
| Anisotropy                                                              | 0.783                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 491.8                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$ | Xtriage          |
| Estimated twinning fraction                                             | 0.086 for k,h,-l                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 8893                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 274.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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: BNG

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     | 0.97         | 5/1866 (0.3%)  | 1.47        | 27/2527 (1.1%)   |
| 1   | B     | 1.03         | 6/1786 (0.3%)  | 1.68        | 42/2408 (1.7%)   |
| 1   | C     | 0.87         | 4/1809 (0.2%)  | 1.56        | 32/2440 (1.3%)   |
| 1   | D     | 0.93         | 2/1821 (0.1%)  | 1.55        | 34/2463 (1.4%)   |
| 1   | E     | 0.87         | 4/1750 (0.2%)  | 1.40        | 19/2366 (0.8%)   |
| All | All   | 0.94         | 21/9032 (0.2%) | 1.53        | 154/12204 (1.3%) |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 99  | GLU  | CA-C  | 6.99  | 1.62        | 1.52     |
| 1   | E     | 77  | ASN  | C-O   | -6.42 | 1.16        | 1.24     |
| 1   | B     | 164 | ALA  | N-CA  | -6.42 | 1.38        | 1.46     |
| 1   | B     | 23  | PHE  | C-O   | 6.21  | 1.31        | 1.24     |
| 1   | E     | 184 | GLY  | C-O   | -6.06 | 1.16        | 1.23     |
| 1   | A     | 182 | SER  | C-O   | 5.80  | 1.30        | 1.24     |
| 1   | A     | 79  | ILE  | C-O   | -5.79 | 1.17        | 1.24     |
| 1   | B     | 40  | ILE  | N-CA  | 5.64  | 1.53        | 1.46     |
| 1   | B     | 31  | ALA  | C-O   | -5.52 | 1.17        | 1.24     |
| 1   | A     | 79  | ILE  | N-CA  | 5.40  | 1.52        | 1.46     |
| 1   | C     | 24  | ILE  | C-O   | -5.30 | 1.18        | 1.24     |
| 1   | C     | 35  | SER  | C-O   | -5.28 | 1.17        | 1.24     |
| 1   | B     | 213 | ASP  | C-O   | 5.27  | 1.30        | 1.24     |
| 1   | A     | 181 | ALA  | C-O   | 5.25  | 1.30        | 1.24     |
| 1   | E     | 31  | ALA  | C-O   | -5.14 | 1.17        | 1.24     |
| 1   | C     | 26  | GLY  | C-O   | 5.09  | 1.29        | 1.23     |
| 1   | B     | 85  | VAL  | C-O   | -5.07 | 1.18        | 1.24     |
| 1   | E     | 238 | THR  | C-O   | 5.07  | 1.29        | 1.24     |
| 1   | D     | 23  | PHE  | C-N   | -5.06 | 1.27        | 1.34     |
| 1   | C     | 23  | PHE  | C-O   | 5.03  | 1.29        | 1.24     |
| 1   | A     | 31  | ALA  | C-O   | -5.00 | 1.17        | 1.24     |

All (154) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | B     | 40  | ILE  | N-CA-C  | 22.89  | 132.50      | 110.30   |
| 1   | B     | 164 | ALA  | N-CA-C  | -19.39 | 79.19       | 108.46   |
| 1   | E     | 103 | THR  | N-CA-C  | 15.28  | 132.22      | 113.12   |
| 1   | B     | 59  | VAL  | N-CA-C  | 12.22  | 134.76      | 109.34   |
| 1   | C     | 68  | TRP  | N-CA-C  | 12.08  | 136.53      | 110.80   |
| 1   | C     | 64  | ILE  | N-CA-C  | -11.85 | 98.17       | 112.98   |
| 1   | D     | 106 | VAL  | CB-CA-C | -11.43 | 94.28       | 110.96   |
| 1   | A     | 102 | MET  | N-CA-C  | -11.28 | 93.66       | 110.24   |
| 1   | C     | 170 | LYS  | N-CA-C  | 10.76  | 127.10      | 113.55   |
| 1   | E     | 101 | LYS  | N-CA-C  | -10.67 | 99.78       | 113.12   |
| 1   | E     | 140 | VAL  | CA-C-N  | 10.60  | 133.09      | 119.84   |
| 1   | E     | 140 | VAL  | C-N-CA  | 10.60  | 133.09      | 119.84   |
| 1   | C     | 140 | VAL  | CA-C-N  | 10.33  | 132.75      | 119.84   |
| 1   | C     | 140 | VAL  | C-N-CA  | 10.33  | 132.75      | 119.84   |
| 1   | E     | 105 | LYS  | N-CA-C  | 10.18  | 124.88      | 109.41   |
| 1   | C     | 113 | PHE  | N-CA-C  | -10.11 | 100.43      | 113.17   |
| 1   | B     | 98  | VAL  | CB-CA-C | -10.09 | 98.29       | 112.22   |
| 1   | A     | 112 | THR  | N-CA-C  | -9.97  | 99.40       | 114.16   |
| 1   | B     | 105 | LYS  | N-CA-C  | 9.91   | 124.89      | 110.42   |
| 1   | D     | 58  | THR  | N-CA-C  | -9.85  | 95.20       | 109.18   |
| 1   | B     | 98  | VAL  | N-CA-C  | 9.80   | 120.62      | 110.72   |
| 1   | D     | 99  | GLU  | N-CA-C  | 9.78   | 131.62      | 110.80   |
| 1   | C     | 224 | ALA  | N-CA-C  | -9.69  | 99.60       | 111.33   |
| 1   | C     | 217 | LYS  | N-CA-C  | -9.35  | 100.45      | 112.23   |
| 1   | C     | 243 | LYS  | N-CA-C  | 9.25   | 122.47      | 109.15   |
| 1   | B     | 165 | LEU  | N-CA-C  | -8.77  | 90.51       | 107.44   |
| 1   | B     | 40  | ILE  | CB-CA-C | -8.66  | 100.99      | 111.81   |
| 1   | D     | 40  | ILE  | N-CA-C  | -8.58  | 91.49       | 109.34   |
| 1   | C     | 104 | LYS  | N-CA-C  | 8.28   | 122.69      | 109.86   |
| 1   | D     | 110 | ASP  | N-CA-C  | 8.17   | 122.18      | 109.52   |
| 1   | A     | 46  | THR  | N-CA-C  | 8.07   | 124.39      | 110.02   |
| 1   | E     | 96  | GLU  | N-CA-C  | -7.99  | 101.27      | 111.02   |
| 1   | A     | 56  | THR  | N-CA-C  | -7.97  | 98.66       | 110.06   |
| 1   | D     | 167 | MET  | CA-C-N  | 7.95   | 129.77      | 119.84   |
| 1   | D     | 167 | MET  | C-N-CA  | 7.95   | 129.77      | 119.84   |
| 1   | C     | 65  | VAL  | CA-C-N  | 7.77   | 135.95      | 121.97   |
| 1   | C     | 65  | VAL  | C-N-CA  | 7.77   | 135.95      | 121.97   |
| 1   | A     | 201 | VAL  | N-CA-C  | -7.69  | 93.34       | 109.34   |
| 1   | D     | 44  | ILE  | N-CA-C  | 7.68   | 118.48      | 110.72   |
| 1   | A     | 187 | LEU  | N-CA-C  | -7.31  | 102.33      | 111.11   |
| 1   | C     | 98  | VAL  | N-CA-C  | -7.24  | 104.24      | 111.77   |
| 1   | D     | 23  | PHE  | CA-C-N  | -7.19  | 110.39      | 120.53   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 23  | PHE  | C-N-CA  | -7.19 | 110.39      | 120.53   |
| 1   | D     | 115 | ARG  | N-CA-C  | 7.17  | 122.42      | 112.45   |
| 1   | A     | 101 | LYS  | N-CA-C  | -7.12 | 104.33      | 112.87   |
| 1   | C     | 70  | ALA  | N-CA-C  | -6.95 | 105.33      | 113.88   |
| 1   | E     | 62  | GLY  | N-CA-C  | -6.95 | 98.16       | 112.34   |
| 1   | E     | 112 | THR  | N-CA-C  | -6.89 | 103.01      | 113.89   |
| 1   | B     | 142 | GLY  | N-CA-C  | -6.83 | 99.52       | 111.46   |
| 1   | A     | 48  | PHE  | N-CA-C  | -6.82 | 103.93      | 111.36   |
| 1   | C     | 167 | MET  | CA-C-N  | 6.78  | 128.32      | 119.84   |
| 1   | C     | 167 | MET  | C-N-CA  | 6.78  | 128.32      | 119.84   |
| 1   | C     | 244 | GLY  | N-CA-C  | 6.77  | 123.28      | 111.50   |
| 1   | B     | 59  | VAL  | CA-C-N  | 6.75  | 134.43      | 121.54   |
| 1   | B     | 59  | VAL  | C-N-CA  | 6.75  | 134.43      | 121.54   |
| 1   | D     | 21  | ILE  | O-C-N   | 6.74  | 128.51      | 121.91   |
| 1   | D     | 56  | THR  | N-CA-C  | -6.74 | 96.23       | 108.02   |
| 1   | D     | 25  | MET  | CA-C-N  | -6.67 | 112.67      | 119.94   |
| 1   | D     | 25  | MET  | C-N-CA  | -6.67 | 112.67      | 119.94   |
| 1   | D     | 22  | ALA  | CA-C-N  | -6.66 | 109.19      | 120.58   |
| 1   | D     | 22  | ALA  | C-N-CA  | -6.66 | 109.19      | 120.58   |
| 1   | A     | 55  | GLU  | N-CA-C  | 6.66  | 120.01      | 108.76   |
| 1   | B     | 217 | LYS  | N-CA-C  | -6.64 | 103.97      | 111.14   |
| 1   | A     | 45  | ILE  | CA-C-N  | -6.62 | 115.33      | 123.21   |
| 1   | A     | 45  | ILE  | C-N-CA  | -6.62 | 115.33      | 123.21   |
| 1   | C     | 151 | LYS  | N-CA-C  | -6.60 | 102.97      | 111.02   |
| 1   | B     | 157 | GLU  | N-CA-C  | -6.58 | 98.51       | 108.52   |
| 1   | D     | 173 | LYS  | N-CA-C  | 6.55  | 118.08      | 111.07   |
| 1   | B     | 59  | VAL  | CB-CA-C | -6.51 | 100.61      | 111.29   |
| 1   | B     | 101 | LYS  | N-CA-C  | 6.46  | 118.91      | 108.32   |
| 1   | A     | 42  | MET  | CA-C-N  | -6.45 | 111.78      | 119.84   |
| 1   | A     | 42  | MET  | C-N-CA  | -6.45 | 111.78      | 119.84   |
| 1   | D     | 224 | ALA  | N-CA-C  | -6.43 | 103.98      | 112.34   |
| 1   | E     | 50  | PRO  | N-CA-C  | -6.42 | 105.50      | 113.84   |
| 1   | B     | 114 | ALA  | N-CA-C  | 6.42  | 118.58      | 110.24   |
| 1   | B     | 112 | THR  | N-CA-C  | -6.36 | 104.98      | 114.64   |
| 1   | C     | 157 | GLU  | N-CA-C  | -6.34 | 99.34       | 108.60   |
| 1   | B     | 141 | PRO  | N-CA-C  | 6.33  | 125.51      | 112.47   |
| 1   | B     | 141 | PRO  | CB-CA-C | -6.29 | 101.18      | 111.56   |
| 1   | B     | 120 | SER  | N-CA-C  | 6.28  | 118.13      | 111.28   |
| 1   | D     | 112 | THR  | N-CA-C  | -6.27 | 105.79      | 113.50   |
| 1   | B     | 108 | ILE  | N-CA-C  | 6.24  | 117.63      | 109.58   |
| 1   | E     | 49  | VAL  | CA-C-N  | -6.20 | 113.24      | 119.56   |
| 1   | E     | 49  | VAL  | C-N-CA  | -6.20 | 113.24      | 119.56   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | E     | 110 | ASP  | N-CA-C     | 6.20  | 119.12      | 109.52   |
| 1   | A     | 225 | GLU  | N-CA-C     | -6.17 | 103.50      | 111.02   |
| 1   | A     | 67  | SER  | N-CA-C     | -6.15 | 97.70       | 110.80   |
| 1   | E     | 40  | ILE  | CB-CA-C    | -6.13 | 101.24      | 111.29   |
| 1   | D     | 82  | ALA  | N-CA-C     | 6.08  | 117.70      | 111.14   |
| 1   | C     | 65  | VAL  | N-CA-C     | 6.07  | 121.97      | 109.34   |
| 1   | D     | 238 | THR  | N-CA-C     | -6.05 | 103.85      | 111.11   |
| 1   | D     | 63  | PRO  | N-CA-C     | -5.98 | 96.55       | 112.10   |
| 1   | B     | 202 | HIS  | N-CA-C     | 5.95  | 117.98      | 110.24   |
| 1   | B     | 185 | LEU  | N-CA-C     | -5.92 | 101.61      | 111.37   |
| 1   | E     | 40  | ILE  | CG1-CB-CG2 | 5.91  | 128.44      | 110.70   |
| 1   | A     | 140 | VAL  | CA-C-N     | 5.82  | 127.12      | 119.84   |
| 1   | A     | 140 | VAL  | C-N-CA     | 5.82  | 127.12      | 119.84   |
| 1   | A     | 157 | GLU  | N-CA-C     | -5.80 | 98.39       | 107.73   |
| 1   | C     | 245 | LEU  | N-CA-C     | 5.76  | 119.59      | 111.52   |
| 1   | D     | 64  | ILE  | N-CA-C     | -5.76 | 103.59      | 111.89   |
| 1   | B     | 59  | VAL  | CA-C-O     | 5.74  | 127.95      | 120.78   |
| 1   | B     | 104 | LYS  | N-CA-C     | 5.72  | 119.24      | 108.65   |
| 1   | E     | 40  | ILE  | N-CA-C     | 5.72  | 121.23      | 109.34   |
| 1   | A     | 65  | VAL  | CB-CA-C    | -5.68 | 104.44      | 111.32   |
| 1   | D     | 66  | ILE  | N-CA-C     | -5.65 | 103.37      | 111.17   |
| 1   | A     | 39  | ASN  | CA-C-N     | -5.65 | 117.44      | 122.97   |
| 1   | A     | 39  | ASN  | C-N-CA     | -5.65 | 117.44      | 122.97   |
| 1   | B     | 58  | THR  | CA-C-N     | -5.64 | 111.82      | 121.97   |
| 1   | B     | 58  | THR  | C-N-CA     | -5.64 | 111.82      | 121.97   |
| 1   | B     | 159 | CYS  | N-CA-C     | -5.62 | 98.83       | 110.80   |
| 1   | B     | 60  | GLU  | N-CA-C     | 5.61  | 122.75      | 110.80   |
| 1   | C     | 27  | ILE  | O-C-N      | 5.61  | 127.41      | 121.91   |
| 1   | D     | 31  | ALA  | N-CA-C     | -5.59 | 104.59      | 111.75   |
| 1   | D     | 140 | VAL  | CA-C-N     | 5.57  | 126.81      | 119.84   |
| 1   | D     | 140 | VAL  | C-N-CA     | 5.57  | 126.81      | 119.84   |
| 1   | B     | 39  | ASN  | CA-C-N     | 5.57  | 127.66      | 120.70   |
| 1   | B     | 39  | ASN  | C-N-CA     | 5.57  | 127.66      | 120.70   |
| 1   | B     | 189 | GLN  | N-CA-C     | -5.56 | 105.14      | 111.14   |
| 1   | A     | 229 | TYR  | N-CA-C     | -5.55 | 104.25      | 111.02   |
| 1   | B     | 216 | ALA  | N-CA-C     | 5.54  | 122.60      | 110.80   |
| 1   | C     | 24  | ILE  | O-C-N      | 5.52  | 127.30      | 121.89   |
| 1   | D     | 146 | LEU  | O-C-N      | 5.52  | 124.74      | 120.38   |
| 1   | A     | 75  | LEU  | N-CA-C     | -5.47 | 104.95      | 111.03   |
| 1   | A     | 110 | ASP  | N-CA-C     | 5.47  | 117.72      | 109.41   |
| 1   | C     | 71  | PHE  | N-CA-C     | -5.42 | 105.02      | 111.03   |
| 1   | A     | 202 | HIS  | N-CA-C     | -5.41 | 101.76      | 110.14   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 238 | THR  | N-CA-C  | -5.32 | 99.46       | 110.80   |
| 1   | D     | 104 | LYS  | N-CA-C  | 5.32  | 117.96      | 110.14   |
| 1   | C     | 67  | SER  | CA-C-N  | 5.31  | 131.68      | 121.54   |
| 1   | C     | 67  | SER  | C-N-CA  | 5.31  | 131.68      | 121.54   |
| 1   | E     | 68  | TRP  | N-CA-C  | -5.28 | 105.58      | 112.23   |
| 1   | B     | 61  | LEU  | N-CA-C  | 5.27  | 122.03      | 110.80   |
| 1   | B     | 140 | VAL  | CA-C-N  | 5.27  | 126.43      | 119.84   |
| 1   | B     | 140 | VAL  | C-N-CA  | 5.27  | 126.43      | 119.84   |
| 1   | E     | 102 | MET  | N-CA-C  | -5.27 | 102.72      | 110.52   |
| 1   | B     | 113 | PHE  | N-CA-C  | -5.24 | 106.73      | 113.23   |
| 1   | A     | 97  | LYS  | CB-CA-C | -5.24 | 102.62      | 110.90   |
| 1   | B     | 243 | LYS  | N-CA-C  | 5.24  | 116.78      | 108.67   |
| 1   | C     | 185 | LEU  | N-CA-C  | -5.20 | 104.67      | 111.02   |
| 1   | A     | 47  | PRO  | N-CA-C  | -5.19 | 101.78      | 112.47   |
| 1   | D     | 100 | LYS  | N-CA-C  | -5.14 | 100.71      | 108.52   |
| 1   | D     | 188 | ALA  | CA-C-N  | 5.06  | 127.33      | 120.65   |
| 1   | D     | 188 | ALA  | C-N-CA  | 5.06  | 127.33      | 120.65   |
| 1   | C     | 66  | ILE  | CB-CA-C | 5.06  | 119.59      | 111.29   |
| 1   | C     | 110 | ASP  | N-CA-C  | 5.06  | 117.09      | 109.41   |
| 1   | C     | 127 | LYS  | N-CA-C  | -5.06 | 105.28      | 111.75   |
| 1   | E     | 206 | ALA  | N-CA-C  | 5.04  | 115.18      | 108.38   |
| 1   | B     | 130 | SER  | CA-C-N  | 5.04  | 126.14      | 119.84   |
| 1   | B     | 130 | SER  | C-N-CA  | 5.04  | 126.14      | 119.84   |
| 1   | C     | 18  | PRO  | O-C-N   | 5.03  | 128.03      | 122.24   |
| 1   | B     | 104 | LYS  | CA-C-N  | 5.03  | 129.41      | 121.56   |
| 1   | B     | 104 | LYS  | C-N-CA  | 5.03  | 129.41      | 121.56   |
| 1   | E     | 81  | ILE  | O-C-N   | 5.02  | 126.74      | 121.87   |
| 1   | D     | 65  | VAL  | CB-CA-C | -5.02 | 103.98      | 112.16   |

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     | 1829  | 0        | 1849     | 354     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 1757  | 0        | 1787     | 312     | 0            |
| 1   | C     | 1778  | 0        | 1801     | 344     | 0            |
| 1   | D     | 1789  | 0        | 1819     | 363     | 2            |
| 1   | E     | 1719  | 0        | 1728     | 346     | 0            |
| 2   | B     | 21    | 0        | 30       | 12      | 0            |
| All | All   | 8893  | 0        | 9014     | 1613    | 2            |

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 90.

All (1613) 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:D:71:PHE:CD1   | 1:E:40:ILE:CD1   | 1.77                     | 1.63              |
| 1:D:71:PHE:CE1   | 1:E:40:ILE:CD1   | 1.75                     | 1.57              |
| 1:D:71:PHE:CG    | 1:E:40:ILE:HD13  | 1.37                     | 1.54              |
| 1:D:71:PHE:CE1   | 1:E:40:ILE:HD11  | 1.02                     | 1.54              |
| 1:D:71:PHE:CD1   | 1:E:40:ILE:HD11  | 1.32                     | 1.47              |
| 1:B:164:ALA:O    | 1:B:199:VAL:CG2  | 1.68                     | 1.38              |
| 1:D:71:PHE:CD2   | 1:E:40:ILE:HD13  | 1.61                     | 1.35              |
| 1:D:71:PHE:CZ    | 1:E:40:ILE:CD1   | 2.16                     | 1.28              |
| 1:A:168:PRO:HD2  | 1:A:201:VAL:O    | 1.31                     | 1.24              |
| 1:B:215:LEU:HD11 | 1:B:219:ARG:HH21 | 1.03                     | 1.17              |
| 1:B:164:ALA:O    | 1:B:199:VAL:HG21 | 1.40                     | 1.16              |
| 1:B:193:ASN:O    | 1:B:194:LYS:HD2  | 1.46                     | 1.12              |
| 1:D:102:MET:HE2  | 1:D:231:LEU:HD23 | 1.19                     | 1.12              |
| 1:B:36:PHE:O     | 1:B:40:ILE:HB    | 1.51                     | 1.11              |
| 1:C:37:VAL:HG22  | 1:C:88:ILE:HG13  | 1.13                     | 1.11              |
| 1:D:187:LEU:HD23 | 1:D:191:MET:HE1  | 1.28                     | 1.09              |
| 1:A:67:SER:O     | 1:A:71:PHE:CD2   | 2.06                     | 1.09              |
| 1:B:243:LYS:HA   | 1:B:254:PRO:HB3  | 1.32                     | 1.09              |
| 1:E:123:ILE:HD12 | 1:E:135:ILE:HD13 | 1.27                     | 1.09              |
| 1:A:123:ILE:HD12 | 1:A:135:ILE:HD13 | 1.20                     | 1.08              |
| 1:B:164:ALA:O    | 1:B:199:VAL:HG23 | 1.40                     | 1.08              |
| 1:D:63:PRO:O     | 1:D:66:ILE:HG13  | 1.50                     | 1.08              |
| 1:D:62:GLY:CA    | 1:D:65:VAL:HG12  | 1.84                     | 1.08              |
| 1:D:62:GLY:HA2   | 1:D:65:VAL:HG12  | 1.13                     | 1.07              |
| 1:D:71:PHE:CZ    | 1:E:40:ILE:HD12  | 1.88                     | 1.07              |
| 1:E:105:LYS:O    | 1:E:159:CYS:HA   | 1.53                     | 1.07              |
| 1:E:121:ILE:HG21 | 1:E:217:LYS:HB2  | 1.35                     | 1.07              |
| 1:A:129:LEU:HD23 | 1:A:228:TYR:CB   | 1.84                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:189:GLN:HB3  | 1:D:148:VAL:HG22 | 1.37                     | 1.07              |
| 1:C:65:VAL:HG22  | 1:C:66:ILE:H     | 0.94                     | 1.07              |
| 1:C:66:ILE:HG12  | 1:C:68:TRP:CD1   | 1.91                     | 1.06              |
| 1:E:68:TRP:O     | 1:E:72:LEU:HG    | 1.55                     | 1.06              |
| 1:A:112:THR:HB   | 1:A:141:PRO:HA   | 1.36                     | 1.05              |
| 1:A:240:MET:HE2  | 1:A:240:MET:HA   | 1.34                     | 1.05              |
| 1:A:186:MET:HE1  | 1:B:180:GLU:HB3  | 1.38                     | 1.05              |
| 1:E:182:SER:HA   | 1:E:185:LEU:HD12 | 1.38                     | 1.05              |
| 1:E:72:LEU:HA    | 1:E:75:LEU:HD23  | 1.38                     | 1.04              |
| 1:D:222:GLU:O    | 1:D:225:GLU:HB3  | 1.58                     | 1.04              |
| 1:C:65:VAL:CG2   | 1:C:66:ILE:H     | 1.67                     | 1.03              |
| 1:D:71:PHE:CG    | 1:E:40:ILE:CD1   | 2.20                     | 1.03              |
| 1:D:68:TRP:HE1   | 1:E:44:ILE:HD13  | 1.20                     | 1.03              |
| 1:A:41:ILE:O     | 1:A:45:ILE:HG12  | 1.58                     | 1.02              |
| 1:B:126:LEU:HG   | 1:B:133:ILE:HD12 | 1.41                     | 1.02              |
| 1:C:87:ILE:HG22  | 1:C:91:LYS:HE2   | 1.38                     | 1.02              |
| 1:E:161:ILE:HG21 | 1:E:231:LEU:HD11 | 1.41                     | 1.02              |
| 1:D:71:PHE:CD1   | 1:E:40:ILE:HD13  | 1.61                     | 1.02              |
| 1:A:151:LYS:HG2  | 1:A:155:GLU:OE2  | 1.60                     | 1.00              |
| 1:E:222:GLU:O    | 1:E:225:GLU:HB3  | 1.59                     | 0.99              |
| 1:A:36:PHE:O     | 1:A:40:ILE:HG12  | 1.62                     | 0.98              |
| 1:B:122:ALA:HB1  | 1:B:224:ALA:HB2  | 1.45                     | 0.98              |
| 1:D:21:ILE:O     | 1:D:24:ILE:HG22  | 1.61                     | 0.98              |
| 1:B:165:LEU:HD23 | 1:B:199:VAL:HG11 | 1.43                     | 0.98              |
| 1:C:183:LEU:O    | 1:C:187:LEU:HD12 | 1.62                     | 0.98              |
| 1:D:160:ASP:O    | 1:D:161:ILE:HG22 | 1.63                     | 0.97              |
| 1:E:154:LEU:HD11 | 1:E:196:ILE:HD11 | 1.44                     | 0.97              |
| 1:C:163:MET:HE2  | 1:C:199:VAL:HG21 | 1.42                     | 0.97              |
| 1:C:134:LYS:H    | 1:C:134:LYS:HD2  | 1.27                     | 0.97              |
| 1:D:123:ILE:HD12 | 1:D:135:ILE:HD13 | 1.45                     | 0.97              |
| 2:B:301:BNG:H5'2 | 1:D:23:PHE:CZ    | 1.99                     | 0.97              |
| 1:D:25:MET:O     | 1:D:29:SER:OG    | 1.82                     | 0.97              |
| 1:A:153:LEU:O    | 1:A:157:GLU:HG3  | 1.65                     | 0.97              |
| 1:C:65:VAL:HG22  | 1:C:66:ILE:N     | 1.79                     | 0.96              |
| 1:D:149:ALA:O    | 1:D:153:LEU:HD12 | 1.66                     | 0.96              |
| 1:A:182:SER:HA   | 1:A:185:LEU:HD12 | 1.47                     | 0.95              |
| 1:D:153:LEU:HB3  | 1:D:159:CYS:SG   | 2.06                     | 0.95              |
| 1:D:71:PHE:CE2   | 1:E:40:ILE:CD1   | 2.50                     | 0.95              |
| 1:C:17:ILE:HD12  | 1:C:17:ILE:H     | 1.32                     | 0.95              |
| 1:D:79:ILE:HG23  | 1:D:83:PHE:CD2   | 2.02                     | 0.94              |
| 1:A:89:ALA:O     | 1:A:92:VAL:HG12  | 1.66                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:161:ILE:HG12 | 1:A:162:VAL:H    | 1.31                     | 0.94              |
| 1:B:185:LEU:O    | 1:B:188:ALA:HB3  | 1.66                     | 0.94              |
| 1:B:222:GLU:O    | 1:B:225:GLU:HB3  | 1.68                     | 0.94              |
| 1:C:115:ARG:HG3  | 1:C:167:MET:SD   | 2.07                     | 0.94              |
| 1:C:150:CYS:HB2  | 1:C:196:ILE:HD11 | 1.50                     | 0.93              |
| 1:E:218:ARG:HA   | 1:E:218:ARG:NH2  | 1.84                     | 0.93              |
| 1:E:218:ARG:HA   | 1:E:218:ARG:HH21 | 1.32                     | 0.93              |
| 1:A:85:VAL:O     | 1:A:88:ILE:HG12  | 1.68                     | 0.93              |
| 1:A:16:VAL:HG11  | 1:E:25:MET:SD    | 2.09                     | 0.93              |
| 1:B:187:LEU:HB3  | 1:B:191:MET:HE1  | 1.49                     | 0.92              |
| 1:B:229:TYR:HB3  | 1:B:237:LEU:HD11 | 1.52                     | 0.92              |
| 1:B:227:VAL:O    | 1:B:231:LEU:HD13 | 1.69                     | 0.92              |
| 1:C:126:LEU:HG   | 1:C:133:ILE:HD12 | 1.50                     | 0.92              |
| 1:D:186:MET:O    | 1:D:190:LEU:HD12 | 1.69                     | 0.92              |
| 1:E:151:LYS:HE3  | 1:E:191:MET:HG2  | 1.51                     | 0.91              |
| 1:A:40:ILE:HG13  | 1:A:41:ILE:N     | 1.83                     | 0.91              |
| 1:B:151:LYS:HG2  | 1:B:155:GLU:OE2  | 1.70                     | 0.91              |
| 1:A:163:MET:HE2  | 1:A:165:LEU:HD21 | 1.53                     | 0.91              |
| 1:B:146:LEU:HD23 | 1:B:146:LEU:H    | 1.34                     | 0.91              |
| 1:B:119:ALA:O    | 1:B:123:ILE:HG12 | 1.69                     | 0.90              |
| 1:E:161:ILE:HD13 | 1:E:227:VAL:HG13 | 1.53                     | 0.90              |
| 1:A:222:GLU:O    | 1:A:225:GLU:HB3  | 1.72                     | 0.90              |
| 1:A:78:PHE:O     | 1:A:81:ILE:HG13  | 1.70                     | 0.90              |
| 1:B:237:LEU:HD12 | 1:B:237:LEU:H    | 1.34                     | 0.90              |
| 1:C:149:ALA:O    | 1:C:153:LEU:HD12 | 1.71                     | 0.90              |
| 1:A:168:PRO:CD   | 1:A:201:VAL:O    | 2.19                     | 0.90              |
| 1:D:73:GLY:O     | 1:D:76:VAL:HG12  | 1.71                     | 0.90              |
| 1:E:193:ASN:O    | 1:E:194:LYS:HD2  | 1.72                     | 0.90              |
| 1:A:126:LEU:HG   | 1:A:133:ILE:HD12 | 1.53                     | 0.90              |
| 1:D:71:PHE:CE2   | 1:E:40:ILE:HD13  | 2.07                     | 0.89              |
| 1:A:94:GLN:O     | 1:A:98:VAL:HG22  | 1.70                     | 0.89              |
| 1:A:61:LEU:HD12  | 1:A:61:LEU:H     | 1.38                     | 0.89              |
| 1:D:119:ALA:O    | 1:D:123:ILE:HG12 | 1.73                     | 0.89              |
| 1:E:98:VAL:HG22  | 1:E:101:LYS:HZ3  | 1.39                     | 0.88              |
| 1:D:71:PHE:CD2   | 1:E:40:ILE:CD1   | 2.50                     | 0.88              |
| 1:E:161:ILE:HD11 | 1:E:227:VAL:HG22 | 1.55                     | 0.88              |
| 1:B:85:VAL:O     | 1:B:88:ILE:HG22  | 1.73                     | 0.88              |
| 1:C:66:ILE:HG13  | 1:C:67:SER:H     | 1.36                     | 0.88              |
| 1:D:23:PHE:O     | 1:D:26:GLY:N     | 2.06                     | 0.88              |
| 1:B:103:THR:C    | 1:B:104:LYS:HD2  | 1.98                     | 0.87              |
| 1:E:226:ASN:HA   | 1:E:229:TYR:CD2  | 2.09                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:63:PRO:HG2   | 1:C:65:VAL:HB    | 1.57                     | 0.87              |
| 1:C:65:VAL:O     | 1:C:66:ILE:HG23  | 1.74                     | 0.87              |
| 1:C:111:THR:CG2  | 1:C:166:GLY:HA2  | 2.05                     | 0.87              |
| 1:A:145:ASP:C    | 1:A:147:PRO:HD2  | 2.00                     | 0.86              |
| 1:B:215:LEU:HD11 | 1:B:219:ARG:NH2  | 1.89                     | 0.86              |
| 1:D:63:PRO:O     | 1:D:66:ILE:CG1   | 2.22                     | 0.86              |
| 1:E:78:PHE:O     | 1:E:81:ILE:HG22  | 1.73                     | 0.86              |
| 1:A:165:LEU:HD23 | 1:A:199:VAL:HG21 | 1.53                     | 0.86              |
| 1:C:161:ILE:O    | 1:C:162:VAL:HG23 | 1.76                     | 0.86              |
| 1:E:85:VAL:O     | 1:E:88:ILE:HG22  | 1.74                     | 0.86              |
| 1:B:125:LYS:HE3  | 1:B:129:LEU:HD11 | 1.57                     | 0.86              |
| 1:C:149:ALA:O    | 1:C:153:LEU:CD1  | 2.24                     | 0.86              |
| 1:D:122:ALA:HB1  | 1:D:224:ALA:HB2  | 1.56                     | 0.86              |
| 1:A:87:ILE:HG22  | 1:A:91:LYS:HE3   | 1.58                     | 0.86              |
| 1:A:154:LEU:HD11 | 1:A:196:ILE:HD11 | 1.55                     | 0.85              |
| 1:B:163:MET:HE2  | 1:B:165:LEU:HD21 | 1.55                     | 0.85              |
| 1:B:246:ARG:HG3  | 1:B:252:ALA:HB3  | 1.57                     | 0.85              |
| 1:D:71:PHE:HA    | 1:E:39:ASN:HD22  | 1.41                     | 0.85              |
| 1:D:46:THR:H     | 1:D:47:PRO:CD    | 1.88                     | 0.85              |
| 1:E:89:ALA:O     | 1:E:92:VAL:HG12  | 1.76                     | 0.85              |
| 1:E:108:ILE:HG13 | 1:E:163:MET:HB2  | 1.59                     | 0.85              |
| 1:E:186:MET:HA   | 1:E:189:GLN:OE1  | 1.76                     | 0.85              |
| 1:A:37:VAL:HG21  | 1:A:85:VAL:HG22  | 1.59                     | 0.85              |
| 1:B:189:GLN:HE21 | 1:B:196:ILE:H    | 1.25                     | 0.85              |
| 1:D:66:ILE:HD12  | 1:D:67:SER:N     | 1.92                     | 0.84              |
| 1:E:185:LEU:HD13 | 1:E:198:GLU:HG2  | 1.57                     | 0.84              |
| 1:A:118:MET:HE1  | 1:A:166:GLY:N    | 1.92                     | 0.84              |
| 1:D:17:ILE:HD12  | 1:D:17:ILE:H     | 1.41                     | 0.84              |
| 1:D:85:VAL:O     | 1:D:88:ILE:HG22  | 1.77                     | 0.84              |
| 1:A:99:GLU:O     | 1:A:100:LYS:HB2  | 1.77                     | 0.84              |
| 1:A:129:LEU:HD23 | 1:A:228:TYR:HB3  | 1.60                     | 0.84              |
| 1:C:154:LEU:HD11 | 1:C:196:ILE:HG13 | 1.59                     | 0.84              |
| 1:E:17:ILE:HD12  | 1:E:17:ILE:H     | 1.42                     | 0.84              |
| 1:D:36:PHE:O     | 1:D:40:ILE:HB    | 1.78                     | 0.84              |
| 1:A:185:LEU:O    | 1:A:188:ALA:HB3  | 1.77                     | 0.83              |
| 1:E:107:GLY:O    | 1:E:162:VAL:HA   | 1.77                     | 0.83              |
| 1:D:43:PRO:O     | 1:D:47:PRO:HD3   | 1.79                     | 0.83              |
| 1:D:187:LEU:HD23 | 1:D:191:MET:CE   | 2.08                     | 0.83              |
| 1:D:143:ILE:HG23 | 1:D:144:LYS:HG3  | 1.60                     | 0.83              |
| 1:E:98:VAL:HA    | 1:E:101:LYS:HD2  | 1.60                     | 0.83              |
| 1:D:63:PRO:HA    | 1:D:66:ILE:HG23  | 1.60                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:69:GLY:HA2   | 1:E:72:LEU:HD12  | 1.57                     | 0.83              |
| 1:A:153:LEU:HA   | 1:A:157:GLU:CD   | 2.04                     | 0.83              |
| 1:A:112:THR:CB   | 1:A:141:PRO:HA   | 2.09                     | 0.82              |
| 1:B:75:LEU:HD12  | 1:B:76:VAL:N     | 1.95                     | 0.82              |
| 1:C:76:VAL:O     | 1:C:80:ILE:HG13  | 1.79                     | 0.82              |
| 1:D:146:LEU:O    | 1:D:149:ALA:HB3  | 1.79                     | 0.82              |
| 1:D:25:MET:O     | 1:D:29:SER:CB    | 2.28                     | 0.82              |
| 1:E:164:ALA:O    | 1:E:199:VAL:HB   | 1.79                     | 0.82              |
| 1:B:112:THR:HB   | 1:B:141:PRO:HA   | 1.62                     | 0.81              |
| 1:B:219:ARG:HG2  | 1:B:223:HIS:NE2  | 1.94                     | 0.81              |
| 1:C:146:LEU:O    | 1:C:149:ALA:HB3  | 1.80                     | 0.81              |
| 1:D:25:MET:SD    | 1:E:16:VAL:HG11  | 2.20                     | 0.81              |
| 1:B:125:LYS:O    | 1:B:129:LEU:HD13 | 1.80                     | 0.81              |
| 1:B:126:LEU:HD23 | 1:B:135:ILE:HD11 | 1.60                     | 0.81              |
| 1:D:62:GLY:HA2   | 1:D:65:VAL:CG1   | 2.05                     | 0.81              |
| 1:A:101:LYS:O    | 1:A:103:THR:HG23 | 1.80                     | 0.81              |
| 1:C:46:THR:O     | 1:C:49:VAL:HG12  | 1.78                     | 0.81              |
| 1:C:110:ASP:C    | 1:C:139:THR:HG23 | 2.06                     | 0.81              |
| 1:C:161:ILE:HG12 | 1:C:162:VAL:N    | 1.95                     | 0.81              |
| 1:E:48:PHE:CD2   | 1:E:49:VAL:HG23  | 2.16                     | 0.81              |
| 1:E:73:GLY:O     | 1:E:76:VAL:HG12  | 1.81                     | 0.81              |
| 1:A:197:ILE:H    | 1:A:197:ILE:HD13 | 1.45                     | 0.81              |
| 1:A:227:VAL:O    | 1:A:231:LEU:HD13 | 1.81                     | 0.81              |
| 1:A:160:ASP:O    | 1:A:194:LYS:HG3  | 1.81                     | 0.81              |
| 1:D:25:MET:O     | 1:D:29:SER:N     | 2.14                     | 0.81              |
| 1:D:108:ILE:HG13 | 1:D:163:MET:HB2  | 1.62                     | 0.80              |
| 1:A:123:ILE:HD12 | 1:A:135:ILE:CD1  | 2.09                     | 0.80              |
| 1:E:150:CYS:O    | 1:E:154:LEU:HG   | 1.81                     | 0.80              |
| 1:D:186:MET:O    | 1:D:189:GLN:HB2  | 1.80                     | 0.80              |
| 1:A:98:VAL:HG23  | 1:A:98:VAL:O     | 1.81                     | 0.80              |
| 1:C:105:LYS:HE3  | 1:C:158:GLY:HA3  | 1.64                     | 0.80              |
| 1:D:187:LEU:CD2  | 1:D:191:MET:HE1  | 2.09                     | 0.80              |
| 1:C:110:ASP:O    | 1:C:139:THR:HG23 | 1.82                     | 0.80              |
| 1:A:197:ILE:HD13 | 1:A:197:ILE:N    | 1.97                     | 0.80              |
| 1:C:213:ASP:O    | 1:C:216:ALA:HB3  | 1.80                     | 0.80              |
| 1:B:153:LEU:O    | 1:B:157:GLU:HG2  | 1.82                     | 0.80              |
| 1:B:161:ILE:HG12 | 1:B:162:VAL:H    | 1.45                     | 0.79              |
| 1:E:182:SER:O    | 1:E:185:LEU:HB2  | 1.82                     | 0.79              |
| 1:B:139:THR:HG22 | 1:B:140:VAL:H    | 1.44                     | 0.79              |
| 1:C:223:HIS:CE1  | 1:C:247:GLN:HB3  | 2.17                     | 0.79              |
| 1:C:85:VAL:O     | 1:C:88:ILE:HG22  | 1.83                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:189:GLN:HB3  | 1:D:148:VAL:CG2  | 2.12                     | 0.79              |
| 1:D:164:ALA:HB3  | 1:D:199:VAL:H    | 1.48                     | 0.79              |
| 1:A:148:VAL:HG22 | 1:E:189:GLN:HB3  | 1.65                     | 0.79              |
| 1:E:98:VAL:CG2   | 1:E:101:LYS:HZ3  | 1.95                     | 0.79              |
| 1:B:232:PHE:O    | 1:B:234:PRO:HD3  | 1.83                     | 0.79              |
| 1:C:159:CYS:O    | 1:C:161:ILE:N    | 2.15                     | 0.79              |
| 1:A:185:LEU:O    | 1:A:189:GLN:HG3  | 1.83                     | 0.79              |
| 1:A:15:LYS:HB3   | 1:A:18:PRO:HG2   | 1.65                     | 0.79              |
| 1:B:145:ASP:C    | 1:B:147:PRO:HD2  | 2.08                     | 0.79              |
| 1:C:102:MET:C    | 1:C:103:THR:CA   | 2.56                     | 0.79              |
| 1:C:245:LEU:CB   | 1:C:245:LEU:CD2  | 2.61                     | 0.79              |
| 1:C:233:LYS:HE2  | 1:C:236:TYR:HB2  | 1.65                     | 0.78              |
| 1:D:46:THR:H     | 1:D:47:PRO:HD2   | 1.48                     | 0.78              |
| 1:A:77:ASN:O     | 1:A:80:ILE:HG22  | 1.83                     | 0.78              |
| 1:E:217:LYS:NZ   | 1:E:217:LYS:HB3  | 1.97                     | 0.78              |
| 1:A:146:LEU:HG   | 1:A:147:PRO:HD3  | 1.66                     | 0.78              |
| 1:C:44:ILE:C     | 1:C:47:PRO:HD2   | 2.08                     | 0.78              |
| 1:D:123:ILE:CD1  | 1:D:135:ILE:HD13 | 2.13                     | 0.78              |
| 1:B:17:ILE:H     | 1:B:17:ILE:HD12  | 1.48                     | 0.78              |
| 1:B:61:LEU:CD1   | 1:B:63:PRO:HB3   | 2.14                     | 0.78              |
| 1:C:37:VAL:CG2   | 1:C:88:ILE:HG13  | 2.06                     | 0.78              |
| 1:C:111:THR:HG21 | 1:C:166:GLY:HA2  | 1.66                     | 0.78              |
| 1:B:213:ASP:O    | 1:B:216:ALA:HB3  | 1.84                     | 0.78              |
| 1:C:66:ILE:HG12  | 1:C:68:TRP:HD1   | 1.49                     | 0.78              |
| 1:E:35:SER:HA    | 1:E:38:ASP:HB3   | 1.66                     | 0.78              |
| 1:E:111:THR:HG21 | 1:E:114:ALA:HB2  | 1.65                     | 0.78              |
| 1:B:111:THR:CG2  | 1:B:114:ALA:HB2  | 2.14                     | 0.78              |
| 1:B:165:LEU:HA   | 1:B:199:VAL:HB   | 1.66                     | 0.78              |
| 1:D:63:PRO:O     | 1:D:66:ILE:N     | 2.16                     | 0.78              |
| 1:D:179:HIS:NE2  | 1:D:183:LEU:HD11 | 1.99                     | 0.78              |
| 1:D:229:TYR:HB3  | 1:D:237:LEU:HD11 | 1.65                     | 0.78              |
| 1:D:79:ILE:HG23  | 1:D:83:PHE:HD2   | 1.48                     | 0.77              |
| 1:C:121:ILE:HG21 | 1:C:217:LYS:O    | 1.84                     | 0.77              |
| 1:C:164:ALA:HB3  | 1:C:199:VAL:H    | 1.48                     | 0.77              |
| 1:B:162:VAL:HG13 | 1:B:163:MET:O    | 1.83                     | 0.77              |
| 1:E:44:ILE:O     | 1:E:47:PRO:HD2   | 1.83                     | 0.77              |
| 1:A:40:ILE:O     | 1:A:44:ILE:HG22  | 1.84                     | 0.77              |
| 1:B:193:ASN:C    | 1:B:194:LYS:HD2  | 2.09                     | 0.76              |
| 1:C:238:THR:O    | 1:C:241:ALA:HB2  | 1.85                     | 0.76              |
| 1:D:94:GLN:O     | 1:D:98:VAL:HG23  | 1.85                     | 0.76              |
| 1:C:118:MET:HB2  | 1:C:165:LEU:HD13 | 1.67                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:164:ALA:HB3  | 1:C:198:GLU:HA   | 1.66                     | 0.76              |
| 1:B:106:VAL:HG12 | 1:B:108:ILE:CD1  | 2.16                     | 0.76              |
| 1:D:182:SER:HA   | 1:D:185:LEU:HD12 | 1.67                     | 0.76              |
| 1:E:81:ILE:O     | 1:E:85:VAL:HG23  | 1.84                     | 0.76              |
| 1:E:36:PHE:O     | 1:E:40:ILE:HG13  | 1.84                     | 0.76              |
| 1:E:87:ILE:O     | 1:E:90:LYS:HG3   | 1.85                     | 0.76              |
| 1:B:36:PHE:C     | 1:B:40:ILE:HB    | 2.11                     | 0.76              |
| 2:B:301:BNG:C6'  | 1:D:23:PHE:HZ    | 1.99                     | 0.76              |
| 1:D:113:PHE:HB2  | 1:D:141:PRO:O    | 1.86                     | 0.76              |
| 1:A:200:PHE:O    | 1:A:201:VAL:HG13 | 1.86                     | 0.76              |
| 1:E:37:VAL:CG1   | 1:E:81:ILE:HG13  | 2.16                     | 0.76              |
| 1:A:146:LEU:H    | 1:A:146:LEU:HD23 | 1.50                     | 0.75              |
| 1:C:232:PHE:O    | 1:C:234:PRO:HD3  | 1.85                     | 0.75              |
| 1:C:121:ILE:HD11 | 1:C:217:LYS:HZ2  | 1.51                     | 0.75              |
| 1:D:77:ASN:O     | 1:D:81:ILE:HG12  | 1.87                     | 0.75              |
| 1:E:151:LYS:HG2  | 1:E:155:GLU:OE2  | 1.87                     | 0.75              |
| 1:D:21:ILE:O     | 1:D:24:ILE:CG2   | 2.34                     | 0.75              |
| 1:E:42:MET:O     | 1:E:46:THR:HG23  | 1.84                     | 0.75              |
| 1:E:98:VAL:HG13  | 1:E:101:LYS:HD2  | 1.69                     | 0.75              |
| 1:C:235:GLU:O    | 1:C:238:THR:HB   | 1.86                     | 0.75              |
| 1:E:187:LEU:HD23 | 1:E:191:MET:HE1  | 1.69                     | 0.75              |
| 1:C:125:LYS:HA   | 1:C:128:GLU:OE1  | 1.85                     | 0.75              |
| 1:D:46:THR:N     | 1:D:47:PRO:HD2   | 2.02                     | 0.75              |
| 1:A:139:THR:HG22 | 1:A:140:VAL:H    | 1.52                     | 0.75              |
| 1:C:243:LYS:HD2  | 1:C:243:LYS:N    | 2.02                     | 0.75              |
| 1:D:71:PHE:CD1   | 1:E:40:ILE:CG1   | 2.69                     | 0.74              |
| 1:D:150:CYS:HB2  | 1:D:196:ILE:HD13 | 1.69                     | 0.74              |
| 1:E:123:ILE:HG23 | 1:E:135:ILE:CD1  | 2.17                     | 0.74              |
| 1:A:15:LYS:C     | 1:A:18:PRO:HD2   | 2.12                     | 0.74              |
| 1:A:150:CYS:HA   | 1:A:153:LEU:HD13 | 1.69                     | 0.74              |
| 1:D:102:MET:HE2  | 1:D:231:LEU:CD2  | 2.12                     | 0.74              |
| 1:B:7:PHE:HE1    | 1:E:86:PHE:HB3   | 1.51                     | 0.74              |
| 1:D:96:GLU:N     | 1:D:96:GLU:OE2   | 2.21                     | 0.74              |
| 1:E:186:MET:O    | 1:E:189:GLN:HB2  | 1.88                     | 0.74              |
| 1:B:110:ASP:O    | 1:B:139:THR:HG23 | 1.87                     | 0.73              |
| 1:B:111:THR:HG21 | 1:B:114:ALA:HB2  | 1.69                     | 0.73              |
| 1:B:161:ILE:HG13 | 1:B:195:HIS:O    | 1.89                     | 0.73              |
| 1:E:110:ASP:O    | 1:E:139:THR:HG23 | 1.87                     | 0.73              |
| 1:A:90:LYS:HE2   | 1:C:7:PHE:HD1    | 1.52                     | 0.73              |
| 1:E:235:GLU:O    | 1:E:238:THR:HB   | 1.89                     | 0.73              |
| 1:A:7:PHE:HE2    | 1:D:90:LYS:HB2   | 1.54                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:61:LEU:H     | 1:A:61:LEU:CD1   | 2.01                     | 0.73              |
| 1:B:108:ILE:HG13 | 1:B:163:MET:HB2  | 1.71                     | 0.73              |
| 1:D:89:ALA:O     | 1:D:92:VAL:HG12  | 1.88                     | 0.73              |
| 1:B:178:ALA:O    | 1:B:182:SER:OG   | 2.04                     | 0.73              |
| 1:C:161:ILE:HG12 | 1:C:162:VAL:H    | 1.54                     | 0.73              |
| 1:E:111:THR:CG2  | 1:E:114:ALA:HB2  | 2.18                     | 0.73              |
| 1:A:129:LEU:HD23 | 1:A:228:TYR:HB2  | 1.69                     | 0.73              |
| 1:B:140:VAL:HG21 | 1:B:145:ASP:HB3  | 1.71                     | 0.73              |
| 2:B:301:BNG:H3'1 | 2:B:301:BNG:H7'2 | 1.71                     | 0.73              |
| 1:A:5:SER:HA     | 1:A:8:LYS:HE2    | 1.69                     | 0.72              |
| 1:D:161:ILE:HG13 | 1:D:195:HIS:O    | 1.89                     | 0.72              |
| 1:A:182:SER:O    | 1:A:185:LEU:HB2  | 1.89                     | 0.72              |
| 1:D:64:ILE:O     | 1:D:67:SER:HB3   | 1.89                     | 0.72              |
| 1:C:145:ASP:C    | 1:C:147:PRO:HD2  | 2.15                     | 0.72              |
| 1:C:237:LEU:HD12 | 1:C:237:LEU:H    | 1.54                     | 0.72              |
| 1:B:161:ILE:HG12 | 1:B:162:VAL:N    | 2.03                     | 0.72              |
| 1:D:65:VAL:HG22  | 1:D:68:TRP:HB2   | 1.71                     | 0.72              |
| 1:A:150:CYS:O    | 1:A:154:LEU:HG   | 1.89                     | 0.72              |
| 1:A:154:LEU:CD1  | 1:A:196:ILE:HD11 | 2.18                     | 0.72              |
| 1:B:7:PHE:CE1    | 1:E:86:PHE:HB3   | 2.24                     | 0.72              |
| 1:B:36:PHE:HA    | 1:B:40:ILE:HG13  | 1.70                     | 0.72              |
| 1:B:222:GLU:OE1  | 1:B:247:GLN:HG3  | 1.89                     | 0.72              |
| 1:A:143:ILE:O    | 1:A:146:LEU:HD21 | 1.89                     | 0.72              |
| 1:C:217:LYS:O    | 1:C:220:ALA:HB3  | 1.89                     | 0.72              |
| 1:A:126:LEU:HG   | 1:A:133:ILE:CD1  | 2.20                     | 0.72              |
| 1:D:40:ILE:HG22  | 1:D:41:ILE:H     | 1.54                     | 0.72              |
| 1:C:157:GLU:HG3  | 1:C:159:CYS:SG   | 2.28                     | 0.72              |
| 1:A:111:THR:HG21 | 1:A:114:ALA:HB2  | 1.70                     | 0.71              |
| 1:A:226:ASN:HA   | 1:A:229:TYR:CD2  | 2.25                     | 0.71              |
| 1:B:42:MET:HB3   | 1:B:43:PRO:HD3   | 1.72                     | 0.71              |
| 1:C:193:ASN:HB3  | 1:D:152:LYS:HG2  | 1.70                     | 0.71              |
| 1:D:35:SER:HA    | 1:D:38:ASP:HB3   | 1.72                     | 0.71              |
| 1:A:229:TYR:HA   | 1:A:233:LYS:HB3  | 1.72                     | 0.71              |
| 1:C:66:ILE:HG12  | 1:C:68:TRP:NE1   | 2.04                     | 0.71              |
| 1:D:161:ILE:O    | 1:D:162:VAL:HG23 | 1.90                     | 0.71              |
| 1:A:139:THR:HG22 | 1:A:140:VAL:N    | 2.06                     | 0.71              |
| 1:B:182:SER:HA   | 1:B:185:LEU:HD12 | 1.71                     | 0.71              |
| 1:B:187:LEU:HB3  | 1:B:191:MET:CE   | 2.20                     | 0.71              |
| 1:D:46:THR:N     | 1:D:47:PRO:CD    | 2.53                     | 0.71              |
| 1:E:68:TRP:HE3   | 1:E:68:TRP:N     | 1.89                     | 0.71              |
| 1:B:76:VAL:O     | 1:B:80:ILE:HG13  | 1.90                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:111:THR:CG2  | 1:C:114:ALA:HB2  | 2.20                     | 0.71              |
| 1:D:123:ILE:HD12 | 1:D:135:ILE:HG21 | 1.73                     | 0.71              |
| 1:B:240:MET:O    | 1:B:243:LYS:HB2  | 1.91                     | 0.71              |
| 1:D:63:PRO:C     | 1:D:66:ILE:HG13  | 2.16                     | 0.71              |
| 1:D:78:PHE:O     | 1:D:82:ALA:N     | 2.16                     | 0.71              |
| 1:D:183:LEU:O    | 1:D:187:LEU:HD12 | 1.91                     | 0.71              |
| 1:E:227:VAL:O    | 1:E:231:LEU:HD13 | 1.91                     | 0.71              |
| 1:C:77:ASN:HA    | 1:C:80:ILE:HD12  | 1.73                     | 0.71              |
| 1:D:164:ALA:O    | 1:D:199:VAL:HB   | 1.91                     | 0.70              |
| 1:E:108:ILE:HG23 | 1:E:165:LEU:HD12 | 1.72                     | 0.70              |
| 1:E:240:MET:O    | 1:E:241:ALA:C    | 2.34                     | 0.70              |
| 1:C:227:VAL:HG12 | 1:C:231:LEU:HD13 | 1.73                     | 0.70              |
| 1:D:61:LEU:HB3   | 1:D:65:VAL:HB    | 1.73                     | 0.70              |
| 1:C:143:ILE:O    | 1:C:146:LEU:HG   | 1.91                     | 0.70              |
| 1:A:186:MET:O    | 1:A:190:LEU:N    | 2.20                     | 0.70              |
| 1:D:193:ASN:HA   | 1:E:148:VAL:HG12 | 1.74                     | 0.70              |
| 1:B:150:CYS:O    | 1:B:154:LEU:HG   | 1.91                     | 0.70              |
| 1:D:68:TRP:NE1   | 1:E:44:ILE:HD13  | 2.01                     | 0.70              |
| 1:D:186:MET:HA   | 1:D:189:GLN:OE1  | 1.91                     | 0.70              |
| 1:E:133:ILE:O    | 1:E:133:ILE:HG13 | 1.89                     | 0.70              |
| 1:B:140:VAL:HB   | 1:B:141:PRO:HD2  | 1.72                     | 0.70              |
| 1:D:25:MET:HG2   | 1:E:16:VAL:CG1   | 2.21                     | 0.70              |
| 1:C:107:GLY:O    | 1:C:162:VAL:HG22 | 1.92                     | 0.70              |
| 1:D:62:GLY:CA    | 1:D:65:VAL:CG1   | 2.66                     | 0.70              |
| 1:A:109:VAL:HG21 | 1:A:153:LEU:HD11 | 1.73                     | 0.70              |
| 1:A:129:LEU:HD23 | 1:A:228:TYR:CG   | 2.27                     | 0.70              |
| 1:A:237:LEU:O    | 1:A:240:MET:N    | 2.25                     | 0.70              |
| 1:B:139:THR:HG22 | 1:B:140:VAL:N    | 2.07                     | 0.70              |
| 1:C:88:ILE:HD13  | 1:C:88:ILE:O     | 1.92                     | 0.70              |
| 1:C:229:TYR:HB3  | 1:C:237:LEU:HD11 | 1.74                     | 0.70              |
| 1:D:23:PHE:O     | 1:D:24:ILE:C     | 2.29                     | 0.69              |
| 1:D:153:LEU:HA   | 1:D:157:GLU:OE2  | 1.92                     | 0.69              |
| 1:B:223:HIS:O    | 1:B:227:VAL:HG23 | 1.92                     | 0.69              |
| 1:C:125:LYS:O    | 1:C:128:GLU:HB3  | 1.92                     | 0.69              |
| 1:C:217:LYS:NZ   | 1:C:217:LYS:HB3  | 2.07                     | 0.69              |
| 1:D:126:LEU:HG   | 1:D:133:ILE:CD1  | 2.23                     | 0.69              |
| 1:E:125:LYS:HG2  | 1:E:221:GLU:HG3  | 1.74                     | 0.69              |
| 1:E:154:LEU:HD11 | 1:E:196:ILE:CD1  | 2.21                     | 0.69              |
| 1:A:180:GLU:HB3  | 1:E:186:MET:HE1  | 1.72                     | 0.69              |
| 2:B:301:BNG:C5'  | 1:D:23:PHE:HZ    | 2.05                     | 0.69              |
| 1:E:112:THR:HB   | 1:E:141:PRO:HA   | 1.73                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:301:BNG:C5'  | 1:D:23:PHE:CZ    | 2.75                     | 0.69              |
| 1:C:148:VAL:O    | 1:C:152:LYS:HG3  | 1.93                     | 0.69              |
| 1:A:68:TRP:HE3   | 1:A:72:LEU:HD21  | 1.57                     | 0.69              |
| 1:E:49:VAL:HG12  | 1:E:49:VAL:O     | 1.91                     | 0.69              |
| 1:A:107:GLY:C    | 1:A:108:ILE:HD12 | 2.18                     | 0.69              |
| 1:A:229:TYR:HB3  | 1:A:233:LYS:O    | 1.92                     | 0.69              |
| 1:E:183:LEU:O    | 1:E:187:LEU:HD12 | 1.92                     | 0.69              |
| 1:A:127:LYS:CA   | 1:A:133:ILE:HD11 | 2.22                     | 0.69              |
| 1:B:183:LEU:O    | 1:B:186:MET:HB3  | 1.92                     | 0.69              |
| 1:A:61:LEU:HD12  | 1:A:61:LEU:N     | 2.08                     | 0.69              |
| 1:C:41:ILE:HG23  | 1:C:91:LYS:HE3   | 1.75                     | 0.69              |
| 1:A:165:LEU:HA   | 1:A:199:VAL:HB   | 1.73                     | 0.68              |
| 1:B:146:LEU:HG   | 1:B:147:PRO:HD3  | 1.75                     | 0.68              |
| 1:C:222:GLU:OE1  | 1:C:248:GLY:N    | 2.27                     | 0.68              |
| 1:B:89:ALA:O     | 1:B:92:VAL:HG12  | 1.93                     | 0.68              |
| 1:C:111:THR:HG22 | 1:C:166:GLY:HA2  | 1.73                     | 0.68              |
| 1:D:71:PHE:HA    | 1:E:39:ASN:ND2   | 2.08                     | 0.68              |
| 1:D:147:PRO:O    | 1:D:148:VAL:C    | 2.36                     | 0.68              |
| 1:C:121:ILE:HG13 | 1:C:217:LYS:HB3  | 1.75                     | 0.68              |
| 1:A:240:MET:HA   | 1:A:240:MET:CE   | 2.18                     | 0.68              |
| 1:B:61:LEU:HD12  | 1:B:63:PRO:HB3   | 1.76                     | 0.68              |
| 1:C:151:LYS:HG2  | 1:C:155:GLU:OE2  | 1.94                     | 0.68              |
| 1:D:67:SER:OG    | 1:E:43:PRO:HB2   | 1.92                     | 0.68              |
| 1:A:121:ILE:HG21 | 1:A:217:LYS:HB2  | 1.75                     | 0.68              |
| 1:A:118:MET:HE1  | 1:A:166:GLY:H    | 1.58                     | 0.68              |
| 1:B:189:GLN:HE21 | 1:B:196:ILE:N    | 1.91                     | 0.68              |
| 1:B:189:GLN:CG   | 1:B:196:ILE:HB   | 2.23                     | 0.68              |
| 1:C:83:PHE:O     | 1:C:87:ILE:HG12  | 1.93                     | 0.68              |
| 1:D:44:ILE:HG23  | 1:D:45:ILE:HG12  | 1.75                     | 0.68              |
| 1:A:127:LYS:N    | 1:A:133:ILE:HD11 | 2.09                     | 0.68              |
| 1:B:75:LEU:HD23  | 1:C:40:ILE:HG13  | 1.76                     | 0.68              |
| 1:C:63:PRO:C     | 1:C:65:VAL:N     | 2.52                     | 0.68              |
| 1:C:140:VAL:HB   | 1:C:141:PRO:HD2  | 1.75                     | 0.67              |
| 1:A:4:PHE:O      | 1:A:8:LYS:HG3    | 1.94                     | 0.67              |
| 1:C:49:VAL:HG13  | 1:C:49:VAL:O     | 1.94                     | 0.67              |
| 1:D:61:LEU:HD12  | 1:D:65:VAL:HG23  | 1.76                     | 0.67              |
| 1:E:161:ILE:O    | 1:E:162:VAL:HG23 | 1.93                     | 0.67              |
| 1:A:67:SER:O     | 1:A:71:PHE:CE2   | 2.47                     | 0.67              |
| 1:B:59:VAL:C     | 1:B:60:GLU:HG3   | 2.18                     | 0.67              |
| 1:D:235:GLU:O    | 1:D:238:THR:HB   | 1.95                     | 0.67              |
| 1:A:68:TRP:CE3   | 1:A:72:LEU:HD21  | 2.28                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:151:LYS:O    | 1:A:155:GLU:HG3  | 1.94                     | 0.67              |
| 1:C:185:LEU:HD13 | 1:C:198:GLU:HG2  | 1.75                     | 0.67              |
| 1:D:187:LEU:O    | 1:D:191:MET:HE3  | 1.95                     | 0.67              |
| 1:A:161:ILE:CG1  | 1:A:162:VAL:H    | 2.08                     | 0.67              |
| 1:D:12:TYR:O     | 1:D:15:LYS:HG3   | 1.95                     | 0.67              |
| 1:E:111:THR:OG1  | 1:E:113:PHE:N    | 2.27                     | 0.67              |
| 1:A:108:ILE:HG13 | 1:A:163:MET:HB2  | 1.75                     | 0.67              |
| 1:A:240:MET:HE2  | 1:A:240:MET:CA   | 2.21                     | 0.67              |
| 1:E:151:LYS:HE2  | 1:E:191:MET:HB3  | 1.75                     | 0.67              |
| 1:C:122:ALA:HB1  | 1:C:224:ALA:HB2  | 1.76                     | 0.67              |
| 1:A:45:ILE:HG22  | 1:A:45:ILE:O     | 1.93                     | 0.67              |
| 1:C:139:THR:HG22 | 1:C:140:VAL:H    | 1.60                     | 0.67              |
| 1:D:79:ILE:HG12  | 1:D:83:PHE:HE2   | 1.60                     | 0.67              |
| 1:D:146:LEU:HG   | 1:D:147:PRO:HD3  | 1.76                     | 0.67              |
| 1:A:127:LYS:HA   | 1:A:133:ILE:HD11 | 1.77                     | 0.66              |
| 1:C:46:THR:O     | 1:C:49:VAL:CG1   | 2.42                     | 0.66              |
| 1:E:37:VAL:HG11  | 1:E:81:ILE:HG13  | 1.77                     | 0.66              |
| 1:A:189:GLN:O    | 1:A:192:THR:O    | 2.12                     | 0.66              |
| 1:B:112:THR:HG1  | 1:B:139:THR:HG22 | 1.61                     | 0.66              |
| 1:D:121:ILE:HG21 | 1:D:217:LYS:O    | 1.93                     | 0.66              |
| 1:A:161:ILE:HG12 | 1:A:162:VAL:N    | 2.09                     | 0.66              |
| 1:D:63:PRO:C     | 1:D:66:ILE:H     | 2.02                     | 0.66              |
| 1:D:58:THR:O     | 1:D:59:VAL:HG13  | 1.95                     | 0.66              |
| 1:A:109:VAL:CG2  | 1:A:153:LEU:HD11 | 2.25                     | 0.66              |
| 1:C:153:LEU:HA   | 1:C:157:GLU:OE2  | 1.95                     | 0.66              |
| 1:C:182:SER:HA   | 1:C:185:LEU:HD12 | 1.76                     | 0.66              |
| 1:D:26:GLY:O     | 1:D:30:THR:HG22  | 1.95                     | 0.66              |
| 1:A:146:LEU:O    | 1:A:149:ALA:HB3  | 1.95                     | 0.66              |
| 1:C:153:LEU:O    | 1:C:157:GLU:HG2  | 1.95                     | 0.66              |
| 1:D:61:LEU:HD12  | 1:D:65:VAL:CG2   | 2.25                     | 0.66              |
| 1:A:234:PRO:HG2  | 1:A:235:GLU:OE2  | 1.94                     | 0.66              |
| 1:B:143:ILE:O    | 1:B:146:LEU:HD21 | 1.95                     | 0.66              |
| 1:A:65:VAL:O     | 1:A:66:ILE:HG13  | 1.96                     | 0.66              |
| 1:A:141:PRO:HD3  | 1:E:230:LEU:HD21 | 1.77                     | 0.66              |
| 1:C:189:GLN:O    | 1:C:192:THR:O    | 2.13                     | 0.66              |
| 1:B:179:HIS:NE2  | 1:B:183:LEU:HD11 | 2.11                     | 0.66              |
| 1:E:121:ILE:CG2  | 1:E:217:LYS:HB2  | 2.22                     | 0.66              |
| 1:B:189:GLN:O    | 1:B:192:THR:O    | 2.13                     | 0.65              |
| 1:C:126:LEU:HG   | 1:C:133:ILE:CD1  | 2.25                     | 0.65              |
| 1:A:149:ALA:O    | 1:A:153:LEU:HD12 | 1.95                     | 0.65              |
| 1:A:42:MET:CE    | 1:A:81:ILE:HG22  | 2.26                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:127:LYS:HA   | 1:D:133:ILE:HD11 | 1.76                     | 0.65              |
| 1:E:118:MET:O    | 1:E:121:ILE:HG12 | 1.95                     | 0.65              |
| 1:B:126:LEU:HG   | 1:B:133:ILE:CD1  | 2.23                     | 0.65              |
| 1:E:98:VAL:HG22  | 1:E:101:LYS:NZ   | 2.09                     | 0.65              |
| 1:B:61:LEU:HD13  | 1:B:63:PRO:HB3   | 1.78                     | 0.65              |
| 1:B:121:ILE:CG1  | 1:B:217:LYS:HZ2  | 2.10                     | 0.65              |
| 1:E:67:SER:OG    | 1:E:68:TRP:HZ3   | 1.79                     | 0.65              |
| 1:E:143:ILE:HD11 | 1:E:167:MET:O    | 1.96                     | 0.65              |
| 1:C:187:LEU:HD23 | 1:C:191:MET:HE1  | 1.77                     | 0.65              |
| 1:D:23:PHE:C     | 1:D:26:GLY:H     | 2.05                     | 0.65              |
| 1:E:48:PHE:HD2   | 1:E:49:VAL:HG23  | 1.60                     | 0.65              |
| 1:C:36:PHE:O     | 1:C:40:ILE:HB    | 1.96                     | 0.65              |
| 1:C:229:TYR:HA   | 1:C:233:LYS:HB3  | 1.79                     | 0.65              |
| 1:D:65:VAL:CG2   | 1:D:68:TRP:HB2   | 2.26                     | 0.65              |
| 1:E:79:ILE:O     | 1:E:83:PHE:N     | 2.24                     | 0.65              |
| 1:E:107:GLY:HA3  | 1:E:162:VAL:HG22 | 1.79                     | 0.65              |
| 1:B:182:SER:HA   | 1:B:185:LEU:CD1  | 2.27                     | 0.65              |
| 1:D:103:THR:C    | 1:D:104:LYS:HD2  | 2.22                     | 0.65              |
| 1:A:190:LEU:HD23 | 1:B:151:LYS:HD2  | 1.77                     | 0.65              |
| 1:A:240:MET:HE2  | 1:A:244:GLY:C    | 2.22                     | 0.65              |
| 1:B:228:TYR:O    | 1:B:232:PHE:HD1  | 1.80                     | 0.65              |
| 1:B:123:ILE:HD12 | 1:B:135:ILE:HG21 | 1.79                     | 0.64              |
| 1:B:243:LYS:HG3  | 1:B:254:PRO:HG3  | 1.78                     | 0.64              |
| 1:E:72:LEU:O     | 1:E:75:LEU:HG    | 1.97                     | 0.64              |
| 1:B:87:ILE:O     | 1:B:90:LYS:HG3   | 1.98                     | 0.64              |
| 1:B:99:GLU:O     | 1:B:100:LYS:HG2  | 1.96                     | 0.64              |
| 1:C:102:MET:O    | 1:C:232:PHE:CE1  | 2.50                     | 0.64              |
| 1:E:149:ALA:O    | 1:E:152:LYS:N    | 2.31                     | 0.64              |
| 1:D:107:GLY:O    | 1:D:162:VAL:HG22 | 1.97                     | 0.64              |
| 1:A:25:MET:HG3   | 1:E:86:PHE:CZ    | 2.32                     | 0.64              |
| 1:A:30:THR:HG23  | 1:A:31:ALA:N     | 2.13                     | 0.64              |
| 1:B:161:ILE:CG1  | 1:B:162:VAL:H    | 2.10                     | 0.64              |
| 1:C:168:PRO:HG2  | 1:C:202:HIS:N    | 2.12                     | 0.64              |
| 1:D:223:HIS:C    | 1:D:225:GLU:N    | 2.51                     | 0.64              |
| 1:A:104:LYS:HB2  | 1:A:134:LYS:CG   | 2.28                     | 0.64              |
| 1:C:107:GLY:C    | 1:C:108:ILE:HD12 | 2.22                     | 0.64              |
| 1:C:121:ILE:HD11 | 1:C:217:LYS:NZ   | 2.12                     | 0.64              |
| 1:A:101:LYS:HB3  | 1:A:101:LYS:NZ   | 2.13                     | 0.64              |
| 2:B:301:BNG:H3'1 | 2:B:301:BNG:C7'  | 2.27                     | 0.64              |
| 1:E:41:ILE:O     | 1:E:45:ILE:HB    | 1.98                     | 0.64              |
| 1:A:236:TYR:O    | 1:A:240:MET:HG2  | 1.98                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:113:PHE:HD1  | 1:B:113:PHE:O    | 1.81                     | 0.63              |
| 1:A:232:PHE:O    | 1:A:234:PRO:HD3  | 1.96                     | 0.63              |
| 1:E:33:ILE:O     | 1:E:36:PHE:HB3   | 1.99                     | 0.63              |
| 1:D:189:GLN:O    | 1:D:192:THR:O    | 2.16                     | 0.63              |
| 1:A:146:LEU:CG   | 1:A:147:PRO:HD3  | 2.28                     | 0.63              |
| 1:C:150:CYS:CB   | 1:C:196:ILE:HD11 | 2.25                     | 0.63              |
| 1:D:62:GLY:N     | 1:D:65:VAL:CG1   | 2.61                     | 0.63              |
| 1:D:93:LEU:HD22  | 1:D:93:LEU:O     | 1.98                     | 0.63              |
| 1:D:104:LYS:HA   | 1:D:104:LYS:HE3  | 1.79                     | 0.63              |
| 1:B:153:LEU:O    | 1:B:157:GLU:CG   | 2.46                     | 0.63              |
| 1:B:184:GLY:O    | 1:B:185:LEU:C    | 2.42                     | 0.63              |
| 1:B:153:LEU:HA   | 1:B:157:GLU:CD   | 2.23                     | 0.63              |
| 1:B:184:GLY:HA2  | 1:B:187:LEU:HD13 | 1.81                     | 0.63              |
| 1:C:164:ALA:CB   | 1:C:198:GLU:HA   | 2.29                     | 0.63              |
| 1:D:227:VAL:HG12 | 1:D:231:LEU:HD12 | 1.81                     | 0.63              |
| 1:E:15:LYS:HB3   | 1:E:18:PRO:HG2   | 1.79                     | 0.63              |
| 1:B:88:ILE:HD13  | 1:B:88:ILE:O     | 1.99                     | 0.63              |
| 1:B:183:LEU:O    | 1:B:187:LEU:HD12 | 1.99                     | 0.62              |
| 1:E:69:GLY:HA2   | 1:E:72:LEU:CD1   | 2.28                     | 0.62              |
| 1:E:168:PRO:HD2  | 1:E:201:VAL:C    | 2.24                     | 0.62              |
| 1:A:87:ILE:HG22  | 1:A:91:LYS:CE    | 2.27                     | 0.62              |
| 1:A:165:LEU:HD23 | 1:A:199:VAL:HG11 | 1.80                     | 0.62              |
| 1:A:15:LYS:O     | 1:A:18:PRO:HD2   | 1.99                     | 0.62              |
| 1:B:121:ILE:HG13 | 1:B:217:LYS:CB   | 2.29                     | 0.62              |
| 1:C:46:THR:H     | 1:C:47:PRO:HD2   | 1.65                     | 0.62              |
| 1:C:187:LEU:O    | 1:C:191:MET:HE3  | 1.99                     | 0.62              |
| 1:A:17:ILE:HD12  | 1:A:17:ILE:H     | 1.63                     | 0.62              |
| 1:A:123:ILE:HG23 | 1:A:135:ILE:HD13 | 1.82                     | 0.62              |
| 1:A:183:LEU:O    | 1:A:187:LEU:HD12 | 1.99                     | 0.62              |
| 1:B:121:ILE:HG13 | 1:B:217:LYS:HB2  | 1.81                     | 0.62              |
| 1:A:164:ALA:O    | 1:A:165:LEU:C    | 2.43                     | 0.62              |
| 1:E:46:THR:C     | 1:E:48:PHE:H     | 2.08                     | 0.62              |
| 1:E:98:VAL:HA    | 1:E:101:LYS:NZ   | 2.14                     | 0.62              |
| 1:D:150:CYS:HA   | 1:D:153:LEU:HD13 | 1.82                     | 0.62              |
| 1:A:41:ILE:O     | 1:A:44:ILE:HG23  | 2.00                     | 0.62              |
| 1:A:189:GLN:HB3  | 1:B:148:VAL:HG13 | 1.81                     | 0.62              |
| 1:D:195:HIS:HE1  | 1:E:149:ALA:HB2  | 1.65                     | 0.62              |
| 1:E:225:GLU:HG2  | 1:E:229:TYR:CE2  | 2.34                     | 0.62              |
| 1:A:32:LEU:HD13  | 1:A:32:LEU:C     | 2.24                     | 0.62              |
| 1:A:101:LYS:HB3  | 1:A:101:LYS:HZ3  | 1.65                     | 0.62              |
| 1:C:107:GLY:HA2  | 1:C:136:ILE:H    | 1.64                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:223:HIS:O    | 1:E:224:ALA:C    | 2.42                     | 0.62              |
| 1:A:90:LYS:HE2   | 1:C:7:PHE:CD1    | 2.35                     | 0.61              |
| 1:C:7:PHE:CZ     | 1:C:11:LEU:HD11  | 2.34                     | 0.61              |
| 1:D:102:MET:CE   | 1:D:231:LEU:HD23 | 2.13                     | 0.61              |
| 1:D:234:PRO:HG2  | 1:D:235:GLU:H    | 1.65                     | 0.61              |
| 1:D:237:LEU:HD12 | 1:D:237:LEU:H    | 1.65                     | 0.61              |
| 1:C:134:LYS:HD2  | 1:C:134:LYS:N    | 2.08                     | 0.61              |
| 1:A:42:MET:HE3   | 1:A:81:ILE:HG22  | 1.82                     | 0.61              |
| 1:A:99:GLU:HA    | 1:A:99:GLU:OE1   | 1.95                     | 0.61              |
| 1:B:126:LEU:HD23 | 1:B:135:ILE:CD1  | 2.29                     | 0.61              |
| 1:D:231:LEU:HD22 | 1:D:232:PHE:CZ   | 2.35                     | 0.61              |
| 1:C:7:PHE:CE1    | 1:C:11:LEU:HG    | 2.36                     | 0.61              |
| 1:C:113:PHE:HB2  | 1:C:142:GLY:HA2  | 1.82                     | 0.61              |
| 1:B:115:ARG:O    | 1:B:116:VAL:HG23 | 2.00                     | 0.61              |
| 1:C:113:PHE:HB2  | 1:C:141:PRO:O    | 2.00                     | 0.61              |
| 1:E:76:VAL:O     | 1:E:80:ILE:HG13  | 2.01                     | 0.61              |
| 1:D:233:LYS:HE2  | 1:D:236:TYR:HB2  | 1.83                     | 0.61              |
| 1:B:148:VAL:O    | 1:B:152:LYS:HG3  | 2.01                     | 0.61              |
| 1:B:199:VAL:O    | 1:B:201:VAL:HG13 | 2.01                     | 0.61              |
| 1:D:37:VAL:CG2   | 1:D:88:ILE:HG13  | 2.30                     | 0.61              |
| 1:A:7:PHE:CE2    | 1:D:90:LYS:HB2   | 2.35                     | 0.61              |
| 1:A:30:THR:HG23  | 1:A:31:ALA:H     | 1.65                     | 0.61              |
| 1:C:125:LYS:O    | 1:C:129:LEU:HD13 | 1.99                     | 0.61              |
| 1:C:154:LEU:HD21 | 1:C:162:VAL:HB   | 1.83                     | 0.61              |
| 1:C:162:VAL:CG1  | 1:C:163:MET:N    | 2.62                     | 0.61              |
| 1:C:186:MET:HE1  | 1:D:180:GLU:HB3  | 1.83                     | 0.61              |
| 1:E:107:GLY:O    | 1:E:108:ILE:HD12 | 2.01                     | 0.61              |
| 1:A:100:LYS:HE2  | 1:B:12:TYR:CG    | 2.36                     | 0.61              |
| 1:B:137:ARG:O    | 1:B:138:LYS:HB2  | 2.00                     | 0.61              |
| 1:B:190:LEU:O    | 1:C:151:LYS:HE3  | 2.01                     | 0.61              |
| 1:C:66:ILE:CG1   | 1:C:68:TRP:HD1   | 2.13                     | 0.61              |
| 1:C:213:ASP:O    | 1:C:217:LYS:HG2  | 2.00                     | 0.61              |
| 1:C:126:LEU:C    | 1:C:133:ILE:HD11 | 2.25                     | 0.60              |
| 1:C:111:THR:OG1  | 1:C:114:ALA:HB2  | 2.01                     | 0.60              |
| 1:C:201:VAL:HG23 | 1:C:201:VAL:O    | 2.00                     | 0.60              |
| 1:B:144:LYS:O    | 1:B:147:PRO:HD2  | 2.01                     | 0.60              |
| 1:C:66:ILE:CG1   | 1:C:68:TRP:CD1   | 2.76                     | 0.60              |
| 1:D:154:LEU:HD11 | 1:D:196:ILE:HG13 | 1.82                     | 0.60              |
| 1:D:88:ILE:HD13  | 1:D:88:ILE:O     | 2.00                     | 0.60              |
| 1:A:197:ILE:N    | 1:A:197:ILE:CD1  | 2.65                     | 0.60              |
| 1:B:23:PHE:CE2   | 2:B:301:BNG:H3   | 2.36                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:77:ASN:HA    | 1:D:80:ILE:HD12  | 1.83                     | 0.60              |
| 1:D:108:ILE:HD11 | 1:D:163:MET:HG3  | 1.83                     | 0.60              |
| 1:A:226:ASN:HA   | 1:A:229:TYR:HD2  | 1.66                     | 0.60              |
| 1:D:229:TYR:CB   | 1:D:237:LEU:HD11 | 2.32                     | 0.60              |
| 1:A:111:THR:HG21 | 1:A:114:ALA:CB   | 2.32                     | 0.60              |
| 1:C:102:MET:O    | 1:C:232:PHE:HE1  | 1.84                     | 0.60              |
| 1:D:111:THR:HG21 | 1:D:166:GLY:HA2  | 1.84                     | 0.60              |
| 1:C:93:LEU:O     | 1:C:96:GLU:HB3   | 2.02                     | 0.60              |
| 1:D:194:LYS:H    | 1:E:148:VAL:HG11 | 1.67                     | 0.60              |
| 1:B:78:PHE:CE1   | 1:C:32:LEU:HA    | 2.37                     | 0.60              |
| 1:C:178:ALA:HA   | 1:C:200:PHE:HE2  | 1.66                     | 0.60              |
| 1:B:193:ASN:O    | 1:B:194:LYS:CD   | 2.35                     | 0.60              |
| 1:C:109:VAL:O    | 1:C:165:LEU:HB2  | 2.01                     | 0.60              |
| 1:D:61:LEU:HB3   | 1:D:65:VAL:CB    | 2.31                     | 0.60              |
| 1:D:81:ILE:O     | 1:D:85:VAL:HG23  | 2.01                     | 0.60              |
| 1:B:182:SER:CA   | 1:B:185:LEU:HD12 | 2.32                     | 0.59              |
| 1:D:79:ILE:HG12  | 1:D:83:PHE:CE2   | 2.37                     | 0.59              |
| 1:D:110:ASP:O    | 1:D:139:THR:HG23 | 2.01                     | 0.59              |
| 1:D:159:CYS:O    | 1:D:161:ILE:N    | 2.34                     | 0.59              |
| 1:A:148:VAL:CG2  | 1:E:189:GLN:HB3  | 2.31                     | 0.59              |
| 1:B:177:CYS:O    | 1:B:180:GLU:HB2  | 2.02                     | 0.59              |
| 1:D:121:ILE:HG21 | 1:D:217:LYS:HB2  | 1.84                     | 0.59              |
| 1:A:39:ASN:HB3   | 1:E:71:PHE:CD2   | 2.38                     | 0.59              |
| 1:B:153:LEU:HA   | 1:B:157:GLU:OE2  | 2.03                     | 0.59              |
| 1:A:100:LYS:O    | 1:A:102:MET:O    | 2.20                     | 0.59              |
| 1:B:226:ASN:HA   | 1:B:229:TYR:HD2  | 1.68                     | 0.59              |
| 1:D:111:THR:HG22 | 1:D:165:LEU:O    | 2.02                     | 0.59              |
| 1:D:127:LYS:CA   | 1:D:133:ILE:HD11 | 2.32                     | 0.59              |
| 1:E:68:TRP:N     | 1:E:68:TRP:CE3   | 2.69                     | 0.59              |
| 1:E:155:GLU:C    | 1:E:156:GLU:HG3  | 2.27                     | 0.59              |
| 1:A:40:ILE:HG13  | 1:A:41:ILE:H     | 1.67                     | 0.59              |
| 1:C:161:ILE:HG13 | 1:C:195:HIS:O    | 2.02                     | 0.59              |
| 1:D:65:VAL:HA    | 1:D:68:TRP:HD1   | 1.68                     | 0.59              |
| 1:D:125:LYS:HG2  | 1:D:221:GLU:HG3  | 1.85                     | 0.59              |
| 1:E:98:VAL:HA    | 1:E:101:LYS:CD   | 2.30                     | 0.59              |
| 1:A:104:LYS:O    | 1:A:105:LYS:HB2  | 2.02                     | 0.59              |
| 1:A:109:VAL:HG21 | 1:A:153:LEU:CD1  | 2.33                     | 0.59              |
| 1:B:146:LEU:HD23 | 1:B:146:LEU:N    | 2.14                     | 0.59              |
| 1:C:46:THR:N     | 1:C:47:PRO:HD2   | 2.18                     | 0.59              |
| 1:E:186:MET:O    | 1:E:190:LEU:HD12 | 2.02                     | 0.59              |
| 1:A:36:PHE:O     | 1:A:40:ILE:CG1   | 2.45                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:176:VAL:O    | 1:B:180:GLU:HG3  | 2.03                     | 0.59              |
| 1:D:11:LEU:O     | 1:D:15:LYS:HA    | 2.03                     | 0.59              |
| 1:D:64:ILE:HG12  | 1:E:44:ILE:HD12  | 1.85                     | 0.59              |
| 1:D:183:LEU:O    | 1:D:187:LEU:CD1  | 2.51                     | 0.58              |
| 1:D:151:LYS:O    | 1:D:155:GLU:N    | 2.33                     | 0.58              |
| 1:A:148:VAL:O    | 1:A:151:LYS:HB3  | 2.02                     | 0.58              |
| 1:B:111:THR:OG1  | 1:B:112:THR:N    | 2.34                     | 0.58              |
| 1:C:214:TRP:HE1  | 1:C:218:ARG:HD2  | 1.68                     | 0.58              |
| 1:E:75:LEU:O     | 1:E:79:ILE:HG13  | 2.03                     | 0.58              |
| 1:A:41:ILE:HG13  | 1:A:88:ILE:HG21  | 1.84                     | 0.58              |
| 1:B:23:PHE:CZ    | 2:B:301:BNG:H3   | 2.39                     | 0.58              |
| 1:D:223:HIS:O    | 1:D:227:VAL:HG23 | 2.04                     | 0.58              |
| 1:E:151:LYS:HZ2  | 1:E:155:GLU:CD   | 2.11                     | 0.58              |
| 1:A:98:VAL:O     | 1:A:99:GLU:HB2   | 2.03                     | 0.58              |
| 1:C:223:HIS:CE1  | 1:C:247:GLN:CB   | 2.86                     | 0.58              |
| 1:D:25:MET:HG2   | 1:D:29:SER:HB3   | 1.83                     | 0.58              |
| 1:D:25:MET:HG2   | 1:E:16:VAL:HG13  | 1.85                     | 0.58              |
| 1:E:185:LEU:O    | 1:E:189:GLN:HG3  | 2.04                     | 0.58              |
| 1:B:121:ILE:HG13 | 1:B:217:LYS:HZ2  | 1.67                     | 0.58              |
| 1:D:166:GLY:O    | 1:D:201:VAL:HG22 | 2.03                     | 0.58              |
| 1:A:98:VAL:O     | 1:A:98:VAL:CG2   | 2.52                     | 0.58              |
| 1:A:165:LEU:CA   | 1:A:199:VAL:HB   | 2.33                     | 0.58              |
| 1:B:165:LEU:CD2  | 1:B:199:VAL:HG11 | 2.28                     | 0.58              |
| 1:A:101:LYS:O    | 1:A:102:MET:C    | 2.44                     | 0.58              |
| 1:B:134:LYS:H    | 1:B:134:LYS:HD2  | 1.69                     | 0.58              |
| 1:D:223:HIS:C    | 1:D:225:GLU:H    | 2.12                     | 0.58              |
| 1:E:88:ILE:HD13  | 1:E:88:ILE:O     | 2.03                     | 0.58              |
| 1:A:163:MET:HE2  | 1:A:165:LEU:CD2  | 2.31                     | 0.58              |
| 1:C:75:LEU:O     | 1:C:79:ILE:HG13  | 2.03                     | 0.58              |
| 1:D:65:VAL:O     | 1:D:68:TRP:N     | 2.37                     | 0.58              |
| 1:A:17:ILE:HB    | 1:A:18:PRO:HD3   | 1.86                     | 0.57              |
| 1:A:107:GLY:O    | 1:A:162:VAL:HG22 | 2.04                     | 0.57              |
| 1:A:111:THR:OG1  | 1:A:114:ALA:N    | 2.34                     | 0.57              |
| 1:B:111:THR:O    | 1:B:139:THR:HG21 | 2.03                     | 0.57              |
| 1:B:122:ALA:CB   | 1:B:224:ALA:HB2  | 2.27                     | 0.57              |
| 1:C:41:ILE:O     | 1:C:45:ILE:HB    | 2.04                     | 0.57              |
| 1:D:37:VAL:O     | 1:D:40:ILE:O     | 2.21                     | 0.57              |
| 1:D:105:LYS:CE   | 1:D:158:GLY:HA3  | 2.34                     | 0.57              |
| 1:A:213:ASP:O    | 1:A:217:LYS:HG2  | 2.04                     | 0.57              |
| 1:A:242:GLY:O    | 1:A:243:LYS:CB   | 2.52                     | 0.57              |
| 1:C:86:PHE:CD1   | 1:E:7:PHE:HZ     | 2.22                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:111:THR:HG21 | 1:D:166:GLY:CA   | 2.35                     | 0.57              |
| 1:B:189:GLN:HG2  | 1:B:196:ILE:HB   | 1.84                     | 0.57              |
| 1:B:233:LYS:HE2  | 1:B:236:TYR:HB2  | 1.86                     | 0.57              |
| 1:C:17:ILE:HD12  | 1:C:17:ILE:N     | 2.13                     | 0.57              |
| 1:C:161:ILE:HD11 | 1:C:197:ILE:CG1  | 2.34                     | 0.57              |
| 1:D:227:VAL:HG12 | 1:D:231:LEU:CD1  | 2.35                     | 0.57              |
| 1:E:68:TRP:C     | 1:E:72:LEU:HG    | 2.27                     | 0.57              |
| 1:E:98:VAL:CA    | 1:E:101:LYS:HZ3  | 2.18                     | 0.57              |
| 1:A:164:ALA:HB3  | 1:A:199:VAL:H    | 1.69                     | 0.57              |
| 1:A:224:ALA:O    | 1:A:227:VAL:HB   | 2.05                     | 0.57              |
| 1:C:110:ASP:O    | 1:C:139:THR:CG2  | 2.51                     | 0.57              |
| 1:A:119:ALA:HA   | 1:A:165:LEU:CD1  | 2.35                     | 0.57              |
| 1:A:163:MET:HE3  | 1:A:223:HIS:HB2  | 1.86                     | 0.57              |
| 1:D:105:LYS:HE2  | 1:D:158:GLY:HA3  | 1.87                     | 0.57              |
| 1:A:146:LEU:H    | 1:A:146:LEU:CD2  | 2.13                     | 0.57              |
| 1:A:202:HIS:N    | 1:A:205:GLU:OE2  | 2.35                     | 0.57              |
| 1:C:42:MET:H     | 1:C:43:PRO:HD2   | 1.69                     | 0.57              |
| 1:D:71:PHE:CE2   | 1:E:40:ILE:HD12  | 2.27                     | 0.57              |
| 1:A:143:ILE:C    | 1:A:146:LEU:HD21 | 2.29                     | 0.57              |
| 1:A:206:ALA:HA   | 1:A:211:GLU:OE2  | 2.05                     | 0.57              |
| 1:D:206:ALA:HA   | 1:D:211:GLU:OE2  | 2.05                     | 0.57              |
| 1:A:105:LYS:HA   | 1:A:134:LYS:O    | 2.05                     | 0.57              |
| 1:C:123:ILE:HD12 | 1:C:135:ILE:HG21 | 1.86                     | 0.57              |
| 1:D:63:PRO:CD    | 1:D:64:ILE:H     | 2.17                     | 0.57              |
| 1:D:164:ALA:HB3  | 1:D:198:GLU:HA   | 1.85                     | 0.57              |
| 1:A:7:PHE:HE1    | 1:A:11:LEU:HD21  | 1.70                     | 0.57              |
| 1:A:143:ILE:HA   | 1:A:146:LEU:HD21 | 1.85                     | 0.57              |
| 1:B:145:ASP:O    | 1:B:148:VAL:HG22 | 2.05                     | 0.57              |
| 1:B:182:SER:N    | 1:B:185:LEU:HD12 | 2.20                     | 0.57              |
| 1:C:113:PHE:HD1  | 1:C:113:PHE:O    | 1.88                     | 0.57              |
| 1:C:213:ASP:OD1  | 1:C:217:LYS:HD2  | 2.05                     | 0.57              |
| 1:E:98:VAL:HA    | 1:E:101:LYS:HZ3  | 1.69                     | 0.57              |
| 1:B:187:LEU:O    | 1:B:190:LEU:N    | 2.37                     | 0.56              |
| 1:C:163:MET:HE2  | 1:C:199:VAL:CG2  | 2.26                     | 0.56              |
| 1:D:222:GLU:C    | 1:D:225:GLU:HB3  | 2.29                     | 0.56              |
| 1:C:42:MET:O     | 1:C:47:PRO:HD3   | 2.05                     | 0.56              |
| 1:D:148:VAL:O    | 1:D:152:LYS:HG3  | 2.04                     | 0.56              |
| 1:A:100:LYS:O    | 1:A:100:LYS:HG2  | 2.05                     | 0.56              |
| 1:C:139:THR:HG22 | 1:C:140:VAL:N    | 2.21                     | 0.56              |
| 1:C:154:LEU:HD11 | 1:C:196:ILE:CG1  | 2.32                     | 0.56              |
| 1:C:164:ALA:HB3  | 1:C:199:VAL:N    | 2.17                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:182:SER:HA   | 1:E:185:LEU:CD1  | 2.26                     | 0.56              |
| 1:C:107:GLY:HA2  | 1:C:136:ILE:O    | 2.04                     | 0.56              |
| 1:A:223:HIS:O    | 1:A:224:ALA:C    | 2.49                     | 0.56              |
| 1:B:161:ILE:CG1  | 1:B:162:VAL:N    | 2.67                     | 0.56              |
| 1:D:126:LEU:HG   | 1:D:133:ILE:HD13 | 1.85                     | 0.56              |
| 1:D:162:VAL:CG1  | 1:D:163:MET:N    | 2.67                     | 0.56              |
| 1:E:83:PHE:O     | 1:E:87:ILE:HG12  | 2.05                     | 0.56              |
| 1:A:145:ASP:C    | 1:A:147:PRO:CD   | 2.75                     | 0.56              |
| 1:E:125:LYS:O    | 1:E:125:LYS:HG3  | 2.05                     | 0.56              |
| 1:C:129:LEU:HD23 | 1:C:228:TYR:CD2  | 2.39                     | 0.56              |
| 1:D:78:PHE:HE2   | 1:E:35:SER:CB    | 2.19                     | 0.56              |
| 1:D:154:LEU:HD11 | 1:D:196:ILE:CG1  | 2.36                     | 0.56              |
| 1:D:194:LYS:H    | 1:E:148:VAL:CG1  | 2.19                     | 0.56              |
| 1:B:98:VAL:O     | 1:B:98:VAL:HG12  | 2.05                     | 0.56              |
| 1:B:105:LYS:HE3  | 1:B:158:GLY:HA3  | 1.86                     | 0.56              |
| 1:B:151:LYS:O    | 1:B:155:GLU:HG3  | 2.05                     | 0.56              |
| 1:B:161:ILE:HG21 | 1:B:231:LEU:HD11 | 1.87                     | 0.56              |
| 1:C:123:ILE:CD1  | 1:C:135:ILE:HG21 | 2.36                     | 0.56              |
| 1:C:87:ILE:CG2   | 1:C:91:LYS:HE2   | 2.24                     | 0.56              |
| 1:C:234:PRO:HG2  | 1:C:235:GLU:H    | 1.71                     | 0.56              |
| 1:E:67:SER:C     | 1:E:68:TRP:HE3   | 2.14                     | 0.56              |
| 1:E:217:LYS:HB3  | 1:E:217:LYS:HZ2  | 1.70                     | 0.56              |
| 1:C:210:LYS:O    | 1:C:213:ASP:HB3  | 2.06                     | 0.55              |
| 1:C:218:ARG:O    | 1:C:222:GLU:HG3  | 2.06                     | 0.55              |
| 1:D:143:ILE:O    | 1:D:146:LEU:HD21 | 2.06                     | 0.55              |
| 1:D:187:LEU:HB3  | 1:D:191:MET:HE1  | 1.87                     | 0.55              |
| 1:D:202:HIS:N    | 1:D:205:GLU:OE2  | 2.39                     | 0.55              |
| 1:E:15:LYS:C     | 1:E:18:PRO:HD2   | 2.31                     | 0.55              |
| 1:E:110:ASP:O    | 1:E:139:THR:CG2  | 2.53                     | 0.55              |
| 1:B:125:LYS:CB   | 1:B:221:GLU:HG3  | 2.36                     | 0.55              |
| 1:B:143:ILE:C    | 1:B:146:LEU:HD21 | 2.31                     | 0.55              |
| 1:C:46:THR:H     | 1:C:47:PRO:CD    | 2.19                     | 0.55              |
| 1:C:230:LEU:HD11 | 1:D:141:PRO:HD3  | 1.88                     | 0.55              |
| 1:B:86:PHE:O     | 1:D:7:PHE:HZ     | 1.89                     | 0.55              |
| 1:B:125:LYS:CE   | 1:B:129:LEU:HD11 | 2.34                     | 0.55              |
| 1:E:123:ILE:HG23 | 1:E:135:ILE:HD13 | 1.87                     | 0.55              |
| 1:B:106:VAL:HG12 | 1:B:108:ILE:HD11 | 1.89                     | 0.55              |
| 1:B:176:VAL:HG12 | 1:B:180:GLU:OE2  | 2.07                     | 0.55              |
| 1:B:185:LEU:O    | 1:B:188:ALA:CB   | 2.50                     | 0.55              |
| 1:D:78:PHE:CE2   | 1:E:35:SER:CB    | 2.90                     | 0.55              |
| 1:D:127:LYS:N    | 1:D:133:ILE:HD11 | 2.22                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:4:PHE:C      | 1:E:6:GLU:H      | 2.15                     | 0.55              |
| 1:E:110:ASP:C    | 1:E:139:THR:HG23 | 2.30                     | 0.55              |
| 1:C:150:CYS:O    | 1:C:154:LEU:HG   | 2.07                     | 0.55              |
| 1:D:78:PHE:CE2   | 1:E:35:SER:HB3   | 2.42                     | 0.55              |
| 1:D:143:ILE:HA   | 1:D:146:LEU:HD21 | 1.88                     | 0.55              |
| 1:E:27:ILE:HA    | 1:E:30:THR:HG22  | 1.88                     | 0.55              |
| 1:E:98:VAL:O     | 1:E:101:LYS:HB2  | 2.06                     | 0.55              |
| 1:B:214:TRP:O    | 1:B:215:LEU:C    | 2.50                     | 0.55              |
| 1:B:222:GLU:OE1  | 1:B:247:GLN:HA   | 2.07                     | 0.55              |
| 1:D:125:LYS:O    | 1:D:129:LEU:HD13 | 2.06                     | 0.55              |
| 1:A:112:THR:HB   | 1:A:141:PRO:CA   | 2.24                     | 0.55              |
| 1:B:78:PHE:C     | 1:B:78:PHE:CD1   | 2.84                     | 0.55              |
| 1:B:217:LYS:O    | 1:B:218:ARG:C    | 2.49                     | 0.55              |
| 1:A:28:ALA:O     | 1:A:32:LEU:HB2   | 2.07                     | 0.55              |
| 1:C:179:HIS:CD2  | 1:C:183:LEU:HD11 | 2.42                     | 0.55              |
| 1:C:233:LYS:O    | 1:C:237:LEU:HD11 | 2.07                     | 0.55              |
| 1:D:30:THR:OG1   | 1:E:24:ILE:HB    | 2.07                     | 0.55              |
| 1:A:226:ASN:O    | 1:A:227:VAL:C    | 2.50                     | 0.55              |
| 1:B:212:LEU:C    | 1:B:212:LEU:HD23 | 2.31                     | 0.55              |
| 1:B:168:PRO:O    | 1:B:203:GLU:OE2  | 2.25                     | 0.54              |
| 1:C:66:ILE:HG13  | 1:C:67:SER:N     | 2.13                     | 0.54              |
| 1:C:102:MET:HE3  | 1:C:102:MET:HA   | 1.88                     | 0.54              |
| 1:D:167:MET:SD   | 1:D:203:GLU:HG2  | 2.47                     | 0.54              |
| 1:E:145:ASP:O    | 1:E:147:PRO:N    | 2.40                     | 0.54              |
| 1:E:206:ALA:HA   | 1:E:211:GLU:OE2  | 2.07                     | 0.54              |
| 1:E:223:HIS:O    | 1:E:226:ASN:N    | 2.40                     | 0.54              |
| 1:A:229:TYR:HB2  | 1:A:237:LEU:HD11 | 1.88                     | 0.54              |
| 1:D:37:VAL:HA    | 1:D:41:ILE:HB    | 1.89                     | 0.54              |
| 1:E:99:GLU:CD    | 1:E:99:GLU:O     | 2.50                     | 0.54              |
| 1:E:156:GLU:O    | 1:E:157:GLU:CB   | 2.56                     | 0.54              |
| 1:A:123:ILE:HG23 | 1:A:135:ILE:CD1  | 2.37                     | 0.54              |
| 1:D:49:VAL:HG13  | 1:D:49:VAL:O     | 2.07                     | 0.54              |
| 1:A:40:ILE:O     | 1:A:44:ILE:CG2   | 2.55                     | 0.54              |
| 1:B:21:ILE:O     | 1:B:24:ILE:HG22  | 2.07                     | 0.54              |
| 1:B:129:LEU:HD12 | 1:B:129:LEU:N    | 2.23                     | 0.54              |
| 1:B:217:LYS:O    | 1:B:220:ALA:N    | 2.40                     | 0.54              |
| 1:B:232:PHE:CD1  | 1:B:232:PHE:N    | 2.75                     | 0.54              |
| 1:E:143:ILE:HG22 | 1:E:144:LYS:HG3  | 1.89                     | 0.54              |
| 1:C:121:ILE:HG21 | 1:C:220:ALA:HB3  | 1.89                     | 0.54              |
| 1:D:164:ALA:H    | 1:D:199:VAL:HG23 | 1.72                     | 0.54              |
| 1:D:227:VAL:O    | 1:D:231:LEU:HD12 | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:179:HIS:O    | 1:E:183:LEU:HG   | 2.08                     | 0.54              |
| 1:A:201:VAL:HG12 | 1:A:219:ARG:NH2  | 2.23                     | 0.54              |
| 1:E:163:MET:HE1  | 1:E:220:ALA:O    | 2.07                     | 0.54              |
| 1:A:146:LEU:HG   | 1:A:147:PRO:CD   | 2.34                     | 0.54              |
| 1:A:164:ALA:HB3  | 1:A:198:GLU:HA   | 1.89                     | 0.54              |
| 1:B:15:LYS:O     | 1:B:18:PRO:HD2   | 2.07                     | 0.54              |
| 1:E:49:VAL:C     | 1:E:51:GLY:N     | 2.64                     | 0.54              |
| 1:E:102:MET:HE3  | 1:E:103:THR:H    | 1.73                     | 0.54              |
| 1:E:234:PRO:O    | 1:E:237:LEU:HD12 | 2.07                     | 0.54              |
| 1:B:33:ILE:O     | 1:B:36:PHE:HB3   | 2.07                     | 0.54              |
| 1:C:78:PHE:CE2   | 1:D:32:LEU:HA    | 2.43                     | 0.54              |
| 1:C:37:VAL:HG22  | 1:C:88:ILE:CG1   | 2.09                     | 0.53              |
| 1:D:162:VAL:O    | 1:D:197:ILE:N    | 2.31                     | 0.53              |
| 1:A:235:GLU:O    | 1:A:238:THR:HB   | 2.08                     | 0.53              |
| 1:B:234:PRO:HG2  | 1:B:235:GLU:N    | 2.24                     | 0.53              |
| 1:E:107:GLY:C    | 1:E:108:ILE:HD12 | 2.33                     | 0.53              |
| 1:E:139:THR:HG22 | 1:E:140:VAL:N    | 2.23                     | 0.53              |
| 1:E:222:GLU:C    | 1:E:225:GLU:HB3  | 2.31                     | 0.53              |
| 1:A:118:MET:O    | 1:A:120:SER:N    | 2.42                     | 0.53              |
| 1:B:224:ALA:O    | 1:B:227:VAL:HB   | 2.08                     | 0.53              |
| 1:D:40:ILE:HG22  | 1:D:41:ILE:N     | 2.21                     | 0.53              |
| 1:D:101:LYS:NZ   | 1:D:101:LYS:HB3  | 2.23                     | 0.53              |
| 1:D:164:ALA:N    | 1:D:197:ILE:O    | 2.37                     | 0.53              |
| 1:E:36:PHE:C     | 1:E:40:ILE:HG13  | 2.32                     | 0.53              |
| 1:E:121:ILE:HG13 | 1:E:217:LYS:HB3  | 1.88                     | 0.53              |
| 1:A:165:LEU:HD23 | 1:A:199:VAL:CG2  | 2.31                     | 0.53              |
| 1:B:75:LEU:HD12  | 1:B:75:LEU:C     | 2.33                     | 0.53              |
| 1:B:87:ILE:HG22  | 1:B:91:LYS:HE2   | 1.89                     | 0.53              |
| 1:C:87:ILE:O     | 1:C:91:LYS:HG3   | 2.08                     | 0.53              |
| 1:C:179:HIS:CD2  | 1:C:183:LEU:HD21 | 2.43                     | 0.53              |
| 1:D:103:THR:H    | 1:D:104:LYS:HD2  | 1.73                     | 0.53              |
| 1:E:168:PRO:HD2  | 1:E:201:VAL:O    | 2.08                     | 0.53              |
| 1:A:223:HIS:O    | 1:A:226:ASN:N    | 2.42                     | 0.53              |
| 1:D:15:LYS:HB3   | 1:D:18:PRO:HG2   | 1.90                     | 0.53              |
| 1:D:186:MET:HE1  | 1:E:180:GLU:O    | 2.08                     | 0.53              |
| 1:A:219:ARG:O    | 1:A:220:ALA:C    | 2.51                     | 0.53              |
| 1:A:228:TYR:CE1  | 1:A:232:PHE:CE1  | 2.97                     | 0.53              |
| 1:C:30:THR:HG23  | 1:C:31:ALA:N     | 2.24                     | 0.53              |
| 1:C:149:ALA:O    | 1:C:153:LEU:HD13 | 2.05                     | 0.53              |
| 1:C:233:LYS:CE   | 1:C:236:TYR:HB2  | 2.37                     | 0.53              |
| 1:D:161:ILE:HG12 | 1:D:162:VAL:N    | 2.22                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:140:VAL:HB   | 1:E:141:PRO:HD2  | 1.90                     | 0.53              |
| 1:B:169:GLY:HA2  | 1:B:203:GLU:OE2  | 2.09                     | 0.53              |
| 1:E:145:ASP:C    | 1:E:147:PRO:HD2  | 2.34                     | 0.53              |
| 1:A:26:GLY:O     | 1:A:30:THR:HG22  | 2.09                     | 0.53              |
| 1:B:161:ILE:HD13 | 1:B:227:VAL:HG13 | 1.90                     | 0.53              |
| 1:D:17:ILE:HG22  | 1:D:21:ILE:HD11  | 1.90                     | 0.53              |
| 1:D:203:GLU:C    | 1:D:205:GLU:H    | 2.17                     | 0.53              |
| 1:A:165:LEU:CD2  | 1:A:199:VAL:HG11 | 2.39                     | 0.53              |
| 1:A:240:MET:CE   | 1:A:244:GLY:C    | 2.82                     | 0.53              |
| 1:C:78:PHE:CD2   | 1:D:35:SER:HB3   | 2.44                     | 0.53              |
| 1:C:121:ILE:HG13 | 1:C:217:LYS:CB   | 2.39                     | 0.53              |
| 1:E:224:ALA:O    | 1:E:225:GLU:C    | 2.52                     | 0.53              |
| 1:A:40:ILE:CG1   | 1:A:41:ILE:N     | 2.67                     | 0.52              |
| 1:B:235:GLU:O    | 1:B:238:THR:HB   | 2.09                     | 0.52              |
| 1:E:146:LEU:O    | 1:E:149:ALA:HB3  | 2.09                     | 0.52              |
| 1:E:229:TYR:N    | 1:E:229:TYR:CD1  | 2.74                     | 0.52              |
| 1:A:29:SER:O     | 1:A:32:LEU:HB3   | 2.10                     | 0.52              |
| 1:A:98:VAL:O     | 1:A:99:GLU:CB    | 2.57                     | 0.52              |
| 1:B:39:ASN:O     | 1:B:43:PRO:HD2   | 2.09                     | 0.52              |
| 1:B:62:GLY:N     | 1:B:63:PRO:HA    | 2.24                     | 0.52              |
| 1:B:181:ALA:C    | 1:B:185:LEU:HD12 | 2.34                     | 0.52              |
| 1:A:118:MET:O    | 1:A:121:ILE:N    | 2.43                     | 0.52              |
| 1:D:160:ASP:O    | 1:D:161:ILE:CG2  | 2.48                     | 0.52              |
| 1:A:33:ILE:O     | 1:A:36:PHE:HB3   | 2.10                     | 0.52              |
| 1:C:179:HIS:O    | 1:C:183:LEU:HG   | 2.08                     | 0.52              |
| 1:C:214:TRP:O    | 1:C:215:LEU:C    | 2.53                     | 0.52              |
| 1:E:170:LYS:O    | 1:E:174:ASP:HB2  | 2.10                     | 0.52              |
| 1:C:122:ALA:CB   | 1:C:224:ALA:HB2  | 2.39                     | 0.52              |
| 1:C:243:LYS:HD2  | 1:C:243:LYS:H    | 1.74                     | 0.52              |
| 1:A:42:MET:C     | 1:A:44:ILE:N     | 2.66                     | 0.52              |
| 1:D:157:GLU:HG3  | 1:D:159:CYS:SG   | 2.50                     | 0.52              |
| 1:E:108:ILE:CG2  | 1:E:165:LEU:HD12 | 2.39                     | 0.52              |
| 1:A:47:PRO:HG2   | 1:A:49:VAL:O     | 2.10                     | 0.52              |
| 1:A:153:LEU:HA   | 1:A:157:GLU:OE2  | 2.08                     | 0.52              |
| 1:B:17:ILE:CD1   | 1:B:18:PRO:HD3   | 2.40                     | 0.52              |
| 1:B:61:LEU:HD12  | 1:B:63:PRO:CB    | 2.39                     | 0.52              |
| 1:C:63:PRO:C     | 1:C:65:VAL:H     | 2.05                     | 0.52              |
| 1:A:100:LYS:C    | 1:A:102:MET:N    | 2.65                     | 0.52              |
| 1:A:129:LEU:CD2  | 1:A:228:TYR:HB3  | 2.37                     | 0.52              |
| 1:A:149:ALA:C    | 1:A:153:LEU:HD12 | 2.34                     | 0.52              |
| 1:A:161:ILE:HD13 | 1:A:231:LEU:HD11 | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:161:ILE:HG21 | 1:A:231:LEU:HD11 | 1.90                     | 0.52              |
| 1:C:19:LEU:HD13  | 1:C:23:PHE:HB2   | 1.92                     | 0.52              |
| 1:C:226:ASN:O    | 1:C:230:LEU:HD12 | 2.10                     | 0.52              |
| 1:D:108:ILE:HG23 | 1:D:165:LEU:HG   | 1.90                     | 0.52              |
| 1:D:111:THR:CG2  | 1:D:166:GLY:HA2  | 2.39                     | 0.52              |
| 1:D:123:ILE:HG23 | 1:D:135:ILE:HD12 | 1.91                     | 0.52              |
| 1:D:161:ILE:CG1  | 1:D:162:VAL:N    | 2.73                     | 0.52              |
| 1:D:179:HIS:O    | 1:D:183:LEU:HG   | 2.09                     | 0.52              |
| 1:E:123:ILE:HD12 | 1:E:135:ILE:HG21 | 1.92                     | 0.52              |
| 1:E:234:PRO:HG2  | 1:E:235:GLU:CD   | 2.35                     | 0.52              |
| 1:A:42:MET:O     | 1:A:44:ILE:N     | 2.43                     | 0.52              |
| 1:D:133:ILE:O    | 1:D:133:ILE:HG13 | 2.10                     | 0.52              |
| 1:D:153:LEU:O    | 1:D:157:GLU:HG2  | 2.10                     | 0.52              |
| 1:E:37:VAL:HG12  | 1:E:81:ILE:HG13  | 1.89                     | 0.52              |
| 1:A:181:ALA:O    | 1:A:182:SER:C    | 2.52                     | 0.51              |
| 1:B:119:ALA:O    | 1:B:123:ILE:CG1  | 2.51                     | 0.51              |
| 1:C:196:ILE:HG22 | 1:C:196:ILE:O    | 2.10                     | 0.51              |
| 1:D:179:HIS:CD2  | 1:D:183:LEU:HD21 | 2.45                     | 0.51              |
| 1:E:107:GLY:CA   | 1:E:162:VAL:HG22 | 2.39                     | 0.51              |
| 1:E:121:ILE:HG13 | 1:E:217:LYS:CB   | 2.40                     | 0.51              |
| 1:A:39:ASN:HD21  | 1:E:68:TRP:HA    | 1.75                     | 0.51              |
| 1:C:242:GLY:HA3  | 1:D:117:ASP:HB2  | 1.91                     | 0.51              |
| 1:D:107:GLY:O    | 1:D:108:ILE:HD12 | 2.11                     | 0.51              |
| 1:A:42:MET:C     | 1:A:44:ILE:H     | 2.17                     | 0.51              |
| 1:A:225:GLU:HG2  | 1:A:229:TYR:OH   | 2.10                     | 0.51              |
| 1:B:77:ASN:HA    | 1:B:80:ILE:HD12  | 1.92                     | 0.51              |
| 1:C:119:ALA:O    | 1:C:123:ILE:HG12 | 2.09                     | 0.51              |
| 1:C:162:VAL:HG12 | 1:C:163:MET:N    | 2.24                     | 0.51              |
| 1:D:109:VAL:O    | 1:D:165:LEU:HB2  | 2.10                     | 0.51              |
| 1:D:161:ILE:HD11 | 1:D:197:ILE:CG1  | 2.41                     | 0.51              |
| 1:E:23:PHE:CD1   | 1:E:23:PHE:C     | 2.88                     | 0.51              |
| 1:B:42:MET:CB    | 1:B:43:PRO:HD3   | 2.40                     | 0.51              |
| 1:A:139:THR:CG2  | 1:A:140:VAL:H    | 2.21                     | 0.51              |
| 1:B:206:ALA:HA   | 1:B:211:GLU:OE2  | 2.10                     | 0.51              |
| 1:C:120:SER:O    | 1:C:121:ILE:C    | 2.53                     | 0.51              |
| 1:C:217:LYS:HZ2  | 1:C:217:LYS:HB3  | 1.73                     | 0.51              |
| 1:D:143:ILE:C    | 1:D:146:LEU:HD21 | 2.35                     | 0.51              |
| 1:E:111:THR:HA   | 1:E:140:VAL:O    | 2.11                     | 0.51              |
| 1:A:7:PHE:HE1    | 1:A:11:LEU:CD2   | 2.23                     | 0.51              |
| 1:D:164:ALA:O    | 1:D:199:VAL:CB   | 2.58                     | 0.51              |
| 1:E:26:GLY:O     | 1:E:30:THR:N     | 2.43                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:46:THR:C     | 1:E:48:PHE:N     | 2.67                     | 0.51              |
| 1:E:161:ILE:CD1  | 1:E:227:VAL:HG13 | 2.35                     | 0.51              |
| 1:E:235:GLU:HA   | 1:E:238:THR:HB   | 1.92                     | 0.51              |
| 1:A:227:VAL:C    | 1:A:231:LEU:HD13 | 2.33                     | 0.51              |
| 1:B:129:LEU:O    | 1:B:130:SER:HB2  | 2.11                     | 0.51              |
| 1:C:44:ILE:HA    | 1:C:47:PRO:CG    | 2.41                     | 0.51              |
| 1:A:84:ALA:O     | 1:A:88:ILE:HG23  | 2.11                     | 0.51              |
| 1:B:111:THR:OG1  | 1:B:114:ALA:HB2  | 2.11                     | 0.51              |
| 1:D:123:ILE:CD1  | 1:D:135:ILE:HG21 | 2.41                     | 0.51              |
| 1:D:158:GLY:O    | 1:D:159:CYS:C    | 2.53                     | 0.51              |
| 1:C:122:ALA:HB1  | 1:C:224:ALA:CB   | 2.40                     | 0.51              |
| 1:E:151:LYS:NZ   | 1:E:155:GLU:CD   | 2.68                     | 0.51              |
| 1:C:65:VAL:C     | 1:C:68:TRP:CD1   | 2.89                     | 0.51              |
| 1:C:168:PRO:HG2  | 1:C:201:VAL:C    | 2.36                     | 0.51              |
| 1:C:245:LEU:O    | 1:C:247:GLN:OE1  | 2.28                     | 0.51              |
| 1:E:67:SER:OG    | 1:E:68:TRP:CZ3   | 2.58                     | 0.51              |
| 1:E:217:LYS:HB3  | 1:E:217:LYS:HZ3  | 1.73                     | 0.51              |
| 1:C:134:LYS:H    | 1:C:134:LYS:CD   | 2.11                     | 0.50              |
| 1:A:112:THR:OG1  | 1:A:140:VAL:O    | 2.27                     | 0.50              |
| 1:A:118:MET:O    | 1:A:119:ALA:C    | 2.55                     | 0.50              |
| 1:B:30:THR:HG23  | 1:B:31:ALA:N     | 2.27                     | 0.50              |
| 1:B:87:ILE:HG23  | 1:B:90:LYS:HZ2   | 1.75                     | 0.50              |
| 1:B:107:GLY:HA2  | 1:B:136:ILE:H    | 1.74                     | 0.50              |
| 1:C:227:VAL:O    | 1:C:231:LEU:HD13 | 2.12                     | 0.50              |
| 1:E:7:PHE:CE2    | 1:E:11:LEU:HD11  | 2.46                     | 0.50              |
| 1:A:240:MET:O    | 1:A:244:GLY:N    | 2.39                     | 0.50              |
| 1:C:125:LYS:HD3  | 1:C:221:GLU:OE1  | 2.10                     | 0.50              |
| 1:D:21:ILE:C     | 1:D:24:ILE:HG22  | 2.33                     | 0.50              |
| 1:D:162:VAL:CG1  | 1:D:163:MET:H    | 2.24                     | 0.50              |
| 1:E:44:ILE:C     | 1:E:46:THR:H     | 2.18                     | 0.50              |
| 1:E:106:VAL:HG11 | 1:E:126:LEU:CD2  | 2.41                     | 0.50              |
| 1:A:19:LEU:HD13  | 1:A:19:LEU:O     | 2.12                     | 0.50              |
| 1:D:70:ALA:O     | 1:D:74:GLU:HG2   | 2.12                     | 0.50              |
| 1:D:235:GLU:HA   | 1:D:238:THR:OG1  | 2.12                     | 0.50              |
| 1:E:123:ILE:HG23 | 1:E:135:ILE:HD12 | 1.91                     | 0.50              |
| 1:E:168:PRO:HB2  | 1:E:202:HIS:HA   | 1.93                     | 0.50              |
| 1:A:129:LEU:CD2  | 1:A:228:TYR:CB   | 2.76                     | 0.50              |
| 1:C:30:THR:HG23  | 1:C:31:ALA:H     | 1.77                     | 0.50              |
| 1:C:207:LYS:H    | 1:C:211:GLU:CD   | 2.20                     | 0.50              |
| 1:D:46:THR:H     | 1:D:47:PRO:HD3   | 1.74                     | 0.50              |
| 1:D:65:VAL:C     | 1:D:67:SER:N     | 2.67                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:95:GLU:OE1   | 1:A:95:GLU:HA    | 2.12                     | 0.50              |
| 1:A:106:VAL:HG12 | 1:A:108:ILE:CD1  | 2.42                     | 0.50              |
| 1:A:119:ALA:HA   | 1:A:165:LEU:HD13 | 1.93                     | 0.50              |
| 1:A:182:SER:CA   | 1:A:185:LEU:HD12 | 2.29                     | 0.50              |
| 1:A:237:LEU:O    | 1:A:238:THR:C    | 2.53                     | 0.50              |
| 1:B:239:ARG:O    | 1:B:240:MET:C    | 2.54                     | 0.50              |
| 1:C:86:PHE:CE1   | 1:D:25:MET:SD    | 3.04                     | 0.50              |
| 1:C:143:ILE:HG21 | 1:C:177:CYS:SG   | 2.51                     | 0.50              |
| 1:D:162:VAL:HG12 | 1:D:163:MET:N    | 2.25                     | 0.50              |
| 1:E:188:ALA:O    | 1:E:191:MET:HB2  | 2.12                     | 0.50              |
| 1:A:154:LEU:HD11 | 1:A:196:ILE:CD1  | 2.34                     | 0.50              |
| 1:A:236:TYR:CZ   | 1:A:240:MET:SD   | 3.05                     | 0.50              |
| 1:C:21:ILE:O     | 1:C:24:ILE:HG22  | 2.12                     | 0.50              |
| 1:C:95:GLU:O     | 1:C:97:LYS:HG3   | 2.12                     | 0.50              |
| 1:D:74:GLU:HG3   | 1:E:39:ASN:ND2   | 2.27                     | 0.50              |
| 1:E:127:LYS:HA   | 1:E:133:ILE:HD11 | 1.93                     | 0.50              |
| 1:A:72:LEU:O     | 1:A:76:VAL:HG12  | 2.12                     | 0.50              |
| 1:A:229:TYR:HB3  | 1:A:233:LYS:HB3  | 1.93                     | 0.50              |
| 1:A:237:LEU:HA   | 1:A:240:MET:HB2  | 1.93                     | 0.50              |
| 1:C:37:VAL:HG13  | 1:C:88:ILE:HB    | 1.94                     | 0.50              |
| 1:C:108:ILE:N    | 1:C:136:ILE:O    | 2.45                     | 0.50              |
| 1:C:233:LYS:HG2  | 1:C:236:TYR:HB3  | 1.92                     | 0.50              |
| 1:C:164:ALA:N    | 1:C:197:ILE:O    | 2.41                     | 0.50              |
| 1:E:5:SER:HA     | 1:E:8:LYS:HE2    | 1.93                     | 0.50              |
| 1:A:107:GLY:O    | 1:A:162:VAL:HA   | 2.11                     | 0.49              |
| 1:A:164:ALA:H    | 1:A:199:VAL:HG23 | 1.76                     | 0.49              |
| 1:B:33:ILE:HD11  | 1:B:88:ILE:HD12  | 1.93                     | 0.49              |
| 1:B:128:GLU:C    | 1:B:130:SER:N    | 2.70                     | 0.49              |
| 1:D:28:ALA:O     | 1:D:32:LEU:HB2   | 2.11                     | 0.49              |
| 1:D:121:ILE:HG13 | 1:D:217:LYS:CB   | 2.42                     | 0.49              |
| 1:D:126:LEU:HD13 | 1:D:224:ALA:O    | 2.11                     | 0.49              |
| 1:D:189:GLN:HB3  | 1:E:148:VAL:HG22 | 1.94                     | 0.49              |
| 1:E:98:VAL:CA    | 1:E:101:LYS:HD2  | 2.37                     | 0.49              |
| 1:E:143:ILE:HG22 | 1:E:144:LYS:N    | 2.27                     | 0.49              |
| 1:C:233:LYS:HG2  | 1:C:236:TYR:CB   | 2.42                     | 0.49              |
| 1:D:58:THR:C     | 1:D:59:VAL:HG22  | 2.36                     | 0.49              |
| 1:D:156:GLU:O    | 1:D:157:GLU:HB3  | 2.10                     | 0.49              |
| 1:E:151:LYS:O    | 1:E:155:GLU:HG3  | 2.11                     | 0.49              |
| 1:E:151:LYS:CE   | 1:E:191:MET:HB3  | 2.40                     | 0.49              |
| 1:C:33:ILE:HG12  | 1:C:88:ILE:HD12  | 1.95                     | 0.49              |
| 1:E:145:ASP:O    | 1:E:146:LEU:C    | 2.56                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:7:PHE:HD1    | 1:A:7:PHE:O      | 1.94                     | 0.49              |
| 1:C:153:LEU:O    | 1:C:157:GLU:CG   | 2.60                     | 0.49              |
| 1:D:61:LEU:C     | 1:D:65:VAL:HG11  | 2.38                     | 0.49              |
| 1:B:125:LYS:HD3  | 1:B:221:GLU:OE1  | 2.12                     | 0.49              |
| 1:B:168:PRO:HD2  | 1:B:202:HIS:HA   | 1.93                     | 0.49              |
| 1:C:46:THR:N     | 1:C:47:PRO:CD    | 2.76                     | 0.49              |
| 1:D:164:ALA:HB3  | 1:D:199:VAL:N    | 2.23                     | 0.49              |
| 1:A:71:PHE:CD2   | 1:B:40:ILE:HA    | 2.47                     | 0.49              |
| 1:A:165:LEU:CD2  | 1:A:199:VAL:HG21 | 2.35                     | 0.49              |
| 1:A:219:ARG:O    | 1:A:222:GLU:N    | 2.45                     | 0.49              |
| 1:A:233:LYS:CG   | 1:A:236:TYR:HB2  | 2.42                     | 0.49              |
| 1:B:217:LYS:O    | 1:B:220:ALA:HB3  | 2.12                     | 0.49              |
| 2:B:301:BNG:H6'2 | 1:D:23:PHE:HZ    | 1.76                     | 0.49              |
| 1:C:125:LYS:C    | 1:C:128:GLU:HB3  | 2.37                     | 0.49              |
| 1:D:227:VAL:O    | 1:D:231:LEU:HB2  | 2.12                     | 0.49              |
| 1:E:96:GLU:O     | 1:E:99:GLU:N     | 2.42                     | 0.49              |
| 1:A:118:MET:O    | 1:A:121:ILE:HG12 | 2.13                     | 0.49              |
| 1:D:45:ILE:O     | 1:D:45:ILE:HG22  | 2.13                     | 0.49              |
| 1:A:41:ILE:O     | 1:A:44:ILE:CG2   | 2.61                     | 0.49              |
| 1:B:79:ILE:HG22  | 1:B:83:PHE:HD2   | 1.78                     | 0.49              |
| 1:B:121:ILE:CD1  | 1:B:217:LYS:HZ2  | 2.26                     | 0.49              |
| 1:B:246:ARG:HB2  | 1:B:252:ALA:H    | 1.77                     | 0.49              |
| 1:D:48:PHE:O     | 1:D:49:VAL:HG12  | 2.13                     | 0.49              |
| 1:E:79:ILE:O     | 1:E:83:PHE:CB    | 2.61                     | 0.49              |
| 1:E:127:LYS:N    | 1:E:133:ILE:HD11 | 2.28                     | 0.49              |
| 1:B:212:LEU:O    | 1:B:213:ASP:C    | 2.56                     | 0.49              |
| 1:C:39:ASN:O     | 1:C:40:ILE:HD13  | 2.13                     | 0.49              |
| 1:C:105:LYS:CE   | 1:C:158:GLY:HA3  | 2.40                     | 0.49              |
| 1:D:170:LYS:O    | 1:D:171:ALA:HB3  | 2.13                     | 0.49              |
| 1:E:119:ALA:HA   | 1:E:165:LEU:HD13 | 1.94                     | 0.49              |
| 1:E:143:ILE:O    | 1:E:146:LEU:CD2  | 2.61                     | 0.49              |
| 1:E:183:LEU:C    | 1:E:187:LEU:HD12 | 2.37                     | 0.49              |
| 1:A:7:PHE:CE1    | 1:A:11:LEU:HD21  | 2.48                     | 0.49              |
| 1:A:196:ILE:O    | 1:A:197:ILE:C    | 2.54                     | 0.49              |
| 1:B:108:ILE:CD1  | 1:B:108:ILE:N    | 2.76                     | 0.49              |
| 1:C:145:ASP:O    | 1:C:146:LEU:C    | 2.56                     | 0.49              |
| 1:D:121:ILE:CG2  | 1:D:217:LYS:O    | 2.60                     | 0.49              |
| 1:A:39:ASN:ND2   | 1:E:68:TRP:HA    | 2.28                     | 0.48              |
| 1:A:225:GLU:HG2  | 1:A:229:TYR:CZ   | 2.48                     | 0.48              |
| 1:B:121:ILE:HD11 | 1:B:217:LYS:HZ2  | 1.78                     | 0.48              |
| 1:C:89:ALA:O     | 1:C:92:VAL:HG12  | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:115:ARG:NE   | 1:C:203:GLU:OE1  | 2.46                     | 0.48              |
| 1:D:39:ASN:O     | 1:D:40:ILE:HD13  | 2.13                     | 0.48              |
| 1:E:156:GLU:O    | 1:E:157:GLU:HB2  | 2.12                     | 0.48              |
| 1:E:224:ALA:O    | 1:E:227:VAL:N    | 2.46                     | 0.48              |
| 1:A:195:HIS:HE1  | 1:B:149:ALA:HB2  | 1.77                     | 0.48              |
| 1:B:15:LYS:HB3   | 1:B:18:PRO:HG2   | 1.95                     | 0.48              |
| 1:B:17:ILE:HD12  | 1:B:18:PRO:HD3   | 1.94                     | 0.48              |
| 1:C:30:THR:O     | 1:C:33:ILE:HG22  | 2.13                     | 0.48              |
| 1:D:78:PHE:CE2   | 1:E:35:SER:HB2   | 2.48                     | 0.48              |
| 1:E:143:ILE:O    | 1:E:146:LEU:HG   | 2.14                     | 0.48              |
| 1:A:104:LYS:O    | 1:A:105:LYS:CB   | 2.61                     | 0.48              |
| 1:B:25:MET:HG2   | 1:C:16:VAL:HG11  | 1.94                     | 0.48              |
| 1:C:7:PHE:CD1    | 1:C:7:PHE:C      | 2.91                     | 0.48              |
| 1:C:7:PHE:C      | 1:C:9:GLU:H      | 2.21                     | 0.48              |
| 1:C:65:VAL:HG13  | 1:C:66:ILE:N     | 2.29                     | 0.48              |
| 1:D:161:ILE:O    | 1:D:162:VAL:CG2  | 2.61                     | 0.48              |
| 1:D:176:VAL:HG12 | 1:D:180:GLU:OE2  | 2.13                     | 0.48              |
| 1:E:126:LEU:C    | 1:E:133:ILE:HD11 | 2.37                     | 0.48              |
| 1:E:149:ALA:O    | 1:E:150:CYS:C    | 2.56                     | 0.48              |
| 1:A:7:PHE:O      | 1:A:10:PHE:HB3   | 2.13                     | 0.48              |
| 1:C:226:ASN:HA   | 1:C:229:TYR:CD2  | 2.48                     | 0.48              |
| 1:D:25:MET:CG    | 1:E:16:VAL:CG1   | 2.91                     | 0.48              |
| 1:A:42:MET:CE    | 1:A:81:ILE:CG2   | 2.90                     | 0.48              |
| 1:A:146:LEU:N    | 1:A:147:PRO:CD   | 2.76                     | 0.48              |
| 1:D:66:ILE:HD12  | 1:D:66:ILE:C     | 2.37                     | 0.48              |
| 1:A:42:MET:HE1   | 1:A:81:ILE:CG2   | 2.44                     | 0.48              |
| 1:A:64:ILE:O     | 1:A:64:ILE:HG23  | 2.13                     | 0.48              |
| 1:A:106:VAL:HG12 | 1:A:108:ILE:HD12 | 1.95                     | 0.48              |
| 1:D:168:PRO:HD2  | 1:D:201:VAL:O    | 2.12                     | 0.48              |
| 1:E:69:GLY:O     | 1:E:72:LEU:N     | 2.46                     | 0.48              |
| 1:A:162:VAL:HG13 | 1:A:163:MET:N    | 2.29                     | 0.48              |
| 1:B:36:PHE:O     | 1:B:40:ILE:CB    | 2.43                     | 0.48              |
| 1:C:65:VAL:C     | 1:C:66:ILE:HG23  | 2.37                     | 0.48              |
| 1:C:115:ARG:CG   | 1:C:167:MET:SD   | 2.92                     | 0.48              |
| 1:C:118:MET:O    | 1:C:119:ALA:C    | 2.56                     | 0.48              |
| 1:A:67:SER:O     | 1:A:71:PHE:CG    | 2.61                     | 0.48              |
| 1:C:193:ASN:O    | 1:C:194:LYS:HD2  | 2.14                     | 0.48              |
| 1:E:94:GLN:O     | 1:E:98:VAL:HG23  | 2.14                     | 0.48              |
| 1:E:111:THR:HG1  | 1:E:114:ALA:H    | 1.61                     | 0.48              |
| 1:A:25:MET:HG3   | 1:E:86:PHE:CE1   | 2.48                     | 0.48              |
| 1:A:237:LEU:HA   | 1:A:240:MET:CG   | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:125:LYS:HE3  | 1:B:129:LEU:CD1  | 2.36                     | 0.48              |
| 2:B:301:BNG:C7'  | 2:B:301:BNG:C3'  | 2.92                     | 0.48              |
| 1:D:78:PHE:HE2   | 1:E:35:SER:HB3   | 1.78                     | 0.48              |
| 1:E:171:ALA:C    | 1:E:173:LYS:H    | 2.22                     | 0.48              |
| 1:A:39:ASN:ND2   | 1:E:71:PHE:CB    | 2.77                     | 0.48              |
| 1:A:226:ASN:HD22 | 1:A:237:LEU:CD2  | 2.27                     | 0.48              |
| 1:A:232:PHE:O    | 1:A:234:PRO:CD   | 2.60                     | 0.48              |
| 1:B:146:LEU:C    | 1:B:150:CYS:SG   | 2.96                     | 0.48              |
| 1:C:32:LEU:HD13  | 1:C:33:ILE:N     | 2.29                     | 0.48              |
| 1:D:15:LYS:C     | 1:D:18:PRO:HD2   | 2.39                     | 0.48              |
| 1:D:25:MET:CG    | 1:D:29:SER:HB3   | 2.44                     | 0.48              |
| 1:D:143:ILE:CA   | 1:D:146:LEU:HD21 | 2.44                     | 0.48              |
| 1:D:149:ALA:O    | 1:D:153:LEU:CD1  | 2.52                     | 0.48              |
| 1:A:11:LEU:HD11  | 1:D:86:PHE:HE1   | 1.77                     | 0.47              |
| 1:A:227:VAL:O    | 1:A:231:LEU:CD1  | 2.56                     | 0.47              |
| 1:B:108:ILE:O    | 1:B:137:ARG:HA   | 2.14                     | 0.47              |
| 1:C:147:PRO:HA   | 1:C:150:CYS:SG   | 2.54                     | 0.47              |
| 1:A:122:ALA:HB2  | 1:A:220:ALA:HB1  | 1.95                     | 0.47              |
| 1:A:229:TYR:HA   | 1:A:233:LYS:CB   | 2.43                     | 0.47              |
| 1:B:236:TYR:O    | 1:B:240:MET:HG2  | 2.13                     | 0.47              |
| 1:C:119:ALA:HA   | 1:C:165:LEU:HD12 | 1.96                     | 0.47              |
| 1:C:162:VAL:HG13 | 1:C:163:MET:H    | 1.79                     | 0.47              |
| 1:D:234:PRO:O    | 1:D:237:LEU:HD12 | 2.13                     | 0.47              |
| 1:E:224:ALA:O    | 1:E:227:VAL:HB   | 2.14                     | 0.47              |
| 1:B:189:GLN:HB3  | 1:C:148:VAL:HG22 | 1.95                     | 0.47              |
| 1:D:123:ILE:HG23 | 1:D:135:ILE:CD1  | 2.44                     | 0.47              |
| 1:A:81:ILE:O     | 1:A:85:VAL:HG23  | 2.14                     | 0.47              |
| 1:A:146:LEU:N    | 1:A:147:PRO:HD2  | 2.29                     | 0.47              |
| 1:A:151:LYS:HE3  | 1:E:190:LEU:O    | 2.14                     | 0.47              |
| 1:B:26:GLY:O     | 1:B:30:THR:HG22  | 2.14                     | 0.47              |
| 1:B:143:ILE:HA   | 1:B:146:LEU:HD21 | 1.95                     | 0.47              |
| 1:C:179:HIS:NE2  | 1:C:183:LEU:HD11 | 2.30                     | 0.47              |
| 1:D:25:MET:CG    | 1:E:16:VAL:HG11  | 2.44                     | 0.47              |
| 1:E:78:PHE:C     | 1:E:81:ILE:HG22  | 2.39                     | 0.47              |
| 1:A:118:MET:HE1  | 1:A:166:GLY:O    | 2.14                     | 0.47              |
| 1:A:149:ALA:O    | 1:A:150:CYS:C    | 2.56                     | 0.47              |
| 1:A:226:ASN:HD22 | 1:A:237:LEU:HD21 | 1.79                     | 0.47              |
| 1:B:45:ILE:O     | 1:B:46:THR:C     | 2.58                     | 0.47              |
| 1:B:154:LEU:HD21 | 1:B:162:VAL:HB   | 1.95                     | 0.47              |
| 1:C:173:LYS:O    | 1:C:176:VAL:HG23 | 2.14                     | 0.47              |
| 1:D:185:LEU:HD13 | 1:D:198:GLU:HG2  | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:168:PRO:HD3  | 1:E:201:VAL:H    | 1.79                     | 0.47              |
| 1:B:32:LEU:HD13  | 1:B:33:ILE:N     | 2.30                     | 0.47              |
| 1:B:139:THR:CG2  | 1:B:140:VAL:H    | 2.20                     | 0.47              |
| 1:C:15:LYS:HB3   | 1:C:18:PRO:HG2   | 1.96                     | 0.47              |
| 1:C:234:PRO:CG   | 1:C:235:GLU:H    | 2.27                     | 0.47              |
| 1:E:140:VAL:CB   | 1:E:141:PRO:HD2  | 2.42                     | 0.47              |
| 1:A:86:PHE:CE2   | 1:C:7:PHE:CE1    | 3.03                     | 0.47              |
| 1:A:111:THR:O    | 1:A:139:THR:CG2  | 2.62                     | 0.47              |
| 1:A:153:LEU:O    | 1:A:157:GLU:CG   | 2.50                     | 0.47              |
| 1:A:160:ASP:O    | 1:A:194:LYS:CG   | 2.59                     | 0.47              |
| 1:B:104:LYS:HB3  | 1:B:105:LYS:H    | 1.53                     | 0.47              |
| 1:B:134:LYS:H    | 1:B:134:LYS:CD   | 2.27                     | 0.47              |
| 1:B:139:THR:CG2  | 1:B:140:VAL:N    | 2.77                     | 0.47              |
| 1:B:143:ILE:O    | 1:B:146:LEU:CD2  | 2.62                     | 0.47              |
| 1:C:107:GLY:O    | 1:C:108:ILE:HD12 | 2.14                     | 0.47              |
| 1:D:94:GLN:O     | 1:D:98:VAL:CG2   | 2.59                     | 0.47              |
| 1:E:107:GLY:HA3  | 1:E:162:VAL:CG2  | 2.45                     | 0.47              |
| 1:E:112:THR:CB   | 1:E:141:PRO:HA   | 2.43                     | 0.47              |
| 1:E:130:SER:O    | 1:E:133:ILE:HG12 | 2.14                     | 0.47              |
| 1:E:228:TYR:CE1  | 1:E:232:PHE:CD2  | 3.02                     | 0.47              |
| 1:B:19:LEU:CD1   | 2:B:301:BNG:H61  | 2.45                     | 0.47              |
| 1:C:153:LEU:HD12 | 1:C:153:LEU:H    | 1.80                     | 0.47              |
| 1:C:162:VAL:CG1  | 1:C:163:MET:H    | 2.28                     | 0.47              |
| 1:C:182:SER:O    | 1:C:183:LEU:C    | 2.58                     | 0.47              |
| 1:D:151:LYS:O    | 1:D:152:LYS:C    | 2.58                     | 0.47              |
| 1:E:187:LEU:O    | 1:E:188:ALA:C    | 2.57                     | 0.47              |
| 1:A:14:TYR:HD2   | 1:A:16:VAL:CG2   | 2.28                     | 0.47              |
| 1:A:189:GLN:HB3  | 1:B:148:VAL:CG1  | 2.45                     | 0.47              |
| 1:A:229:TYR:CB   | 1:A:233:LYS:HB3  | 2.45                     | 0.47              |
| 1:B:226:ASN:HA   | 1:B:229:TYR:CD2  | 2.48                     | 0.47              |
| 1:C:202:HIS:N    | 1:C:205:GLU:OE2  | 2.48                     | 0.47              |
| 1:D:42:MET:O     | 1:D:43:PRO:C     | 2.58                     | 0.47              |
| 1:E:107:GLY:C    | 1:E:162:VAL:HG22 | 2.39                     | 0.47              |
| 1:E:147:PRO:C    | 1:E:149:ALA:N    | 2.69                     | 0.47              |
| 1:A:19:LEU:HD13  | 1:A:19:LEU:C     | 2.40                     | 0.47              |
| 1:B:125:LYS:O    | 1:B:129:LEU:CD1  | 2.58                     | 0.47              |
| 1:C:146:LEU:O    | 1:C:150:CYS:SG   | 2.72                     | 0.47              |
| 1:E:15:LYS:HD3   | 1:E:18:PRO:HG2   | 1.96                     | 0.47              |
| 1:E:39:ASN:C     | 1:E:43:PRO:HG3   | 2.39                     | 0.47              |
| 1:E:123:ILE:CD1  | 1:E:135:ILE:HG21 | 2.45                     | 0.47              |
| 1:A:21:ILE:O     | 1:A:24:ILE:HG22  | 2.14                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:121:ILE:HG13 | 1:B:217:LYS:HB3  | 1.97                     | 0.46              |
| 1:B:250:GLU:O    | 1:B:251:ASP:C    | 2.57                     | 0.46              |
| 1:C:126:LEU:C    | 1:C:128:GLU:N    | 2.71                     | 0.46              |
| 1:C:217:LYS:HB3  | 1:C:217:LYS:HZ3  | 1.80                     | 0.46              |
| 1:C:243:LYS:N    | 1:C:243:LYS:CD   | 2.73                     | 0.46              |
| 1:D:212:LEU:C    | 1:D:212:LEU:HD23 | 2.39                     | 0.46              |
| 1:E:92:VAL:O     | 1:E:96:GLU:HG2   | 2.14                     | 0.46              |
| 1:E:103:THR:O    | 1:E:104:LYS:HB2  | 2.14                     | 0.46              |
| 1:E:149:ALA:O    | 1:E:151:LYS:N    | 2.48                     | 0.46              |
| 1:A:19:LEU:O     | 1:A:23:PHE:HB2   | 2.14                     | 0.46              |
| 1:A:87:ILE:CG2   | 1:A:91:LYS:HE3   | 2.39                     | 0.46              |
| 1:B:7:PHE:C      | 1:B:9:GLU:N      | 2.73                     | 0.46              |
| 1:B:78:PHE:O     | 1:B:81:ILE:HG22  | 2.16                     | 0.46              |
| 1:B:125:LYS:HB2  | 1:B:221:GLU:OE1  | 2.14                     | 0.46              |
| 1:C:63:PRO:HB2   | 1:C:65:VAL:CA    | 2.44                     | 0.46              |
| 1:D:121:ILE:HG21 | 1:D:217:LYS:C    | 2.40                     | 0.46              |
| 1:D:150:CYS:HB2  | 1:D:196:ILE:CD1  | 2.42                     | 0.46              |
| 1:D:189:GLN:O    | 1:D:192:THR:C    | 2.58                     | 0.46              |
| 1:E:44:ILE:O     | 1:E:44:ILE:HG13  | 2.15                     | 0.46              |
| 1:A:71:PHE:O     | 1:A:75:LEU:CB    | 2.63                     | 0.46              |
| 1:B:15:LYS:C     | 1:B:18:PRO:HD2   | 2.40                     | 0.46              |
| 1:D:123:ILE:HD12 | 1:D:135:ILE:CD1  | 2.33                     | 0.46              |
| 1:E:26:GLY:HA2   | 1:E:29:SER:OG    | 2.16                     | 0.46              |
| 1:E:111:THR:OG1  | 1:E:112:THR:N    | 2.45                     | 0.46              |
| 1:E:120:SER:O    | 1:E:121:ILE:C    | 2.58                     | 0.46              |
| 1:E:126:LEU:O    | 1:E:133:ILE:HD13 | 2.15                     | 0.46              |
| 1:A:226:ASN:O    | 1:A:230:LEU:N    | 2.43                     | 0.46              |
| 1:B:140:VAL:HB   | 1:B:141:PRO:CD   | 2.44                     | 0.46              |
| 1:C:104:LYS:N    | 1:C:104:LYS:CD   | 2.77                     | 0.46              |
| 1:D:151:LYS:HG2  | 1:D:155:GLU:OE2  | 2.15                     | 0.46              |
| 1:A:56:THR:O     | 1:A:58:THR:N     | 2.49                     | 0.46              |
| 1:B:110:ASP:OD1  | 1:B:138:LYS:O    | 2.34                     | 0.46              |
| 1:C:32:LEU:HD13  | 1:C:32:LEU:C     | 2.41                     | 0.46              |
| 1:C:145:ASP:C    | 1:C:147:PRO:CD   | 2.87                     | 0.46              |
| 1:C:168:PRO:HB2  | 1:C:202:HIS:HA   | 1.97                     | 0.46              |
| 1:C:184:GLY:O    | 1:C:185:LEU:C    | 2.58                     | 0.46              |
| 1:C:214:TRP:C    | 1:C:216:ALA:N    | 2.69                     | 0.46              |
| 1:D:63:PRO:CA    | 1:D:66:ILE:HG23  | 2.40                     | 0.46              |
| 1:D:150:CYS:HA   | 1:D:153:LEU:CD1  | 2.45                     | 0.46              |
| 1:E:121:ILE:CD1  | 1:E:217:LYS:HZ2  | 2.28                     | 0.46              |
| 1:A:183:LEU:O    | 1:A:187:LEU:CD1  | 2.64                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:225:GLU:HG2  | 1:A:229:TYR:CE2  | 2.50                     | 0.46              |
| 1:B:19:LEU:HD11  | 2:B:301:BNG:H61  | 1.97                     | 0.46              |
| 1:B:75:LEU:HD23  | 1:C:40:ILE:CG1   | 2.43                     | 0.46              |
| 1:B:90:LYS:HB3   | 1:D:7:PHE:CZ     | 2.50                     | 0.46              |
| 1:B:121:ILE:HG21 | 1:B:217:LYS:HB2  | 1.98                     | 0.46              |
| 1:C:121:ILE:CD1  | 1:C:217:LYS:HZ2  | 2.25                     | 0.46              |
| 1:E:40:ILE:HG22  | 1:E:41:ILE:N     | 2.30                     | 0.46              |
| 1:E:98:VAL:CG1   | 1:E:101:LYS:HD2  | 2.41                     | 0.46              |
| 1:B:246:ARG:O    | 1:B:247:GLN:C    | 2.58                     | 0.46              |
| 1:C:34:LYS:O     | 1:C:37:VAL:HG23  | 2.15                     | 0.46              |
| 1:D:33:ILE:HD11  | 1:D:88:ILE:HD12  | 1.98                     | 0.46              |
| 1:D:152:LYS:HB3  | 1:D:156:GLU:OE2  | 2.16                     | 0.46              |
| 1:E:96:GLU:O     | 1:E:99:GLU:HB3   | 2.15                     | 0.46              |
| 1:C:17:ILE:HB    | 1:C:18:PRO:HD3   | 1.98                     | 0.46              |
| 1:D:64:ILE:CG1   | 1:E:44:ILE:HD12  | 2.44                     | 0.46              |
| 1:E:26:GLY:O     | 1:E:30:THR:HG22  | 2.15                     | 0.46              |
| 1:E:44:ILE:O     | 1:E:47:PRO:CD    | 2.60                     | 0.46              |
| 1:E:160:ASP:OD2  | 1:E:194:LYS:HE3  | 2.15                     | 0.46              |
| 1:B:187:LEU:O    | 1:B:191:MET:N    | 2.40                     | 0.46              |
| 1:C:7:PHE:C      | 1:C:9:GLU:N      | 2.74                     | 0.46              |
| 1:C:16:VAL:HG12  | 1:C:16:VAL:O     | 2.15                     | 0.46              |
| 1:C:161:ILE:HD13 | 1:C:227:VAL:HG13 | 1.97                     | 0.46              |
| 1:C:233:LYS:O    | 1:C:237:LEU:CD1  | 2.64                     | 0.46              |
| 1:D:160:ASP:C    | 1:D:161:ILE:HG22 | 2.36                     | 0.46              |
| 1:D:193:ASN:ND2  | 1:E:155:GLU:OE2  | 2.47                     | 0.46              |
| 1:A:127:LYS:HA   | 1:A:133:ILE:CD1  | 2.46                     | 0.46              |
| 1:A:148:VAL:O    | 1:A:151:LYS:CB   | 2.64                     | 0.46              |
| 1:B:108:ILE:N    | 1:B:108:ILE:HD12 | 2.30                     | 0.46              |
| 1:B:111:THR:OG1  | 1:B:114:ALA:N    | 2.44                     | 0.46              |
| 1:B:146:LEU:N    | 1:B:147:PRO:HD2  | 2.30                     | 0.46              |
| 1:C:93:LEU:HD13  | 1:C:93:LEU:C     | 2.41                     | 0.46              |
| 1:D:189:GLN:HB3  | 1:E:148:VAL:CG2  | 2.45                     | 0.46              |
| 1:D:201:VAL:O    | 1:D:201:VAL:HG23 | 2.16                     | 0.46              |
| 1:B:234:PRO:CG   | 1:B:235:GLU:N    | 2.79                     | 0.45              |
| 1:C:44:ILE:HA    | 1:C:47:PRO:HG3   | 1.98                     | 0.45              |
| 1:C:152:LYS:O    | 1:C:156:GLU:N    | 2.39                     | 0.45              |
| 1:D:239:ARG:C    | 1:D:241:ALA:H    | 2.22                     | 0.45              |
| 1:E:127:LYS:CA   | 1:E:133:ILE:HD11 | 2.46                     | 0.45              |
| 1:A:36:PHE:CZ    | 1:A:40:ILE:HD11  | 2.50                     | 0.45              |
| 1:C:111:THR:HG23 | 1:C:114:ALA:HB2  | 1.95                     | 0.45              |
| 1:D:122:ALA:HB2  | 1:D:220:ALA:O    | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:93:LEU:HD22  | 1:E:93:LEU:HA    | 1.82                     | 0.45              |
| 1:A:14:TYR:HD2   | 1:A:16:VAL:HG23  | 1.81                     | 0.45              |
| 1:A:143:ILE:O    | 1:A:146:LEU:CD2  | 2.60                     | 0.45              |
| 1:A:196:ILE:O    | 1:A:196:ILE:HG22 | 2.16                     | 0.45              |
| 1:B:112:THR:CB   | 1:B:140:VAL:O    | 2.63                     | 0.45              |
| 1:C:214:TRP:O    | 1:C:216:ALA:N    | 2.49                     | 0.45              |
| 1:C:214:TRP:NE1  | 1:C:218:ARG:HD2  | 2.31                     | 0.45              |
| 1:E:19:LEU:HD13  | 1:E:19:LEU:O     | 2.16                     | 0.45              |
| 1:E:30:THR:HG23  | 1:E:31:ALA:N     | 2.31                     | 0.45              |
| 1:E:121:ILE:HD13 | 1:E:121:ILE:H    | 1.81                     | 0.45              |
| 1:E:229:TYR:HB3  | 1:E:237:LEU:HD11 | 1.99                     | 0.45              |
| 1:B:7:PHE:HE2    | 1:B:11:LEU:HD11  | 1.82                     | 0.45              |
| 1:B:223:HIS:O    | 1:B:224:ALA:C    | 2.60                     | 0.45              |
| 1:C:41:ILE:CG2   | 1:C:91:LYS:HE3   | 2.44                     | 0.45              |
| 1:C:71:PHE:CZ    | 1:D:43:PRO:HG2   | 2.52                     | 0.45              |
| 1:C:213:ASP:OD1  | 1:C:213:ASP:C    | 2.59                     | 0.45              |
| 1:D:25:MET:HG2   | 1:E:16:VAL:HG11  | 1.97                     | 0.45              |
| 1:D:179:HIS:HD2  | 1:D:183:LEU:HD21 | 1.80                     | 0.45              |
| 1:A:130:SER:HA   | 1:A:131:PRO:HD3  | 1.70                     | 0.45              |
| 1:B:58:THR:HG22  | 1:B:59:VAL:N     | 2.32                     | 0.45              |
| 1:B:146:LEU:O    | 1:B:149:ALA:N    | 2.50                     | 0.45              |
| 1:B:244:GLY:HA2  | 1:B:253:GLY:C    | 2.41                     | 0.45              |
| 1:C:159:CYS:C    | 1:C:161:ILE:H    | 2.16                     | 0.45              |
| 1:C:167:MET:HA   | 1:C:168:PRO:HD3  | 1.65                     | 0.45              |
| 1:C:183:LEU:N    | 1:C:183:LEU:HD23 | 2.32                     | 0.45              |
| 1:C:206:ALA:HA   | 1:C:211:GLU:OE2  | 2.15                     | 0.45              |
| 1:D:129:LEU:HD23 | 1:D:228:TYR:CD2  | 2.51                     | 0.45              |
| 1:E:183:LEU:N    | 1:E:183:LEU:HD23 | 2.31                     | 0.45              |
| 1:E:228:TYR:O    | 1:E:231:LEU:HB2  | 2.16                     | 0.45              |
| 1:A:109:VAL:CG2  | 1:A:153:LEU:CD1  | 2.92                     | 0.45              |
| 1:A:222:GLU:O    | 1:A:225:GLU:CB   | 2.56                     | 0.45              |
| 1:B:111:THR:HG1  | 1:B:114:ALA:H    | 1.60                     | 0.45              |
| 1:E:126:LEU:HD13 | 1:E:224:ALA:HB1  | 1.99                     | 0.45              |
| 1:A:39:ASN:CB    | 1:E:71:PHE:CD2   | 3.00                     | 0.45              |
| 1:B:7:PHE:CE2    | 1:B:11:LEU:HG    | 2.52                     | 0.45              |
| 1:D:61:LEU:CB    | 1:D:65:VAL:HG21  | 2.47                     | 0.45              |
| 1:D:61:LEU:HB2   | 1:D:65:VAL:HG21  | 1.98                     | 0.45              |
| 1:D:101:LYS:HB3  | 1:D:101:LYS:HZ3  | 1.82                     | 0.45              |
| 1:D:118:MET:SD   | 1:D:220:ALA:HB2  | 2.56                     | 0.45              |
| 1:E:146:LEU:HD12 | 1:E:185:LEU:HD21 | 1.97                     | 0.45              |
| 1:A:229:TYR:CA   | 1:A:233:LYS:HB3  | 2.45                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:163:MET:HE2  | 1:B:165:LEU:CD2  | 2.38                     | 0.45              |
| 1:C:42:MET:N     | 1:C:43:PRO:HD2   | 2.29                     | 0.45              |
| 1:E:186:MET:HA   | 1:E:189:GLN:CD   | 2.40                     | 0.45              |
| 1:A:30:THR:CG2   | 1:A:31:ALA:N     | 2.79                     | 0.45              |
| 1:A:37:VAL:HG11  | 1:A:85:VAL:HG22  | 1.99                     | 0.45              |
| 1:A:143:ILE:CA   | 1:A:146:LEU:HD21 | 2.47                     | 0.45              |
| 1:B:106:VAL:CG1  | 1:B:108:ILE:HD11 | 2.47                     | 0.45              |
| 1:B:229:TYR:HD1  | 1:B:233:LYS:HB3  | 1.81                     | 0.45              |
| 1:C:149:ALA:C    | 1:C:153:LEU:CD1  | 2.89                     | 0.45              |
| 1:C:161:ILE:O    | 1:C:162:VAL:CG2  | 2.58                     | 0.45              |
| 1:E:146:LEU:CD1  | 1:E:185:LEU:HD21 | 2.47                     | 0.45              |
| 1:A:101:LYS:C    | 1:A:102:MET:O    | 2.54                     | 0.45              |
| 1:B:32:LEU:HD13  | 1:B:32:LEU:C     | 2.41                     | 0.45              |
| 1:B:189:GLN:NE2  | 1:C:145:ASP:OD1  | 2.50                     | 0.45              |
| 1:B:244:GLY:N    | 1:B:254:PRO:HD3  | 2.32                     | 0.45              |
| 1:E:125:LYS:HB2  | 1:E:221:GLU:CD   | 2.41                     | 0.45              |
| 1:A:158:GLY:O    | 1:A:159:CYS:C    | 2.60                     | 0.44              |
| 1:B:162:VAL:HG13 | 1:B:163:MET:N    | 2.31                     | 0.44              |
| 1:B:165:LEU:HD23 | 1:B:199:VAL:CG1  | 2.32                     | 0.44              |
| 1:C:154:LEU:CD1  | 1:C:196:ILE:HG13 | 2.39                     | 0.44              |
| 1:D:37:VAL:HG22  | 1:D:88:ILE:HG13  | 2.00                     | 0.44              |
| 1:D:169:GLY:HA2  | 1:D:203:GLU:OE2  | 2.17                     | 0.44              |
| 1:E:106:VAL:HG12 | 1:E:107:GLY:H    | 1.82                     | 0.44              |
| 1:A:36:PHE:HD2   | 1:A:88:ILE:HD12  | 1.82                     | 0.44              |
| 1:A:163:MET:HE3  | 1:A:223:HIS:CB   | 2.48                     | 0.44              |
| 1:C:102:MET:O    | 1:C:232:PHE:CD1  | 2.70                     | 0.44              |
| 1:D:102:MET:HG2  | 1:D:231:LEU:O    | 2.17                     | 0.44              |
| 1:D:152:LYS:O    | 1:D:156:GLU:N    | 2.50                     | 0.44              |
| 1:E:46:THR:O     | 1:E:48:PHE:N     | 2.50                     | 0.44              |
| 1:E:102:MET:HE3  | 1:E:103:THR:N    | 2.32                     | 0.44              |
| 1:E:146:LEU:CG   | 1:E:147:PRO:HD3  | 2.47                     | 0.44              |
| 1:E:147:PRO:O    | 1:E:148:VAL:C    | 2.58                     | 0.44              |
| 1:E:156:GLU:O    | 1:E:157:GLU:CG   | 2.65                     | 0.44              |
| 1:A:188:ALA:O    | 1:A:189:GLN:C    | 2.60                     | 0.44              |
| 1:B:90:LYS:HA    | 1:B:93:LEU:HD12  | 2.00                     | 0.44              |
| 1:B:187:LEU:CB   | 1:B:191:MET:HE1  | 2.35                     | 0.44              |
| 1:D:158:GLY:O    | 1:D:160:ASP:N    | 2.50                     | 0.44              |
| 1:D:167:MET:HA   | 1:D:168:PRO:HD3  | 1.59                     | 0.44              |
| 1:D:226:ASN:HD22 | 1:D:229:TYR:HD2  | 1.64                     | 0.44              |
| 1:E:111:THR:OG1  | 1:E:114:ALA:N    | 2.46                     | 0.44              |
| 1:E:165:LEU:HD23 | 1:E:199:VAL:HG11 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:145:ASP:O    | 1:A:146:LEU:C    | 2.59                     | 0.44              |
| 1:A:171:ALA:C    | 1:A:173:LYS:H    | 2.25                     | 0.44              |
| 1:B:122:ALA:HB1  | 1:B:224:ALA:CB   | 2.33                     | 0.44              |
| 1:C:239:ARG:O    | 1:C:240:MET:C    | 2.59                     | 0.44              |
| 1:D:30:THR:HG23  | 1:D:31:ALA:N     | 2.33                     | 0.44              |
| 1:D:65:VAL:HA    | 1:D:68:TRP:CD1   | 2.49                     | 0.44              |
| 1:D:157:GLU:O    | 1:D:159:CYS:N    | 2.50                     | 0.44              |
| 1:E:32:LEU:C     | 1:E:32:LEU:HD13  | 2.41                     | 0.44              |
| 1:A:93:LEU:HD13  | 1:A:93:LEU:C     | 2.42                     | 0.44              |
| 1:B:106:VAL:CG1  | 1:B:108:ILE:CD1  | 2.93                     | 0.44              |
| 1:B:110:ASP:OD1  | 1:B:110:ASP:N    | 2.49                     | 0.44              |
| 1:B:112:THR:OG1  | 1:B:139:THR:HG22 | 2.15                     | 0.44              |
| 1:B:145:ASP:O    | 1:B:148:VAL:CG2  | 2.65                     | 0.44              |
| 1:D:63:PRO:C     | 1:D:65:VAL:N     | 2.72                     | 0.44              |
| 1:D:110:ASP:N    | 1:D:110:ASP:OD1  | 2.50                     | 0.44              |
| 1:E:111:THR:HG1  | 1:E:114:ALA:N    | 2.16                     | 0.44              |
| 1:A:74:GLU:OE2   | 1:A:74:GLU:HA    | 2.18                     | 0.44              |
| 1:A:111:THR:OG1  | 1:A:112:THR:N    | 2.51                     | 0.44              |
| 1:B:112:THR:OG1  | 1:B:140:VAL:O    | 2.26                     | 0.44              |
| 1:E:125:LYS:CG   | 1:E:221:GLU:HG3  | 2.47                     | 0.44              |
| 1:A:66:ILE:HG22  | 1:A:67:SER:H     | 1.83                     | 0.44              |
| 1:C:145:ASP:O    | 1:C:147:PRO:N    | 2.51                     | 0.44              |
| 1:C:223:HIS:C    | 1:C:225:GLU:N    | 2.73                     | 0.44              |
| 1:C:231:LEU:HD23 | 1:C:232:PHE:CZ   | 2.52                     | 0.44              |
| 1:B:75:LEU:O     | 1:B:79:ILE:HG13  | 2.17                     | 0.44              |
| 1:B:213:ASP:C    | 1:B:213:ASP:OD1  | 2.60                     | 0.44              |
| 1:C:88:ILE:HD13  | 1:C:88:ILE:C     | 2.42                     | 0.44              |
| 1:C:240:MET:O    | 1:C:241:ALA:O    | 2.36                     | 0.44              |
| 1:E:167:MET:HA   | 1:E:168:PRO:HD3  | 1.89                     | 0.44              |
| 1:B:59:VAL:O     | 1:B:60:GLU:HG3   | 2.17                     | 0.44              |
| 1:C:130:SER:HA   | 1:C:131:PRO:HD3  | 1.83                     | 0.44              |
| 1:C:182:SER:O    | 1:C:185:LEU:N    | 2.51                     | 0.44              |
| 1:D:164:ALA:N    | 1:D:199:VAL:HG23 | 2.32                     | 0.44              |
| 1:D:179:HIS:CD2  | 1:D:183:LEU:HD11 | 2.51                     | 0.44              |
| 1:E:111:THR:HG23 | 1:E:114:ALA:HB2  | 1.96                     | 0.44              |
| 1:A:19:LEU:HD13  | 1:A:23:PHE:HB2   | 2.00                     | 0.43              |
| 1:A:67:SER:HB3   | 1:A:71:PHE:HE2   | 1.83                     | 0.43              |
| 1:A:106:VAL:HG11 | 1:A:126:LEU:HD21 | 2.00                     | 0.43              |
| 1:A:165:LEU:H    | 1:A:165:LEU:HG   | 1.57                     | 0.43              |
| 1:B:111:THR:O    | 1:B:139:THR:CG2  | 2.65                     | 0.43              |
| 1:D:30:THR:HA    | 1:D:33:ILE:HG22  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:187:LEU:CB   | 1:D:191:MET:HE1  | 2.47                     | 0.43              |
| 1:D:237:LEU:O    | 1:D:238:THR:C    | 2.61                     | 0.43              |
| 1:E:113:PHE:HB2  | 1:E:141:PRO:O    | 2.18                     | 0.43              |
| 1:E:118:MET:HE1  | 1:E:199:VAL:O    | 2.18                     | 0.43              |
| 1:A:66:ILE:HG22  | 1:A:67:SER:N     | 2.33                     | 0.43              |
| 1:A:186:MET:HB3  | 1:A:190:LEU:HD12 | 1.99                     | 0.43              |
| 1:B:113:PHE:O    | 1:B:113:PHE:CD1  | 2.66                     | 0.43              |
| 1:B:118:MET:O    | 1:B:119:ALA:C    | 2.61                     | 0.43              |
| 1:C:66:ILE:HG12  | 1:C:68:TRP:HE1   | 1.80                     | 0.43              |
| 1:C:187:LEU:C    | 1:C:191:MET:HE3  | 2.42                     | 0.43              |
| 1:A:37:VAL:HG11  | 1:A:85:VAL:CG2   | 2.48                     | 0.43              |
| 1:A:83:PHE:O     | 1:A:87:ILE:HG12  | 2.18                     | 0.43              |
| 1:A:113:PHE:CD2  | 1:A:143:ILE:HG22 | 2.54                     | 0.43              |
| 1:B:128:GLU:C    | 1:B:130:SER:H    | 2.27                     | 0.43              |
| 1:B:228:TYR:O    | 1:B:232:PHE:CD1  | 2.65                     | 0.43              |
| 1:C:123:ILE:HD12 | 1:C:135:ILE:HD13 | 2.00                     | 0.43              |
| 1:C:161:ILE:HD11 | 1:C:197:ILE:HG13 | 1.99                     | 0.43              |
| 1:C:237:LEU:O    | 1:C:238:THR:C    | 2.61                     | 0.43              |
| 1:D:221:GLU:O    | 1:D:222:GLU:C    | 2.59                     | 0.43              |
| 1:E:119:ALA:HA   | 1:E:165:LEU:CD1  | 2.48                     | 0.43              |
| 1:A:163:MET:HE1  | 1:A:220:ALA:O    | 2.18                     | 0.43              |
| 1:B:199:VAL:O    | 1:B:199:VAL:HG12 | 2.17                     | 0.43              |
| 1:D:178:ALA:O    | 1:D:179:HIS:C    | 2.61                     | 0.43              |
| 1:A:119:ALA:O    | 1:A:123:ILE:HG12 | 2.18                     | 0.43              |
| 1:A:223:HIS:C    | 1:A:225:GLU:N    | 2.76                     | 0.43              |
| 1:A:234:PRO:HD2  | 1:A:235:GLU:OE1  | 2.18                     | 0.43              |
| 1:B:4:PHE:C      | 1:B:6:GLU:H      | 2.26                     | 0.43              |
| 1:B:126:LEU:O    | 1:B:133:ILE:HD11 | 2.19                     | 0.43              |
| 1:C:125:LYS:HE3  | 1:C:129:LEU:HD11 | 2.01                     | 0.43              |
| 1:C:152:LYS:HB3  | 1:C:156:GLU:OE2  | 2.18                     | 0.43              |
| 1:D:93:LEU:HD22  | 1:D:93:LEU:C     | 2.44                     | 0.43              |
| 1:D:186:MET:HA   | 1:D:189:GLN:CD   | 2.42                     | 0.43              |
| 1:E:148:VAL:O    | 1:E:152:LYS:HG3  | 2.17                     | 0.43              |
| 1:E:164:ALA:HB3  | 1:E:198:GLU:HA   | 2.00                     | 0.43              |
| 1:A:187:LEU:O    | 1:A:191:MET:N    | 2.51                     | 0.43              |
| 1:B:165:LEU:HD23 | 1:B:199:VAL:HG21 | 2.01                     | 0.43              |
| 1:C:189:GLN:O    | 1:C:190:LEU:C    | 2.61                     | 0.43              |
| 1:D:74:GLU:OE1   | 1:D:74:GLU:HA    | 2.19                     | 0.43              |
| 1:D:83:PHE:O     | 1:D:87:ILE:HG12  | 2.18                     | 0.43              |
| 1:D:165:LEU:CD2  | 1:D:199:VAL:HG21 | 2.48                     | 0.43              |
| 1:E:23:PHE:CD1   | 1:E:24:ILE:N     | 2.87                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:113:PHE:O    | 1:E:113:PHE:HD1  | 2.01                     | 0.43              |
| 1:E:125:LYS:HB2  | 1:E:221:GLU:OE1  | 2.18                     | 0.43              |
| 1:B:145:ASP:O    | 1:B:146:LEU:C    | 2.62                     | 0.43              |
| 1:B:182:SER:O    | 1:B:185:LEU:HB2  | 2.18                     | 0.43              |
| 1:E:80:ILE:O     | 1:E:84:ALA:N     | 2.38                     | 0.43              |
| 1:A:229:TYR:O    | 1:A:232:PHE:N    | 2.52                     | 0.43              |
| 1:B:146:LEU:C    | 1:B:150:CYS:HG   | 2.27                     | 0.43              |
| 1:B:187:LEU:HA   | 1:B:190:LEU:HB2  | 2.00                     | 0.43              |
| 1:B:193:ASN:HB3  | 1:C:152:LYS:HG2  | 2.01                     | 0.43              |
| 1:C:113:PHE:CB   | 1:C:142:GLY:HA2  | 2.48                     | 0.43              |
| 1:C:159:CYS:C    | 1:C:161:ILE:N    | 2.77                     | 0.43              |
| 1:D:167:MET:CE   | 1:D:212:LEU:HD21 | 2.49                     | 0.43              |
| 1:E:234:PRO:HG2  | 1:E:235:GLU:H    | 1.83                     | 0.43              |
| 1:B:189:GLN:HB3  | 1:C:148:VAL:CG2  | 2.48                     | 0.43              |
| 1:C:176:VAL:HG12 | 1:C:180:GLU:HG3  | 2.00                     | 0.43              |
| 1:D:15:LYS:O     | 1:D:18:PRO:HD2   | 2.19                     | 0.43              |
| 1:D:237:LEU:HA   | 1:D:240:MET:HB2  | 2.00                     | 0.43              |
| 1:E:131:PRO:O    | 1:E:133:ILE:N    | 2.52                     | 0.43              |
| 1:A:156:GLU:C    | 1:A:157:GLU:HG2  | 2.42                     | 0.43              |
| 1:C:127:LYS:HA   | 1:C:133:ILE:HD11 | 2.00                     | 0.43              |
| 1:C:151:LYS:O    | 1:C:152:LYS:C    | 2.62                     | 0.43              |
| 1:D:120:SER:O    | 1:D:122:ALA:N    | 2.52                     | 0.43              |
| 1:D:121:ILE:HG13 | 1:D:217:LYS:HB2  | 1.99                     | 0.43              |
| 1:D:122:ALA:C    | 1:D:124:LYS:N    | 2.76                     | 0.43              |
| 1:D:195:HIS:HA   | 1:E:148:VAL:HG21 | 2.01                     | 0.43              |
| 1:A:236:TYR:CE1  | 1:A:240:MET:SD   | 3.12                     | 0.42              |
| 1:C:65:VAL:O     | 1:C:68:TRP:CD1   | 2.72                     | 0.42              |
| 1:C:245:LEU:CD2  | 1:C:245:LEU:N    | 2.82                     | 0.42              |
| 1:D:25:MET:O     | 1:D:29:SER:CA    | 2.67                     | 0.42              |
| 1:D:39:ASN:O     | 1:D:40:ILE:HG12  | 2.19                     | 0.42              |
| 1:D:125:LYS:CB   | 1:D:221:GLU:HG3  | 2.49                     | 0.42              |
| 1:E:186:MET:O    | 1:E:190:LEU:CD1  | 2.66                     | 0.42              |
| 1:B:60:GLU:HB2   | 1:B:61:LEU:H     | 1.05                     | 0.42              |
| 1:B:146:LEU:O    | 1:B:150:CYS:SG   | 2.75                     | 0.42              |
| 1:B:149:ALA:O    | 1:B:153:LEU:HD12 | 2.19                     | 0.42              |
| 1:C:208:ASP:OD1  | 1:C:208:ASP:C    | 2.62                     | 0.42              |
| 1:E:78:PHE:HA    | 1:E:81:ILE:HG22  | 2.01                     | 0.42              |
| 1:E:96:GLU:O     | 1:E:99:GLU:CB    | 2.68                     | 0.42              |
| 1:E:118:MET:O    | 1:E:119:ALA:C    | 2.61                     | 0.42              |
| 1:E:125:LYS:NZ   | 1:E:129:LEU:HD11 | 2.34                     | 0.42              |
| 1:B:25:MET:SD    | 1:C:16:VAL:HG21  | 2.59                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:229:TYR:CD1  | 1:B:233:LYS:HD3  | 2.54                     | 0.42              |
| 1:B:244:GLY:HA2  | 1:B:252:ALA:O    | 2.18                     | 0.42              |
| 1:C:111:THR:HG21 | 1:C:114:ALA:HB2  | 1.98                     | 0.42              |
| 1:A:121:ILE:HG21 | 1:A:217:LYS:CB   | 2.47                     | 0.42              |
| 1:D:21:ILE:HA    | 1:D:24:ILE:HG22  | 2.01                     | 0.42              |
| 1:D:79:ILE:HG23  | 1:D:83:PHE:CE2   | 2.51                     | 0.42              |
| 1:D:96:GLU:OE2   | 1:D:96:GLU:CA    | 2.67                     | 0.42              |
| 1:A:71:PHE:O     | 1:A:75:LEU:N     | 2.41                     | 0.42              |
| 1:B:198:GLU:OE1  | 1:C:144:LYS:HB3  | 2.18                     | 0.42              |
| 1:C:26:GLY:O     | 1:C:30:THR:HG22  | 2.19                     | 0.42              |
| 1:C:63:PRO:CG    | 1:C:65:VAL:HB    | 2.36                     | 0.42              |
| 1:C:160:ASP:C    | 1:C:161:ILE:HG22 | 2.44                     | 0.42              |
| 1:E:90:LYS:HZ3   | 1:E:91:LYS:CG    | 2.33                     | 0.42              |
| 1:E:121:ILE:HD13 | 1:E:121:ILE:N    | 2.33                     | 0.42              |
| 1:E:125:LYS:O    | 1:E:125:LYS:CG   | 2.67                     | 0.42              |
| 1:E:151:LYS:HG2  | 1:E:155:GLU:CD   | 2.43                     | 0.42              |
| 1:A:7:PHE:CD1    | 1:A:7:PHE:C      | 2.96                     | 0.42              |
| 1:A:189:GLN:HE21 | 1:A:196:ILE:N    | 2.17                     | 0.42              |
| 1:A:229:TYR:HA   | 1:A:233:LYS:H    | 1.85                     | 0.42              |
| 1:B:129:LEU:CD1  | 1:B:129:LEU:H    | 2.32                     | 0.42              |
| 1:B:130:SER:HA   | 1:B:131:PRO:HD3  | 1.67                     | 0.42              |
| 1:C:122:ALA:HB2  | 1:C:220:ALA:O    | 2.20                     | 0.42              |
| 1:C:128:GLU:OE2  | 1:C:129:LEU:CD1  | 2.67                     | 0.42              |
| 1:C:171:ALA:C    | 1:C:173:LYS:H    | 2.27                     | 0.42              |
| 1:D:66:ILE:C     | 1:D:66:ILE:CD1   | 2.93                     | 0.42              |
| 1:D:124:LYS:C    | 1:D:126:LEU:N    | 2.76                     | 0.42              |
| 1:D:164:ALA:CB   | 1:D:198:GLU:HA   | 2.48                     | 0.42              |
| 1:E:147:PRO:O    | 1:E:149:ALA:N    | 2.53                     | 0.42              |
| 1:A:108:ILE:O    | 1:A:108:ILE:HG22 | 2.19                     | 0.42              |
| 1:B:158:GLY:O    | 1:B:160:ASP:N    | 2.53                     | 0.42              |
| 1:B:159:CYS:C    | 1:B:161:ILE:H    | 2.27                     | 0.42              |
| 1:C:42:MET:C     | 1:C:44:ILE:H     | 2.26                     | 0.42              |
| 1:C:168:PRO:HG2  | 1:C:202:HIS:HA   | 2.01                     | 0.42              |
| 1:D:119:ALA:CB   | 1:D:137:ARG:NH2  | 2.83                     | 0.42              |
| 1:E:126:LEU:C    | 1:E:133:ILE:CD1  | 2.92                     | 0.42              |
| 1:E:222:GLU:O    | 1:E:226:ASN:OD1  | 2.37                     | 0.42              |
| 1:A:165:LEU:HA   | 1:A:199:VAL:CB   | 2.48                     | 0.42              |
| 1:B:40:ILE:HG22  | 1:B:41:ILE:N     | 2.26                     | 0.42              |
| 1:B:190:LEU:HD23 | 1:C:151:LYS:HD2  | 2.01                     | 0.42              |
| 1:C:240:MET:O    | 1:C:241:ALA:C    | 2.62                     | 0.42              |
| 1:E:90:LYS:O     | 1:E:94:GLN:HG3   | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:118:MET:HB2  | 1:E:165:LEU:HD22 | 2.00                     | 0.42              |
| 1:A:183:LEU:O    | 1:A:184:GLY:C    | 2.61                     | 0.42              |
| 1:A:189:GLN:HE21 | 1:A:196:ILE:H    | 1.68                     | 0.42              |
| 1:B:240:MET:HA   | 1:B:240:MET:HE2  | 2.01                     | 0.42              |
| 1:C:42:MET:O     | 1:C:44:ILE:N     | 2.47                     | 0.42              |
| 1:C:127:LYS:N    | 1:C:133:ILE:HD11 | 2.35                     | 0.42              |
| 1:D:63:PRO:CD    | 1:D:64:ILE:N     | 2.78                     | 0.42              |
| 1:D:239:ARG:C    | 1:D:241:ALA:N    | 2.75                     | 0.42              |
| 1:E:149:ALA:C    | 1:E:151:LYS:N    | 2.76                     | 0.42              |
| 1:A:219:ARG:O    | 1:A:221:GLU:N    | 2.53                     | 0.42              |
| 1:B:98:VAL:O     | 1:B:98:VAL:CG1   | 2.66                     | 0.42              |
| 1:C:33:ILE:CG1   | 1:C:88:ILE:HD12  | 2.50                     | 0.42              |
| 1:C:100:LYS:HA   | 1:C:100:LYS:HD3  | 1.71                     | 0.42              |
| 1:C:112:THR:O    | 1:C:112:THR:HG22 | 2.19                     | 0.42              |
| 1:D:122:ALA:CB   | 1:D:224:ALA:HB2  | 2.38                     | 0.42              |
| 1:D:125:LYS:CG   | 1:D:221:GLU:HG3  | 2.48                     | 0.42              |
| 1:E:164:ALA:O    | 1:E:199:VAL:CB   | 2.60                     | 0.42              |
| 1:A:88:ILE:CG1   | 1:A:89:ALA:N     | 2.82                     | 0.41              |
| 1:A:229:TYR:O    | 1:A:233:LYS:N    | 2.53                     | 0.41              |
| 1:B:144:LYS:O    | 1:B:147:PRO:HG2  | 2.20                     | 0.41              |
| 1:D:65:VAL:O     | 1:D:69:GLY:N     | 2.41                     | 0.41              |
| 1:A:240:MET:CE   | 1:A:240:MET:CA   | 2.91                     | 0.41              |
| 1:C:7:PHE:O      | 1:C:9:GLU:N      | 2.53                     | 0.41              |
| 1:C:230:LEU:HD11 | 1:D:141:PRO:CD   | 2.49                     | 0.41              |
| 1:D:25:MET:SD    | 1:E:16:VAL:CG1   | 3.00                     | 0.41              |
| 1:D:65:VAL:O     | 1:D:66:ILE:C     | 2.61                     | 0.41              |
| 1:D:221:GLU:O    | 1:D:223:HIS:N    | 2.53                     | 0.41              |
| 1:A:30:THR:CG2   | 1:A:31:ALA:H     | 2.30                     | 0.41              |
| 1:B:74:GLU:C     | 1:B:74:GLU:OE2   | 2.63                     | 0.41              |
| 1:B:112:THR:OG1  | 1:B:139:THR:CG2  | 2.68                     | 0.41              |
| 1:C:110:ASP:CG   | 1:C:139:THR:OG1  | 2.63                     | 0.41              |
| 1:D:68:TRP:NE1   | 1:E:44:ILE:HG21  | 2.35                     | 0.41              |
| 1:A:146:LEU:C    | 1:A:150:CYS:HG   | 2.27                     | 0.41              |
| 1:A:233:LYS:O    | 1:A:237:LEU:HD12 | 2.21                     | 0.41              |
| 1:C:17:ILE:O     | 1:C:21:ILE:HG13  | 2.20                     | 0.41              |
| 1:C:99:GLU:HG3   | 1:C:100:LYS:HG2  | 2.03                     | 0.41              |
| 1:C:128:GLU:HG2  | 1:C:129:LEU:HD12 | 2.02                     | 0.41              |
| 1:C:161:ILE:CG1  | 1:C:162:VAL:N    | 2.75                     | 0.41              |
| 1:D:110:ASP:OD1  | 1:D:138:LYS:O    | 2.38                     | 0.41              |
| 1:E:39:ASN:O     | 1:E:43:PRO:HG3   | 2.21                     | 0.41              |
| 1:A:42:MET:HE2   | 1:A:46:THR:HG21  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:129:LEU:CD2  | 1:A:228:TYR:HB2  | 2.46                     | 0.41              |
| 1:B:18:PRO:HB3   | 1:C:14:TYR:HE2   | 1.85                     | 0.41              |
| 1:B:107:GLY:HA2  | 1:B:136:ILE:O    | 2.21                     | 0.41              |
| 1:B:112:THR:HB   | 1:B:140:VAL:O    | 2.20                     | 0.41              |
| 1:B:125:LYS:O    | 1:B:125:LYS:HG3  | 2.19                     | 0.41              |
| 1:C:63:PRO:HB2   | 1:C:65:VAL:HA    | 2.03                     | 0.41              |
| 1:D:11:LEU:O     | 1:D:15:LYS:CA    | 2.69                     | 0.41              |
| 1:D:39:ASN:O     | 1:D:40:ILE:CD1   | 2.69                     | 0.41              |
| 1:D:111:THR:CG2  | 1:D:166:GLY:CA   | 2.97                     | 0.41              |
| 1:D:173:LYS:C    | 1:D:175:LYS:H    | 2.28                     | 0.41              |
| 1:E:103:THR:C    | 1:E:104:LYS:O    | 2.62                     | 0.41              |
| 1:A:15:LYS:HA    | 1:A:17:ILE:HD12  | 2.03                     | 0.41              |
| 1:A:72:LEU:O     | 1:A:76:VAL:N     | 2.44                     | 0.41              |
| 1:A:140:VAL:HB   | 1:A:141:PRO:HD2  | 2.01                     | 0.41              |
| 1:B:7:PHE:C      | 1:B:9:GLU:H      | 2.27                     | 0.41              |
| 1:B:146:LEU:CG   | 1:B:147:PRO:HD3  | 2.48                     | 0.41              |
| 1:C:15:LYS:C     | 1:C:18:PRO:HD2   | 2.45                     | 0.41              |
| 1:C:85:VAL:HG11  | 1:D:28:ALA:CB    | 2.51                     | 0.41              |
| 1:D:71:PHE:CD1   | 1:E:40:ILE:HG12  | 2.52                     | 0.41              |
| 1:E:25:MET:O     | 1:E:29:SER:N     | 2.46                     | 0.41              |
| 1:E:179:HIS:C    | 1:E:179:HIS:CD2  | 2.99                     | 0.41              |
| 1:B:158:GLY:O    | 1:B:160:ASP:OD1  | 2.39                     | 0.41              |
| 1:B:202:HIS:HB3  | 1:B:204:ASP:OD1  | 2.20                     | 0.41              |
| 1:C:65:VAL:HG22  | 1:C:66:ILE:O     | 2.21                     | 0.41              |
| 1:D:113:PHE:CD1  | 1:D:113:PHE:C    | 2.99                     | 0.41              |
| 1:D:162:VAL:HG13 | 1:D:163:MET:H    | 1.85                     | 0.41              |
| 1:E:109:VAL:O    | 1:E:165:LEU:HB2  | 2.19                     | 0.41              |
| 1:E:150:CYS:HB3  | 1:E:196:ILE:CD1  | 2.51                     | 0.41              |
| 1:E:225:GLU:HG2  | 1:E:229:TYR:CZ   | 2.56                     | 0.41              |
| 1:A:106:VAL:CG1  | 1:A:108:ILE:HD11 | 2.50                     | 0.41              |
| 1:B:149:ALA:O    | 1:B:152:LYS:N    | 2.54                     | 0.41              |
| 1:C:19:LEU:HD13  | 1:C:19:LEU:O     | 2.20                     | 0.41              |
| 1:C:71:PHE:HZ    | 1:D:43:PRO:HG2   | 1.84                     | 0.41              |
| 1:E:90:LYS:HD2   | 1:E:90:LYS:C     | 2.45                     | 0.41              |
| 1:E:108:ILE:HG23 | 1:E:165:LEU:CD1  | 2.47                     | 0.41              |
| 1:E:233:LYS:O    | 1:E:233:LYS:HG2  | 2.21                     | 0.41              |
| 1:A:7:PHE:CD1    | 1:A:11:LEU:HG    | 2.56                     | 0.41              |
| 1:A:143:ILE:O    | 1:A:146:LEU:HD11 | 2.20                     | 0.41              |
| 1:A:164:ALA:N    | 1:A:199:VAL:HG23 | 2.36                     | 0.41              |
| 1:A:228:TYR:CE1  | 1:A:232:PHE:CD1  | 3.08                     | 0.41              |
| 1:A:234:PRO:HG2  | 1:A:235:GLU:CD   | 2.45                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:115:ARG:O    | 1:B:116:VAL:CG2  | 2.66                     | 0.41              |
| 1:B:144:LYS:H    | 1:B:144:LYS:HG3  | 1.67                     | 0.41              |
| 1:B:179:HIS:CD2  | 1:B:183:LEU:HD11 | 2.55                     | 0.41              |
| 1:C:17:ILE:N     | 1:C:18:PRO:CD    | 2.84                     | 0.41              |
| 1:C:86:PHE:HB3   | 1:E:7:PHE:CZ     | 2.56                     | 0.41              |
| 1:C:111:THR:OG1  | 1:C:112:THR:N    | 2.54                     | 0.41              |
| 1:C:241:ALA:O    | 1:C:242:GLY:C    | 2.64                     | 0.41              |
| 1:D:213:ASP:O    | 1:D:217:LYS:HG2  | 2.21                     | 0.41              |
| 1:D:230:LEU:HD11 | 1:E:141:PRO:CD   | 2.50                     | 0.41              |
| 1:E:44:ILE:C     | 1:E:46:THR:N     | 2.79                     | 0.41              |
| 1:E:122:ALA:O    | 1:E:123:ILE:C    | 2.63                     | 0.41              |
| 1:E:146:LEU:CB   | 1:E:147:PRO:HD3  | 2.51                     | 0.41              |
| 1:E:151:LYS:CG   | 1:E:155:GLU:OE2  | 2.64                     | 0.41              |
| 1:A:17:ILE:N     | 1:A:18:PRO:CD    | 2.84                     | 0.41              |
| 1:A:45:ILE:O     | 1:A:45:ILE:CG2   | 2.64                     | 0.41              |
| 1:B:61:LEU:CD1   | 1:B:63:PRO:CB    | 2.91                     | 0.41              |
| 1:B:90:LYS:HD2   | 1:B:90:LYS:C     | 2.46                     | 0.41              |
| 1:B:165:LEU:HA   | 1:B:199:VAL:CB   | 2.42                     | 0.41              |
| 1:B:229:TYR:CE1  | 1:B:233:LYS:HD3  | 2.56                     | 0.41              |
| 1:B:237:LEU:HA   | 1:B:240:MET:CG   | 2.51                     | 0.41              |
| 1:C:15:LYS:O     | 1:C:18:PRO:HD2   | 2.21                     | 0.41              |
| 1:C:78:PHE:HE2   | 1:D:32:LEU:HA    | 1.86                     | 0.41              |
| 1:C:94:GLN:OE1   | 1:C:94:GLN:HA    | 2.20                     | 0.41              |
| 1:C:149:ALA:C    | 1:C:153:LEU:HD13 | 2.45                     | 0.41              |
| 1:C:168:PRO:HG2  | 1:C:202:HIS:CA   | 2.50                     | 0.41              |
| 1:E:46:THR:OG1   | 1:E:47:PRO:HD3   | 2.21                     | 0.41              |
| 1:E:99:GLU:CD    | 1:E:99:GLU:C     | 2.89                     | 0.41              |
| 1:E:152:LYS:O    | 1:E:153:LEU:C    | 2.64                     | 0.41              |
| 1:E:214:TRP:O    | 1:E:218:ARG:HB2  | 2.20                     | 0.41              |
| 1:A:66:ILE:O     | 1:A:67:SER:OG    | 2.29                     | 0.40              |
| 1:A:75:LEU:HD11  | 1:B:32:LEU:HD22  | 2.03                     | 0.40              |
| 1:A:86:PHE:CE2   | 1:C:7:PHE:HE1    | 2.38                     | 0.40              |
| 1:A:225:GLU:CG   | 1:A:229:TYR:OH   | 2.69                     | 0.40              |
| 1:C:63:PRO:HB2   | 1:C:65:VAL:H     | 1.86                     | 0.40              |
| 1:D:95:GLU:HB2   | 1:D:96:GLU:OE2   | 2.21                     | 0.40              |
| 1:D:161:ILE:HD11 | 1:D:197:ILE:HG12 | 2.03                     | 0.40              |
| 1:D:202:HIS:O    | 1:D:205:GLU:HG3  | 2.21                     | 0.40              |
| 1:D:223:HIS:O    | 1:D:225:GLU:N    | 2.54                     | 0.40              |
| 1:E:69:GLY:HA2   | 1:E:72:LEU:CG    | 2.51                     | 0.40              |
| 1:E:75:LEU:HG    | 1:E:76:VAL:N     | 2.36                     | 0.40              |
| 1:E:171:ALA:C    | 1:E:173:LYS:N    | 2.79                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:27:ILE:HA    | 1:A:30:THR:HG22  | 2.04                     | 0.40              |
| 1:A:169:GLY:HA2  | 1:A:203:GLU:OE2  | 2.21                     | 0.40              |
| 1:A:219:ARG:C    | 1:A:221:GLU:N    | 2.78                     | 0.40              |
| 1:A:228:TYR:O    | 1:A:229:TYR:C    | 2.65                     | 0.40              |
| 1:B:228:TYR:CD1  | 1:B:232:PHE:CE1  | 3.09                     | 0.40              |
| 1:C:40:ILE:HG22  | 1:C:41:ILE:HD13  | 2.03                     | 0.40              |
| 1:C:235:GLU:O    | 1:C:238:THR:CB   | 2.63                     | 0.40              |
| 1:D:146:LEU:O    | 1:D:149:ALA:CB   | 2.62                     | 0.40              |
| 1:E:106:VAL:HG12 | 1:E:107:GLY:N    | 2.37                     | 0.40              |
| 1:A:12:TYR:O     | 1:A:13:GLU:HB3   | 2.21                     | 0.40              |
| 1:A:105:LYS:N    | 1:A:134:LYS:HB2  | 2.36                     | 0.40              |
| 1:A:162:VAL:CG1  | 1:A:163:MET:N    | 2.84                     | 0.40              |
| 1:B:125:LYS:HB3  | 1:B:221:GLU:HG3  | 2.04                     | 0.40              |
| 1:B:187:LEU:O    | 1:B:188:ALA:C    | 2.63                     | 0.40              |
| 1:C:4:PHE:C      | 1:C:6:GLU:H      | 2.30                     | 0.40              |
| 1:C:121:ILE:CG2  | 1:C:220:ALA:HB3  | 2.52                     | 0.40              |
| 1:D:61:LEU:HD12  | 1:D:65:VAL:HG21  | 2.03                     | 0.40              |
| 1:D:105:LYS:HE3  | 1:D:158:GLY:HA3  | 2.02                     | 0.40              |
| 1:E:7:PHE:CZ     | 1:E:11:LEU:HD21  | 2.56                     | 0.40              |
| 1:E:120:SER:C    | 1:E:122:ALA:N    | 2.79                     | 0.40              |
| 1:A:108:ILE:CG2  | 1:A:165:LEU:HD12 | 2.52                     | 0.40              |
| 1:B:103:THR:O    | 1:B:104:LYS:HD2  | 2.21                     | 0.40              |
| 1:B:129:LEU:N    | 1:B:129:LEU:CD1  | 2.84                     | 0.40              |
| 1:B:145:ASP:O    | 1:B:147:PRO:HD2  | 2.21                     | 0.40              |
| 1:C:93:LEU:O     | 1:C:96:GLU:CB    | 2.69                     | 0.40              |
| 1:C:125:LYS:HB2  | 1:C:221:GLU:HG3  | 2.03                     | 0.40              |
| 1:E:121:ILE:CD1  | 1:E:121:ILE:H    | 2.35                     | 0.40              |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1       | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------|---------------------|--------------------------|-------------------|
| 1:D:62:GLY:N | 1:D:62:GLY:O[2_645] | 2.13                     | 0.07              |
| 1:D:62:GLY:O | 1:D:62:GLY:O[2_645] | 2.15                     | 0.05              |



## 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     | 239/277 (86%)   | 168 (70%) | 49 (20%)  | 22 (9%)  | 0           | 10 |
| 1   | B     | 224/277 (81%)   | 143 (64%) | 66 (30%)  | 15 (7%)  | 1           | 14 |
| 1   | C     | 228/277 (82%)   | 161 (71%) | 45 (20%)  | 22 (10%) | 0           | 8  |
| 1   | D     | 229/277 (83%)   | 167 (73%) | 46 (20%)  | 16 (7%)  | 1           | 13 |
| 1   | E     | 223/277 (80%)   | 163 (73%) | 46 (21%)  | 14 (6%)  | 1           | 15 |
| All | All   | 1143/1385 (82%) | 802 (70%) | 252 (22%) | 89 (8%)  | 1           | 12 |

All (89) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 67  | SER  |
| 1   | A     | 99  | GLU  |
| 1   | A     | 100 | LYS  |
| 1   | A     | 105 | LYS  |
| 1   | A     | 119 | ALA  |
| 1   | A     | 243 | LYS  |
| 1   | B     | 61  | LEU  |
| 1   | B     | 161 | ILE  |
| 1   | C     | 44  | ILE  |
| 1   | C     | 65  | VAL  |
| 1   | C     | 66  | ILE  |
| 1   | C     | 160 | ASP  |
| 1   | C     | 161 | ILE  |
| 1   | C     | 241 | ALA  |
| 1   | D     | 59  | VAL  |
| 1   | D     | 157 | GLU  |
| 1   | D     | 161 | ILE  |
| 1   | D     | 194 | LYS  |
| 1   | E     | 119 | ALA  |
| 1   | E     | 157 | GLU  |
| 1   | E     | 161 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 193 | ASN  |
| 1   | A     | 159 | CYS  |
| 1   | A     | 233 | LYS  |
| 1   | B     | 44  | ILE  |
| 1   | B     | 102 | MET  |
| 1   | B     | 138 | LYS  |
| 1   | B     | 245 | LEU  |
| 1   | C     | 8   | LYS  |
| 1   | C     | 145 | ASP  |
| 1   | C     | 247 | GLN  |
| 1   | D     | 40  | ILE  |
| 1   | D     | 46  | THR  |
| 1   | D     | 121 | ILE  |
| 1   | D     | 160 | ASP  |
| 1   | A     | 57  | ALA  |
| 1   | A     | 171 | ALA  |
| 1   | A     | 220 | ALA  |
| 1   | B     | 60  | GLU  |
| 1   | B     | 100 | LYS  |
| 1   | B     | 193 | ASN  |
| 1   | B     | 251 | ASP  |
| 1   | C     | 119 | ALA  |
| 1   | C     | 168 | PRO  |
| 1   | C     | 172 | GLU  |
| 1   | D     | 159 | CYS  |
| 1   | E     | 146 | LEU  |
| 1   | E     | 171 | ALA  |
| 1   | A     | 64  | ILE  |
| 1   | C     | 121 | ILE  |
| 1   | D     | 99  | GLU  |
| 1   | D     | 147 | PRO  |
| 1   | D     | 158 | GLY  |
| 1   | E     | 132 | ASN  |
| 1   | E     | 150 | CYS  |
| 1   | E     | 172 | GLU  |
| 1   | A     | 162 | VAL  |
| 1   | A     | 188 | ALA  |
| 1   | B     | 130 | SER  |
| 1   | B     | 146 | LEU  |
| 1   | B     | 247 | GLN  |
| 1   | C     | 46  | THR  |
| 1   | C     | 146 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 215 | LEU  |
| 1   | C     | 234 | PRO  |
| 1   | C     | 238 | THR  |
| 1   | E     | 147 | PRO  |
| 1   | A     | 47  | PRO  |
| 1   | A     | 141 | PRO  |
| 1   | A     | 146 | LEU  |
| 1   | A     | 224 | ALA  |
| 1   | E     | 42  | MET  |
| 1   | E     | 201 | VAL  |
| 1   | A     | 196 | ILE  |
| 1   | C     | 233 | LYS  |
| 1   | D     | 201 | VAL  |
| 1   | A     | 161 | ILE  |
| 1   | D     | 41  | ILE  |
| 1   | E     | 133 | ILE  |
| 1   | B     | 234 | PRO  |
| 1   | C     | 43  | PRO  |
| 1   | D     | 148 | VAL  |
| 1   | E     | 162 | VAL  |
| 1   | A     | 147 | PRO  |
| 1   | B     | 45  | ILE  |
| 1   | C     | 147 | PRO  |
| 1   | C     | 42  | MET  |
| 1   | D     | 42  | MET  |
| 1   | A     | 63  | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 185/231 (80%) | 160 (86%) | 25 (14%) | 4           | 17 |
| 1   | B     | 181/231 (78%) | 153 (84%) | 28 (16%) | 2           | 14 |
| 1   | C     | 178/231 (77%) | 150 (84%) | 28 (16%) | 2           | 14 |
| 1   | D     | 184/231 (80%) | 158 (86%) | 26 (14%) | 3           | 17 |

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| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |    |
|-----|-------|----------------|-----------|-----------|-------------|----|
| 1   | E     | 171/231 (74%)  | 140 (82%) | 31 (18%)  | 2           | 11 |
| All | All   | 899/1155 (78%) | 761 (85%) | 138 (15%) | 2           | 14 |

All (138) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 17  | ILE  |
| 1   | A     | 18  | PRO  |
| 1   | A     | 40  | ILE  |
| 1   | A     | 42  | MET  |
| 1   | A     | 61  | LEU  |
| 1   | A     | 72  | LEU  |
| 1   | A     | 88  | ILE  |
| 1   | A     | 99  | GLU  |
| 1   | A     | 100 | LYS  |
| 1   | A     | 101 | LYS  |
| 1   | A     | 111 | THR  |
| 1   | A     | 129 | LEU  |
| 1   | A     | 146 | LEU  |
| 1   | A     | 150 | CYS  |
| 1   | A     | 157 | GLU  |
| 1   | A     | 162 | VAL  |
| 1   | A     | 191 | MET  |
| 1   | A     | 192 | THR  |
| 1   | A     | 197 | ILE  |
| 1   | A     | 201 | VAL  |
| 1   | A     | 204 | ASP  |
| 1   | A     | 217 | LYS  |
| 1   | A     | 237 | LEU  |
| 1   | A     | 238 | THR  |
| 1   | A     | 240 | MET  |
| 1   | B     | 17  | ILE  |
| 1   | B     | 38  | ASP  |
| 1   | B     | 46  | THR  |
| 1   | B     | 59  | VAL  |
| 1   | B     | 60  | GLU  |
| 1   | B     | 61  | LEU  |
| 1   | B     | 75  | LEU  |
| 1   | B     | 88  | ILE  |
| 1   | B     | 90  | LYS  |
| 1   | B     | 96  | GLU  |
| 1   | B     | 101 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 108 | ILE  |
| 1   | B     | 111 | THR  |
| 1   | B     | 134 | LYS  |
| 1   | B     | 146 | LEU  |
| 1   | B     | 147 | PRO  |
| 1   | B     | 148 | VAL  |
| 1   | B     | 150 | CYS  |
| 1   | B     | 160 | ASP  |
| 1   | B     | 162 | VAL  |
| 1   | B     | 191 | MET  |
| 1   | B     | 192 | THR  |
| 1   | B     | 196 | ILE  |
| 1   | B     | 204 | ASP  |
| 1   | B     | 217 | LYS  |
| 1   | B     | 232 | PHE  |
| 1   | B     | 234 | PRO  |
| 1   | B     | 249 | PHE  |
| 1   | C     | 17  | ILE  |
| 1   | C     | 32  | LEU  |
| 1   | C     | 37  | VAL  |
| 1   | C     | 44  | ILE  |
| 1   | C     | 75  | LEU  |
| 1   | C     | 76  | VAL  |
| 1   | C     | 88  | ILE  |
| 1   | C     | 98  | VAL  |
| 1   | C     | 99  | GLU  |
| 1   | C     | 105 | LYS  |
| 1   | C     | 111 | THR  |
| 1   | C     | 134 | LYS  |
| 1   | C     | 146 | LEU  |
| 1   | C     | 147 | PRO  |
| 1   | C     | 148 | VAL  |
| 1   | C     | 150 | CYS  |
| 1   | C     | 161 | ILE  |
| 1   | C     | 165 | LEU  |
| 1   | C     | 177 | CYS  |
| 1   | C     | 187 | LEU  |
| 1   | C     | 191 | MET  |
| 1   | C     | 192 | THR  |
| 1   | C     | 196 | ILE  |
| 1   | C     | 204 | ASP  |
| 1   | C     | 217 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 231 | LEU  |
| 1   | C     | 240 | MET  |
| 1   | C     | 246 | ARG  |
| 1   | D     | 7   | PHE  |
| 1   | D     | 17  | ILE  |
| 1   | D     | 59  | VAL  |
| 1   | D     | 61  | LEU  |
| 1   | D     | 64  | ILE  |
| 1   | D     | 65  | VAL  |
| 1   | D     | 66  | ILE  |
| 1   | D     | 88  | ILE  |
| 1   | D     | 91  | LYS  |
| 1   | D     | 92  | VAL  |
| 1   | D     | 93  | LEU  |
| 1   | D     | 96  | GLU  |
| 1   | D     | 105 | LYS  |
| 1   | D     | 111 | THR  |
| 1   | D     | 112 | THR  |
| 1   | D     | 146 | LEU  |
| 1   | D     | 150 | CYS  |
| 1   | D     | 154 | LEU  |
| 1   | D     | 165 | LEU  |
| 1   | D     | 187 | LEU  |
| 1   | D     | 191 | MET  |
| 1   | D     | 192 | THR  |
| 1   | D     | 199 | VAL  |
| 1   | D     | 204 | ASP  |
| 1   | D     | 231 | LEU  |
| 1   | D     | 237 | LEU  |
| 1   | E     | 17  | ILE  |
| 1   | E     | 18  | PRO  |
| 1   | E     | 23  | PHE  |
| 1   | E     | 37  | VAL  |
| 1   | E     | 40  | ILE  |
| 1   | E     | 67  | SER  |
| 1   | E     | 68  | TRP  |
| 1   | E     | 75  | LEU  |
| 1   | E     | 78  | PHE  |
| 1   | E     | 88  | ILE  |
| 1   | E     | 90  | LYS  |
| 1   | E     | 93  | LEU  |
| 1   | E     | 102 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 105 | LYS  |
| 1   | E     | 111 | THR  |
| 1   | E     | 121 | ILE  |
| 1   | E     | 143 | ILE  |
| 1   | E     | 145 | ASP  |
| 1   | E     | 146 | LEU  |
| 1   | E     | 148 | VAL  |
| 1   | E     | 156 | GLU  |
| 1   | E     | 162 | VAL  |
| 1   | E     | 183 | LEU  |
| 1   | E     | 187 | LEU  |
| 1   | E     | 191 | MET  |
| 1   | E     | 192 | THR  |
| 1   | E     | 201 | VAL  |
| 1   | E     | 204 | ASP  |
| 1   | E     | 217 | LYS  |
| 1   | E     | 218 | ARG  |
| 1   | E     | 237 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 39  | ASN  |
| 1   | A     | 226 | ASN  |
| 1   | B     | 132 | ASN  |
| 1   | B     | 189 | GLN  |
| 1   | B     | 226 | ASN  |
| 1   | C     | 179 | HIS  |
| 1   | C     | 223 | HIS  |
| 1   | C     | 226 | ASN  |
| 1   | D     | 179 | HIS  |
| 1   | D     | 195 | HIS  |
| 1   | D     | 226 | ASN  |
| 1   | E     | 39  | ASN  |
| 1   | E     | 179 | HIS  |
| 1   | E     | 195 | HIS  |
| 1   | E     | 226 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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 | $\# Z  > 2$ |
| 2   | BNG  | B     | 301 | -    | 21,21,21     | 0.44 | 0           | 26,26,26    | 0.70 | 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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | BNG  | B     | 301 | -    | -       | 7/12/32/32 | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | B     | 301 | BNG  | C4-C5-C6-O6     |
| 2   | B     | 301 | BNG  | O5-C5-C6-O6     |
| 2   | B     | 301 | BNG  | C3'-C4'-C5'-C6' |
| 2   | B     | 301 | BNG  | O1-C1'-C2'-C3'  |

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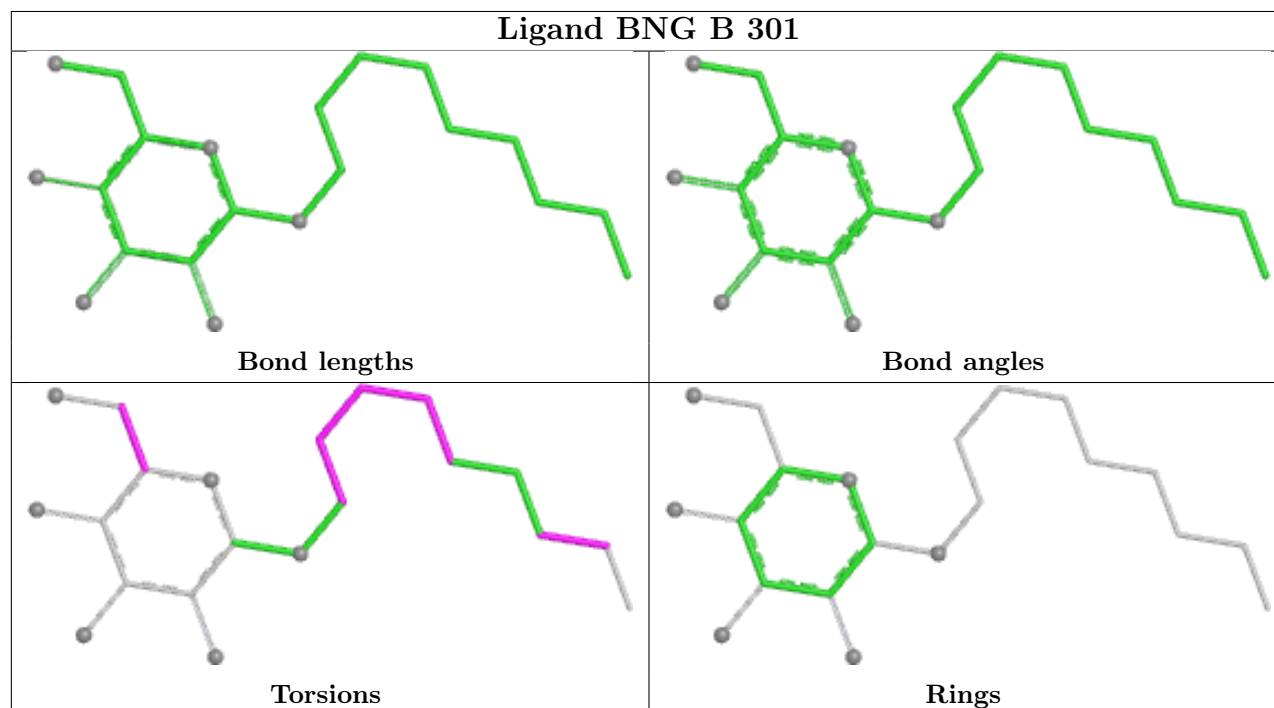
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | B     | 301 | BNG  | C1'-C2'-C3'-C4' |
| 2   | B     | 301 | BNG  | C2'-C3'-C4'-C5' |
| 2   | B     | 301 | BNG  | C6'-C7'-C8'-C9' |

There are no ring outliers.

1 monomer is involved in 12 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 301 | BNG  | 12      | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 241/277 (87%)   | 0.55   | 23 (9%) 14 16  | 87, 254, 449, 499     | 0     |
| 1   | B     | 230/277 (83%)   | 0.36   | 17 (7%) 20 20  | 90, 231, 472, 500     | 0     |
| 1   | C     | 234/277 (84%)   | 0.54   | 21 (8%) 15 17  | 107, 227, 437, 500    | 0     |
| 1   | D     | 235/277 (84%)   | 0.42   | 16 (6%) 23 22  | 97, 243, 483, 500     | 0     |
| 1   | E     | 231/277 (83%)   | 0.69   | 26 (11%) 10 13 | 89, 292, 475, 500     | 0     |
| All | All   | 1171/1385 (84%) | 0.51   | 103 (8%) 15 18 | 87, 247, 463, 500     | 0     |

All (103) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 106 | VAL  | 8.9  |
| 1   | A     | 83  | PHE  | 7.0  |
| 1   | A     | 74  | GLU  | 6.9  |
| 1   | E     | 160 | ASP  | 6.8  |
| 1   | E     | 103 | THR  | 6.3  |
| 1   | E     | 230 | LEU  | 5.8  |
| 1   | D     | 198 | GLU  | 5.8  |
| 1   | E     | 142 | GLY  | 5.8  |
| 1   | E     | 105 | LYS  | 5.6  |
| 1   | A     | 192 | THR  | 5.4  |
| 1   | E     | 141 | PRO  | 5.2  |
| 1   | C     | 175 | LYS  | 5.0  |
| 1   | C     | 32  | LEU  | 4.9  |
| 1   | E     | 195 | HIS  | 4.6  |
| 1   | D     | 17  | ILE  | 4.2  |
| 1   | B     | 83  | PHE  | 4.1  |
| 1   | C     | 163 | MET  | 4.0  |
| 1   | D     | 137 | ARG  | 4.0  |
| 1   | B     | 198 | GLU  | 3.9  |
| 1   | E     | 104 | LYS  | 3.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 157 | GLU  | 3.8  |
| 1   | E     | 140 | VAL  | 3.7  |
| 1   | B     | 200 | PHE  | 3.7  |
| 1   | A     | 137 | ARG  | 3.6  |
| 1   | A     | 119 | ALA  | 3.5  |
| 1   | D     | 216 | ALA  | 3.5  |
| 1   | B     | 167 | MET  | 3.5  |
| 1   | B     | 158 | GLY  | 3.4  |
| 1   | E     | 161 | ILE  | 3.4  |
| 1   | A     | 154 | LEU  | 3.4  |
| 1   | E     | 14  | TYR  | 3.4  |
| 1   | E     | 132 | ASN  | 3.3  |
| 1   | A     | 91  | LYS  | 3.3  |
| 1   | C     | 28  | ALA  | 3.3  |
| 1   | B     | 113 | PHE  | 3.2  |
| 1   | D     | 86  | PHE  | 3.2  |
| 1   | A     | 87  | ILE  | 3.2  |
| 1   | B     | 156 | GLU  | 3.2  |
| 1   | D     | 120 | SER  | 3.1  |
| 1   | B     | 160 | ASP  | 3.1  |
| 1   | C     | 248 | GLY  | 3.1  |
| 1   | E     | 77  | ASN  | 3.1  |
| 1   | D     | 118 | MET  | 3.1  |
| 1   | C     | 215 | LEU  | 3.1  |
| 1   | D     | 223 | HIS  | 3.0  |
| 1   | A     | 151 | LYS  | 2.9  |
| 1   | D     | 83  | PHE  | 2.8  |
| 1   | C     | 74  | GLU  | 2.8  |
| 1   | E     | 176 | VAL  | 2.8  |
| 1   | D     | 220 | ALA  | 2.8  |
| 1   | C     | 192 | THR  | 2.7  |
| 1   | A     | 190 | LEU  | 2.7  |
| 1   | D     | 119 | ALA  | 2.7  |
| 1   | B     | 143 | ILE  | 2.7  |
| 1   | D     | 219 | ARG  | 2.7  |
| 1   | A     | 152 | LYS  | 2.6  |
| 1   | C     | 205 | GLU  | 2.6  |
| 1   | D     | 147 | PRO  | 2.6  |
| 1   | E     | 128 | GLU  | 2.5  |
| 1   | E     | 78  | PHE  | 2.5  |
| 1   | B     | 168 | PRO  | 2.5  |
| 1   | A     | 17  | ILE  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 80  | ILE  | 2.5  |
| 1   | A     | 33  | ILE  | 2.4  |
| 1   | A     | 85  | VAL  | 2.4  |
| 1   | E     | 198 | GLU  | 2.4  |
| 1   | A     | 155 | GLU  | 2.4  |
| 1   | C     | 180 | GLU  | 2.4  |
| 1   | C     | 29  | SER  | 2.4  |
| 1   | A     | 11  | LEU  | 2.4  |
| 1   | C     | 200 | PHE  | 2.4  |
| 1   | C     | 246 | ARG  | 2.4  |
| 1   | A     | 36  | PHE  | 2.3  |
| 1   | A     | 191 | MET  | 2.3  |
| 1   | B     | 114 | ALA  | 2.3  |
| 1   | E     | 157 | GLU  | 2.3  |
| 1   | E     | 56  | THR  | 2.3  |
| 1   | A     | 135 | ILE  | 2.3  |
| 1   | B     | 159 | CYS  | 2.2  |
| 1   | A     | 156 | GLU  | 2.2  |
| 1   | B     | 105 | LYS  | 2.2  |
| 1   | B     | 163 | MET  | 2.2  |
| 1   | C     | 150 | CYS  | 2.2  |
| 1   | A     | 13  | GLU  | 2.2  |
| 1   | E     | 38  | ASP  | 2.2  |
| 1   | E     | 138 | LYS  | 2.1  |
| 1   | E     | 42  | MET  | 2.1  |
| 1   | D     | 196 | ILE  | 2.1  |
| 1   | C     | 68  | TRP  | 2.1  |
| 1   | C     | 229 | TYR  | 2.1  |
| 1   | C     | 189 | GLN  | 2.1  |
| 1   | E     | 57  | ALA  | 2.1  |
| 1   | A     | 128 | GLU  | 2.1  |
| 1   | C     | 87  | ILE  | 2.1  |
| 1   | C     | 109 | VAL  | 2.1  |
| 1   | E     | 109 | VAL  | 2.1  |
| 1   | C     | 160 | ASP  | 2.1  |
| 1   | B     | 155 | GLU  | 2.1  |
| 1   | A     | 232 | PHE  | 2.0  |
| 1   | D     | 179 | HIS  | 2.0  |
| 1   | B     | 185 | LEU  | 2.0  |
| 1   | C     | 198 | GLU  | 2.0  |
| 1   | D     | 243 | LYS  | 2.0  |

## 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](#)

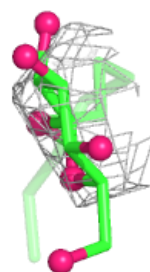
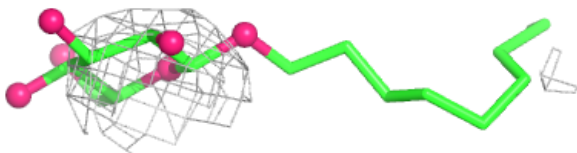
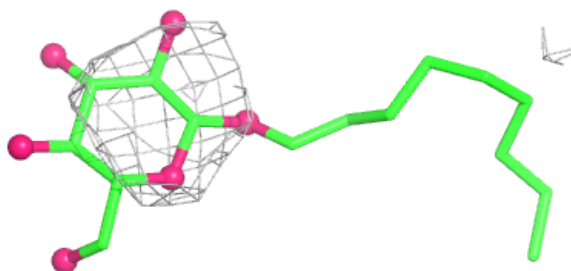
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | BNG  | B     | 301 | 21/21 | 0.81 | 0.19 | 302,345,374,378             | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around BNG B 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.