



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:02 PM UTC

PDB ID : 3K1B / pdb\_00003k1b  
Title : Structure of OmpF porin  
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Center for Structures of Membrane Proteins (CSMP)  
Deposited on : 2009-09-26  
Resolution : 4.39 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  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

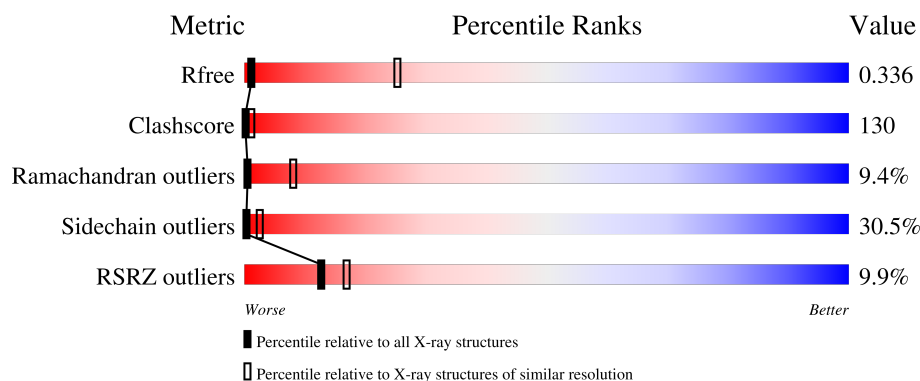
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.39 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                      | 1085 (4.84-3.90)                                      |
| Clashscore            | 190562                      | 1132 (4.84-3.90)                                      |
| Ramachandran outliers | 187476                      | 1024 (4.84-3.90)                                      |
| Sidechain outliers    | 187428                      | 1008 (4.84-3.90)                                      |
| RSRZ outliers         | 180081                      | 1081 (4.84-3.90)                                      |

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     | 340    | <div> <div>10%</div> <div>13% 42% 32% 13%</div> </div> |
| 1   | B     | 340    | <div> <div>9%</div> <div>11% 49% 31% 10%</div> </div>  |
| 1   | C     | 340    | <div> <div>11%</div> <div>13% 47% 32% 8%</div> </div>  |
| 1   | D     | 340    | <div> <div>10%</div> <div>11% 49% 34% 6%</div> </div>  |

## 2 Entry composition

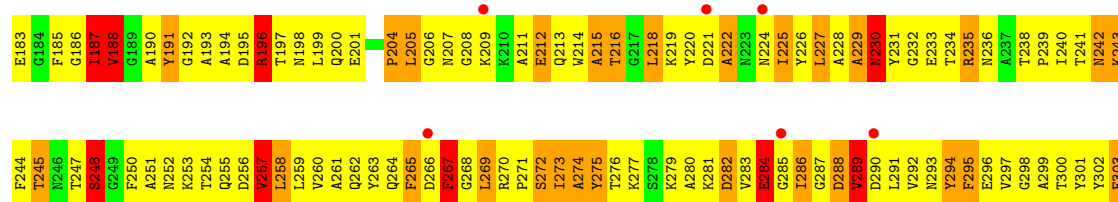
There is only 1 type of molecule in this entry. The entry contains 10508 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

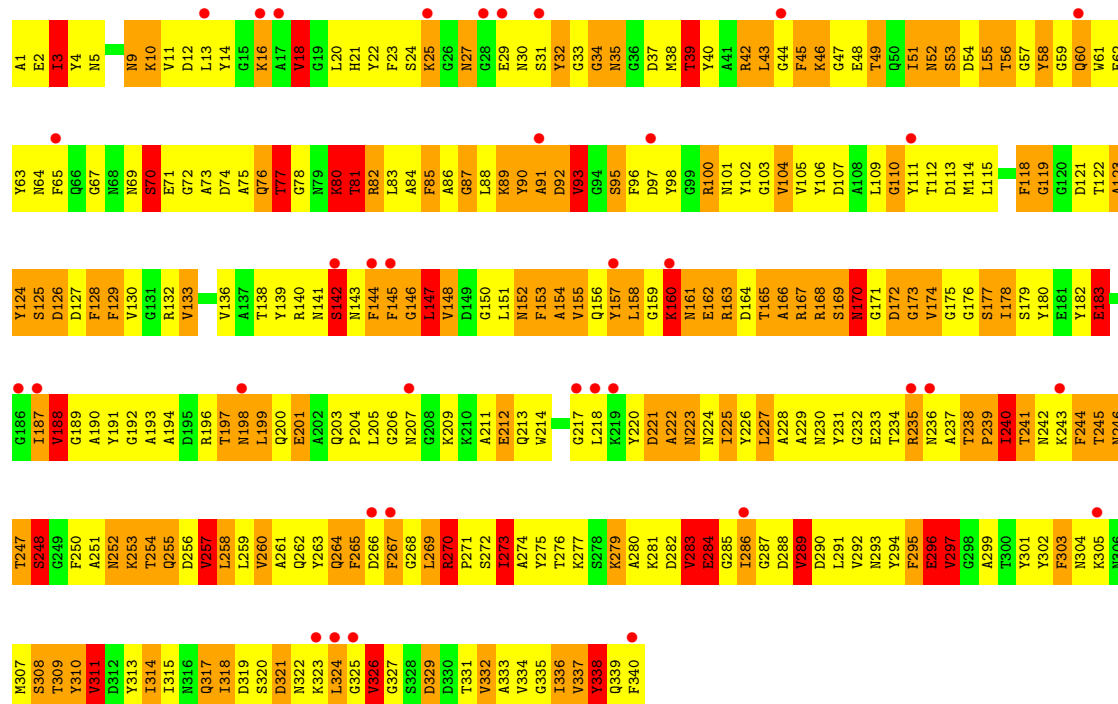
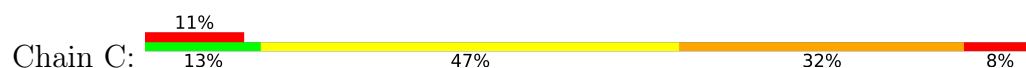
- Molecule 1 is a protein called Outer membrane protein F.

| Mol | Chain | Residues | Atoms         |           |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 1   | A     | 340      | Total<br>2627 | C<br>1654 | N<br>438 | O<br>532 | S<br>3 | 8       | 0       | 0     |
| 1   | B     | 340      | Total<br>2627 | C<br>1654 | N<br>438 | O<br>532 | S<br>3 | 0       | 0       | 0     |
| 1   | C     | 340      | Total<br>2627 | C<br>1654 | N<br>438 | O<br>532 | S<br>3 | 0       | 0       | 0     |
| 1   | D     | 340      | Total<br>2627 | C<br>1654 | N<br>438 | O<br>532 | S<br>3 | 0       | 0       | 0     |

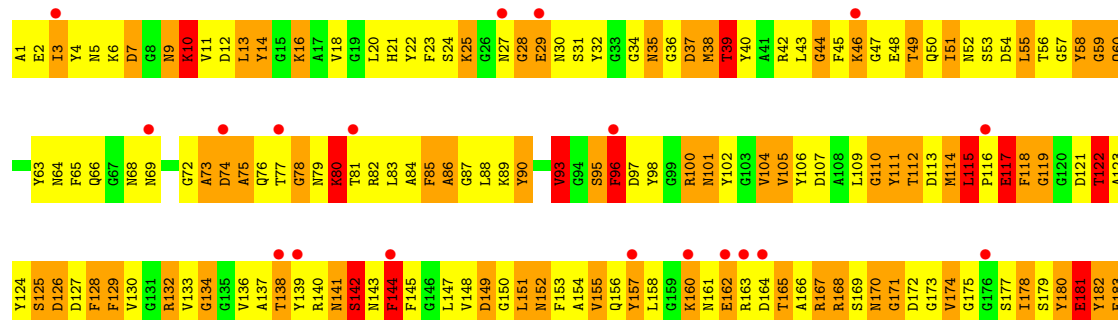
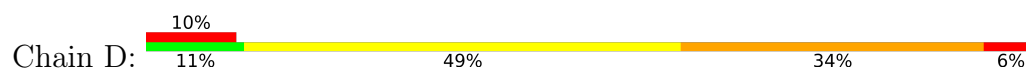


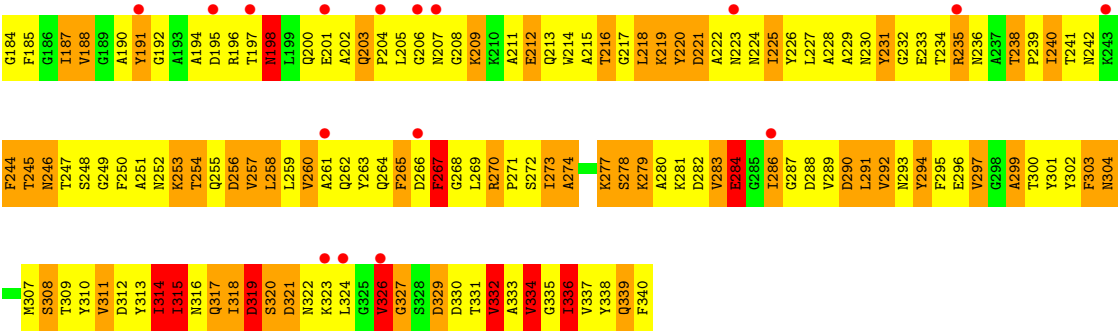


● Molecule 1: Outer membrane protein F



● Molecule 1: Outer membrane protein F





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 3 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 215.53Å 215.53Å 137.47Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 50.00 – 4.39<br>50.00 – 4.39                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.0 (50.00-4.39)<br>99.0 (50.00-4.39)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.21                                                        | Depositor        |
| $R_{sym}$                                                               | 0.21                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.90 (at 4.45Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.5.0066                                             | Depositor        |
| R, $R_{free}$                                                           | 0.264 , 0.329<br>0.273 , 0.336                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1211 reflections (5.09%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 91.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.084                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 114.1                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | 0.003 for -h,-k,l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.78                                                        | EDS              |
| Total number of atoms                                                   | 10508                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 126.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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

### 5.1 Standard geometry

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     | 1.66         | 41/2683 (1.5%)   | 1.82        | 87/3628 (2.4%)   |
| 1   | B     | 1.63         | 37/2683 (1.4%)   | 1.86        | 86/3628 (2.4%)   |
| 1   | C     | 1.61         | 29/2683 (1.1%)   | 1.86        | 89/3628 (2.5%)   |
| 1   | D     | 1.54         | 25/2683 (0.9%)   | 1.75        | 72/3628 (2.0%)   |
| All | All   | 1.61         | 132/10732 (1.2%) | 1.82        | 334/14512 (2.3%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 3                   |
| 1   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 2                   |
| All | All   | 0                   | 7                   |

All (132) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | A     | 311 | VAL  | CA-CB | -12.59 | 1.38        | 1.54     |
| 1   | D     | 225 | ILE  | CA-CB | 12.58  | 1.69        | 1.53     |
| 1   | D     | 59  | GLY  | CA-C  | 10.78  | 1.67        | 1.51     |
| 1   | C     | 18  | VAL  | CA-CB | 9.61   | 1.65        | 1.53     |
| 1   | D     | 225 | ILE  | CA-C  | 9.47   | 1.64        | 1.52     |
| 1   | A     | 3   | ILE  | CA-CB | -9.00  | 1.42        | 1.54     |
| 1   | A     | 334 | VAL  | CA-CB | -8.90  | 1.39        | 1.55     |
| 1   | B     | 257 | VAL  | CA-CB | -8.38  | 1.43        | 1.54     |
| 1   | B     | 332 | VAL  | CA-CB | -8.34  | 1.43        | 1.54     |
| 1   | C     | 315 | ILE  | CA-CB | -8.22  | 1.44        | 1.53     |
| 1   | C     | 257 | VAL  | CA-CB | -8.11  | 1.43        | 1.54     |
| 1   | A     | 289 | VAL  | CA-C  | -8.10  | 1.42        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 238 | THR  | CA-CB  | 8.07  | 1.66        | 1.53     |
| 1   | B     | 282 | ASP  | CA-C   | -8.01 | 1.42        | 1.52     |
| 1   | B     | 157 | TYR  | N-CA   | 7.98  | 1.55        | 1.45     |
| 1   | B     | 93  | VAL  | CA-CB  | -7.94 | 1.43        | 1.54     |
| 1   | A     | 157 | TYR  | N-CA   | 7.72  | 1.55        | 1.46     |
| 1   | A     | 289 | VAL  | CA-CB  | -7.47 | 1.44        | 1.54     |
| 1   | D     | 315 | ILE  | CA-CB  | -7.47 | 1.44        | 1.53     |
| 1   | C     | 165 | THR  | CA-CB  | 7.41  | 1.62        | 1.53     |
| 1   | C     | 311 | VAL  | CA-CB  | -7.30 | 1.44        | 1.54     |
| 1   | A     | 311 | VAL  | N-CA   | -7.25 | 1.37        | 1.46     |
| 1   | A     | 260 | VAL  | CA-CB  | -7.24 | 1.47        | 1.55     |
| 1   | D     | 9   | ASN  | N-CA   | 7.17  | 1.54        | 1.46     |
| 1   | B     | 216 | THR  | CA-CB  | -7.04 | 1.42        | 1.53     |
| 1   | D     | 152 | ASN  | N-CA   | 6.93  | 1.54        | 1.46     |
| 1   | A     | 93  | VAL  | CA-CB  | -6.84 | 1.45        | 1.54     |
| 1   | A     | 21  | HIS  | N-CA   | 6.77  | 1.54        | 1.46     |
| 1   | D     | 216 | THR  | CA-CB  | -6.73 | 1.42        | 1.53     |
| 1   | B     | 101 | ASN  | CA-C   | 6.63  | 1.59        | 1.53     |
| 1   | B     | 17  | ALA  | CA-C   | -6.60 | 1.44        | 1.52     |
| 1   | C     | 290 | ASP  | CA-C   | -6.55 | 1.44        | 1.52     |
| 1   | B     | 105 | VAL  | CA-CB  | -6.54 | 1.45        | 1.54     |
| 1   | B     | 133 | VAL  | CA-CB  | -6.52 | 1.48        | 1.55     |
| 1   | A     | 262 | GLN  | CA-C   | -6.50 | 1.44        | 1.52     |
| 1   | B     | 257 | VAL  | CA-C   | -6.49 | 1.44        | 1.52     |
| 1   | D     | 168 | ARG  | CZ-NH1 | 6.47  | 1.41        | 1.32     |
| 1   | A     | 82  | ARG  | CA-C   | -6.44 | 1.44        | 1.53     |
| 1   | B     | 283 | VAL  | N-CA   | -6.44 | 1.38        | 1.46     |
| 1   | A     | 270 | ARG  | CA-C   | -6.43 | 1.44        | 1.52     |
| 1   | C     | 49  | THR  | N-CA   | -6.37 | 1.37        | 1.46     |
| 1   | B     | 101 | ASN  | N-CA   | 6.34  | 1.53        | 1.46     |
| 1   | A     | 299 | ALA  | CA-C   | 6.31  | 1.60        | 1.52     |
| 1   | C     | 30  | ASN  | N-CA   | -6.28 | 1.39        | 1.46     |
| 1   | D     | 138 | THR  | CA-CB  | 6.28  | 1.61        | 1.53     |
| 1   | C     | 187 | ILE  | CA-C   | 6.25  | 1.60        | 1.52     |
| 1   | C     | 329 | ASP  | CA-C   | -6.25 | 1.44        | 1.53     |
| 1   | B     | 197 | THR  | CA-CB  | -6.24 | 1.43        | 1.53     |
| 1   | D     | 165 | THR  | CA-C   | -6.21 | 1.45        | 1.52     |
| 1   | B     | 63  | TYR  | CA-C   | -6.21 | 1.44        | 1.53     |
| 1   | B     | 72  | GLY  | N-CA   | 6.21  | 1.50        | 1.45     |
| 1   | D     | 332 | VAL  | CA-CB  | -6.19 | 1.46        | 1.54     |
| 1   | C     | 283 | VAL  | CA-CB  | -6.18 | 1.46        | 1.54     |
| 1   | B     | 133 | VAL  | CA-C   | -6.12 | 1.44        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 32  | TYR  | CA-C  | -6.12 | 1.44        | 1.52     |
| 1   | A     | 152 | ASN  | N-CA  | 6.10  | 1.53        | 1.46     |
| 1   | C     | 174 | VAL  | CA-C  | -6.08 | 1.45        | 1.52     |
| 1   | A     | 257 | VAL  | CA-CB | -6.06 | 1.44        | 1.54     |
| 1   | A     | 39  | THR  | CA-CB | -6.01 | 1.45        | 1.53     |
| 1   | D     | 283 | VAL  | N-CA  | -5.96 | 1.40        | 1.46     |
| 1   | A     | 334 | VAL  | CA-C  | -5.95 | 1.45        | 1.52     |
| 1   | D     | 46  | LYS  | CA-C  | 5.93  | 1.60        | 1.52     |
| 1   | B     | 46  | LYS  | CA-C  | -5.93 | 1.45        | 1.52     |
| 1   | C     | 257 | VAL  | CA-C  | -5.90 | 1.45        | 1.52     |
| 1   | A     | 254 | THR  | N-CA  | 5.83  | 1.53        | 1.45     |
| 1   | B     | 289 | VAL  | CA-C  | -5.83 | 1.46        | 1.52     |
| 1   | D     | 134 | GLY  | N-CA  | 5.82  | 1.50        | 1.44     |
| 1   | B     | 148 | VAL  | CA-C  | -5.77 | 1.48        | 1.53     |
| 1   | A     | 292 | VAL  | CA-CB | -5.76 | 1.46        | 1.54     |
| 1   | D     | 220 | TYR  | CA-CB | 5.75  | 1.61        | 1.53     |
| 1   | A     | 334 | VAL  | N-CA  | -5.75 | 1.39        | 1.46     |
| 1   | A     | 133 | VAL  | CA-CB | -5.75 | 1.45        | 1.54     |
| 1   | A     | 102 | TYR  | CA-C  | -5.75 | 1.45        | 1.52     |
| 1   | C     | 77  | THR  | CA-CB | -5.73 | 1.44        | 1.53     |
| 1   | C     | 174 | VAL  | CA-CB | -5.71 | 1.46        | 1.54     |
| 1   | D     | 334 | VAL  | CA-CB | -5.70 | 1.47        | 1.54     |
| 1   | C     | 172 | ASP  | CA-C  | -5.70 | 1.46        | 1.52     |
| 1   | A     | 157 | TYR  | CA-C  | -5.69 | 1.46        | 1.52     |
| 1   | D     | 44  | GLY  | N-CA  | 5.67  | 1.51        | 1.45     |
| 1   | A     | 155 | VAL  | CA-CB | -5.67 | 1.46        | 1.54     |
| 1   | D     | 164 | ASP  | CA-C  | -5.66 | 1.44        | 1.52     |
| 1   | C     | 84  | ALA  | CA-C  | -5.64 | 1.46        | 1.52     |
| 1   | A     | 104 | VAL  | CA-CB | -5.62 | 1.47        | 1.54     |
| 1   | B     | 164 | ASP  | CA-C  | -5.61 | 1.45        | 1.52     |
| 1   | B     | 286 | ILE  | CA-C  | -5.61 | 1.45        | 1.52     |
| 1   | C     | 89  | LYS  | N-CA  | 5.59  | 1.52        | 1.45     |
| 1   | B     | 87  | GLY  | CA-C  | 5.56  | 1.59        | 1.52     |
| 1   | C     | 164 | ASP  | CA-C  | -5.56 | 1.45        | 1.53     |
| 1   | C     | 260 | VAL  | CA-C  | -5.55 | 1.46        | 1.52     |
| 1   | C     | 103 | GLY  | N-CA  | 5.54  | 1.51        | 1.45     |
| 1   | B     | 11  | VAL  | CA-CB | -5.54 | 1.47        | 1.54     |
| 1   | B     | 174 | VAL  | CA-C  | -5.52 | 1.46        | 1.52     |
| 1   | B     | 79  | ASN  | CA-C  | -5.50 | 1.45        | 1.52     |
| 1   | A     | 86  | ALA  | N-CA  | 5.49  | 1.52        | 1.45     |
| 1   | B     | 267 | PHE  | CA-C  | -5.48 | 1.45        | 1.52     |
| 1   | A     | 241 | THR  | N-CA  | 5.46  | 1.52        | 1.45     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 51  | ILE  | N-CA  | -5.45 | 1.39        | 1.46     |
| 1   | C     | 81  | THR  | CA-CB | -5.45 | 1.45        | 1.53     |
| 1   | D     | 117 | GLU  | N-CA  | 5.45  | 1.53        | 1.46     |
| 1   | B     | 290 | ASP  | N-CA  | -5.42 | 1.39        | 1.46     |
| 1   | B     | 56  | THR  | CA-CB | -5.41 | 1.45        | 1.53     |
| 1   | D     | 38  | MET  | N-CA  | 5.40  | 1.52        | 1.46     |
| 1   | D     | 220 | TYR  | CA-C  | 5.40  | 1.59        | 1.52     |
| 1   | A     | 193 | ALA  | CA-C  | -5.38 | 1.45        | 1.52     |
| 1   | B     | 290 | ASP  | CA-C  | -5.37 | 1.46        | 1.52     |
| 1   | D     | 22  | TYR  | CA-C  | -5.33 | 1.46        | 1.52     |
| 1   | B     | 191 | TYR  | N-CA  | -5.32 | 1.40        | 1.46     |
| 1   | B     | 330 | ASP  | CA-C  | -5.32 | 1.45        | 1.52     |
| 1   | B     | 294 | TYR  | CA-C  | 5.29  | 1.58        | 1.52     |
| 1   | B     | 5   | ASN  | CA-C  | -5.29 | 1.46        | 1.52     |
| 1   | A     | 314 | ILE  | N-CA  | -5.29 | 1.38        | 1.46     |
| 1   | B     | 215 | ALA  | N-CA  | -5.29 | 1.39        | 1.46     |
| 1   | A     | 235 | ARG  | N-CA  | -5.27 | 1.40        | 1.46     |
| 1   | A     | 122 | THR  | CA-C  | -5.26 | 1.45        | 1.52     |
| 1   | A     | 109 | LEU  | CA-C  | 5.25  | 1.59        | 1.52     |
| 1   | B     | 315 | ILE  | CA-CB | -5.24 | 1.47        | 1.53     |
| 1   | D     | 290 | ASP  | CA-C  | -5.23 | 1.46        | 1.52     |
| 1   | A     | 123 | ALA  | CA-CB | -5.22 | 1.46        | 1.53     |
| 1   | A     | 16  | LYS  | CA-C  | -5.22 | 1.46        | 1.52     |
| 1   | C     | 118 | PHE  | CA-C  | 5.21  | 1.59        | 1.52     |
| 1   | A     | 241 | THR  | CA-C  | 5.14  | 1.58        | 1.52     |
| 1   | C     | 309 | THR  | CA-CB | -5.14 | 1.45        | 1.53     |
| 1   | B     | 188 | VAL  | CA-CB | -5.12 | 1.46        | 1.55     |
| 1   | A     | 308 | SER  | CA-C  | -5.10 | 1.46        | 1.52     |
| 1   | C     | 297 | VAL  | CA-CB | -5.10 | 1.48        | 1.54     |
| 1   | A     | 101 | ASN  | CA-C  | 5.08  | 1.59        | 1.52     |
| 1   | D     | 86  | ALA  | C-N   | 5.08  | 1.39        | 1.33     |
| 1   | D     | 49  | THR  | N-CA  | -5.06 | 1.40        | 1.46     |
| 1   | A     | 188 | VAL  | N-CA  | 5.05  | 1.51        | 1.46     |
| 1   | C     | 77  | THR  | CA-C  | -5.05 | 1.46        | 1.52     |
| 1   | C     | 157 | TYR  | N-CA  | 5.03  | 1.52        | 1.46     |
| 1   | C     | 297 | VAL  | CA-C  | -5.03 | 1.46        | 1.52     |

All (334) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 270 | ARG  | CA-C-N | 18.87 | 138.63      | 119.76   |
| 1   | C     | 270 | ARG  | C-N-CA | 18.87 | 138.63      | 119.76   |

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| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | B     | 87  | GLY  | N-CA-C   | 13.40  | 127.53      | 110.38   |
| 1   | A     | 133 | VAL  | CB-CA-C  | -10.67 | 94.33       | 110.55   |
| 1   | D     | 260 | VAL  | CB-CA-C  | -10.65 | 94.76       | 110.62   |
| 1   | B     | 207 | ASN  | N-CA-C   | 10.34  | 128.46      | 107.69   |
| 1   | B     | 133 | VAL  | CB-CA-C  | -10.01 | 97.29       | 111.40   |
| 1   | D     | 182 | TYR  | N-CA-C   | 10.00  | 127.61      | 107.41   |
| 1   | C     | 209 | LYS  | N-CA-C   | -9.94  | 101.94      | 114.56   |
| 1   | D     | 182 | TYR  | CA-CB-CG | -9.86  | 96.14       | 113.90   |
| 1   | D     | 90  | TYR  | N-CA-C   | 9.73   | 124.64      | 107.80   |
| 1   | A     | 188 | VAL  | N-CA-C   | 9.49   | 124.33      | 108.86   |
| 1   | B     | 148 | VAL  | CB-CA-C  | -9.47  | 101.66      | 111.23   |
| 1   | C     | 159 | GLY  | N-CA-C   | 9.36   | 122.69      | 111.93   |
| 1   | A     | 241 | THR  | N-CA-C   | 9.25   | 122.74      | 108.96   |
| 1   | A     | 250 | PHE  | N-CA-C   | 9.17   | 123.44      | 109.23   |
| 1   | B     | 250 | PHE  | N-CA-C   | 9.02   | 122.00      | 109.18   |
| 1   | D     | 326 | VAL  | N-CA-C   | -8.97  | 97.26       | 109.37   |
| 1   | B     | 155 | VAL  | CB-CA-C  | -8.72  | 95.56       | 110.30   |
| 1   | D     | 164 | ASP  | CA-C-N   | -8.70  | 108.86      | 122.87   |
| 1   | D     | 164 | ASP  | C-N-CA   | -8.70  | 108.86      | 122.87   |
| 1   | B     | 106 | TYR  | N-CA-C   | -8.54  | 103.00      | 113.50   |
| 1   | A     | 322 | ASN  | N-CA-C   | 8.42   | 122.14      | 109.25   |
| 1   | C     | 201 | GLU  | N-CA-C   | -8.41  | 102.06      | 111.82   |
| 1   | C     | 268 | GLY  | N-CA-C   | 8.36   | 127.06      | 115.27   |
| 1   | B     | 107 | ASP  | N-CA-C   | -8.34  | 101.08      | 111.75   |
| 1   | C     | 76  | GLN  | CA-C-N   | -8.32  | 111.51      | 123.00   |
| 1   | C     | 76  | GLN  | C-N-CA   | -8.32  | 111.51      | 123.00   |
| 1   | B     | 265 | PHE  | N-CA-C   | 8.31   | 122.22      | 110.50   |
| 1   | C     | 248 | SER  | N-CA-C   | 8.31   | 122.11      | 109.23   |
| 1   | C     | 128 | PHE  | CB-CA-C  | -8.25  | 107.06      | 116.63   |
| 1   | D     | 319 | ASP  | N-CA-C   | 8.12   | 118.98      | 108.34   |
| 1   | C     | 160 | LYS  | N-CA-C   | -7.98  | 98.07       | 109.96   |
| 1   | A     | 288 | ASP  | CA-C-N   | -7.98  | 111.85      | 122.94   |
| 1   | A     | 288 | ASP  | C-N-CA   | -7.98  | 111.85      | 122.94   |
| 1   | D     | 16  | LYS  | N-CA-C   | 7.96   | 120.22      | 108.60   |
| 1   | B     | 337 | VAL  | CB-CA-C  | -7.92  | 98.30       | 111.29   |
| 1   | A     | 61  | TRP  | N-CA-C   | 7.92   | 120.46      | 107.23   |
| 1   | C     | 267 | PHE  | N-CA-C   | -7.92  | 103.34      | 113.16   |
| 1   | B     | 174 | VAL  | N-CA-C   | -7.89  | 97.28       | 108.80   |
| 1   | A     | 334 | VAL  | N-CA-C   | -7.88  | 96.01       | 108.86   |
| 1   | A     | 209 | LYS  | N-CA-C   | -7.88  | 104.27      | 114.04   |
| 1   | D     | 270 | ARG  | CA-C-N   | 7.85   | 129.65      | 119.84   |
| 1   | D     | 270 | ARG  | C-N-CA   | 7.85   | 129.65      | 119.84   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 165 | THR  | CB-CA-C   | -7.84 | 93.59       | 110.45   |
| 1   | B     | 6   | LYS  | N-CA-C    | 7.84  | 121.30      | 108.99   |
| 1   | B     | 142 | SER  | N-CA-C    | 7.73  | 121.22      | 109.23   |
| 1   | D     | 277 | LYS  | N-CA-C    | 7.66  | 121.05      | 107.80   |
| 1   | D     | 107 | ASP  | N-CA-C    | -7.64 | 103.03      | 111.36   |
| 1   | B     | 269 | LEU  | CA-CB-CG  | -7.63 | 89.59       | 116.30   |
| 1   | B     | 77  | THR  | CB-CA-C   | -7.62 | 95.26       | 110.42   |
| 1   | D     | 168 | ARG  | NE-CZ-NH1 | -7.58 | 113.92      | 121.50   |
| 1   | B     | 115 | LEU  | CA-C-N    | 7.58  | 128.53      | 120.12   |
| 1   | B     | 115 | LEU  | C-N-CA    | 7.58  | 128.53      | 120.12   |
| 1   | C     | 34  | GLY  | N-CA-C    | -7.54 | 103.94      | 111.56   |
| 1   | D     | 115 | LEU  | CA-C-N    | 7.51  | 129.23      | 119.84   |
| 1   | D     | 115 | LEU  | C-N-CA    | 7.51  | 129.23      | 119.84   |
| 1   | A     | 174 | VAL  | N-CA-C    | -7.50 | 98.31       | 108.96   |
| 1   | A     | 299 | ALA  | N-CA-C    | 7.47  | 120.22      | 108.79   |
| 1   | C     | 198 | ASN  | N-CA-C    | 7.44  | 119.17      | 111.14   |
| 1   | A     | 172 | ASP  | N-CA-C    | 7.42  | 120.38      | 109.69   |
| 1   | B     | 99  | GLY  | CA-C-N    | -7.42 | 112.53      | 122.85   |
| 1   | B     | 99  | GLY  | C-N-CA    | -7.42 | 112.53      | 122.85   |
| 1   | C     | 169 | SER  | N-CA-C    | 7.39  | 119.71      | 109.29   |
| 1   | D     | 142 | SER  | N-CA-C    | 7.38  | 121.06      | 107.99   |
| 1   | D     | 203 | GLN  | CA-C-N    | 7.34  | 129.02      | 119.84   |
| 1   | D     | 203 | GLN  | C-N-CA    | 7.34  | 129.02      | 119.84   |
| 1   | B     | 330 | ASP  | N-CA-C    | -7.29 | 99.69       | 110.48   |
| 1   | C     | 297 | VAL  | CB-CA-C   | -7.28 | 98.78       | 110.28   |
| 1   | B     | 122 | THR  | CA-C-N    | -7.24 | 113.21      | 123.20   |
| 1   | B     | 122 | THR  | C-N-CA    | -7.24 | 113.21      | 123.20   |
| 1   | C     | 329 | ASP  | N-CA-C    | 7.24  | 121.17      | 110.46   |
| 1   | A     | 260 | VAL  | CB-CA-C   | -7.20 | 100.72      | 111.80   |
| 1   | B     | 309 | THR  | CB-CA-C   | -7.19 | 97.54       | 111.78   |
| 1   | A     | 334 | VAL  | CB-CA-C   | -7.17 | 99.21       | 110.69   |
| 1   | A     | 93  | VAL  | N-CA-C    | -7.17 | 103.48      | 110.72   |
| 1   | B     | 82  | ARG  | N-CA-C    | -7.16 | 104.17      | 113.12   |
| 1   | D     | 225 | ILE  | CB-CA-C   | 7.15  | 121.13      | 111.19   |
| 1   | A     | 105 | VAL  | CB-CA-C   | -7.15 | 101.61      | 112.05   |
| 1   | D     | 148 | VAL  | N-CA-C    | 7.14  | 118.88      | 107.73   |
| 1   | C     | 289 | VAL  | CB-CA-C   | -7.08 | 99.41       | 110.52   |
| 1   | C     | 77  | THR  | N-CA-C    | 7.04  | 120.40      | 109.07   |
| 1   | D     | 93  | VAL  | CB-CA-C   | -7.04 | 102.81      | 112.24   |
| 1   | A     | 180 | TYR  | N-CA-C    | 7.02  | 119.51      | 107.93   |
| 1   | D     | 294 | TYR  | N-CA-C    | 7.01  | 118.80      | 108.14   |
| 1   | A     | 338 | TYR  | N-CA-C    | -7.01 | 101.48      | 110.53   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 79  | ASN  | N-CA-C   | -6.99 | 97.84       | 109.24   |
| 1   | C     | 317 | GLN  | CA-C-N   | -6.93 | 109.49      | 121.97   |
| 1   | C     | 317 | GLN  | C-N-CA   | -6.93 | 109.49      | 121.97   |
| 1   | C     | 290 | ASP  | N-CA-C   | 6.93  | 120.03      | 108.73   |
| 1   | A     | 165 | THR  | N-CA-C   | 6.92  | 119.59      | 109.07   |
| 1   | D     | 141 | ASN  | N-CA-C   | 6.89  | 120.47      | 109.24   |
| 1   | A     | 39  | THR  | N-CA-CB  | -6.88 | 98.60       | 110.17   |
| 1   | A     | 53  | SER  | N-CA-C   | 6.88  | 119.66      | 111.33   |
| 1   | B     | 332 | VAL  | CB-CA-C  | -6.87 | 100.77      | 110.12   |
| 1   | C     | 129 | PHE  | N-CA-C   | 6.87  | 121.51      | 113.20   |
| 1   | C     | 70  | SER  | CA-C-N   | -6.86 | 112.95      | 123.17   |
| 1   | C     | 70  | SER  | C-N-CA   | -6.86 | 112.95      | 123.17   |
| 1   | A     | 207 | ASN  | N-CA-C   | 6.85  | 123.16      | 107.48   |
| 1   | A     | 222 | ALA  | N-CA-C   | 6.85  | 118.93      | 108.52   |
| 1   | C     | 264 | GLN  | N-CA-C   | 6.84  | 118.82      | 109.11   |
| 1   | B     | 216 | THR  | CB-CA-C  | -6.83 | 97.92       | 110.62   |
| 1   | D     | 174 | VAL  | CB-CA-C  | -6.80 | 100.21      | 110.55   |
| 1   | B     | 3   | ILE  | CB-CA-C  | -6.77 | 100.93      | 110.95   |
| 1   | C     | 80  | LYS  | N-CA-C   | 6.73  | 118.35      | 108.86   |
| 1   | C     | 125 | SER  | CA-C-N   | -6.68 | 112.52      | 122.07   |
| 1   | C     | 125 | SER  | C-N-CA   | -6.68 | 112.52      | 122.07   |
| 1   | A     | 248 | SER  | N-CA-C   | 6.67  | 117.29      | 107.88   |
| 1   | B     | 182 | TYR  | CA-CB-CG | -6.63 | 101.97      | 113.90   |
| 1   | A     | 317 | GLN  | N-CA-C   | 6.63  | 121.20      | 113.18   |
| 1   | D     | 9   | ASN  | N-CA-C   | 6.62  | 119.32      | 108.52   |
| 1   | A     | 288 | ASP  | N-CA-C   | 6.61  | 119.79      | 108.02   |
| 1   | B     | 159 | GLY  | N-CA-C   | 6.60  | 120.99      | 112.54   |
| 1   | C     | 303 | PHE  | N-CA-C   | -6.57 | 102.58      | 112.04   |
| 1   | C     | 260 | VAL  | CB-CA-C  | -6.55 | 100.21      | 110.69   |
| 1   | A     | 315 | ILE  | CB-CA-C  | -6.54 | 104.17      | 111.23   |
| 1   | A     | 81  | THR  | N-CA-C   | -6.53 | 98.25       | 108.90   |
| 1   | A     | 137 | ALA  | N-CA-C   | 6.53  | 118.78      | 108.79   |
| 1   | D     | 315 | ILE  | N-CA-C   | 6.51  | 116.10      | 106.85   |
| 1   | B     | 85  | PHE  | N-CA-C   | 6.51  | 117.72      | 108.74   |
| 1   | B     | 313 | TYR  | CA-C-N   | -6.50 | 115.13      | 123.19   |
| 1   | B     | 313 | TYR  | C-N-CA   | -6.50 | 115.13      | 123.19   |
| 1   | D     | 207 | ASN  | N-CA-C   | 6.49  | 121.51      | 107.49   |
| 1   | C     | 161 | ASN  | N-CA-C   | 6.48  | 121.94      | 108.53   |
| 1   | B     | 77  | THR  | CA-C-N   | -6.48 | 116.44      | 123.30   |
| 1   | B     | 77  | THR  | C-N-CA   | -6.48 | 116.44      | 123.30   |
| 1   | C     | 188 | VAL  | N-CA-C   | 6.47  | 117.67      | 108.42   |
| 1   | D     | 157 | TYR  | N-CA-C   | -6.47 | 100.63      | 110.14   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 337 | VAL  | CB-CA-C | -6.46 | 100.70      | 111.29   |
| 1   | C     | 238 | THR  | CA-C-N  | 6.43  | 128.14      | 120.23   |
| 1   | C     | 238 | THR  | C-N-CA  | 6.43  | 128.14      | 120.23   |
| 1   | B     | 133 | VAL  | N-CA-C  | -6.43 | 98.62       | 107.75   |
| 1   | D     | 80  | LYS  | N-CA-C  | 6.42  | 118.53      | 108.96   |
| 1   | C     | 288 | ASP  | N-CA-C  | 6.41  | 118.60      | 108.67   |
| 1   | C     | 95  | SER  | N-CA-C  | 6.39  | 118.22      | 108.07   |
| 1   | B     | 153 | PHE  | N-CA-C  | 6.38  | 116.70      | 108.34   |
| 1   | C     | 5   | ASN  | N-CA-C  | 6.37  | 124.37      | 110.80   |
| 1   | C     | 90  | TYR  | N-CA-C  | 6.36  | 118.68      | 107.61   |
| 1   | B     | 230 | ASN  | N-CA-C  | 6.36  | 119.86      | 109.06   |
| 1   | D     | 96  | PHE  | N-CA-C  | 6.35  | 118.17      | 108.52   |
| 1   | B     | 274 | ALA  | N-CA-C  | 6.33  | 118.71      | 108.32   |
| 1   | C     | 93  | VAL  | N-CA-C  | -6.33 | 96.17       | 109.34   |
| 1   | A     | 148 | VAL  | N-CA-C  | 6.33  | 117.23      | 108.12   |
| 1   | B     | 275 | TYR  | CB-CA-C | -6.32 | 99.10       | 110.36   |
| 1   | C     | 81  | THR  | N-CA-C  | -6.32 | 98.94       | 109.24   |
| 1   | B     | 245 | THR  | CB-CA-C | 6.31  | 121.23      | 110.56   |
| 1   | D     | 149 | ASP  | N-CA-C  | 6.29  | 118.97      | 108.96   |
| 1   | C     | 326 | VAL  | CB-CA-C | -6.28 | 100.99      | 111.29   |
| 1   | D     | 330 | ASP  | N-CA-C  | -6.27 | 100.35      | 110.32   |
| 1   | B     | 79  | ASN  | N-CA-C  | -6.27 | 101.14      | 110.23   |
| 1   | A     | 300 | THR  | N-CA-C  | -6.27 | 100.71      | 110.42   |
| 1   | C     | 338 | TYR  | N-CA-C  | -6.26 | 100.43      | 110.14   |
| 1   | D     | 148 | VAL  | CB-CA-C | -6.25 | 103.31      | 111.25   |
| 1   | D     | 321 | ASP  | CB-CA-C | -6.22 | 98.28       | 110.11   |
| 1   | D     | 179 | SER  | N-CA-C  | 6.19  | 118.86      | 108.02   |
| 1   | B     | 81  | THR  | N-CA-C  | -6.17 | 100.52      | 110.32   |
| 1   | B     | 121 | ASP  | CA-C-N  | -6.16 | 111.97      | 122.56   |
| 1   | B     | 121 | ASP  | C-N-CA  | -6.16 | 111.97      | 122.56   |
| 1   | A     | 266 | ASP  | N-CA-C  | 6.12  | 117.95      | 111.28   |
| 1   | D     | 314 | ILE  | CB-CA-C | -6.11 | 102.70      | 111.19   |
| 1   | B     | 182 | TYR  | N-CA-C  | 6.07  | 119.16      | 107.44   |
| 1   | D     | 10  | LYS  | CA-C-N  | -6.06 | 115.29      | 122.93   |
| 1   | D     | 10  | LYS  | C-N-CA  | -6.06 | 115.29      | 122.93   |
| 1   | A     | 174 | VAL  | CB-CA-C | -6.06 | 102.89      | 111.19   |
| 1   | C     | 43  | LEU  | N-CA-C  | -6.05 | 98.77       | 109.06   |
| 1   | B     | 141 | ASN  | CA-C-N  | -6.04 | 112.33      | 122.29   |
| 1   | B     | 141 | ASN  | C-N-CA  | -6.04 | 112.33      | 122.29   |
| 1   | C     | 240 | ILE  | N-CA-C  | 6.04  | 117.17      | 108.48   |
| 1   | B     | 248 | SER  | N-CA-C  | 6.02  | 117.73      | 109.18   |
| 1   | A     | 187 | ILE  | CB-CA-C | -6.00 | 102.25      | 110.77   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 269 | LEU  | N-CA-C   | -5.99 | 100.80      | 110.32   |
| 1   | B     | 34  | GLY  | N-CA-C   | -5.99 | 101.88      | 110.38   |
| 1   | C     | 321 | ASP  | CB-CA-C  | -5.97 | 99.75       | 110.37   |
| 1   | A     | 17  | ALA  | CA-C-N   | -5.97 | 114.99      | 123.11   |
| 1   | A     | 17  | ALA  | C-N-CA   | -5.97 | 114.99      | 123.11   |
| 1   | A     | 254 | THR  | N-CA-C   | 5.96  | 118.35      | 108.99   |
| 1   | A     | 101 | ASN  | N-CA-C   | 5.96  | 115.95      | 108.45   |
| 1   | B     | 294 | TYR  | N-CA-C   | 5.92  | 117.85      | 108.79   |
| 1   | A     | 307 | MET  | CB-CG-SD | -5.92 | 94.94       | 112.70   |
| 1   | C     | 289 | VAL  | N-CA-C   | 5.92  | 117.23      | 108.65   |
| 1   | B     | 304 | ASN  | N-CA-C   | 5.92  | 116.39      | 108.23   |
| 1   | C     | 178 | ILE  | CB-CA-C  | -5.89 | 102.83      | 110.84   |
| 1   | D     | 129 | PHE  | N-CA-C   | 5.86  | 120.71      | 113.50   |
| 1   | A     | 332 | VAL  | CB-CA-C  | -5.86 | 102.52      | 110.42   |
| 1   | C     | 93  | VAL  | CB-CA-C  | -5.84 | 101.71      | 111.29   |
| 1   | A     | 274 | ALA  | N-CA-C   | 5.83  | 118.98      | 109.06   |
| 1   | D     | 225 | ILE  | N-CA-C   | 5.82  | 115.99      | 107.37   |
| 1   | C     | 282 | ASP  | CB-CA-C  | -5.82 | 102.32      | 111.51   |
| 1   | C     | 296 | GLU  | N-CA-C   | 5.80  | 119.00      | 109.72   |
| 1   | D     | 29  | GLU  | CB-CA-C  | -5.80 | 101.17      | 110.79   |
| 1   | A     | 211 | ALA  | N-CA-C   | 5.79  | 118.50      | 109.52   |
| 1   | C     | 44  | GLY  | N-CA-C   | 5.75  | 119.98      | 110.55   |
| 1   | C     | 32  | TYR  | N-CA-C   | -5.72 | 104.65      | 111.69   |
| 1   | C     | 155 | VAL  | CB-CA-C  | -5.70 | 101.78      | 110.95   |
| 1   | B     | 283 | VAL  | N-CA-C   | -5.69 | 97.50       | 109.34   |
| 1   | C     | 16  | LYS  | N-CA-C   | 5.69  | 115.62      | 108.45   |
| 1   | A     | 156 | GLN  | N-CA-CB  | -5.69 | 101.25      | 110.81   |
| 1   | B     | 188 | VAL  | N-CA-C   | 5.68  | 118.00      | 108.81   |
| 1   | B     | 307 | MET  | N-CA-C   | 5.67  | 118.81      | 110.59   |
| 1   | C     | 70  | SER  | CB-CA-C  | -5.67 | 99.14       | 110.42   |
| 1   | B     | 32  | TYR  | N-CA-C   | -5.66 | 106.73      | 113.97   |
| 1   | B     | 91  | ALA  | CA-C-N   | -5.66 | 112.70      | 122.14   |
| 1   | B     | 91  | ALA  | C-N-CA   | -5.66 | 112.70      | 122.14   |
| 1   | C     | 324 | LEU  | CA-C-N   | -5.63 | 116.77      | 123.08   |
| 1   | C     | 324 | LEU  | C-N-CA   | -5.63 | 116.77      | 123.08   |
| 1   | B     | 288 | ASP  | N-CA-C   | 5.63  | 118.08      | 108.90   |
| 1   | D     | 44  | GLY  | N-CA-C   | 5.63  | 118.97      | 110.75   |
| 1   | B     | 13  | LEU  | N-CA-C   | -5.61 | 100.10      | 109.24   |
| 1   | D     | 126 | ASP  | N-CA-C   | -5.60 | 106.03      | 112.86   |
| 1   | A     | 85  | PHE  | N-CA-C   | 5.58  | 117.01      | 108.42   |
| 1   | C     | 2   | GLU  | N-CA-C   | -5.56 | 101.62      | 109.96   |
| 1   | A     | 245 | THR  | N-CA-C   | -5.56 | 106.27      | 113.16   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 29  | GLU  | N-CA-C   | -5.56 | 105.22      | 111.28   |
| 1   | B     | 188 | VAL  | CB-CA-C  | -5.55 | 100.78      | 110.71   |
| 1   | A     | 18  | VAL  | N-CA-C   | 5.54  | 115.57      | 107.37   |
| 1   | D     | 114 | MET  | N-CA-C   | 5.54  | 120.54      | 113.18   |
| 1   | A     | 238 | THR  | CA-C-N   | -5.53 | 112.93      | 119.84   |
| 1   | A     | 238 | THR  | C-N-CA   | -5.53 | 112.93      | 119.84   |
| 1   | C     | 173 | GLY  | N-CA-C   | 5.52  | 119.68      | 111.18   |
| 1   | D     | 29  | GLU  | CA-CB-CG | -5.51 | 103.08      | 114.10   |
| 1   | B     | 332 | VAL  | N-CA-C   | 5.50  | 115.97      | 107.78   |
| 1   | B     | 187 | ILE  | N-CA-C   | 5.49  | 115.76      | 107.80   |
| 1   | C     | 168 | ARG  | N-CA-C   | -5.49 | 104.52      | 113.19   |
| 1   | A     | 325 | GLY  | CA-C-N   | -5.49 | 113.50      | 122.33   |
| 1   | A     | 325 | GLY  | C-N-CA   | -5.49 | 113.50      | 122.33   |
| 1   | C     | 3   | ILE  | CA-C-N   | -5.49 | 113.84      | 122.73   |
| 1   | C     | 3   | ILE  | C-N-CA   | -5.49 | 113.84      | 122.73   |
| 1   | A     | 310 | TYR  | N-CA-C   | 5.48  | 117.51      | 109.24   |
| 1   | C     | 27  | ASN  | N-CA-C   | 5.45  | 119.68      | 113.19   |
| 1   | A     | 225 | ILE  | CB-CA-C  | 5.45  | 118.66      | 110.98   |
| 1   | A     | 91  | ALA  | CB-CA-C  | -5.45 | 110.31      | 116.63   |
| 1   | A     | 142 | SER  | N-CA-C   | 5.45  | 117.53      | 107.73   |
| 1   | D     | 39  | THR  | CB-CA-C  | -5.44 | 99.59       | 110.42   |
| 1   | A     | 256 | ASP  | CA-C-N   | -5.44 | 114.09      | 122.68   |
| 1   | A     | 256 | ASP  | C-N-CA   | -5.44 | 114.09      | 122.68   |
| 1   | D     | 221 | ASP  | N-CA-C   | 5.43  | 116.28      | 107.32   |
| 1   | C     | 337 | VAL  | N-CA-C   | 5.41  | 115.65      | 107.75   |
| 1   | D     | 329 | ASP  | N-CA-C   | 5.40  | 118.51      | 110.52   |
| 1   | A     | 102 | TYR  | CB-CA-C  | -5.39 | 101.77      | 110.77   |
| 1   | D     | 254 | THR  | CB-CA-C  | -5.39 | 97.60       | 109.56   |
| 1   | B     | 196 | ARG  | N-CA-C   | -5.38 | 102.55      | 110.52   |
| 1   | C     | 239 | PRO  | CB-CA-C  | -5.38 | 105.69      | 111.56   |
| 1   | B     | 324 | LEU  | N-CA-C   | -5.38 | 105.85      | 112.90   |
| 1   | D     | 256 | ASP  | N-CA-C   | 5.37  | 117.16      | 108.41   |
| 1   | A     | 283 | VAL  | N-CA-C   | -5.37 | 102.66      | 109.58   |
| 1   | C     | 121 | ASP  | CA-C-N   | -5.35 | 113.00      | 122.26   |
| 1   | C     | 121 | ASP  | C-N-CA   | -5.35 | 113.00      | 122.26   |
| 1   | B     | 39  | THR  | CB-CA-C  | -5.35 | 99.78       | 110.42   |
| 1   | A     | 122 | THR  | CB-CA-C  | -5.34 | 100.41      | 110.67   |
| 1   | B     | 173 | GLY  | N-CA-C   | 5.34  | 119.93      | 110.80   |
| 1   | A     | 25  | LYS  | CA-C-O   | -5.33 | 115.87      | 120.88   |
| 1   | D     | 218 | LEU  | CA-CB-CG | -5.33 | 97.65       | 116.30   |
| 1   | C     | 9   | ASN  | N-CA-C   | 5.33  | 117.40      | 109.25   |
| 1   | D     | 238 | THR  | CA-C-N   | 5.32  | 127.70      | 120.79   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 238 | THR  | C-N-CA     | 5.32  | 127.70      | 120.79   |
| 1   | D     | 274 | ALA  | N-CA-C     | 5.31  | 117.15      | 108.76   |
| 1   | A     | 39  | THR  | N-CA-C     | 5.30  | 117.39      | 108.96   |
| 1   | A     | 45  | PHE  | N-CA-C     | 5.29  | 116.82      | 107.61   |
| 1   | B     | 132 | ARG  | N-CA-C     | -5.28 | 103.56      | 110.53   |
| 1   | D     | 278 | SER  | N-CA-C     | -5.28 | 100.64      | 109.24   |
| 1   | C     | 78  | GLY  | N-CA-C     | -5.28 | 107.51      | 115.32   |
| 1   | C     | 273 | ILE  | N-CA-C     | 5.28  | 115.45      | 107.80   |
| 1   | D     | 315 | ILE  | CB-CA-C    | -5.27 | 104.67      | 111.53   |
| 1   | A     | 112 | THR  | CB-CA-C    | -5.27 | 101.29      | 110.09   |
| 1   | A     | 132 | ARG  | NE-CZ-NH2  | 5.27  | 123.94      | 119.20   |
| 1   | B     | 204 | PRO  | N-CA-C     | -5.27 | 105.94      | 113.47   |
| 1   | A     | 319 | ASP  | N-CA-C     | 5.26  | 117.39      | 109.23   |
| 1   | A     | 287 | GLY  | N-CA-C     | -5.26 | 100.71      | 113.18   |
| 1   | C     | 188 | VAL  | CB-CA-C    | -5.26 | 101.72      | 111.18   |
| 1   | C     | 207 | ASN  | N-CA-C     | 5.25  | 117.29      | 107.99   |
| 1   | A     | 199 | LEU  | N-CA-C     | -5.25 | 104.81      | 111.11   |
| 1   | B     | 227 | LEU  | CA-CB-CG   | -5.25 | 97.91       | 116.30   |
| 1   | D     | 316 | ASN  | N-CA-C     | 5.25  | 116.86      | 108.41   |
| 1   | A     | 308 | SER  | N-CA-C     | -5.24 | 100.95      | 108.60   |
| 1   | D     | 168 | ARG  | NH1-CZ-NH2 | 5.22  | 126.08      | 119.30   |
| 1   | A     | 292 | VAL  | N-CA-C     | 5.20  | 120.16      | 109.34   |
| 1   | A     | 32  | TYR  | N-CA-C     | 5.20  | 117.85      | 111.82   |
| 1   | C     | 158 | LEU  | CA-C-N     | 5.19  | 125.03      | 120.10   |
| 1   | C     | 158 | LEU  | C-N-CA     | 5.19  | 125.03      | 120.10   |
| 1   | C     | 337 | VAL  | CB-CA-C    | -5.18 | 103.42      | 110.77   |
| 1   | C     | 241 | THR  | N-CA-C     | 5.17  | 117.74      | 110.14   |
| 1   | A     | 224 | ASN  | CA-C-N     | -5.17 | 115.51      | 122.91   |
| 1   | A     | 224 | ASN  | C-N-CA     | -5.17 | 115.51      | 122.91   |
| 1   | C     | 33  | GLY  | N-CA-C     | 5.17  | 125.43      | 113.18   |
| 1   | A     | 127 | ASP  | CA-C-N     | -5.16 | 111.68      | 121.54   |
| 1   | A     | 127 | ASP  | C-N-CA     | -5.16 | 111.68      | 121.54   |
| 1   | C     | 265 | PHE  | CA-C-N     | -5.16 | 114.39      | 122.65   |
| 1   | C     | 265 | PHE  | C-N-CA     | -5.16 | 114.39      | 122.65   |
| 1   | C     | 295 | PHE  | N-CA-C     | -5.16 | 101.28      | 109.59   |
| 1   | B     | 229 | ALA  | N-CA-C     | 5.15  | 116.82      | 109.14   |
| 1   | D     | 14  | TYR  | N-CA-C     | 5.15  | 116.13      | 108.86   |
| 1   | D     | 180 | TYR  | N-CA-C     | 5.15  | 116.92      | 108.52   |
| 1   | A     | 145 | PHE  | CB-CA-C    | -5.15 | 103.37      | 111.51   |
| 1   | C     | 126 | ASP  | N-CA-C     | -5.14 | 104.55      | 111.54   |
| 1   | C     | 239 | PRO  | N-CA-C     | 5.14  | 118.57      | 110.50   |
| 1   | B     | 167 | ARG  | CA-C-N     | -5.13 | 113.92      | 122.08   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 167 | ARG  | C-N-CA    | -5.13 | 113.92      | 122.08   |
| 1   | B     | 338 | TYR  | N-CA-C    | -5.12 | 103.84      | 110.19   |
| 1   | D     | 181 | GLU  | CB-CA-C   | -5.12 | 102.63      | 111.23   |
| 1   | B     | 90  | TYR  | N-CA-C    | 5.12  | 117.75      | 107.41   |
| 1   | D     | 78  | GLY  | N-CA-C    | -5.12 | 108.56      | 115.21   |
| 1   | A     | 191 | TYR  | N-CA-CB   | -5.12 | 103.63      | 111.56   |
| 1   | C     | 162 | GLU  | N-CA-C    | 5.11  | 117.46      | 108.56   |
| 1   | A     | 61  | TRP  | CB-CA-C   | -5.11 | 104.73      | 111.42   |
| 1   | B     | 317 | GLN  | CA-C-N    | -5.11 | 112.78      | 121.97   |
| 1   | B     | 317 | GLN  | C-N-CA    | -5.11 | 112.78      | 121.97   |
| 1   | B     | 126 | ASP  | N-CA-C    | -5.10 | 99.94       | 110.80   |
| 1   | B     | 26  | GLY  | N-CA-C    | -5.09 | 101.12      | 113.18   |
| 1   | C     | 87  | GLY  | N-CA-C    | 5.09  | 117.48      | 110.56   |
| 1   | B     | 16  | LYS  | N-CA-C    | 5.08  | 115.25      | 108.23   |
| 1   | A     | 318 | ILE  | CB-CA-C   | -5.07 | 102.97      | 111.29   |
| 1   | C     | 142 | SER  | N-CA-C    | 5.07  | 118.47      | 109.96   |
| 1   | A     | 187 | ILE  | N-CA-CB   | -5.06 | 105.07      | 111.64   |
| 1   | D     | 112 | THR  | CA-C-O    | 5.05  | 124.46      | 118.90   |
| 1   | D     | 122 | THR  | CA-C-N    | -5.05 | 116.03      | 122.79   |
| 1   | D     | 122 | THR  | C-N-CA    | -5.05 | 116.03      | 122.79   |
| 1   | C     | 123 | ALA  | N-CA-C    | 5.05  | 117.19      | 109.62   |
| 1   | A     | 24  | SER  | N-CA-C    | 5.04  | 116.18      | 108.52   |
| 1   | A     | 305 | LYS  | N-CA-C    | -5.04 | 107.30      | 113.50   |
| 1   | D     | 185 | PHE  | N-CA-C    | 5.04  | 118.28      | 110.17   |
| 1   | D     | 101 | ASN  | N-CA-C    | -5.04 | 101.45      | 108.96   |
| 1   | B     | 324 | LEU  | CB-CG-CD2 | -5.04 | 95.59       | 110.70   |
| 1   | B     | 164 | ASP  | CB-CA-C   | -5.03 | 101.50      | 110.70   |
| 1   | C     | 197 | THR  | N-CA-C    | -5.03 | 103.89      | 110.53   |
| 1   | B     | 180 | TYR  | CA-CB-CG  | -5.02 | 104.87      | 113.90   |
| 1   | A     | 316 | ASN  | N-CA-C    | 5.01  | 116.93      | 108.96   |
| 1   | B     | 124 | TYR  | CA-C-N    | -5.01 | 116.09      | 123.00   |
| 1   | B     | 124 | TYR  | C-N-CA    | -5.01 | 116.09      | 123.00   |
| 1   | D     | 144 | PHE  | N-CA-C    | 5.01  | 121.47      | 110.80   |
| 1   | D     | 299 | ALA  | N-CA-C    | 5.01  | 115.92      | 108.86   |
| 1   | B     | 17  | ALA  | CA-C-N    | -5.01 | 116.76      | 123.17   |
| 1   | B     | 17  | ALA  | C-N-CA    | -5.01 | 116.76      | 123.17   |
| 1   | C     | 39  | THR  | CB-CA-C   | -5.01 | 100.46      | 110.42   |
| 1   | D     | 46  | LYS  | N-CA-C    | 5.00  | 117.39      | 107.98   |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 137 | ALA  | Peptide |
| 1   | A     | 164 | ASP  | Peptide |
| 1   | A     | 321 | ASP  | Peptide |
| 1   | B     | 176 | GLY  | Peptide |
| 1   | C     | 255 | GLN  | Peptide |
| 1   | D     | 315 | ILE  | Peptide |
| 1   | D     | 336 | ILE  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2627  | 0        | 2442     | 789     | 0            |
| 1   | B     | 2627  | 0        | 2443     | 711     | 5            |
| 1   | C     | 2627  | 0        | 2444     | 668     | 2            |
| 1   | D     | 2627  | 0        | 2444     | 627     | 1            |
| All | All   | 10508 | 0        | 9773     | 2631    | 6            |

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 130.

All (2631) 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:A:114:MET:HE1  | 1:A:226:TYR:CE1  | 1.18                     | 1.63              |
| 1:A:258:LEU:CD1  | 1:A:276:THR:HG23 | 1.28                     | 1.58              |
| 1:A:313:TYR:CD1  | 1:A:332:VAL:CG2  | 1.86                     | 1.58              |
| 1:A:191:TYR:HD2  | 1:A:192:GLY:N    | 1.06                     | 1.53              |
| 1:A:313:TYR:HD1  | 1:A:332:VAL:CG2  | 1.19                     | 1.52              |
| 1:A:114:MET:CE   | 1:A:226:TYR:CE1  | 1.93                     | 1.52              |
| 1:C:269:LEU:CD1  | 1:C:270:ARG:H    | 1.25                     | 1.47              |
| 1:D:311:VAL:HG13 | 1:D:334:VAL:CG2  | 1.42                     | 1.47              |
| 1:D:311:VAL:CG1  | 1:D:334:VAL:HG23 | 1.44                     | 1.46              |
| 1:A:115:LEU:H    | 1:A:115:LEU:CD2  | 0.94                     | 1.45              |
| 1:B:115:LEU:H    | 1:B:115:LEU:CD2  | 0.99                     | 1.45              |
| 1:A:307:MET:CE   | 1:B:88:LEU:CD2   | 1.96                     | 1.42              |
| 1:D:51:ILE:CD1   | 1:D:55:LEU:HD23  | 1.46                     | 1.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:21:HIS:HD2   | 1:B:23:PHE:CE2   | 1.36                     | 1.41              |
| 1:A:104:VAL:CG1  | 1:A:156:GLN:OE1  | 1.68                     | 1.41              |
| 1:A:231:TYR:HD2  | 1:A:232:GLY:N    | 1.18                     | 1.40              |
| 1:C:204:PRO:HG2  | 1:C:247:THR:CG2  | 1.50                     | 1.39              |
| 1:A:51:ILE:CG1   | 1:A:55:LEU:HD23  | 1.54                     | 1.38              |
| 1:D:229:ALA:HB2  | 1:D:259:LEU:CD2  | 1.49                     | 1.38              |
| 1:B:151:LEU:C    | 1:B:151:LEU:HD12 | 1.18                     | 1.37              |
| 1:A:294:TYR:CD2  | 1:A:314:ILE:HD12 | 1.59                     | 1.37              |
| 1:A:211:ALA:HB1  | 1:A:235:ARG:O    | 1.19                     | 1.36              |
| 1:A:170:ASN:O    | 1:A:170:ASN:ND2  | 1.56                     | 1.36              |
| 1:A:4:TYR:CE1    | 1:C:1:ALA:HB1    | 1.59                     | 1.35              |
| 1:A:20:LEU:CD2   | 1:A:117:GLU:OE1  | 1.75                     | 1.35              |
| 1:D:104:VAL:CG1  | 1:D:156:GLN:OE1  | 1.73                     | 1.35              |
| 1:D:144:PHE:CD2  | 1:D:144:PHE:O    | 1.80                     | 1.34              |
| 1:A:51:ILE:CD1   | 1:A:55:LEU:HD23  | 1.58                     | 1.34              |
| 1:A:51:ILE:CD1   | 1:A:55:LEU:CD2   | 2.04                     | 1.33              |
| 1:A:285:GLY:C    | 1:A:286:ILE:HD12 | 1.53                     | 1.33              |
| 1:B:21:HIS:CD2   | 1:B:23:PHE:HE2   | 1.45                     | 1.33              |
| 1:D:132:ARG:HH11 | 1:D:132:ARG:CG   | 1.32                     | 1.33              |
| 1:D:115:LEU:H    | 1:D:115:LEU:CD2  | 1.15                     | 1.32              |
| 1:A:114:MET:HE1  | 1:A:226:TYR:CD1  | 1.63                     | 1.32              |
| 1:D:229:ALA:CB   | 1:D:259:LEU:CD2  | 2.08                     | 1.31              |
| 1:A:191:TYR:CD2  | 1:A:192:GLY:N    | 1.96                     | 1.30              |
| 1:A:90:TYR:O     | 1:A:93:VAL:HG23  | 1.26                     | 1.30              |
| 1:C:269:LEU:HD12 | 1:C:269:LEU:C    | 1.48                     | 1.29              |
| 1:B:276:THR:CG2  | 1:B:294:TYR:HE2  | 1.44                     | 1.29              |
| 1:C:172:ASP:O    | 1:C:194:ALA:HB1  | 1.24                     | 1.29              |
| 1:C:269:LEU:HD12 | 1:C:270:ARG:N    | 0.96                     | 1.28              |
| 1:A:258:LEU:O    | 1:A:259:LEU:HD23 | 1.15                     | 1.28              |
| 1:C:45:PHE:HD1   | 1:C:45:PHE:O     | 1.16                     | 1.28              |
| 1:A:20:LEU:HD21  | 1:A:117:GLU:OE1  | 1.21                     | 1.27              |
| 1:D:104:VAL:HG13 | 1:D:156:GLN:OE1  | 1.15                     | 1.27              |
| 1:B:258:LEU:O    | 1:B:259:LEU:HD23 | 1.30                     | 1.27              |
| 1:A:285:GLY:O    | 1:A:286:ILE:HD12 | 1.21                     | 1.27              |
| 1:C:286:ILE:CD1  | 1:C:286:ILE:H    | 1.46                     | 1.26              |
| 1:C:112:THR:HG23 | 1:C:230:ASN:OD1  | 1.34                     | 1.26              |
| 1:C:269:LEU:CD1  | 1:C:270:ARG:N    | 1.87                     | 1.26              |
| 1:A:313:TYR:CD1  | 1:A:332:VAL:HG22 | 1.59                     | 1.26              |
| 1:B:87:GLY:O     | 1:B:88:LEU:HD23  | 1.13                     | 1.26              |
| 1:B:115:LEU:HD12 | 1:B:119:GLY:CA   | 1.63                     | 1.25              |
| 1:B:276:THR:CG2  | 1:B:294:TYR:CE2  | 2.18                     | 1.25              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:172:ASP:O    | 1:A:194:ALA:CB   | 1.85                     | 1.25              |
| 1:C:63:TYR:CD1   | 1:C:80:LYS:O     | 1.89                     | 1.25              |
| 1:B:21:HIS:CD2   | 1:B:23:PHE:CE2   | 2.23                     | 1.24              |
| 1:A:258:LEU:CD1  | 1:A:276:THR:CG2  | 2.16                     | 1.24              |
| 1:A:294:TYR:CD2  | 1:A:314:ILE:CD1  | 2.20                     | 1.23              |
| 1:D:279:LYS:HB2  | 1:D:279:LYS:NZ   | 1.24                     | 1.23              |
| 1:A:1:ALA:HB3    | 1:B:4:TYR:CE1    | 1.73                     | 1.23              |
| 1:A:337:VAL:O    | 1:A:337:VAL:CG1  | 1.74                     | 1.23              |
| 1:B:229:ALA:CB   | 1:B:259:LEU:CD2  | 2.17                     | 1.23              |
| 1:D:115:LEU:CD2  | 1:D:115:LEU:N    | 1.80                     | 1.22              |
| 1:A:258:LEU:C    | 1:A:259:LEU:HD23 | 1.62                     | 1.22              |
| 1:B:96:PHE:HD2   | 1:B:97:ASP:N     | 1.33                     | 1.22              |
| 1:D:309:THR:CG2  | 1:D:336:ILE:HB   | 1.67                     | 1.22              |
| 1:B:151:LEU:C    | 1:B:151:LEU:CD1  | 1.98                     | 1.22              |
| 1:D:170:ASN:O    | 1:D:170:ASN:ND2  | 1.71                     | 1.22              |
| 1:B:229:ALA:HB1  | 1:B:259:LEU:CD2  | 1.71                     | 1.21              |
| 1:B:45:PHE:CD1   | 1:B:45:PHE:O     | 1.94                     | 1.20              |
| 1:A:141:ASN:O    | 1:A:152:ASN:HB3  | 1.40                     | 1.20              |
| 1:B:151:LEU:HD12 | 1:B:152:ASN:N    | 1.56                     | 1.20              |
| 1:C:174:VAL:HG12 | 1:C:175:GLY:N    | 1.56                     | 1.20              |
| 1:D:29:GLU:CG    | 1:D:30:ASN:N     | 2.01                     | 1.20              |
| 1:D:144:PHE:O    | 1:D:144:PHE:HD2  | 0.91                     | 1.20              |
| 1:C:172:ASP:O    | 1:C:194:ALA:CB   | 1.89                     | 1.20              |
| 1:A:61:TRP:CZ2   | 1:C:65:PHE:CD1   | 2.29                     | 1.19              |
| 1:A:231:TYR:CD2  | 1:A:232:GLY:N    | 2.11                     | 1.19              |
| 1:B:96:PHE:CD2   | 1:B:97:ASP:N     | 2.10                     | 1.19              |
| 1:D:315:ILE:N    | 1:D:315:ILE:HD12 | 1.48                     | 1.19              |
| 1:B:313:TYR:CD1  | 1:B:332:VAL:HG23 | 1.77                     | 1.19              |
| 1:A:111:TYR:CE2  | 1:A:219:LYS:HG2  | 1.77                     | 1.18              |
| 1:B:45:PHE:O     | 1:B:45:PHE:HD1   | 1.22                     | 1.18              |
| 1:B:113:ASP:C    | 1:B:114:MET:HG2  | 1.66                     | 1.18              |
| 1:C:286:ILE:HD12 | 1:C:286:ILE:N    | 1.47                     | 1.18              |
| 1:B:115:LEU:CD1  | 1:B:119:GLY:HA3  | 1.72                     | 1.18              |
| 1:A:22:TYR:CE2   | 1:A:38:MET:HE2   | 1.78                     | 1.18              |
| 1:A:262:GLN:OE1  | 1:A:270:ARG:NH1  | 1.76                     | 1.18              |
| 1:B:242:ASN:OD1  | 1:B:242:ASN:O    | 1.62                     | 1.18              |
| 1:B:276:THR:HG21 | 1:B:294:TYR:CE2  | 1.78                     | 1.18              |
| 1:B:114:MET:HE2  | 1:B:226:TYR:CE1  | 1.78                     | 1.18              |
| 1:A:309:THR:CG2  | 1:A:336:ILE:HB   | 1.74                     | 1.17              |
| 1:A:258:LEU:O    | 1:A:259:LEU:CD2  | 1.92                     | 1.17              |
| 1:A:271:PRO:HA   | 1:A:299:ALA:CB   | 1.74                     | 1.17              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:167:ARG:CG   | 1:C:167:ARG:O    | 1.91                     | 1.17              |
| 1:B:180:TYR:C    | 1:B:180:TYR:HD2  | 1.47                     | 1.17              |
| 1:C:338:TYR:CD2  | 1:C:339:GLN:N    | 2.13                     | 1.16              |
| 1:D:51:ILE:CD1   | 1:D:55:LEU:CD2   | 2.22                     | 1.16              |
| 1:A:267:PHE:N    | 1:A:267:PHE:HD1  | 1.42                     | 1.16              |
| 1:A:307:MET:HE2  | 1:B:88:LEU:HD22  | 1.27                     | 1.16              |
| 1:B:105:VAL:O    | 1:B:105:VAL:CG1  | 1.89                     | 1.16              |
| 1:D:96:PHE:CD2   | 1:D:97:ASP:N     | 2.14                     | 1.16              |
| 1:B:87:GLY:C     | 1:B:88:LEU:HD23  | 1.70                     | 1.16              |
| 1:B:143:ASN:OD1  | 1:B:150:GLY:N    | 1.79                     | 1.15              |
| 1:B:64:ASN:O     | 1:B:64:ASN:ND2   | 1.77                     | 1.15              |
| 1:D:226:TYR:O    | 1:D:227:LEU:HD23 | 1.47                     | 1.15              |
| 1:A:275:TYR:O    | 1:A:276:THR:OG1  | 1.61                     | 1.14              |
| 1:B:285:GLY:C    | 1:B:286:ILE:HD12 | 1.72                     | 1.14              |
| 1:B:313:TYR:HD1  | 1:B:332:VAL:CG2  | 1.56                     | 1.14              |
| 1:B:112:THR:HG21 | 1:B:230:ASN:HB2  | 1.18                     | 1.14              |
| 1:B:332:VAL:O    | 1:B:332:VAL:CG1  | 1.91                     | 1.14              |
| 1:C:291:LEU:O    | 1:C:292:VAL:HG23 | 1.46                     | 1.14              |
| 1:C:204:PRO:HG2  | 1:C:247:THR:HG22 | 1.22                     | 1.14              |
| 1:A:22:TYR:CD2   | 1:A:38:MET:HG3   | 1.82                     | 1.14              |
| 1:A:45:PHE:HD1   | 1:A:45:PHE:O     | 1.29                     | 1.14              |
| 1:A:118:PHE:O    | 1:A:119:GLY:O    | 1.63                     | 1.14              |
| 1:C:307:MET:HG3  | 1:C:308:SER:H    | 1.12                     | 1.13              |
| 1:A:69:ASN:HD21  | 1:A:77:THR:HB    | 0.97                     | 1.13              |
| 1:C:27:ASN:OD1   | 1:C:27:ASN:O     | 1.65                     | 1.13              |
| 1:A:307:MET:CE   | 1:B:88:LEU:HD21  | 1.64                     | 1.13              |
| 1:A:313:TYR:CD1  | 1:A:332:VAL:HG23 | 1.63                     | 1.13              |
| 1:A:258:LEU:HD13 | 1:A:276:THR:HG23 | 1.30                     | 1.12              |
| 1:B:113:ASP:O    | 1:B:114:MET:HG2  | 1.48                     | 1.12              |
| 1:A:45:PHE:O     | 1:A:45:PHE:CD1   | 2.00                     | 1.12              |
| 1:A:114:MET:O    | 1:A:115:LEU:O    | 1.66                     | 1.12              |
| 1:C:224:ASN:O    | 1:C:263:TYR:HD1  | 1.30                     | 1.12              |
| 1:A:158:LEU:C    | 1:A:158:LEU:HD12 | 1.73                     | 1.12              |
| 1:A:51:ILE:HG13  | 1:A:55:LEU:HD23  | 1.13                     | 1.11              |
| 1:B:255:GLN:OE1  | 1:B:281:LYS:HE2  | 1.50                     | 1.11              |
| 1:D:144:PHE:HD2  | 1:D:144:PHE:C    | 1.58                     | 1.11              |
| 1:C:204:PRO:HG2  | 1:C:247:THR:HG21 | 1.25                     | 1.11              |
| 1:A:172:ASP:O    | 1:A:194:ALA:HB1  | 1.39                     | 1.11              |
| 1:A:187:ILE:CG2  | 1:A:187:ILE:O    | 1.99                     | 1.11              |
| 1:A:141:ASN:OD1  | 1:A:153:PHE:HE1  | 1.32                     | 1.10              |
| 1:B:276:THR:HG21 | 1:B:294:TYR:HE2  | 0.99                     | 1.10              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:129:PHE:HE2  | 1:A:193:ALA:N    | 1.48                     | 1.10              |
| 1:B:115:LEU:HD23 | 1:B:115:LEU:N    | 0.97                     | 1.10              |
| 1:D:203:GLN:HB3  | 1:D:204:PRO:HD2  | 1.34                     | 1.10              |
| 1:A:211:ALA:CB   | 1:A:236:ASN:HB2  | 1.81                     | 1.10              |
| 1:B:180:TYR:C    | 1:B:180:TYR:CD2  | 2.24                     | 1.09              |
| 1:C:82:ARG:O     | 1:C:100:ARG:HD3  | 1.51                     | 1.09              |
| 1:D:20:LEU:HD12  | 1:D:21:HIS:H     | 1.03                     | 1.09              |
| 1:B:23:PHE:HA    | 1:B:35:ASN:HD21  | 1.04                     | 1.09              |
| 1:B:311:VAL:HG13 | 1:B:334:VAL:HG22 | 1.31                     | 1.09              |
| 1:A:104:VAL:HG13 | 1:A:156:GLN:OE1  | 0.91                     | 1.09              |
| 1:A:113:ASP:O    | 1:A:114:MET:HG2  | 1.53                     | 1.09              |
| 1:B:27:ASN:OD1   | 1:B:27:ASN:O     | 1.71                     | 1.09              |
| 1:B:277:LYS:HD2  | 1:B:293:ASN:ND2  | 1.65                     | 1.09              |
| 1:A:22:TYR:HE2   | 1:A:38:MET:HE2   | 0.93                     | 1.09              |
| 1:C:174:VAL:CG1  | 1:C:175:GLY:N    | 2.15                     | 1.08              |
| 1:D:132:ARG:HG3  | 1:D:132:ARG:NH1  | 1.11                     | 1.08              |
| 1:D:279:LYS:NZ   | 1:D:279:LYS:CB   | 2.10                     | 1.08              |
| 1:A:115:LEU:HD22 | 1:A:115:LEU:N    | 1.67                     | 1.08              |
| 1:A:258:LEU:HD12 | 1:A:276:THR:HG23 | 1.11                     | 1.08              |
| 1:B:242:ASN:O    | 1:B:244:PHE:N    | 1.85                     | 1.08              |
| 1:B:114:MET:CE   | 1:B:226:TYR:CE1  | 2.35                     | 1.08              |
| 1:D:13:LEU:HD12  | 1:D:14:TYR:N     | 1.69                     | 1.08              |
| 1:D:51:ILE:HD13  | 1:D:55:LEU:CD2   | 1.80                     | 1.08              |
| 1:D:51:ILE:HD13  | 1:D:55:LEU:HD23  | 1.24                     | 1.07              |
| 1:D:338:TYR:CD2  | 1:D:339:GLN:N    | 2.22                     | 1.07              |
| 1:A:51:ILE:HD11  | 1:A:55:LEU:CD2   | 1.78                     | 1.07              |
| 1:A:158:LEU:HD12 | 1:A:159:GLY:N    | 1.70                     | 1.07              |
| 1:B:115:LEU:CD2  | 1:B:115:LEU:N    | 1.73                     | 1.07              |
| 1:B:229:ALA:CB   | 1:B:259:LEU:HD22 | 1.85                     | 1.07              |
| 1:D:122:THR:HG21 | 1:D:256:ASP:OD2  | 1.53                     | 1.07              |
| 1:A:276:THR:HB   | 1:A:294:TYR:HE1  | 1.18                     | 1.07              |
| 1:A:293:ASN:HD22 | 1:A:317:GLN:HB3  | 1.14                     | 1.07              |
| 1:D:271:PRO:HA   | 1:D:299:ALA:HB2  | 1.32                     | 1.07              |
| 1:A:318:ILE:HD13 | 1:A:318:ILE:N    | 1.68                     | 1.06              |
| 1:C:179:SER:HA   | 1:C:188:VAL:HG12 | 1.13                     | 1.06              |
| 1:A:313:TYR:HD1  | 1:A:332:VAL:HG23 | 0.95                     | 1.06              |
| 1:D:20:LEU:HD12  | 1:D:21:HIS:N     | 1.70                     | 1.06              |
| 1:D:51:ILE:HD12  | 1:D:55:LEU:HD23  | 1.32                     | 1.06              |
| 1:A:167:ARG:CG   | 1:A:167:ARG:HH11 | 1.68                     | 1.06              |
| 1:A:285:GLY:C    | 1:A:286:ILE:CD1  | 2.28                     | 1.06              |
| 1:B:114:MET:C    | 1:B:115:LEU:HD23 | 1.79                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:144:PHE:CD2  | 1:D:144:PHE:C    | 2.26                     | 1.06              |
| 1:A:307:MET:HE2  | 1:B:88:LEU:CD2   | 1.76                     | 1.06              |
| 1:A:271:PRO:CA   | 1:A:299:ALA:HB2  | 1.86                     | 1.06              |
| 1:B:64:ASN:HD22  | 1:B:64:ASN:C     | 1.59                     | 1.06              |
| 1:B:87:GLY:O     | 1:B:88:LEU:CD2   | 2.03                     | 1.06              |
| 1:B:276:THR:CB   | 1:B:294:TYR:CE2  | 2.39                     | 1.06              |
| 1:D:286:ILE:HD12 | 1:D:286:ILE:H    | 1.17                     | 1.06              |
| 1:A:129:PHE:CD2  | 1:A:192:GLY:HA3  | 1.90                     | 1.05              |
| 1:B:276:THR:HB   | 1:B:294:TYR:CE2  | 1.90                     | 1.05              |
| 1:B:69:ASN:HD21  | 1:B:77:THR:HB    | 1.21                     | 1.05              |
| 1:D:309:THR:HG22 | 1:D:336:ILE:HA   | 1.38                     | 1.05              |
| 1:A:191:TYR:HD2  | 1:A:191:TYR:C    | 1.62                     | 1.05              |
| 1:B:205:LEU:HD11 | 1:B:247:THR:HG22 | 1.37                     | 1.05              |
| 1:B:332:VAL:O    | 1:B:332:VAL:HG12 | 1.32                     | 1.05              |
| 1:C:167:ARG:O    | 1:C:167:ARG:HG3  | 1.27                     | 1.05              |
| 1:C:297:VAL:O    | 1:C:297:VAL:HG12 | 1.48                     | 1.05              |
| 1:A:1:ALA:CB     | 1:B:4:TYR:CE1    | 2.38                     | 1.05              |
| 1:B:30:ASN:O     | 1:B:30:ASN:OD1   | 1.75                     | 1.05              |
| 1:C:42:ARG:NH1   | 1:C:82:ARG:NH2   | 2.04                     | 1.05              |
| 1:C:179:SER:CA   | 1:C:188:VAL:HG12 | 1.86                     | 1.05              |
| 1:B:167:ARG:HH11 | 1:B:167:ARG:HG3  | 1.15                     | 1.05              |
| 1:C:45:PHE:O     | 1:C:45:PHE:CD1   | 2.08                     | 1.04              |
| 1:D:115:LEU:N    | 1:D:115:LEU:HD23 | 1.01                     | 1.04              |
| 1:D:286:ILE:H    | 1:D:286:ILE:CD1  | 1.71                     | 1.04              |
| 1:A:51:ILE:HD12  | 1:A:55:LEU:CD2   | 1.87                     | 1.04              |
| 1:A:165:THR:CG2  | 1:A:166:ALA:N    | 2.19                     | 1.04              |
| 1:D:40:TYR:HE2   | 1:D:42:ARG:NH2   | 1.51                     | 1.04              |
| 1:B:115:LEU:HD12 | 1:B:119:GLY:HA3  | 1.05                     | 1.04              |
| 1:B:229:ALA:HB1  | 1:B:259:LEU:HD23 | 1.40                     | 1.04              |
| 1:A:303:PHE:HD2  | 1:A:307:MET:HG2  | 1.21                     | 1.04              |
| 1:D:229:ALA:HB2  | 1:D:259:LEU:HD22 | 1.33                     | 1.04              |
| 1:D:274:ALA:HB3  | 1:D:296:GLU:HB3  | 1.35                     | 1.04              |
| 1:A:127:ASP:O    | 1:A:128:PHE:CB   | 2.01                     | 1.04              |
| 1:B:125:SER:O    | 1:B:126:ASP:HB2  | 1.55                     | 1.04              |
| 1:B:130:VAL:CG1  | 1:B:213:GLN:NE2  | 2.19                     | 1.04              |
| 1:D:229:ALA:CB   | 1:D:259:LEU:HD21 | 1.84                     | 1.04              |
| 1:A:69:ASN:ND2   | 1:A:77:THR:HB    | 1.72                     | 1.03              |
| 1:B:28:GLY:O     | 1:B:31:SER:N     | 1.89                     | 1.03              |
| 1:C:309:THR:HG22 | 1:C:336:ILE:HA   | 1.37                     | 1.03              |
| 1:D:187:ILE:HG13 | 1:D:218:LEU:HD21 | 1.36                     | 1.03              |
| 1:B:20:LEU:HD21  | 1:B:117:GLU:OE1  | 1.56                     | 1.03              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:40:TYR:CE2   | 1:D:42:ARG:NH2   | 2.25                     | 1.03              |
| 1:D:315:ILE:N    | 1:D:315:ILE:CD1  | 2.21                     | 1.03              |
| 1:B:302:TYR:O    | 1:B:303:PHE:C    | 1.98                     | 1.03              |
| 1:B:112:THR:HG23 | 1:B:230:ASN:OD1  | 1.58                     | 1.03              |
| 1:B:313:TYR:CD1  | 1:B:332:VAL:CG2  | 2.39                     | 1.03              |
| 1:A:170:ASN:ND2  | 1:A:170:ASN:C    | 2.17                     | 1.02              |
| 1:D:74:ASP:O     | 1:D:76:GLN:N     | 1.92                     | 1.02              |
| 1:A:61:TRP:HZ2   | 1:C:65:PHE:CD1   | 1.69                     | 1.02              |
| 1:A:86:ALA:O     | 1:A:97:ASP:HB2   | 1.58                     | 1.02              |
| 1:C:241:THR:HG22 | 1:C:242:ASN:H    | 1.22                     | 1.02              |
| 1:B:241:THR:HG22 | 1:B:242:ASN:N    | 1.63                     | 1.02              |
| 1:A:4:TYR:CE1    | 1:C:1:ALA:CB     | 2.41                     | 1.02              |
| 1:C:229:ALA:CB   | 1:C:259:LEU:CD2  | 2.38                     | 1.02              |
| 1:A:132:ARG:HG3  | 1:A:132:ARG:HH11 | 1.22                     | 1.02              |
| 1:D:229:ALA:CB   | 1:D:259:LEU:HD23 | 1.87                     | 1.02              |
| 1:A:71:GLU:HG3   | 1:B:100:ARG:NH2  | 1.75                     | 1.01              |
| 1:C:112:THR:CG2  | 1:C:230:ASN:OD1  | 2.07                     | 1.01              |
| 1:A:22:TYR:CD1   | 1:A:333:ALA:HB2  | 1.94                     | 1.01              |
| 1:A:115:LEU:N    | 1:A:115:LEU:HD23 | 1.21                     | 1.01              |
| 1:A:170:ASN:C    | 1:A:170:ASN:HD22 | 1.69                     | 1.01              |
| 1:B:130:VAL:HG13 | 1:B:213:GLN:NE2  | 1.75                     | 1.01              |
| 1:B:311:VAL:HG13 | 1:B:334:VAL:CG2  | 1.90                     | 1.01              |
| 1:D:13:LEU:HD12  | 1:D:13:LEU:C     | 1.84                     | 1.01              |
| 1:A:231:TYR:HD2  | 1:A:231:TYR:C    | 1.67                     | 1.01              |
| 1:C:289:VAL:CG1  | 1:C:323:LYS:HB2  | 1.91                     | 1.01              |
| 1:A:1:ALA:CB     | 1:B:4:TYR:OH     | 2.07                     | 1.01              |
| 1:A:127:ASP:OD1  | 1:A:239:PRO:HD3  | 1.61                     | 1.01              |
| 1:A:258:LEU:HD12 | 1:A:276:THR:CG2  | 1.86                     | 1.01              |
| 1:B:101:ASN:OD1  | 1:B:102:TYR:N    | 1.93                     | 1.01              |
| 1:B:285:GLY:O    | 1:B:286:ILE:HD12 | 1.58                     | 1.01              |
| 1:C:39:THR:HG22  | 1:C:39:THR:O     | 1.58                     | 1.01              |
| 1:A:51:ILE:HG23  | 1:C:304:ASN:ND2  | 1.76                     | 1.00              |
| 1:B:229:ALA:HB2  | 1:B:259:LEU:HD22 | 1.39                     | 1.00              |
| 1:D:294:TYR:CD1  | 1:D:314:ILE:HD12 | 1.94                     | 1.00              |
| 1:D:311:VAL:CG1  | 1:D:334:VAL:CG2  | 2.18                     | 1.00              |
| 1:A:180:TYR:HD2  | 1:A:180:TYR:C    | 1.68                     | 1.00              |
| 1:A:204:PRO:HG2  | 1:A:247:THR:HG22 | 1.43                     | 1.00              |
| 1:B:306:ASN:OD1  | 1:C:9:ASN:HB2    | 1.59                     | 1.00              |
| 1:B:338:TYR:O    | 1:B:339:GLN:HB3  | 1.62                     | 1.00              |
| 1:D:105:VAL:O    | 1:D:105:VAL:CG1  | 2.09                     | 1.00              |
| 1:A:241:THR:CG2  | 1:A:242:ASN:H    | 1.73                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:55:LEU:HD12  | 1:D:90:TYR:HD1   | 1.23                     | 1.00              |
| 1:A:61:TRP:CZ2   | 1:C:65:PHE:CE1   | 2.49                     | 1.00              |
| 1:B:105:VAL:O    | 1:B:105:VAL:HG13 | 1.18                     | 1.00              |
| 1:A:294:TYR:HD2  | 1:A:314:ILE:HD12 | 0.87                     | 1.00              |
| 1:A:211:ALA:HB2  | 1:A:236:ASN:HB2  | 1.00                     | 0.99              |
| 1:A:100:ARG:NH2  | 1:C:71:GLU:OE2   | 1.94                     | 0.99              |
| 1:A:129:PHE:CE2  | 1:A:193:ALA:N    | 2.29                     | 0.99              |
| 1:A:309:THR:HG21 | 1:A:336:ILE:HB   | 1.43                     | 0.99              |
| 1:C:104:VAL:HG11 | 1:C:176:GLY:CA   | 1.91                     | 0.99              |
| 1:C:229:ALA:HB1  | 1:C:259:LEU:CD2  | 1.92                     | 0.99              |
| 1:B:294:TYR:CD1  | 1:B:314:ILE:HD12 | 1.97                     | 0.99              |
| 1:C:277:LYS:HE2  | 1:C:279:LYS:HD2  | 1.40                     | 0.99              |
| 1:A:104:VAL:CG1  | 1:A:156:GLN:CD   | 2.35                     | 0.99              |
| 1:A:231:TYR:CD2  | 1:A:231:TYR:C    | 2.38                     | 0.99              |
| 1:C:224:ASN:O    | 1:C:263:TYR:CD1  | 2.14                     | 0.99              |
| 1:B:23:PHE:HA    | 1:B:35:ASN:ND2   | 1.77                     | 0.99              |
| 1:C:338:TYR:HD2  | 1:C:339:GLN:N    | 1.56                     | 0.99              |
| 1:D:66:GLN:HG3   | 1:D:78:GLY:HA3   | 1.42                     | 0.99              |
| 1:B:24:SER:H     | 1:B:35:ASN:ND2   | 1.60                     | 0.99              |
| 1:B:51:ILE:O     | 1:B:52:ASN:HB3   | 1.61                     | 0.99              |
| 1:D:132:ARG:CG   | 1:D:132:ARG:NH1  | 1.99                     | 0.99              |
| 1:A:24:SER:H     | 1:A:35:ASN:HD22  | 1.07                     | 0.99              |
| 1:A:122:THR:HG23 | 1:A:256:ASP:OD2  | 1.61                     | 0.99              |
| 1:B:64:ASN:ND2   | 1:B:64:ASN:C     | 2.17                     | 0.99              |
| 1:A:307:MET:HE3  | 1:B:88:LEU:HD21  | 1.01                     | 0.99              |
| 1:C:144:PHE:HD2  | 1:C:144:PHE:O    | 1.44                     | 0.99              |
| 1:D:309:THR:HG21 | 1:D:336:ILE:HB   | 1.41                     | 0.99              |
| 1:D:112:THR:HG23 | 1:D:230:ASN:OD1  | 1.63                     | 0.98              |
| 1:C:163:ARG:HD2  | 1:C:168:ARG:O    | 1.64                     | 0.98              |
| 1:D:299:ALA:O    | 1:D:310:TYR:HB2  | 1.62                     | 0.98              |
| 1:C:167:ARG:HG3  | 1:C:167:ARG:HH11 | 1.27                     | 0.98              |
| 1:C:286:ILE:CD1  | 1:C:286:ILE:N    | 2.09                     | 0.98              |
| 1:A:289:VAL:CG1  | 1:A:323:LYS:HB2  | 1.94                     | 0.98              |
| 1:D:124:TYR:HE2  | 1:D:238:THR:HG23 | 1.26                     | 0.98              |
| 1:A:51:ILE:HD11  | 1:A:55:LEU:HD21  | 1.45                     | 0.98              |
| 1:A:125:SER:O    | 1:A:126:ASP:HB2  | 1.57                     | 0.98              |
| 1:A:211:ALA:HB2  | 1:A:236:ASN:CB   | 1.93                     | 0.98              |
| 1:C:18:VAL:HG22  | 1:C:337:VAL:HG22 | 1.42                     | 0.98              |
| 1:A:104:VAL:HG13 | 1:A:156:GLN:CD   | 1.88                     | 0.98              |
| 1:C:307:MET:O    | 1:C:308:SER:HB3  | 1.64                     | 0.98              |
| 1:D:29:GLU:HG3   | 1:D:30:ASN:N     | 1.37                     | 0.98              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:309:THR:HG22 | 1:A:336:ILE:HB   | 1.43                     | 0.98              |
| 1:C:104:VAL:CG1  | 1:C:176:GLY:HA2  | 1.92                     | 0.98              |
| 1:A:90:TYR:O     | 1:A:93:VAL:CG2   | 2.11                     | 0.98              |
| 1:D:286:ILE:HD12 | 1:D:286:ILE:N    | 1.77                     | 0.97              |
| 1:A:112:THR:HG23 | 1:A:230:ASN:OD1  | 1.61                     | 0.97              |
| 1:A:127:ASP:O    | 1:A:128:PHE:HB2  | 1.17                     | 0.97              |
| 1:D:314:ILE:C    | 1:D:315:ILE:HD12 | 1.88                     | 0.97              |
| 1:A:241:THR:CG2  | 1:A:242:ASN:N    | 2.28                     | 0.97              |
| 1:B:269:LEU:HG   | 1:B:270:ARG:N    | 1.79                     | 0.97              |
| 1:C:307:MET:HG3  | 1:C:308:SER:N    | 1.75                     | 0.97              |
| 1:A:307:MET:HE1  | 1:B:87:GLY:O     | 1.64                     | 0.97              |
| 1:A:318:ILE:HG21 | 1:A:322:ASN:HD22 | 1.29                     | 0.97              |
| 1:D:111:TYR:CZ   | 1:D:188:VAL:CG2  | 2.48                     | 0.97              |
| 1:D:229:ALA:HB1  | 1:D:259:LEU:HD21 | 1.43                     | 0.97              |
| 1:A:211:ALA:CB   | 1:A:235:ARG:O    | 2.13                     | 0.97              |
| 1:B:54:ASP:HB3   | 1:B:91:ALA:HB2   | 1.42                     | 0.97              |
| 1:A:241:THR:HG23 | 1:A:242:ASN:H    | 1.27                     | 0.97              |
| 1:D:111:TYR:CE2  | 1:D:188:VAL:CG2  | 2.48                     | 0.97              |
| 1:B:180:TYR:CD2  | 1:B:181:GLU:N    | 2.33                     | 0.96              |
| 1:A:1:ALA:CB     | 1:B:4:TYR:HE1    | 1.75                     | 0.96              |
| 1:A:141:ASN:OD1  | 1:A:153:PHE:CE1  | 2.19                     | 0.96              |
| 1:D:82:ARG:O     | 1:D:132:ARG:HD2  | 1.64                     | 0.96              |
| 1:D:122:THR:CG2  | 1:D:256:ASP:OD2  | 2.13                     | 0.96              |
| 1:A:284:GLU:N    | 1:A:284:GLU:OE2  | 1.98                     | 0.96              |
| 1:C:51:ILE:CD1   | 1:C:55:LEU:HD23  | 1.94                     | 0.96              |
| 1:C:104:VAL:HG11 | 1:C:176:GLY:HA2  | 0.98                     | 0.96              |
| 1:A:276:THR:HB   | 1:A:294:TYR:CE1  | 1.99                     | 0.96              |
| 1:D:51:ILE:HD12  | 1:D:55:LEU:CD2   | 1.90                     | 0.96              |
| 1:B:127:ASP:O    | 1:B:128:PHE:HB2  | 1.63                     | 0.96              |
| 1:D:311:VAL:HG13 | 1:D:334:VAL:HG22 | 1.48                     | 0.96              |
| 1:C:54:ASP:HB2   | 1:C:90:TYR:HE1   | 1.29                     | 0.96              |
| 1:D:180:TYR:HD2  | 1:D:181:GLU:N    | 1.63                     | 0.95              |
| 1:D:196:ARG:NH2  | 1:D:250:PHE:HD1  | 1.63                     | 0.95              |
| 1:D:229:ALA:HB1  | 1:D:259:LEU:CD2  | 1.95                     | 0.95              |
| 1:A:130:VAL:CG1  | 1:A:213:GLN:NE2  | 2.29                     | 0.95              |
| 1:A:141:ASN:CB   | 1:A:153:PHE:CE1  | 2.50                     | 0.95              |
| 1:A:322:ASN:C    | 1:A:322:ASN:OD1  | 2.06                     | 0.95              |
| 1:B:18:VAL:HG11  | 1:B:40:TYR:HE1   | 1.32                     | 0.95              |
| 1:D:226:TYR:C    | 1:D:227:LEU:HD23 | 1.89                     | 0.95              |
| 1:D:337:VAL:O    | 1:D:337:VAL:HG12 | 1.64                     | 0.95              |
| 1:A:63:TYR:CD1   | 1:A:80:LYS:O     | 2.20                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:226:TYR:O    | 1:A:227:LEU:HD23 | 1.67                     | 0.95              |
| 1:A:318:ILE:HD13 | 1:A:318:ILE:H    | 1.31                     | 0.95              |
| 1:B:58:TYR:H     | 1:B:58:TYR:HD2   | 1.11                     | 0.95              |
| 1:C:222:ALA:O    | 1:C:223:ASN:HB2  | 1.63                     | 0.95              |
| 1:A:115:LEU:CD2  | 1:A:115:LEU:N    | 1.70                     | 0.95              |
| 1:D:96:PHE:CD2   | 1:D:96:PHE:C     | 2.45                     | 0.95              |
| 1:B:5:ASN:C      | 1:B:6:LYS:HG2    | 1.91                     | 0.94              |
| 1:D:96:PHE:HD2   | 1:D:97:ASP:N     | 1.65                     | 0.94              |
| 1:A:24:SER:OG    | 1:A:331:THR:OG1  | 1.83                     | 0.94              |
| 1:B:14:TYR:C     | 1:B:340:PHE:HE2  | 1.75                     | 0.94              |
| 1:B:129:PHE:HE2  | 1:B:193:ALA:N    | 1.66                     | 0.94              |
| 1:D:196:ARG:HH21 | 1:D:250:PHE:HD1  | 1.07                     | 0.94              |
| 1:D:277:LYS:HB2  | 1:D:293:ASN:OD1  | 1.68                     | 0.94              |
| 1:A:167:ARG:HH11 | 1:A:167:ARG:HG3  | 1.31                     | 0.94              |
| 1:C:258:LEU:O    | 1:C:259:LEU:HD23 | 1.67                     | 0.94              |
| 1:D:171:GLY:HA3  | 1:D:195:ASP:HB2  | 1.50                     | 0.94              |
| 1:A:114:MET:CE   | 1:A:226:TYR:CZ   | 2.50                     | 0.94              |
| 1:C:240:ILE:HD11 | 1:C:251:ALA:N    | 1.83                     | 0.94              |
| 1:D:309:THR:CG2  | 1:D:336:ILE:CB   | 2.46                     | 0.94              |
| 1:C:167:ARG:O    | 1:C:168:ARG:HD3  | 1.68                     | 0.93              |
| 1:B:310:TYR:HD1  | 1:B:310:TYR:O    | 1.50                     | 0.93              |
| 1:C:139:TYR:O    | 1:C:154:ALA:HB1  | 1.67                     | 0.93              |
| 1:D:100:ARG:CG   | 1:D:100:ARG:HH11 | 1.82                     | 0.93              |
| 1:D:83:LEU:HD21  | 1:D:102:TYR:CE2  | 2.04                     | 0.93              |
| 1:A:61:TRP:CZ2   | 1:C:65:PHE:HD1   | 1.79                     | 0.93              |
| 1:B:112:THR:HG21 | 1:B:230:ASN:CB   | 1.99                     | 0.93              |
| 1:B:303:PHE:HB3  | 1:C:51:ILE:HG21  | 1.49                     | 0.93              |
| 1:C:240:ILE:CD1  | 1:C:251:ALA:N    | 2.32                     | 0.93              |
| 1:D:60:GLN:HB3   | 1:D:85:PHE:CE2   | 2.03                     | 0.93              |
| 1:D:318:ILE:CG2  | 1:D:319:ASP:N    | 2.29                     | 0.93              |
| 1:B:241:THR:CG2  | 1:B:242:ASN:N    | 2.30                     | 0.93              |
| 1:C:18:VAL:HG11  | 1:C:40:TYR:CZ    | 2.03                     | 0.93              |
| 1:C:21:HIS:CD2   | 1:C:23:PHE:CZ    | 2.56                     | 0.93              |
| 1:C:160:LYS:HA   | 1:C:160:LYS:HE3  | 1.46                     | 0.93              |
| 1:C:169:SER:O    | 1:C:170:ASN:HB3  | 1.66                     | 0.93              |
| 1:B:294:TYR:CE1  | 1:B:314:ILE:HD12 | 2.03                     | 0.93              |
| 1:D:105:VAL:O    | 1:D:105:VAL:HG13 | 1.69                     | 0.93              |
| 1:D:309:THR:HG22 | 1:D:336:ILE:CA   | 1.98                     | 0.93              |
| 1:C:23:PHE:HA    | 1:C:35:ASN:HD22  | 1.30                     | 0.93              |
| 1:A:309:THR:HG22 | 1:A:336:ILE:CB   | 1.97                     | 0.93              |
| 1:C:172:ASP:C    | 1:C:194:ALA:HB1  | 1.94                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:20:LEU:CD1   | 1:D:21:HIS:H     | 1.81                     | 0.92              |
| 1:C:241:THR:HG22 | 1:C:242:ASN:N    | 1.85                     | 0.92              |
| 1:A:129:PHE:HE2  | 1:A:193:ALA:H    | 1.03                     | 0.92              |
| 1:A:114:MET:HE1  | 1:A:226:TYR:HE1  | 1.28                     | 0.92              |
| 1:B:180:TYR:HD2  | 1:B:181:GLU:N    | 1.67                     | 0.92              |
| 1:A:22:TYR:HD1   | 1:A:333:ALA:HB2  | 1.34                     | 0.92              |
| 1:A:180:TYR:HD2  | 1:A:181:GLU:N    | 1.67                     | 0.92              |
| 1:B:15:GLY:N     | 1:B:340:PHE:CE2  | 2.38                     | 0.92              |
| 1:B:241:THR:CG2  | 1:B:242:ASN:H    | 1.81                     | 0.92              |
| 1:C:223:ASN:O    | 1:C:224:ASN:HB2  | 1.66                     | 0.92              |
| 1:C:283:VAL:HG23 | 1:C:287:GLY:O    | 1.70                     | 0.92              |
| 1:D:111:TYR:CZ   | 1:D:188:VAL:HG21 | 2.03                     | 0.92              |
| 1:C:10:LYS:HG3   | 1:C:10:LYS:O     | 1.67                     | 0.92              |
| 1:C:297:VAL:O    | 1:C:297:VAL:CG1  | 2.15                     | 0.92              |
| 1:B:110:GLY:O    | 1:B:112:THR:N    | 2.02                     | 0.92              |
| 1:D:24:SER:H     | 1:D:35:ASN:HD22  | 0.95                     | 0.92              |
| 1:D:118:PHE:CD2  | 1:D:314:ILE:HG12 | 2.05                     | 0.92              |
| 1:D:258:LEU:O    | 1:D:259:LEU:HD23 | 1.70                     | 0.92              |
| 1:A:18:VAL:HB    | 1:A:40:TYR:CE1   | 2.04                     | 0.91              |
| 1:B:20:LEU:HD12  | 1:B:21:HIS:H     | 1.34                     | 0.91              |
| 1:B:309:THR:HG22 | 1:B:336:ILE:HA   | 1.51                     | 0.91              |
| 1:C:60:GLN:HG2   | 1:C:61:TRP:N     | 1.85                     | 0.91              |
| 1:C:204:PRO:CG   | 1:C:247:THR:CG2  | 2.46                     | 0.91              |
| 1:D:104:VAL:HG12 | 1:D:156:GLN:OE1  | 1.69                     | 0.91              |
| 1:B:98:TYR:HD2   | 1:B:98:TYR:C     | 1.77                     | 0.91              |
| 1:A:165:THR:HG23 | 1:A:166:ALA:N    | 1.84                     | 0.91              |
| 1:B:4:TYR:CE2    | 1:B:6:LYS:HB2    | 2.04                     | 0.91              |
| 1:C:45:PHE:HD1   | 1:C:45:PHE:C     | 1.77                     | 0.91              |
| 1:D:279:LYS:HB2  | 1:D:279:LYS:HZ3  | 1.12                     | 0.91              |
| 1:A:22:TYR:HE2   | 1:A:38:MET:CE    | 1.83                     | 0.91              |
| 1:A:268:GLY:O    | 1:A:301:TYR:HD2  | 1.53                     | 0.91              |
| 1:B:112:THR:CG2  | 1:B:230:ASN:HB2  | 2.00                     | 0.91              |
| 1:A:61:TRP:CE3   | 1:A:61:TRP:O     | 2.23                     | 0.91              |
| 1:C:144:PHE:O    | 1:C:144:PHE:CD2  | 2.23                     | 0.91              |
| 1:D:60:GLN:HG2   | 1:D:85:PHE:HE2   | 1.36                     | 0.91              |
| 1:A:289:VAL:HG11 | 1:A:323:LYS:HB2  | 1.49                     | 0.91              |
| 1:D:215:ALA:C    | 1:D:216:THR:HG23 | 1.95                     | 0.91              |
| 1:A:85:PHE:HD2   | 1:A:101:ASN:HB2  | 1.36                     | 0.91              |
| 1:A:114:MET:C    | 1:A:115:LEU:O    | 2.11                     | 0.91              |
| 1:C:274:ALA:HB3  | 1:C:296:GLU:HB3  | 1.53                     | 0.91              |
| 1:D:307:MET:HG3  | 1:D:308:SER:H    | 1.36                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:318:ILE:HG23 | 1:D:319:ASP:H    | 1.34                     | 0.91              |
| 1:A:1:ALA:HB3    | 1:B:4:TYR:CZ     | 2.05                     | 0.90              |
| 1:D:223:ASN:O    | 1:D:224:ASN:HB2  | 1.68                     | 0.90              |
| 1:A:51:ILE:CG2   | 1:C:304:ASN:ND2  | 2.33                     | 0.90              |
| 1:A:100:ARG:HG2  | 1:A:134:GLY:HA2  | 1.51                     | 0.90              |
| 1:B:241:THR:HG22 | 1:B:242:ASN:H    | 1.30                     | 0.90              |
| 1:D:279:LYS:CB   | 1:D:279:LYS:HZ3  | 1.77                     | 0.90              |
| 1:C:101:ASN:OD1  | 1:C:102:TYR:N    | 2.04                     | 0.90              |
| 1:D:167:ARG:HG3  | 1:D:167:ARG:O    | 1.72                     | 0.90              |
| 1:D:46:LYS:HD3   | 1:D:60:GLN:HE22  | 1.35                     | 0.90              |
| 1:A:237:ALA:O    | 1:A:238:THR:C    | 2.11                     | 0.90              |
| 1:A:187:ILE:O    | 1:A:187:ILE:HG23 | 1.68                     | 0.90              |
| 1:B:58:TYR:CD2   | 1:B:58:TYR:O     | 2.25                     | 0.90              |
| 1:B:151:LEU:CG   | 1:B:151:LEU:O    | 2.17                     | 0.90              |
| 1:C:51:ILE:HD12  | 1:C:55:LEU:HD23  | 1.49                     | 0.90              |
| 1:B:87:GLY:C     | 1:B:88:LEU:CD2   | 2.44                     | 0.90              |
| 1:B:277:LYS:CD   | 1:B:293:ASN:ND2  | 2.34                     | 0.90              |
| 1:C:54:ASP:HB2   | 1:C:90:TYR:CE1   | 2.06                     | 0.90              |
| 1:A:226:TYR:HE2  | 1:A:228:ALA:HB2  | 1.37                     | 0.90              |
| 1:A:275:TYR:CD2  | 1:A:276:THR:N    | 2.40                     | 0.90              |
| 1:B:269:LEU:HG   | 1:B:271:PRO:HD3  | 1.51                     | 0.90              |
| 1:C:21:HIS:HD2   | 1:C:23:PHE:CZ    | 1.89                     | 0.90              |
| 1:A:4:TYR:CD1    | 1:C:1:ALA:CB     | 2.55                     | 0.90              |
| 1:A:257:VAL:O    | 1:A:258:LEU:HD13 | 1.72                     | 0.90              |
| 1:C:18:VAL:HG11  | 1:C:40:TYR:CE1   | 2.07                     | 0.90              |
| 1:D:55:LEU:CD1   | 1:D:90:TYR:HD1   | 1.84                     | 0.89              |
| 1:D:114:MET:C    | 1:D:115:LEU:HD23 | 1.97                     | 0.89              |
| 1:A:153:PHE:HD1  | 1:A:153:PHE:H    | 1.17                     | 0.89              |
| 1:D:180:TYR:HD2  | 1:D:180:TYR:C    | 1.80                     | 0.89              |
| 1:A:180:TYR:C    | 1:A:180:TYR:CD2  | 2.46                     | 0.89              |
| 1:B:101:ASN:CG   | 1:B:102:TYR:H    | 1.80                     | 0.89              |
| 1:C:18:VAL:CG2   | 1:C:337:VAL:HG22 | 2.03                     | 0.89              |
| 1:A:114:MET:HE2  | 1:A:226:TYR:CE1  | 2.08                     | 0.89              |
| 1:A:115:LEU:HG   | 1:A:119:GLY:HA3  | 1.52                     | 0.89              |
| 1:A:114:MET:HE2  | 1:A:226:TYR:CZ   | 2.08                     | 0.89              |
| 1:B:5:ASN:O      | 1:B:6:LYS:HG2    | 1.72                     | 0.89              |
| 1:B:130:VAL:HG13 | 1:B:213:GLN:HE22 | 1.38                     | 0.89              |
| 1:A:313:TYR:CG   | 1:A:332:VAL:HG22 | 2.08                     | 0.89              |
| 1:C:223:ASN:HB3  | 1:C:225:ILE:HD11 | 1.53                     | 0.89              |
| 1:C:269:LEU:HD11 | 1:C:270:ARG:H    | 1.36                     | 0.89              |
| 1:B:90:TYR:HB3   | 1:B:93:VAL:HG23  | 1.52                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:170:ASN:HD22 | 1:D:170:ASN:C    | 1.78                     | 0.88              |
| 1:A:102:TYR:O    | 1:A:103:GLY:O    | 1.89                     | 0.88              |
| 1:C:42:ARG:HH12  | 1:C:82:ARG:NH2   | 1.71                     | 0.88              |
| 1:D:24:SER:HB2   | 1:D:34:GLY:O     | 1.73                     | 0.88              |
| 1:A:258:LEU:HD11 | 1:A:276:THR:HG23 | 1.56                     | 0.88              |
| 1:B:141:ASN:ND2  | 1:B:145:PHE:CD1  | 2.41                     | 0.88              |
| 1:C:274:ALA:O    | 1:C:296:GLU:N    | 2.07                     | 0.88              |
| 1:D:96:PHE:C     | 1:D:96:PHE:HD2   | 1.79                     | 0.88              |
| 1:D:144:PHE:HB2  | 1:D:151:LEU:HD23 | 1.54                     | 0.88              |
| 1:A:293:ASN:ND2  | 1:A:317:GLN:HB3  | 1.87                     | 0.88              |
| 1:B:161:ASN:HB2  | 1:B:170:ASN:OD1  | 1.74                     | 0.88              |
| 1:D:215:ALA:O    | 1:D:216:THR:CG2  | 2.21                     | 0.88              |
| 1:B:151:LEU:O    | 1:B:151:LEU:HG   | 1.72                     | 0.88              |
| 1:D:124:TYR:HE2  | 1:D:238:THR:CG2  | 1.87                     | 0.88              |
| 1:D:231:TYR:CD2  | 1:D:232:GLY:N    | 2.41                     | 0.88              |
| 1:A:51:ILE:HG21  | 1:C:303:PHE:HB3  | 1.56                     | 0.88              |
| 1:A:129:PHE:CE2  | 1:A:192:GLY:HA3  | 2.09                     | 0.88              |
| 1:B:151:LEU:CD1  | 1:B:151:LEU:O    | 2.20                     | 0.88              |
| 1:D:187:ILE:CG1  | 1:D:218:LEU:HD21 | 2.04                     | 0.87              |
| 1:A:187:ILE:O    | 1:A:187:ILE:HG22 | 1.74                     | 0.87              |
| 1:A:271:PRO:HA   | 1:A:299:ALA:HB2  | 0.90                     | 0.87              |
| 1:A:130:VAL:HG12 | 1:A:213:GLN:NE2  | 1.90                     | 0.87              |
| 1:B:18:VAL:HG11  | 1:B:40:TYR:CE1   | 2.08                     | 0.87              |
| 1:C:286:ILE:H    | 1:C:286:ILE:HD13 | 1.38                     | 0.87              |
| 1:B:23:PHE:CA    | 1:B:35:ASN:HD21  | 1.87                     | 0.87              |
| 1:B:125:SER:O    | 1:B:126:ASP:CB   | 2.19                     | 0.87              |
| 1:C:141:ASN:HB3  | 1:C:153:PHE:CE1  | 2.10                     | 0.87              |
| 1:A:336:ILE:HG13 | 1:A:337:VAL:N    | 1.90                     | 0.87              |
| 1:B:111:TYR:CZ   | 1:B:188:VAL:HG21 | 2.10                     | 0.87              |
| 1:B:130:VAL:CG1  | 1:B:213:GLN:CD   | 2.48                     | 0.87              |
| 1:A:281:LYS:O    | 1:A:282:ASP:HB2  | 1.74                     | 0.86              |
| 1:D:6:LYS:O      | 1:D:7:ASP:HB2    | 1.74                     | 0.86              |
| 1:A:141:ASN:CG   | 1:A:153:PHE:HE1  | 1.82                     | 0.86              |
| 1:B:71:GLU:HG3   | 1:C:100:ARG:NH2  | 1.88                     | 0.86              |
| 1:C:310:TYR:O    | 1:C:310:TYR:HD1  | 1.58                     | 0.86              |
| 1:C:318:ILE:HG22 | 1:C:319:ASP:H    | 1.39                     | 0.86              |
| 1:A:4:TYR:CD1    | 1:C:1:ALA:HB1    | 2.10                     | 0.86              |
| 1:A:276:THR:CB   | 1:A:294:TYR:HE1  | 1.88                     | 0.86              |
| 1:C:174:VAL:CG1  | 1:C:175:GLY:H    | 1.84                     | 0.86              |
| 1:D:40:TYR:HE2   | 1:D:42:ARG:HH22  | 1.20                     | 0.86              |
| 1:D:267:PHE:N    | 1:D:267:PHE:HD1  | 1.70                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:132:ARG:HG3  | 1:A:132:ARG:NH1  | 1.87                     | 0.86              |
| 1:B:162:GLU:O    | 1:B:163:ARG:O    | 1.94                     | 0.86              |
| 1:A:20:LEU:HD13  | 1:A:335:GLY:HA3  | 1.55                     | 0.86              |
| 1:B:1:ALA:O      | 1:B:12:ASP:OD1   | 1.93                     | 0.86              |
| 1:B:155:VAL:HG23 | 1:B:156:GLN:N    | 1.91                     | 0.86              |
| 1:A:326:VAL:O    | 1:A:326:VAL:HG12 | 1.73                     | 0.86              |
| 1:C:144:PHE:O    | 1:C:145:PHE:HB2  | 1.76                     | 0.86              |
| 1:C:229:ALA:HB2  | 1:C:259:LEU:HD22 | 1.58                     | 0.86              |
| 1:B:98:TYR:HD2   | 1:B:99:GLY:N     | 1.73                     | 0.86              |
| 1:A:231:TYR:HD2  | 1:A:232:GLY:H    | 1.20                     | 0.86              |
| 1:C:129:PHE:HE2  | 1:C:193:ALA:N    | 1.73                     | 0.86              |
| 1:B:98:TYR:CD2   | 1:B:99:GLY:N     | 2.44                     | 0.86              |
| 1:C:139:TYR:O    | 1:C:154:ALA:CB   | 2.23                     | 0.86              |
| 1:B:112:THR:CG2  | 1:B:230:ASN:OD1  | 2.24                     | 0.85              |
| 1:D:83:LEU:HD21  | 1:D:102:TYR:HE2  | 1.37                     | 0.85              |
| 1:A:172:ASP:O    | 1:A:194:ALA:CA   | 2.23                     | 0.85              |
| 1:C:229:ALA:HB2  | 1:C:259:LEU:CD2  | 2.05                     | 0.85              |
| 1:A:51:ILE:HD12  | 1:A:55:LEU:HD22  | 1.55                     | 0.85              |
| 1:D:21:HIS:CD2   | 1:D:23:PHE:CE1   | 2.63                     | 0.85              |
| 1:D:180:TYR:CD2  | 1:D:181:GLU:N    | 2.44                     | 0.85              |
| 1:A:204:PRO:HG2  | 1:A:247:THR:CG2  | 2.06                     | 0.85              |
| 1:A:307:MET:CE   | 1:B:88:LEU:HD23  | 2.06                     | 0.85              |
| 1:B:274:ALA:HB3  | 1:B:296:GLU:OE1  | 1.76                     | 0.85              |
| 1:D:111:TYR:CE2  | 1:D:188:VAL:HG23 | 2.10                     | 0.85              |
| 1:B:167:ARG:HG3  | 1:B:167:ARG:O    | 1.73                     | 0.85              |
| 1:A:100:ARG:CG   | 1:A:134:GLY:HA2  | 2.06                     | 0.85              |
| 1:B:30:ASN:O     | 1:B:30:ASN:CG    | 2.17                     | 0.85              |
| 1:B:167:ARG:HH11 | 1:B:167:ARG:CG   | 1.89                     | 0.85              |
| 1:A:51:ILE:HD13  | 1:C:303:PHE:HB3  | 1.59                     | 0.85              |
| 1:B:269:LEU:CD2  | 1:B:271:PRO:HD3  | 2.07                     | 0.85              |
| 1:C:338:TYR:CD2  | 1:C:338:TYR:C    | 2.53                     | 0.85              |
| 1:D:141:ASN:OD1  | 1:D:145:PHE:N    | 2.08                     | 0.85              |
| 1:A:241:THR:HG22 | 1:A:242:ASN:N    | 1.89                     | 0.85              |
| 1:B:151:LEU:HD12 | 1:B:151:LEU:O    | 1.75                     | 0.85              |
| 1:C:85:PHE:HD2   | 1:C:101:ASN:HB2  | 1.42                     | 0.84              |
| 1:A:57:GLY:HA2   | 1:A:88:LEU:HD23  | 1.59                     | 0.84              |
| 1:A:303:PHE:HB2  | 1:A:307:MET:HB3  | 1.58                     | 0.84              |
| 1:B:123:ALA:HA   | 1:B:130:VAL:HG23 | 1.58                     | 0.84              |
| 1:C:286:ILE:H    | 1:C:286:ILE:HD12 | 1.13                     | 0.84              |
| 1:B:310:TYR:O    | 1:B:310:TYR:CD1  | 2.30                     | 0.84              |
| 1:C:124:TYR:H    | 1:C:124:TYR:HD2  | 1.24                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:86:ALA:HB3   | 1:C:336:ILE:HG12 | 1.59                     | 0.84              |
| 1:B:296:GLU:HB2  | 1:B:314:ILE:HD13 | 1.57                     | 0.84              |
| 1:C:172:ASP:C    | 1:C:194:ALA:CB   | 2.48                     | 0.84              |
| 1:A:61:TRP:O     | 1:A:61:TRP:CD2   | 2.30                     | 0.84              |
| 1:A:191:TYR:CD2  | 1:A:191:TYR:C    | 2.40                     | 0.84              |
| 1:B:155:VAL:CG2  | 1:B:156:GLN:N    | 2.37                     | 0.84              |
| 1:B:340:PHE:HE1  | 1:C:45:PHE:CD2   | 1.93                     | 0.84              |
| 1:D:279:LYS:HE3  | 1:D:281:LYS:NZ   | 1.93                     | 0.84              |
| 1:D:309:THR:HG22 | 1:D:336:ILE:CB   | 2.07                     | 0.84              |
| 1:A:139:TYR:O    | 1:A:154:ALA:HB1  | 1.78                     | 0.84              |
| 1:B:5:ASN:C      | 1:B:5:ASN:OD1    | 2.18                     | 0.84              |
| 1:C:179:SER:HA   | 1:C:188:VAL:CG1  | 2.04                     | 0.84              |
| 1:D:111:TYR:CE2  | 1:D:219:LYS:HG2  | 2.13                     | 0.84              |
| 1:D:215:ALA:O    | 1:D:216:THR:HG23 | 1.78                     | 0.84              |
| 1:A:307:MET:HE3  | 1:B:88:LEU:CD2   | 1.76                     | 0.84              |
| 1:A:336:ILE:HG13 | 1:A:337:VAL:H    | 1.40                     | 0.84              |
| 1:C:204:PRO:CG   | 1:C:247:THR:HG21 | 2.07                     | 0.84              |
| 1:D:90:TYR:O     | 1:D:93:VAL:HG23  | 1.77                     | 0.84              |
| 1:D:112:THR:CG2  | 1:D:230:ASN:OD1  | 2.25                     | 0.84              |
| 1:D:311:VAL:HG13 | 1:D:334:VAL:HG23 | 0.86                     | 0.84              |
| 1:A:311:VAL:O    | 1:A:311:VAL:HG12 | 1.71                     | 0.83              |
| 1:D:244:PHE:O    | 1:D:246:ASN:N    | 2.10                     | 0.83              |
| 1:C:70:SER:OG    | 1:C:72:GLY:N     | 2.10                     | 0.83              |
| 1:A:22:TYR:CE2   | 1:A:38:MET:CE    | 2.60                     | 0.83              |
| 1:C:310:TYR:O    | 1:C:310:TYR:CD1  | 2.30                     | 0.83              |
| 1:D:299:ALA:O    | 1:D:310:TYR:CB   | 2.26                     | 0.83              |
| 1:A:58:TYR:HA    | 1:C:338:TYR:CD1  | 2.13                     | 0.83              |
| 1:C:204:PRO:CG   | 1:C:247:THR:HG22 | 2.08                     | 0.83              |
| 1:A:303:PHE:HE2  | 1:B:88:LEU:CD1   | 1.90                     | 0.83              |
| 1:D:82:ARG:O     | 1:D:132:ARG:CD   | 2.25                     | 0.83              |
| 1:D:141:ASN:ND2  | 1:D:142:SER:H    | 1.75                     | 0.83              |
| 1:A:174:VAL:HG13 | 1:A:175:GLY:N    | 1.92                     | 0.83              |
| 1:A:191:TYR:HE2  | 1:A:192:GLY:O    | 1.59                     | 0.83              |
| 1:B:111:TYR:CZ   | 1:B:188:VAL:CG2  | 2.61                     | 0.83              |
| 1:B:205:LEU:HD21 | 1:B:247:THR:HG21 | 1.61                     | 0.83              |
| 1:A:289:VAL:HG21 | 1:A:324:LEU:HG   | 1.60                     | 0.83              |
| 1:D:334:VAL:O    | 1:D:334:VAL:HG12 | 1.77                     | 0.83              |
| 1:A:18:VAL:HG13  | 1:A:337:VAL:HG23 | 1.59                     | 0.83              |
| 1:B:216:THR:O    | 1:B:230:ASN:ND2  | 2.10                     | 0.83              |
| 1:C:18:VAL:HG22  | 1:C:337:VAL:CG2  | 2.09                     | 0.83              |
| 1:D:60:GLN:CG    | 1:D:85:PHE:HE2   | 1.91                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:267:PHE:N    | 1:D:267:PHE:CD1  | 2.46                     | 0.83              |
| 1:B:258:LEU:C    | 1:B:259:LEU:HD23 | 2.04                     | 0.82              |
| 1:C:100:ARG:HH11 | 1:C:100:ARG:HG3  | 1.41                     | 0.82              |
| 1:C:197:THR:O    | 1:C:200:GLN:HB2  | 1.79                     | 0.82              |
| 1:A:39:THR:O     | 1:A:39:THR:HG22  | 1.78                     | 0.82              |
| 1:A:1:ALA:CB     | 1:B:4:TYR:CZ     | 2.61                     | 0.82              |
| 1:A:51:ILE:HG13  | 1:A:55:LEU:CD2   | 2.04                     | 0.82              |
| 1:A:51:ILE:O     | 1:A:52:ASN:HB3   | 1.78                     | 0.82              |
| 1:B:4:TYR:HE2    | 1:B:6:LYS:HB2    | 1.43                     | 0.82              |
| 1:C:220:TYR:CE1  | 1:C:222:ALA:HB3  | 2.15                     | 0.82              |
| 1:A:241:THR:O    | 1:A:324:LEU:HB3  | 1.79                     | 0.82              |
| 1:C:141:ASN:O    | 1:C:152:ASN:HB3  | 1.79                     | 0.82              |
| 1:C:144:PHE:HB3  | 1:C:148:VAL:HG23 | 1.62                     | 0.82              |
| 1:A:303:PHE:CE2  | 1:B:88:LEU:HD13  | 2.15                     | 0.82              |
| 1:C:173:GLY:HA2  | 1:C:194:ALA:HB2  | 1.62                     | 0.82              |
| 1:C:291:LEU:O    | 1:C:292:VAL:CG2  | 2.27                     | 0.82              |
| 1:D:55:LEU:HD12  | 1:D:90:TYR:CD1   | 2.14                     | 0.82              |
| 1:D:109:LEU:O    | 1:D:110:GLY:C    | 2.23                     | 0.82              |
| 1:D:208:GLY:HA3  | 1:D:236:ASN:ND2  | 1.95                     | 0.82              |
| 1:A:1:ALA:HB3    | 1:B:4:TYR:HE1    | 1.31                     | 0.82              |
| 1:A:315:ILE:HA   | 1:A:330:ASP:OD1  | 1.80                     | 0.82              |
| 1:B:307:MET:HG3  | 1:B:308:SER:N    | 1.94                     | 0.82              |
| 1:D:172:ASP:O    | 1:D:194:ALA:HB1  | 1.79                     | 0.82              |
| 1:B:20:LEU:HD12  | 1:B:21:HIS:N     | 1.95                     | 0.82              |
| 1:C:173:GLY:CA   | 1:C:194:ALA:HB2  | 2.10                     | 0.82              |
| 1:D:104:VAL:CG1  | 1:D:156:GLN:CB   | 2.58                     | 0.82              |
| 1:D:231:TYR:CD2  | 1:D:231:TYR:C    | 2.56                     | 0.82              |
| 1:A:111:TYR:CD2  | 1:A:219:LYS:HG2  | 2.13                     | 0.82              |
| 1:A:313:TYR:CE1  | 1:A:332:VAL:HG23 | 2.15                     | 0.82              |
| 1:B:183:GLU:O    | 1:B:183:GLU:HG3  | 1.79                     | 0.82              |
| 1:D:245:THR:HG1  | 1:D:247:THR:HG1  | 0.95                     | 0.81              |
| 1:D:294:TYR:CD1  | 1:D:314:ILE:CD1  | 2.62                     | 0.81              |
| 1:A:1:ALA:HB1    | 1:B:4:TYR:OH     | 1.79                     | 0.81              |
| 1:A:114:MET:O    | 1:A:115:LEU:C    | 2.21                     | 0.81              |
| 1:A:172:ASP:H    | 1:A:195:ASP:HB2  | 1.43                     | 0.81              |
| 1:B:192:GLY:O    | 1:B:193:ALA:HB2  | 1.79                     | 0.81              |
| 1:C:153:PHE:HD1  | 1:C:153:PHE:H    | 1.28                     | 0.81              |
| 1:C:257:VAL:O    | 1:C:258:LEU:HD13 | 1.80                     | 0.81              |
| 1:A:229:ALA:HB2  | 1:A:259:LEU:HD22 | 1.60                     | 0.81              |
| 1:B:205:LEU:CD1  | 1:B:247:THR:HG22 | 2.08                     | 0.81              |
| 1:C:234:THR:HB   | 1:C:237:ALA:HB3  | 1.61                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:255:GLN:C    | 1:C:256:ASP:OD1  | 2.22                     | 0.81              |
| 1:A:284:GLU:O    | 1:A:286:ILE:HD13 | 1.79                     | 0.81              |
| 1:B:274:ALA:CB   | 1:B:296:GLU:OE1  | 2.27                     | 0.81              |
| 1:C:326:VAL:O    | 1:C:326:VAL:HG12 | 1.81                     | 0.81              |
| 1:A:40:TYR:H     | 1:A:40:TYR:HD1   | 1.25                     | 0.81              |
| 1:A:275:TYR:C    | 1:A:276:THR:HG1  | 1.89                     | 0.81              |
| 1:D:5:ASN:O      | 1:D:6:LYS:HD3    | 1.81                     | 0.81              |
| 1:A:24:SER:H     | 1:A:35:ASN:ND2   | 1.77                     | 0.81              |
| 1:D:5:ASN:O      | 1:D:6:LYS:CD     | 2.29                     | 0.81              |
| 1:D:111:TYR:OH   | 1:D:188:VAL:HG22 | 1.81                     | 0.81              |
| 1:B:255:GLN:OE1  | 1:B:281:LYS:CE   | 2.29                     | 0.81              |
| 1:C:90:TYR:HD2   | 1:C:93:VAL:HG21  | 1.46                     | 0.80              |
| 1:C:289:VAL:HG11 | 1:C:323:LYS:HB2  | 1.63                     | 0.80              |
| 1:A:58:TYR:HA    | 1:C:338:TYR:HD1  | 1.44                     | 0.80              |
| 1:B:58:TYR:CD2   | 1:B:58:TYR:N     | 2.42                     | 0.80              |
| 1:B:113:ASP:O    | 1:B:114:MET:CG   | 2.29                     | 0.80              |
| 1:C:90:TYR:O     | 1:C:92:ASP:N     | 2.14                     | 0.80              |
| 1:B:267:PHE:H    | 1:B:267:PHE:HD1  | 1.29                     | 0.80              |
| 1:A:274:ALA:HB3  | 1:A:296:GLU:OE1  | 1.80                     | 0.80              |
| 1:A:275:TYR:HD2  | 1:A:276:THR:N    | 1.78                     | 0.80              |
| 1:A:65:PHE:CD1   | 1:B:61:TRP:HZ2   | 2.00                     | 0.80              |
| 1:D:294:TYR:CE1  | 1:D:314:ILE:CD1  | 2.64                     | 0.80              |
| 1:A:141:ASN:HB3  | 1:A:153:PHE:CE1  | 2.16                     | 0.80              |
| 1:B:4:TYR:HD2    | 1:B:4:TYR:C      | 1.89                     | 0.80              |
| 1:B:300:THR:HG21 | 1:B:302:TYR:CE1  | 2.16                     | 0.80              |
| 1:C:182:TYR:HD1  | 1:C:183:GLU:N    | 1.80                     | 0.80              |
| 1:C:289:VAL:HG13 | 1:C:323:LYS:HB2  | 1.61                     | 0.80              |
| 1:A:70:SER:OG    | 1:A:71:GLU:N     | 2.11                     | 0.80              |
| 1:B:222:ALA:O    | 1:B:225:ILE:HG13 | 1.80                     | 0.80              |
| 1:C:18:VAL:CG1   | 1:C:40:TYR:CE1   | 2.64                     | 0.80              |
| 1:B:229:ALA:HB1  | 1:B:258:LEU:O    | 1.81                     | 0.80              |
| 1:A:268:GLY:O    | 1:A:301:TYR:CD2  | 2.34                     | 0.80              |
| 1:C:240:ILE:HD11 | 1:C:250:PHE:C    | 2.06                     | 0.80              |
| 1:A:82:ARG:NH1   | 1:A:82:ARG:HG2   | 1.97                     | 0.79              |
| 1:B:21:HIS:HD2   | 1:B:23:PHE:CZ    | 1.99                     | 0.79              |
| 1:B:66:GLN:HG3   | 1:B:78:GLY:HA3   | 1.63                     | 0.79              |
| 1:C:223:ASN:CB   | 1:C:225:ILE:CD1  | 2.60                     | 0.79              |
| 1:A:129:PHE:CE2  | 1:A:192:GLY:CA   | 2.66                     | 0.79              |
| 1:C:182:TYR:C    | 1:C:182:TYR:CD1  | 2.57                     | 0.79              |
| 1:D:29:GLU:CG    | 1:D:30:ASN:H     | 1.96                     | 0.79              |
| 1:D:118:PHE:HD2  | 1:D:314:ILE:HG12 | 1.43                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:60:GLN:HG2   | 1:D:85:PHE:CE2   | 2.18                     | 0.79              |
| 1:D:180:TYR:C    | 1:D:180:TYR:CD2  | 2.59                     | 0.79              |
| 1:D:338:TYR:O    | 1:D:339:GLN:HB3  | 1.82                     | 0.79              |
| 1:A:85:PHE:CD2   | 1:A:101:ASN:HB2  | 2.17                     | 0.79              |
| 1:A:161:ASN:O    | 1:A:169:SER:HB3  | 1.80                     | 0.79              |
| 1:B:258:LEU:O    | 1:B:259:LEU:CD2  | 2.24                     | 0.79              |
| 1:D:24:SER:H     | 1:D:35:ASN:ND2   | 1.78                     | 0.79              |
| 1:A:114:MET:H    | 1:A:115:LEU:HD23 | 1.45                     | 0.79              |
| 1:D:231:TYR:C    | 1:D:231:TYR:HD2  | 1.91                     | 0.79              |
| 1:A:262:GLN:HG2  | 1:A:272:SER:HB2  | 1.64                     | 0.79              |
| 1:C:274:ALA:CB   | 1:C:296:GLU:OE1  | 2.31                     | 0.79              |
| 1:A:112:THR:CG2  | 1:A:230:ASN:OD1  | 2.29                     | 0.79              |
| 1:A:226:TYR:C    | 1:A:227:LEU:HD23 | 2.07                     | 0.79              |
| 1:B:158:LEU:HD12 | 1:B:159:GLY:N    | 1.98                     | 0.79              |
| 1:B:226:TYR:O    | 1:B:227:LEU:HD23 | 1.82                     | 0.79              |
| 1:B:231:TYR:CD1  | 1:B:232:GLY:N    | 2.50                     | 0.79              |
| 1:B:24:SER:N     | 1:B:35:ASN:ND2   | 2.30                     | 0.79              |
| 1:D:51:ILE:HD12  | 1:D:55:LEU:CG    | 2.12                     | 0.79              |
| 1:A:113:ASP:C    | 1:A:114:MET:HG2  | 2.07                     | 0.78              |
| 1:A:122:THR:CG2  | 1:A:256:ASP:OD2  | 2.30                     | 0.78              |
| 1:A:71:GLU:CG    | 1:B:100:ARG:NH2  | 2.46                     | 0.78              |
| 1:D:267:PHE:HD1  | 1:D:267:PHE:H    | 1.31                     | 0.78              |
| 1:A:170:ASN:O    | 1:A:170:ASN:CG   | 2.25                     | 0.78              |
| 1:B:310:TYR:CD1  | 1:B:310:TYR:C    | 2.59                     | 0.78              |
| 1:D:124:TYR:CE2  | 1:D:238:THR:HG23 | 2.15                     | 0.78              |
| 1:D:318:ILE:HG22 | 1:D:319:ASP:N    | 1.99                     | 0.78              |
| 1:A:86:ALA:HB1   | 1:C:336:ILE:CG1  | 2.13                     | 0.78              |
| 1:A:125:SER:O    | 1:A:126:ASP:CB   | 2.31                     | 0.78              |
| 1:A:303:PHE:CD2  | 1:A:307:MET:HG2  | 2.13                     | 0.78              |
| 1:B:310:TYR:HD1  | 1:B:310:TYR:C    | 1.91                     | 0.78              |
| 1:C:90:TYR:O     | 1:C:91:ALA:C     | 2.24                     | 0.78              |
| 1:B:240:ILE:CG2  | 1:B:291:LEU:CD2  | 2.62                     | 0.78              |
| 1:B:96:PHE:HD2   | 1:B:96:PHE:C     | 1.91                     | 0.78              |
| 1:A:102:TYR:CD1  | 1:A:106:TYR:CD2  | 2.72                     | 0.78              |
| 1:D:100:ARG:HH11 | 1:D:100:ARG:HG3  | 1.46                     | 0.78              |
| 1:D:279:LYS:HB2  | 1:D:279:LYS:HZ2  | 0.96                     | 0.78              |
| 1:B:221:ASP:O    | 1:B:222:ALA:CB   | 2.32                     | 0.78              |
| 1:A:69:ASN:HD21  | 1:A:77:THR:CB    | 1.90                     | 0.77              |
| 1:B:90:TYR:O     | 1:B:92:ASP:N     | 2.17                     | 0.77              |
| 1:B:300:THR:CG2  | 1:B:302:TYR:CE1  | 2.67                     | 0.77              |
| 1:C:318:ILE:HG13 | 1:C:326:VAL:HG11 | 1.66                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:331:THR:HG22 | 1:C:332:VAL:N    | 1.96                     | 0.77              |
| 1:A:191:TYR:CE2  | 1:A:192:GLY:O    | 2.37                     | 0.77              |
| 1:A:267:PHE:CZ   | 1:A:269:LEU:HD12 | 2.18                     | 0.77              |
| 1:B:269:LEU:HG   | 1:B:270:ARG:H    | 1.48                     | 0.77              |
| 1:A:59:GLY:N     | 1:C:338:TYR:CD1  | 2.53                     | 0.77              |
| 1:A:141:ASN:HB3  | 1:A:153:PHE:CD1  | 2.20                     | 0.77              |
| 1:A:285:GLY:O    | 1:A:286:ILE:CD1  | 2.17                     | 0.77              |
| 1:A:337:VAL:O    | 1:A:337:VAL:HG12 | 1.00                     | 0.77              |
| 1:B:4:TYR:C      | 1:B:4:TYR:CD2    | 2.57                     | 0.77              |
| 1:D:313:TYR:CD1  | 1:D:332:VAL:HG22 | 2.19                     | 0.77              |
| 1:B:130:VAL:HG11 | 1:B:213:GLN:NE2  | 1.99                     | 0.77              |
| 1:C:179:SER:CB   | 1:C:188:VAL:CG1  | 2.63                     | 0.77              |
| 1:A:51:ILE:CG1   | 1:A:55:LEU:CD2   | 2.46                     | 0.77              |
| 1:C:70:SER:HG    | 1:C:72:GLY:H     | 1.32                     | 0.77              |
| 1:D:51:ILE:CB    | 1:D:55:LEU:HD23  | 2.14                     | 0.77              |
| 1:D:265:PHE:HB2  | 1:D:269:LEU:O    | 1.85                     | 0.77              |
| 1:A:121:ASP:OD1  | 1:A:294:TYR:OH   | 2.03                     | 0.77              |
| 1:B:263:TYR:O    | 1:B:270:ARG:HA   | 1.84                     | 0.77              |
| 1:C:125:SER:O    | 1:C:126:ASP:C    | 2.22                     | 0.77              |
| 1:A:174:VAL:CG1  | 1:A:175:GLY:N    | 2.46                     | 0.77              |
| 1:B:238:THR:O    | 1:B:238:THR:HG22 | 1.84                     | 0.77              |
| 1:D:121:ASP:O    | 1:D:123:ALA:N    | 2.18                     | 0.77              |
| 1:A:20:LEU:CD1   | 1:A:335:GLY:HA3  | 2.13                     | 0.76              |
| 1:A:307:MET:HE1  | 1:B:88:LEU:CD2   | 2.12                     | 0.76              |
| 1:C:284:GLU:H    | 1:C:284:GLU:CD   | 1.91                     | 0.76              |
| 1:D:104:VAL:HG11 | 1:D:156:GLN:HB3  | 1.66                     | 0.76              |
| 1:C:263:TYR:O    | 1:C:270:ARG:HA   | 1.86                     | 0.76              |
| 1:A:326:VAL:O    | 1:A:326:VAL:CG1  | 2.33                     | 0.76              |
| 1:C:229:ALA:CB   | 1:C:259:LEU:HD23 | 2.14                     | 0.76              |
| 1:D:226:TYR:HE2  | 1:D:228:ALA:HB2  | 1.51                     | 0.76              |
| 1:B:16:LYS:HB3   | 1:B:339:GLN:CB   | 2.16                     | 0.76              |
| 1:B:229:ALA:HB2  | 1:B:259:LEU:CD2  | 2.01                     | 0.76              |
| 1:B:242:ASN:HB3  | 1:B:247:THR:HB   | 1.66                     | 0.76              |
| 1:D:24:SER:N     | 1:D:35:ASN:HD22  | 1.79                     | 0.76              |
| 1:D:128:PHE:O    | 1:D:133:VAL:HG21 | 1.86                     | 0.76              |
| 1:A:58:TYR:CA    | 1:C:338:TYR:HD1  | 1.97                     | 0.76              |
| 1:A:294:TYR:CE2  | 1:A:314:ILE:HD11 | 2.20                     | 0.76              |
| 1:B:240:ILE:CG2  | 1:B:291:LEU:HD22 | 2.15                     | 0.76              |
| 1:A:294:TYR:CE2  | 1:A:314:ILE:CD1  | 2.69                     | 0.76              |
| 1:B:28:GLY:O     | 1:B:29:GLU:C     | 2.23                     | 0.76              |
| 1:C:179:SER:CB   | 1:C:188:VAL:HG12 | 2.14                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:273:ILE:HD11 | 1:D:297:VAL:CG2  | 2.16                     | 0.76              |
| 1:A:88:LEU:HD11  | 1:C:303:PHE:HE2  | 1.50                     | 0.76              |
| 1:B:307:MET:HG3  | 1:B:308:SER:H    | 1.50                     | 0.76              |
| 1:D:271:PRO:HA   | 1:D:299:ALA:CB   | 2.15                     | 0.76              |
| 1:A:242:ASN:O    | 1:A:244:PHE:N    | 2.18                     | 0.75              |
| 1:D:144:PHE:HB2  | 1:D:151:LEU:CD2  | 2.16                     | 0.75              |
| 1:D:315:ILE:HD12 | 1:D:315:ILE:H    | 1.48                     | 0.75              |
| 1:A:307:MET:CE   | 1:B:87:GLY:O     | 2.33                     | 0.75              |
| 1:B:129:PHE:HE2  | 1:B:193:ALA:H    | 1.32                     | 0.75              |
| 1:B:221:ASP:O    | 1:B:222:ALA:HB2  | 1.86                     | 0.75              |
| 1:B:339:GLN:HG3  | 1:B:339:GLN:O    | 1.85                     | 0.75              |
| 1:C:85:PHE:CE2   | 1:C:101:ASN:ND2  | 2.54                     | 0.75              |
| 1:C:314:ILE:O    | 1:C:314:ILE:HG22 | 1.85                     | 0.75              |
| 1:C:338:TYR:HD2  | 1:C:338:TYR:C    | 1.91                     | 0.75              |
| 1:D:236:ASN:OD1  | 1:D:252:ASN:HA   | 1.86                     | 0.75              |
| 1:B:185:PHE:CE2  | 1:B:220:TYR:CE1  | 2.75                     | 0.75              |
| 1:B:236:ASN:OD1  | 1:B:252:ASN:HA   | 1.85                     | 0.75              |
| 1:C:45:PHE:CD1   | 1:C:45:PHE:C     | 2.52                     | 0.75              |
| 1:C:241:THR:CG2  | 1:C:242:ASN:H    | 1.99                     | 0.75              |
| 1:A:167:ARG:CG   | 1:A:167:ARG:NH1  | 2.41                     | 0.75              |
| 1:A:167:ARG:HH11 | 1:A:167:ARG:HG2  | 1.49                     | 0.75              |
| 1:A:22:TYR:CE1   | 1:A:333:ALA:HB2  | 2.21                     | 0.75              |
| 1:C:274:ALA:HB3  | 1:C:296:GLU:OE1  | 1.85                     | 0.75              |
| 1:A:318:ILE:N    | 1:A:318:ILE:CD1  | 2.42                     | 0.75              |
| 1:A:104:VAL:HG12 | 1:A:156:GLN:OE1  | 1.84                     | 0.75              |
| 1:A:167:ARG:HG2  | 1:A:167:ARG:O    | 1.87                     | 0.75              |
| 1:A:86:ALA:CB    | 1:C:336:ILE:CG1  | 2.64                     | 0.74              |
| 1:A:129:PHE:HD2  | 1:A:192:GLY:HA3  | 1.49                     | 0.74              |
| 1:B:65:PHE:CD2   | 1:C:61:TRP:CZ2   | 2.74                     | 0.74              |
| 1:B:72:GLY:O     | 1:B:74:ASP:N     | 2.20                     | 0.74              |
| 1:B:269:LEU:CG   | 1:B:271:PRO:HD3  | 2.16                     | 0.74              |
| 1:D:48:GLU:CD    | 1:D:56:THR:CG2   | 2.60                     | 0.74              |
| 1:D:303:PHE:HB2  | 1:D:307:MET:HB3  | 1.69                     | 0.74              |
| 1:A:61:TRP:CZ2   | 1:A:63:TYR:HB2   | 2.21                     | 0.74              |
| 1:B:296:GLU:HB2  | 1:B:314:ILE:CD1  | 2.17                     | 0.74              |
| 1:C:63:TYR:CD1   | 1:C:80:LYS:C     | 2.65                     | 0.74              |
| 1:C:222:ALA:O    | 1:C:225:ILE:HD12 | 1.87                     | 0.74              |
| 1:A:258:LEU:HD11 | 1:A:276:THR:CG2  | 2.10                     | 0.74              |
| 1:B:23:PHE:CA    | 1:B:35:ASN:ND2   | 2.45                     | 0.74              |
| 1:B:124:TYR:O    | 1:B:131:GLY:HA3  | 1.87                     | 0.74              |
| 1:D:29:GLU:HG3   | 1:D:30:ASN:CA    | 2.18                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:51:ILE:HD12  | 1:C:55:LEU:CD2   | 2.17                     | 0.74              |
| 1:D:205:LEU:HG   | 1:D:247:THR:HG22 | 1.70                     | 0.74              |
| 1:B:141:ASN:CG   | 1:B:153:PHE:HE1  | 1.94                     | 0.74              |
| 1:B:167:ARG:HG3  | 1:B:167:ARG:NH1  | 1.97                     | 0.74              |
| 1:B:338:TYR:O    | 1:B:339:GLN:CB   | 2.33                     | 0.74              |
| 1:C:203:GLN:HB3  | 1:C:248:SER:O    | 1.88                     | 0.74              |
| 1:C:223:ASN:HB2  | 1:C:225:ILE:CD1  | 2.18                     | 0.74              |
| 1:A:61:TRP:HZ2   | 1:C:65:PHE:CE1   | 1.99                     | 0.74              |
| 1:C:174:VAL:HG13 | 1:C:175:GLY:H    | 1.53                     | 0.74              |
| 1:D:174:VAL:CG1  | 1:D:175:GLY:N    | 2.50                     | 0.74              |
| 1:A:113:ASP:C    | 1:A:114:MET:CG   | 2.60                     | 0.74              |
| 1:B:98:TYR:C     | 1:B:98:TYR:CD2   | 2.54                     | 0.74              |
| 1:A:263:TYR:O    | 1:A:271:PRO:HD2  | 1.87                     | 0.74              |
| 1:C:11:VAL:HG12  | 1:C:12:ASP:N     | 2.01                     | 0.74              |
| 1:C:32:TYR:CE2   | 1:C:314:ILE:HG13 | 2.23                     | 0.74              |
| 1:B:141:ASN:HB3  | 1:B:153:PHE:CE1  | 2.23                     | 0.74              |
| 1:C:139:TYR:CE1  | 1:C:140:ARG:O    | 2.41                     | 0.74              |
| 1:C:286:ILE:CG2  | 1:C:323:LYS:HB3  | 2.17                     | 0.74              |
| 1:D:28:GLY:O     | 1:D:31:SER:OG    | 2.06                     | 0.74              |
| 1:D:124:TYR:CE2  | 1:D:238:THR:CG2  | 2.71                     | 0.74              |
| 1:A:336:ILE:CG1  | 1:A:337:VAL:N    | 2.51                     | 0.74              |
| 1:A:4:TYR:CD1    | 1:C:1:ALA:HB3    | 2.23                     | 0.73              |
| 1:A:153:PHE:HD1  | 1:A:153:PHE:N    | 1.84                     | 0.73              |
| 1:A:319:ASP:O    | 1:A:321:ASP:N    | 2.21                     | 0.73              |
| 1:B:111:TYR:CZ   | 1:B:219:LYS:HE2  | 2.23                     | 0.73              |
| 1:B:336:ILE:CD1  | 1:C:87:GLY:HA2   | 2.17                     | 0.73              |
| 1:A:86:ALA:CB    | 1:C:336:ILE:HG12 | 2.18                     | 0.73              |
| 1:A:336:ILE:HD11 | 1:B:87:GLY:N     | 2.03                     | 0.73              |
| 1:C:32:TYR:CD2   | 1:C:314:ILE:HG13 | 2.23                     | 0.73              |
| 1:C:48:GLU:HG2   | 1:C:48:GLU:O     | 1.81                     | 0.73              |
| 1:C:90:TYR:CD2   | 1:C:93:VAL:HG21  | 2.22                     | 0.73              |
| 1:C:104:VAL:N    | 1:C:156:GLN:OE1  | 2.20                     | 0.73              |
| 1:D:34:GLY:O     | 1:D:35:ASN:HB2   | 1.87                     | 0.73              |
| 1:D:303:PHE:HD2  | 1:D:307:MET:HG2  | 1.53                     | 0.73              |
| 1:A:24:SER:N     | 1:A:35:ASN:HD22  | 1.83                     | 0.73              |
| 1:A:65:PHE:CE1   | 1:B:61:TRP:HZ2   | 2.07                     | 0.73              |
| 1:C:229:ALA:HB1  | 1:C:259:LEU:HD23 | 1.66                     | 0.73              |
| 1:D:51:ILE:CG1   | 1:D:55:LEU:HD23  | 2.17                     | 0.73              |
| 1:A:4:TYR:HE1    | 1:C:1:ALA:HB1    | 1.45                     | 0.73              |
| 1:B:1:ALA:HB2    | 1:C:4:TYR:CE2    | 2.23                     | 0.73              |
| 1:C:21:HIS:CD2   | 1:C:23:PHE:CE2   | 2.77                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:319:ASP:O    | 1:A:320:SER:C    | 2.31                     | 0.73              |
| 1:C:141:ASN:CG   | 1:C:153:PHE:HE1  | 1.97                     | 0.73              |
| 1:D:205:LEU:HD23 | 1:D:284:GLU:HG3  | 1.69                     | 0.73              |
| 1:D:258:LEU:CD2  | 1:D:258:LEU:N    | 2.51                     | 0.73              |
| 1:A:232:GLY:O    | 1:A:256:ASP:HB2  | 1.87                     | 0.73              |
| 1:B:126:ASP:OD2  | 1:B:168:ARG:NH1  | 2.21                     | 0.73              |
| 1:C:223:ASN:CB   | 1:C:225:ILE:HD11 | 2.19                     | 0.73              |
| 1:D:182:TYR:CD2  | 1:D:182:TYR:O    | 2.41                     | 0.73              |
| 1:A:161:ASN:O    | 1:A:169:SER:CB   | 2.37                     | 0.73              |
| 1:C:132:ARG:HG3  | 1:C:132:ARG:NH1  | 2.02                     | 0.73              |
| 1:D:300:THR:HA   | 1:D:310:TYR:HB3  | 1.70                     | 0.73              |
| 1:B:16:LYS:HB3   | 1:B:339:GLN:HB3  | 1.69                     | 0.73              |
| 1:B:51:ILE:HB    | 1:B:55:LEU:O     | 1.88                     | 0.73              |
| 1:C:82:ARG:O     | 1:C:100:ARG:CD   | 2.33                     | 0.73              |
| 1:B:160:LYS:NZ   | 1:B:162:GLU:OE2  | 2.17                     | 0.73              |
| 1:C:229:ALA:HB1  | 1:C:259:LEU:HD21 | 1.70                     | 0.73              |
| 1:D:52:ASN:OD1   | 1:D:53:SER:N     | 2.22                     | 0.73              |
| 1:A:292:VAL:O    | 1:A:292:VAL:HG12 | 1.88                     | 0.73              |
| 1:B:158:LEU:HD12 | 1:B:158:LEU:C    | 2.13                     | 0.73              |
| 1:A:130:VAL:HG12 | 1:A:213:GLN:CD   | 2.13                     | 0.72              |
| 1:B:174:VAL:HG13 | 1:B:175:GLY:N    | 2.02                     | 0.72              |
| 1:C:105:VAL:HG23 | 1:C:129:PHE:HB3  | 1.69                     | 0.72              |
| 1:D:66:GLN:HG3   | 1:D:78:GLY:CA    | 2.18                     | 0.72              |
| 1:B:240:ILE:HG22 | 1:B:291:LEU:HD22 | 1.71                     | 0.72              |
| 1:C:23:PHE:HA    | 1:C:35:ASN:ND2   | 2.04                     | 0.72              |
| 1:C:223:ASN:O    | 1:C:224:ASN:CB   | 2.36                     | 0.72              |
| 1:D:29:GLU:HG2   | 1:D:30:ASN:H     | 1.54                     | 0.72              |
| 1:D:60:GLN:HB3   | 1:D:85:PHE:HE2   | 1.54                     | 0.72              |
| 1:C:21:HIS:HD2   | 1:C:23:PHE:CE2   | 2.07                     | 0.72              |
| 1:A:182:TYR:CG   | 1:A:182:TYR:O    | 2.36                     | 0.72              |
| 1:B:15:GLY:N     | 1:B:340:PHE:HE2  | 1.81                     | 0.72              |
| 1:C:285:GLY:C    | 1:C:286:ILE:HD12 | 2.14                     | 0.72              |
| 1:A:58:TYR:C     | 1:C:338:TYR:HD1  | 1.97                     | 0.72              |
| 1:C:165:THR:O    | 1:C:166:ALA:C    | 2.30                     | 0.72              |
| 1:A:167:ARG:HG3  | 1:A:167:ARG:NH1  | 2.04                     | 0.72              |
| 1:C:83:LEU:HD11  | 1:C:102:TYR:HE2  | 1.55                     | 0.72              |
| 1:A:61:TRP:CH2   | 1:C:65:PHE:CE1   | 2.76                     | 0.72              |
| 1:B:139:TYR:C    | 1:B:139:TYR:CD2  | 2.67                     | 0.72              |
| 1:C:58:TYR:HE2   | 1:C:89:LYS:HE3   | 1.55                     | 0.72              |
| 1:D:167:ARG:HG3  | 1:D:167:ARG:HH11 | 1.55                     | 0.72              |
| 1:D:229:ALA:HB2  | 1:D:259:LEU:HD23 | 1.50                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:132:ARG:NH1  | 1:A:132:ARG:CG   | 2.50                     | 0.72              |
| 1:D:172:ASP:O    | 1:D:194:ALA:CB   | 2.37                     | 0.72              |
| 1:D:263:TYR:O    | 1:D:270:ARG:HA   | 1.88                     | 0.72              |
| 1:A:16:LYS:HB3   | 1:A:339:GLN:HB3  | 1.70                     | 0.72              |
| 1:D:29:GLU:HG2   | 1:D:30:ASN:N     | 1.99                     | 0.72              |
| 1:D:240:ILE:HG21 | 1:D:251:ALA:HB2  | 1.70                     | 0.72              |
| 1:A:82:ARG:HG2   | 1:A:82:ARG:HH11  | 1.54                     | 0.71              |
| 1:A:118:PHE:O    | 1:A:119:GLY:C    | 2.33                     | 0.71              |
| 1:A:129:PHE:HE2  | 1:A:192:GLY:C    | 1.97                     | 0.71              |
| 1:B:69:ASN:ND2   | 1:B:77:THR:HB    | 2.03                     | 0.71              |
| 1:B:114:MET:HE1  | 1:B:226:TYR:CE1  | 2.24                     | 0.71              |
| 1:B:229:ALA:HB1  | 1:B:259:LEU:HD21 | 1.72                     | 0.71              |
| 1:D:255:GLN:O    | 1:D:278:SER:HA   | 1.89                     | 0.71              |
| 1:B:315:ILE:HG22 | 1:B:315:ILE:O    | 1.89                     | 0.71              |
| 1:C:230:ASN:HB2  | 1:C:258:LEU:HB2  | 1.71                     | 0.71              |
| 1:A:279:LYS:CB   | 1:A:279:LYS:NZ   | 2.53                     | 0.71              |
| 1:A:309:THR:HG22 | 1:A:336:ILE:CA   | 2.20                     | 0.71              |
| 1:B:141:ASN:ND2  | 1:B:145:PHE:CE1  | 2.58                     | 0.71              |
| 1:C:308:SER:O    | 1:C:309:THR:HG23 | 1.90                     | 0.71              |
| 1:B:196:ARG:HA   | 1:B:200:GLN:OE1  | 1.90                     | 0.71              |
| 1:A:104:VAL:HG12 | 1:A:156:GLN:CD   | 2.15                     | 0.71              |
| 1:B:226:TYR:HE2  | 1:B:228:ALA:HB2  | 1.53                     | 0.71              |
| 1:D:48:GLU:HG3   | 1:D:56:THR:CG2   | 2.20                     | 0.71              |
| 1:D:303:PHE:O    | 1:D:304:ASN:CB   | 2.38                     | 0.71              |
| 1:A:86:ALA:HB1   | 1:C:336:ILE:HG13 | 1.70                     | 0.71              |
| 1:A:139:TYR:O    | 1:A:154:ALA:CB   | 2.38                     | 0.71              |
| 1:B:141:ASN:OD1  | 1:B:153:PHE:HE1  | 1.73                     | 0.71              |
| 1:D:239:PRO:HA   | 1:D:250:PHE:HD2  | 1.54                     | 0.71              |
| 1:A:18:VAL:HG22  | 1:A:337:VAL:HG22 | 1.72                     | 0.71              |
| 1:A:104:VAL:HG11 | 1:A:156:GLN:CB   | 2.21                     | 0.71              |
| 1:B:9:ASN:CG     | 1:B:9:ASN:O      | 2.33                     | 0.71              |
| 1:D:51:ILE:HD13  | 1:D:55:LEU:HD21  | 1.70                     | 0.71              |
| 1:D:60:GLN:CB    | 1:D:85:PHE:HE2   | 2.04                     | 0.71              |
| 1:D:144:PHE:CB   | 1:D:151:LEU:HD23 | 2.21                     | 0.71              |
| 1:D:337:VAL:O    | 1:D:337:VAL:CG1  | 2.38                     | 0.71              |
| 1:C:25:LYS:HB2   | 1:C:25:LYS:NZ    | 2.05                     | 0.71              |
| 1:C:308:SER:O    | 1:C:309:THR:CG2  | 2.39                     | 0.71              |
| 1:C:310:TYR:CD1  | 1:C:310:TYR:C    | 2.69                     | 0.71              |
| 1:D:257:VAL:C    | 1:D:258:LEU:HD22 | 2.16                     | 0.71              |
| 1:C:141:ASN:CB   | 1:C:153:PHE:CE1  | 2.74                     | 0.71              |
| 1:D:21:HIS:HD2   | 1:D:23:PHE:CE1   | 2.08                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:114:MET:CE   | 1:A:226:TYR:CD1  | 2.45                     | 0.70              |
| 1:B:336:ILE:HD11 | 1:C:87:GLY:N     | 2.06                     | 0.70              |
| 1:C:283:VAL:O    | 1:C:286:ILE:HD13 | 1.90                     | 0.70              |
| 1:D:310:TYR:O    | 1:D:310:TYR:CD1  | 2.44                     | 0.70              |
| 1:B:129:PHE:CE2  | 1:B:193:ALA:N    | 2.56                     | 0.70              |
| 1:B:340:PHE:CE1  | 1:C:45:PHE:CD2   | 2.78                     | 0.70              |
| 1:D:273:ILE:CD1  | 1:D:297:VAL:HG23 | 2.20                     | 0.70              |
| 1:D:310:TYR:CD1  | 1:D:310:TYR:C    | 2.69                     | 0.70              |
| 1:B:315:ILE:HA   | 1:B:330:ASP:OD2  | 1.91                     | 0.70              |
| 1:C:303:PHE:HD2  | 1:C:307:MET:HG2  | 1.54                     | 0.70              |
| 1:D:18:VAL:O     | 1:D:18:VAL:HG12  | 1.89                     | 0.70              |
| 1:D:158:LEU:HB3  | 1:D:173:GLY:HA3  | 1.73                     | 0.70              |
| 1:A:18:VAL:HB    | 1:A:40:TYR:HE1   | 1.50                     | 0.70              |
| 1:A:51:ILE:HD13  | 1:C:303:PHE:CB   | 2.22                     | 0.70              |
| 1:D:174:VAL:HG12 | 1:D:175:GLY:N    | 2.05                     | 0.70              |
| 1:A:11:VAL:CG2   | 1:C:340:PHE:HB2  | 2.22                     | 0.70              |
| 1:B:18:VAL:CG1   | 1:B:40:TYR:CE1   | 2.75                     | 0.70              |
| 1:B:70:SER:O     | 1:B:75:ALA:HB2   | 1.91                     | 0.70              |
| 1:B:114:MET:HE2  | 1:B:226:TYR:CZ   | 2.26                     | 0.70              |
| 1:B:277:LYS:CE   | 1:B:293:ASN:ND2  | 2.55                     | 0.70              |
| 1:C:262:GLN:OE1  | 1:C:270:ARG:NH1  | 2.25                     | 0.70              |
| 1:A:141:ASN:CG   | 1:A:153:PHE:CE1  | 2.65                     | 0.70              |
| 1:A:309:THR:CG2  | 1:A:336:ILE:CB   | 2.58                     | 0.70              |
| 1:B:58:TYR:HE2   | 1:B:87:GLY:C     | 2.00                     | 0.70              |
| 1:B:129:PHE:CD2  | 1:B:192:GLY:HA3  | 2.26                     | 0.70              |
| 1:B:285:GLY:C    | 1:B:286:ILE:CD1  | 2.60                     | 0.70              |
| 1:C:100:ARG:HG2  | 1:C:133:VAL:O    | 1.92                     | 0.70              |
| 1:D:239:PRO:HA   | 1:D:250:PHE:CD2  | 2.26                     | 0.70              |
| 1:A:51:ILE:HG23  | 1:C:304:ASN:HD21 | 1.57                     | 0.70              |
| 1:A:303:PHE:CE2  | 1:B:88:LEU:CD1   | 2.71                     | 0.70              |
| 1:B:123:ALA:HA   | 1:B:130:VAL:CG2  | 2.21                     | 0.70              |
| 1:C:100:ARG:HG3  | 1:C:100:ARG:NH1  | 2.06                     | 0.70              |
| 1:D:25:LYS:HE2   | 1:D:329:ASP:OD1  | 1.91                     | 0.70              |
| 1:D:24:SER:OG    | 1:D:331:THR:OG1  | 2.09                     | 0.70              |
| 1:D:303:PHE:O    | 1:D:304:ASN:CG   | 2.35                     | 0.70              |
| 1:A:336:ILE:CD1  | 1:B:87:GLY:HA2   | 2.22                     | 0.70              |
| 1:B:71:GLU:HG3   | 1:C:100:ARG:HH21 | 1.54                     | 0.70              |
| 1:B:224:ASN:O    | 1:B:263:TYR:CD1  | 2.44                     | 0.70              |
| 1:C:214:TRP:CH2  | 1:C:231:TYR:HE2  | 2.10                     | 0.70              |
| 1:C:58:TYR:CE2   | 1:C:89:LYS:HE3   | 2.26                     | 0.69              |
| 1:D:130:VAL:HG13 | 1:D:213:GLN:CD   | 2.17                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:21:HIS:CD2   | 1:A:23:PHE:CE2   | 2.79                     | 0.69              |
| 1:C:115:LEU:HD12 | 1:C:119:GLY:CA   | 2.21                     | 0.69              |
| 1:C:303:PHE:HB2  | 1:C:307:MET:HB3  | 1.73                     | 0.69              |
| 1:D:104:VAL:CG1  | 1:D:156:GLN:HB3  | 2.19                     | 0.69              |
| 1:D:294:TYR:CE1  | 1:D:314:ILE:HD12 | 2.27                     | 0.69              |
| 1:D:311:VAL:HG11 | 1:D:334:VAL:HG23 | 1.65                     | 0.69              |
| 1:A:274:ALA:O    | 1:A:296:GLU:N    | 2.23                     | 0.69              |
| 1:A:320:SER:O    | 1:A:322:ASN:N    | 2.26                     | 0.69              |
| 1:B:240:ILE:HG21 | 1:B:291:LEU:HD21 | 1.75                     | 0.69              |
| 1:A:156:GLN:N    | 1:A:175:GLY:O    | 2.23                     | 0.69              |
| 1:B:191:TYR:CD1  | 1:B:192:GLY:N    | 2.60                     | 0.69              |
| 1:C:167:ARG:CG   | 1:C:167:ARG:HH11 | 2.01                     | 0.69              |
| 1:D:56:THR:HB    | 1:D:89:LYS:HB2   | 1.74                     | 0.69              |
| 1:C:182:TYR:HD1  | 1:C:182:TYR:C    | 1.99                     | 0.69              |
| 1:D:105:VAL:O    | 1:D:105:VAL:HG12 | 1.90                     | 0.69              |
| 1:B:18:VAL:CG1   | 1:B:40:TYR:HE1   | 2.05                     | 0.69              |
| 1:C:240:ILE:HD12 | 1:C:251:ALA:HB2  | 1.74                     | 0.69              |
| 1:C:307:MET:O    | 1:C:308:SER:CB   | 2.39                     | 0.69              |
| 1:A:316:ASN:N    | 1:A:330:ASP:OD1  | 2.25                     | 0.69              |
| 1:B:91:ALA:C     | 1:B:92:ASP:OD1   | 2.36                     | 0.69              |
| 1:C:170:ASN:O    | 1:C:170:ASN:ND2  | 2.26                     | 0.69              |
| 1:D:86:ALA:O     | 1:D:97:ASP:HB2   | 1.92                     | 0.69              |
| 1:A:267:PHE:N    | 1:A:267:PHE:CD1  | 2.19                     | 0.69              |
| 1:A:313:TYR:CB   | 1:A:332:VAL:HG22 | 2.23                     | 0.69              |
| 1:B:318:ILE:HG22 | 1:B:319:ASP:N    | 2.07                     | 0.69              |
| 1:C:27:ASN:OD1   | 1:C:27:ASN:C     | 2.35                     | 0.69              |
| 1:C:96:PHE:HD1   | 1:C:138:THR:O    | 1.75                     | 0.69              |
| 1:C:124:TYR:N    | 1:C:124:TYR:CD2  | 2.54                     | 0.69              |
| 1:D:27:ASN:O     | 1:D:29:GLU:N     | 2.25                     | 0.69              |
| 1:D:307:MET:O    | 1:D:308:SER:HB3  | 1.90                     | 0.69              |
| 1:B:274:ALA:HB3  | 1:B:296:GLU:HB3  | 1.74                     | 0.69              |
| 1:C:240:ILE:CD1  | 1:C:251:ALA:HB2  | 2.23                     | 0.69              |
| 1:B:32:TYR:C     | 1:B:32:TYR:CD2   | 2.71                     | 0.69              |
| 1:C:211:ALA:C    | 1:C:212:GLU:CG   | 2.66                     | 0.69              |
| 1:D:27:ASN:C     | 1:D:29:GLU:H     | 2.01                     | 0.69              |
| 1:A:123:ALA:HA   | 1:A:130:VAL:CG2  | 2.23                     | 0.68              |
| 1:A:223:ASN:O    | 1:A:224:ASN:HB2  | 1.92                     | 0.68              |
| 1:A:303:PHE:HE2  | 1:B:88:LEU:HD11  | 1.56                     | 0.68              |
| 1:B:165:THR:HG22 | 1:B:166:ALA:N    | 2.08                     | 0.68              |
| 1:B:295:PHE:N    | 1:B:295:PHE:CD1  | 2.59                     | 0.68              |
| 1:C:308:SER:C    | 1:C:309:THR:HG23 | 2.18                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:100:ARG:CG   | 1:D:100:ARG:NH1  | 2.51                     | 0.68              |
| 1:A:102:TYR:C    | 1:A:103:GLY:O    | 2.37                     | 0.68              |
| 1:B:18:VAL:HG22  | 1:B:337:VAL:HG13 | 1.76                     | 0.68              |
| 1:B:296:GLU:CB   | 1:B:314:ILE:HD13 | 2.23                     | 0.68              |
| 1:C:145:PHE:C    | 1:C:147:LEU:H    | 2.01                     | 0.68              |
| 1:D:104:VAL:HG11 | 1:D:156:GLN:CB   | 2.21                     | 0.68              |
| 1:D:258:LEU:O    | 1:D:259:LEU:CD2  | 2.40                     | 0.68              |
| 1:C:130:VAL:HG13 | 1:C:213:GLN:NE2  | 2.09                     | 0.68              |
| 1:D:308:SER:O    | 1:D:309:THR:HG23 | 1.93                     | 0.68              |
| 1:A:163:ARG:N    | 1:A:169:SER:OG   | 2.21                     | 0.68              |
| 1:C:196:ARG:NH2  | 1:C:250:PHE:HB2  | 2.09                     | 0.68              |
| 1:A:26:GLY:C     | 1:A:28:GLY:H     | 2.01                     | 0.68              |
| 1:A:309:THR:HG22 | 1:A:336:ILE:HA   | 1.75                     | 0.68              |
| 1:D:203:GLN:HB3  | 1:D:204:PRO:CD   | 2.19                     | 0.68              |
| 1:D:231:TYR:HD2  | 1:D:232:GLY:N    | 1.87                     | 0.68              |
| 1:A:20:LEU:HD22  | 1:A:117:GLU:OE1  | 1.87                     | 0.68              |
| 1:A:39:THR:O     | 1:A:67:GLY:N     | 2.27                     | 0.68              |
| 1:A:66:GLN:HG3   | 1:A:78:GLY:O     | 1.94                     | 0.68              |
| 1:B:229:ALA:CB   | 1:B:259:LEU:HD23 | 2.04                     | 0.68              |
| 1:B:309:THR:HG22 | 1:B:336:ILE:HB   | 1.76                     | 0.68              |
| 1:C:182:TYR:CD1  | 1:C:183:GLU:N    | 2.62                     | 0.68              |
| 1:C:198:ASN:C    | 1:C:200:GLN:H    | 2.01                     | 0.68              |
| 1:C:206:GLY:CA   | 1:C:250:PHE:O    | 2.42                     | 0.68              |
| 1:D:74:ASP:O     | 1:D:75:ALA:C     | 2.35                     | 0.68              |
| 1:A:55:LEU:HG    | 1:A:56:THR:N     | 2.08                     | 0.68              |
| 1:B:220:TYR:N    | 1:B:227:LEU:O    | 2.20                     | 0.68              |
| 1:D:238:THR:OG1  | 1:D:254:THR:HG21 | 1.94                     | 0.68              |
| 1:D:258:LEU:N    | 1:D:258:LEU:HD23 | 2.09                     | 0.68              |
| 1:D:279:LYS:CB   | 1:D:279:LYS:HZ2  | 1.86                     | 0.68              |
| 1:B:243:LYS:H    | 1:B:243:LYS:HD2  | 1.57                     | 0.68              |
| 1:C:273:ILE:HG22 | 1:C:273:ILE:O    | 1.94                     | 0.68              |
| 1:D:60:GLN:CB    | 1:D:85:PHE:CE2   | 2.76                     | 0.68              |
| 1:A:114:MET:N    | 1:A:115:LEU:HD23 | 2.09                     | 0.68              |
| 1:A:137:ALA:O    | 1:A:156:GLN:HA   | 1.94                     | 0.68              |
| 1:A:152:ASN:HD22 | 1:A:152:ASN:N    | 1.92                     | 0.68              |
| 1:A:313:TYR:CD1  | 1:A:332:VAL:HG21 | 2.17                     | 0.68              |
| 1:B:72:GLY:O     | 1:B:73:ALA:C     | 2.36                     | 0.68              |
| 1:C:25:LYS:HB2   | 1:C:25:LYS:HZ2   | 1.59                     | 0.68              |
| 1:B:214:TRP:HE1  | 1:B:233:GLU:HB2  | 1.59                     | 0.67              |
| 1:B:337:VAL:HG12 | 1:B:338:TYR:O    | 1.94                     | 0.67              |
| 1:D:215:ALA:O    | 1:D:216:THR:HG22 | 1.94                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:313:TYR:CE1  | 1:A:332:VAL:CG2  | 2.68                     | 0.67              |
| 1:B:14:TYR:C     | 1:B:340:PHE:CE2  | 2.65                     | 0.67              |
| 1:B:90:TYR:HB3   | 1:B:93:VAL:CG2   | 2.23                     | 0.67              |
| 1:B:295:PHE:N    | 1:B:295:PHE:HD1  | 1.91                     | 0.67              |
| 1:C:222:ALA:O    | 1:C:225:ILE:CD1  | 2.42                     | 0.67              |
| 1:A:104:VAL:HG11 | 1:A:156:GLN:HB3  | 1.74                     | 0.67              |
| 1:C:139:TYR:HE1  | 1:C:140:ARG:O    | 1.77                     | 0.67              |
| 1:C:338:TYR:HD2  | 1:C:339:GLN:CA   | 2.08                     | 0.67              |
| 1:A:45:PHE:CD1   | 1:A:45:PHE:C     | 2.72                     | 0.67              |
| 1:A:113:ASP:O    | 1:A:114:MET:CG   | 2.39                     | 0.67              |
| 1:A:167:ARG:CG   | 1:A:167:ARG:O    | 2.41                     | 0.67              |
| 1:C:24:SER:OG    | 1:C:331:THR:OG1  | 2.12                     | 0.67              |
| 1:C:206:GLY:H    | 1:C:284:GLU:CD   | 2.03                     | 0.67              |
| 1:A:61:TRP:HZ2   | 1:C:65:PHE:HD1   | 1.15                     | 0.67              |
| 1:B:115:LEU:HD12 | 1:B:119:GLY:HA2  | 1.71                     | 0.67              |
| 1:C:3:ILE:HD11   | 1:C:13:LEU:HB2   | 1.75                     | 0.67              |
| 1:D:315:ILE:CD1  | 1:D:315:ILE:H    | 2.02                     | 0.67              |
| 1:A:171:GLY:C    | 1:A:172:ASP:OD1  | 2.38                     | 0.67              |
| 1:A:245:THR:OG1  | 1:A:247:THR:OG1  | 2.12                     | 0.67              |
| 1:C:69:ASN:HD21  | 1:C:77:THR:HB    | 1.60                     | 0.67              |
| 1:C:37:ASP:OD1   | 1:C:38:MET:N     | 2.28                     | 0.67              |
| 1:C:63:TYR:CE1   | 1:C:80:LYS:O     | 2.48                     | 0.67              |
| 1:C:136:VAL:HG12 | 1:C:158:LEU:CD1  | 2.25                     | 0.67              |
| 1:C:267:PHE:CZ   | 1:C:269:LEU:HB3  | 2.29                     | 0.67              |
| 1:D:118:PHE:CZ   | 1:D:333:ALA:HB2  | 2.28                     | 0.67              |
| 1:A:20:LEU:HD21  | 1:A:117:GLU:CD   | 2.16                     | 0.67              |
| 1:A:122:THR:OG1  | 1:A:258:LEU:HD21 | 1.95                     | 0.67              |
| 1:A:172:ASP:O    | 1:A:194:ALA:HA   | 1.93                     | 0.67              |
| 1:A:293:ASN:HB3  | 1:A:317:GLN:HB2  | 1.76                     | 0.67              |
| 1:B:309:THR:HG22 | 1:B:336:ILE:CA   | 2.24                     | 0.67              |
| 1:C:235:ARG:O    | 1:C:236:ASN:C    | 2.38                     | 0.67              |
| 1:D:48:GLU:CD    | 1:D:56:THR:HG21  | 2.18                     | 0.67              |
| 1:C:63:TYR:HD1   | 1:C:80:LYS:O     | 1.72                     | 0.67              |
| 1:D:13:LEU:HD12  | 1:D:14:TYR:H     | 1.60                     | 0.67              |
| 1:D:257:VAL:C    | 1:D:258:LEU:CD2  | 2.68                     | 0.67              |
| 1:B:277:LYS:CD   | 1:B:293:ASN:HD21 | 2.07                     | 0.67              |
| 1:C:31:SER:HA    | 1:C:329:ASP:HB2  | 1.77                     | 0.67              |
| 1:C:65:PHE:HD2   | 1:C:65:PHE:N     | 1.91                     | 0.67              |
| 1:C:226:TYR:O    | 1:C:227:LEU:HD23 | 1.95                     | 0.67              |
| 1:D:118:PHE:O    | 1:D:119:GLY:O    | 2.12                     | 0.67              |
| 1:A:39:THR:O     | 1:A:67:GLY:CA    | 2.43                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:28:GLY:O     | 1:B:30:ASN:N     | 2.28                     | 0.66              |
| 1:C:13:LEU:HD12  | 1:C:14:TYR:H     | 1.60                     | 0.66              |
| 1:C:318:ILE:HG22 | 1:C:319:ASP:N    | 2.08                     | 0.66              |
| 1:A:208:GLY:HA3  | 1:A:236:ASN:HD22 | 1.60                     | 0.66              |
| 1:A:279:LYS:HZ2  | 1:A:279:LYS:HB2  | 1.60                     | 0.66              |
| 1:A:289:VAL:HG13 | 1:A:323:LYS:HB2  | 1.75                     | 0.66              |
| 1:B:185:PHE:HE2  | 1:B:220:TYR:CE1  | 2.12                     | 0.66              |
| 1:B:240:ILE:HG21 | 1:B:291:LEU:CD2  | 2.26                     | 0.66              |
| 1:D:104:VAL:CG1  | 1:D:156:GLN:HB2  | 2.23                     | 0.66              |
| 1:A:292:VAL:O    | 1:A:292:VAL:CG1  | 2.38                     | 0.66              |
| 1:A:296:GLU:HG2  | 1:A:297:VAL:N    | 2.09                     | 0.66              |
| 1:B:303:PHE:HB2  | 1:B:307:MET:HB3  | 1.75                     | 0.66              |
| 1:D:18:VAL:HG22  | 1:D:337:VAL:HG22 | 1.78                     | 0.66              |
| 1:C:46:LYS:HA    | 1:C:60:GLN:HB2   | 1.77                     | 0.66              |
| 1:C:198:ASN:C    | 1:C:200:GLN:N    | 2.49                     | 0.66              |
| 1:C:294:TYR:CD1  | 1:C:314:ILE:HD12 | 2.31                     | 0.66              |
| 1:D:24:SER:CB    | 1:D:34:GLY:O     | 2.43                     | 0.66              |
| 1:D:119:GLY:HA2  | 1:D:294:TYR:OH   | 1.96                     | 0.66              |
| 1:A:124:TYR:O    | 1:A:131:GLY:HA3  | 1.95                     | 0.66              |
| 1:B:114:MET:CE   | 1:B:226:TYR:HE1  | 2.06                     | 0.66              |
| 1:D:273:ILE:HD11 | 1:D:297:VAL:HG23 | 1.77                     | 0.66              |
| 1:D:302:TYR:C    | 1:D:304:ASN:H    | 2.03                     | 0.66              |
| 1:A:229:ALA:HB2  | 1:A:259:LEU:CD2  | 2.26                     | 0.66              |
| 1:C:10:LYS:O     | 1:C:10:LYS:CG    | 2.44                     | 0.66              |
| 1:C:144:PHE:CD1  | 1:C:151:LEU:HD23 | 2.30                     | 0.66              |
| 1:D:74:ASP:C     | 1:D:76:GLN:H     | 2.03                     | 0.66              |
| 1:D:112:THR:O    | 1:D:114:MET:N    | 2.28                     | 0.66              |
| 1:A:322:ASN:OD1  | 1:A:323:LYS:N    | 2.28                     | 0.66              |
| 1:A:70:SER:HG    | 1:A:72:GLY:H     | 1.44                     | 0.66              |
| 1:A:229:ALA:CB   | 1:A:259:LEU:CD2  | 2.74                     | 0.66              |
| 1:C:37:ASP:C     | 1:C:38:MET:HG2   | 2.21                     | 0.66              |
| 1:D:111:TYR:OH   | 1:D:188:VAL:CG2  | 2.41                     | 0.66              |
| 1:B:90:TYR:O     | 1:B:91:ALA:C     | 2.39                     | 0.66              |
| 1:B:141:ASN:CB   | 1:B:153:PHE:CE1  | 2.79                     | 0.66              |
| 1:C:70:SER:OG    | 1:C:71:GLU:N     | 2.18                     | 0.66              |
| 1:C:96:PHE:CD1   | 1:C:138:THR:O    | 2.49                     | 0.65              |
| 1:C:217:GLY:HA3  | 1:C:230:ASN:ND2  | 2.11                     | 0.65              |
| 1:D:182:TYR:CE2  | 1:D:183:GLU:HB3  | 2.30                     | 0.65              |
| 1:A:42:ARG:NH1   | 1:A:82:ARG:NH2   | 2.44                     | 0.65              |
| 1:D:51:ILE:HB    | 1:D:55:LEU:HD23  | 1.77                     | 0.65              |
| 1:D:205:LEU:HD22 | 1:D:284:GLU:HG2  | 1.77                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:13:LEU:HD12  | 1:C:14:TYR:N     | 2.11                     | 0.65              |
| 1:D:48:GLU:CG    | 1:D:56:THR:CG2   | 2.74                     | 0.65              |
| 1:D:205:LEU:CD2  | 1:D:284:GLU:HG3  | 2.27                     | 0.65              |
| 1:A:208:GLY:HA3  | 1:A:236:ASN:ND2  | 2.12                     | 0.65              |
| 1:A:242:ASN:O    | 1:A:246:ASN:N    | 2.29                     | 0.65              |
| 1:B:111:TYR:OH   | 1:B:188:VAL:HG22 | 1.97                     | 0.65              |
| 1:B:158:LEU:HD11 | 1:B:170:ASN:ND2  | 2.12                     | 0.65              |
| 1:D:224:ASN:ND2  | 1:D:264:GLN:O    | 2.30                     | 0.65              |
| 1:A:340:PHE:HE1  | 1:B:45:PHE:CE2   | 2.15                     | 0.65              |
| 1:B:113:ASP:C    | 1:B:114:MET:CG   | 2.53                     | 0.65              |
| 1:B:183:GLU:O    | 1:B:183:GLU:CG   | 2.44                     | 0.65              |
| 1:B:242:ASN:O    | 1:B:242:ASN:CG   | 2.39                     | 0.65              |
| 1:B:310:TYR:CE1  | 1:B:335:GLY:HA3  | 2.31                     | 0.65              |
| 1:C:172:ASP:O    | 1:C:194:ALA:HB2  | 1.88                     | 0.65              |
| 1:A:35:ASN:C     | 1:A:35:ASN:OD1   | 2.39                     | 0.65              |
| 1:A:39:THR:O     | 1:A:39:THR:CG2   | 2.45                     | 0.65              |
| 1:A:71:GLU:CD    | 1:B:132:ARG:HH21 | 2.05                     | 0.65              |
| 1:C:240:ILE:HD13 | 1:C:251:ALA:N    | 2.11                     | 0.65              |
| 1:A:50:GLN:HA    | 1:A:56:THR:HA    | 1.78                     | 0.65              |
| 1:A:82:ARG:HG3   | 1:A:132:ARG:HH21 | 1.62                     | 0.65              |
| 1:B:21:HIS:HD1   | 1:C:98:TYR:HH    | 1.43                     | 0.65              |
| 1:B:165:THR:CG2  | 1:B:166:ALA:N    | 2.59                     | 0.65              |
| 1:C:236:ASN:OD1  | 1:C:252:ASN:HA   | 1.97                     | 0.65              |
| 1:D:20:LEU:CD1   | 1:D:21:HIS:N     | 2.49                     | 0.65              |
| 1:D:273:ILE:CD1  | 1:D:297:VAL:CG2  | 2.75                     | 0.65              |
| 1:A:203:GLN:NE2  | 1:A:203:GLN:HA   | 2.11                     | 0.65              |
| 1:A:300:THR:HA   | 1:A:310:TYR:HB3  | 1.79                     | 0.65              |
| 1:B:54:ASP:HB3   | 1:B:91:ALA:CB    | 2.21                     | 0.65              |
| 1:B:220:TYR:HB3  | 1:B:227:LEU:HB2  | 1.77                     | 0.65              |
| 1:B:301:TYR:C    | 1:B:301:TYR:CD2  | 2.72                     | 0.65              |
| 1:B:340:PHE:CB   | 1:C:11:VAL:HG21  | 2.26                     | 0.65              |
| 1:C:231:TYR:C    | 1:C:231:TYR:CD2  | 2.74                     | 0.65              |
| 1:A:105:VAL:HB   | 1:A:129:PHE:O    | 1.97                     | 0.65              |
| 1:A:144:PHE:O    | 1:A:145:PHE:HB2  | 1.96                     | 0.65              |
| 1:B:148:VAL:O    | 1:B:148:VAL:HG12 | 1.94                     | 0.65              |
| 1:B:293:ASN:OD1  | 1:B:317:GLN:HB3  | 1.97                     | 0.65              |
| 1:D:158:LEU:O    | 1:D:158:LEU:HG   | 1.96                     | 0.65              |
| 1:B:5:ASN:O      | 1:B:6:LYS:CG     | 2.44                     | 0.65              |
| 1:B:336:ILE:HD11 | 1:C:87:GLY:HA2   | 1.78                     | 0.65              |
| 1:C:48:GLU:HG3   | 1:C:56:THR:HG23  | 1.78                     | 0.65              |
| 1:D:314:ILE:O    | 1:D:314:ILE:HG22 | 1.96                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:14:TYR:OH    | 1:A:62:GLU:HB2   | 1.97                     | 0.64              |
| 1:A:57:GLY:HA2   | 1:A:88:LEU:CD2   | 2.27                     | 0.64              |
| 1:A:115:LEU:H    | 1:A:115:LEU:HD23 | 0.48                     | 0.64              |
| 1:B:2:GLU:OE2    | 1:B:5:ASN:HB2    | 1.98                     | 0.64              |
| 1:B:281:LYS:O    | 1:B:282:ASP:HB2  | 1.97                     | 0.64              |
| 1:C:232:GLY:O    | 1:C:256:ASP:HB2  | 1.97                     | 0.64              |
| 1:A:86:ALA:O     | 1:A:97:ASP:CB    | 2.39                     | 0.64              |
| 1:A:102:TYR:O    | 1:A:103:GLY:C    | 2.37                     | 0.64              |
| 1:B:49:THR:N     | 1:B:57:GLY:O     | 2.27                     | 0.64              |
| 1:B:276:THR:HG22 | 1:B:294:TYR:CE2  | 2.24                     | 0.64              |
| 1:C:331:THR:CG2  | 1:C:332:VAL:N    | 2.61                     | 0.64              |
| 1:D:13:LEU:C     | 1:D:13:LEU:CD1   | 2.52                     | 0.64              |
| 1:D:102:TYR:HD2  | 1:D:102:TYR:H    | 1.45                     | 0.64              |
| 1:A:40:TYR:HD1   | 1:A:40:TYR:N     | 1.89                     | 0.64              |
| 1:A:43:LEU:HG    | 1:A:43:LEU:O     | 1.92                     | 0.64              |
| 1:A:179:SER:HB2  | 1:A:188:VAL:HG13 | 1.80                     | 0.64              |
| 1:B:54:ASP:O     | 1:B:90:TYR:HA    | 1.98                     | 0.64              |
| 1:D:307:MET:HG3  | 1:D:308:SER:N    | 2.09                     | 0.64              |
| 1:A:71:GLU:HG3   | 1:B:100:ARG:HH22 | 1.59                     | 0.64              |
| 1:D:51:ILE:HB    | 1:D:55:LEU:HB3   | 1.79                     | 0.64              |
| 1:D:104:VAL:CG1  | 1:D:156:GLN:CD   | 2.67                     | 0.64              |
| 1:B:45:PHE:CD1   | 1:B:45:PHE:C     | 2.74                     | 0.64              |
| 1:C:338:TYR:CD2  | 1:C:339:GLN:CA   | 2.80                     | 0.64              |
| 1:A:22:TYR:CD2   | 1:A:38:MET:CG    | 2.73                     | 0.64              |
| 1:A:157:TYR:HA   | 1:A:173:GLY:O    | 1.97                     | 0.64              |
| 1:B:242:ASN:ND2  | 1:B:245:THR:OG1  | 2.29                     | 0.64              |
| 1:A:80:LYS:HD2   | 1:C:71:GLU:HB3   | 1.79                     | 0.64              |
| 1:A:338:TYR:CD2  | 1:A:339:GLN:N    | 2.66                     | 0.64              |
| 1:B:58:TYR:HD2   | 1:B:58:TYR:O     | 1.77                     | 0.64              |
| 1:B:273:ILE:HD11 | 1:B:297:VAL:HG22 | 1.80                     | 0.64              |
| 1:C:45:PHE:O     | 1:C:60:GLN:HG3   | 1.97                     | 0.64              |
| 1:A:152:ASN:N    | 1:A:152:ASN:ND2  | 2.46                     | 0.64              |
| 1:B:27:ASN:OD1   | 1:B:27:ASN:C     | 2.35                     | 0.64              |
| 1:C:179:SER:HB2  | 1:C:188:VAL:CG1  | 2.27                     | 0.64              |
| 1:C:263:TYR:CE2  | 1:C:265:PHE:CE1  | 2.86                     | 0.64              |
| 1:C:270:ARG:HD2  | 1:C:302:TYR:HE2  | 1.63                     | 0.64              |
| 1:D:129:PHE:CE2  | 1:D:192:GLY:HA3  | 2.33                     | 0.64              |
| 1:A:283:VAL:HB   | 1:A:286:ILE:HB   | 1.80                     | 0.64              |
| 1:B:6:LYS:C      | 1:B:8:GLY:N      | 2.54                     | 0.64              |
| 1:B:22:TYR:O     | 1:B:23:PHE:CD2   | 2.50                     | 0.64              |
| 1:B:205:LEU:HA   | 1:B:284:GLU:OE2  | 1.97                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:74:ASP:C     | 1:D:76:GLN:N     | 2.57                     | 0.64              |
| 1:A:129:PHE:CE2  | 1:A:192:GLY:C    | 2.74                     | 0.63              |
| 1:B:4:TYR:HD2    | 1:B:5:ASN:N      | 1.95                     | 0.63              |
| 1:B:58:TYR:CD2   | 1:B:58:TYR:C     | 2.60                     | 0.63              |
| 1:B:309:THR:CG2  | 1:B:336:ILE:HB   | 2.28                     | 0.63              |
| 1:C:191:TYR:CD1  | 1:C:192:GLY:N    | 2.65                     | 0.63              |
| 1:D:102:TYR:CD2  | 1:D:102:TYR:N    | 2.65                     | 0.63              |
| 1:D:104:VAL:HG12 | 1:D:156:GLN:HB2  | 1.81                     | 0.63              |
| 1:A:104:VAL:CG1  | 1:A:156:GLN:CB   | 2.75                     | 0.63              |
| 1:A:251:ALA:O    | 1:A:252:ASN:C    | 2.37                     | 0.63              |
| 1:A:308:SER:O    | 1:A:309:THR:HG23 | 1.98                     | 0.63              |
| 1:C:141:ASN:CB   | 1:C:153:PHE:HE1  | 2.11                     | 0.63              |
| 1:D:90:TYR:CD2   | 1:D:90:TYR:C     | 2.75                     | 0.63              |
| 1:B:5:ASN:C      | 1:B:6:LYS:CG     | 2.71                     | 0.63              |
| 1:B:108:ALA:O    | 1:B:109:LEU:C    | 2.41                     | 0.63              |
| 1:B:174:VAL:CG1  | 1:B:175:GLY:N    | 2.59                     | 0.63              |
| 1:A:18:VAL:HG13  | 1:A:337:VAL:CG2  | 2.29                     | 0.63              |
| 1:B:1:ALA:HB1    | 1:C:4:TYR:CD1    | 2.33                     | 0.63              |
| 1:C:54:ASP:CB    | 1:C:90:TYR:CE1   | 2.81                     | 0.63              |
| 1:D:122:THR:HG21 | 1:D:256:ASP:CG   | 2.22                     | 0.63              |
| 1:D:205:LEU:HD22 | 1:D:284:GLU:CG   | 2.28                     | 0.63              |
| 1:A:51:ILE:HG22  | 1:C:304:ASN:ND2  | 2.14                     | 0.63              |
| 1:A:229:ALA:HB1  | 1:A:259:LEU:HD21 | 1.79                     | 0.63              |
| 1:B:240:ILE:HG22 | 1:B:291:LEU:CD2  | 2.28                     | 0.63              |
| 1:C:289:VAL:HG21 | 1:C:324:LEU:HG   | 1.81                     | 0.63              |
| 1:A:3:ILE:O      | 1:A:3:ILE:HG13   | 1.90                     | 0.63              |
| 1:A:320:SER:C    | 1:A:322:ASN:H    | 2.05                     | 0.63              |
| 1:C:65:PHE:N     | 1:C:65:PHE:CD2   | 2.60                     | 0.63              |
| 1:A:114:MET:H    | 1:A:115:LEU:CD2  | 2.11                     | 0.63              |
| 1:B:1:ALA:HB1    | 1:C:4:TYR:CE1    | 2.34                     | 0.63              |
| 1:B:6:LYS:O      | 1:B:8:GLY:N      | 2.32                     | 0.63              |
| 1:B:162:GLU:O    | 1:B:163:ARG:C    | 2.42                     | 0.63              |
| 1:B:257:VAL:O    | 1:B:258:LEU:HD13 | 1.99                     | 0.63              |
| 1:C:136:VAL:HG12 | 1:C:158:LEU:HD12 | 1.81                     | 0.63              |
| 1:C:139:TYR:CD1  | 1:C:140:ARG:N    | 2.67                     | 0.63              |
| 1:C:264:GLN:HG3  | 1:C:264:GLN:O    | 1.98                     | 0.63              |
| 1:A:293:ASN:C    | 1:A:317:GLN:HB2  | 2.24                     | 0.62              |
| 1:B:129:PHE:CE2  | 1:B:192:GLY:HA3  | 2.34                     | 0.62              |
| 1:A:172:ASP:N    | 1:A:195:ASP:HB2  | 2.14                     | 0.62              |
| 1:B:101:ASN:CG   | 1:B:102:TYR:N    | 2.44                     | 0.62              |
| 1:B:274:ALA:O    | 1:B:295:PHE:HA   | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:125:SER:O    | 1:C:126:ASP:HB2  | 1.99                     | 0.62              |
| 1:C:167:ARG:O    | 1:C:167:ARG:HG2  | 1.95                     | 0.62              |
| 1:C:16:LYS:HB3   | 1:C:339:GLN:HB3  | 1.80                     | 0.62              |
| 1:C:257:VAL:C    | 1:C:258:LEU:HD13 | 2.23                     | 0.62              |
| 1:D:127:ASP:O    | 1:D:128:PHE:HB2  | 1.99                     | 0.62              |
| 1:D:263:TYR:O    | 1:D:271:PRO:HD2  | 2.00                     | 0.62              |
| 1:A:267:PHE:HD1  | 1:A:267:PHE:H    | 0.72                     | 0.62              |
| 1:B:110:GLY:O    | 1:B:111:TYR:C    | 2.41                     | 0.62              |
| 1:B:304:ASN:ND2  | 1:C:51:ILE:HG23  | 2.14                     | 0.62              |
| 1:D:122:THR:HG22 | 1:D:256:ASP:OD2  | 2.00                     | 0.62              |
| 1:D:200:GLN:O    | 1:D:201:GLU:C    | 2.42                     | 0.62              |
| 1:D:270:ARG:HB3  | 1:D:302:TYR:HE2  | 1.64                     | 0.62              |
| 1:D:311:VAL:HG11 | 1:D:334:VAL:CG2  | 2.22                     | 0.62              |
| 1:A:49:THR:O     | 1:A:49:THR:OG1   | 2.10                     | 0.62              |
| 1:A:223:ASN:O    | 1:A:224:ASN:CB   | 2.47                     | 0.62              |
| 1:A:275:TYR:C    | 1:A:276:THR:OG1  | 2.38                     | 0.62              |
| 1:B:114:MET:HE1  | 1:B:226:TYR:HE1  | 1.61                     | 0.62              |
| 1:B:185:PHE:CE2  | 1:B:220:TYR:CD1  | 2.87                     | 0.62              |
| 1:C:260:VAL:HG12 | 1:C:261:ALA:N    | 2.15                     | 0.62              |
| 1:C:284:GLU:O    | 1:C:286:ILE:CD1  | 2.47                     | 0.62              |
| 1:D:72:GLY:O     | 1:D:73:ALA:C     | 2.42                     | 0.62              |
| 1:D:85:PHE:N     | 1:D:85:PHE:HD2   | 1.96                     | 0.62              |
| 1:A:179:SER:CB   | 1:A:188:VAL:HG13 | 2.30                     | 0.62              |
| 1:B:140:ARG:HG2  | 1:B:154:ALA:HB2  | 1.81                     | 0.62              |
| 1:B:270:ARG:HG2  | 1:B:270:ARG:O    | 1.98                     | 0.62              |
| 1:B:309:THR:HG22 | 1:B:336:ILE:CB   | 2.29                     | 0.62              |
| 1:B:340:PHE:HB3  | 1:C:11:VAL:HG21  | 1.81                     | 0.62              |
| 1:C:161:ASN:HB2  | 1:C:170:ASN:HD21 | 1.64                     | 0.62              |
| 1:D:40:TYR:CD2   | 1:D:42:ARG:NH2   | 2.67                     | 0.62              |
| 1:A:1:ALA:HB1    | 1:B:4:TYR:CE1    | 2.31                     | 0.62              |
| 1:C:214:TRP:CH2  | 1:C:231:TYR:CE2  | 2.86                     | 0.62              |
| 1:A:165:THR:HG23 | 1:A:166:ALA:H    | 1.64                     | 0.62              |
| 1:C:60:GLN:CG    | 1:C:61:TRP:N     | 2.60                     | 0.62              |
| 1:D:165:THR:HG22 | 1:D:166:ALA:N    | 2.13                     | 0.62              |
| 1:D:297:VAL:O    | 1:D:313:TYR:HB3  | 2.00                     | 0.62              |
| 1:A:88:LEU:HD11  | 1:C:303:PHE:CE2  | 2.34                     | 0.62              |
| 1:A:273:ILE:O    | 1:A:273:ILE:HG22 | 1.98                     | 0.62              |
| 1:B:234:THR:C    | 1:B:235:ARG:HD3  | 2.25                     | 0.62              |
| 1:D:102:TYR:CD1  | 1:D:106:TYR:CE2  | 2.87                     | 0.62              |
| 1:D:134:GLY:O    | 1:D:136:VAL:HG13 | 2.00                     | 0.62              |
| 1:A:39:THR:HG22  | 1:A:67:GLY:HA3   | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:163:ARG:HG2  | 1:B:163:ARG:NH1  | 2.15                     | 0.62              |
| 1:D:270:ARG:O    | 1:D:270:ARG:HG2  | 1.99                     | 0.62              |
| 1:A:22:TYR:CD1   | 1:A:333:ALA:CB   | 2.77                     | 0.61              |
| 1:A:87:GLY:N     | 1:C:336:ILE:HD11 | 2.15                     | 0.61              |
| 1:A:293:ASN:HB3  | 1:A:317:GLN:CB   | 2.29                     | 0.61              |
| 1:B:83:LEU:HD22  | 1:B:85:PHE:HE2   | 1.65                     | 0.61              |
| 1:B:259:LEU:HB2  | 1:B:275:TYR:HB3  | 1.81                     | 0.61              |
| 1:D:3:ILE:HD11   | 1:D:11:VAL:HG12  | 1.82                     | 0.61              |
| 1:D:111:TYR:CZ   | 1:D:219:LYS:HG2  | 2.35                     | 0.61              |
| 1:B:42:ARG:HE    | 1:B:64:ASN:HB2   | 1.65                     | 0.61              |
| 1:C:145:PHE:O    | 1:C:147:LEU:N    | 2.28                     | 0.61              |
| 1:D:295:PHE:O    | 1:D:315:ILE:HD13 | 1.99                     | 0.61              |
| 1:B:336:ILE:HD11 | 1:C:87:GLY:CA    | 2.30                     | 0.61              |
| 1:D:157:TYR:HA   | 1:D:173:GLY:O    | 1.99                     | 0.61              |
| 1:A:197:THR:O    | 1:A:200:GLN:HB2  | 2.01                     | 0.61              |
| 1:A:260:VAL:HG12 | 1:A:261:ALA:N    | 2.13                     | 0.61              |
| 1:C:274:ALA:HB3  | 1:C:296:GLU:CB   | 2.29                     | 0.61              |
| 1:D:106:TYR:HB2  | 1:D:130:VAL:O    | 1.99                     | 0.61              |
| 1:A:65:PHE:CZ    | 1:B:61:TRP:CZ2   | 2.87                     | 0.61              |
| 1:B:63:TYR:CD2   | 1:B:65:PHE:CE1   | 2.88                     | 0.61              |
| 1:B:276:THR:HB   | 1:B:294:TYR:CD2  | 2.33                     | 0.61              |
| 1:D:24:SER:HB2   | 1:D:35:ASN:HB2   | 1.83                     | 0.61              |
| 1:D:294:TYR:CE1  | 1:D:314:ILE:HD11 | 2.36                     | 0.61              |
| 1:C:132:ARG:HG3  | 1:C:132:ARG:HH11 | 1.64                     | 0.61              |
| 1:C:240:ILE:CD1  | 1:C:251:ALA:CA   | 2.78                     | 0.61              |
| 1:D:144:PHE:CE2  | 1:D:145:PHE:HD2  | 2.19                     | 0.61              |
| 1:B:128:PHE:O    | 1:B:133:VAL:HG11 | 2.01                     | 0.61              |
| 1:D:143:ASN:HB3  | 1:D:149:ASP:HA   | 1.83                     | 0.61              |
| 1:A:22:TYR:HE1   | 1:A:118:PHE:CZ   | 2.19                     | 0.61              |
| 1:A:61:TRP:O     | 1:A:61:TRP:CG    | 2.52                     | 0.61              |
| 1:A:71:GLU:HB3   | 1:B:80:LYS:HD2   | 1.82                     | 0.61              |
| 1:C:16:LYS:HB3   | 1:C:339:GLN:CB   | 2.30                     | 0.61              |
| 1:C:105:VAL:HA   | 1:C:190:ALA:HB3  | 1.83                     | 0.61              |
| 1:A:65:PHE:CE1   | 1:B:61:TRP:CZ2   | 2.89                     | 0.61              |
| 1:A:245:THR:O    | 1:A:246:ASN:C    | 2.39                     | 0.61              |
| 1:B:338:TYR:CD2  | 1:B:339:GLN:N    | 2.68                     | 0.61              |
| 1:B:340:PHE:CE1  | 1:C:45:PHE:CE2   | 2.89                     | 0.61              |
| 1:D:117:GLU:HG3  | 1:D:118:PHE:CD1  | 2.36                     | 0.61              |
| 1:D:143:ASN:OD1  | 1:D:150:GLY:N    | 2.34                     | 0.61              |
| 1:D:338:TYR:CG   | 1:D:339:GLN:N    | 2.68                     | 0.61              |
| 1:A:13:LEU:HD11  | 1:A:43:LEU:HD11  | 1.81                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:58:TYR:C     | 1:C:338:TYR:CD1  | 2.78                     | 0.60              |
| 1:A:100:ARG:HG3  | 1:C:67:GLY:O     | 2.01                     | 0.60              |
| 1:A:118:PHE:C    | 1:A:119:GLY:O    | 2.40                     | 0.60              |
| 1:A:300:THR:HG21 | 1:A:302:TYR:CE1  | 2.36                     | 0.60              |
| 1:B:90:TYR:O     | 1:B:93:VAL:HG23  | 2.00                     | 0.60              |
| 1:C:112:THR:HG21 | 1:C:230:ASN:HB2  | 1.82                     | 0.60              |
| 1:C:310:TYR:HD1  | 1:C:310:TYR:C    | 2.05                     | 0.60              |
| 1:B:162:GLU:C    | 1:B:163:ARG:O    | 2.42                     | 0.60              |
| 1:B:219:LYS:HG3  | 1:B:219:LYS:O    | 1.99                     | 0.60              |
| 1:C:179:SER:HB2  | 1:C:188:VAL:HG11 | 1.83                     | 0.60              |
| 1:D:48:GLU:HG3   | 1:D:57:GLY:O     | 2.02                     | 0.60              |
| 1:D:205:LEU:CD2  | 1:D:284:GLU:CG   | 2.79                     | 0.60              |
| 1:D:254:THR:HA   | 1:D:279:LYS:O    | 2.00                     | 0.60              |
| 1:D:338:TYR:O    | 1:D:339:GLN:CB   | 2.49                     | 0.60              |
| 1:A:129:PHE:HE2  | 1:A:192:GLY:CA   | 2.12                     | 0.60              |
| 1:B:9:ASN:HB2    | 1:B:49:THR:HB    | 1.83                     | 0.60              |
| 1:C:193:ALA:HB1  | 1:C:211:ALA:O    | 2.01                     | 0.60              |
| 1:D:141:ASN:ND2  | 1:D:142:SER:N    | 2.48                     | 0.60              |
| 1:D:177:SER:C    | 1:D:178:ILE:HG13 | 2.25                     | 0.60              |
| 1:A:40:TYR:N     | 1:A:40:TYR:CD1   | 2.67                     | 0.60              |
| 1:C:169:SER:O    | 1:C:170:ASN:CB   | 2.42                     | 0.60              |
| 1:D:313:TYR:CE1  | 1:D:332:VAL:HG22 | 2.37                     | 0.60              |
| 1:A:109:LEU:O    | 1:A:110:GLY:C    | 2.43                     | 0.60              |
| 1:B:6:LYS:C      | 1:B:8:GLY:H      | 2.08                     | 0.60              |
| 1:B:340:PHE:HB3  | 1:C:11:VAL:CG2   | 2.30                     | 0.60              |
| 1:C:24:SER:HB2   | 1:C:34:GLY:O     | 2.01                     | 0.60              |
| 1:D:40:TYR:N     | 1:D:40:TYR:CD1   | 2.67                     | 0.60              |
| 1:C:118:PHE:O    | 1:C:119:GLY:O    | 2.20                     | 0.60              |
| 1:C:160:LYS:HE3  | 1:C:160:LYS:CA   | 2.19                     | 0.60              |
| 1:C:214:TRP:HH2  | 1:C:231:TYR:HE2  | 1.47                     | 0.60              |
| 1:D:30:ASN:OD1   | 1:D:30:ASN:O     | 2.19                     | 0.60              |
| 1:A:157:TYR:CD2  | 1:A:157:TYR:N    | 2.70                     | 0.60              |
| 1:A:307:MET:HE1  | 1:B:88:LEU:HD23  | 1.75                     | 0.60              |
| 1:C:142:SER:O    | 1:C:143:ASN:C    | 2.44                     | 0.60              |
| 1:A:11:VAL:HG22  | 1:C:340:PHE:HB2  | 1.83                     | 0.60              |
| 1:B:224:ASN:O    | 1:B:263:TYR:HD1  | 1.82                     | 0.60              |
| 1:C:11:VAL:CG1   | 1:C:12:ASP:N     | 2.65                     | 0.60              |
| 1:C:77:THR:O     | 1:C:77:THR:HG22  | 2.01                     | 0.60              |
| 1:C:139:TYR:CD1  | 1:C:139:TYR:C    | 2.76                     | 0.60              |
| 1:D:48:GLU:HG3   | 1:D:56:THR:HG22  | 1.83                     | 0.60              |
| 1:D:87:GLY:O     | 1:D:88:LEU:HD23  | 2.02                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:262:GLN:OE1  | 1:B:270:ARG:NH1  | 2.35                     | 0.60              |
| 1:A:141:ASN:O    | 1:A:152:ASN:CB   | 2.33                     | 0.60              |
| 1:B:111:TYR:CE2  | 1:B:219:LYS:HE2  | 2.37                     | 0.60              |
| 1:B:226:TYR:O    | 1:B:227:LEU:CD2  | 2.48                     | 0.60              |
| 1:C:3:ILE:CD1    | 1:C:13:LEU:HB2   | 2.31                     | 0.60              |
| 1:C:167:ARG:HD2  | 1:C:239:PRO:CB   | 2.31                     | 0.59              |
| 1:A:205:LEU:O    | 1:A:250:PHE:O    | 2.19                     | 0.59              |
| 1:C:45:PHE:HE1   | 1:C:60:GLN:HA    | 1.67                     | 0.59              |
| 1:C:144:PHE:O    | 1:C:145:PHE:CB   | 2.49                     | 0.59              |
| 1:D:127:ASP:O    | 1:D:127:ASP:OD1  | 2.20                     | 0.59              |
| 1:A:22:TYR:CE1   | 1:A:118:PHE:CE1  | 2.91                     | 0.59              |
| 1:A:22:TYR:CE1   | 1:A:118:PHE:CZ   | 2.91                     | 0.59              |
| 1:A:63:TYR:CE1   | 1:A:80:LYS:O     | 2.55                     | 0.59              |
| 1:A:158:LEU:HD12 | 1:A:159:GLY:H    | 1.65                     | 0.59              |
| 1:D:167:ARG:HH11 | 1:D:167:ARG:CG   | 2.16                     | 0.59              |
| 1:D:49:THR:O     | 1:D:49:THR:HG23  | 2.01                     | 0.59              |
| 1:D:52:ASN:CG    | 1:D:53:SER:H     | 2.10                     | 0.59              |
| 1:D:203:GLN:CB   | 1:D:204:PRO:HD2  | 2.13                     | 0.59              |
| 1:D:262:GLN:HG2  | 1:D:272:SER:HB2  | 1.84                     | 0.59              |
| 1:A:28:GLY:O     | 1:A:31:SER:N     | 2.28                     | 0.59              |
| 1:A:180:TYR:CD2  | 1:A:181:GLU:N    | 2.58                     | 0.59              |
| 1:A:254:THR:HB   | 1:A:279:LYS:O    | 2.03                     | 0.59              |
| 1:B:71:GLU:CG    | 1:C:100:ARG:NH2  | 2.63                     | 0.59              |
| 1:B:71:GLU:CG    | 1:C:100:ARG:HH21 | 2.16                     | 0.59              |
| 1:B:233:GLU:HG2  | 1:B:254:THR:O    | 2.02                     | 0.59              |
| 1:B:269:LEU:CD2  | 1:B:271:PRO:CD   | 2.80                     | 0.59              |
| 1:C:303:PHE:CD2  | 1:C:307:MET:HG2  | 2.37                     | 0.59              |
| 1:D:257:VAL:HG23 | 1:D:277:LYS:O    | 2.02                     | 0.59              |
| 1:A:242:ASN:C    | 1:A:244:PHE:H    | 2.11                     | 0.59              |
| 1:B:5:ASN:O      | 1:B:6:LYS:HE2    | 2.03                     | 0.59              |
| 1:B:259:LEU:HB2  | 1:B:275:TYR:CB   | 2.32                     | 0.59              |
| 1:C:109:LEU:O    | 1:C:111:TYR:N    | 2.36                     | 0.59              |
| 1:C:153:PHE:HD1  | 1:C:153:PHE:N    | 1.99                     | 0.59              |
| 1:A:284:GLU:C    | 1:A:286:ILE:HD13 | 2.26                     | 0.59              |
| 1:B:111:TYR:OH   | 1:B:188:VAL:CG2  | 2.51                     | 0.59              |
| 1:B:334:VAL:O    | 1:B:334:VAL:HG12 | 2.03                     | 0.59              |
| 1:C:115:LEU:HD12 | 1:C:119:GLY:HA3  | 1.83                     | 0.59              |
| 1:C:141:ASN:HB3  | 1:C:153:PHE:CD1  | 2.38                     | 0.59              |
| 1:D:196:ARG:NH2  | 1:D:250:PHE:CD1  | 2.54                     | 0.59              |
| 1:D:278:SER:HB3  | 1:D:292:VAL:HG23 | 1.85                     | 0.59              |
| 1:A:165:THR:HG22 | 1:A:166:ALA:N    | 1.93                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:249:GLY:C    | 1:A:250:PHE:CD1  | 2.81                     | 0.59              |
| 1:A:274:ALA:CB   | 1:A:296:GLU:OE1  | 2.50                     | 0.59              |
| 1:B:16:LYS:HB3   | 1:B:339:GLN:HB2  | 1.85                     | 0.59              |
| 1:C:18:VAL:HG11  | 1:C:40:TYR:OH    | 2.02                     | 0.59              |
| 1:D:211:ALA:HB2  | 1:D:236:ASN:O    | 2.02                     | 0.59              |
| 1:A:258:LEU:C    | 1:A:259:LEU:CD2  | 2.56                     | 0.59              |
| 1:A:279:LYS:NZ   | 1:A:279:LYS:HB2  | 2.16                     | 0.59              |
| 1:A:51:ILE:HG22  | 1:C:304:ASN:HD22 | 1.67                     | 0.59              |
| 1:A:65:PHE:CE2   | 1:B:61:TRP:CZ2   | 2.91                     | 0.59              |
| 1:A:71:GLU:OE2   | 1:B:132:ARG:NH2  | 2.35                     | 0.59              |
| 1:A:182:TYR:O    | 1:A:183:GLU:HB3  | 2.02                     | 0.59              |
| 1:B:157:TYR:HA   | 1:B:173:GLY:O    | 2.03                     | 0.59              |
| 1:B:338:TYR:CZ   | 1:C:47:GLY:HA3   | 2.38                     | 0.59              |
| 1:D:1:ALA:HB2    | 1:D:340:PHE:C    | 2.28                     | 0.59              |
| 1:D:114:MET:O    | 1:D:115:LEU:O    | 2.21                     | 0.59              |
| 1:A:130:VAL:CG2  | 1:A:130:VAL:O    | 2.51                     | 0.58              |
| 1:A:132:ARG:NH2  | 1:C:71:GLU:OE1   | 2.36                     | 0.58              |
| 1:A:284:GLU:O    | 1:A:286:ILE:CD1  | 2.50                     | 0.58              |
| 1:C:132:ARG:HH11 | 1:C:132:ARG:CG   | 2.14                     | 0.58              |
| 1:A:71:GLU:OE1   | 1:B:132:ARG:NH2  | 2.36                     | 0.58              |
| 1:A:259:LEU:HB2  | 1:A:275:TYR:HB3  | 1.85                     | 0.58              |
| 1:B:165:THR:CG2  | 1:B:166:ALA:H    | 2.16                     | 0.58              |
| 1:C:144:PHE:HB3  | 1:C:148:VAL:CG2  | 2.33                     | 0.58              |
| 1:D:58:TYR:HE2   | 1:D:87:GLY:C     | 2.10                     | 0.58              |
| 1:A:242:ASN:C    | 1:A:244:PHE:N    | 2.60                     | 0.58              |
| 1:C:325:GLY:O    | 1:C:326:VAL:C    | 2.44                     | 0.58              |
| 1:D:5:ASN:O      | 1:D:6:LYS:CE     | 2.52                     | 0.58              |
| 1:A:23:PHE:HB2   | 1:A:332:VAL:O    | 2.04                     | 0.58              |
| 1:B:96:PHE:CD2   | 1:B:96:PHE:C     | 2.64                     | 0.58              |
| 1:C:74:ASP:O     | 1:C:75:ALA:C     | 2.41                     | 0.58              |
| 1:C:174:VAL:HG12 | 1:C:175:GLY:CA   | 2.33                     | 0.58              |
| 1:D:266:ASP:C    | 1:D:268:GLY:H    | 2.09                     | 0.58              |
| 1:D:290:ASP:HB2  | 1:D:318:ILE:HD11 | 1.85                     | 0.58              |
| 1:A:24:SER:O     | 1:A:25:LYS:C     | 2.45                     | 0.58              |
| 1:B:230:ASN:O    | 1:B:257:VAL:HA   | 2.03                     | 0.58              |
| 1:C:24:SER:HB3   | 1:C:31:SER:HB3   | 1.85                     | 0.58              |
| 1:C:114:MET:O    | 1:C:115:LEU:C    | 2.44                     | 0.58              |
| 1:A:314:ILE:HB   | 1:A:331:THR:O    | 2.03                     | 0.58              |
| 1:B:24:SER:OG    | 1:B:331:THR:OG1  | 2.17                     | 0.58              |
| 1:B:277:LYS:CE   | 1:B:293:ASN:HD21 | 2.15                     | 0.58              |
| 1:C:24:SER:HB2   | 1:C:35:ASN:HB2   | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:251:ALA:O    | 1:C:252:ASN:C    | 2.47                     | 0.58              |
| 1:D:14:TYR:CE2   | 1:D:44:GLY:C     | 2.82                     | 0.58              |
| 1:D:85:PHE:CE1   | 1:D:101:ASN:ND2  | 2.71                     | 0.58              |
| 1:D:187:ILE:HG13 | 1:D:218:LEU:CD2  | 2.23                     | 0.58              |
| 1:B:111:TYR:HD1  | 1:B:111:TYR:H    | 1.52                     | 0.58              |
| 1:B:274:ALA:HB2  | 1:B:296:GLU:OE1  | 2.02                     | 0.58              |
| 1:D:314:ILE:CA   | 1:D:315:ILE:HD12 | 2.34                     | 0.58              |
| 1:A:21:HIS:HD2   | 1:A:23:PHE:CZ    | 2.21                     | 0.58              |
| 1:A:136:VAL:HG21 | 1:A:156:GLN:NE2  | 2.18                     | 0.58              |
| 1:B:87:GLY:C     | 1:B:88:LEU:CG    | 2.77                     | 0.58              |
| 1:C:74:ASP:O     | 1:C:76:GLN:N     | 2.37                     | 0.58              |
| 1:C:167:ARG:O    | 1:C:167:ARG:NH1  | 2.32                     | 0.58              |
| 1:C:191:TYR:CG   | 1:C:192:GLY:N    | 2.71                     | 0.58              |
| 1:C:214:TRP:HH2  | 1:C:231:TYR:CE2  | 2.22                     | 0.58              |
| 1:C:226:TYR:C    | 1:C:227:LEU:HD23 | 2.29                     | 0.58              |
| 1:D:47:GLY:O     | 1:D:58:TYR:HA    | 2.04                     | 0.58              |
| 1:D:85:PHE:N     | 1:D:85:PHE:CD2   | 2.69                     | 0.58              |
| 1:D:253:LYS:HE3  | 1:D:254:THR:O    | 2.03                     | 0.58              |
| 1:C:114:MET:HE2  | 1:C:226:TYR:CZ   | 2.39                     | 0.58              |
| 1:C:163:ARG:NH1  | 1:C:163:ARG:HG2  | 2.19                     | 0.58              |
| 1:A:21:HIS:ND1   | 1:A:36:GLY:O     | 2.36                     | 0.58              |
| 1:A:108:ALA:O    | 1:A:109:LEU:C    | 2.46                     | 0.58              |
| 1:B:185:PHE:HE2  | 1:B:220:TYR:HE1  | 1.50                     | 0.58              |
| 1:D:114:MET:O    | 1:D:115:LEU:C    | 2.46                     | 0.58              |
| 1:D:165:THR:HG22 | 1:D:167:ARG:H    | 1.68                     | 0.58              |
| 1:A:114:MET:C    | 1:A:115:LEU:HD23 | 2.17                     | 0.57              |
| 1:A:128:PHE:CE1  | 1:A:170:ASN:HB2  | 2.39                     | 0.57              |
| 1:A:308:SER:O    | 1:A:309:THR:CG2  | 2.52                     | 0.57              |
| 1:A:152:ASN:HD22 | 1:A:152:ASN:H    | 1.49                     | 0.57              |
| 1:A:267:PHE:CZ   | 1:A:269:LEU:CD1  | 2.87                     | 0.57              |
| 1:B:321:ASP:OD1  | 1:D:282:ASP:HA   | 2.03                     | 0.57              |
| 1:C:182:TYR:CE1  | 1:C:183:GLU:HB3  | 2.39                     | 0.57              |
| 1:D:102:TYR:HD1  | 1:D:106:TYR:CD2  | 2.22                     | 0.57              |
| 1:D:111:TYR:CE2  | 1:D:188:VAL:HG21 | 2.31                     | 0.57              |
| 1:A:18:VAL:CB    | 1:A:40:TYR:CE1   | 2.82                     | 0.57              |
| 1:A:172:ASP:C    | 1:A:194:ALA:HB1  | 2.24                     | 0.57              |
| 1:B:64:ASN:O     | 1:B:79:ASN:HA    | 2.05                     | 0.57              |
| 1:C:105:VAL:HA   | 1:C:190:ALA:CB   | 2.33                     | 0.57              |
| 1:C:234:THR:OG1  | 1:C:254:THR:HG23 | 2.05                     | 0.57              |
| 1:D:232:GLY:C    | 1:D:233:GLU:HG3  | 2.29                     | 0.57              |
| 1:D:313:TYR:CB   | 1:D:332:VAL:HG13 | 2.33                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:151:LEU:O    | 1:A:151:LEU:HD23 | 2.05                     | 0.57              |
| 1:C:74:ASP:C     | 1:C:76:GLN:H     | 2.10                     | 0.57              |
| 1:C:182:TYR:O    | 1:C:183:GLU:C    | 2.47                     | 0.57              |
| 1:C:206:GLY:HA2  | 1:C:250:PHE:O    | 2.03                     | 0.57              |
| 1:D:96:PHE:HA    | 1:D:138:THR:O    | 2.04                     | 0.57              |
| 1:D:266:ASP:C    | 1:D:268:GLY:N    | 2.63                     | 0.57              |
| 1:A:98:TYR:HE2   | 1:C:20:LEU:O     | 1.88                     | 0.57              |
| 1:A:141:ASN:HB2  | 1:A:153:PHE:CE1  | 2.39                     | 0.57              |
| 1:B:48:GLU:HG3   | 1:B:56:THR:CG2   | 2.34                     | 0.57              |
| 1:B:205:LEU:HD11 | 1:B:247:THR:CG2  | 2.25                     | 0.57              |
| 1:B:276:THR:CB   | 1:B:294:TYR:CZ   | 2.88                     | 0.57              |
| 1:D:25:LYS:HE2   | 1:D:329:ASP:CG   | 2.30                     | 0.57              |
| 1:D:100:ARG:NH1  | 1:D:100:ARG:HG2  | 2.19                     | 0.57              |
| 1:D:211:ALA:CB   | 1:D:236:ASN:O    | 2.52                     | 0.57              |
| 1:D:303:PHE:O    | 1:D:304:ASN:HB3  | 2.04                     | 0.57              |
| 1:A:1:ALA:O      | 1:A:3:ILE:HG22   | 2.04                     | 0.57              |
| 1:A:4:TYR:HE2    | 1:A:6:LYS:H      | 1.51                     | 0.57              |
| 1:A:100:ARG:HG3  | 1:A:134:GLY:HA2  | 1.85                     | 0.57              |
| 1:B:300:THR:HG22 | 1:B:302:TYR:CE1  | 2.40                     | 0.57              |
| 1:C:51:ILE:HD11  | 1:C:55:LEU:HD23  | 1.81                     | 0.57              |
| 1:C:234:THR:CB   | 1:C:237:ALA:HB3  | 2.34                     | 0.57              |
| 1:D:27:ASN:C     | 1:D:29:GLU:N     | 2.62                     | 0.57              |
| 1:D:58:TYR:CE2   | 1:D:87:GLY:C     | 2.83                     | 0.57              |
| 1:A:129:PHE:CD2  | 1:A:192:GLY:CA   | 2.76                     | 0.57              |
| 1:B:180:TYR:CE2  | 1:B:182:TYR:HB2  | 2.39                     | 0.57              |
| 1:B:276:THR:HB   | 1:B:294:TYR:CZ   | 2.38                     | 0.57              |
| 1:B:293:ASN:OD1  | 1:B:317:GLN:CB   | 2.51                     | 0.57              |
| 1:B:302:TYR:O    | 1:B:303:PHE:O    | 2.22                     | 0.57              |
| 1:D:315:ILE:O    | 1:D:317:GLN:NE2  | 2.37                     | 0.57              |
| 1:A:216:THR:O    | 1:A:230:ASN:HA   | 2.05                     | 0.57              |
| 1:A:226:TYR:CE2  | 1:A:228:ALA:HB2  | 2.29                     | 0.57              |
| 1:B:66:GLN:CG    | 1:B:78:GLY:HA3   | 2.35                     | 0.57              |
| 1:A:18:VAL:CB    | 1:A:40:TYR:HE1   | 2.16                     | 0.57              |
| 1:B:115:LEU:CG   | 1:B:119:GLY:HA3  | 2.34                     | 0.57              |
| 1:C:155:VAL:O    | 1:C:155:VAL:CG1  | 2.50                     | 0.57              |
| 1:C:313:TYR:CD1  | 1:C:332:VAL:HG23 | 2.39                     | 0.57              |
| 1:D:265:PHE:HB3  | 1:D:267:PHE:HE1  | 1.69                     | 0.57              |
| 1:D:301:TYR:N    | 1:D:309:THR:O    | 2.36                     | 0.57              |
| 1:A:129:PHE:CZ   | 1:A:174:VAL:O    | 2.57                     | 0.56              |
| 1:A:226:TYR:C    | 1:A:226:TYR:HD2  | 2.13                     | 0.56              |
| 1:A:314:ILE:O    | 1:A:314:ILE:HG22 | 2.04                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:179:SER:CB   | 1:C:188:VAL:HG11 | 2.35                     | 0.56              |
| 1:D:48:GLU:CG    | 1:D:56:THR:HG23  | 2.35                     | 0.56              |
| 1:D:64:ASN:ND2   | 1:D:78:GLY:O     | 2.38                     | 0.56              |
| 1:D:182:TYR:CD2  | 1:D:182:TYR:C    | 2.77                     | 0.56              |
| 1:A:114:MET:SD   | 1:A:226:TYR:CE1  | 2.99                     | 0.56              |
| 1:A:115:LEU:HG   | 1:A:119:GLY:CA   | 2.31                     | 0.56              |
| 1:A:267:PHE:HZ   | 1:A:269:LEU:HD12 | 1.66                     | 0.56              |
| 1:B:294:TYR:CD1  | 1:B:314:ILE:HG23 | 2.40                     | 0.56              |
| 1:C:129:PHE:HE2  | 1:C:193:ALA:H    | 1.51                     | 0.56              |
| 1:C:258:LEU:HD11 | 1:C:276:THR:HG23 | 1.85                     | 0.56              |
| 1:A:200:GLN:HE21 | 1:A:250:PHE:HZ   | 1.53                     | 0.56              |
| 1:A:334:VAL:O    | 1:A:334:VAL:HG12 | 1.88                     | 0.56              |
| 1:B:141:ASN:HB3  | 1:B:153:PHE:CD1  | 2.40                     | 0.56              |
| 1:B:180:TYR:HE2  | 1:B:182:TYR:HB2  | 1.69                     | 0.56              |
| 1:B:226:TYR:CE2  | 1:B:228:ALA:HB2  | 2.38                     | 0.56              |
| 1:C:45:PHE:CE1   | 1:C:60:GLN:HA    | 2.40                     | 0.56              |
| 1:C:127:ASP:O    | 1:C:128:PHE:HB2  | 2.05                     | 0.56              |
| 1:C:270:ARG:N    | 1:C:271:PRO:CD   | 2.67                     | 0.56              |
| 1:C:274:ALA:HB2  | 1:C:296:GLU:OE1  | 2.05                     | 0.56              |
| 1:D:244:PHE:C    | 1:D:246:ASN:H    | 2.12                     | 0.56              |
| 1:A:21:HIS:HD2   | 1:A:23:PHE:CE2   | 2.22                     | 0.56              |
| 1:A:141:ASN:CB   | 1:A:153:PHE:HE1  | 2.02                     | 0.56              |
| 1:C:3:ILE:HD13   | 1:C:13:LEU:HB3   | 1.88                     | 0.56              |
| 1:C:22:TYR:CE2   | 1:C:38:MET:HE2   | 2.40                     | 0.56              |
| 1:D:32:TYR:C     | 1:D:32:TYR:CD2   | 2.83                     | 0.56              |
| 1:D:100:ARG:HH11 | 1:D:100:ARG:HG2  | 1.66                     | 0.56              |
| 1:B:2:GLU:OE2    | 1:B:5:ASN:CB     | 2.53                     | 0.56              |
| 1:C:140:ARG:HA   | 1:C:154:ALA:HB2  | 1.88                     | 0.56              |
| 1:D:55:LEU:CD1   | 1:D:90:TYR:CD1   | 2.76                     | 0.56              |
| 1:B:291:LEU:C    | 1:B:292:VAL:CG2  | 2.79                     | 0.56              |
| 1:B:311:VAL:HG13 | 1:B:334:VAL:HG23 | 1.85                     | 0.56              |
| 1:C:90:TYR:HB3   | 1:C:93:VAL:HB    | 1.88                     | 0.56              |
| 1:D:32:TYR:CE2   | 1:D:314:ILE:HG13 | 2.40                     | 0.56              |
| 1:D:48:GLU:HA    | 1:D:57:GLY:O     | 2.06                     | 0.56              |
| 1:A:11:VAL:HG21  | 1:C:340:PHE:HB2  | 1.86                     | 0.56              |
| 1:A:40:TYR:HE2   | 1:A:42:ARG:NH2   | 2.04                     | 0.56              |
| 1:A:45:PHE:HD1   | 1:A:45:PHE:C     | 2.07                     | 0.56              |
| 1:A:65:PHE:CZ    | 1:B:61:TRP:CH2   | 2.93                     | 0.56              |
| 1:A:240:ILE:HG22 | 1:A:291:LEU:HD22 | 1.88                     | 0.56              |
| 1:B:4:TYR:CD2    | 1:B:5:ASN:N      | 2.73                     | 0.56              |
| 1:C:18:VAL:HG12  | 1:C:40:TYR:CE1   | 2.40                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:129:PHE:CE2  | 1:C:193:ALA:N    | 2.65                     | 0.56              |
| 1:D:205:LEU:HA   | 1:D:284:GLU:HG3  | 1.86                     | 0.56              |
| 1:A:201:GLU:OE1  | 1:A:208:GLY:O    | 2.23                     | 0.56              |
| 1:A:279:LYS:CB   | 1:A:279:LYS:HZ3  | 2.18                     | 0.56              |
| 1:B:148:VAL:O    | 1:B:149:ASP:C    | 2.49                     | 0.56              |
| 1:B:167:ARG:HD2  | 1:B:239:PRO:CB   | 2.36                     | 0.56              |
| 1:B:187:ILE:CG2  | 1:B:187:ILE:O    | 2.54                     | 0.56              |
| 1:D:309:THR:CG2  | 1:D:336:ILE:HA   | 2.25                     | 0.56              |
| 1:B:143:ASN:O    | 1:B:147:LEU:N    | 2.39                     | 0.56              |
| 1:B:234:THR:O    | 1:B:235:ARG:HD3  | 2.05                     | 0.56              |
| 1:D:66:GLN:NE2   | 1:D:68:ASN:HD21  | 2.04                     | 0.56              |
| 1:D:104:VAL:HG12 | 1:D:156:GLN:CD   | 2.30                     | 0.56              |
| 1:D:151:LEU:HG   | 1:D:151:LEU:O    | 1.93                     | 0.56              |
| 1:D:313:TYR:HA   | 1:D:332:VAL:HG13 | 1.88                     | 0.56              |
| 1:A:82:ARG:CG    | 1:A:132:ARG:HH21 | 2.19                     | 0.56              |
| 1:A:113:ASP:C    | 1:A:113:ASP:OD1  | 2.49                     | 0.56              |
| 1:B:251:ALA:O    | 1:B:252:ASN:C    | 2.47                     | 0.56              |
| 1:B:276:THR:HG22 | 1:B:294:TYR:HE2  | 1.52                     | 0.56              |
| 1:C:60:GLN:HE21  | 1:C:85:PHE:HE1   | 1.54                     | 0.56              |
| 1:C:145:PHE:C    | 1:C:147:LEU:N    | 2.64                     | 0.56              |
| 1:C:271:PRO:HA   | 1:C:299:ALA:HB2  | 1.88                     | 0.56              |
| 1:D:205:LEU:HG   | 1:D:247:THR:CG2  | 2.36                     | 0.56              |
| 1:A:21:HIS:CE1   | 1:A:36:GLY:C     | 2.85                     | 0.55              |
| 1:B:206:GLY:N    | 1:B:284:GLU:OE2  | 2.38                     | 0.55              |
| 1:C:144:PHE:CD2  | 1:C:144:PHE:C    | 2.84                     | 0.55              |
| 1:C:179:SER:CA   | 1:C:188:VAL:CG1  | 2.70                     | 0.55              |
| 1:C:231:TYR:CD2  | 1:C:232:GLY:N    | 2.74                     | 0.55              |
| 1:D:51:ILE:HD12  | 1:D:55:LEU:HG    | 1.88                     | 0.55              |
| 1:A:11:VAL:HG11  | 1:C:340:PHE:CD2  | 2.41                     | 0.55              |
| 1:B:214:TRP:O    | 1:B:215:ALA:HB2  | 2.06                     | 0.55              |
| 1:B:215:ALA:C    | 1:B:216:THR:CG2  | 2.79                     | 0.55              |
| 1:C:113:ASP:N    | 1:C:114:MET:HG2  | 2.20                     | 0.55              |
| 1:C:326:VAL:HG12 | 1:C:327:GLY:O    | 2.05                     | 0.55              |
| 1:D:271:PRO:HG2  | 1:D:271:PRO:O    | 2.05                     | 0.55              |
| 1:A:127:ASP:OD1  | 1:A:239:PRO:CD   | 2.44                     | 0.55              |
| 1:A:250:PHE:CD1  | 1:A:250:PHE:N    | 2.73                     | 0.55              |
| 1:A:307:MET:HG3  | 1:A:308:SER:N    | 2.21                     | 0.55              |
| 1:B:301:TYR:CD2  | 1:B:302:TYR:N    | 2.75                     | 0.55              |
| 1:B:313:TYR:CE1  | 1:B:332:VAL:HG23 | 2.37                     | 0.55              |
| 1:D:226:TYR:HE2  | 1:D:228:ALA:CB   | 2.18                     | 0.55              |
| 1:A:40:TYR:CE2   | 1:A:42:ARG:NH2   | 2.74                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:74:ASP:C     | 1:C:76:GLN:N     | 2.58                     | 0.55              |
| 1:B:24:SER:H     | 1:B:35:ASN:CG    | 2.14                     | 0.55              |
| 1:A:200:GLN:NE2  | 1:A:250:PHE:CZ   | 2.75                     | 0.55              |
| 1:A:271:PRO:CA   | 1:A:299:ALA:CB   | 2.66                     | 0.55              |
| 1:B:14:TYR:CA    | 1:B:340:PHE:HE2  | 2.18                     | 0.55              |
| 1:B:264:GLN:HA   | 1:B:270:ARG:HB2  | 1.89                     | 0.55              |
| 1:A:166:ALA:O    | 1:A:168:ARG:N    | 2.39                     | 0.55              |
| 1:B:155:VAL:HG22 | 1:B:155:VAL:O    | 1.94                     | 0.55              |
| 1:C:115:LEU:HD22 | 1:C:296:GLU:OE2  | 2.07                     | 0.55              |
| 1:D:191:TYR:HD1  | 1:D:213:GLN:O    | 1.89                     | 0.55              |
| 1:A:130:VAL:O    | 1:A:130:VAL:HG23 | 2.06                     | 0.55              |
| 1:C:153:PHE:N    | 1:C:153:PHE:CD1  | 2.72                     | 0.55              |
| 1:C:211:ALA:C    | 1:C:212:GLU:HG3  | 2.30                     | 0.55              |
| 1:D:40:TYR:N     | 1:D:40:TYR:HD1   | 2.04                     | 0.55              |
| 1:A:86:ALA:CB    | 1:C:336:ILE:HG13 | 2.33                     | 0.55              |
| 1:A:104:VAL:N    | 1:A:156:GLN:OE1  | 2.39                     | 0.55              |
| 1:A:219:LYS:HA   | 1:A:227:LEU:O    | 2.07                     | 0.55              |
| 1:D:13:LEU:HG    | 1:D:13:LEU:O     | 2.07                     | 0.55              |
| 1:D:111:TYR:CD2  | 1:D:219:LYS:HG2  | 2.42                     | 0.55              |
| 1:A:22:TYR:HD2   | 1:A:38:MET:HG3   | 1.63                     | 0.54              |
| 1:A:85:PHE:CE2   | 1:A:101:ASN:ND2  | 2.76                     | 0.54              |
| 1:B:2:GLU:CD     | 1:B:5:ASN:HB2    | 2.32                     | 0.54              |
| 1:C:24:SER:HB3   | 1:C:31:SER:CB    | 2.37                     | 0.54              |
| 1:C:69:ASN:ND2   | 1:C:77:THR:H     | 2.05                     | 0.54              |
| 1:C:85:PHE:CD2   | 1:C:101:ASN:ND2  | 2.76                     | 0.54              |
| 1:D:270:ARG:HD2  | 1:D:302:TYR:OH   | 2.07                     | 0.54              |
| 1:D:313:TYR:CD1  | 1:D:332:VAL:HG13 | 2.42                     | 0.54              |
| 1:A:71:GLU:CD    | 1:B:100:ARG:HH21 | 2.15                     | 0.54              |
| 1:B:242:ASN:C    | 1:B:244:PHE:H    | 2.12                     | 0.54              |
| 1:C:198:ASN:O    | 1:C:200:GLN:N    | 2.40                     | 0.54              |
| 1:A:105:VAL:O    | 1:A:105:VAL:HG13 | 2.07                     | 0.54              |
| 1:A:318:ILE:HG13 | 1:A:326:VAL:HG12 | 1.88                     | 0.54              |
| 1:B:76:GLN:O     | 1:B:77:THR:C     | 2.47                     | 0.54              |
| 1:C:20:LEU:HB3   | 1:C:38:MET:HB2   | 1.90                     | 0.54              |
| 1:C:144:PHE:HB2  | 1:C:151:LEU:HD23 | 1.88                     | 0.54              |
| 1:C:167:ARG:HD2  | 1:C:239:PRO:HB3  | 1.90                     | 0.54              |
| 1:D:86:ALA:O     | 1:D:97:ASP:CB    | 2.55                     | 0.54              |
| 1:D:167:ARG:O    | 1:D:167:ARG:CG   | 2.48                     | 0.54              |
| 1:A:1:ALA:O      | 1:A:3:ILE:CG2    | 2.55                     | 0.54              |
| 1:B:4:TYR:CE2    | 1:B:6:LYS:CB     | 2.86                     | 0.54              |
| 1:C:220:TYR:HE1  | 1:C:222:ALA:HB3  | 1.66                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:144:PHE:CE2  | 1:D:145:PHE:HB2  | 2.42                     | 0.54              |
| 1:D:167:ARG:CG   | 1:D:167:ARG:NH1  | 2.68                     | 0.54              |
| 1:B:231:TYR:CD1  | 1:B:231:TYR:C    | 2.79                     | 0.54              |
| 1:C:242:ASN:CG   | 1:C:245:THR:OG1  | 2.51                     | 0.54              |
| 1:C:308:SER:C    | 1:C:309:THR:CG2  | 2.81                     | 0.54              |
| 1:D:137:ALA:O    | 1:D:156:GLN:HA   | 2.07                     | 0.54              |
| 1:A:39:THR:O     | 1:A:67:GLY:HA3   | 2.06                     | 0.54              |
| 1:B:1:ALA:HB2    | 1:C:4:TYR:CD2    | 2.43                     | 0.54              |
| 1:B:141:ASN:OD1  | 1:B:153:PHE:CE1  | 2.59                     | 0.54              |
| 1:C:42:ARG:NH1   | 1:C:82:ARG:HH21  | 1.96                     | 0.54              |
| 1:C:274:ALA:HB3  | 1:C:296:GLU:CD   | 2.33                     | 0.54              |
| 1:D:115:LEU:HD12 | 1:D:296:GLU:HG3  | 1.89                     | 0.54              |
| 1:D:223:ASN:O    | 1:D:224:ASN:CB   | 2.41                     | 0.54              |
| 1:A:52:ASN:C     | 1:A:52:ASN:OD1   | 2.50                     | 0.54              |
| 1:A:226:TYR:C    | 1:A:226:TYR:CD2  | 2.82                     | 0.54              |
| 1:A:296:GLU:HG2  | 1:A:297:VAL:H    | 1.72                     | 0.54              |
| 1:B:271:PRO:HA   | 1:B:299:ALA:CB   | 2.37                     | 0.54              |
| 1:C:51:ILE:O     | 1:C:52:ASN:HB3   | 2.08                     | 0.54              |
| 1:D:157:TYR:CD2  | 1:D:157:TYR:N    | 2.75                     | 0.54              |
| 1:D:163:ARG:HD2  | 1:D:168:ARG:O    | 2.08                     | 0.54              |
| 1:D:280:ALA:O    | 1:D:288:ASP:HA   | 2.07                     | 0.54              |
| 1:A:4:TYR:CD2    | 1:A:5:ASN:N      | 2.76                     | 0.54              |
| 1:A:65:PHE:CG    | 1:B:61:TRP:CZ2   | 2.95                     | 0.54              |
| 1:B:109:LEU:HD11 | 1:B:122:THR:HB   | 1.90                     | 0.54              |
| 1:B:110:GLY:C    | 1:B:112:THR:H    | 2.15                     | 0.54              |
| 1:B:167:ARG:HD2  | 1:B:239:PRO:HB2  | 1.90                     | 0.54              |
| 1:B:277:LYS:HE3  | 1:B:293:ASN:HD21 | 1.72                     | 0.54              |
| 1:C:90:TYR:CD2   | 1:C:93:VAL:CG2   | 2.90                     | 0.54              |
| 1:C:114:MET:HE2  | 1:C:226:TYR:CE1  | 2.43                     | 0.54              |
| 1:A:223:ASN:HD22 | 1:A:223:ASN:N    | 2.06                     | 0.54              |
| 1:A:336:ILE:HD11 | 1:B:87:GLY:CA    | 2.37                     | 0.54              |
| 1:B:115:LEU:CD1  | 1:B:119:GLY:CA   | 2.50                     | 0.54              |
| 1:B:265:PHE:HB2  | 1:B:269:LEU:O    | 2.08                     | 0.54              |
| 1:C:240:ILE:HD13 | 1:C:251:ALA:H    | 1.70                     | 0.54              |
| 1:C:263:TYR:CD2  | 1:C:265:PHE:CZ   | 2.95                     | 0.54              |
| 1:D:102:TYR:CD1  | 1:D:106:TYR:CD2  | 2.96                     | 0.54              |
| 1:D:279:LYS:HE3  | 1:D:281:LYS:HZ3  | 1.69                     | 0.54              |
| 1:A:26:GLY:O     | 1:A:28:GLY:N     | 2.41                     | 0.54              |
| 1:A:318:ILE:HG13 | 1:A:326:VAL:CG1  | 2.38                     | 0.54              |
| 1:B:48:GLU:HA    | 1:B:58:TYR:HA    | 1.90                     | 0.54              |
| 1:D:319:ASP:CG   | 1:D:320:SER:N    | 2.61                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:21:HIS:ND1   | 1:A:36:GLY:C     | 2.66                     | 0.53              |
| 1:A:311:VAL:CG2  | 1:A:334:VAL:HG22 | 2.38                     | 0.53              |
| 1:B:65:PHE:CE2   | 1:C:61:TRP:CZ2   | 2.96                     | 0.53              |
| 1:B:112:THR:CG2  | 1:B:230:ASN:CG   | 2.81                     | 0.53              |
| 1:B:141:ASN:CG   | 1:B:153:PHE:CE1  | 2.83                     | 0.53              |
| 1:B:208:GLY:HA3  | 1:B:236:ASN:ND2  | 2.23                     | 0.53              |
| 1:B:235:ARG:HD3  | 1:B:235:ARG:N    | 2.19                     | 0.53              |
| 1:A:65:PHE:CD1   | 1:B:61:TRP:CZ2   | 2.89                     | 0.53              |
| 1:A:96:PHE:O     | 1:A:97:ASP:HB3   | 2.07                     | 0.53              |
| 1:A:293:ASN:ND2  | 1:A:317:GLN:CB   | 2.66                     | 0.53              |
| 1:B:63:TYR:HE2   | 1:B:79:ASN:HB3   | 1.73                     | 0.53              |
| 1:C:23:PHE:CA    | 1:C:35:ASN:HD22  | 2.15                     | 0.53              |
| 1:C:85:PHE:CD2   | 1:C:101:ASN:HB2  | 2.33                     | 0.53              |
| 1:D:302:TYR:C    | 1:D:304:ASN:N    | 2.61                     | 0.53              |
| 1:A:4:TYR:CD2    | 1:A:4:TYR:C      | 2.86                     | 0.53              |
| 1:B:268:GLY:O    | 1:B:301:TYR:HD2  | 1.92                     | 0.53              |
| 1:C:37:ASP:O     | 1:C:38:MET:HG2   | 2.07                     | 0.53              |
| 1:D:211:ALA:C    | 1:D:212:GLU:HG3  | 2.33                     | 0.53              |
| 1:D:208:GLY:HA3  | 1:D:236:ASN:HD22 | 1.72                     | 0.53              |
| 1:B:4:TYR:HE2    | 1:B:6:LYS:CB     | 2.19                     | 0.53              |
| 1:C:223:ASN:CB   | 1:C:225:ILE:HD12 | 2.37                     | 0.53              |
| 1:C:286:ILE:HG21 | 1:C:323:LYS:HB3  | 1.91                     | 0.53              |
| 1:D:155:VAL:O    | 1:D:155:VAL:CG1  | 2.54                     | 0.53              |
| 1:A:166:ALA:C    | 1:A:168:ARG:H    | 2.16                     | 0.53              |
| 1:B:27:ASN:O     | 1:B:27:ASN:CG    | 2.50                     | 0.53              |
| 1:B:196:ARG:HD3  | 1:B:208:GLY:O    | 2.08                     | 0.53              |
| 1:B:204:PRO:HD2  | 1:B:248:SER:O    | 2.09                     | 0.53              |
| 1:D:100:ARG:HA   | 1:D:134:GLY:HA2  | 1.89                     | 0.53              |
| 1:D:160:LYS:CB   | 1:D:172:ASP:OD1  | 2.57                     | 0.53              |
| 1:D:293:ASN:HD22 | 1:D:317:GLN:HB3  | 1.73                     | 0.53              |
| 1:A:62:GLU:OE2   | 1:A:82:ARG:NH2   | 2.41                     | 0.53              |
| 1:A:82:ARG:HH11  | 1:A:82:ARG:CG    | 2.21                     | 0.53              |
| 1:B:205:LEU:HD21 | 1:B:247:THR:CG2  | 2.36                     | 0.53              |
| 1:D:127:ASP:O    | 1:D:127:ASP:CG   | 2.45                     | 0.53              |
| 1:D:182:TYR:CZ   | 1:D:183:GLU:HB3  | 2.44                     | 0.53              |
| 1:A:16:LYS:HG2   | 1:A:42:ARG:HB2   | 1.91                     | 0.53              |
| 1:A:51:ILE:CG2   | 1:C:304:ASN:HD22 | 2.15                     | 0.53              |
| 1:A:72:GLY:O     | 1:A:74:ASP:N     | 2.42                     | 0.53              |
| 1:A:163:ARG:NH1  | 1:C:70:SER:H     | 2.07                     | 0.53              |
| 1:B:273:ILE:HG23 | 1:B:274:ALA:N    | 2.23                     | 0.53              |
| 1:B:25:LYS:O     | 1:B:27:ASN:N     | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:118:PHE:CZ   | 1:B:333:ALA:HB2  | 2.43                     | 0.53              |
| 1:D:208:GLY:HA3  | 1:D:236:ASN:HD21 | 1.73                     | 0.53              |
| 1:D:273:ILE:HD13 | 1:D:297:VAL:HG23 | 1.89                     | 0.53              |
| 1:B:18:VAL:O     | 1:B:39:THR:HA    | 2.09                     | 0.53              |
| 1:B:54:ASP:HB2   | 1:B:90:TYR:CE1   | 2.44                     | 0.53              |
| 1:B:85:PHE:CD2   | 1:B:101:ASN:HB2  | 2.44                     | 0.53              |
| 1:B:265:PHE:N    | 1:B:269:LEU:O    | 2.38                     | 0.53              |
| 1:C:18:VAL:CG1   | 1:C:40:TYR:CZ    | 2.82                     | 0.53              |
| 1:C:283:VAL:CG2  | 1:C:287:GLY:O    | 2.52                     | 0.53              |
| 1:D:115:LEU:H    | 1:D:115:LEU:HD23 | 0.44                     | 0.53              |
| 1:A:136:VAL:CG2  | 1:A:156:GLN:HE21 | 2.23                     | 0.52              |
| 1:B:300:THR:HG21 | 1:B:302:TYR:HE1  | 1.69                     | 0.52              |
| 1:D:158:LEU:HB3  | 1:D:173:GLY:CA   | 2.39                     | 0.52              |
| 1:D:165:THR:CG2  | 1:D:166:ALA:N    | 2.72                     | 0.52              |
| 1:D:278:SER:HB3  | 1:D:292:VAL:CG2  | 2.38                     | 0.52              |
| 1:A:23:PHE:O     | 1:A:24:SER:OG    | 2.22                     | 0.52              |
| 1:A:83:LEU:HD23  | 1:A:101:ASN:HA   | 1.91                     | 0.52              |
| 1:A:100:ARG:HG2  | 1:A:134:GLY:CA   | 2.31                     | 0.52              |
| 1:A:279:LYS:HZ3  | 1:A:279:LYS:HB3  | 1.72                     | 0.52              |
| 1:A:301:TYR:O    | 1:A:308:SER:HA   | 2.09                     | 0.52              |
| 1:B:291:LEU:C    | 1:B:292:VAL:HG23 | 2.32                     | 0.52              |
| 1:C:172:ASP:C    | 1:C:194:ALA:HB2  | 2.29                     | 0.52              |
| 1:C:269:LEU:HD11 | 1:C:299:ALA:HB1  | 1.92                     | 0.52              |
| 1:C:294:TYR:CD1  | 1:C:314:ILE:CD1  | 2.92                     | 0.52              |
| 1:C:318:ILE:CG2  | 1:C:319:ASP:H    | 2.17                     | 0.52              |
| 1:A:161:ASN:HB2  | 1:A:170:ASN:OD1  | 2.09                     | 0.52              |
| 1:A:214:TRP:CE2  | 1:A:233:GLU:HB2  | 2.44                     | 0.52              |
| 1:A:313:TYR:HB2  | 1:A:332:VAL:HG22 | 1.90                     | 0.52              |
| 1:B:5:ASN:HA     | 1:B:10:LYS:HA    | 1.91                     | 0.52              |
| 1:B:48:GLU:OE1   | 1:B:56:THR:HG21  | 2.08                     | 0.52              |
| 1:B:306:ASN:CG   | 1:C:9:ASN:HB2    | 2.33                     | 0.52              |
| 1:C:58:TYR:O     | 1:C:58:TYR:HD1   | 1.92                     | 0.52              |
| 1:D:36:GLY:O     | 1:D:37:ASP:C     | 2.52                     | 0.52              |
| 1:D:121:ASP:C    | 1:D:123:ALA:H    | 2.16                     | 0.52              |
| 1:A:340:PHE:CE1  | 1:B:45:PHE:CE2   | 2.97                     | 0.52              |
| 1:A:242:ASN:O    | 1:A:243:LYS:C    | 2.50                     | 0.52              |
| 1:B:267:PHE:CD1  | 1:B:267:PHE:N    | 2.73                     | 0.52              |
| 1:C:82:ARG:HG2   | 1:C:82:ARG:HH11  | 1.74                     | 0.52              |
| 1:D:12:ASP:HB3   | 1:D:46:LYS:O     | 2.08                     | 0.52              |
| 1:A:116:PRO:O    | 1:A:310:TYR:CE2  | 2.63                     | 0.52              |
| 1:A:214:TRP:CZ2  | 1:A:233:GLU:HB2  | 2.44                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:110:GLY:C    | 1:B:112:THR:N    | 2.67                     | 0.52              |
| 1:B:130:VAL:HG13 | 1:B:213:GLN:CD   | 2.25                     | 0.52              |
| 1:B:212:GLU:H    | 1:B:235:ARG:HB2  | 1.75                     | 0.52              |
| 1:A:71:GLU:CD    | 1:B:132:ARG:NH2  | 2.68                     | 0.52              |
| 1:A:197:THR:O    | 1:A:200:GLN:N    | 2.43                     | 0.52              |
| 1:B:172:ASP:O    | 1:B:194:ALA:HA   | 2.10                     | 0.52              |
| 1:C:64:ASN:ND2   | 1:C:80:LYS:HE2   | 2.24                     | 0.52              |
| 1:A:331:THR:CG2  | 1:A:332:VAL:N    | 2.71                     | 0.52              |
| 1:B:104:VAL:HG21 | 1:B:176:GLY:HA2  | 1.92                     | 0.52              |
| 1:C:193:ALA:HB2  | 1:C:212:GLU:HB3  | 1.91                     | 0.52              |
| 1:B:1:ALA:CB     | 1:C:4:TYR:CD2    | 2.93                     | 0.52              |
| 1:B:269:LEU:HD21 | 1:B:271:PRO:HD3  | 1.91                     | 0.52              |
| 1:C:318:ILE:HG13 | 1:C:326:VAL:CG1  | 2.39                     | 0.52              |
| 1:D:104:VAL:N    | 1:D:156:GLN:OE1  | 2.43                     | 0.52              |
| 1:B:118:PHE:C    | 1:B:119:GLY:O    | 2.52                     | 0.52              |
| 1:B:186:GLY:HA3  | 1:B:219:LYS:HE3  | 1.92                     | 0.52              |
| 1:C:63:TYR:CE1   | 1:C:80:LYS:C     | 2.87                     | 0.52              |
| 1:C:196:ARG:NH2  | 1:C:250:PHE:CD1  | 2.78                     | 0.52              |
| 1:D:286:ILE:CG2  | 1:D:323:LYS:HB3  | 2.39                     | 0.52              |
| 1:A:163:ARG:NH1  | 1:C:70:SER:N     | 2.58                     | 0.51              |
| 1:A:286:ILE:CD1  | 1:A:286:ILE:N    | 2.71                     | 0.51              |
| 1:C:203:GLN:CB   | 1:C:248:SER:O    | 2.58                     | 0.51              |
| 1:C:240:ILE:CD1  | 1:C:251:ALA:CB   | 2.88                     | 0.51              |
| 1:C:242:ASN:ND2  | 1:C:245:THR:OG1  | 2.43                     | 0.51              |
| 1:D:48:GLU:CD    | 1:D:56:THR:HG23  | 2.33                     | 0.51              |
| 1:D:130:VAL:CG1  | 1:D:213:GLN:CD   | 2.83                     | 0.51              |
| 1:A:102:TYR:CE1  | 1:A:106:TYR:CE2  | 2.99                     | 0.51              |
| 1:D:48:GLU:HG2   | 1:D:49:THR:N     | 2.24                     | 0.51              |
| 1:A:90:TYR:C     | 1:A:90:TYR:CD1   | 2.87                     | 0.51              |
| 1:A:284:GLU:H    | 1:A:284:GLU:CD   | 2.09                     | 0.51              |
| 1:B:63:TYR:CE2   | 1:B:79:ASN:HB3   | 2.45                     | 0.51              |
| 1:B:215:ALA:C    | 1:B:216:THR:HG23 | 2.34                     | 0.51              |
| 1:B:294:TYR:CE1  | 1:B:314:ILE:CD1  | 2.87                     | 0.51              |
| 1:D:160:LYS:HD3  | 1:D:162:GLU:OE2  | 2.11                     | 0.51              |
| 1:A:22:TYR:CE1   | 1:A:333:ALA:CB   | 2.91                     | 0.51              |
| 1:A:56:THR:O     | 1:A:88:LEU:HA    | 2.10                     | 0.51              |
| 1:A:132:ARG:NH2  | 1:C:71:GLU:CD    | 2.68                     | 0.51              |
| 1:B:14:TYR:HA    | 1:B:340:PHE:CE2  | 2.46                     | 0.51              |
| 1:D:31:SER:HA    | 1:D:329:ASP:H    | 1.74                     | 0.51              |
| 1:A:72:GLY:O     | 1:A:73:ALA:C     | 2.54                     | 0.51              |
| 1:A:82:ARG:CG    | 1:A:132:ARG:NH2  | 2.73                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:139:TYR:CD1  | 1:A:140:ARG:N    | 2.79                     | 0.51              |
| 1:A:163:ARG:HG3  | 1:A:169:SER:OG   | 2.11                     | 0.51              |
| 1:B:5:ASN:O      | 1:B:5:ASN:OD1    | 2.27                     | 0.51              |
| 1:B:48:GLU:HG3   | 1:B:56:THR:HG22  | 1.93                     | 0.51              |
| 1:B:167:ARG:O    | 1:B:167:ARG:CG   | 2.55                     | 0.51              |
| 1:B:169:SER:O    | 1:B:170:ASN:HB3  | 2.09                     | 0.51              |
| 1:B:273:ILE:HD12 | 1:B:296:GLU:O    | 2.10                     | 0.51              |
| 1:C:152:ASN:ND2  | 1:C:152:ASN:N    | 2.58                     | 0.51              |
| 1:C:167:ARG:HD2  | 1:C:239:PRO:HB2  | 1.92                     | 0.51              |
| 1:D:18:VAL:HG11  | 1:D:40:TYR:CE1   | 2.45                     | 0.51              |
| 1:A:272:SER:N    | 1:A:298:GLY:O    | 2.42                     | 0.51              |
| 1:A:293:ASN:CB   | 1:A:317:GLN:HB2  | 2.40                     | 0.51              |
| 1:C:3:ILE:HD13   | 1:C:13:LEU:CB    | 2.40                     | 0.51              |
| 1:C:296:GLU:HG2  | 1:C:297:VAL:N    | 2.26                     | 0.51              |
| 1:D:3:ILE:HD13   | 1:D:13:LEU:HB3   | 1.92                     | 0.51              |
| 1:D:241:THR:HG22 | 1:D:242:ASN:N    | 2.25                     | 0.51              |
| 1:B:54:ASP:O     | 1:B:90:TYR:HD1   | 1.92                     | 0.51              |
| 1:B:229:ALA:CB   | 1:B:258:LEU:O    | 2.55                     | 0.51              |
| 1:B:318:ILE:CG2  | 1:B:319:ASP:N    | 2.73                     | 0.51              |
| 1:B:332:VAL:O    | 1:B:332:VAL:HG13 | 1.97                     | 0.51              |
| 1:C:58:TYR:HD1   | 1:C:58:TYR:C     | 2.18                     | 0.51              |
| 1:D:30:ASN:O     | 1:D:30:ASN:CG    | 2.53                     | 0.51              |
| 1:A:172:ASP:O    | 1:A:194:ALA:HB2  | 1.99                     | 0.51              |
| 1:A:237:ALA:O    | 1:A:239:PRO:HD3  | 2.11                     | 0.51              |
| 1:A:245:THR:O    | 1:A:246:ASN:O    | 2.28                     | 0.51              |
| 1:B:130:VAL:HG12 | 1:B:213:GLN:CD   | 2.33                     | 0.51              |
| 1:B:138:THR:OG1  | 1:B:156:GLN:NE2  | 2.42                     | 0.51              |
| 1:B:167:ARG:CG   | 1:B:167:ARG:NH1  | 2.55                     | 0.51              |
| 1:B:284:GLU:O    | 1:B:286:ILE:HD13 | 2.10                     | 0.51              |
| 1:C:113:ASP:C    | 1:C:114:MET:HG2  | 2.35                     | 0.51              |
| 1:C:309:THR:HG22 | 1:C:336:ILE:CA   | 2.26                     | 0.51              |
| 1:D:76:GLN:O     | 1:D:79:ASN:HB2   | 2.11                     | 0.51              |
| 1:D:109:LEU:O    | 1:D:110:GLY:O    | 2.29                     | 0.51              |
| 1:D:265:PHE:HB3  | 1:D:267:PHE:CE1  | 2.46                     | 0.51              |
| 1:D:313:TYR:CZ   | 1:D:315:ILE:HG13 | 2.46                     | 0.51              |
| 1:B:9:ASN:HA     | 1:B:49:THR:HA    | 1.92                     | 0.51              |
| 1:C:196:ARG:HH22 | 1:C:250:PHE:HB2  | 1.74                     | 0.51              |
| 1:C:205:LEU:HA   | 1:C:284:GLU:HG3  | 1.92                     | 0.51              |
| 1:C:123:ALA:HB1  | 1:C:130:VAL:O    | 2.11                     | 0.51              |
| 1:C:161:ASN:HB2  | 1:C:170:ASN:ND2  | 2.26                     | 0.51              |
| 1:A:32:TYR:CD2   | 1:A:32:TYR:C     | 2.87                     | 0.50              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:65:PHE:CD2  | 1:B:61:TRP:CZ2   | 2.99                     | 0.50              |
| 1:A:105:VAL:O   | 1:A:105:VAL:CG1  | 2.50                     | 0.50              |
| 1:A:153:PHE:CD1 | 1:A:153:PHE:N    | 2.54                     | 0.50              |
| 1:B:114:MET:CE  | 1:B:226:TYR:CD1  | 2.92                     | 0.50              |
| 1:B:275:TYR:HE1 | 1:B:295:PHE:CE1  | 2.29                     | 0.50              |
| 1:D:90:TYR:HD2  | 1:D:93:VAL:HG23  | 1.76                     | 0.50              |
| 1:A:170:ASN:ND2 | 1:A:171:GLY:O    | 2.44                     | 0.50              |
| 1:B:242:ASN:O   | 1:B:243:LYS:C    | 2.51                     | 0.50              |
| 1:B:296:GLU:CG  | 1:B:314:ILE:HD13 | 2.42                     | 0.50              |
| 1:C:339:GLN:HG3 | 1:C:339:GLN:O    | 2.07                     | 0.50              |
| 1:D:102:TYR:HD2 | 1:D:102:TYR:N    | 2.07                     | 0.50              |
| 1:D:127:ASP:OD1 | 1:D:127:ASP:C    | 2.53                     | 0.50              |
| 1:A:139:TYR:O   | 1:A:154:ALA:CA   | 2.60                     | 0.50              |
| 1:B:231:TYR:HA  | 1:B:256:ASP:O    | 2.11                     | 0.50              |
| 1:B:263:TYR:HD1 | 1:B:264:GLN:H    | 1.58                     | 0.50              |
| 1:C:25:LYS:NZ   | 1:C:25:LYS:CB    | 2.71                     | 0.50              |
| 1:C:85:PHE:HE2  | 1:C:101:ASN:ND2  | 2.10                     | 0.50              |
| 1:C:160:LYS:CA  | 1:C:160:LYS:CE   | 2.88                     | 0.50              |
| 1:C:263:TYR:CD1 | 1:C:264:GLN:N    | 2.78                     | 0.50              |
| 1:C:307:MET:CG  | 1:C:308:SER:N    | 2.51                     | 0.50              |
| 1:D:293:ASN:O   | 1:D:317:GLN:N    | 2.44                     | 0.50              |
| 1:A:61:TRP:CH2  | 1:C:65:PHE:HE1   | 2.26                     | 0.50              |
| 1:A:319:ASP:C   | 1:A:321:ASP:N    | 2.68                     | 0.50              |
| 1:B:220:TYR:C   | 1:B:220:TYR:CD2  | 2.89                     | 0.50              |
| 1:B:338:TYR:CG  | 1:B:339:GLN:N    | 2.79                     | 0.50              |
| 1:D:87:GLY:HA3  | 1:D:97:ASP:HB3   | 1.93                     | 0.50              |
| 1:B:191:TYR:CD1 | 1:B:191:TYR:C    | 2.84                     | 0.50              |
| 1:D:204:PRO:HG2 | 1:D:248:SER:O    | 2.11                     | 0.50              |
| 1:D:229:ALA:HA  | 1:D:258:LEU:O    | 2.12                     | 0.50              |
| 1:D:307:MET:CG  | 1:D:308:SER:H    | 2.16                     | 0.50              |
| 1:A:1:ALA:HB1   | 1:B:4:TYR:CZ     | 2.40                     | 0.50              |
| 1:A:167:ARG:NH1 | 1:A:167:ARG:HG2  | 2.17                     | 0.50              |
| 1:B:58:TYR:CE2  | 1:B:87:GLY:C     | 2.86                     | 0.50              |
| 1:B:137:ALA:O   | 1:B:156:GLN:HA   | 2.11                     | 0.50              |
| 1:B:179:SER:CB  | 1:B:188:VAL:HG13 | 2.42                     | 0.50              |
| 1:A:65:PHE:CE2  | 1:B:61:TRP:CH2   | 3.00                     | 0.50              |
| 1:A:66:GLN:CG   | 1:A:78:GLY:O     | 2.58                     | 0.50              |
| 1:D:85:PHE:HE1  | 1:D:101:ASN:ND2  | 2.09                     | 0.50              |
| 1:D:239:PRO:HB3 | 1:D:250:PHE:HE2  | 1.77                     | 0.50              |
| 1:D:280:ALA:HB2 | 1:D:291:LEU:HD11 | 1.94                     | 0.50              |
| 1:A:74:ASP:C    | 1:A:76:GLN:H     | 2.20                     | 0.50              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:1:ALA:CB    | 1:C:4:TYR:CE2    | 2.93                     | 0.50              |
| 1:B:63:TYR:CD2  | 1:B:64:ASN:N     | 2.80                     | 0.50              |
| 1:B:106:TYR:CD2 | 1:B:106:TYR:O    | 2.64                     | 0.50              |
| 1:B:123:ALA:CA  | 1:B:130:VAL:HG23 | 2.37                     | 0.50              |
| 1:B:143:ASN:OD1 | 1:B:149:ASP:HA   | 2.12                     | 0.50              |
| 1:B:231:TYR:HD1 | 1:B:232:GLY:H    | 1.58                     | 0.50              |
| 1:C:112:THR:CG2 | 1:C:230:ASN:CG   | 2.82                     | 0.50              |
| 1:C:136:VAL:CG1 | 1:C:158:LEU:CD1  | 2.90                     | 0.50              |
| 1:C:262:GLN:HG2 | 1:C:272:SER:HB2  | 1.92                     | 0.50              |
| 1:D:160:LYS:HA  | 1:D:171:GLY:O    | 2.12                     | 0.50              |
| 1:A:123:ALA:HA  | 1:A:130:VAL:HG21 | 1.94                     | 0.50              |
| 1:B:52:ASN:C    | 1:B:52:ASN:OD1   | 2.55                     | 0.50              |
| 1:C:85:PHE:CD1  | 1:C:85:PHE:C     | 2.90                     | 0.50              |
| 1:C:309:THR:CG2 | 1:C:336:ILE:HA   | 2.25                     | 0.50              |
| 1:D:229:ALA:CA  | 1:D:259:LEU:HD23 | 2.40                     | 0.50              |
| 1:A:319:ASP:O   | 1:A:322:ASN:N    | 2.45                     | 0.49              |
| 1:B:205:LEU:CA  | 1:B:284:GLU:OE2  | 2.59                     | 0.49              |
| 1:D:1:ALA:HB2   | 1:D:340:PHE:OXT  | 2.12                     | 0.49              |
| 1:A:20:LEU:CD1  | 1:A:335:GLY:CA   | 2.87                     | 0.49              |
| 1:A:179:SER:CB  | 1:A:188:VAL:CG1  | 2.90                     | 0.49              |
| 1:A:322:ASN:OD1 | 1:A:322:ASN:O    | 2.28                     | 0.49              |
| 1:B:193:ALA:HB2 | 1:B:212:GLU:HB3  | 1.94                     | 0.49              |
| 1:C:58:TYR:C    | 1:C:58:TYR:CD1   | 2.88                     | 0.49              |
| 1:C:144:PHE:CD1 | 1:C:151:LEU:CD2  | 2.95                     | 0.49              |
| 1:C:222:ALA:O   | 1:C:223:ASN:CB   | 2.47                     | 0.49              |
| 1:D:268:GLY:O   | 1:D:302:TYR:HD2  | 1.95                     | 0.49              |
| 1:D:312:ASP:O   | 1:D:332:VAL:HG12 | 2.12                     | 0.49              |
| 1:A:211:ALA:CB  | 1:A:236:ASN:CB   | 2.71                     | 0.49              |
| 1:A:315:ILE:CA  | 1:A:330:ASP:OD1  | 2.55                     | 0.49              |
| 1:B:6:LYS:O     | 1:B:7:ASP:C      | 2.54                     | 0.49              |
| 1:B:219:LYS:HA  | 1:B:227:LEU:O    | 2.12                     | 0.49              |
| 1:C:141:ASN:OD1 | 1:C:153:PHE:HE1  | 1.94                     | 0.49              |
| 1:D:21:HIS:ND1  | 1:D:37:ASP:HA    | 2.27                     | 0.49              |
| 1:D:115:LEU:CB  | 1:D:116:PRO:CD   | 2.90                     | 0.49              |
| 1:D:301:TYR:CD1 | 1:D:303:PHE:CE1  | 3.01                     | 0.49              |
| 1:A:58:TYR:HA   | 1:C:338:TYR:CE1  | 2.47                     | 0.49              |
| 1:B:22:TYR:C    | 1:B:23:PHE:CD2   | 2.90                     | 0.49              |
| 1:C:83:LEU:HD11 | 1:C:102:TYR:CE2  | 2.43                     | 0.49              |
| 1:C:165:THR:HB  | 1:C:168:ARG:HG2  | 1.94                     | 0.49              |
| 1:C:196:ARG:NH2 | 1:C:250:PHE:HD1  | 2.11                     | 0.49              |
| 1:A:155:VAL:CG2 | 1:A:156:GLN:N    | 2.71                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:119:GLY:HA2  | 1:B:294:TYR:OH   | 2.13                     | 0.49              |
| 1:B:139:TYR:HB3  | 1:B:155:VAL:HG13 | 1.95                     | 0.49              |
| 1:B:226:TYR:HD2  | 1:B:227:LEU:N    | 2.10                     | 0.49              |
| 1:C:130:VAL:HG13 | 1:C:213:GLN:CD   | 2.37                     | 0.49              |
| 1:D:242:ASN:ND2  | 1:D:245:THR:OG1  | 2.45                     | 0.49              |
| 1:D:293:ASN:C    | 1:D:317:GLN:HB2  | 2.38                     | 0.49              |
| 1:A:83:LEU:O     | 1:A:84:ALA:HB2   | 2.11                     | 0.49              |
| 1:A:132:ARG:HH11 | 1:A:132:ARG:CG   | 1.94                     | 0.49              |
| 1:B:179:SER:HB2  | 1:B:188:VAL:HG13 | 1.95                     | 0.49              |
| 1:B:297:VAL:HG12 | 1:B:298:GLY:N    | 2.26                     | 0.49              |
| 1:B:308:SER:O    | 1:B:309:THR:HG23 | 2.12                     | 0.49              |
| 1:C:22:TYR:CZ    | 1:C:38:MET:HE2   | 2.47                     | 0.49              |
| 1:A:55:LEU:HG    | 1:A:56:THR:H     | 1.76                     | 0.49              |
| 1:A:74:ASP:C     | 1:A:76:GLN:N     | 2.70                     | 0.49              |
| 1:A:88:LEU:CD1   | 1:C:303:PHE:HE2  | 2.21                     | 0.49              |
| 1:C:42:ARG:NH1   | 1:C:82:ARG:CZ    | 2.72                     | 0.49              |
| 1:C:100:ARG:CG   | 1:C:133:VAL:O    | 2.59                     | 0.49              |
| 1:C:146:GLY:O    | 1:C:147:LEU:C    | 2.56                     | 0.49              |
| 1:D:198:ASN:O    | 1:D:202:ALA:N    | 2.35                     | 0.49              |
| 1:A:132:ARG:NH2  | 1:C:71:GLU:OE2   | 2.46                     | 0.49              |
| 1:A:151:LEU:HA   | 1:A:179:SER:O    | 2.13                     | 0.49              |
| 1:B:302:TYR:O    | 1:B:304:ASN:N    | 2.43                     | 0.49              |
| 1:B:313:TYR:HE2  | 1:B:315:ILE:HG13 | 1.75                     | 0.49              |
| 1:C:80:LYS:HD3   | 1:C:80:LYS:N     | 2.28                     | 0.49              |
| 1:C:217:GLY:HA3  | 1:C:230:ASN:HD21 | 1.78                     | 0.49              |
| 1:A:259:LEU:O    | 1:A:260:VAL:HG22 | 2.13                     | 0.49              |
| 1:C:86:ALA:O     | 1:C:97:ASP:HA    | 2.12                     | 0.49              |
| 1:C:160:LYS:HA   | 1:C:160:LYS:CE   | 2.31                     | 0.49              |
| 1:C:289:VAL:HG11 | 1:C:323:LYS:CB   | 2.41                     | 0.49              |
| 1:C:314:ILE:HD13 | 1:C:314:ILE:HA   | 1.69                     | 0.49              |
| 1:D:144:PHE:CE2  | 1:D:145:PHE:CD2  | 3.00                     | 0.49              |
| 1:D:307:MET:O    | 1:D:308:SER:CB   | 2.60                     | 0.49              |
| 1:A:24:SER:CB    | 1:A:331:THR:OG1  | 2.61                     | 0.49              |
| 1:A:306:ASN:HD21 | 1:B:9:ASN:ND2    | 2.10                     | 0.49              |
| 1:C:115:LEU:N    | 1:C:115:LEU:HD23 | 2.18                     | 0.49              |
| 1:C:235:ARG:O    | 1:C:237:ALA:HB2  | 2.12                     | 0.49              |
| 1:D:117:GLU:HG2  | 1:D:333:ALA:CB   | 2.43                     | 0.49              |
| 1:D:319:ASP:CG   | 1:D:321:ASP:H    | 2.20                     | 0.48              |
| 1:A:214:TRP:HZ2  | 1:A:233:GLU:OE2  | 1.96                     | 0.48              |
| 1:B:63:TYR:CD2   | 1:B:65:PHE:CD1   | 3.01                     | 0.48              |
| 1:B:118:PHE:O    | 1:B:119:GLY:O    | 2.30                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:313:TYR:CD1  | 1:D:313:TYR:C    | 2.87                     | 0.48              |
| 1:A:18:VAL:HB    | 1:A:40:TYR:CD1   | 2.45                     | 0.48              |
| 1:A:240:ILE:HD13 | 1:A:251:ALA:HB2  | 1.95                     | 0.48              |
| 1:C:139:TYR:HD1  | 1:C:140:ARG:N    | 2.10                     | 0.48              |
| 1:C:144:PHE:HD1  | 1:C:151:LEU:HD23 | 1.78                     | 0.48              |
| 1:C:153:PHE:O    | 1:C:154:ALA:CB   | 2.60                     | 0.48              |
| 1:D:132:ARG:NH1  | 1:D:132:ARG:CB   | 2.75                     | 0.48              |
| 1:D:144:PHE:CD2  | 1:D:145:PHE:HB2  | 2.47                     | 0.48              |
| 1:A:61:TRP:CZ2   | 1:C:65:PHE:HE1   | 2.25                     | 0.48              |
| 1:A:277:LYS:HA   | 1:A:292:VAL:O    | 2.12                     | 0.48              |
| 1:B:304:ASN:ND2  | 1:C:51:ILE:CG2   | 2.77                     | 0.48              |
| 1:A:124:TYR:HB2  | 1:A:127:ASP:HB2  | 1.93                     | 0.48              |
| 1:A:171:GLY:HA3  | 1:A:195:ASP:HB2  | 1.94                     | 0.48              |
| 1:A:281:LYS:O    | 1:A:282:ASP:CB   | 2.51                     | 0.48              |
| 1:B:276:THR:HG21 | 1:B:294:TYR:CZ   | 2.40                     | 0.48              |
| 1:C:139:TYR:O    | 1:C:154:ALA:CA   | 2.61                     | 0.48              |
| 1:C:153:PHE:O    | 1:C:154:ALA:HB2  | 2.12                     | 0.48              |
| 1:C:167:ARG:HG3  | 1:C:167:ARG:NH1  | 2.06                     | 0.48              |
| 1:C:284:GLU:O    | 1:C:286:ILE:HD11 | 2.13                     | 0.48              |
| 1:D:212:GLU:O    | 1:D:234:THR:HA   | 2.13                     | 0.48              |
| 1:D:264:GLN:NE2  | 1:D:268:GLY:HA2  | 2.28                     | 0.48              |
| 1:D:273:ILE:HG23 | 1:D:274:ALA:N    | 2.27                     | 0.48              |
| 1:D:318:ILE:HG23 | 1:D:319:ASP:N    | 1.98                     | 0.48              |
| 1:A:24:SER:OG    | 1:A:331:THR:CB   | 2.60                     | 0.48              |
| 1:A:182:TYR:CD1  | 1:A:182:TYR:C    | 2.88                     | 0.48              |
| 1:B:86:ALA:O     | 1:B:97:ASP:HA    | 2.14                     | 0.48              |
| 1:C:48:GLU:HA    | 1:C:57:GLY:O     | 2.13                     | 0.48              |
| 1:C:163:ARG:CG   | 1:C:163:ARG:HH11 | 2.26                     | 0.48              |
| 1:C:309:THR:HB   | 1:C:335:GLY:O    | 2.14                     | 0.48              |
| 1:D:304:ASN:OD1  | 1:D:307:MET:N    | 2.37                     | 0.48              |
| 1:A:4:TYR:OH     | 1:A:6:LYS:HB2    | 2.14                     | 0.48              |
| 1:A:111:TYR:CZ   | 1:A:188:VAL:CG2  | 2.97                     | 0.48              |
| 1:C:109:LEU:C    | 1:C:111:TYR:H    | 2.21                     | 0.48              |
| 1:D:10:LYS:O     | 1:D:47:GLY:HA2   | 2.13                     | 0.48              |
| 1:B:271:PRO:HA   | 1:B:299:ALA:HB2  | 1.93                     | 0.48              |
| 1:C:136:VAL:HG12 | 1:C:158:LEU:HD13 | 1.96                     | 0.48              |
| 1:C:217:GLY:CA   | 1:C:230:ASN:ND2  | 2.76                     | 0.48              |
| 1:C:275:TYR:CE1  | 1:C:295:PHE:CE1  | 3.02                     | 0.48              |
| 1:A:259:LEU:HD23 | 1:A:259:LEU:N    | 1.83                     | 0.48              |
| 1:A:259:LEU:O    | 1:A:260:VAL:CG2  | 2.62                     | 0.48              |
| 1:A:295:PHE:N    | 1:A:295:PHE:HD1  | 2.10                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:78:GLY:O     | 1:B:79:ASN:C     | 2.51                     | 0.48              |
| 1:B:167:ARG:C    | 1:B:168:ARG:HG2  | 2.39                     | 0.48              |
| 1:B:313:TYR:CE2  | 1:B:315:ILE:HG13 | 2.48                     | 0.48              |
| 1:C:52:ASN:OD1   | 1:C:53:SER:N     | 2.47                     | 0.48              |
| 1:C:60:GLN:HG2   | 1:C:61:TRP:H     | 1.72                     | 0.48              |
| 1:C:251:ALA:O    | 1:C:253:LYS:N    | 2.46                     | 0.48              |
| 1:D:18:VAL:CG1   | 1:D:40:TYR:CE1   | 2.96                     | 0.48              |
| 1:D:112:THR:HG21 | 1:D:230:ASN:OD1  | 2.12                     | 0.48              |
| 1:D:291:LEU:C    | 1:D:292:VAL:HG22 | 2.39                     | 0.48              |
| 1:A:136:VAL:HG23 | 1:A:137:ALA:N    | 2.23                     | 0.48              |
| 1:C:3:ILE:CD1    | 1:C:13:LEU:CB    | 2.91                     | 0.48              |
| 1:D:5:ASN:C      | 1:D:6:LYS:HG2    | 2.38                     | 0.48              |
| 1:D:118:PHE:HZ   | 1:D:333:ALA:HB2  | 1.79                     | 0.48              |
| 1:A:82:ARG:HG2   | 1:A:132:ARG:NH2  | 2.29                     | 0.47              |
| 1:B:264:GLN:OE1  | 1:B:270:ARG:NE   | 2.44                     | 0.47              |
| 1:D:16:LYS:HG2   | 1:D:42:ARG:HB2   | 1.96                     | 0.47              |
| 1:D:340:PHE:CD1  | 1:D:340:PHE:N    | 2.82                     | 0.47              |
| 1:A:88:LEU:CD1   | 1:C:303:PHE:CE2  | 2.97                     | 0.47              |
| 1:A:104:VAL:O    | 1:A:105:VAL:C    | 2.57                     | 0.47              |
| 1:A:192:GLY:O    | 1:A:193:ALA:HB2  | 2.14                     | 0.47              |
| 1:A:295:PHE:N    | 1:A:295:PHE:CD1  | 2.80                     | 0.47              |
| 1:C:332:VAL:CG1  | 1:C:333:ALA:N    | 2.76                     | 0.47              |
| 1:D:37:ASP:OD1   | 1:D:38:MET:N     | 2.48                     | 0.47              |
| 1:D:124:TYR:CD2  | 1:D:239:PRO:HD2  | 2.50                     | 0.47              |
| 1:D:273:ILE:HD11 | 1:D:297:VAL:HG22 | 1.95                     | 0.47              |
| 1:A:104:VAL:HG11 | 1:A:156:GLN:HB2  | 1.94                     | 0.47              |
| 1:A:116:PRO:O    | 1:A:117:GLU:HB2  | 2.14                     | 0.47              |
| 1:B:54:ASP:HB2   | 1:B:90:TYR:HE1   | 1.79                     | 0.47              |
| 1:B:322:ASN:OD1  | 1:B:325:GLY:N    | 2.45                     | 0.47              |
| 1:A:109:LEU:HD13 | 1:A:122:THR:HB   | 1.95                     | 0.47              |
| 1:C:211:ALA:C    | 1:C:212:GLU:HG2  | 2.38                     | 0.47              |
| 1:C:229:ALA:HA   | 1:C:258:LEU:O    | 2.14                     | 0.47              |
| 1:D:253:LYS:HD2  | 1:D:254:THR:H    | 1.80                     | 0.47              |
| 1:D:130:VAL:HG13 | 1:D:213:GLN:NE2  | 2.29                     | 0.47              |
| 1:D:160:LYS:HB3  | 1:D:172:ASP:OD1  | 2.14                     | 0.47              |
| 1:D:161:ASN:H    | 1:D:170:ASN:ND2  | 2.13                     | 0.47              |
| 1:A:7:ASP:OD2    | 1:C:305:LYS:NZ   | 2.47                     | 0.47              |
| 1:A:22:TYR:CE1   | 1:A:118:PHE:HE1  | 2.33                     | 0.47              |
| 1:A:76:GLN:HE22  | 1:B:79:ASN:HB2   | 1.79                     | 0.47              |
| 1:A:85:PHE:CD1   | 1:A:85:PHE:C     | 2.92                     | 0.47              |
| 1:A:161:ASN:ND2  | 1:A:163:ARG:NH2  | 2.63                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:115:LEU:H    | 1:B:115:LEU:HD23 | 0.56                     | 0.47              |
| 1:B:139:TYR:C    | 1:B:139:TYR:HD2  | 2.16                     | 0.47              |
| 1:B:303:PHE:HB3  | 1:C:51:ILE:HD13  | 1.96                     | 0.47              |
| 1:C:11:VAL:CG1   | 1:C:12:ASP:H     | 2.28                     | 0.47              |
| 1:D:84:ALA:O     | 1:D:100:ARG:N    | 2.43                     | 0.47              |
| 1:A:51:ILE:HD13  | 1:C:303:PHE:CG   | 2.50                     | 0.47              |
| 1:A:130:VAL:CG1  | 1:A:213:GLN:HE22 | 2.18                     | 0.47              |
| 1:A:141:ASN:CB   | 1:A:153:PHE:CD1  | 2.90                     | 0.47              |
| 1:A:258:LEU:O    | 1:A:259:LEU:HD21 | 2.04                     | 0.47              |
| 1:A:270:ARG:HD2  | 1:A:302:TYR:CE2  | 2.49                     | 0.47              |
| 1:A:320:SER:C    | 1:A:322:ASN:N    | 2.64                     | 0.47              |
| 1:B:63:TYR:CE2   | 1:B:65:PHE:CD1   | 3.03                     | 0.47              |
| 1:B:104:VAL:HG11 | 1:B:176:GLY:HA2  | 1.96                     | 0.47              |
| 1:B:112:THR:CG2  | 1:B:230:ASN:CB   | 2.75                     | 0.47              |
| 1:B:255:GLN:C    | 1:B:256:ASP:OD1  | 2.58                     | 0.47              |
| 1:C:105:VAL:O    | 1:C:106:TYR:C    | 2.57                     | 0.47              |
| 1:C:313:TYR:CD1  | 1:C:332:VAL:CG2  | 2.97                     | 0.47              |
| 1:D:83:LEU:HD21  | 1:D:102:TYR:CD2  | 2.48                     | 0.47              |
| 1:D:111:TYR:HE2  | 1:D:188:VAL:HG23 | 1.75                     | 0.47              |
| 1:B:188:VAL:O    | 1:B:216:THR:HA   | 2.15                     | 0.47              |
| 1:C:223:ASN:HB2  | 1:C:225:ILE:HD12 | 1.95                     | 0.47              |
| 1:C:293:ASN:HD22 | 1:C:317:GLN:HB3  | 1.80                     | 0.47              |
| 1:D:184:GLY:O    | 1:D:221:ASP:N    | 2.44                     | 0.47              |
| 1:A:52:ASN:CG    | 1:A:53:SER:N     | 2.71                     | 0.47              |
| 1:B:182:TYR:CD1  | 1:B:182:TYR:C    | 2.87                     | 0.47              |
| 1:C:24:SER:O     | 1:C:25:LYS:C     | 2.58                     | 0.47              |
| 1:C:85:PHE:C     | 1:C:85:PHE:HD1   | 2.23                     | 0.47              |
| 1:A:26:GLY:C     | 1:A:28:GLY:N     | 2.63                     | 0.47              |
| 1:B:241:THR:HG23 | 1:B:242:ASN:H    | 1.74                     | 0.47              |
| 1:B:242:ASN:C    | 1:B:244:PHE:N    | 2.62                     | 0.47              |
| 1:B:257:VAL:C    | 1:B:258:LEU:HD13 | 2.40                     | 0.47              |
| 1:C:224:ASN:HA   | 1:C:264:GLN:HB3  | 1.97                     | 0.47              |
| 1:D:117:GLU:HG3  | 1:D:118:PHE:CE1  | 2.49                     | 0.47              |
| 1:D:118:PHE:CD2  | 1:D:314:ILE:CG1  | 2.90                     | 0.47              |
| 1:A:289:VAL:HG21 | 1:A:324:LEU:CG   | 2.36                     | 0.46              |
| 1:B:104:VAL:N    | 1:B:156:GLN:OE1  | 2.48                     | 0.46              |
| 1:B:111:TYR:CE2  | 1:B:188:VAL:CG2  | 2.98                     | 0.46              |
| 1:B:196:ARG:CA   | 1:B:200:GLN:OE1  | 2.60                     | 0.46              |
| 1:C:294:TYR:CD1  | 1:C:294:TYR:C    | 2.94                     | 0.46              |
| 1:D:139:TYR:HB3  | 1:D:155:VAL:HG12 | 1.97                     | 0.46              |
| 1:A:220:TYR:O    | 1:A:220:TYR:CG   | 2.64                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:259:LEU:O    | 1:B:274:ALA:HA   | 2.15                     | 0.46              |
| 1:B:262:GLN:HE21 | 1:B:272:SER:HB2  | 1.80                     | 0.46              |
| 1:C:106:TYR:O    | 1:C:110:GLY:N    | 2.42                     | 0.46              |
| 1:C:144:PHE:HD1  | 1:C:151:LEU:CD2  | 2.29                     | 0.46              |
| 1:D:2:GLU:OE2    | 1:D:5:ASN:HB2    | 2.15                     | 0.46              |
| 1:D:170:ASN:ND2  | 1:D:170:ASN:C    | 2.49                     | 0.46              |
| 1:A:22:TYR:CE1   | 1:A:118:PHE:HZ   | 2.33                     | 0.46              |
| 1:A:57:GLY:HA3   | 1:C:307:MET:SD   | 2.55                     | 0.46              |
| 1:A:155:VAL:HG22 | 1:A:156:GLN:N    | 2.28                     | 0.46              |
| 1:A:207:ASN:O    | 1:A:252:ASN:OD1  | 2.32                     | 0.46              |
| 1:A:260:VAL:CG1  | 1:A:261:ALA:N    | 2.78                     | 0.46              |
| 1:B:65:PHE:CE2   | 1:C:61:TRP:CH2   | 3.04                     | 0.46              |
| 1:D:116:PRO:HB2  | 1:D:312:ASP:HB2  | 1.97                     | 0.46              |
| 1:D:264:GLN:HE21 | 1:D:268:GLY:HA2  | 1.80                     | 0.46              |
| 1:A:129:PHE:CE2  | 1:A:174:VAL:O    | 2.69                     | 0.46              |
| 1:B:263:TYR:CD1  | 1:B:264:GLN:N    | 2.84                     | 0.46              |
| 1:D:25:LYS:O     | 1:D:25:LYS:HG3   | 2.14                     | 0.46              |
| 1:D:313:TYR:CA   | 1:D:332:VAL:HG13 | 2.45                     | 0.46              |
| 1:D:318:ILE:HD13 | 1:D:318:ILE:HA   | 1.55                     | 0.46              |
| 1:A:24:SER:CB    | 1:A:331:THR:HG1  | 2.19                     | 0.46              |
| 1:A:136:VAL:O    | 1:A:137:ALA:HB2  | 2.16                     | 0.46              |
| 1:A:274:ALA:HB3  | 1:A:296:GLU:HB3  | 1.97                     | 0.46              |
| 1:B:25:LYS:HB2   | 1:B:25:LYS:NZ    | 2.30                     | 0.46              |
| 1:B:262:GLN:HG2  | 1:B:272:SER:HB2  | 1.97                     | 0.46              |
| 1:B:293:ASN:CG   | 1:B:317:GLN:HB3  | 2.40                     | 0.46              |
| 1:C:223:ASN:HB3  | 1:C:225:ILE:CD1  | 2.24                     | 0.46              |
| 1:D:140:ARG:HH11 | 1:D:154:ALA:HB2  | 1.80                     | 0.46              |
| 1:D:301:TYR:CD1  | 1:D:303:PHE:HE1  | 2.33                     | 0.46              |
| 1:A:160:LYS:HD3  | 1:A:162:GLU:OE2  | 2.14                     | 0.46              |
| 1:A:229:ALA:CB   | 1:A:259:LEU:HD21 | 2.39                     | 0.46              |
| 1:C:126:ASP:OD2  | 1:C:168:ARG:NH1  | 2.48                     | 0.46              |
| 1:C:156:GLN:N    | 1:C:175:GLY:O    | 2.47                     | 0.46              |
| 1:D:48:GLU:CG    | 1:D:49:THR:N     | 2.77                     | 0.46              |
| 1:D:121:ASP:C    | 1:D:123:ALA:N    | 2.74                     | 0.46              |
| 1:D:125:SER:C    | 1:D:127:ASP:N    | 2.68                     | 0.46              |
| 1:A:136:VAL:HG21 | 1:A:156:GLN:HE21 | 1.79                     | 0.46              |
| 1:B:166:ALA:C    | 1:B:168:ARG:H    | 2.23                     | 0.46              |
| 1:C:226:TYR:O    | 1:C:261:ALA:HA   | 2.15                     | 0.46              |
| 1:C:269:LEU:HG   | 1:C:271:PRO:HD3  | 1.97                     | 0.46              |
| 1:C:273:ILE:HD12 | 1:C:296:GLU:O    | 2.16                     | 0.46              |
| 1:D:14:TYR:HE2   | 1:D:45:PHE:N     | 2.14                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:43:LEU:HD12  | 1:D:43:LEU:HA    | 1.61                     | 0.46              |
| 1:D:90:TYR:HD2   | 1:D:93:VAL:CG2   | 2.29                     | 0.46              |
| 1:D:309:THR:HG22 | 1:D:335:GLY:O    | 2.15                     | 0.46              |
| 1:B:142:SER:HG   | 1:B:152:ASN:CG   | 2.21                     | 0.46              |
| 1:D:125:SER:O    | 1:D:126:ASP:C    | 2.58                     | 0.46              |
| 1:D:313:TYR:CD1  | 1:D:314:ILE:N    | 2.84                     | 0.46              |
| 1:A:179:SER:HB2  | 1:A:188:VAL:CG1  | 2.45                     | 0.46              |
| 1:B:131:GLY:O    | 1:B:133:VAL:HG22 | 2.15                     | 0.46              |
| 1:C:87:GLY:HA3   | 1:C:96:PHE:O     | 2.16                     | 0.46              |
| 1:D:30:ASN:HD21  | 1:D:327:GLY:HA2  | 1.81                     | 0.46              |
| 1:B:15:GLY:HA3   | 1:B:42:ARG:O     | 2.15                     | 0.46              |
| 1:C:177:SER:HA   | 1:C:189:GLY:O    | 2.16                     | 0.46              |
| 1:C:262:GLN:HG2  | 1:C:272:SER:CB   | 2.46                     | 0.46              |
| 1:D:37:ASP:OD2   | 1:D:68:ASN:HA    | 2.15                     | 0.46              |
| 1:D:72:GLY:O     | 1:D:73:ALA:O     | 2.34                     | 0.46              |
| 1:D:95:SER:O     | 1:D:139:TYR:HD1  | 1.98                     | 0.46              |
| 1:A:238:THR:HG21 | 1:A:291:LEU:HD12 | 1.98                     | 0.45              |
| 1:B:3:ILE:HG22   | 1:C:4:TYR:HB2    | 1.98                     | 0.45              |
| 1:B:132:ARG:C    | 1:B:133:VAL:HG22 | 2.41                     | 0.45              |
| 1:B:257:VAL:HG23 | 1:B:277:LYS:HB3  | 1.98                     | 0.45              |
| 1:B:269:LEU:HA   | 1:B:269:LEU:HD12 | 1.25                     | 0.45              |
| 1:C:234:THR:HB   | 1:C:237:ALA:CB   | 2.40                     | 0.45              |
| 1:D:222:ALA:O    | 1:D:223:ASN:HB2  | 2.16                     | 0.45              |
| 1:D:274:ALA:O    | 1:D:295:PHE:HA   | 2.16                     | 0.45              |
| 1:D:309:THR:HG23 | 1:D:336:ILE:HB   | 1.84                     | 0.45              |
| 1:A:58:TYR:CA    | 1:C:338:TYR:CD1  | 2.82                     | 0.45              |
| 1:A:104:VAL:CG1  | 1:A:156:GLN:HB3  | 2.40                     | 0.45              |
| 1:A:140:ARG:HG3  | 1:A:154:ALA:HB2  | 1.97                     | 0.45              |
| 1:A:203:GLN:HA   | 1:A:203:GLN:HE21 | 1.79                     | 0.45              |
| 1:B:28:GLY:C     | 1:B:30:ASN:N     | 2.73                     | 0.45              |
| 1:B:95:SER:O     | 1:B:96:PHE:CB    | 2.64                     | 0.45              |
| 1:B:294:TYR:HD1  | 1:B:314:ILE:HG23 | 1.80                     | 0.45              |
| 1:D:30:ASN:O     | 1:D:329:ASP:HB2  | 2.16                     | 0.45              |
| 1:A:337:VAL:O    | 1:A:337:VAL:HG13 | 1.97                     | 0.45              |
| 1:B:293:ASN:HB3  | 1:B:317:GLN:HB3  | 1.98                     | 0.45              |
| 1:C:123:ALA:O    | 1:C:124:TYR:O    | 2.35                     | 0.45              |
| 1:D:51:ILE:HB    | 1:D:55:LEU:CD2   | 2.46                     | 0.45              |
| 1:D:59:GLY:O     | 1:D:60:GLN:HB2   | 2.16                     | 0.45              |
| 1:D:129:PHE:CD2  | 1:D:192:GLY:HA3  | 2.52                     | 0.45              |
| 1:A:97:ASP:O     | 1:A:137:ALA:HB1  | 2.15                     | 0.45              |
| 1:A:310:TYR:HE1  | 1:A:335:GLY:HA3  | 1.82                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:111:TYR:CE1  | 1:B:188:VAL:HG21 | 2.49                     | 0.45              |
| 1:B:269:LEU:HD23 | 1:B:271:PRO:CD   | 2.46                     | 0.45              |
| 1:B:336:ILE:HG13 | 1:B:337:VAL:N    | 2.31                     | 0.45              |
| 1:C:60:GLN:CG    | 1:C:61:TRP:H     | 2.28                     | 0.45              |
| 1:C:275:TYR:C    | 1:C:275:TYR:CD2  | 2.94                     | 0.45              |
| 1:C:277:LYS:HE2  | 1:C:279:LYS:CD   | 2.29                     | 0.45              |
| 1:B:13:LEU:HD12  | 1:B:14:TYR:N     | 2.32                     | 0.45              |
| 1:B:196:ARG:H    | 1:B:196:ARG:HG3  | 1.46                     | 0.45              |
| 1:C:43:LEU:HD12  | 1:C:43:LEU:HA    | 1.82                     | 0.45              |
| 1:C:227:LEU:HD23 | 1:C:227:LEU:N    | 2.31                     | 0.45              |
| 1:D:283:VAL:O    | 1:D:286:ILE:HD13 | 2.17                     | 0.45              |
| 1:A:63:TYR:HD1   | 1:A:81:THR:HG1   | 1.63                     | 0.45              |
| 1:A:86:ALA:HB3   | 1:C:336:ILE:CG1  | 2.33                     | 0.45              |
| 1:A:96:PHE:CG    | 1:A:97:ASP:N     | 2.85                     | 0.45              |
| 1:A:303:PHE:O    | 1:A:304:ASN:CB   | 2.62                     | 0.45              |
| 1:B:16:LYS:HB2   | 1:B:17:ALA:H     | 1.61                     | 0.45              |
| 1:B:187:ILE:O    | 1:B:187:ILE:HG23 | 2.16                     | 0.45              |
| 1:B:268:GLY:O    | 1:B:301:TYR:HA   | 2.16                     | 0.45              |
| 1:B:273:ILE:HD12 | 1:B:273:ILE:HA   | 1.77                     | 0.45              |
| 1:B:313:TYR:CD1  | 1:B:332:VAL:HG21 | 2.43                     | 0.45              |
| 1:C:24:SER:OG    | 1:C:331:THR:HA   | 2.16                     | 0.45              |
| 1:C:231:TYR:CG   | 1:C:232:GLY:N    | 2.84                     | 0.45              |
| 1:D:205:LEU:O    | 1:D:250:PHE:N    | 2.44                     | 0.45              |
| 1:D:253:LYS:HD2  | 1:D:253:LYS:HA   | 1.54                     | 0.45              |
| 1:D:253:LYS:O    | 1:D:280:ALA:HA   | 2.16                     | 0.45              |
| 1:D:338:TYR:HD2  | 1:D:339:GLN:N    | 2.01                     | 0.45              |
| 1:A:22:TYR:HD1   | 1:A:333:ALA:CB   | 2.17                     | 0.45              |
| 1:A:24:SER:O     | 1:A:26:GLY:O     | 2.34                     | 0.45              |
| 1:A:130:VAL:HG11 | 1:A:213:GLN:NE2  | 2.26                     | 0.45              |
| 1:A:165:THR:HG22 | 1:A:166:ALA:C    | 2.41                     | 0.45              |
| 1:C:14:TYR:CD1   | 1:C:14:TYR:C     | 2.94                     | 0.45              |
| 1:D:114:MET:HE2  | 1:D:226:TYR:CD1  | 2.51                     | 0.45              |
| 1:A:60:GLN:HG2   | 1:A:61:TRP:N     | 2.32                     | 0.45              |
| 1:A:79:ASN:HB2   | 1:C:76:GLN:NE2   | 2.31                     | 0.45              |
| 1:A:109:LEU:HD23 | 1:A:109:LEU:HA   | 1.47                     | 0.45              |
| 1:B:272:SER:O    | 1:B:272:SER:OG   | 2.34                     | 0.45              |
| 1:B:318:ILE:HA   | 1:B:318:ILE:HD13 | 1.79                     | 0.45              |
| 1:A:16:LYS:H     | 1:A:42:ARG:HB2   | 1.81                     | 0.45              |
| 1:A:166:ALA:C    | 1:A:168:ARG:N    | 2.75                     | 0.45              |
| 1:A:263:TYR:O    | 1:A:270:ARG:HA   | 2.17                     | 0.45              |
| 1:B:3:ILE:HG13   | 1:B:4:TYR:N      | 2.31                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:262:GLN:CG   | 1:B:272:SER:HB2  | 2.47                     | 0.45              |
| 1:C:109:LEU:C    | 1:C:111:TYR:N    | 2.75                     | 0.45              |
| 1:C:284:GLU:C    | 1:C:286:ILE:CD1  | 2.90                     | 0.45              |
| 1:D:69:ASN:ND2   | 1:D:74:ASP:O     | 2.50                     | 0.45              |
| 1:D:307:MET:CG   | 1:D:308:SER:N    | 2.71                     | 0.45              |
| 1:A:20:LEU:HD12  | 1:A:21:HIS:H     | 1.81                     | 0.45              |
| 1:A:114:MET:CE   | 1:A:226:TYR:HE1  | 2.00                     | 0.45              |
| 1:A:340:PHE:CE1  | 1:B:45:PHE:CD2   | 3.05                     | 0.45              |
| 1:B:48:GLU:O     | 1:B:48:GLU:HG2   | 2.14                     | 0.45              |
| 1:B:63:TYR:CE2   | 1:B:65:PHE:CE1   | 3.04                     | 0.45              |
| 1:B:129:PHE:CE2  | 1:B:192:GLY:CA   | 3.00                     | 0.45              |
| 1:B:243:LYS:HD2  | 1:B:243:LYS:N    | 2.30                     | 0.45              |
| 1:C:18:VAL:HG23  | 1:C:337:VAL:HG22 | 1.95                     | 0.45              |
| 1:C:163:ARG:HG2  | 1:C:163:ARG:HH11 | 1.82                     | 0.45              |
| 1:C:221:ASP:C    | 1:C:221:ASP:OD1  | 2.60                     | 0.45              |
| 1:D:34:GLY:O     | 1:D:35:ASN:CB    | 2.53                     | 0.45              |
| 1:D:58:TYR:N     | 1:D:58:TYR:HD2   | 2.16                     | 0.45              |
| 1:D:281:LYS:HA   | 1:D:288:ASP:OD1  | 2.17                     | 0.45              |
| 1:D:313:TYR:HB2  | 1:D:332:VAL:HG13 | 1.97                     | 0.45              |
| 1:A:54:ASP:OD1   | 1:A:54:ASP:N     | 2.51                     | 0.44              |
| 1:B:139:TYR:CE2  | 1:B:140:ARG:O    | 2.70                     | 0.44              |
| 1:B:226:TYR:C    | 1:B:227:LEU:HD23 | 2.42                     | 0.44              |
| 1:B:307:MET:HE2  | 1:C:88:LEU:CD2   | 2.46                     | 0.44              |
| 1:C:235:ARG:HD3  | 1:C:235:ARG:HA   | 1.77                     | 0.44              |
| 1:C:256:ASP:C    | 1:C:257:VAL:CG2  | 2.82                     | 0.44              |
| 1:D:30:ASN:ND2   | 1:D:327:GLY:HA2  | 2.32                     | 0.44              |
| 1:D:83:LEU:HD23  | 1:D:101:ASN:HA   | 1.99                     | 0.44              |
| 1:A:105:VAL:O    | 1:A:106:TYR:C    | 2.60                     | 0.44              |
| 1:B:22:TYR:CE1   | 1:B:38:MET:HG3   | 2.53                     | 0.44              |
| 1:B:143:ASN:OD1  | 1:B:149:ASP:C    | 2.56                     | 0.44              |
| 1:C:14:TYR:OH    | 1:C:62:GLU:HG3   | 2.17                     | 0.44              |
| 1:C:92:ASP:O     | 1:C:93:VAL:O     | 2.35                     | 0.44              |
| 1:D:63:TYR:CD1   | 1:D:80:LYS:O     | 2.70                     | 0.44              |
| 1:D:85:PHE:CE1   | 1:D:101:ASN:CG   | 2.95                     | 0.44              |
| 1:A:4:TYR:CE2    | 1:A:6:LYS:N      | 2.74                     | 0.44              |
| 1:A:128:PHE:HB3  | 1:A:129:PHE:H    | 1.61                     | 0.44              |
| 1:A:285:GLY:C    | 1:A:286:ILE:HD13 | 2.34                     | 0.44              |
| 1:A:294:TYR:HA   | 1:A:317:GLN:HG2  | 1.98                     | 0.44              |
| 1:A:316:ASN:C    | 1:A:317:GLN:NE2  | 2.74                     | 0.44              |
| 1:C:104:VAL:HG22 | 1:C:156:GLN:OE1  | 2.17                     | 0.44              |
| 1:C:167:ARG:NH1  | 1:C:168:ARG:HD3  | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:114:MET:CE   | 1:D:270:ARG:HH12 | 2.30                     | 0.44              |
| 1:A:106:TYR:O    | 1:A:108:ALA:N    | 2.50                     | 0.44              |
| 1:A:172:ASP:OD1  | 1:A:172:ASP:N    | 2.42                     | 0.44              |
| 1:A:291:LEU:O    | 1:A:292:VAL:HG23 | 2.18                     | 0.44              |
| 1:B:62:GLU:HB3   | 1:B:83:LEU:HB2   | 2.00                     | 0.44              |
| 1:B:124:TYR:HB2  | 1:B:127:ASP:HB2  | 1.98                     | 0.44              |
| 1:C:23:PHE:O     | 1:C:332:VAL:N    | 2.37                     | 0.44              |
| 1:C:24:SER:OG    | 1:C:331:THR:CB   | 2.65                     | 0.44              |
| 1:C:82:ARG:HG2   | 1:C:82:ARG:NH1   | 2.32                     | 0.44              |
| 1:C:255:GLN:O    | 1:C:256:ASP:OD1  | 2.35                     | 0.44              |
| 1:D:5:ASN:O      | 1:D:6:LYS:HE2    | 2.18                     | 0.44              |
| 1:D:111:TYR:HE2  | 1:D:217:GLY:O    | 2.00                     | 0.44              |
| 1:D:118:PHE:O    | 1:D:119:GLY:C    | 2.59                     | 0.44              |
| 1:D:167:ARG:HG3  | 1:D:167:ARG:NH1  | 2.27                     | 0.44              |
| 1:D:219:LYS:HA   | 1:D:227:LEU:O    | 2.17                     | 0.44              |
| 1:A:20:LEU:CD2   | 1:A:117:GLU:CD   | 2.76                     | 0.44              |
| 1:A:225:ILE:HD13 | 1:A:225:ILE:HG23 | 1.71                     | 0.44              |
| 1:B:111:TYR:CE2  | 1:B:219:LYS:HG2  | 2.53                     | 0.44              |
| 1:B:227:LEU:CD2  | 1:B:261:ALA:HA   | 2.48                     | 0.44              |
| 1:C:115:LEU:HD23 | 1:C:115:LEU:HA   | 1.44                     | 0.44              |
| 1:C:203:GLN:H    | 1:C:203:GLN:HG2  | 1.56                     | 0.44              |
| 1:D:45:PHE:O     | 1:D:60:GLN:HA    | 2.17                     | 0.44              |
| 1:D:104:VAL:HG12 | 1:D:156:GLN:CB   | 2.40                     | 0.44              |
| 1:D:150:GLY:O    | 1:D:181:GLU:HG3  | 2.17                     | 0.44              |
| 1:A:13:LEU:HD21  | 1:B:13:LEU:HD22  | 1.99                     | 0.44              |
| 1:A:112:THR:CG2  | 1:A:230:ASN:CG   | 2.91                     | 0.44              |
| 1:A:251:ALA:O    | 1:A:252:ASN:O    | 2.36                     | 0.44              |
| 1:A:338:TYR:CG   | 1:A:339:GLN:N    | 2.86                     | 0.44              |
| 1:B:105:VAL:HG23 | 1:B:190:ALA:C    | 2.42                     | 0.44              |
| 1:B:157:TYR:N    | 1:B:157:TYR:CD2  | 2.85                     | 0.44              |
| 1:B:216:THR:O    | 1:B:216:THR:OG1  | 2.21                     | 0.44              |
| 1:B:294:TYR:HD1  | 1:B:314:ILE:HD12 | 1.68                     | 0.44              |
| 1:C:55:LEU:HD12  | 1:C:90:TYR:CD1   | 2.53                     | 0.44              |
| 1:C:114:MET:HB3  | 1:C:262:GLN:HE22 | 1.82                     | 0.44              |
| 1:C:160:LYS:HA   | 1:C:172:ASP:OD1  | 2.17                     | 0.44              |
| 1:C:198:ASN:O    | 1:C:199:LEU:C    | 2.60                     | 0.44              |
| 1:D:20:LEU:CG    | 1:D:21:HIS:N     | 2.81                     | 0.44              |
| 1:B:48:GLU:CD    | 1:B:56:THR:HG21  | 2.43                     | 0.44              |
| 1:B:98:TYR:HA    | 1:B:136:VAL:O    | 2.18                     | 0.44              |
| 1:B:211:ALA:HA   | 1:B:235:ARG:O    | 2.17                     | 0.44              |
| 1:B:233:GLU:HG2  | 1:B:255:GLN:HG2  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:163:ARG:HD2  | 1:C:168:ARG:C    | 2.40                     | 0.44              |
| 1:C:275:TYR:HE1  | 1:C:295:PHE:CE1  | 2.36                     | 0.44              |
| 1:D:36:GLY:O     | 1:D:37:ASP:O     | 2.36                     | 0.44              |
| 1:D:219:LYS:O    | 1:D:219:LYS:CG   | 2.66                     | 0.44              |
| 1:D:301:TYR:O    | 1:D:308:SER:HB2  | 2.17                     | 0.44              |
| 1:A:71:GLU:CD    | 1:B:100:ARG:NH2  | 2.74                     | 0.44              |
| 1:A:85:PHE:C     | 1:A:85:PHE:HD1   | 2.26                     | 0.44              |
| 1:A:95:SER:O     | 1:A:139:TYR:HD1  | 2.00                     | 0.44              |
| 1:A:139:TYR:O    | 1:A:154:ALA:HA   | 2.18                     | 0.44              |
| 1:A:220:TYR:C    | 1:A:220:TYR:CD1  | 2.94                     | 0.44              |
| 1:A:307:MET:CE   | 1:B:57:GLY:HA3   | 2.48                     | 0.44              |
| 1:B:60:GLN:HG3   | 1:B:61:TRP:N     | 2.31                     | 0.44              |
| 1:B:227:LEU:HD21 | 1:B:261:ALA:HA   | 1.99                     | 0.44              |
| 1:C:167:ARG:CG   | 1:C:167:ARG:NH1  | 2.69                     | 0.44              |
| 1:C:192:GLY:O    | 1:C:193:ALA:HB2  | 2.18                     | 0.44              |
| 1:A:29:GLU:O     | 1:A:29:GLU:CG    | 2.63                     | 0.44              |
| 1:A:306:ASN:ND2  | 1:A:339:GLN:O    | 2.41                     | 0.44              |
| 1:A:310:TYR:O    | 1:A:310:TYR:HD1  | 2.01                     | 0.44              |
| 1:C:22:TYR:CB    | 1:C:35:ASN:HA    | 2.48                     | 0.44              |
| 1:C:27:ASN:O     | 1:C:27:ASN:CG    | 2.52                     | 0.44              |
| 1:C:112:THR:HG21 | 1:C:230:ASN:OD1  | 2.11                     | 0.44              |
| 1:C:129:PHE:CE2  | 1:C:192:GLY:HA3  | 2.53                     | 0.44              |
| 1:D:38:MET:O     | 1:D:39:THR:C     | 2.60                     | 0.44              |
| 1:D:218:LEU:HD23 | 1:D:218:LEU:HA   | 1.33                     | 0.44              |
| 1:D:219:LYS:O    | 1:D:219:LYS:HG3  | 2.18                     | 0.44              |
| 1:D:266:ASP:O    | 1:D:268:GLY:N    | 2.51                     | 0.44              |
| 1:D:273:ILE:CG2  | 1:D:274:ALA:N    | 2.80                     | 0.44              |
| 1:B:122:THR:CG2  | 1:B:256:ASP:OD2  | 2.66                     | 0.43              |
| 1:B:262:GLN:HG2  | 1:B:272:SER:HA   | 1.99                     | 0.43              |
| 1:D:125:SER:O    | 1:D:127:ASP:N    | 2.51                     | 0.43              |
| 1:D:245:THR:HG1  | 1:D:247:THR:CB   | 2.21                     | 0.43              |
| 1:A:11:VAL:HG21  | 1:C:340:PHE:CD2  | 2.52                     | 0.43              |
| 1:A:115:LEU:CG   | 1:A:119:GLY:HA3  | 2.35                     | 0.43              |
| 1:A:289:VAL:HG21 | 1:A:324:LEU:CD1  | 2.48                     | 0.43              |
| 1:A:311:VAL:HG23 | 1:A:334:VAL:HG22 | 1.98                     | 0.43              |
| 1:B:54:ASP:O     | 1:B:90:TYR:CD1   | 2.71                     | 0.43              |
| 1:B:196:ARG:HB3  | 1:B:200:GLN:OE1  | 2.18                     | 0.43              |
| 1:D:66:GLN:NE2   | 1:D:68:ASN:ND2   | 2.66                     | 0.43              |
| 1:D:323:LYS:HD2  | 1:D:323:LYS:HA   | 1.64                     | 0.43              |
| 1:A:240:ILE:CG2  | 1:A:291:LEU:HD22 | 2.49                     | 0.43              |
| 1:B:185:PHE:CE2  | 1:B:220:TYR:HE1  | 2.26                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:282:ASP:O    | 1:B:284:GLU:N    | 2.51                     | 0.43              |
| 1:B:316:ASN:HD22 | 1:B:329:ASP:N    | 2.16                     | 0.43              |
| 1:C:14:TYR:HA    | 1:C:340:PHE:CE2  | 2.53                     | 0.43              |
| 1:D:212:GLU:OE1  | 1:D:235:ARG:HB2  | 2.19                     | 0.43              |
| 1:A:104:VAL:CG1  | 1:A:156:GLN:HB2  | 2.48                     | 0.43              |
| 1:A:294:TYR:O    | 1:A:294:TYR:HD1  | 2.01                     | 0.43              |
| 1:B:208:GLY:HA3  | 1:B:236:ASN:HD22 | 1.83                     | 0.43              |
| 1:B:263:TYR:HD1  | 1:B:264:GLN:N    | 2.15                     | 0.43              |
| 1:B:285:GLY:O    | 1:B:286:ILE:CD1  | 2.48                     | 0.43              |
| 1:B:294:TYR:C    | 1:B:295:PHE:HD1  | 2.26                     | 0.43              |
| 1:C:45:PHE:O     | 1:C:60:GLN:CG    | 2.65                     | 0.43              |
| 1:C:49:THR:HG23  | 1:C:49:THR:O     | 2.18                     | 0.43              |
| 1:D:45:PHE:O     | 1:D:45:PHE:CD1   | 2.71                     | 0.43              |
| 1:D:240:ILE:O    | 1:D:240:ILE:HG12 | 2.14                     | 0.43              |
| 1:A:69:ASN:HD22  | 1:A:77:THR:H     | 1.65                     | 0.43              |
| 1:A:178:ILE:CG2  | 1:A:179:SER:N    | 2.78                     | 0.43              |
| 1:C:170:ASN:ND2  | 1:C:170:ASN:C    | 2.75                     | 0.43              |
| 1:D:20:LEU:HD21  | 1:D:117:GLU:CD   | 2.44                     | 0.43              |
| 1:D:129:PHE:HB2  | 1:D:213:GLN:OE1  | 2.19                     | 0.43              |
| 1:D:161:ASN:H    | 1:D:170:ASN:HD21 | 1.66                     | 0.43              |
| 1:A:69:ASN:ND2   | 1:A:77:THR:CB    | 2.63                     | 0.43              |
| 1:B:22:TYR:O     | 1:B:23:PHE:HD2   | 1.97                     | 0.43              |
| 1:B:310:TYR:C    | 1:B:311:VAL:CG2  | 2.90                     | 0.43              |
| 1:C:92:ASP:O     | 1:C:93:VAL:C     | 2.53                     | 0.43              |
| 1:C:115:LEU:HD12 | 1:C:119:GLY:N    | 2.32                     | 0.43              |
| 1:C:163:ARG:NH1  | 1:C:163:ARG:CG   | 2.78                     | 0.43              |
| 1:C:163:ARG:CD   | 1:C:168:ARG:O    | 2.52                     | 0.43              |
| 1:D:58:TYR:HD2   | 1:D:58:TYR:H     | 1.67                     | 0.43              |
| 1:D:260:VAL:HG12 | 1:D:261:ALA:N    | 2.33                     | 0.43              |
| 1:D:286:ILE:HG23 | 1:D:323:LYS:HB3  | 2.00                     | 0.43              |
| 1:A:102:TYR:CD1  | 1:A:106:TYR:HD2  | 2.30                     | 0.43              |
| 1:B:22:TYR:N     | 1:B:22:TYR:CD1   | 2.86                     | 0.43              |
| 1:A:6:LYS:O      | 1:A:7:ASP:HB2    | 2.17                     | 0.43              |
| 1:C:60:GLN:NE2   | 1:C:85:PHE:CE1   | 2.80                     | 0.43              |
| 1:D:24:SER:OG    | 1:D:331:THR:HG23 | 2.18                     | 0.43              |
| 1:D:114:MET:HE1  | 1:D:270:ARG:HH12 | 1.83                     | 0.43              |
| 1:D:124:TYR:CE2  | 1:D:238:THR:HG22 | 2.51                     | 0.43              |
| 1:D:190:ALA:O    | 1:D:191:TYR:HB2  | 2.18                     | 0.43              |
| 1:D:273:ILE:CD1  | 1:D:297:VAL:HG22 | 2.48                     | 0.43              |
| 1:D:274:ALA:HB3  | 1:D:296:GLU:OE1  | 2.18                     | 0.43              |
| 1:B:104:VAL:HG21 | 1:B:176:GLY:CA   | 2.49                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:122:THR:HG21 | 1:B:256:ASP:OD2  | 2.19                     | 0.43              |
| 1:B:242:ASN:CB   | 1:B:247:THR:HB   | 2.45                     | 0.43              |
| 1:B:277:LYS:HE3  | 1:B:293:ASN:ND2  | 2.31                     | 0.43              |
| 1:B:318:ILE:HD12 | 1:B:318:ILE:HG23 | 1.60                     | 0.43              |
| 1:C:301:TYR:C    | 1:C:301:TYR:CD2  | 2.89                     | 0.43              |
| 1:C:322:ASN:O    | 1:C:323:LYS:C    | 2.62                     | 0.43              |
| 1:D:226:TYR:C    | 1:D:227:LEU:CD2  | 2.77                     | 0.43              |
| 1:A:106:TYR:C    | 1:A:108:ALA:N    | 2.76                     | 0.43              |
| 1:A:151:LEU:HD23 | 1:A:151:LEU:C    | 2.44                     | 0.43              |
| 1:A:188:VAL:O    | 1:A:216:THR:HA   | 2.19                     | 0.43              |
| 1:A:294:TYR:O    | 1:A:294:TYR:CD1  | 2.72                     | 0.43              |
| 1:B:1:ALA:CB     | 1:C:4:TYR:CG     | 3.02                     | 0.43              |
| 1:B:318:ILE:HG22 | 1:B:319:ASP:H    | 1.82                     | 0.43              |
| 1:C:13:LEU:HD12  | 1:C:13:LEU:HA    | 1.56                     | 0.43              |
| 1:C:176:GLY:O    | 1:C:190:ALA:HA   | 2.19                     | 0.43              |
| 1:C:303:PHE:HD1  | 1:C:303:PHE:HA   | 1.68                     | 0.43              |
| 1:D:52:ASN:CG    | 1:D:53:SER:N     | 2.76                     | 0.43              |
| 1:D:206:GLY:N    | 1:D:284:GLU:OE2  | 2.50                     | 0.43              |
| 1:D:314:ILE:HD13 | 1:D:314:ILE:HA   | 1.84                     | 0.43              |
| 1:D:318:ILE:HG23 | 1:D:318:ILE:HD12 | 1.70                     | 0.43              |
| 1:A:112:THR:HG21 | 1:A:230:ASN:HB2  | 2.00                     | 0.42              |
| 1:A:225:ILE:HD12 | 1:A:225:ILE:HG21 | 1.78                     | 0.42              |
| 1:C:205:LEU:HA   | 1:C:284:GLU:CG   | 2.49                     | 0.42              |
| 1:C:269:LEU:HD13 | 1:C:269:LEU:HA   | 1.55                     | 0.42              |
| 1:C:311:VAL:HA   | 1:C:333:ALA:O    | 2.19                     | 0.42              |
| 1:D:151:LEU:O    | 1:D:151:LEU:CG   | 2.62                     | 0.42              |
| 1:D:209:LYS:HE3  | 1:D:209:LYS:HB3  | 1.42                     | 0.42              |
| 1:A:24:SER:HG    | 1:A:331:THR:HA   | 1.83                     | 0.42              |
| 1:A:74:ASP:N     | 1:A:74:ASP:OD1   | 2.30                     | 0.42              |
| 1:A:226:TYR:HD2  | 1:A:227:LEU:N    | 2.17                     | 0.42              |
| 1:A:237:ALA:O    | 1:A:239:PRO:N    | 2.52                     | 0.42              |
| 1:C:267:PHE:CZ   | 1:C:269:LEU:CB   | 3.01                     | 0.42              |
| 1:C:296:GLU:HB2  | 1:C:314:ILE:HD13 | 2.00                     | 0.42              |
| 1:D:5:ASN:C      | 1:D:6:LYS:CG     | 2.92                     | 0.42              |
| 1:A:2:GLU:OE2    | 1:A:5:ASN:ND2    | 2.42                     | 0.42              |
| 1:A:203:GLN:HB3  | 1:A:204:PRO:CD   | 2.49                     | 0.42              |
| 1:B:20:LEU:HD13  | 1:B:20:LEU:HA    | 1.56                     | 0.42              |
| 1:B:39:THR:O     | 1:B:39:THR:HG22  | 2.11                     | 0.42              |
| 1:B:196:ARG:CD   | 1:B:208:GLY:O    | 2.67                     | 0.42              |
| 1:D:338:TYR:CD2  | 1:D:339:GLN:CA   | 3.00                     | 0.42              |
| 1:A:35:ASN:OD1   | 1:A:36:GLY:N     | 2.51                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:47:GLY:O     | 1:A:58:TYR:HB2   | 2.20                     | 0.42              |
| 1:A:340:PHE:HE1  | 1:B:45:PHE:CZ    | 2.38                     | 0.42              |
| 1:B:51:ILE:HG21  | 1:B:51:ILE:HD13  | 1.84                     | 0.42              |
| 1:B:114:MET:CA   | 1:B:115:LEU:HD23 | 2.47                     | 0.42              |
| 1:B:163:ARG:HG2  | 1:B:163:ARG:HH11 | 1.84                     | 0.42              |
| 1:D:58:TYR:CE2   | 1:D:87:GLY:HA3   | 2.54                     | 0.42              |
| 1:D:154:ALA:HB3  | 1:D:177:SER:OG   | 2.20                     | 0.42              |
| 1:D:229:ALA:HA   | 1:D:259:LEU:HD23 | 2.01                     | 0.42              |
| 1:D:235:ARG:O    | 1:D:236:ASN:C    | 2.60                     | 0.42              |
| 1:D:257:VAL:C    | 1:D:258:LEU:HD23 | 2.39                     | 0.42              |
| 1:A:22:TYR:CZ    | 1:A:118:PHE:HE1  | 2.37                     | 0.42              |
| 1:A:334:VAL:HG13 | 1:A:335:GLY:N    | 2.34                     | 0.42              |
| 1:B:277:LYS:HA   | 1:B:292:VAL:O    | 2.18                     | 0.42              |
| 1:B:287:GLY:C    | 1:B:288:ASP:OD1  | 2.63                     | 0.42              |
| 1:C:105:VAL:C    | 1:C:107:ASP:N    | 2.75                     | 0.42              |
| 1:D:21:HIS:CD2   | 1:D:23:PHE:CZ    | 3.07                     | 0.42              |
| 1:D:100:ARG:NH1  | 1:D:133:VAL:C    | 2.78                     | 0.42              |
| 1:D:156:GLN:O    | 1:D:175:GLY:N    | 2.53                     | 0.42              |
| 1:D:165:THR:O    | 1:D:166:ALA:C    | 2.63                     | 0.42              |
| 1:D:183:GLU:O    | 1:D:183:GLU:HG2  | 2.19                     | 0.42              |
| 1:A:21:HIS:CD2   | 1:A:23:PHE:CZ    | 3.03                     | 0.42              |
| 1:A:277:LYS:HB2  | 1:A:293:ASN:OD1  | 2.19                     | 0.42              |
| 1:A:303:PHE:O    | 1:A:304:ASN:HB3  | 2.20                     | 0.42              |
| 1:B:22:TYR:CD1   | 1:B:38:MET:HG3   | 2.54                     | 0.42              |
| 1:B:139:TYR:HE2  | 1:B:141:ASN:HB2  | 1.85                     | 0.42              |
| 1:B:186:GLY:O    | 1:B:218:LEU:HA   | 2.20                     | 0.42              |
| 1:B:280:ALA:HB2  | 1:B:291:LEU:HD11 | 2.01                     | 0.42              |
| 1:C:198:ASN:HA   | 1:C:201:GLU:HG2  | 2.02                     | 0.42              |
| 1:D:82:ARG:O     | 1:D:132:ARG:HD3  | 2.11                     | 0.42              |
| 1:D:205:LEU:O    | 1:D:249:GLY:HA3  | 2.19                     | 0.42              |
| 1:D:270:ARG:HA   | 1:D:271:PRO:HD2  | 1.76                     | 0.42              |
| 1:D:277:LYS:CB   | 1:D:293:ASN:OD1  | 2.53                     | 0.42              |
| 1:A:51:ILE:CD1   | 1:C:303:PHE:HB3  | 2.39                     | 0.42              |
| 1:A:226:TYR:HE2  | 1:A:228:ALA:CB   | 2.21                     | 0.42              |
| 1:A:237:ALA:C    | 1:A:238:THR:O    | 2.61                     | 0.42              |
| 1:A:336:ILE:CD1  | 1:B:87:GLY:CA    | 2.92                     | 0.42              |
| 1:C:111:TYR:O    | 1:C:228:ALA:CB   | 2.68                     | 0.42              |
| 1:D:5:ASN:O      | 1:D:6:LYS:CG     | 2.68                     | 0.42              |
| 1:D:231:TYR:HA   | 1:D:256:ASP:O    | 2.20                     | 0.42              |
| 1:A:34:GLY:O     | 1:A:35:ASN:HB2   | 2.20                     | 0.42              |
| 1:A:111:TYR:CD2  | 1:A:219:LYS:CG   | 2.95                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:237:ALA:O    | 1:A:238:THR:O    | 2.35                     | 0.42              |
| 1:A:320:SER:O    | 1:A:321:ASP:C    | 2.62                     | 0.42              |
| 1:B:324:LEU:N    | 1:B:324:LEU:HD23 | 2.27                     | 0.42              |
| 1:C:61:TRP:HE1   | 1:C:81:THR:CG2   | 2.33                     | 0.42              |
| 1:C:244:PHE:C    | 1:C:246:ASN:H    | 2.28                     | 0.42              |
| 1:D:9:ASN:HA     | 1:D:48:GLU:O     | 2.20                     | 0.42              |
| 1:D:300:THR:HA   | 1:D:310:TYR:CB   | 2.44                     | 0.42              |
| 1:A:23:PHE:C     | 1:A:24:SER:HG    | 2.24                     | 0.42              |
| 1:A:31:SER:HA    | 1:A:329:ASP:H    | 1.85                     | 0.42              |
| 1:A:303:PHE:CB   | 1:A:307:MET:HB3  | 2.41                     | 0.42              |
| 1:B:51:ILE:O     | 1:B:52:ASN:CB    | 2.42                     | 0.42              |
| 1:B:128:PHE:O    | 1:B:133:VAL:CG1  | 2.66                     | 0.42              |
| 1:C:191:TYR:CE1  | 1:C:192:GLY:O    | 2.72                     | 0.42              |
| 1:D:24:SER:OG    | 1:D:331:THR:CB   | 2.68                     | 0.42              |
| 1:A:65:PHE:CD1   | 1:B:63:TYR:CD1   | 3.08                     | 0.42              |
| 1:A:168:ARG:HD3  | 1:C:70:SER:HB2   | 2.01                     | 0.42              |
| 1:B:95:SER:O     | 1:B:96:PHE:HB2   | 2.20                     | 0.42              |
| 1:B:127:ASP:O    | 1:B:129:PHE:N    | 2.53                     | 0.42              |
| 1:B:182:TYR:HD1  | 1:B:182:TYR:HA   | 1.59                     | 0.42              |
| 1:C:235:ARG:CZ   | 1:C:253:LYS:HD3  | 2.49                     | 0.41              |
| 1:D:227:LEU:HD23 | 1:D:227:LEU:N    | 2.24                     | 0.41              |
| 1:A:15:GLY:C     | 1:A:16:LYS:HG2   | 2.43                     | 0.41              |
| 1:A:23:PHE:C     | 1:A:24:SER:OG    | 2.64                     | 0.41              |
| 1:A:318:ILE:CG1  | 1:A:326:VAL:HG12 | 2.50                     | 0.41              |
| 1:C:140:ARG:HG2  | 1:C:154:ALA:CB   | 2.50                     | 0.41              |
| 1:D:75:ALA:C     | 1:D:76:GLN:HG2   | 2.44                     | 0.41              |
| 1:D:160:LYS:HB2  | 1:D:160:LYS:HE2  | 1.29                     | 0.41              |
| 1:D:232:GLY:O    | 1:D:233:GLU:HG3  | 2.20                     | 0.41              |
| 1:D:264:GLN:O    | 1:D:264:GLN:HG3  | 2.18                     | 0.41              |
| 1:A:22:TYR:OH    | 1:A:118:PHE:HE1  | 2.02                     | 0.41              |
| 1:A:85:PHE:HD1   | 1:A:85:PHE:O     | 2.02                     | 0.41              |
| 1:A:171:GLY:HA3  | 1:A:195:ASP:CB   | 2.50                     | 0.41              |
| 1:B:201:GLU:OE1  | 1:B:208:GLY:O    | 2.37                     | 0.41              |
| 1:B:251:ALA:O    | 1:B:253:LYS:N    | 2.53                     | 0.41              |
| 1:B:296:GLU:CG   | 1:B:314:ILE:CD1  | 2.98                     | 0.41              |
| 1:C:52:ASN:OD1   | 1:C:54:ASP:N     | 2.53                     | 0.41              |
| 1:C:118:PHE:O    | 1:C:119:GLY:C    | 2.63                     | 0.41              |
| 1:C:260:VAL:HG12 | 1:C:261:ALA:H    | 1.85                     | 0.41              |
| 1:C:280:ALA:HB2  | 1:C:291:LEU:HD12 | 2.03                     | 0.41              |
| 1:D:141:ASN:OD1  | 1:D:145:PHE:CA   | 2.67                     | 0.41              |
| 1:D:190:ALA:O    | 1:D:191:TYR:CB   | 2.68                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:265:PHE:HD1  | 1:D:265:PHE:HA   | 1.72                     | 0.41              |
| 1:A:174:VAL:HG13 | 1:A:175:GLY:H    | 1.76                     | 0.41              |
| 1:B:148:VAL:O    | 1:B:148:VAL:CG1  | 2.57                     | 0.41              |
| 1:B:178:ILE:CG2  | 1:B:179:SER:N    | 2.83                     | 0.41              |
| 1:B:205:LEU:CG   | 1:B:247:THR:HG22 | 2.49                     | 0.41              |
| 1:B:245:THR:C    | 1:B:247:THR:H    | 2.28                     | 0.41              |
| 1:C:105:VAL:HG23 | 1:C:129:PHE:CB   | 2.46                     | 0.41              |
| 1:C:240:ILE:HD11 | 1:C:251:ALA:CA   | 2.44                     | 0.41              |
| 1:D:3:ILE:CD1    | 1:D:13:LEU:HB3   | 2.50                     | 0.41              |
| 1:A:20:LEU:HD12  | 1:A:21:HIS:N     | 2.35                     | 0.41              |
| 1:A:42:ARG:HD3   | 1:A:42:ARG:HA    | 1.36                     | 0.41              |
| 1:A:326:VAL:O    | 1:A:327:GLY:C    | 2.62                     | 0.41              |
| 1:B:94:GLY:HA3   | 1:B:140:ARG:O    | 2.20                     | 0.41              |
| 1:B:275:TYR:CG   | 1:B:276:THR:N    | 2.87                     | 0.41              |
| 1:B:307:MET:CG   | 1:B:308:SER:N    | 2.71                     | 0.41              |
| 1:C:11:VAL:HG12  | 1:C:12:ASP:H     | 1.76                     | 0.41              |
| 1:D:98:TYR:CD2   | 1:D:98:TYR:C     | 2.99                     | 0.41              |
| 1:D:241:THR:O    | 1:D:324:LEU:HD22 | 2.21                     | 0.41              |
| 1:A:336:ILE:CD1  | 1:B:87:GLY:N     | 2.80                     | 0.41              |
| 1:B:129:PHE:HB2  | 1:B:213:GLN:OE1  | 2.21                     | 0.41              |
| 1:B:166:ALA:C    | 1:B:168:ARG:N    | 2.75                     | 0.41              |
| 1:C:48:GLU:HG3   | 1:C:56:THR:CG2   | 2.48                     | 0.41              |
| 1:C:130:VAL:CG1  | 1:C:213:GLN:NE2  | 2.80                     | 0.41              |
| 1:C:153:PHE:HA   | 1:C:177:SER:O    | 2.21                     | 0.41              |
| 1:D:293:ASN:ND2  | 1:D:317:GLN:HB3  | 2.34                     | 0.41              |
| 1:D:303:PHE:CD2  | 1:D:307:MET:HG2  | 2.42                     | 0.41              |
| 1:A:240:ILE:CD1  | 1:A:251:ALA:HB2  | 2.50                     | 0.41              |
| 1:B:158:LEU:CD1  | 1:B:170:ASN:ND2  | 2.82                     | 0.41              |
| 1:B:316:ASN:ND2  | 1:B:328:SER:C    | 2.79                     | 0.41              |
| 1:C:140:ARG:HG2  | 1:C:154:ALA:HB2  | 2.02                     | 0.41              |
| 1:C:141:ASN:CG   | 1:C:153:PHE:CE1  | 2.87                     | 0.41              |
| 1:C:155:VAL:O    | 1:C:155:VAL:HG12 | 2.21                     | 0.41              |
| 1:D:114:MET:C    | 1:D:115:LEU:O    | 2.64                     | 0.41              |
| 1:A:111:TYR:O    | 1:A:226:TYR:OH   | 2.37                     | 0.41              |
| 1:A:198:ASN:O    | 1:A:199:LEU:C    | 2.62                     | 0.41              |
| 1:B:265:PHE:CD2  | 1:B:267:PHE:HE1  | 2.39                     | 0.41              |
| 1:D:100:ARG:HH12 | 1:D:133:VAL:CA   | 2.34                     | 0.41              |
| 1:D:123:ALA:HA   | 1:D:130:VAL:HG23 | 2.02                     | 0.41              |
| 1:D:191:TYR:HB2  | 1:D:214:TRP:CB   | 2.51                     | 0.41              |
| 1:A:14:TYR:HH    | 1:A:62:GLU:HB2   | 1.85                     | 0.41              |
| 1:A:22:TYR:HE1   | 1:A:118:PHE:HZ   | 1.67                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:203:GLN:NE2  | 1:A:203:GLN:CA   | 2.83                     | 0.41              |
| 1:B:216:THR:C    | 1:B:230:ASN:ND2  | 2.76                     | 0.41              |
| 1:B:265:PHE:HB3  | 1:B:267:PHE:CE1  | 2.56                     | 0.41              |
| 1:B:289:VAL:HG21 | 1:B:324:LEU:HG   | 2.02                     | 0.41              |
| 1:B:321:ASP:CG   | 1:D:287:GLY:HA2  | 2.46                     | 0.41              |
| 1:B:321:ASP:HB3  | 1:D:287:GLY:HA2  | 2.03                     | 0.41              |
| 1:C:12:ASP:O     | 1:C:45:PHE:HA    | 2.20                     | 0.41              |
| 1:C:48:GLU:O     | 1:C:48:GLU:CG    | 2.58                     | 0.41              |
| 1:C:294:TYR:CG   | 1:C:314:ILE:HD12 | 2.56                     | 0.41              |
| 1:C:340:PHE:CD2  | 1:C:340:PHE:C    | 2.98                     | 0.41              |
| 1:D:65:PHE:HA    | 1:D:79:ASN:OD1   | 2.20                     | 0.41              |
| 1:D:115:LEU:CD1  | 1:D:296:GLU:HG3  | 2.51                     | 0.41              |
| 1:D:144:PHE:N    | 1:D:151:LEU:O    | 2.51                     | 0.41              |
| 1:D:172:ASP:H    | 1:D:195:ASP:HB2  | 1.86                     | 0.41              |
| 1:D:205:LEU:HA   | 1:D:284:GLU:CG   | 2.51                     | 0.41              |
| 1:D:313:TYR:HB2  | 1:D:332:VAL:CG1  | 2.51                     | 0.41              |
| 1:D:322:ASN:OD1  | 1:D:326:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:161:ASN:O    | 1:A:169:SER:OG   | 2.39                     | 0.41              |
| 1:A:277:LYS:HE3  | 1:A:279:LYS:HD2  | 2.03                     | 0.41              |
| 1:B:338:TYR:HB3  | 1:C:59:GLY:HA3   | 2.04                     | 0.41              |
| 1:C:90:TYR:HD1   | 1:C:90:TYR:HA    | 1.60                     | 0.41              |
| 1:C:114:MET:HE2  | 1:C:226:TYR:CE2  | 2.55                     | 0.41              |
| 1:C:238:THR:HA   | 1:C:239:PRO:HD2  | 1.82                     | 0.41              |
| 1:C:283:VAL:O    | 1:C:284:GLU:C    | 2.64                     | 0.41              |
| 1:D:4:TYR:CD2    | 1:D:4:TYR:C      | 2.99                     | 0.41              |
| 1:A:259:LEU:C    | 1:A:260:VAL:CG2  | 2.94                     | 0.40              |
| 1:A:317:GLN:NE2  | 1:A:317:GLN:N    | 2.69                     | 0.40              |
| 1:B:1:ALA:CB     | 1:C:4:TYR:CZ     | 3.04                     | 0.40              |
| 1:B:104:VAL:H    | 1:B:104:VAL:HG22 | 1.64                     | 0.40              |
| 1:C:42:ARG:HH12  | 1:C:82:ARG:HH22  | 1.59                     | 0.40              |
| 1:C:111:TYR:CZ   | 1:C:188:VAL:CG2  | 3.04                     | 0.40              |
| 1:C:112:THR:HG21 | 1:C:230:ASN:CB   | 2.51                     | 0.40              |
| 1:C:255:GLN:HE22 | 1:C:281:LYS:NZ   | 2.19                     | 0.40              |
| 1:C:326:VAL:CG1  | 1:C:327:GLY:O    | 2.69                     | 0.40              |
| 1:D:14:TYR:CD2   | 1:D:44:GLY:O     | 2.73                     | 0.40              |
| 1:D:20:LEU:HD21  | 1:D:117:GLU:OE2  | 2.21                     | 0.40              |
| 1:D:235:ARG:HD3  | 1:D:252:ASN:O    | 2.21                     | 0.40              |
| 1:D:269:LEU:HG   | 1:D:271:PRO:HD3  | 2.03                     | 0.40              |
| 1:A:104:VAL:CG2  | 1:A:105:VAL:N    | 2.79                     | 0.40              |
| 1:A:314:ILE:O    | 1:A:330:ASP:OD1  | 2.40                     | 0.40              |
| 1:B:14:TYR:CA    | 1:B:340:PHE:CE2  | 2.99                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:316:ASN:HB3  | 1:B:328:SER:O    | 2.21                     | 0.40              |
| 1:C:180:TYR:C    | 1:C:180:TYR:CD1  | 2.99                     | 0.40              |
| 1:D:184:GLY:O    | 1:D:220:TYR:HA   | 2.21                     | 0.40              |
| 1:A:32:TYR:O     | 1:A:32:TYR:CG    | 2.72                     | 0.40              |
| 1:A:50:GLN:H     | 1:A:50:GLN:HG3   | 1.29                     | 0.40              |
| 1:A:165:THR:HG22 | 1:A:165:THR:O    | 1.99                     | 0.40              |
| 1:B:76:GLN:O     | 1:B:78:GLY:N     | 2.54                     | 0.40              |
| 1:B:109:LEU:O    | 1:B:109:LEU:HD23 | 2.21                     | 0.40              |
| 1:C:111:TYR:CZ   | 1:C:188:VAL:HG21 | 2.56                     | 0.40              |
| 1:C:165:THR:O    | 1:C:166:ALA:O    | 2.40                     | 0.40              |
| 1:C:169:SER:HB3  | 1:C:170:ASN:H    | 1.43                     | 0.40              |
| 1:C:198:ASN:O    | 1:C:201:GLU:N    | 2.54                     | 0.40              |
| 1:C:241:THR:HG23 | 1:C:247:THR:O    | 2.20                     | 0.40              |
| 1:A:105:VAL:HG12 | 1:A:106:TYR:N    | 2.24                     | 0.40              |
| 1:A:340:PHE:HE1  | 1:B:45:PHE:CD2   | 2.39                     | 0.40              |
| 1:B:129:PHE:CZ   | 1:B:174:VAL:O    | 2.75                     | 0.40              |
| 1:B:139:TYR:CE2  | 1:B:141:ASN:HB2  | 2.56                     | 0.40              |
| 1:B:340:PHE:C    | 1:B:340:PHE:CD2  | 2.99                     | 0.40              |
| 1:C:106:TYR:O    | 1:C:109:LEU:N    | 2.55                     | 0.40              |
| 1:C:233:GLU:HG2  | 1:C:255:GLN:HG2  | 2.04                     | 0.40              |
| 1:C:323:LYS:HA   | 1:C:323:LYS:HD3  | 1.73                     | 0.40              |
| 1:D:122:THR:CG2  | 1:D:256:ASP:CG   | 2.90                     | 0.40              |
| 1:D:197:THR:O    | 1:D:198:ASN:C    | 2.64                     | 0.40              |
| 1:D:258:LEU:C    | 1:D:259:LEU:HG   | 2.47                     | 0.40              |
| 1:A:200:GLN:HG2  | 1:A:250:PHE:CE1  | 2.57                     | 0.40              |
| 1:B:3:ILE:HD13   | 1:B:13:LEU:HD23  | 2.03                     | 0.40              |
| 1:B:21:HIS:ND1   | 1:C:98:TYR:OH    | 2.38                     | 0.40              |
| 1:B:23:PHE:C     | 1:B:35:ASN:ND2   | 2.78                     | 0.40              |
| 1:B:39:THR:HG22  | 1:B:67:GLY:HA3   | 2.02                     | 0.40              |
| 1:B:180:TYR:CE2  | 1:B:181:GLU:C    | 2.99                     | 0.40              |
| 1:C:147:LEU:HD22 | 1:C:147:LEU:HA   | 1.43                     | 0.40              |
| 1:C:308:SER:O    | 1:C:309:THR:HG22 | 2.17                     | 0.40              |
| 1:D:14:TYR:CD2   | 1:D:44:GLY:C     | 2.99                     | 0.40              |
| 1:D:161:ASN:N    | 1:D:170:ASN:HD21 | 2.20                     | 0.40              |
| 1:D:239:PRO:CA   | 1:D:250:PHE:HD2  | 2.27                     | 0.40              |

All (6) 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:B:6:LYS:CB | 1:B:6:LYS:NZ[5_555] | 1.70                     | 0.50              |

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| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:B:6:LYS:C    | 1:B:6:LYS:NZ[5_555]    | 1.91                     | 0.29              |
| 1:B:6:LYS:CA   | 1:B:6:LYS:NZ[5_555]    | 1.96                     | 0.24              |
| 1:C:287:GLY:CA | 1:D:321:ASP:OD1[2_565] | 1.97                     | 0.23              |
| 1:B:287:GLY:CA | 1:C:321:ASP:OD1[3_455] | 2.07                     | 0.13              |
| 1:B:6:LYS:CD   | 1:B:6:LYS:CD[5_555]    | 2.09                     | 0.11              |

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 338/340 (99%)   | 255 (75%)  | 47 (14%)  | 36 (11%) | 0           | 6 |
| 1   | B     | 338/340 (99%)   | 270 (80%)  | 41 (12%)  | 27 (8%)  | 1           | 9 |
| 1   | C     | 338/340 (99%)   | 255 (75%)  | 53 (16%)  | 30 (9%)  | 0           | 8 |
| 1   | D     | 338/340 (99%)   | 256 (76%)  | 48 (14%)  | 34 (10%) | 0           | 7 |
| All | All   | 1352/1360 (99%) | 1036 (77%) | 189 (14%) | 127 (9%) | 0           | 8 |

All (127) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | GLU  |
| 1   | A     | 52  | ASN  |
| 1   | A     | 73  | ALA  |
| 1   | A     | 115 | LEU  |
| 1   | A     | 119 | GLY  |
| 1   | A     | 126 | ASP  |
| 1   | A     | 135 | GLY  |
| 1   | A     | 166 | ALA  |
| 1   | A     | 276 | THR  |
| 1   | A     | 304 | ASN  |
| 1   | A     | 320 | SER  |
| 1   | A     | 321 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 327 | GLY  |
| 1   | B     | 39  | THR  |
| 1   | B     | 52  | ASN  |
| 1   | B     | 73  | ALA  |
| 1   | B     | 75  | ALA  |
| 1   | B     | 91  | ALA  |
| 1   | B     | 111 | TYR  |
| 1   | B     | 163 | ARG  |
| 1   | B     | 222 | ALA  |
| 1   | B     | 243 | LYS  |
| 1   | C     | 91  | ALA  |
| 1   | C     | 110 | GLY  |
| 1   | C     | 154 | ALA  |
| 1   | C     | 170 | ASN  |
| 1   | C     | 183 | GLU  |
| 1   | C     | 244 | PHE  |
| 1   | C     | 252 | ASN  |
| 1   | C     | 284 | GLU  |
| 1   | C     | 308 | SER  |
| 1   | C     | 326 | VAL  |
| 1   | D     | 7   | ASP  |
| 1   | D     | 60  | GLN  |
| 1   | D     | 73  | ALA  |
| 1   | D     | 75  | ALA  |
| 1   | D     | 113 | ASP  |
| 1   | D     | 119 | GLY  |
| 1   | D     | 122 | THR  |
| 1   | D     | 245 | THR  |
| 1   | D     | 265 | PHE  |
| 1   | D     | 304 | ASN  |
| 1   | D     | 339 | GLN  |
| 1   | A     | 103 | GLY  |
| 1   | A     | 107 | ASP  |
| 1   | A     | 109 | LEU  |
| 1   | A     | 110 | GLY  |
| 1   | A     | 117 | GLU  |
| 1   | A     | 163 | ARG  |
| 1   | A     | 167 | ARG  |
| 1   | A     | 170 | ASN  |
| 1   | A     | 200 | GLN  |
| 1   | A     | 243 | LYS  |
| 1   | A     | 252 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 282 | ASP  |
| 1   | B     | 7   | ASP  |
| 1   | B     | 26  | GLY  |
| 1   | B     | 29  | GLU  |
| 1   | B     | 170 | ASN  |
| 1   | B     | 303 | PHE  |
| 1   | B     | 339 | GLN  |
| 1   | C     | 39  | THR  |
| 1   | C     | 124 | TYR  |
| 1   | C     | 146 | GLY  |
| 1   | C     | 150 | GLY  |
| 1   | C     | 166 | ALA  |
| 1   | C     | 171 | GLY  |
| 1   | C     | 177 | SER  |
| 1   | C     | 223 | ASN  |
| 1   | D     | 28  | GLY  |
| 1   | D     | 35  | ASN  |
| 1   | D     | 37  | ASP  |
| 1   | D     | 74  | ASP  |
| 1   | D     | 111 | TYR  |
| 1   | D     | 118 | PHE  |
| 1   | D     | 144 | PHE  |
| 1   | D     | 183 | GLU  |
| 1   | D     | 244 | PHE  |
| 1   | D     | 284 | GLU  |
| 1   | D     | 308 | SER  |
| 1   | D     | 327 | GLY  |
| 1   | A     | 27  | ASN  |
| 1   | A     | 128 | PHE  |
| 1   | A     | 337 | VAL  |
| 1   | B     | 96  | PHE  |
| 1   | B     | 97  | ASP  |
| 1   | B     | 117 | GLU  |
| 1   | B     | 149 | ASP  |
| 1   | B     | 167 | ARG  |
| 1   | B     | 284 | GLU  |
| 1   | C     | 145 | PHE  |
| 1   | C     | 199 | LEU  |
| 1   | C     | 222 | ALA  |
| 1   | D     | 50  | GLN  |
| 1   | D     | 117 | GLU  |
| 1   | D     | 171 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 303 | PHE  |
| 1   | A     | 177 | SER  |
| 1   | A     | 183 | GLU  |
| 1   | A     | 221 | ASP  |
| 1   | A     | 303 | PHE  |
| 1   | B     | 77  | THR  |
| 1   | B     | 114 | MET  |
| 1   | B     | 126 | ASP  |
| 1   | C     | 52  | ASN  |
| 1   | C     | 70  | SER  |
| 1   | C     | 73  | ALA  |
| 1   | C     | 93  | VAL  |
| 1   | C     | 119 | GLY  |
| 1   | C     | 147 | LEU  |
| 1   | C     | 245 | THR  |
| 1   | D     | 110 | GLY  |
| 1   | D     | 191 | TYR  |
| 1   | D     | 198 | ASN  |
| 1   | D     | 267 | PHE  |
| 1   | B     | 128 | PHE  |
| 1   | C     | 35  | ASN  |
| 1   | C     | 144 | PHE  |
| 1   | D     | 39  | THR  |
| 1   | D     | 115 | LEU  |
| 1   | D     | 128 | PHE  |
| 1   | A     | 114 | MET  |
| 1   | A     | 171 | GLY  |
| 1   | B     | 51  | ILE  |
| 1   | B     | 105 | VAL  |
| 1   | A     | 28  | GLY  |
| 1   | A     | 286 | ILE  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

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| Mol | Chain | Analysed         | Rotameric | Outliers  | Percentiles |   |
|-----|-------|------------------|-----------|-----------|-------------|---|
| 1   | A     | 263/263 (100%)   | 169 (64%) | 94 (36%)  | 0           | 1 |
| 1   | B     | 263/263 (100%)   | 182 (69%) | 81 (31%)  | 0           | 2 |
| 1   | C     | 263/263 (100%)   | 187 (71%) | 76 (29%)  | 0           | 3 |
| 1   | D     | 263/263 (100%)   | 193 (73%) | 70 (27%)  | 0           | 3 |
| All | All   | 1052/1052 (100%) | 731 (70%) | 321 (30%) | 0           | 2 |

All (321) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | GLU  |
| 1   | A     | 3   | ILE  |
| 1   | A     | 4   | TYR  |
| 1   | A     | 11  | VAL  |
| 1   | A     | 16  | LYS  |
| 1   | A     | 20  | LEU  |
| 1   | A     | 30  | ASN  |
| 1   | A     | 32  | TYR  |
| 1   | A     | 39  | THR  |
| 1   | A     | 40  | TYR  |
| 1   | A     | 42  | ARG  |
| 1   | A     | 45  | PHE  |
| 1   | A     | 46  | LYS  |
| 1   | A     | 49  | THR  |
| 1   | A     | 50  | GLN  |
| 1   | A     | 51  | ILE  |
| 1   | A     | 54  | ASP  |
| 1   | A     | 70  | SER  |
| 1   | A     | 80  | LYS  |
| 1   | A     | 81  | THR  |
| 1   | A     | 82  | ARG  |
| 1   | A     | 89  | LYS  |
| 1   | A     | 92  | ASP  |
| 1   | A     | 93  | VAL  |
| 1   | A     | 96  | PHE  |
| 1   | A     | 101 | ASN  |
| 1   | A     | 104 | VAL  |
| 1   | A     | 105 | VAL  |
| 1   | A     | 115 | LEU  |
| 1   | A     | 122 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 130 | VAL  |
| 1   | A     | 133 | VAL  |
| 1   | A     | 136 | VAL  |
| 1   | A     | 142 | SER  |
| 1   | A     | 144 | PHE  |
| 1   | A     | 148 | VAL  |
| 1   | A     | 152 | ASN  |
| 1   | A     | 153 | PHE  |
| 1   | A     | 157 | TYR  |
| 1   | A     | 158 | LEU  |
| 1   | A     | 160 | LYS  |
| 1   | A     | 162 | GLU  |
| 1   | A     | 165 | THR  |
| 1   | A     | 167 | ARG  |
| 1   | A     | 170 | ASN  |
| 1   | A     | 172 | ASP  |
| 1   | A     | 174 | VAL  |
| 1   | A     | 181 | GLU  |
| 1   | A     | 183 | GLU  |
| 1   | A     | 187 | ILE  |
| 1   | A     | 188 | VAL  |
| 1   | A     | 191 | TYR  |
| 1   | A     | 197 | THR  |
| 1   | A     | 198 | ASN  |
| 1   | A     | 199 | LEU  |
| 1   | A     | 216 | THR  |
| 1   | A     | 225 | ILE  |
| 1   | A     | 230 | ASN  |
| 1   | A     | 231 | TYR  |
| 1   | A     | 243 | LYS  |
| 1   | A     | 245 | THR  |
| 1   | A     | 247 | THR  |
| 1   | A     | 248 | SER  |
| 1   | A     | 253 | LYS  |
| 1   | A     | 254 | THR  |
| 1   | A     | 257 | VAL  |
| 1   | A     | 258 | LEU  |
| 1   | A     | 259 | LEU  |
| 1   | A     | 265 | PHE  |
| 1   | A     | 267 | PHE  |
| 1   | A     | 271 | PRO  |
| 1   | A     | 272 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 273 | ILE  |
| 1   | A     | 279 | LYS  |
| 1   | A     | 284 | GLU  |
| 1   | A     | 286 | ILE  |
| 1   | A     | 289 | VAL  |
| 1   | A     | 292 | VAL  |
| 1   | A     | 294 | TYR  |
| 1   | A     | 296 | GLU  |
| 1   | A     | 297 | VAL  |
| 1   | A     | 305 | LYS  |
| 1   | A     | 308 | SER  |
| 1   | A     | 310 | TYR  |
| 1   | A     | 311 | VAL  |
| 1   | A     | 314 | ILE  |
| 1   | A     | 318 | ILE  |
| 1   | A     | 320 | SER  |
| 1   | A     | 321 | ASP  |
| 1   | A     | 326 | VAL  |
| 1   | A     | 331 | THR  |
| 1   | A     | 334 | VAL  |
| 1   | A     | 336 | ILE  |
| 1   | A     | 337 | VAL  |
| 1   | B     | 4   | TYR  |
| 1   | B     | 5   | ASN  |
| 1   | B     | 9   | ASN  |
| 1   | B     | 13  | LEU  |
| 1   | B     | 20  | LEU  |
| 1   | B     | 25  | LYS  |
| 1   | B     | 32  | TYR  |
| 1   | B     | 35  | ASN  |
| 1   | B     | 45  | PHE  |
| 1   | B     | 46  | LYS  |
| 1   | B     | 48  | GLU  |
| 1   | B     | 49  | THR  |
| 1   | B     | 52  | ASN  |
| 1   | B     | 54  | ASP  |
| 1   | B     | 58  | TYR  |
| 1   | B     | 64  | ASN  |
| 1   | B     | 88  | LEU  |
| 1   | B     | 89  | LYS  |
| 1   | B     | 93  | VAL  |
| 1   | B     | 96  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 98  | TYR  |
| 1   | B     | 104 | VAL  |
| 1   | B     | 105 | VAL  |
| 1   | B     | 109 | LEU  |
| 1   | B     | 115 | LEU  |
| 1   | B     | 122 | THR  |
| 1   | B     | 125 | SER  |
| 1   | B     | 130 | VAL  |
| 1   | B     | 133 | VAL  |
| 1   | B     | 138 | THR  |
| 1   | B     | 139 | TYR  |
| 1   | B     | 149 | ASP  |
| 1   | B     | 151 | LEU  |
| 1   | B     | 153 | PHE  |
| 1   | B     | 155 | VAL  |
| 1   | B     | 156 | GLN  |
| 1   | B     | 157 | TYR  |
| 1   | B     | 158 | LEU  |
| 1   | B     | 160 | LYS  |
| 1   | B     | 167 | ARG  |
| 1   | B     | 169 | SER  |
| 1   | B     | 174 | VAL  |
| 1   | B     | 178 | ILE  |
| 1   | B     | 180 | TYR  |
| 1   | B     | 187 | ILE  |
| 1   | B     | 188 | VAL  |
| 1   | B     | 195 | ASP  |
| 1   | B     | 196 | ARG  |
| 1   | B     | 198 | ASN  |
| 1   | B     | 199 | LEU  |
| 1   | B     | 205 | LEU  |
| 1   | B     | 209 | LYS  |
| 1   | B     | 212 | GLU  |
| 1   | B     | 218 | LEU  |
| 1   | B     | 225 | ILE  |
| 1   | B     | 230 | ASN  |
| 1   | B     | 235 | ARG  |
| 1   | B     | 242 | ASN  |
| 1   | B     | 248 | SER  |
| 1   | B     | 257 | VAL  |
| 1   | B     | 258 | LEU  |
| 1   | B     | 260 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 266 | ASP  |
| 1   | B     | 267 | PHE  |
| 1   | B     | 272 | SER  |
| 1   | B     | 273 | ILE  |
| 1   | B     | 279 | LYS  |
| 1   | B     | 284 | GLU  |
| 1   | B     | 289 | VAL  |
| 1   | B     | 295 | PHE  |
| 1   | B     | 305 | LYS  |
| 1   | B     | 310 | TYR  |
| 1   | B     | 311 | VAL  |
| 1   | B     | 317 | GLN  |
| 1   | B     | 320 | SER  |
| 1   | B     | 323 | LYS  |
| 1   | B     | 330 | ASP  |
| 1   | B     | 331 | THR  |
| 1   | B     | 332 | VAL  |
| 1   | B     | 334 | VAL  |
| 1   | B     | 336 | ILE  |
| 1   | C     | 3   | ILE  |
| 1   | C     | 10  | LYS  |
| 1   | C     | 18  | VAL  |
| 1   | C     | 25  | LYS  |
| 1   | C     | 29  | GLU  |
| 1   | C     | 42  | ARG  |
| 1   | C     | 45  | PHE  |
| 1   | C     | 46  | LYS  |
| 1   | C     | 51  | ILE  |
| 1   | C     | 53  | SER  |
| 1   | C     | 55  | LEU  |
| 1   | C     | 56  | THR  |
| 1   | C     | 58  | TYR  |
| 1   | C     | 60  | GLN  |
| 1   | C     | 70  | SER  |
| 1   | C     | 77  | THR  |
| 1   | C     | 80  | LYS  |
| 1   | C     | 81  | THR  |
| 1   | C     | 82  | ARG  |
| 1   | C     | 85  | PHE  |
| 1   | C     | 92  | ASP  |
| 1   | C     | 95  | SER  |
| 1   | C     | 100 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 104 | VAL  |
| 1   | C     | 122 | THR  |
| 1   | C     | 133 | VAL  |
| 1   | C     | 142 | SER  |
| 1   | C     | 147 | LEU  |
| 1   | C     | 148 | VAL  |
| 1   | C     | 152 | ASN  |
| 1   | C     | 153 | PHE  |
| 1   | C     | 157 | TYR  |
| 1   | C     | 160 | LYS  |
| 1   | C     | 162 | GLU  |
| 1   | C     | 163 | ARG  |
| 1   | C     | 167 | ARG  |
| 1   | C     | 170 | ASN  |
| 1   | C     | 178 | ILE  |
| 1   | C     | 183 | GLU  |
| 1   | C     | 187 | ILE  |
| 1   | C     | 188 | VAL  |
| 1   | C     | 212 | GLU  |
| 1   | C     | 218 | LEU  |
| 1   | C     | 221 | ASP  |
| 1   | C     | 225 | ILE  |
| 1   | C     | 227 | LEU  |
| 1   | C     | 235 | ARG  |
| 1   | C     | 240 | ILE  |
| 1   | C     | 243 | LYS  |
| 1   | C     | 246 | ASN  |
| 1   | C     | 247 | THR  |
| 1   | C     | 248 | SER  |
| 1   | C     | 253 | LYS  |
| 1   | C     | 254 | THR  |
| 1   | C     | 257 | VAL  |
| 1   | C     | 258 | LEU  |
| 1   | C     | 266 | ASP  |
| 1   | C     | 269 | LEU  |
| 1   | C     | 270 | ARG  |
| 1   | C     | 273 | ILE  |
| 1   | C     | 279 | LYS  |
| 1   | C     | 283 | VAL  |
| 1   | C     | 284 | GLU  |
| 1   | C     | 286 | ILE  |
| 1   | C     | 289 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 296 | GLU  |
| 1   | C     | 297 | VAL  |
| 1   | C     | 310 | TYR  |
| 1   | C     | 311 | VAL  |
| 1   | C     | 314 | ILE  |
| 1   | C     | 318 | ILE  |
| 1   | C     | 320 | SER  |
| 1   | C     | 332 | VAL  |
| 1   | C     | 334 | VAL  |
| 1   | C     | 336 | ILE  |
| 1   | C     | 338 | TYR  |
| 1   | D     | 3   | ILE  |
| 1   | D     | 10  | LYS  |
| 1   | D     | 13  | LEU  |
| 1   | D     | 25  | LYS  |
| 1   | D     | 51  | ILE  |
| 1   | D     | 54  | ASP  |
| 1   | D     | 55  | LEU  |
| 1   | D     | 58  | TYR  |
| 1   | D     | 77  | THR  |
| 1   | D     | 80  | LYS  |
| 1   | D     | 81  | THR  |
| 1   | D     | 85  | PHE  |
| 1   | D     | 93  | VAL  |
| 1   | D     | 95  | SER  |
| 1   | D     | 96  | PHE  |
| 1   | D     | 100 | ARG  |
| 1   | D     | 104 | VAL  |
| 1   | D     | 105 | VAL  |
| 1   | D     | 115 | LEU  |
| 1   | D     | 122 | THR  |
| 1   | D     | 125 | SER  |
| 1   | D     | 132 | ARG  |
| 1   | D     | 142 | SER  |
| 1   | D     | 144 | PHE  |
| 1   | D     | 147 | LEU  |
| 1   | D     | 151 | LEU  |
| 1   | D     | 152 | ASN  |
| 1   | D     | 153 | PHE  |
| 1   | D     | 155 | VAL  |
| 1   | D     | 160 | LYS  |
| 1   | D     | 162 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 167 | ARG  |
| 1   | D     | 169 | SER  |
| 1   | D     | 170 | ASN  |
| 1   | D     | 178 | ILE  |
| 1   | D     | 181 | GLU  |
| 1   | D     | 187 | ILE  |
| 1   | D     | 188 | VAL  |
| 1   | D     | 198 | ASN  |
| 1   | D     | 209 | LYS  |
| 1   | D     | 212 | GLU  |
| 1   | D     | 219 | LYS  |
| 1   | D     | 225 | ILE  |
| 1   | D     | 231 | TYR  |
| 1   | D     | 235 | ARG  |
| 1   | D     | 240 | ILE  |
| 1   | D     | 246 | ASN  |
| 1   | D     | 253 | LYS  |
| 1   | D     | 257 | VAL  |
| 1   | D     | 258 | LEU  |
| 1   | D     | 267 | PHE  |
| 1   | D     | 273 | ILE  |
| 1   | D     | 279 | LYS  |
| 1   | D     | 284 | GLU  |
| 1   | D     | 286 | ILE  |
| 1   | D     | 289 | VAL  |
| 1   | D     | 291 | LEU  |
| 1   | D     | 292 | VAL  |
| 1   | D     | 297 | VAL  |
| 1   | D     | 311 | VAL  |
| 1   | D     | 314 | ILE  |
| 1   | D     | 315 | ILE  |
| 1   | D     | 317 | GLN  |
| 1   | D     | 318 | ILE  |
| 1   | D     | 319 | ASP  |
| 1   | D     | 320 | SER  |
| 1   | D     | 326 | VAL  |
| 1   | D     | 332 | VAL  |
| 1   | D     | 334 | VAL  |
| 1   | D     | 336 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 21  | HIS  |
| 1   | A     | 35  | ASN  |
| 1   | A     | 60  | GLN  |
| 1   | A     | 69  | ASN  |
| 1   | A     | 76  | GLN  |
| 1   | A     | 141 | ASN  |
| 1   | A     | 152 | ASN  |
| 1   | A     | 161 | ASN  |
| 1   | A     | 203 | GLN  |
| 1   | A     | 223 | ASN  |
| 1   | A     | 246 | ASN  |
| 1   | A     | 252 | ASN  |
| 1   | A     | 293 | ASN  |
| 1   | A     | 306 | ASN  |
| 1   | A     | 317 | GLN  |
| 1   | A     | 339 | GLN  |
| 1   | B     | 21  | HIS  |
| 1   | B     | 35  | ASN  |
| 1   | B     | 60  | GLN  |
| 1   | B     | 66  | GLN  |
| 1   | B     | 246 | ASN  |
| 1   | B     | 306 | ASN  |
| 1   | B     | 316 | ASN  |
| 1   | C     | 35  | ASN  |
| 1   | C     | 64  | ASN  |
| 1   | C     | 66  | GLN  |
| 1   | C     | 69  | ASN  |
| 1   | C     | 76  | GLN  |
| 1   | C     | 152 | ASN  |
| 1   | C     | 170 | ASN  |
| 1   | C     | 242 | ASN  |
| 1   | C     | 255 | GLN  |
| 1   | C     | 293 | ASN  |
| 1   | D     | 9   | ASN  |
| 1   | D     | 21  | HIS  |
| 1   | D     | 30  | ASN  |
| 1   | D     | 35  | ASN  |
| 1   | D     | 60  | GLN  |
| 1   | D     | 66  | GLN  |
| 1   | D     | 101 | ASN  |
| 1   | D     | 161 | ASN  |
| 1   | D     | 170 | ASN  |
| 1   | D     | 223 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 264 | GLN  |
| 1   | D     | 306 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 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     | 339/340 (99%)   | 0.71   | 33 (9%) 13 17  | 71, 125, 137, 149     | 0     |
| 1   | B     | 340/340 (100%)  | 0.63   | 30 (8%) 15 19  | 99, 122, 134, 139     | 0     |
| 1   | C     | 340/340 (100%)  | 0.71   | 36 (10%) 11 15 | 101, 124, 138, 146    | 0     |
| 1   | D     | 340/340 (100%)  | 0.75   | 35 (10%) 12 16 | 118, 135, 147, 157    | 0     |
| All | All   | 1359/1360 (99%) | 0.70   | 134 (9%) 13 17 | 71, 126, 142, 157     | 0     |

All (134) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 162 | GLU  | 10.0 |
| 1   | C     | 29  | GLU  | 8.3  |
| 1   | A     | 29  | GLU  | 7.8  |
| 1   | C     | 323 | LYS  | 7.0  |
| 1   | A     | 28  | GLY  | 6.4  |
| 1   | D     | 243 | LYS  | 5.1  |
| 1   | C     | 218 | LEU  | 4.8  |
| 1   | D     | 323 | LYS  | 4.7  |
| 1   | B     | 323 | LYS  | 4.6  |
| 1   | B     | 16  | LYS  | 4.6  |
| 1   | B     | 44  | GLY  | 4.5  |
| 1   | A     | 299 | ALA  | 4.3  |
| 1   | B     | 29  | GLU  | 4.2  |
| 1   | A     | 325 | GLY  | 4.0  |
| 1   | B     | 42  | ARG  | 4.0  |
| 1   | A     | 26  | GLY  | 3.9  |
| 1   | A     | 298 | GLY  | 3.9  |
| 1   | D     | 160 | LYS  | 3.9  |
| 1   | D     | 223 | ASN  | 3.8  |
| 1   | D     | 164 | ASP  | 3.8  |
| 1   | A     | 273 | ILE  | 3.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 285 | GLY  | 3.7  |
| 1   | D     | 74  | ASP  | 3.7  |
| 1   | D     | 163 | ARG  | 3.6  |
| 1   | C     | 340 | PHE  | 3.6  |
| 1   | A     | 243 | LYS  | 3.5  |
| 1   | B     | 43  | LEU  | 3.4  |
| 1   | D     | 157 | TYR  | 3.4  |
| 1   | B     | 25  | LYS  | 3.4  |
| 1   | A     | 221 | ASP  | 3.3  |
| 1   | D     | 326 | VAL  | 3.2  |
| 1   | B     | 324 | LEU  | 3.2  |
| 1   | C     | 28  | GLY  | 3.2  |
| 1   | A     | 13  | LEU  | 3.1  |
| 1   | B     | 14  | TYR  | 3.1  |
| 1   | D     | 27  | ASN  | 3.1  |
| 1   | B     | 340 | PHE  | 3.1  |
| 1   | B     | 13  | LEU  | 3.1  |
| 1   | A     | 326 | VAL  | 3.1  |
| 1   | C     | 13  | LEU  | 3.0  |
| 1   | C     | 187 | ILE  | 3.0  |
| 1   | B     | 326 | VAL  | 3.0  |
| 1   | A     | 157 | TYR  | 3.0  |
| 1   | C     | 186 | GLY  | 3.0  |
| 1   | C     | 217 | GLY  | 3.0  |
| 1   | C     | 111 | TYR  | 3.0  |
| 1   | D     | 96  | PHE  | 3.0  |
| 1   | C     | 266 | ASP  | 2.9  |
| 1   | C     | 157 | TYR  | 2.9  |
| 1   | C     | 235 | ARG  | 2.9  |
| 1   | A     | 272 | SER  | 2.9  |
| 1   | A     | 340 | PHE  | 2.9  |
| 1   | A     | 305 | LYS  | 2.8  |
| 1   | B     | 327 | GLY  | 2.8  |
| 1   | B     | 61  | TRP  | 2.8  |
| 1   | B     | 157 | TYR  | 2.8  |
| 1   | C     | 60  | GLN  | 2.8  |
| 1   | C     | 44  | GLY  | 2.8  |
| 1   | C     | 145 | PHE  | 2.8  |
| 1   | B     | 60  | GLN  | 2.7  |
| 1   | B     | 45  | PHE  | 2.7  |
| 1   | D     | 204 | PRO  | 2.7  |
| 1   | D     | 324 | LEU  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 62  | GLU  | 2.7  |
| 1   | A     | 43  | LEU  | 2.7  |
| 1   | C     | 142 | SER  | 2.7  |
| 1   | A     | 37  | ASP  | 2.7  |
| 1   | D     | 206 | GLY  | 2.7  |
| 1   | B     | 290 | ASP  | 2.7  |
| 1   | B     | 89  | LYS  | 2.7  |
| 1   | D     | 77  | THR  | 2.7  |
| 1   | B     | 329 | ASP  | 2.6  |
| 1   | C     | 31  | SER  | 2.6  |
| 1   | C     | 91  | ALA  | 2.6  |
| 1   | D     | 191 | TYR  | 2.6  |
| 1   | C     | 305 | LYS  | 2.6  |
| 1   | A     | 96  | PHE  | 2.6  |
| 1   | A     | 178 | ILE  | 2.6  |
| 1   | D     | 46  | LYS  | 2.6  |
| 1   | B     | 15  | GLY  | 2.6  |
| 1   | D     | 29  | GLU  | 2.6  |
| 1   | C     | 243 | LYS  | 2.5  |
| 1   | A     | 266 | ASP  | 2.5  |
| 1   | D     | 197 | THR  | 2.5  |
| 1   | C     | 324 | LEU  | 2.5  |
| 1   | A     | 229 | ALA  | 2.5  |
| 1   | D     | 286 | ILE  | 2.5  |
| 1   | D     | 139 | TYR  | 2.5  |
| 1   | D     | 207 | ASN  | 2.5  |
| 1   | B     | 31  | SER  | 2.5  |
| 1   | A     | 234 | THR  | 2.4  |
| 1   | D     | 81  | THR  | 2.4  |
| 1   | C     | 286 | ILE  | 2.4  |
| 1   | B     | 224 | ASN  | 2.4  |
| 1   | B     | 266 | ASP  | 2.4  |
| 1   | D     | 3   | ILE  | 2.4  |
| 1   | A     | 235 | ARG  | 2.4  |
| 1   | A     | 117 | GLU  | 2.4  |
| 1   | A     | 44  | GLY  | 2.4  |
| 1   | A     | 269 | LEU  | 2.3  |
| 1   | A     | 113 | ASP  | 2.3  |
| 1   | D     | 266 | ASP  | 2.3  |
| 1   | B     | 209 | LYS  | 2.3  |
| 1   | C     | 219 | LYS  | 2.3  |
| 1   | B     | 221 | ASP  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 116 | PRO  | 2.2  |
| 1   | C     | 160 | LYS  | 2.2  |
| 1   | D     | 195 | ASP  | 2.2  |
| 1   | A     | 78  | GLY  | 2.2  |
| 1   | B     | 161 | ASN  | 2.2  |
| 1   | D     | 176 | GLY  | 2.2  |
| 1   | A     | 80  | LYS  | 2.2  |
| 1   | D     | 235 | ARG  | 2.2  |
| 1   | C     | 325 | GLY  | 2.2  |
| 1   | A     | 207 | ASN  | 2.2  |
| 1   | A     | 189 | GLY  | 2.1  |
| 1   | A     | 210 | LYS  | 2.1  |
| 1   | B     | 147 | LEU  | 2.1  |
| 1   | C     | 25  | LYS  | 2.1  |
| 1   | C     | 16  | LYS  | 2.1  |
| 1   | C     | 144 | PHE  | 2.1  |
| 1   | D     | 261 | ALA  | 2.1  |
| 1   | C     | 267 | PHE  | 2.1  |
| 1   | D     | 144 | PHE  | 2.1  |
| 1   | A     | 1   | ALA  | 2.1  |
| 1   | D     | 69  | ASN  | 2.1  |
| 1   | D     | 201 | GLU  | 2.1  |
| 1   | C     | 17  | ALA  | 2.0  |
| 1   | D     | 138 | THR  | 2.0  |
| 1   | C     | 97  | ASP  | 2.0  |
| 1   | C     | 198 | ASN  | 2.0  |
| 1   | C     | 65  | PHE  | 2.0  |
| 1   | C     | 207 | ASN  | 2.0  |
| 1   | C     | 236 | ASN  | 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.