



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:40 AM UTC

PDB ID : 1LDK / pdb\_00001ldk  
Title : Structure of the Cul1-Rbx1-Skp1-F boxSkp2 SCF Ubiquitin Ligase Complex  
Authors : Zheng, N.; Schulman, B.A.; Song, L.; Miller, J.J.; Jeffrey, P.D.; Wang, P.; Chu, C.; Koepp, D.M.; Elledge, S.J.; Pagano, M.; Conaway, R.C.; Conaway, J.W.; Harper, J.W.; Pavletich, N.P.  
Deposited on : 2002-04-08  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

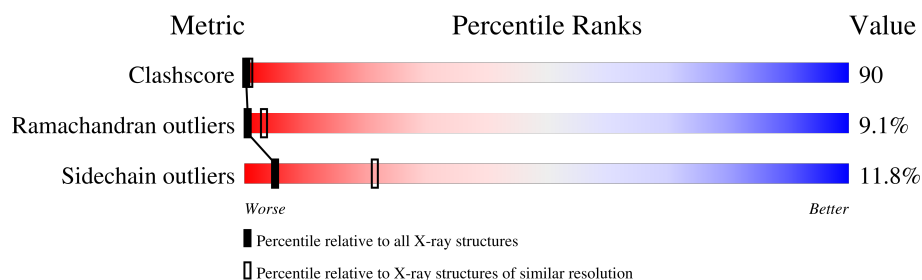
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |

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  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 396    |                  |
| 2   | B     | 366    |                  |
| 3   | C     | 90     |                  |
| 4   | D     | 133    |                  |
| 5   | E     | 41     |                  |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7922 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 CULLIN HOMOLOG.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 358      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2950  | 1870 | 508 | 558 | 14 |         |         |       |

- Molecule 2 is a protein called CULLIN HOMOLOG.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 366      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2981  | 1894 | 503 | 569 | 15 |         |         |       |

- Molecule 3 is a protein called ring-box protein 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | C     | 88       | Total | C   | N   | O   | S | 574     | 0       | 0     |
|     |       |          | 731   | 464 | 133 | 125 | 9 |         |         |       |

- Molecule 4 is a protein called CYCLIN A/CDK2-ASSOCIATED PROTEIN P19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 926   | 594 | 149 | 178 | 5 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | ?       | -        | ASP    | deletion | UNP P63208 |
| D     | ?       | -        | ASP    | deletion | UNP P63208 |
| D     | ?       | -        | GLU    | deletion | UNP P63208 |
| D     | ?       | -        | GLY    | deletion | UNP P63208 |
| D     | ?       | -        | ASP    | deletion | UNP P63208 |
| D     | ?       | -        | ASP    | deletion | UNP P63208 |

- Molecule 5 is a protein called SKP2-like protein type gamma.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 5   | E     | 41       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 331   | 218 | 52 | 58 | 3 |         |         |       |

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

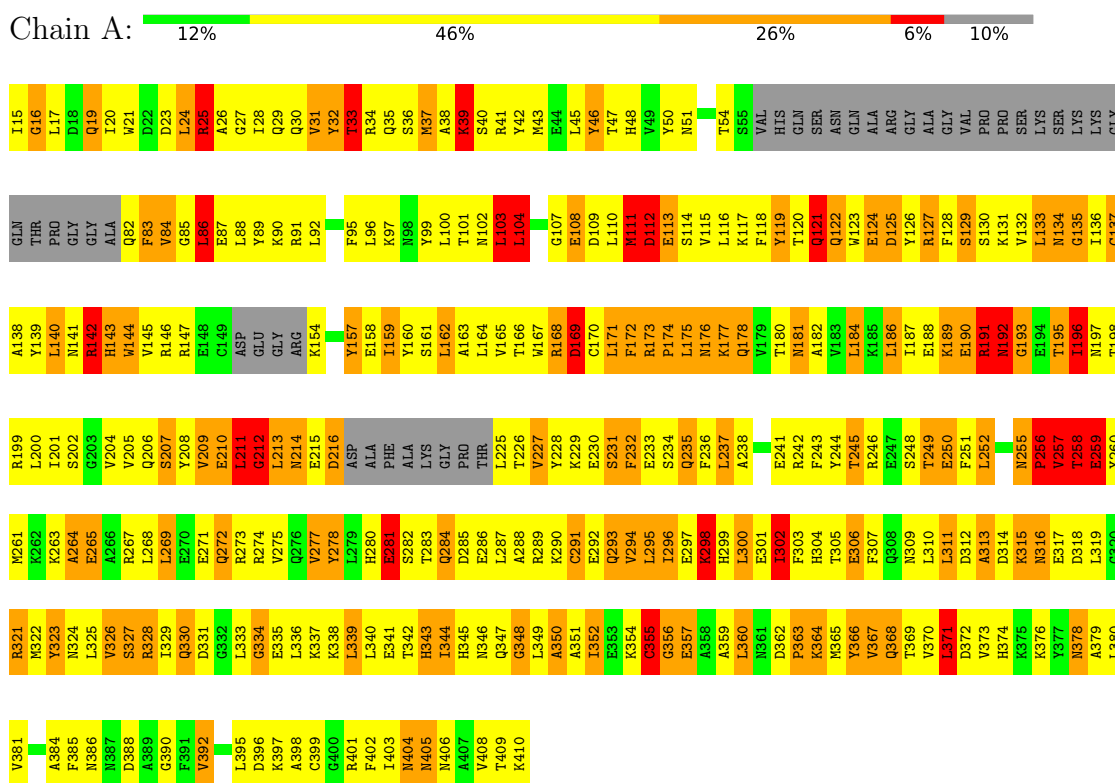
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | C     | 3        | Total | Zn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |

### 3 Residue-property plots

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

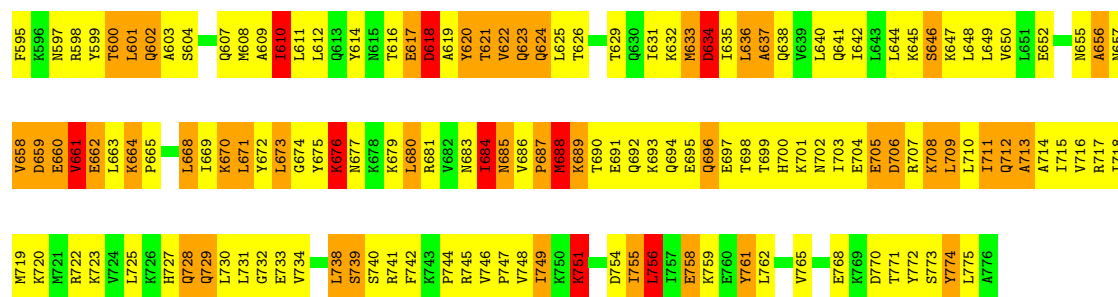
Note EDS was not executed.

#### • Molecule 1: CULLIN HOMOLOG



#### • Molecule 2: CULLIN HOMOLOG

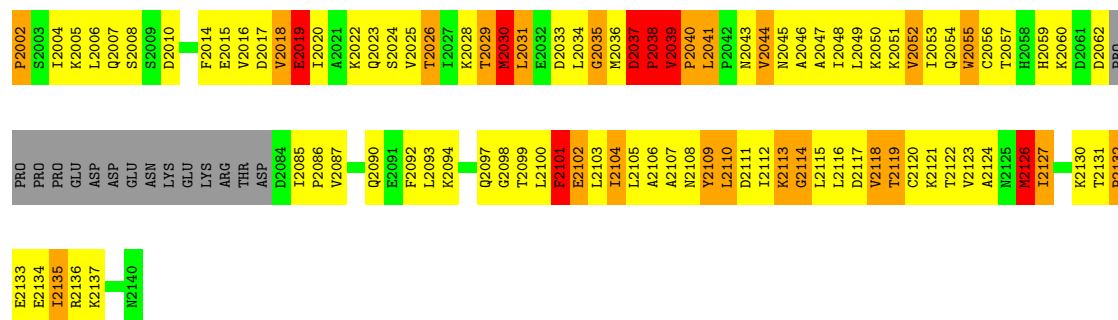
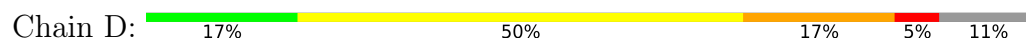




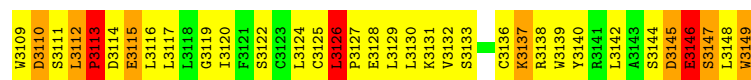
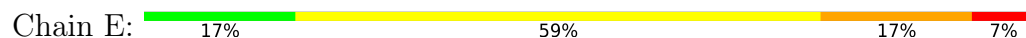
• Molecule 3: ring-box protein 1



• Molecule 4: CYCLIN A/CDK2-ASSOCIATED PROTEIN P19



• Molecule 5: SKP2-like protein type gamma



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                          | Source    |
|----------------------------------------------------------|------------------------------------------------|-----------|
| Space group                                              | P 21 21 2                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 219.38Å 50.53Å 158.61Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 20.00 – 3.10                                   | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (20.00-3.10)                   | Depositor |
| $R_{merge}$                                              | (Not available)                                | Depositor |
| $R_{sym}$                                                | (Not available)                                | Depositor |
| Refinement program                                       | CNS 1.0                                        | Depositor |
| R, $R_{free}$                                            | 0.289 , 0.331                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 7922                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 77.0                                           | wwPDB-VP  |

## 5 Model quality [i](#)

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

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 1.09         | 25/2999 (0.8%) | 1.90        | 109/4039 (2.7%)  |
| 2   | B     | 1.16         | 35/3027 (1.2%) | 1.80        | 113/4069 (2.8%)  |
| 3   | C     | 0.39         | 0/752          | 0.96        | 3/1020 (0.3%)    |
| 4   | D     | 1.29         | 9/940 (1.0%)   | 1.73        | 28/1271 (2.2%)   |
| 5   | E     | 0.99         | 3/340 (0.9%)   | 1.65        | 7/461 (1.5%)     |
| All | All   | 1.10         | 72/8058 (0.9%) | 1.76        | 260/10860 (2.4%) |

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                   | 5                   |
| 2   | B     | 0                   | 3                   |
| 4   | D     | 0                   | 1                   |
| All | All   | 0                   | 9                   |

All (72) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | D     | 2102 | GLU  | N-CA    | 28.38 | 1.82        | 1.46     |
| 2   | B     | 453  | PHE  | N-CA    | 15.62 | 1.65        | 1.46     |
| 2   | B     | 489  | ILE  | N-CA    | 15.25 | 1.65        | 1.46     |
| 2   | B     | 443  | GLU  | C-N     | 15.12 | 1.53        | 1.33     |
| 1   | A     | 210  | GLU  | N-CA    | 13.22 | 1.63        | 1.46     |
| 1   | A     | 367  | VAL  | N-CA    | 12.59 | 1.63        | 1.46     |
| 1   | A     | 135  | GLY  | N-CA    | 11.74 | 1.62        | 1.45     |
| 2   | B     | 426  | CYS  | N-CA    | 10.96 | 1.60        | 1.46     |
| 2   | B     | 523  | LYS  | N-CA    | 10.81 | 1.60        | 1.46     |
| 1   | A     | 196  | ILE  | CG1-CD1 | 10.42 | 1.92        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 344  | ILE  | N-CA    | 10.32 | 1.60        | 1.46     |
| 4   | D     | 2110 | LEU  | N-CA    | 10.26 | 1.59        | 1.46     |
| 2   | B     | 580  | THR  | N-CA    | -9.71 | 1.34        | 1.46     |
| 2   | B     | 637  | ALA  | N-CA    | 9.25  | 1.58        | 1.46     |
| 2   | B     | 661  | VAL  | C-N     | -8.72 | 1.21        | 1.33     |
| 2   | B     | 579  | LEU  | C-N     | -8.64 | 1.22        | 1.33     |
| 1   | A     | 296  | ILE  | CG1-CD1 | 8.58  | 1.85        | 1.51     |
| 1   | A     | 99   | TYR  | N-CA    | 8.24  | 1.56        | 1.46     |
| 4   | D     | 2126 | MET  | N-CA    | 7.90  | 1.56        | 1.46     |
| 2   | B     | 712  | GLN  | C-N     | -7.76 | 1.22        | 1.33     |
| 1   | A     | 371  | LEU  | N-CA    | 7.67  | 1.55        | 1.46     |
| 5   | E     | 3145 | ASP  | C-N     | -7.57 | 1.24        | 1.33     |
| 1   | A     | 108  | GLU  | C-N     | 7.56  | 1.43        | 1.33     |
| 2   | B     | 580  | THR  | CA-C    | -7.50 | 1.44        | 1.52     |
| 1   | A     | 231  | SER  | N-CA    | -7.48 | 1.37        | 1.46     |
| 2   | B     | 424  | ARG  | N-CA    | 7.39  | 1.55        | 1.46     |
| 2   | B     | 662  | GLU  | C-N     | -6.87 | 1.24        | 1.33     |
| 2   | B     | 684  | ILE  | N-CA    | -6.86 | 1.37        | 1.46     |
| 1   | A     | 143  | HIS  | N-CA    | -6.86 | 1.37        | 1.46     |
| 1   | A     | 142  | ARG  | C-N     | -6.81 | 1.24        | 1.33     |
| 1   | A     | 207  | SER  | N-CA    | 6.73  | 1.54        | 1.46     |
| 2   | B     | 706  | ASP  | N-CA    | 6.63  | 1.54        | 1.46     |
| 2   | B     | 685  | ASN  | C-N     | 6.53  | 1.40        | 1.33     |
| 1   | A     | 295  | LEU  | C-N     | 6.42  | 1.42        | 1.33     |
| 1   | A     | 216  | ASP  | C-O     | -6.38 | 1.10        | 1.23     |
| 1   | A     | 256  | PRO  | CA-C    | -6.37 | 1.44        | 1.52     |
| 5   | E     | 3149 | TRP  | C-OXT   | 6.36  | 1.36        | 1.23     |
| 2   | B     | 712  | GLN  | CA-C    | -6.33 | 1.45        | 1.53     |
| 1   | A     | 214  | ASN  | N-CA    | -6.24 | 1.39        | 1.46     |
| 5   | E     | 3114 | ASP  | CA-C    | -5.96 | 1.45        | 1.53     |
| 2   | B     | 436  | ASN  | CA-C    | 5.84  | 1.58        | 1.52     |
| 1   | A     | 256  | PRO  | C-N     | -5.82 | 1.27        | 1.33     |
| 2   | B     | 686  | VAL  | N-CA    | 5.75  | 1.53        | 1.46     |
| 1   | A     | 257  | VAL  | N-CA    | -5.71 | 1.40        | 1.46     |
| 1   | A     | 192  | ASN  | CA-C    | 5.63  | 1.60        | 1.52     |
| 1   | A     | 113  | GLU  | C-O     | -5.61 | 1.17        | 1.24     |
| 2   | B     | 495  | ALA  | N-CA    | 5.57  | 1.53        | 1.46     |
| 2   | B     | 709  | LEU  | C-N     | -5.54 | 1.26        | 1.33     |
| 2   | B     | 713  | ALA  | N-CA    | -5.53 | 1.39        | 1.46     |
| 4   | D     | 2029 | THR  | C-N     | -5.51 | 1.25        | 1.33     |
| 2   | B     | 465  | PHE  | N-CA    | 5.50  | 1.53        | 1.46     |
| 2   | B     | 437  | PRO  | CA-C    | -5.48 | 1.45        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 633  | MET  | C-N     | -5.48 | 1.26        | 1.33     |
| 1   | A     | 32   | TYR  | C-N     | -5.48 | 1.26        | 1.33     |
| 1   | A     | 255  | ASN  | C-N     | 5.47  | 1.40        | 1.33     |
| 1   | A     | 293  | GLN  | C-N     | -5.46 | 1.27        | 1.33     |
| 4   | D     | 2002 | PRO  | C-N     | -5.46 | 1.27        | 1.33     |
| 2   | B     | 579  | LEU  | CA-C    | -5.42 | 1.45        | 1.52     |
| 2   | B     | 755  | ILE  | CA-C    | 5.38  | 1.59        | 1.52     |
| 2   | B     | 436  | ASN  | CA-CB   | -5.28 | 1.47        | 1.54     |
| 4   | D     | 2119 | THR  | N-CA    | -5.26 | 1.40        | 1.46     |
| 2   | B     | 573  | ARG  | C-N     | -5.22 | 1.26        | 1.33     |
| 2   | B     | 711  | ILE  | CG1-CD1 | 5.19  | 1.72        | 1.51     |
| 4   | D     | 2040 | PRO  | C-N     | -5.17 | 1.29        | 1.33     |
| 2   | B     | 687  | PRO  | C-N     | -5.14 | 1.26        | 1.33     |
| 4   | D     | 2030 | MET  | N-CA    | -5.13 | 1.39        | 1.46     |
| 4   | D     | 2119 | THR  | CA-C    | -5.10 | 1.46        | 1.52     |
| 2   | B     | 659  | ASP  | C-N     | -5.09 | 1.26        | 1.33     |
| 1   | A     | 298  | LYS  | C-N     | -5.07 | 1.26        | 1.33     |
| 2   | B     | 756  | LEU  | N-CA    | 5.07  | 1.52        | 1.46     |
| 2   | B     | 503  | LYS  | C-N     | -5.03 | 1.26        | 1.33     |
| 2   | B     | 688  | MET  | N-CA    | -5.00 | 1.39        | 1.46     |

All (260) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 5   | E     | 3146 | GLU  | N-CA-C | -22.34 | 79.08       | 108.34   |
| 4   | D     | 2102 | GLU  | N-CA-C | 20.95  | 139.58      | 112.34   |
| 4   | D     | 2110 | LEU  | N-CA-C | -20.85 | 85.37       | 113.30   |
| 1   | A     | 212  | GLY  | CA-C-N | -20.45 | 92.19       | 122.65   |
| 1   | A     | 212  | GLY  | C-N-CA | -20.45 | 92.19       | 122.65   |
| 1   | A     | 112  | ASP  | O-C-N  | -19.43 | 95.86       | 122.68   |
| 2   | B     | 476  | HIS  | N-CA-C | -17.77 | 87.61       | 110.53   |
| 2   | B     | 523  | LYS  | N-CA-C | -16.81 | 89.09       | 112.45   |
| 1   | A     | 213  | LEU  | CA-C-O | 16.44  | 139.05      | 120.80   |
| 1   | A     | 213  | LEU  | CA-C-N | 16.43  | 142.98      | 120.63   |
| 1   | A     | 213  | LEU  | C-N-CA | 16.43  | 142.98      | 120.63   |
| 2   | B     | 706  | ASP  | N-CA-C | 16.39  | 133.21      | 112.89   |
| 1   | A     | 190  | GLU  | N-CA-C | -15.46 | 93.69       | 113.17   |
| 1   | A     | 127  | ARG  | N-CA-C | -15.31 | 93.91       | 112.89   |
| 1   | A     | 367  | VAL  | N-CA-C | -15.11 | 91.19       | 111.44   |
| 2   | B     | 701  | LYS  | N-CA-C | -14.81 | 94.53       | 112.89   |
| 2   | B     | 424  | ARG  | N-CA-C | -14.39 | 94.09       | 112.23   |
| 1   | A     | 344  | ILE  | N-CA-C | -14.05 | 93.83       | 113.07   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | A     | 112  | ASP  | CA-C-N     | 13.83  | 147.95      | 121.54   |
| 1   | A     | 112  | ASP  | C-N-CA     | 13.83  | 147.95      | 121.54   |
| 3   | C     | 1023 | GLU  | N-CA-CB    | -13.82 | 88.73       | 110.85   |
| 2   | B     | 646  | SER  | N-CA-C     | -13.78 | 92.38       | 110.43   |
| 2   | B     | 637  | ALA  | N-CA-C     | -13.67 | 95.01       | 112.23   |
| 1   | A     | 195  | THR  | N-CA-C     | 13.41  | 129.12      | 112.23   |
| 1   | A     | 350  | ALA  | N-CA-C     | -13.30 | 96.86       | 111.36   |
| 1   | A     | 196  | ILE  | CB-CG1-CD1 | -12.82 | 86.89       | 113.80   |
| 1   | A     | 210  | GLU  | N-CA-C     | -12.68 | 97.83       | 113.18   |
| 1   | A     | 129  | SER  | N-CA-C     | -12.53 | 96.44       | 112.23   |
| 4   | D     | 2101 | PHE  | CA-C-N     | -12.38 | 100.70      | 120.63   |
| 4   | D     | 2101 | PHE  | C-N-CA     | -12.38 | 100.70      | 120.63   |
| 1   | A     | 371  | LEU  | N-CA-C     | -12.37 | 97.78       | 111.14   |
| 2   | B     | 436  | ASN  | CA-CB-CG   | -12.25 | 100.35      | 112.60   |
| 2   | B     | 426  | CYS  | N-CA-C     | -11.92 | 97.02       | 111.69   |
| 2   | B     | 479  | SER  | CB-CA-C    | -10.90 | 96.14       | 111.95   |
| 2   | B     | 494  | GLN  | OE1-CD-NE2 | -10.78 | 111.82      | 122.60   |
| 1   | A     | 33   | THR  | N-CA-C     | -10.77 | 90.34       | 108.75   |
| 1   | A     | 16   | GLY  | N-CA-C     | -10.75 | 87.71       | 113.18   |
| 1   | A     | 296  | ILE  | CB-CG1-CD1 | -10.70 | 91.33       | 113.80   |
| 2   | B     | 706  | ASP  | N-CA-CB    | -10.64 | 93.06       | 110.40   |
| 1   | A     | 99   | TYR  | N-CA-C     | -10.60 | 99.69       | 111.14   |
| 2   | B     | 412  | ALA  | N-CA-C     | -10.60 | 96.54       | 110.53   |
| 1   | A     | 378  | ASN  | N-CA-C     | -10.58 | 99.71       | 111.14   |
| 2   | B     | 465  | PHE  | N-CA-C     | -10.56 | 99.77       | 111.28   |
| 2   | B     | 505  | GLN  | OE1-CD-NE2 | -10.52 | 112.08      | 122.60   |
| 2   | B     | 549  | GLN  | OE1-CD-NE2 | -10.49 | 112.11      | 122.60   |
| 2   | B     | 696  | GLN  | OE1-CD-NE2 | -10.36 | 112.24      | 122.60   |
| 4   | D     | 2102 | GLU  | N-CA-CB    | -10.27 | 91.70       | 110.18   |
| 1   | A     | 35   | GLN  | OE1-CD-NE2 | -10.24 | 112.36      | 122.60   |
| 1   | A     | 19   | GLN  | OE1-CD-NE2 | -10.20 | 112.40      | 122.60   |
| 1   | A     | 293  | GLN  | OE1-CD-NE2 | -10.18 | 112.42      | 122.60   |
| 2   | B     | 477  | GLN  | OE1-CD-NE2 | -10.15 | 112.45      | 122.60   |
| 1   | A     | 135  | GLY  | N-CA-C     | -10.11 | 89.22       | 113.18   |
| 2   | B     | 520  | GLN  | OE1-CD-NE2 | -9.93  | 112.67      | 122.60   |
| 2   | B     | 624  | GLN  | OE1-CD-NE2 | -9.90  | 112.70      | 122.60   |
| 2   | B     | 728  | GLN  | OE1-CD-NE2 | -9.83  | 112.77      | 122.60   |
| 1   | A     | 121  | GLN  | OE1-CD-NE2 | -9.76  | 112.84      | 122.60   |
| 2   | B     | 602  | GLN  | OE1-CD-NE2 | -9.75  | 112.85      | 122.60   |
| 1   | A     | 213  | LEU  | O-C-N      | 9.74   | 134.59      | 123.19   |
| 2   | B     | 548  | GLN  | OE1-CD-NE2 | -9.69  | 112.91      | 122.60   |
| 2   | B     | 584  | GLN  | OE1-CD-NE2 | -9.67  | 112.93      | 122.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2   | B     | 712  | GLN  | OE1-CD-NE2 | -9.54 | 113.06      | 122.60   |
| 1   | A     | 178  | GLN  | OE1-CD-NE2 | -9.50 | 113.10      | 122.60   |
| 2   | B     | 623  | GLN  | OE1-CD-NE2 | -9.44 | 113.16      | 122.60   |
| 1   | A     | 265  | GLU  | N-CA-C     | -9.33 | 101.00      | 111.82   |
| 1   | A     | 122  | GLN  | OE1-CD-NE2 | -9.29 | 113.31      | 122.60   |
| 2   | B     | 633  | MET  | CA-C-N     | -9.28 | 104.71      | 120.58   |
| 2   | B     | 633  | MET  | C-N-CA     | -9.28 | 104.71      | 120.58   |
| 2   | B     | 634  | ASP  | CA-CB-CG   | 9.12  | 121.72      | 112.60   |
| 1   | A     | 172  | PHE  | CA-CB-CG   | -9.11 | 104.69      | 113.80   |
| 1   | A     | 256  | PRO  | CA-N-CD    | -9.06 | 99.32       | 112.00   |
| 1   | A     | 191  | ARG  | N-CA-C     | -8.91 | 96.66       | 109.31   |
| 2   | B     | 729  | GLN  | OE1-CD-NE2 | -8.90 | 113.70      | 122.60   |
| 1   | A     | 104  | LEU  | N-CA-C     | -8.83 | 100.83      | 111.69   |
| 2   | B     | 774  | TYR  | CA-C-N     | 8.75  | 134.12      | 122.30   |
| 2   | B     | 774  | TYR  | C-N-CA     | 8.75  | 134.12      | 122.30   |
| 2   | B     | 521  | PHE  | N-CA-CB    | -8.64 | 96.89       | 110.46   |
| 1   | A     | 360  | LEU  | N-CA-C     | -8.64 | 102.18      | 112.89   |
| 2   | B     | 413  | GLN  | OE1-CD-NE2 | -8.58 | 114.02      | 122.60   |
| 1   | A     | 291  | CYS  | N-CA-C     | -8.52 | 102.07      | 111.36   |
| 1   | A     | 189  | LYS  | N-CA-C     | -8.49 | 97.54       | 110.70   |
| 1   | A     | 356  | GLY  | N-CA-C     | 8.47  | 125.68      | 110.95   |
| 2   | B     | 489  | ILE  | N-CA-C     | 8.45  | 126.92      | 109.34   |
| 2   | B     | 692  | GLN  | N-CA-C     | -8.44 | 102.03      | 111.82   |
| 2   | B     | 687  | PRO  | CB-CA-C    | 8.30  | 122.02      | 111.39   |
| 2   | B     | 495  | ALA  | N-CA-C     | 8.23  | 128.34      | 110.80   |
| 2   | B     | 453  | PHE  | N-CA-C     | -8.14 | 101.47      | 111.40   |
| 2   | B     | 437  | PRO  | CA-N-CD    | -8.09 | 100.67      | 112.00   |
| 5   | E     | 3113 | PRO  | CA-N-CD    | -8.02 | 100.78      | 112.00   |
| 4   | D     | 2118 | VAL  | N-CA-C     | 7.85  | 118.40      | 110.23   |
| 2   | B     | 660  | GLU  | CA-C-N     | -7.79 | 107.96      | 121.97   |
| 2   | B     | 660  | GLU  | C-N-CA     | -7.79 | 107.96      | 121.97   |
| 2   | B     | 610  | ILE  | N-CA-C     | -7.78 | 101.69      | 112.50   |
| 1   | A     | 207  | SER  | N-CA-C     | -7.75 | 102.47      | 112.23   |
| 4   | D     | 2002 | PRO  | N-CA-CB    | 7.62  | 111.39      | 103.00   |
| 4   | D     | 2105 | LEU  | CA-C-N     | -7.59 | 108.30      | 121.66   |
| 4   | D     | 2105 | LEU  | C-N-CA     | -7.59 | 108.30      | 121.66   |
| 1   | A     | 313  | ALA  | N-CA-C     | -7.51 | 94.81       | 110.80   |
| 2   | B     | 618  | ASP  | CA-CB-CG   | -7.47 | 105.13      | 112.60   |
| 1   | A     | 257  | VAL  | CA-C-N     | 7.45  | 135.76      | 121.54   |
| 1   | A     | 257  | VAL  | C-N-CA     | 7.45  | 135.76      | 121.54   |
| 4   | D     | 2104 | ILE  | N-CA-C     | -7.44 | 103.61      | 110.82   |
| 4   | D     | 2126 | MET  | N-CA-C     | 7.43  | 126.62      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 5   | E     | 3147 | SER  | N-CA-C    | 7.42  | 126.60      | 110.80   |
| 2   | B     | 684  | ILE  | CA-C-N    | -7.38 | 109.82      | 122.14   |
| 2   | B     | 684  | ILE  | C-N-CA    | -7.38 | 109.82      | 122.14   |
| 2   | B     | 488  | MET  | CA-C-N    | -7.25 | 108.93      | 121.97   |
| 2   | B     | 488  | MET  | C-N-CA    | -7.25 | 108.93      | 121.97   |
| 2   | B     | 696  | GLN  | CG-CD-NE2 | 7.23  | 127.25      | 116.40   |
| 2   | B     | 756  | LEU  | N-CA-C    | 7.23  | 121.19      | 112.38   |
| 2   | B     | 505  | GLN  | CG-CD-NE2 | 7.19  | 127.19      | 116.40   |
| 2   | B     | 436  | ASN  | CA-C-N    | 7.15  | 127.72      | 120.14   |
| 2   | B     | 436  | ASN  | C-N-CA    | 7.15  | 127.72      | 120.14   |
| 2   | B     | 494  | GLN  | CG-CD-NE2 | 7.14  | 127.11      | 116.40   |
| 1   | A     | 392  | VAL  | N-CA-C    | -7.12 | 102.88      | 110.36   |
| 4   | D     | 2055 | TRP  | N-CA-C    | -7.12 | 103.45      | 111.07   |
| 2   | B     | 521  | PHE  | CA-C-N    | -7.09 | 109.39      | 122.09   |
| 2   | B     | 521  | PHE  | C-N-CA    | -7.09 | 109.39      | 122.09   |
| 2   | B     | 548  | GLN  | CG-CD-NE2 | 7.07  | 127.01      | 116.40   |
| 4   | D     | 2033 | ASP  | N-CA-C    | -7.06 | 104.80      | 113.41   |
| 2   | B     | 549  | GLN  | CG-CD-NE2 | 7.03  | 126.94      | 116.40   |
| 1   | A     | 269  | LEU  | N-CA-C    | -6.99 | 103.35      | 110.97   |
| 2   | B     | 477  | GLN  | CG-CD-NE2 | 6.94  | 126.81      | 116.40   |
| 2   | B     | 712  | GLN  | CG-CD-NE2 | 6.92  | 126.77      | 116.40   |
| 1   | A     | 35   | GLN  | CG-CD-NE2 | 6.89  | 126.74      | 116.40   |
| 1   | A     | 122  | GLN  | CG-CD-NE2 | 6.86  | 126.69      | 116.40   |
| 1   | A     | 99   | TYR  | N-CA-CB   | -6.86 | 100.12      | 110.07   |
| 2   | B     | 729  | GLN  | CG-CD-NE2 | 6.85  | 126.67      | 116.40   |
| 1   | A     | 192  | ASN  | CA-CB-CG  | 6.84  | 119.44      | 112.60   |
| 2   | B     | 455  | TYR  | N-CA-C    | -6.81 | 105.91      | 114.56   |
| 2   | B     | 413  | GLN  | CG-CD-NE2 | 6.79  | 126.59      | 116.40   |
| 2   | B     | 451  | VAL  | N-CA-C    | -6.79 | 103.70      | 110.62   |
| 2   | B     | 537  | ILE  | N-CA-C    | -6.74 | 100.15      | 109.46   |
| 2   | B     | 618  | ASP  | CB-CA-C   | 6.72  | 123.80      | 110.42   |
| 4   | D     | 2109 | TYR  | CA-C-N    | -6.71 | 112.08      | 122.49   |
| 4   | D     | 2109 | TYR  | C-N-CA    | -6.71 | 112.08      | 122.49   |
| 1   | A     | 181  | ASN  | N-CA-C    | -6.70 | 104.05      | 111.36   |
| 2   | B     | 571  | ALA  | CA-C-N    | 6.70  | 129.93      | 120.28   |
| 2   | B     | 571  | ALA  | C-N-CA    | 6.70  | 129.93      | 120.28   |
| 2   | B     | 520  | GLN  | CG-CD-NE2 | 6.67  | 126.41      | 116.40   |
| 2   | B     | 624  | GLN  | CG-CD-NE2 | 6.67  | 126.41      | 116.40   |
| 2   | B     | 602  | GLN  | CG-CD-NE2 | 6.61  | 126.31      | 116.40   |
| 2   | B     | 728  | GLN  | CG-CD-NE2 | 6.58  | 126.28      | 116.40   |
| 1   | A     | 293  | GLN  | CG-CD-NE2 | 6.58  | 126.27      | 116.40   |
| 1   | A     | 19   | GLN  | CG-CD-NE2 | 6.58  | 126.27      | 116.40   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 134  | ASN  | CA-C-N    | -6.56 | 108.56      | 121.41   |
| 1   | A     | 134  | ASN  | C-N-CA    | -6.56 | 108.56      | 121.41   |
| 2   | B     | 585  | LEU  | N-CA-C    | 6.53  | 123.82      | 114.16   |
| 1   | A     | 119  | TYR  | N-CA-C    | -6.53 | 97.90       | 110.56   |
| 4   | D     | 2108 | ASN  | N-CA-C    | -6.47 | 104.31      | 111.36   |
| 1   | A     | 255  | ASN  | CA-C-N    | 6.46  | 126.42      | 119.76   |
| 1   | A     | 255  | ASN  | C-N-CA    | 6.46  | 126.42      | 119.76   |
| 1   | A     | 121  | GLN  | CG-CD-NE2 | 6.43  | 126.05      | 116.40   |
| 4   | D     | 2041 | LEU  | CA-C-N    | 6.43  | 126.56      | 119.87   |
| 4   | D     | 2041 | LEU  | C-N-CA    | 6.43  | 126.56      | 119.87   |
| 2   | B     | 584  | GLN  | CG-CD-NE2 | 6.42  | 126.03      | 116.40   |
| 2   | B     | 623  | GLN  | CG-CD-NE2 | 6.41  | 126.02      | 116.40   |
| 4   | D     | 2118 | VAL  | O-C-N     | 6.40  | 128.87      | 121.96   |
| 1   | A     | 178  | GLN  | CG-CD-NE2 | 6.39  | 125.99      | 116.40   |
| 5   | E     | 3112 | LEU  | CA-C-N    | 6.35  | 127.78      | 119.84   |
| 5   | E     | 3112 | LEU  | C-N-CA    | 6.35  | 127.78      | 119.84   |
| 2   | B     | 696  | GLN  | N-CA-C    | 6.33  | 117.87      | 110.97   |
| 1   | A     | 232  | PHE  | CA-CB-CG  | -6.28 | 107.52      | 113.80   |
| 1   | A     | 366  | TYR  | CA-C-N    | -6.27 | 109.51      | 120.29   |
| 1   | A     | 366  | TYR  | C-N-CA    | -6.27 | 109.51      | 120.29   |
| 1   | A     | 326  | VAL  | CB-CA-C   | -6.26 | 103.99      | 111.81   |
| 2   | B     | 528  | SER  | N-CA-C    | -6.26 | 97.47       | 110.80   |
| 2   | B     | 662  | GLU  | CA-C-O    | -6.25 | 111.57      | 120.51   |
| 1   | A     | 177  | LYS  | CA-C-N    | 6.24  | 131.12      | 121.19   |
| 1   | A     | 177  | LYS  | C-N-CA    | 6.24  | 131.12      | 121.19   |
| 1   | A     | 142  | ARG  | N-CA-C    | 6.23  | 120.88      | 113.16   |
| 5   | E     | 3112 | LEU  | O-C-N     | 6.20  | 126.94      | 121.18   |
| 1   | A     | 133  | LEU  | N-CA-C    | -6.16 | 104.11      | 111.69   |
| 1   | A     | 404  | ASN  | CA-CB-CG  | 6.16  | 118.75      | 112.60   |
| 1   | A     | 256  | PRO  | N-CA-CB   | 6.15  | 108.78      | 103.31   |
| 1   | A     | 302  | ILE  | N-CA-C    | -6.14 | 104.52      | 110.72   |
| 2   | B     | 774  | TYR  | N-CA-C    | 6.10  | 119.58      | 109.46   |
| 2   | B     | 687  | PRO  | CA-C-N    | -6.08 | 109.94      | 121.54   |
| 2   | B     | 687  | PRO  | C-N-CA    | -6.08 | 109.94      | 121.54   |
| 2   | B     | 688  | MET  | CB-CA-C   | 6.08  | 122.51      | 110.42   |
| 1   | A     | 364  | LYS  | N-CA-C    | 6.07  | 117.59      | 110.97   |
| 1   | A     | 157  | TYR  | N-CA-C    | 6.06  | 123.70      | 110.80   |
| 4   | D     | 2127 | ILE  | N-CA-C    | -6.05 | 107.96      | 113.71   |
| 1   | A     | 108  | GLU  | O-C-N     | 6.05  | 130.35      | 122.97   |
| 1   | A     | 278  | TYR  | N-CA-C    | 6.03  | 123.64      | 110.80   |
| 2   | B     | 688  | MET  | N-CA-C    | -5.98 | 98.06       | 110.80   |
| 1   | A     | 316  | ASN  | CB-CA-C   | 5.97  | 120.42      | 110.92   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 664  | LYS  | CA-C-N  | 5.96  | 126.73      | 120.12   |
| 2   | B     | 664  | LYS  | C-N-CA  | 5.96  | 126.73      | 120.12   |
| 1   | A     | 169  | ASP  | N-CA-C  | -5.95 | 98.14       | 110.80   |
| 2   | B     | 585  | LEU  | CB-CA-C | -5.92 | 101.25      | 110.37   |
| 1   | A     | 281  | GLU  | N-CA-C  | 5.91  | 118.48      | 111.33   |
| 1   | A     | 211  | LEU  | N-CA-C  | -5.90 | 105.34      | 112.54   |
| 1   | A     | 255  | ASN  | O-C-N   | 5.90  | 125.95      | 121.65   |
| 2   | B     | 462  | PHE  | N-CA-C  | -5.87 | 104.96      | 111.71   |
| 4   | D     | 2044 | VAL  | N-CA-C  | 5.87  | 115.19      | 106.85   |
| 2   | B     | 435  | LYS  | N-CA-C  | -5.86 | 98.31       | 110.80   |
| 4   | D     | 2038 | PRO  | N-CA-C  | 5.85  | 124.53      | 112.47   |
| 1   | A     | 306  | GLU  | N-CA-C  | -5.82 | 104.86      | 111.14   |
| 5   | E     | 3114 | ASP  | CB-CA-C | -5.80 | 99.95       | 110.56   |
| 3   | C     | 1043 | ALA  | N-CA-C  | -5.79 | 105.51      | 113.56   |
| 1   | A     | 343  | HIS  | CA-C-N  | -5.71 | 112.32      | 121.35   |
| 1   | A     | 343  | HIS  | C-N-CA  | -5.71 | 112.32      | 121.35   |
| 1   | A     | 46   | TYR  | N-CA-C  | -5.70 | 102.02      | 111.37   |
| 1   | A     | 355  | CYS  | CA-C-N  | -5.70 | 116.79      | 122.20   |
| 1   | A     | 355  | CYS  | C-N-CA  | -5.70 | 116.79      | 122.20   |
| 1   | A     | 211  | LEU  | CA-C-N  | 5.67  | 132.52      | 121.41   |
| 1   | A     | 211  | LEU  | C-N-CA  | 5.67  | 132.52      | 121.41   |
| 3   | C     | 1022 | PHE  | CB-CA-C | -5.66 | 101.98      | 110.24   |
| 2   | B     | 452  | VAL  | CA-C-N  | -5.64 | 111.29      | 120.71   |
| 2   | B     | 452  | VAL  | C-N-CA  | -5.64 | 111.29      | 120.71   |
| 1   | A     | 25   | ARG  | N-CA-C  | -5.63 | 105.15      | 111.28   |
| 2   | B     | 754  | ASP  | CA-C-N  | -5.62 | 114.03      | 120.88   |
| 2   | B     | 754  | ASP  | C-N-CA  | -5.62 | 114.03      | 120.88   |
| 2   | B     | 661  | VAL  | CA-C-O  | -5.60 | 113.78      | 120.78   |
| 4   | D     | 2002 | PRO  | CA-C-N  | -5.57 | 112.96      | 121.26   |
| 4   | D     | 2002 | PRO  | C-N-CA  | -5.57 | 112.96      | 121.26   |
| 2   | B     | 555  | LEU  | O-C-N   | 5.55  | 127.45      | 121.12   |
| 1   | A     | 189  | LYS  | CA-C-N  | 5.49  | 131.60      | 122.54   |
| 1   | A     | 189  | LYS  | C-N-CA  | 5.49  | 131.60      | 122.54   |
| 2   | B     | 573  | ARG  | CB-CA-C | -5.44 | 101.30      | 110.44   |
| 2   | B     | 664  | LYS  | CA-C-O  | 5.44  | 126.03      | 120.64   |
| 2   | B     | 510  | ASP  | N-CA-C  | -5.43 | 105.44      | 111.36   |
| 1   | A     | 357  | GLU  | N-CA-C  | -5.43 | 99.23       | 110.80   |
| 4   | D     | 2037 | ASP  | CA-C-N  | -5.42 | 113.07      | 119.84   |
| 4   | D     | 2037 | ASP  | C-N-CA  | -5.42 | 113.07      | 119.84   |
| 1   | A     | 209  | VAL  | CA-C-N  | -5.40 | 111.06      | 121.58   |
| 1   | A     | 209  | VAL  | C-N-CA  | -5.40 | 111.06      | 121.58   |
| 2   | B     | 633  | MET  | N-CA-C  | 5.39  | 117.91      | 111.71   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 494  | GLN  | CA-C-N  | 5.34  | 131.74      | 121.54   |
| 2   | B     | 494  | GLN  | C-N-CA  | 5.34  | 131.74      | 121.54   |
| 1   | A     | 32   | TYR  | CA-C-N  | 5.33  | 131.33      | 121.94   |
| 1   | A     | 32   | TYR  | C-N-CA  | 5.33  | 131.33      | 121.94   |
| 2   | B     | 452  | VAL  | N-CA-C  | -5.33 | 105.19      | 110.62   |
| 1   | A     | 264  | ALA  | N-CA-C  | -5.33 | 105.16      | 110.97   |
| 2   | B     | 705  | GLU  | CA-C-N  | -5.33 | 111.82      | 121.14   |
| 2   | B     | 705  | GLU  | C-N-CA  | -5.33 | 111.82      | 121.14   |
| 1   | A     | 19   | GLN  | N-CA-C  | -5.29 | 106.72      | 114.39   |
| 1   | A     | 348  | GLY  | N-CA-C  | -5.27 | 107.25      | 113.99   |
| 1   | A     | 259  | GLU  | N-CA-C  | -5.25 | 99.61       | 110.80   |
| 1   | A     | 232  | PHE  | N-CA-C  | 5.24  | 119.14      | 112.12   |
| 2   | B     | 761  | TYR  | CB-CA-C | -5.24 | 108.83      | 116.53   |
| 4   | D     | 2126 | MET  | N-CA-CB | -5.24 | 101.64      | 110.49   |
| 2   | B     | 659  | ASP  | O-C-N   | 5.22  | 127.73      | 122.09   |
| 2   | B     | 521  | PHE  | CB-CA-C | 5.20  | 119.69      | 109.72   |
| 1   | A     | 404  | ASN  | N-CA-C  | 5.19  | 117.53      | 110.88   |
| 2   | B     | 561  | ARG  | N-CA-C  | -5.19 | 107.12      | 113.50   |
| 2   | B     | 504  | LEU  | CB-CA-C | 5.18  | 120.73      | 110.42   |
| 4   | D     | 2135 | ILE  | N-CA-C  | -5.17 | 105.29      | 110.30   |
| 2   | B     | 774  | TYR  | O-C-N   | 5.13  | 129.07      | 123.22   |
| 1   | A     | 272  | GLN  | N-CA-C  | -5.11 | 105.60      | 111.07   |
| 1   | A     | 293  | GLN  | CA-C-N  | 5.09  | 127.44      | 120.77   |
| 1   | A     | 293  | GLN  | C-N-CA  | 5.09  | 127.44      | 120.77   |
| 1   | A     | 31   | VAL  | N-CA-C  | 5.07  | 119.89      | 109.34   |
| 2   | B     | 453  | PHE  | N-CA-CB | -5.07 | 102.62      | 110.13   |
| 1   | A     | 277  | VAL  | N-CA-C  | 5.07  | 116.40      | 110.62   |
| 1   | A     | 111  | MET  | O-C-N   | -5.06 | 117.02      | 122.79   |
| 2   | B     | 437  | PRO  | CA-C-N  | -5.05 | 114.28      | 121.50   |
| 2   | B     | 437  | PRO  | C-N-CA  | -5.05 | 114.28      | 121.50   |
| 1   | A     | 330  | GLN  | N-CA-C  | 5.05  | 118.11      | 110.64   |
| 2   | B     | 676  | LYS  | N-CA-C  | -5.04 | 103.94      | 110.19   |

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 111 | MET  | Mainchain         |
| 1   | A     | 112 | ASP  | Mainchain,Peptide |
| 1   | A     | 113 | GLU  | Mainchain         |
| 1   | A     | 323 | TYR  | Sidechain         |
| 2   | B     | 443 | GLU  | Mainchain         |

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| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | B     | 452  | VAL  | Peptide |
| 2   | B     | 488  | MET  | Peptide |
| 4   | D     | 2101 | PHE  | 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     | 2950  | 0        | 2915     | 571     | 1            |
| 2   | B     | 2981  | 0        | 3049     | 573     | 3            |
| 3   | C     | 731   | 0        | 689      | 28      | 1            |
| 4   | D     | 926   | 0        | 944      | 175     | 0            |
| 5   | E     | 331   | 0        | 331      | 44      | 0            |
| 6   | C     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 7922  | 0        | 7928     | 1320    | 4            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 90.

All (1320) 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:409:THR:CG2  | 2:B:415:SER:HA    | 1.32                     | 1.58              |
| 2:B:555:LEU:CD2  | 2:B:559:LEU:HD22  | 1.11                     | 1.55              |
| 1:A:296:ILE:CD1  | 1:A:296:ILE:CG1   | 1.85                     | 1.55              |
| 2:B:553:PHE:CD1  | 2:B:631:ILE:HG12  | 1.37                     | 1.53              |
| 4:D:2002:PRO:CB  | 4:D:2018:VAL:HG13 | 1.41                     | 1.47              |
| 4:D:2038:PRO:O   | 4:D:2040:PRO:CD   | 1.63                     | 1.47              |
| 1:A:196:ILE:CD1  | 1:A:196:ILE:CG1   | 1.92                     | 1.46              |
| 4:D:2102:GLU:N   | 4:D:2102:GLU:CA   | 1.82                     | 1.41              |
| 1:A:409:THR:CG2  | 2:B:415:SER:CA    | 1.88                     | 1.40              |
| 1:A:144:TRP:O    | 1:A:144:TRP:CE3   | 1.72                     | 1.40              |
| 2:B:555:LEU:HD23 | 2:B:559:LEU:CD2   | 0.91                     | 1.39              |
| 1:A:196:ILE:CD1  | 1:A:196:ILE:CG2   | 2.04                     | 1.35              |
| 1:A:409:THR:HG21 | 2:B:415:SER:CA    | 1.40                     | 1.34              |
| 2:B:712:GLN:HB3  | 2:B:756:LEU:CD2   | 1.60                     | 1.30              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:719:MET:HE3  | 2:B:774:TYR:CD1  | 1.67                     | 1.29              |
| 1:A:107:GLY:O    | 1:A:110:LEU:HG   | 1.10                     | 1.28              |
| 2:B:555:LEU:CD2  | 2:B:559:LEU:CD2  | 1.77                     | 1.27              |
| 2:B:577:ARG:O    | 2:B:577:ARG:HD3  | 1.32                     | 1.26              |
| 4:D:2038:PRO:O   | 4:D:2040:PRO:HD3 | 1.14                     | 1.25              |
| 2:B:578:LYS:O    | 2:B:579:LEU:HD23 | 1.24                     | 1.25              |
| 1:A:196:ILE:CD1  | 1:A:196:ILE:HG21 | 1.61                     | 1.25              |
| 1:A:297:GLU:O    | 1:A:300:LEU:HB2  | 1.32                     | 1.23              |
| 1:A:142:ARG:O    | 1:A:146:ARG:NH2  | 1.71                     | 1.23              |
| 1:A:211:LEU:O    | 1:A:213:LEU:HD23 | 1.07                     | 1.22              |
| 2:B:553:PHE:CD1  | 2:B:631:ILE:CG1  | 2.24                     | 1.21              |
| 4:D:2002:PRO:CB  | 4:D:2018:VAL:CG1 | 2.21                     | 1.19              |
| 1:A:293:GLN:HG3  | 1:A:297:GLU:OE2  | 1.42                     | 1.18              |
| 1:A:111:MET:HB2  | 1:A:114:SER:OG   | 1.41                     | 1.18              |
| 2:B:553:PHE:CE1  | 2:B:631:ILE:HD11 | 1.80                     | 1.16              |
| 2:B:712:GLN:HB3  | 2:B:756:LEU:HD21 | 1.23                     | 1.15              |
| 1:A:402:PHE:O    | 1:A:406:ASN:ND2  | 1.81                     | 1.14              |
| 1:A:30:GLN:O     | 1:A:33:THR:O     | 1.62                     | 1.14              |
| 1:A:211:LEU:O    | 1:A:213:LEU:CD2  | 1.96                     | 1.14              |
| 2:B:569:PHE:O    | 2:B:572:SER:OG   | 1.66                     | 1.13              |
| 2:B:620:TYR:CD2  | 2:B:624:GLN:HG2  | 1.82                     | 1.13              |
| 2:B:551:CYS:SG   | 2:B:632:LYS:HD2  | 1.89                     | 1.12              |
| 2:B:521:PHE:O    | 2:B:525:LEU:HB2  | 1.50                     | 1.11              |
| 2:B:619:ALA:HB2  | 2:B:670:LYS:CB   | 1.80                     | 1.11              |
| 1:A:100:LEU:HA   | 1:A:103:LEU:HD23 | 1.30                     | 1.11              |
| 1:A:296:ILE:HG12 | 1:A:325:LEU:HD22 | 1.31                     | 1.10              |
| 1:A:196:ILE:HG21 | 1:A:196:ILE:HD12 | 1.24                     | 1.10              |
| 2:B:727:HIS:O    | 2:B:727:HIS:ND1  | 1.85                     | 1.10              |
| 2:B:637:ALA:HB1  | 2:B:663:LEU:HD12 | 1.34                     | 1.09              |
| 2:B:474:LEU:O    | 2:B:476:HIS:O    | 1.71                     | 1.09              |
| 2:B:638:GLN:OE1  | 2:B:688:MET:CE   | 1.99                     | 1.09              |
| 1:A:186:LEU:HD21 | 1:A:197:ASN:HD22 | 0.96                     | 1.09              |
| 1:A:297:GLU:O    | 1:A:300:LEU:N    | 1.86                     | 1.09              |
| 2:B:555:LEU:HD21 | 2:B:559:LEU:HD22 | 1.27                     | 1.09              |
| 5:E:3145:ASP:OD2 | 5:E:3146:GLU:O   | 1.71                     | 1.08              |
| 1:A:196:ILE:CG2  | 1:A:196:ILE:HD13 | 1.73                     | 1.08              |
| 2:B:553:PHE:HD1  | 2:B:631:ILE:CG1  | 1.60                     | 1.08              |
| 2:B:469:MET:HB3  | 2:B:473:ARG:HH12 | 1.12                     | 1.07              |
| 2:B:574:HIS:HB2  | 2:B:577:ARG:HG3  | 1.31                     | 1.07              |
| 1:A:39:LYS:HE2   | 4:D:2037:ASP:H   | 1.12                     | 1.06              |
| 1:A:107:GLY:O    | 1:A:110:LEU:CG   | 2.02                     | 1.06              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:566:PHE:O    | 2:B:569:PHE:N     | 1.89                     | 1.06              |
| 2:B:553:PHE:CE1  | 2:B:629:THR:HB    | 1.91                     | 1.06              |
| 2:B:712:GLN:CB   | 2:B:756:LEU:HD21  | 1.85                     | 1.05              |
| 1:A:107:GLY:HA2  | 1:A:110:LEU:HD11  | 1.36                     | 1.05              |
| 1:A:168:ARG:HH11 | 1:A:213:LEU:HD22  | 1.20                     | 1.04              |
| 1:A:409:THR:HG21 | 2:B:415:SER:C     | 1.82                     | 1.04              |
| 1:A:186:LEU:HD21 | 1:A:197:ASN:ND2   | 1.69                     | 1.04              |
| 1:A:404:ASN:O    | 1:A:405:ASN:OD1   | 1.76                     | 1.03              |
| 1:A:144:TRP:O    | 1:A:144:TRP:CD2   | 2.11                     | 1.03              |
| 1:A:297:GLU:O    | 1:A:300:LEU:CB    | 2.07                     | 1.03              |
| 4:D:2038:PRO:O   | 4:D:2040:PRO:HD2  | 1.50                     | 1.03              |
| 2:B:555:LEU:HD23 | 2:B:559:LEU:HD23  | 1.09                     | 1.02              |
| 2:B:553:PHE:CE1  | 2:B:631:ILE:CD1   | 2.41                     | 1.02              |
| 2:B:619:ALA:CB   | 2:B:670:LYS:HB3   | 1.90                     | 1.02              |
| 2:B:660:GLU:O    | 2:B:661:VAL:O     | 1.76                     | 1.02              |
| 1:A:112:ASP:HB3  | 1:A:182:ALA:HA    | 1.39                     | 1.02              |
| 1:A:173:ARG:H    | 1:A:174:PRO:HD2   | 1.26                     | 1.01              |
| 1:A:142:ARG:O    | 1:A:146:ARG:CZ    | 2.09                     | 1.01              |
| 1:A:158:GLU:HG3  | 1:A:159:ILE:H     | 1.24                     | 1.01              |
| 2:B:474:LEU:C    | 2:B:476:HIS:O     | 2.04                     | 1.01              |
| 1:A:196:ILE:CD1  | 1:A:196:ILE:CB    | 2.39                     | 1.00              |
| 1:A:186:LEU:CD1  | 1:A:197:ASN:HB3   | 1.93                     | 0.99              |
| 1:A:196:ILE:HD13 | 1:A:196:ILE:HG23  | 1.39                     | 0.98              |
| 2:B:553:PHE:CE1  | 2:B:631:ILE:CG1   | 2.46                     | 0.98              |
| 2:B:758:GLU:OE1  | 2:B:759:LYS:HG3   | 1.63                     | 0.98              |
| 2:B:453:PHE:HA   | 2:B:456:ILE:HD13  | 1.46                     | 0.98              |
| 2:B:477:GLN:O    | 2:B:477:GLN:HG2   | 1.63                     | 0.98              |
| 1:A:186:LEU:HD13 | 1:A:197:ASN:HB3   | 1.47                     | 0.97              |
| 1:A:118:PHE:O    | 1:A:122:GLN:HG2   | 1.65                     | 0.96              |
| 1:A:296:ILE:CD1  | 1:A:296:ILE:CB    | 2.43                     | 0.96              |
| 1:A:197:ASN:CB   | 1:A:200:LEU:HD12  | 1.97                     | 0.95              |
| 2:B:577:ARG:O    | 2:B:577:ARG:CD    | 2.15                     | 0.95              |
| 1:A:256:PRO:HB2  | 1:A:259:GLU:HB2   | 1.49                     | 0.95              |
| 1:A:409:THR:C    | 2:B:414:SER:O     | 2.03                     | 0.94              |
| 2:B:571:ALA:CA   | 2:B:577:ARG:HH21  | 1.80                     | 0.94              |
| 2:B:719:MET:SD   | 2:B:774:TYR:CG    | 2.60                     | 0.94              |
| 4:D:2100:LEU:HA  | 4:D:2103:LEU:HD12 | 1.47                     | 0.94              |
| 1:A:100:LEU:HD12 | 1:A:166:THR:HG22  | 1.48                     | 0.94              |
| 1:A:142:ARG:O    | 1:A:146:ARG:NE    | 2.00                     | 0.94              |
| 4:D:2040:PRO:O   | 4:D:2041:LEU:HD23 | 1.68                     | 0.94              |
| 1:A:197:ASN:CG   | 1:A:200:LEU:HD12  | 1.91                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:577:ARG:HD3   | 2:B:577:ARG:C     | 1.90                     | 0.94              |
| 2:B:719:MET:SD    | 2:B:774:TYR:CB    | 2.56                     | 0.94              |
| 2:B:553:PHE:CE1   | 2:B:631:ILE:HG12  | 2.04                     | 0.93              |
| 2:B:553:PHE:HE1   | 2:B:631:ILE:HD11  | 1.17                     | 0.93              |
| 1:A:111:MET:HB2   | 1:A:114:SER:HG    | 1.18                     | 0.92              |
| 1:A:17:LEU:HA     | 1:A:20:ILE:HB     | 1.51                     | 0.92              |
| 2:B:610:ILE:HD13  | 2:B:610:ILE:H     | 1.34                     | 0.91              |
| 1:A:39:LYS:HE2    | 4:D:2037:ASP:N    | 1.84                     | 0.91              |
| 2:B:719:MET:SD    | 2:B:774:TYR:HB3   | 2.10                     | 0.91              |
| 2:B:541:SER:H     | 2:B:545:TRP:NE1   | 1.68                     | 0.91              |
| 1:A:157:TYR:C     | 1:A:157:TYR:CD2   | 2.45                     | 0.90              |
| 1:A:352:ILE:HD11  | 1:A:406:ASN:HB3   | 1.52                     | 0.90              |
| 1:A:235:GLN:H     | 1:A:235:GLN:NE2   | 1.68                     | 0.90              |
| 2:B:430:LEU:O     | 2:B:431:LYS:O     | 1.89                     | 0.90              |
| 5:E:3126:LEU:HD12 | 5:E:3126:LEU:H    | 1.35                     | 0.90              |
| 1:A:100:LEU:HA    | 1:A:103:LEU:CD2   | 2.01                     | 0.90              |
| 2:B:660:GLU:O     | 2:B:661:VAL:C     | 2.11                     | 0.90              |
| 1:A:15:ILE:HG22   | 1:A:20:ILE:HG13   | 1.50                     | 0.90              |
| 4:D:2038:PRO:C    | 4:D:2040:PRO:HD3  | 1.95                     | 0.90              |
| 1:A:257:VAL:O     | 1:A:260:TYR:HB3   | 1.72                     | 0.90              |
| 2:B:719:MET:CE    | 2:B:774:TYR:CD1   | 2.55                     | 0.89              |
| 4:D:2031:LEU:HA   | 4:D:2035:GLY:HA2  | 1.52                     | 0.89              |
| 2:B:712:GLN:HB3   | 2:B:756:LEU:HD22  | 1.53                     | 0.89              |
| 4:D:2101:PHE:C    | 4:D:2102:GLU:CA   | 2.45                     | 0.89              |
| 1:A:297:GLU:C     | 1:A:300:LEU:HB2   | 1.97                     | 0.89              |
| 2:B:578:LYS:C     | 2:B:579:LEU:HD23  | 1.96                     | 0.89              |
| 4:D:2102:GLU:H    | 4:D:2102:GLU:HG3  | 1.37                     | 0.88              |
| 1:A:409:THR:HG22  | 2:B:415:SER:HA    | 1.34                     | 0.88              |
| 2:B:638:GLN:OE1   | 2:B:688:MET:SD    | 2.31                     | 0.88              |
| 2:B:574:HIS:HB2   | 2:B:577:ARG:CG    | 2.04                     | 0.88              |
| 2:B:722:ARG:O     | 2:B:774:TYR:CE2   | 2.25                     | 0.88              |
| 2:B:727:HIS:HB3   | 2:B:770:ASP:HB3   | 1.56                     | 0.88              |
| 1:A:296:ILE:CG1   | 1:A:325:LEU:HD22  | 2.03                     | 0.87              |
| 2:B:660:GLU:C     | 2:B:661:VAL:O     | 2.17                     | 0.87              |
| 2:B:427:ASP:OD1   | 2:B:431:LYS:HD2   | 1.75                     | 0.87              |
| 2:B:711:ILE:HG22  | 2:B:711:ILE:O     | 1.74                     | 0.87              |
| 4:D:2014:PHE:O    | 4:D:2016:VAL:HG23 | 1.72                     | 0.87              |
| 2:B:711:ILE:HA    | 2:B:714:ALA:HB3   | 1.57                     | 0.87              |
| 1:A:366:TYR:CD2   | 1:A:408:VAL:HG21  | 2.10                     | 0.87              |
| 1:A:54:THR:HG23   | 5:E:3113:PRO:HG3  | 1.55                     | 0.87              |
| 2:B:582:LEU:HD21  | 3:C:1032:LEU:HG   | 1.58                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:321:ARG:HH11  | 1:A:321:ARG:HG2   | 1.41                     | 0.86              |
| 2:B:578:LYS:HG3   | 2:B:579:LEU:H     | 1.37                     | 0.86              |
| 4:D:2018:VAL:HG23 | 4:D:2019:GLU:H    | 1.40                     | 0.86              |
| 1:A:187:ILE:O     | 1:A:190:GLU:HB2   | 1.76                     | 0.86              |
| 1:A:107:GLY:HA2   | 1:A:110:LEU:CD1   | 2.06                     | 0.85              |
| 2:B:619:ALA:CB    | 2:B:670:LYS:CB    | 2.49                     | 0.85              |
| 4:D:2048:ILE:O    | 4:D:2052:VAL:HG23 | 1.75                     | 0.85              |
| 2:B:730:LEU:HD12  | 2:B:733:GLU:HB2   | 1.57                     | 0.85              |
| 1:A:235:GLN:N     | 1:A:235:GLN:HE21  | 1.74                     | 0.85              |
| 1:A:158:GLU:HG3   | 1:A:159:ILE:N     | 1.89                     | 0.85              |
| 1:A:326:VAL:HG21  | 1:A:336:LEU:HD11  | 1.59                     | 0.85              |
| 1:A:355:CYS:O     | 1:A:359:ALA:HB3   | 1.76                     | 0.85              |
| 1:A:101:THR:C     | 1:A:102:ASN:HD22  | 1.83                     | 0.84              |
| 1:A:107:GLY:C     | 1:A:110:LEU:HG    | 2.01                     | 0.84              |
| 2:B:566:PHE:O     | 2:B:567:THR:C     | 2.19                     | 0.84              |
| 2:B:430:LEU:O     | 2:B:431:LYS:C     | 2.18                     | 0.84              |
| 1:A:197:ASN:OD1   | 1:A:200:LEU:CD1   | 2.25                     | 0.84              |
| 1:A:111:MET:CB    | 1:A:114:SER:OG    | 2.23                     | 0.84              |
| 1:A:111:MET:HE3   | 1:A:114:SER:HB3   | 1.57                     | 0.84              |
| 2:B:661:VAL:HG12  | 2:B:662:GLU:O     | 1.78                     | 0.84              |
| 1:A:235:GLN:H     | 1:A:235:GLN:HE21  | 1.21                     | 0.84              |
| 2:B:708:LYS:HD2   | 2:B:708:LYS:N     | 1.94                     | 0.83              |
| 2:B:719:MET:CE    | 2:B:774:TYR:HB2   | 2.08                     | 0.83              |
| 1:A:39:LYS:HB2    | 1:A:39:LYS:NZ     | 1.94                     | 0.83              |
| 2:B:578:LYS:O     | 2:B:579:LEU:CD2   | 2.19                     | 0.83              |
| 2:B:534:ASP:HB2   | 3:C:1026:LYS:HG3  | 1.57                     | 0.83              |
| 2:B:571:ALA:HA    | 2:B:577:ARG:NH2   | 1.92                     | 0.83              |
| 2:B:638:GLN:OE1   | 2:B:688:MET:HE3   | 1.79                     | 0.83              |
| 1:A:144:TRP:CD2   | 1:A:144:TRP:C     | 2.56                     | 0.82              |
| 4:D:2102:GLU:N    | 4:D:2102:GLU:HG3  | 1.94                     | 0.82              |
| 2:B:719:MET:HE1   | 2:B:774:TYR:HB2   | 1.60                     | 0.82              |
| 1:A:157:TYR:CD2   | 1:A:157:TYR:O     | 2.33                     | 0.82              |
| 2:B:542:SER:HA    | 3:C:1032:LEU:HD22 | 1.60                     | 0.82              |
| 2:B:620:TYR:CD2   | 2:B:624:GLN:CG    | 2.62                     | 0.82              |
| 4:D:2102:GLU:N    | 4:D:2102:GLU:CB   | 2.42                     | 0.82              |
| 4:D:2107:ALA:HB2  | 4:D:2115:LEU:HD22 | 1.60                     | 0.82              |
| 1:A:300:LEU:HD13  | 1:A:304:HIS:NE2   | 1.94                     | 0.81              |
| 1:A:168:ARG:HH11  | 1:A:213:LEU:CD2   | 1.93                     | 0.81              |
| 1:A:168:ARG:NH1   | 1:A:213:LEU:HD22  | 1.94                     | 0.81              |
| 2:B:553:PHE:HE1   | 2:B:631:ILE:CD1   | 1.85                     | 0.81              |
| 2:B:571:ALA:HA    | 2:B:577:ARG:HH21  | 1.42                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:147:ARG:HH22 | 5:E:3146:GLU:HG2 | 1.46                     | 0.81              |
| 2:B:616:THR:HG22 | 2:B:617:GLU:H    | 1.43                     | 0.81              |
| 1:A:188:GLU:C    | 1:A:190:GLU:H    | 1.88                     | 0.81              |
| 2:B:765:VAL:HG22 | 2:B:773:SER:HB2  | 1.63                     | 0.81              |
| 1:A:209:VAL:O    | 1:A:212:GLY:N    | 2.12                     | 0.81              |
| 2:B:620:TYR:CD1  | 2:B:624:GLN:OE1  | 2.34                     | 0.80              |
| 2:B:662:GLU:O    | 2:B:663:LEU:HD23 | 1.81                     | 0.80              |
| 2:B:719:MET:HE3  | 2:B:774:TYR:CG   | 2.17                     | 0.80              |
| 2:B:641:GLN:HA   | 2:B:644:LEU:HD12 | 1.61                     | 0.80              |
| 1:A:244:TYR:HB3  | 1:A:295:LEU:HD21 | 1.63                     | 0.80              |
| 2:B:432:LYS:HD2  | 2:B:480:ALA:HB2  | 1.62                     | 0.80              |
| 2:B:571:ALA:HB2  | 2:B:577:ARG:NH2  | 1.97                     | 0.80              |
| 2:B:574:HIS:CB   | 2:B:577:ARG:HG3  | 2.09                     | 0.80              |
| 1:A:34:ARG:C     | 1:A:36:SER:H     | 1.90                     | 0.79              |
| 1:A:363:PRO:HA   | 2:B:421:LEU:HD12 | 1.64                     | 0.79              |
| 1:A:110:LEU:HB2  | 1:A:115:VAL:HG23 | 1.63                     | 0.79              |
| 2:B:469:MET:HB3  | 2:B:473:ARG:NH1  | 1.94                     | 0.79              |
| 2:B:547:PHE:CE1  | 2:B:585:LEU:HD21 | 2.17                     | 0.79              |
| 2:B:719:MET:CE   | 2:B:774:TYR:CG   | 2.65                     | 0.79              |
| 1:A:211:LEU:C    | 1:A:214:ASN:HD21 | 1.91                     | 0.79              |
| 2:B:578:LYS:HG3  | 2:B:579:LEU:N    | 1.90                     | 0.79              |
| 1:A:409:THR:HG21 | 2:B:415:SER:HA   | 0.84                     | 0.79              |
| 2:B:573:ARG:O    | 2:B:574:HIS:CG   | 2.36                     | 0.79              |
| 2:B:571:ALA:CB   | 2:B:577:ARG:NH2  | 2.46                     | 0.78              |
| 2:B:712:GLN:CG   | 2:B:756:LEU:HD21 | 2.13                     | 0.78              |
| 1:A:356:GLY:HA2  | 1:A:359:ALA:HB3  | 1.64                     | 0.78              |
| 2:B:619:ALA:HB2  | 2:B:670:LYS:HB2  | 1.65                     | 0.78              |
| 4:D:2119:THR:O   | 4:D:2122:THR:OG1 | 2.01                     | 0.78              |
| 1:A:296:ILE:CD1  | 1:A:296:ILE:HB   | 2.11                     | 0.78              |
| 1:A:134:ASN:O    | 1:A:138:ALA:N    | 2.16                     | 0.78              |
| 1:A:212:GLY:O    | 1:A:214:ASN:CG   | 2.26                     | 0.77              |
| 2:B:637:ALA:HB1  | 2:B:663:LEU:CD1  | 2.12                     | 0.77              |
| 4:D:2131:THR:H   | 4:D:2134:GLU:HB3 | 1.47                     | 0.77              |
| 2:B:541:SER:H    | 2:B:545:TRP:HE1  | 1.27                     | 0.77              |
| 2:B:719:MET:CE   | 2:B:774:TYR:CB   | 2.62                     | 0.77              |
| 1:A:173:ARG:N    | 1:A:174:PRO:HD2  | 1.99                     | 0.77              |
| 1:A:197:ASN:HB3  | 1:A:200:LEU:HD12 | 1.63                     | 0.77              |
| 2:B:522:LYS:NZ   | 2:B:525:LEU:HD23 | 2.00                     | 0.77              |
| 1:A:286:GLU:O    | 1:A:289:ARG:N    | 2.18                     | 0.77              |
| 2:B:551:CYS:SG   | 2:B:632:LYS:CD   | 2.72                     | 0.77              |
| 1:A:186:LEU:CD2  | 1:A:197:ASN:HD22 | 1.88                     | 0.77              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:640:LEU:HD11 | 2:B:669:ILE:HG12  | 1.65                     | 0.77              |
| 2:B:582:LEU:HB2  | 3:C:1030:VAL:HG23 | 1.66                     | 0.77              |
| 5:E:3109:TRP:HA  | 5:E:3138:ARG:HH22 | 1.50                     | 0.77              |
| 1:A:231:SER:O    | 1:A:235:GLN:OE1   | 2.04                     | 0.76              |
| 1:A:100:LEU:CA   | 1:A:103:LEU:HD23  | 2.12                     | 0.76              |
| 2:B:473:ARG:HB3  | 2:B:479:SER:OG    | 1.86                     | 0.76              |
| 2:B:708:LYS:HD2  | 2:B:708:LYS:H     | 1.48                     | 0.76              |
| 4:D:2038:PRO:C   | 4:D:2040:PRO:CD   | 2.56                     | 0.76              |
| 1:A:404:ASN:O    | 1:A:405:ASN:CG    | 2.28                     | 0.76              |
| 2:B:427:ASP:O    | 2:B:431:LYS:HG3   | 1.86                     | 0.76              |
| 1:A:211:LEU:O    | 1:A:214:ASN:ND2   | 2.18                     | 0.76              |
| 2:B:547:PHE:CD1  | 2:B:585:LEU:HD21  | 2.21                     | 0.76              |
| 1:A:171:LEU:O    | 1:A:176:ASN:HB2   | 1.86                     | 0.76              |
| 1:A:293:GLN:CG   | 1:A:297:GLU:OE2   | 2.29                     | 0.76              |
| 2:B:427:ASP:CG   | 2:B:431:LYS:HD2   | 2.12                     | 0.75              |
| 2:B:620:TYR:CG   | 2:B:624:GLN:OE1   | 2.39                     | 0.75              |
| 2:B:668:LEU:C    | 2:B:669:ILE:HD12  | 2.11                     | 0.75              |
| 2:B:671:LEU:HD22 | 2:B:672:TYR:N     | 2.01                     | 0.75              |
| 1:A:175:LEU:O    | 1:A:178:GLN:HB3   | 1.86                     | 0.75              |
| 1:A:292:GLU:O    | 1:A:296:ILE:HD12  | 1.86                     | 0.75              |
| 2:B:604:SER:O    | 2:B:608:MET:HG2   | 1.85                     | 0.75              |
| 1:A:257:VAL:HG11 | 1:A:306:GLU:CD    | 2.11                     | 0.75              |
| 2:B:436:ASN:OD1  | 2:B:437:PRO:O     | 2.03                     | 0.75              |
| 1:A:211:LEU:C    | 1:A:214:ASN:ND2   | 2.45                     | 0.75              |
| 1:A:212:GLY:O    | 1:A:214:ASN:ND2   | 2.20                     | 0.75              |
| 1:A:297:GLU:C    | 1:A:300:LEU:H     | 1.94                     | 0.75              |
| 1:A:197:ASN:HA   | 1:A:200:LEU:HG    | 1.67                     | 0.75              |
| 2:B:712:GLN:OE1  | 2:B:756:LEU:HD21  | 1.87                     | 0.75              |
| 2:B:695:GLU:O    | 2:B:699:THR:HG22  | 1.87                     | 0.75              |
| 2:B:566:PHE:O    | 2:B:568:ALA:N     | 2.20                     | 0.75              |
| 1:A:197:ASN:OD1  | 1:A:200:LEU:HD12  | 1.86                     | 0.74              |
| 2:B:716:VAL:HA   | 2:B:719:MET:HB3   | 1.67                     | 0.74              |
| 1:A:132:VAL:HG23 | 4:D:2034:LEU:HD21 | 1.68                     | 0.74              |
| 1:A:296:ILE:HG21 | 1:A:325:LEU:O     | 1.86                     | 0.74              |
| 2:B:719:MET:HE3  | 2:B:774:TYR:HD1   | 1.48                     | 0.74              |
| 2:B:620:TYR:CE2  | 2:B:624:GLN:HG2   | 2.23                     | 0.74              |
| 2:B:587:LYS:HD3  | 2:B:587:LYS:N     | 2.03                     | 0.74              |
| 4:D:2024:SER:HA  | 4:D:2112:ILE:HG12 | 1.68                     | 0.74              |
| 1:A:157:TYR:O    | 1:A:157:TYR:HD2   | 1.70                     | 0.74              |
| 2:B:642:ILE:HD11 | 2:B:688:MET:N     | 2.01                     | 0.74              |
| 2:B:711:ILE:O    | 2:B:715:ILE:HG13  | 1.88                     | 0.74              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:111:MET:O    | 1:A:115:VAL:HB    | 1.87                     | 0.74              |
| 2:B:538:GLN:HB2  | 3:C:1030:VAL:HG12 | 1.69                     | 0.73              |
| 2:B:722:ARG:HD3  | 2:B:725:LEU:HD23  | 1.70                     | 0.73              |
| 2:B:520:GLN:OE1  | 2:B:573:ARG:NH2   | 2.22                     | 0.73              |
| 1:A:144:TRP:CE3  | 1:A:144:TRP:C     | 2.64                     | 0.73              |
| 1:A:177:LYS:O    | 1:A:181:ASN:OD1   | 2.06                     | 0.73              |
| 1:A:307:PHE:CD1  | 1:A:336:LEU:HD22  | 2.24                     | 0.73              |
| 1:A:348:GLY:O    | 1:A:352:ILE:HG23  | 1.88                     | 0.73              |
| 1:A:24:LEU:HD23  | 1:A:45:LEU:HD22   | 1.71                     | 0.73              |
| 2:B:745:ARG:O    | 2:B:749:ILE:HG12  | 1.88                     | 0.73              |
| 1:A:159:ILE:HG22 | 1:A:160:TYR:N     | 2.04                     | 0.73              |
| 1:A:257:VAL:HG11 | 1:A:306:GLU:CG    | 2.18                     | 0.73              |
| 1:A:108:GLU:O    | 1:A:109:ASP:HB2   | 1.87                     | 0.73              |
| 1:A:327:SER:HA   | 1:A:333:LEU:HD11  | 1.71                     | 0.73              |
| 2:B:442:LEU:O    | 2:B:446:LEU:CD2   | 2.36                     | 0.73              |
| 2:B:676:LYS:HE3  | 2:B:676:LYS:N     | 2.04                     | 0.73              |
| 1:A:186:LEU:HD11 | 1:A:197:ASN:HB3   | 1.69                     | 0.72              |
| 2:B:555:LEU:HD22 | 2:B:559:LEU:CD2   | 2.14                     | 0.72              |
| 1:A:257:VAL:HG13 | 1:A:258:THR:H     | 1.54                     | 0.72              |
| 1:A:234:SER:HB3  | 1:A:235:GLN:NE2   | 2.04                     | 0.72              |
| 2:B:491:LYS:H    | 2:B:491:LYS:HD2   | 1.54                     | 0.72              |
| 1:A:186:LEU:CD1  | 1:A:197:ASN:CB    | 2.65                     | 0.72              |
| 4:D:2102:GLU:N   | 4:D:2102:GLU:CG   | 2.52                     | 0.72              |
| 1:A:32:TYR:OH    | 1:A:130:SER:HA    | 1.89                     | 0.72              |
| 1:A:54:THR:HG23  | 5:E:3113:PRO:CG   | 2.19                     | 0.72              |
| 2:B:460:ASP:O    | 2:B:463:GLN:HB3   | 1.90                     | 0.72              |
| 5:E:3111:SER:O   | 5:E:3113:PRO:HD3  | 1.89                     | 0.72              |
| 1:A:39:LYS:HG2   | 4:D:2036:MET:HB3  | 1.72                     | 0.72              |
| 1:A:197:ASN:OD1  | 1:A:200:LEU:HD11  | 1.89                     | 0.72              |
| 2:B:464:LYS:HZ2  | 2:B:703:ILE:HA    | 1.54                     | 0.72              |
| 2:B:577:ARG:CD   | 2:B:577:ARG:C     | 2.61                     | 0.71              |
| 2:B:727:HIS:O    | 2:B:727:HIS:CG    | 2.43                     | 0.71              |
| 4:D:2005:LYS:O   | 4:D:2006:LEU:HD22 | 1.90                     | 0.71              |
| 1:A:168:ARG:NH1  | 1:A:213:LEU:HD13  | 2.05                     | 0.71              |
| 2:B:589:GLU:HA   | 2:B:602:GLN:HA    | 1.72                     | 0.71              |
| 2:B:603:ALA:HA   | 2:B:685:ASN:OD1   | 1.91                     | 0.71              |
| 1:A:227:VAL:HA   | 1:A:230:GLU:HG2   | 1.72                     | 0.71              |
| 2:B:762:LEU:HD13 | 2:B:772:TYR:HD2   | 1.55                     | 0.71              |
| 2:B:696:GLN:O    | 2:B:700:HIS:N     | 2.24                     | 0.71              |
| 2:B:742:PHE:O    | 2:B:744:PRO:HD3   | 1.90                     | 0.71              |
| 1:A:86:LEU:HD11  | 1:A:90:LYS:HE3    | 1.73                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:537:ILE:HG13  | 3:C:1029:ALA:C    | 2.16                     | 0.71              |
| 4:D:2005:LYS:C    | 4:D:2006:LEU:HD22 | 2.16                     | 0.71              |
| 2:B:599:TYR:CE2   | 2:B:677:ASN:HB3   | 2.25                     | 0.71              |
| 2:B:761:TYR:O     | 2:B:775:LEU:HD12  | 1.91                     | 0.71              |
| 4:D:2037:ASP:HB3  | 4:D:2038:PRO:HD2  | 1.72                     | 0.71              |
| 1:A:188:GLU:C     | 1:A:190:GLU:N     | 2.49                     | 0.70              |
| 2:B:586:SER:C     | 2:B:587:LYS:HD3   | 2.16                     | 0.70              |
| 1:A:154:LYS:HD2   | 1:A:154:LYS:N     | 2.05                     | 0.70              |
| 4:D:2118:VAL:HG13 | 4:D:2119:THR:H    | 1.56                     | 0.70              |
| 1:A:145:VAL:CG1   | 1:A:157:TYR:HD2   | 2.04                     | 0.70              |
| 2:B:633:MET:SD    | 2:B:633:MET:C     | 2.74                     | 0.70              |
| 1:A:378:ASN:HA    | 1:A:395:LEU:HD11  | 1.72                     | 0.70              |
| 2:B:626:THR:HG23  | 2:B:636:LEU:HD22  | 1.72                     | 0.70              |
| 2:B:619:ALA:HB2   | 2:B:670:LYS:HB3   | 1.55                     | 0.70              |
| 4:D:2037:ASP:HB3  | 4:D:2038:PRO:CD   | 2.21                     | 0.70              |
| 1:A:241:GLU:HG3   | 1:A:290:LYS:HD2   | 1.73                     | 0.70              |
| 5:E:3126:LEU:HB3  | 5:E:3149:TRP:CZ3  | 2.27                     | 0.70              |
| 1:A:257:VAL:CG1   | 1:A:306:GLU:OE2   | 2.40                     | 0.70              |
| 1:A:376:LYS:O     | 1:A:379:ALA:HB3   | 1.91                     | 0.70              |
| 1:A:207:SER:O     | 1:A:211:LEU:HB2   | 1.91                     | 0.70              |
| 1:A:245:THR:O     | 1:A:249:THR:HG22  | 1.92                     | 0.69              |
| 2:B:696:GLN:O     | 2:B:700:HIS:HB2   | 1.92                     | 0.69              |
| 1:A:281:GLU:HG2   | 1:A:282:SER:N     | 2.07                     | 0.69              |
| 1:A:246:ARG:HG3   | 1:A:246:ARG:HH11  | 1.57                     | 0.69              |
| 1:A:293:GLN:O     | 1:A:297:GLU:HG2   | 1.91                     | 0.69              |
| 1:A:409:THR:CG2   | 2:B:415:SER:C     | 2.54                     | 0.69              |
| 2:B:506:ARG:HA    | 2:B:509:GLN:HG2   | 1.74                     | 0.69              |
| 4:D:2023:GLN:HE22 | 4:D:2056:CYS:HA   | 1.57                     | 0.69              |
| 2:B:571:ALA:CA    | 2:B:577:ARG:NH2   | 2.48                     | 0.69              |
| 4:D:2031:LEU:HD23 | 4:D:2031:LEU:O    | 1.93                     | 0.69              |
| 1:A:111:MET:CB    | 1:A:114:SER:HG    | 2.02                     | 0.69              |
| 2:B:592:THR:HG21  | 2:B:599:TYR:HB2   | 1.73                     | 0.69              |
| 2:B:714:ALA:HA    | 2:B:717:ARG:HD2   | 1.73                     | 0.69              |
| 2:B:427:ASP:OD1   | 2:B:431:LYS:CD    | 2.41                     | 0.69              |
| 2:B:487:SER:OG    | 2:B:491:LYS:HE2   | 1.93                     | 0.69              |
| 2:B:579:LEU:C     | 2:B:580:THR:HG22  | 2.17                     | 0.68              |
| 1:A:92:LEU:HD11   | 1:A:137:CYS:SG    | 2.33                     | 0.68              |
| 1:A:15:ILE:CG2    | 1:A:20:ILE:HG13   | 2.21                     | 0.68              |
| 2:B:711:ILE:O     | 2:B:711:ILE:CG2   | 2.41                     | 0.68              |
| 1:A:173:ARG:H     | 1:A:174:PRO:CD    | 2.04                     | 0.68              |
| 2:B:503:LYS:O     | 2:B:504:LEU:C     | 2.34                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:515:LYS:HA    | 2:B:518:ASN:HD22  | 1.57                     | 0.68              |
| 1:A:142:ARG:C     | 1:A:146:ARG:HH21  | 1.99                     | 0.68              |
| 1:A:205:VAL:HG13  | 1:A:228:TYR:CE2   | 2.28                     | 0.68              |
| 2:B:577:ARG:H     | 2:B:577:ARG:HD2   | 1.57                     | 0.68              |
| 2:B:571:ALA:CB    | 2:B:577:ARG:HH21  | 2.05                     | 0.68              |
| 2:B:592:THR:CG2   | 2:B:599:TYR:HB2   | 2.24                     | 0.68              |
| 1:A:300:LEU:O     | 1:A:304:HIS:CD2   | 2.47                     | 0.67              |
| 2:B:473:ARG:HD2   | 2:B:479:SER:OG    | 1.94                     | 0.67              |
| 2:B:645:LYS:O     | 2:B:647:LYS:HD2   | 1.94                     | 0.67              |
| 2:B:431:LYS:HA    | 2:B:479:SER:HA    | 1.75                     | 0.67              |
| 2:B:540:LEU:HB2   | 3:C:1032:LEU:HD23 | 1.75                     | 0.67              |
| 2:B:633:MET:SD    | 2:B:634:ASP:HA    | 2.34                     | 0.67              |
| 2:B:555:LEU:CD2   | 2:B:559:LEU:HD21  | 2.13                     | 0.67              |
| 2:B:619:ALA:HB2   | 2:B:670:LYS:CA    | 2.24                     | 0.67              |
| 1:A:104:LEU:HD22  | 1:A:108:GLU:HG3   | 1.77                     | 0.67              |
| 5:E:3109:TRP:HA   | 5:E:3138:ARG:NH2  | 2.09                     | 0.67              |
| 2:B:578:LYS:C     | 2:B:579:LEU:CD2   | 2.68                     | 0.67              |
| 2:B:633:MET:SD    | 2:B:634:ASP:CA    | 2.83                     | 0.67              |
| 2:B:719:MET:HA    | 2:B:722:ARG:HB2   | 1.76                     | 0.67              |
| 4:D:2017:ASP:HB3  | 4:D:2020:ILE:CG1  | 2.25                     | 0.67              |
| 1:A:50:TYR:CE2    | 4:D:2109:TYR:HA   | 2.30                     | 0.66              |
| 2:B:453:PHE:C     | 2:B:455:TYR:H     | 2.03                     | 0.66              |
| 1:A:297:GLU:O     | 1:A:300:LEU:CA    | 2.43                     | 0.66              |
| 2:B:574:HIS:O     | 2:B:577:ARG:HG3   | 1.96                     | 0.66              |
| 1:A:176:ASN:O     | 1:A:177:LYS:C     | 2.34                     | 0.66              |
| 2:B:433:SER:O     | 2:B:435:LYS:O     | 2.14                     | 0.66              |
| 1:A:145:VAL:CG1   | 1:A:157:TYR:CD2   | 2.79                     | 0.66              |
| 2:B:553:PHE:CD1   | 2:B:631:ILE:CD1   | 2.71                     | 0.66              |
| 2:B:577:ARG:HD2   | 2:B:577:ARG:N     | 2.11                     | 0.66              |
| 1:A:186:LEU:HD13  | 1:A:197:ASN:CB    | 2.24                     | 0.66              |
| 2:B:574:HIS:HB3   | 2:B:577:ARG:HB3   | 1.77                     | 0.66              |
| 2:B:642:ILE:HD11  | 2:B:688:MET:CA    | 2.26                     | 0.66              |
| 4:D:2049:LEU:CD2  | 4:D:2053:ILE:HB   | 2.25                     | 0.66              |
| 1:A:168:ARG:NH1   | 1:A:215:GLU:HG3   | 2.11                     | 0.66              |
| 2:B:712:GLN:CD    | 2:B:756:LEU:HD21  | 2.21                     | 0.66              |
| 2:B:723:LYS:HB3   | 2:B:774:TYR:HE2   | 1.59                     | 0.66              |
| 2:B:705:GLU:O     | 2:B:709:LEU:HB2   | 1.96                     | 0.66              |
| 1:A:261:MET:HB3   | 1:A:325:LEU:HD12  | 1.78                     | 0.65              |
| 2:B:579:LEU:C     | 2:B:580:THR:CG2   | 2.69                     | 0.65              |
| 2:B:590:LEU:HB2   | 2:B:601:LEU:HB2   | 1.77                     | 0.65              |
| 4:D:2004:ILE:HG12 | 4:D:2031:LEU:HD11 | 1.77                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:2049:LEU:HD23 | 4:D:2049:LEU:O    | 1.96                     | 0.65              |
| 1:A:399:CYS:O     | 1:A:403:ILE:HG13  | 1.96                     | 0.65              |
| 4:D:2044:VAL:HG21 | 4:D:2106:ALA:HB1  | 1.77                     | 0.65              |
| 1:A:401:ARG:HG3   | 1:A:401:ARG:HH11  | 1.62                     | 0.65              |
| 1:A:409:THR:HG22  | 2:B:415:SER:CA    | 1.90                     | 0.65              |
| 2:B:442:LEU:O     | 2:B:446:LEU:HD23  | 1.96                     | 0.65              |
| 1:A:285:ASP:O     | 1:A:288:ALA:HB3   | 1.96                     | 0.65              |
| 2:B:476:HIS:N     | 2:B:476:HIS:CD2   | 2.64                     | 0.65              |
| 2:B:516:ASP:O     | 2:B:520:GLN:HG3   | 1.97                     | 0.65              |
| 2:B:707:ARG:NH1   | 2:B:742:PHE:HB2   | 2.11                     | 0.65              |
| 1:A:360:LEU:C     | 1:A:360:LEU:HD12  | 2.22                     | 0.65              |
| 4:D:2017:ASP:OD2  | 4:D:2018:VAL:HG22 | 1.97                     | 0.65              |
| 4:D:2024:SER:OG   | 4:D:2110:LEU:HB3  | 1.96                     | 0.65              |
| 2:B:640:LEU:CD1   | 2:B:644:LEU:HD11  | 2.27                     | 0.65              |
| 2:B:683:ASN:OD1   | 2:B:684:ILE:N     | 2.29                     | 0.65              |
| 2:B:541:SER:HA    | 3:C:1033:TRP:CZ2  | 2.31                     | 0.64              |
| 1:A:144:TRP:O     | 1:A:144:TRP:HE3   | 1.69                     | 0.64              |
| 1:A:366:TYR:CE2   | 1:A:408:VAL:HG21  | 2.31                     | 0.64              |
| 2:B:640:LEU:O     | 2:B:644:LEU:HG    | 1.96                     | 0.64              |
| 5:E:3117:LEU:HD22 | 5:E:3142:LEU:HD13 | 1.79                     | 0.64              |
| 1:A:364:LYS:O     | 1:A:367:VAL:N     | 2.29                     | 0.64              |
| 2:B:525:LEU:O     | 2:B:529:GLU:HB2   | 1.97                     | 0.64              |
| 2:B:756:LEU:HA    | 2:B:759:LYS:HE2   | 1.77                     | 0.64              |
| 1:A:355:CYS:O     | 1:A:359:ALA:CB    | 2.46                     | 0.64              |
| 2:B:644:LEU:O     | 2:B:646:SER:O     | 2.15                     | 0.64              |
| 2:B:723:LYS:HD3   | 2:B:723:LYS:N     | 2.12                     | 0.64              |
| 1:A:132:VAL:O     | 1:A:136:ILE:HG13  | 1.98                     | 0.64              |
| 2:B:635:ILE:HG13  | 2:B:638:GLN:NE2   | 2.13                     | 0.64              |
| 2:B:684:ILE:O     | 2:B:685:ASN:OD1   | 2.16                     | 0.64              |
| 2:B:729:GLN:O     | 2:B:733:GLU:HG3   | 1.98                     | 0.64              |
| 1:A:130:SER:O     | 1:A:133:LEU:HB3   | 1.98                     | 0.64              |
| 1:A:296:ILE:HG12  | 1:A:325:LEU:CD2   | 2.19                     | 0.64              |
| 1:A:294:VAL:HG12  | 1:A:295:LEU:HG    | 1.78                     | 0.63              |
| 2:B:595:PHE:CE2   | 2:B:671:LEU:HD21  | 2.33                     | 0.63              |
| 4:D:2045:ASN:OD1  | 4:D:2048:ILE:HG13 | 1.98                     | 0.63              |
| 1:A:141:ASN:HD21  | 1:A:159:ILE:HB    | 1.63                     | 0.63              |
| 2:B:620:TYR:CE2   | 2:B:624:GLN:CG    | 2.81                     | 0.63              |
| 2:B:739:SER:C     | 2:B:741:ARG:H     | 2.07                     | 0.63              |
| 1:A:27:GLY:O      | 1:A:31:VAL:HG12   | 1.97                     | 0.63              |
| 1:A:157:TYR:C     | 1:A:157:TYR:HD2   | 2.04                     | 0.63              |
| 1:A:244:TYR:HE2   | 1:A:267:ARG:HD2   | 1.64                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:442:LEU:HG    | 2:B:446:LEU:HD21  | 1.80                     | 0.63              |
| 2:B:522:LYS:HZ2   | 2:B:522:LYS:HB3   | 1.62                     | 0.63              |
| 1:A:366:TYR:HD2   | 1:A:408:VAL:HG21  | 1.60                     | 0.63              |
| 2:B:723:LYS:HA    | 2:B:774:TYR:CE2   | 2.34                     | 0.63              |
| 2:B:762:LEU:HD22  | 2:B:772:TYR:HB3   | 1.81                     | 0.63              |
| 2:B:620:TYR:CE2   | 2:B:624:GLN:CD    | 2.77                     | 0.63              |
| 4:D:2085:ILE:HD12 | 4:D:2085:ILE:H    | 1.63                     | 0.63              |
| 1:A:297:GLU:CA    | 1:A:300:LEU:HB2   | 2.29                     | 0.62              |
| 2:B:756:LEU:HD23  | 2:B:759:LYS:NZ    | 2.14                     | 0.62              |
| 1:A:306:GLU:O     | 1:A:309:ASN:HB2   | 1.99                     | 0.62              |
| 2:B:468:LYS:HE2   | 2:B:699:THR:HB    | 1.79                     | 0.62              |
| 1:A:258:THR:O     | 1:A:258:THR:OG1   | 2.11                     | 0.62              |
| 2:B:619:ALA:CB    | 2:B:670:LYS:HA    | 2.29                     | 0.62              |
| 2:B:758:GLU:OE1   | 2:B:759:LYS:CG    | 2.43                     | 0.62              |
| 4:D:2019:GLU:N    | 4:D:2019:GLU:OE2  | 2.31                     | 0.62              |
| 1:A:248:SER:HB2   | 1:A:299:HIS:NE2   | 2.14                     | 0.62              |
| 2:B:578:LYS:CG    | 2:B:579:LEU:N     | 2.63                     | 0.62              |
| 2:B:690:THR:O     | 2:B:693:LYS:HB3   | 2.00                     | 0.62              |
| 5:E:3129:LEU:HA   | 5:E:3132:VAL:HG22 | 1.81                     | 0.62              |
| 1:A:168:ARG:HH12  | 1:A:215:GLU:HG3   | 1.64                     | 0.62              |
| 1:A:283:THR:HG22  | 1:A:283:THR:O     | 1.99                     | 0.62              |
| 1:A:311:LEU:HD12  | 1:A:343:HIS:CG    | 2.35                     | 0.62              |
| 1:A:111:MET:O     | 1:A:115:VAL:CB    | 2.48                     | 0.62              |
| 1:A:173:ARG:N     | 1:A:174:PRO:CD    | 2.60                     | 0.62              |
| 2:B:417:LYS:O     | 2:B:420:GLU:HB3   | 2.00                     | 0.62              |
| 4:D:2107:ALA:CB   | 4:D:2115:LEU:HD22 | 2.30                     | 0.62              |
| 1:A:111:MET:CE    | 1:A:114:SER:HB3   | 2.26                     | 0.62              |
| 1:A:159:ILE:O     | 1:A:160:TYR:C     | 2.43                     | 0.61              |
| 2:B:450:MET:HB3   | 2:B:454:LYS:HE3   | 1.82                     | 0.61              |
| 2:B:622:VAL:O     | 2:B:626:THR:N     | 2.33                     | 0.61              |
| 2:B:730:LEU:O     | 2:B:732:GLY:N     | 2.33                     | 0.61              |
| 4:D:2054:GLN:HA   | 4:D:2057:THR:OG1  | 2.00                     | 0.61              |
| 1:A:323:TYR:O     | 1:A:323:TYR:CD2   | 2.53                     | 0.61              |
| 4:D:2115:LEU:HD23 | 4:D:2115:LEU:C    | 2.25                     | 0.61              |
| 2:B:427:ASP:OD1   | 2:B:431:LYS:CG    | 2.49                     | 0.61              |
| 2:B:559:LEU:HD11  | 3:C:1027:TRP:CE3  | 2.35                     | 0.61              |
| 1:A:39:LYS:HB2    | 1:A:39:LYS:HZ3    | 1.64                     | 0.61              |
| 1:A:39:LYS:HE3    | 4:D:2037:ASP:HB2  | 1.82                     | 0.61              |
| 1:A:294:VAL:HG12  | 1:A:295:LEU:N     | 2.14                     | 0.61              |
| 2:B:746:VAL:CG2   | 2:B:747:PRO:HD3   | 2.30                     | 0.61              |
| 1:A:371:LEU:HD11  | 2:B:448:GLN:HB3   | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:619:ALA:CB   | 2:B:670:LYS:CA   | 2.79                     | 0.61              |
| 4:D:2049:LEU:HA  | 4:D:2052:VAL:CG2 | 2.30                     | 0.61              |
| 2:B:569:PHE:O    | 2:B:572:SER:CB   | 2.48                     | 0.61              |
| 2:B:638:GLN:OE1  | 2:B:688:MET:HE1  | 1.93                     | 0.61              |
| 1:A:118:PHE:O    | 1:A:122:GLN:CG   | 2.42                     | 0.61              |
| 1:A:145:VAL:HG12 | 1:A:157:TYR:CD2  | 2.36                     | 0.61              |
| 1:A:208:TYR:HB3  | 1:A:228:TYR:HA   | 1.82                     | 0.61              |
| 2:B:453:PHE:O    | 2:B:455:TYR:N    | 2.34                     | 0.61              |
| 1:A:386:ASN:O    | 1:A:386:ASN:ND2  | 2.34                     | 0.61              |
| 2:B:586:SER:OG   | 3:C:1028:ASN:O   | 2.18                     | 0.61              |
| 2:B:609:ALA:HB1  | 2:B:629:THR:HG21 | 1.81                     | 0.61              |
| 2:B:723:LYS:CB   | 2:B:774:TYR:HE2  | 2.13                     | 0.61              |
| 1:A:111:MET:HE3  | 1:A:114:SER:CB   | 2.30                     | 0.61              |
| 1:A:337:LYS:HD3  | 1:A:338:LYS:N    | 2.15                     | 0.61              |
| 1:A:21:TRP:CZ2   | 1:A:25:ARG:HG3   | 2.36                     | 0.61              |
| 1:A:311:LEU:HD11 | 1:A:340:LEU:HD13 | 1.83                     | 0.61              |
| 2:B:586:SER:OG   | 3:C:1029:ALA:HA  | 2.01                     | 0.61              |
| 2:B:442:LEU:O    | 2:B:446:LEU:HD22 | 1.99                     | 0.60              |
| 1:A:39:LYS:CE    | 4:D:2037:ASP:H   | 2.01                     | 0.60              |
| 2:B:745:ARG:HB2  | 2:B:748:VAL:HG22 | 1.83                     | 0.60              |
| 1:A:233:GLU:O    | 1:A:237:LEU:HB2  | 2.01                     | 0.60              |
| 2:B:498:PHE:CZ   | 2:B:501:THR:HG21 | 2.36                     | 0.60              |
| 2:B:521:PHE:O    | 2:B:525:LEU:CB   | 2.38                     | 0.60              |
| 5:E:3111:SER:O   | 5:E:3113:PRO:CD  | 2.48                     | 0.60              |
| 2:B:689:LYS:HA   | 2:B:689:LYS:HE2  | 1.83                     | 0.60              |
| 2:B:697:GLU:HA   | 2:B:700:HIS:HB3  | 1.83                     | 0.60              |
| 2:B:746:VAL:HG23 | 2:B:747:PRO:HD3  | 1.83                     | 0.60              |
| 2:B:491:LYS:HD2  | 2:B:491:LYS:N    | 2.16                     | 0.60              |
| 2:B:522:LYS:HZ3  | 2:B:525:LEU:HD23 | 1.64                     | 0.60              |
| 1:A:209:VAL:O    | 1:A:212:GLY:CA   | 2.49                     | 0.60              |
| 2:B:430:LEU:HD13 | 2:B:442:LEU:HD11 | 1.83                     | 0.60              |
| 4:D:2031:LEU:CA  | 4:D:2035:GLY:HA2 | 2.28                     | 0.60              |
| 4:D:2090:GLN:O   | 4:D:2094:LYS:HB2 | 2.02                     | 0.60              |
| 1:A:186:LEU:HD11 | 1:A:197:ASN:CB   | 2.30                     | 0.60              |
| 1:A:252:LEU:HD13 | 1:A:302:ILE:CD1  | 2.32                     | 0.60              |
| 1:A:388:ASP:O    | 1:A:392:VAL:HG23 | 2.01                     | 0.60              |
| 2:B:723:LYS:CA   | 2:B:774:TYR:HE2  | 2.14                     | 0.60              |
| 1:A:242:ARG:HG3  | 1:A:242:ARG:HH11 | 1.65                     | 0.60              |
| 1:A:311:LEU:CD2  | 1:A:319:LEU:HD21 | 2.32                     | 0.60              |
| 2:B:718:ILE:N    | 2:B:718:ILE:HD12 | 2.17                     | 0.60              |
| 2:B:723:LYS:HB3  | 2:B:774:TYR:CE2  | 2.36                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:2109:TYR:HD2  | 4:D:2110:LEU:HD23 | 1.67                     | 0.60              |
| 5:E:3113:PRO:HB3  | 5:E:3115:GLU:OE1  | 2.02                     | 0.60              |
| 1:A:344:ILE:HA    | 1:A:347:GLN:HB2   | 1.84                     | 0.60              |
| 2:B:424:ARG:HG3   | 2:B:424:ARG:HH11  | 1.66                     | 0.60              |
| 2:B:595:PHE:CZ    | 2:B:671:LEU:HD21  | 2.37                     | 0.60              |
| 2:B:511:ILE:O     | 2:B:515:LYS:HG3   | 2.02                     | 0.59              |
| 2:B:566:PHE:C     | 2:B:568:ALA:N     | 2.60                     | 0.59              |
| 2:B:746:VAL:HA    | 2:B:749:ILE:HD11  | 1.84                     | 0.59              |
| 4:D:2127:ILE:HD12 | 4:D:2135:ILE:HD12 | 1.84                     | 0.59              |
| 1:A:378:ASN:HA    | 1:A:395:LEU:CD1   | 2.32                     | 0.59              |
| 4:D:2131:THR:O    | 4:D:2134:GLU:HB3  | 2.02                     | 0.59              |
| 4:D:2025:VAL:HG22 | 4:D:2111:ASP:O    | 2.02                     | 0.59              |
| 4:D:2085:ILE:HD12 | 4:D:2085:ILE:N    | 2.18                     | 0.59              |
| 1:A:294:VAL:HA    | 1:A:298:LYS:HD2   | 1.82                     | 0.59              |
| 2:B:524:HIS:O     | 2:B:527:ASN:HB2   | 2.01                     | 0.59              |
| 4:D:2017:ASP:HB3  | 4:D:2020:ILE:HG13 | 1.85                     | 0.59              |
| 1:A:24:LEU:HD22   | 1:A:28:ILE:HG13   | 1.83                     | 0.59              |
| 1:A:197:ASN:O     | 1:A:200:LEU:HB2   | 2.03                     | 0.59              |
| 1:A:201:ILE:HG21  | 1:A:278:TYR:CE1   | 2.38                     | 0.59              |
| 1:A:202:SER:HB3   | 1:A:278:TYR:HB2   | 1.83                     | 0.59              |
| 1:A:246:ARG:HG3   | 1:A:246:ARG:NH1   | 2.15                     | 0.59              |
| 1:A:248:SER:HB2   | 1:A:299:HIS:HE2   | 1.65                     | 0.59              |
| 1:A:15:ILE:HG22   | 1:A:16:GLY:N      | 2.17                     | 0.59              |
| 2:B:635:ILE:O     | 2:B:638:GLN:HB2   | 2.03                     | 0.59              |
| 4:D:2133:GLU:N    | 4:D:2136:ARG:HH21 | 2.01                     | 0.59              |
| 1:A:39:LYS:HB2    | 1:A:39:LYS:HZ2    | 1.68                     | 0.59              |
| 1:A:299:HIS:O     | 1:A:302:ILE:HG13  | 2.02                     | 0.59              |
| 1:A:112:ASP:CB    | 1:A:182:ALA:HA    | 2.25                     | 0.59              |
| 2:B:458:ASP:C     | 2:B:460:ASP:H     | 2.11                     | 0.59              |
| 1:A:274:ARG:HD2   | 1:A:278:TYR:CE2   | 2.37                     | 0.58              |
| 1:A:19:GLN:O      | 1:A:23:ASP:OD1    | 2.21                     | 0.58              |
| 1:A:24:LEU:O      | 1:A:28:ILE:HG13   | 2.02                     | 0.58              |
| 1:A:87:GLU:OE2    | 1:A:87:GLU:HA     | 2.03                     | 0.58              |
| 1:A:310:LEU:O     | 1:A:313:ALA:O     | 2.21                     | 0.58              |
| 2:B:537:ILE:HG13  | 3:C:1030:VAL:N    | 2.19                     | 0.58              |
| 2:B:668:LEU:N     | 2:B:668:LEU:HD12  | 2.19                     | 0.58              |
| 1:A:335:GLU:O     | 1:A:339:LEU:HB2   | 2.03                     | 0.58              |
| 2:B:696:GLN:O     | 2:B:700:HIS:CB    | 2.51                     | 0.58              |
| 1:A:51:ASN:HD21   | 4:D:2043:ASN:HD21 | 1.52                     | 0.58              |
| 1:A:274:ARG:NH1   | 1:A:278:TYR:OH    | 2.35                     | 0.58              |
| 4:D:2087:VAL:O    | 4:D:2090:GLN:HB2  | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:213:LEU:HG    | 1:A:227:VAL:CG2   | 2.33                     | 0.58              |
| 2:B:515:LYS:HA    | 2:B:518:ASN:ND2   | 2.19                     | 0.58              |
| 2:B:553:PHE:HD1   | 2:B:631:ILE:HG12  | 0.66                     | 0.58              |
| 2:B:677:ASN:ND2   | 2:B:679:LYS:O     | 2.37                     | 0.58              |
| 1:A:205:VAL:O     | 1:A:209:VAL:HG23  | 2.03                     | 0.58              |
| 1:A:286:GLU:HG3   | 1:A:289:ARG:NH1   | 2.19                     | 0.58              |
| 2:B:614:TYR:CD1   | 2:B:671:LEU:HB2   | 2.38                     | 0.58              |
| 4:D:2118:VAL:HG13 | 4:D:2119:THR:N    | 2.18                     | 0.58              |
| 1:A:197:ASN:HA    | 1:A:200:LEU:CG    | 2.32                     | 0.58              |
| 2:B:526:THR:O     | 2:B:527:ASN:C     | 2.45                     | 0.58              |
| 2:B:599:TYR:HE2   | 2:B:677:ASN:HB3   | 1.69                     | 0.58              |
| 2:B:712:GLN:CB    | 2:B:756:LEU:CD2   | 2.49                     | 0.58              |
| 1:A:360:LEU:C     | 1:A:362:ASP:H     | 2.12                     | 0.57              |
| 2:B:607:GLN:O     | 2:B:610:ILE:HD13  | 2.04                     | 0.57              |
| 2:B:610:ILE:HD13  | 2:B:610:ILE:N     | 2.12                     | 0.57              |
| 2:B:649:LEU:HA    | 2:B:670:LYS:O     | 2.03                     | 0.57              |
| 2:B:703:ILE:HG12  | 2:B:707:ARG:HH21  | 1.68                     | 0.57              |
| 5:E:3140:TYR:C    | 5:E:3140:TYR:CD2  | 2.82                     | 0.57              |
| 1:A:91:ARG:HG3    | 1:A:91:ARG:HH11   | 1.67                     | 0.57              |
| 1:A:158:GLU:CG    | 1:A:159:ILE:H     | 2.10                     | 0.57              |
| 1:A:175:LEU:O     | 1:A:178:GLN:CB    | 2.52                     | 0.57              |
| 2:B:717:ARG:O     | 2:B:720:LYS:HD3   | 2.04                     | 0.57              |
| 2:B:727:HIS:ND1   | 2:B:727:HIS:C     | 2.62                     | 0.57              |
| 2:B:738:LEU:C     | 2:B:740:SER:H     | 2.12                     | 0.57              |
| 1:A:17:LEU:C      | 1:A:19:GLN:H      | 2.12                     | 0.57              |
| 2:B:453:PHE:HA    | 2:B:456:ILE:CD1   | 2.29                     | 0.57              |
| 2:B:644:LEU:C     | 2:B:646:SER:O     | 2.48                     | 0.57              |
| 1:A:45:LEU:O      | 1:A:46:TYR:C      | 2.48                     | 0.57              |
| 1:A:214:ASN:O     | 1:A:215:GLU:C     | 2.44                     | 0.57              |
| 1:A:244:TYR:CE2   | 1:A:267:ARG:HD2   | 2.38                     | 0.57              |
| 1:A:171:LEU:O     | 1:A:172:PHE:C     | 2.47                     | 0.57              |
| 4:D:2023:GLN:NE2  | 4:D:2056:CYS:HA   | 2.20                     | 0.57              |
| 4:D:2130:LYS:H    | 5:E:3131:LYS:NZ   | 2.03                     | 0.57              |
| 1:A:197:ASN:O     | 1:A:200:LEU:N     | 2.38                     | 0.57              |
| 1:A:213:LEU:HG    | 1:A:227:VAL:HG23  | 1.86                     | 0.57              |
| 1:A:50:TYR:HA     | 1:A:139:TYR:CD2   | 2.39                     | 0.56              |
| 1:A:143:HIS:ND1   | 1:A:146:ARG:NH2   | 2.53                     | 0.56              |
| 2:B:483:ASP:O     | 2:B:486:ALA:HB3   | 2.05                     | 0.56              |
| 2:B:620:TYR:CD2   | 2:B:624:GLN:CD    | 2.82                     | 0.56              |
| 4:D:2002:PRO:CB   | 4:D:2018:VAL:HG11 | 2.31                     | 0.56              |
| 4:D:2123:VAL:CG1  | 5:E:3120:ILE:HD13 | 2.34                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:180:THR:O     | 1:A:184:LEU:HD23  | 2.05                     | 0.56              |
| 1:A:257:VAL:HG13  | 1:A:258:THR:HG22  | 1.88                     | 0.56              |
| 1:A:306:GLU:O     | 1:A:309:ASN:N     | 2.36                     | 0.56              |
| 1:A:326:VAL:O     | 1:A:328:ARG:N     | 2.39                     | 0.56              |
| 1:A:378:ASN:CA    | 1:A:395:LEU:HD11  | 2.35                     | 0.56              |
| 4:D:2014:PHE:O    | 4:D:2016:VAL:N    | 2.39                     | 0.56              |
| 1:A:42:TYR:HD2    | 4:D:2030:MET:SD   | 2.28                     | 0.56              |
| 1:A:226:THR:O     | 1:A:229:LYS:N     | 2.39                     | 0.56              |
| 2:B:555:LEU:HD23  | 2:B:559:LEU:HD22  | 0.64                     | 0.56              |
| 2:B:622:VAL:HG21  | 2:B:664:LYS:O     | 2.05                     | 0.56              |
| 1:A:380:LEU:O     | 1:A:384:ALA:HB3   | 2.06                     | 0.56              |
| 2:B:545:TRP:HB3   | 2:B:547:PHE:CD2   | 2.40                     | 0.56              |
| 2:B:545:TRP:HB3   | 2:B:547:PHE:CE2   | 2.41                     | 0.56              |
| 2:B:704:GLU:OE1   | 2:B:707:ARG:HG3   | 2.06                     | 0.56              |
| 2:B:662:GLU:O     | 2:B:663:LEU:CD2   | 2.53                     | 0.56              |
| 1:A:287:LEU:CD2   | 1:A:291:CYS:SG    | 2.93                     | 0.56              |
| 2:B:765:VAL:CG2   | 2:B:773:SER:HB2   | 2.35                     | 0.56              |
| 1:A:251:PHE:CE2   | 1:A:255:ASN:HB2   | 2.41                     | 0.56              |
| 4:D:2017:ASP:HB3  | 4:D:2020:ILE:HG12 | 1.86                     | 0.56              |
| 5:E:3126:LEU:H    | 5:E:3126:LEU:CD1  | 2.13                     | 0.56              |
| 1:A:47:THR:O      | 1:A:48:HIS:C      | 2.47                     | 0.56              |
| 2:B:562:SER:HA    | 2:B:565:ARG:HB3   | 1.88                     | 0.56              |
| 4:D:2044:VAL:HG22 | 4:D:2106:ALA:CB   | 2.36                     | 0.56              |
| 1:A:311:LEU:HD22  | 1:A:319:LEU:HD21  | 1.88                     | 0.55              |
| 2:B:423:ALA:HA    | 2:B:462:PHE:CE1   | 2.40                     | 0.55              |
| 2:B:517:LEU:O     | 2:B:520:GLN:HB2   | 2.06                     | 0.55              |
| 4:D:2010:ASP:CG   | 4:D:2046:ALA:H    | 2.13                     | 0.55              |
| 1:A:37:MET:O      | 1:A:37:MET:HG2    | 2.07                     | 0.55              |
| 1:A:177:LYS:C     | 1:A:181:ASN:OD1   | 2.48                     | 0.55              |
| 2:B:601:LEU:HD11  | 2:B:648:LEU:HD21  | 1.87                     | 0.55              |
| 2:B:728:GLN:HE21  | 2:B:728:GLN:HA    | 1.70                     | 0.55              |
| 1:A:348:GLY:HA2   | 1:A:373:VAL:HG21  | 1.88                     | 0.55              |
| 1:A:403:ILE:HD12  | 2:B:455:TYR:HB3   | 1.87                     | 0.55              |
| 2:B:717:ARG:C     | 2:B:720:LYS:HD3   | 2.32                     | 0.55              |
| 2:B:745:ARG:HH21  | 2:B:748:VAL:HG11  | 1.71                     | 0.55              |
| 4:D:2121:LYS:O    | 4:D:2124:ALA:HB3  | 2.06                     | 0.55              |
| 2:B:751:LYS:NZ    | 2:B:755:ILE:HD11  | 2.22                     | 0.55              |
| 4:D:2044:VAL:CG2  | 4:D:2106:ALA:HB1  | 2.36                     | 0.55              |
| 1:A:104:LEU:CD2   | 1:A:108:GLU:HG3   | 2.36                     | 0.55              |
| 4:D:2044:VAL:CG2  | 4:D:2106:ALA:CB   | 2.84                     | 0.55              |
| 2:B:430:LEU:C     | 2:B:431:LYS:O     | 2.49                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:2133:GLU:O    | 4:D:2137:LYS:HG3  | 2.07                     | 0.55              |
| 2:B:553:PHE:CE1   | 2:B:629:THR:CB    | 2.80                     | 0.55              |
| 2:B:722:ARG:O     | 2:B:774:TYR:HE2   | 1.89                     | 0.55              |
| 1:A:307:PHE:CG    | 1:A:336:LEU:HD22  | 2.41                     | 0.55              |
| 2:B:590:LEU:N     | 2:B:601:LEU:O     | 2.40                     | 0.55              |
| 2:B:610:ILE:H     | 2:B:610:ILE:CD1   | 2.13                     | 0.55              |
| 2:B:475:VAL:C     | 2:B:476:HIS:O     | 2.33                     | 0.55              |
| 2:B:645:LYS:C     | 2:B:646:SER:O     | 2.38                     | 0.55              |
| 1:A:96:LEU:HD23   | 1:A:163:ALA:HA    | 1.87                     | 0.55              |
| 1:A:131:LYS:O     | 1:A:134:ASN:HB2   | 2.07                     | 0.55              |
| 1:A:350:ALA:O     | 1:A:354:LYS:HG3   | 2.07                     | 0.55              |
| 2:B:485:GLU:O     | 2:B:489:ILE:HG12  | 2.07                     | 0.55              |
| 2:B:542:SER:HB2   | 3:C:1032:LEU:HB3  | 1.89                     | 0.55              |
| 2:B:704:GLU:OE1   | 2:B:708:LYS:HE2   | 2.06                     | 0.55              |
| 4:D:2044:VAL:HG22 | 4:D:2106:ALA:HB2  | 1.88                     | 0.55              |
| 2:B:442:LEU:HD23  | 2:B:484:ALA:HB1   | 1.89                     | 0.54              |
| 2:B:466:TYR:OH    | 2:B:488:MET:HE3   | 2.07                     | 0.54              |
| 2:B:619:ALA:HB2   | 2:B:670:LYS:HA    | 1.89                     | 0.54              |
| 4:D:2017:ASP:OD2  | 4:D:2018:VAL:N    | 2.40                     | 0.54              |
| 2:B:540:LEU:HD12  | 2:B:582:LEU:HD11  | 1.87                     | 0.54              |
| 2:B:559:LEU:HD11  | 3:C:1027:TRP:CD2  | 2.41                     | 0.54              |
| 2:B:535:PHE:O     | 2:B:536:SER:HB2   | 2.05                     | 0.54              |
| 2:B:730:LEU:HA    | 2:B:733:GLU:HB2   | 1.90                     | 0.54              |
| 4:D:2131:THR:O    | 4:D:2135:ILE:HG12 | 2.08                     | 0.54              |
| 5:E:3125:CYS:O    | 5:E:3128:GLU:N    | 2.39                     | 0.54              |
| 1:A:180:THR:HG22  | 1:A:184:LEU:HD23  | 1.90                     | 0.54              |
| 1:A:380:LEU:CD1   | 1:A:384:ALA:HB2   | 2.38                     | 0.54              |
| 2:B:745:ARG:NH2   | 2:B:748:VAL:HG11  | 2.22                     | 0.54              |
| 1:A:115:VAL:O     | 1:A:118:PHE:HB3   | 2.08                     | 0.54              |
| 1:A:257:VAL:HG11  | 1:A:306:GLU:HG2   | 1.87                     | 0.54              |
| 2:B:432:LYS:HD2   | 2:B:480:ALA:CB    | 2.34                     | 0.54              |
| 4:D:2123:VAL:HG11 | 5:E:3120:ILE:HD13 | 1.88                     | 0.54              |
| 2:B:424:ARG:HG3   | 2:B:424:ARG:NH1   | 2.22                     | 0.54              |
| 2:B:545:TRP:CD1   | 2:B:545:TRP:H     | 2.26                     | 0.54              |
| 4:D:2133:GLU:HA   | 4:D:2136:ARG:HE   | 1.73                     | 0.54              |
| 1:A:39:LYS:HE2    | 4:D:2037:ASP:CA   | 2.38                     | 0.54              |
| 4:D:2019:GLU:HA   | 4:D:2022:LYS:HB2  | 1.88                     | 0.54              |
| 1:A:86:LEU:HD23   | 1:A:87:GLU:N      | 2.23                     | 0.54              |
| 1:A:272:GLN:HG3   | 1:A:284:GLN:HE22  | 1.73                     | 0.54              |
| 1:A:275:VAL:HG21  | 1:A:284:GLN:HG2   | 1.88                     | 0.54              |
| 1:A:286:GLU:CD    | 1:A:289:ARG:HH22  | 2.15                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:756:LEU:HA   | 2:B:759:LYS:CE    | 2.38                     | 0.54              |
| 1:A:96:LEU:CD2   | 1:A:163:ALA:HA    | 2.38                     | 0.54              |
| 1:A:321:ARG:HH11 | 1:A:321:ARG:CG    | 2.18                     | 0.54              |
| 2:B:616:THR:HG22 | 2:B:617:GLU:N     | 2.19                     | 0.53              |
| 2:B:621:THR:O    | 2:B:622:VAL:C     | 2.50                     | 0.53              |
| 2:B:719:MET:SD   | 2:B:774:TYR:CD2   | 3.01                     | 0.53              |
| 1:A:39:LYS:HE2   | 4:D:2037:ASP:C    | 2.32                     | 0.53              |
| 1:A:159:ILE:CG2  | 1:A:160:TYR:N     | 2.71                     | 0.53              |
| 1:A:235:GLN:NE2  | 1:A:235:GLN:N     | 2.41                     | 0.53              |
| 2:B:476:HIS:CD2  | 2:B:476:HIS:H     | 2.26                     | 0.53              |
| 2:B:593:ASN:OD1  | 2:B:598:ARG:NH1   | 2.41                     | 0.53              |
| 2:B:604:SER:OG   | 2:B:607:GLN:HG3   | 2.07                     | 0.53              |
| 2:B:734:VAL:HG12 | 2:B:738:LEU:HD23  | 1.90                     | 0.53              |
| 4:D:2119:THR:O   | 4:D:2120:CYS:C    | 2.52                     | 0.53              |
| 1:A:129:SER:HA   | 1:A:132:VAL:HG12  | 1.90                     | 0.53              |
| 1:A:340:LEU:HD22 | 1:A:385:PHE:CE2   | 2.43                     | 0.53              |
| 2:B:449:VAL:O    | 2:B:452:VAL:HB    | 2.08                     | 0.53              |
| 2:B:621:THR:O    | 2:B:625:LEU:N     | 2.41                     | 0.53              |
| 5:E:3113:PRO:CB  | 5:E:3115:GLU:OE1  | 2.56                     | 0.53              |
| 1:A:17:LEU:C     | 1:A:20:ILE:H      | 2.17                     | 0.53              |
| 1:A:142:ARG:HB2  | 1:A:146:ARG:HH21  | 1.73                     | 0.53              |
| 1:A:17:LEU:C     | 1:A:19:GLN:N      | 2.66                     | 0.53              |
| 2:B:522:LYS:HZ3  | 2:B:522:LYS:HA    | 1.74                     | 0.53              |
| 2:B:727:HIS:HB3  | 2:B:770:ASP:CB    | 2.35                     | 0.53              |
| 5:E:3109:TRP:O   | 5:E:3110:ASP:C    | 2.51                     | 0.53              |
| 5:E:3125:CYS:C   | 5:E:3127:PRO:HD2  | 2.34                     | 0.53              |
| 1:A:196:ILE:C    | 1:A:198:THR:N     | 2.64                     | 0.53              |
| 2:B:418:SER:N    | 2:B:419:PRO:HD2   | 2.23                     | 0.53              |
| 2:B:474:LEU:HD13 | 2:B:507:MET:O     | 2.08                     | 0.53              |
| 2:B:623:GLN:HA   | 2:B:626:THR:HB    | 1.90                     | 0.53              |
| 1:A:260:TYR:OH   | 1:A:295:LEU:O     | 2.26                     | 0.53              |
| 1:A:269:LEU:O    | 1:A:272:GLN:HB3   | 2.09                     | 0.53              |
| 2:B:589:GLU:HG2  | 2:B:602:GLN:HG2   | 1.90                     | 0.53              |
| 4:D:2118:VAL:HA  | 4:D:2121:LYS:HD3  | 1.91                     | 0.53              |
| 1:A:82:GLN:O     | 1:A:82:GLN:HG2    | 2.09                     | 0.53              |
| 1:A:115:VAL:HG13 | 1:A:116:LEU:N     | 2.22                     | 0.53              |
| 1:A:173:ARG:HB3  | 1:A:174:PRO:HD3   | 1.90                     | 0.53              |
| 2:B:578:LYS:C    | 2:B:579:LEU:CG    | 2.82                     | 0.53              |
| 2:B:707:ARG:HB2  | 2:B:708:LYS:HD2   | 1.89                     | 0.53              |
| 2:B:716:VAL:HA   | 2:B:719:MET:HE2   | 1.90                     | 0.53              |
| 4:D:2127:ILE:CD1 | 4:D:2135:ILE:HD12 | 2.39                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:257:VAL:HG11 | 1:A:306:GLU:OE2   | 2.07                     | 0.53              |
| 1:A:271:GLU:O    | 1:A:275:VAL:HG23  | 2.09                     | 0.53              |
| 1:A:333:LEU:O    | 1:A:334:GLY:C     | 2.51                     | 0.53              |
| 2:B:573:ARG:O    | 2:B:574:HIS:CD2   | 2.61                     | 0.53              |
| 2:B:640:LEU:HD12 | 2:B:644:LEU:HD11  | 1.91                     | 0.53              |
| 2:B:714:ALA:HB1  | 2:B:738:LEU:CD2   | 2.38                     | 0.53              |
| 4:D:2049:LEU:O   | 4:D:2053:ILE:HG22 | 2.09                     | 0.53              |
| 1:A:110:LEU:CD1  | 1:A:118:PHE:CG    | 2.91                     | 0.52              |
| 1:A:24:LEU:HD22  | 1:A:24:LEU:O      | 2.09                     | 0.52              |
| 1:A:297:GLU:HA   | 1:A:300:LEU:HB2   | 1.92                     | 0.52              |
| 1:A:321:ARG:HG2  | 1:A:321:ARG:NH1   | 2.14                     | 0.52              |
| 2:B:442:LEU:HG   | 2:B:446:LEU:CD2   | 2.40                     | 0.52              |
| 2:B:464:LYS:NZ   | 2:B:703:ILE:HA    | 2.22                     | 0.52              |
| 2:B:522:LYS:NZ   | 2:B:522:LYS:HB3   | 2.24                     | 0.52              |
| 2:B:706:ASP:O    | 2:B:710:LEU:HB2   | 2.09                     | 0.52              |
| 1:A:244:TYR:HE2  | 1:A:267:ARG:CD    | 2.23                     | 0.52              |
| 2:B:458:ASP:O    | 2:B:460:ASP:N     | 2.42                     | 0.52              |
| 2:B:584:GLN:C    | 2:B:585:LEU:HD12  | 2.34                     | 0.52              |
| 1:A:100:LEU:HD13 | 1:A:167:TRP:HA    | 1.91                     | 0.52              |
| 1:A:227:VAL:HA   | 1:A:230:GLU:CG    | 2.38                     | 0.52              |
| 2:B:592:THR:OG1  | 2:B:599:TYR:N     | 2.42                     | 0.52              |
| 4:D:2043:ASN:HB2 | 4:D:2109:TYR:CE1  | 2.44                     | 0.52              |
| 4:D:2131:THR:HB  | 4:D:2132:PRO:HD2  | 1.91                     | 0.52              |
| 5:E:3146:GLU:O   | 5:E:3148:LEU:N    | 2.42                     | 0.52              |
| 1:A:234:SER:HB3  | 1:A:235:GLN:HE22  | 1.73                     | 0.52              |
| 2:B:442:LEU:C    | 2:B:446:LEU:HD23  | 2.34                     | 0.52              |
| 2:B:484:ALA:O    | 2:B:487:SER:HB3   | 2.09                     | 0.52              |
| 1:A:34:ARG:C     | 1:A:36:SER:N      | 2.55                     | 0.52              |
| 1:A:234:SER:CB   | 1:A:235:GLN:NE2   | 2.73                     | 0.52              |
| 2:B:475:VAL:HG13 | 3:C:1030:VAL:HG11 | 1.92                     | 0.52              |
| 1:A:38:ALA:C     | 1:A:40:SER:N      | 2.66                     | 0.52              |
| 2:B:427:ASP:OD2  | 2:B:431:LYS:HD2   | 2.10                     | 0.52              |
| 1:A:83:PHE:O     | 1:A:84:VAL:C      | 2.53                     | 0.52              |
| 1:A:111:MET:O    | 1:A:115:VAL:N     | 2.40                     | 0.52              |
| 1:A:115:VAL:CG1  | 1:A:116:LEU:N     | 2.73                     | 0.52              |
| 1:A:135:GLY:C    | 1:A:137:CYS:N     | 2.62                     | 0.52              |
| 2:B:588:GLY:HA3  | 2:B:608:MET:HE2   | 1.91                     | 0.52              |
| 2:B:707:ARG:HH11 | 2:B:742:PHE:HB2   | 1.74                     | 0.52              |
| 4:D:2099:THR:HA  | 4:D:2102:GLU:OE1  | 2.10                     | 0.52              |
| 4:D:2113:LYS:O   | 4:D:2114:GLY:C    | 2.53                     | 0.52              |
| 1:A:38:ALA:C     | 1:A:40:SER:H      | 2.18                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:2086:PRO:O    | 4:D:2090:GLN:HG3  | 2.10                     | 0.51              |
| 4:D:2131:THR:N    | 4:D:2134:GLU:HB3  | 2.20                     | 0.51              |
| 1:A:117:LYS:O     | 1:A:121:GLN:CB    | 2.58                     | 0.51              |
| 1:A:314:ASP:O     | 1:A:316:ASN:N     | 2.43                     | 0.51              |
| 1:A:372:ASP:O     | 1:A:373:VAL:C     | 2.53                     | 0.51              |
| 2:B:633:MET:SD    | 2:B:634:ASP:N     | 2.83                     | 0.51              |
| 4:D:2016:VAL:CG1  | 4:D:2053:ILE:HD11 | 2.40                     | 0.51              |
| 1:A:304:HIS:CE1   | 1:A:335:GLU:HB3   | 2.45                     | 0.51              |
| 2:B:438:GLU:O     | 2:B:441:GLU:HB3   | 2.10                     | 0.51              |
| 4:D:2104:ILE:HG21 | 5:E:3112:LEU:HD11 | 1.92                     | 0.51              |
| 5:E:3140:TYR:C    | 5:E:3140:TYR:HD2  | 2.17                     | 0.51              |
| 1:A:39:LYS:CG     | 4:D:2036:MET:HE2  | 2.40                     | 0.51              |
| 2:B:427:ASP:CG    | 2:B:431:LYS:CD    | 2.84                     | 0.51              |
| 2:B:513:VAL:HG13  | 2:B:514:SER:N     | 2.26                     | 0.51              |
| 4:D:2031:LEU:O    | 4:D:2031:LEU:CD2  | 2.59                     | 0.51              |
| 1:A:39:LYS:CE     | 4:D:2037:ASP:N    | 2.67                     | 0.51              |
| 1:A:227:VAL:O     | 1:A:228:TYR:C     | 2.52                     | 0.51              |
| 1:A:100:LEU:CD1   | 1:A:166:THR:HG22  | 2.31                     | 0.51              |
| 1:A:233:GLU:HG2   | 1:A:237:LEU:HD12  | 1.93                     | 0.51              |
| 2:B:574:HIS:CB    | 2:B:577:ARG:HB3   | 2.41                     | 0.51              |
| 3:C:1033:TRP:HE3  | 3:C:1033:TRP:C    | 2.19                     | 0.51              |
| 4:D:2117:ASP:O    | 4:D:2120:CYS:HB3  | 2.10                     | 0.51              |
| 2:B:470:LEU:O     | 2:B:474:LEU:HG    | 2.11                     | 0.51              |
| 4:D:2055:TRP:CD2  | 4:D:2115:LEU:HD12 | 2.46                     | 0.51              |
| 1:A:225:LEU:O     | 1:A:229:LYS:HB2   | 2.10                     | 0.51              |
| 1:A:275:VAL:HG11  | 1:A:284:GLN:HG2   | 1.93                     | 0.51              |
| 2:B:510:ASP:O     | 2:B:513:VAL:HG12  | 2.10                     | 0.51              |
| 4:D:2025:VAL:HG22 | 4:D:2111:ASP:HB3  | 1.91                     | 0.51              |
| 1:A:351:ALA:HA    | 1:A:354:LYS:HE2   | 1.93                     | 0.50              |
| 2:B:445:THR:O     | 2:B:448:GLN:HB2   | 2.12                     | 0.50              |
| 2:B:554:ALA:O     | 2:B:556:PRO:HD2   | 2.11                     | 0.50              |
| 2:B:680:LEU:HD12  | 2:B:680:LEU:H     | 1.75                     | 0.50              |
| 2:B:756:LEU:HB3   | 2:B:761:TYR:CG    | 2.46                     | 0.50              |
| 1:A:158:GLU:CG    | 1:A:159:ILE:N     | 2.68                     | 0.50              |
| 1:A:158:GLU:HB3   | 1:A:161:SER:OG    | 2.11                     | 0.50              |
| 1:A:284:GLN:O     | 1:A:285:ASP:C     | 2.54                     | 0.50              |
| 2:B:501:THR:O     | 2:B:501:THR:HG22  | 2.09                     | 0.50              |
| 2:B:587:LYS:N     | 2:B:587:LYS:CD    | 2.74                     | 0.50              |
| 1:A:92:LEU:O      | 1:A:95:PHE:HB3    | 2.11                     | 0.50              |
| 1:A:180:THR:HG23  | 1:A:232:PHE:CD1   | 2.47                     | 0.50              |
| 1:A:275:VAL:HG11  | 1:A:284:GLN:CG    | 2.41                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:300:LEU:CD1   | 1:A:304:HIS:NE2   | 2.70                     | 0.50              |
| 1:A:323:TYR:HB2   | 1:A:385:PHE:HD1   | 1.76                     | 0.50              |
| 1:A:352:ILE:HA    | 1:A:369:THR:HG21  | 1.92                     | 0.50              |
| 2:B:559:LEU:C     | 2:B:561:ARG:H     | 2.17                     | 0.50              |
| 2:B:657:ASN:O     | 2:B:659:ASP:N     | 2.45                     | 0.50              |
| 4:D:2050:LYS:O    | 4:D:2054:GLN:HG2  | 2.11                     | 0.50              |
| 4:D:2093:LEU:HD13 | 4:D:2119:THR:HA   | 1.93                     | 0.50              |
| 1:A:159:ILE:O     | 1:A:162:LEU:N     | 2.44                     | 0.50              |
| 2:B:436:ASN:OD1   | 2:B:436:ASN:C     | 2.51                     | 0.50              |
| 2:B:522:LYS:HZ1   | 2:B:525:LEU:HD23  | 1.75                     | 0.50              |
| 2:B:616:THR:HG22  | 2:B:617:GLU:HG3   | 1.93                     | 0.50              |
| 5:E:3117:LEU:C    | 5:E:3117:LEU:HD23 | 2.36                     | 0.50              |
| 1:A:145:VAL:HG12  | 1:A:157:TYR:CE2   | 2.47                     | 0.50              |
| 1:A:402:PHE:CD1   | 1:A:402:PHE:C     | 2.89                     | 0.50              |
| 2:B:474:LEU:HD12  | 2:B:507:MET:HB3   | 1.93                     | 0.50              |
| 4:D:2018:VAL:O    | 4:D:2020:ILE:N    | 2.45                     | 0.50              |
| 4:D:2029:THR:O    | 4:D:2031:LEU:N    | 2.45                     | 0.50              |
| 1:A:196:ILE:C     | 1:A:198:THR:H     | 2.19                     | 0.50              |
| 1:A:256:PRO:HB3   | 1:A:258:THR:HG23  | 1.94                     | 0.50              |
| 1:A:323:TYR:O     | 1:A:323:TYR:CG    | 2.65                     | 0.50              |
| 2:B:717:ARG:HA    | 2:B:720:LYS:HE3   | 1.93                     | 0.50              |
| 4:D:2087:VAL:HA   | 4:D:2090:GLN:NE2  | 2.27                     | 0.50              |
| 1:A:117:LYS:O     | 1:A:121:GLN:HB2   | 2.11                     | 0.50              |
| 2:B:768:GLU:HB2   | 2:B:771:THR:HG23  | 1.94                     | 0.50              |
| 4:D:2117:ASP:O    | 4:D:2121:LYS:HG3  | 2.10                     | 0.50              |
| 1:A:116:LEU:O     | 1:A:117:LYS:C     | 2.54                     | 0.50              |
| 1:A:226:THR:O     | 1:A:227:VAL:C     | 2.54                     | 0.50              |
| 2:B:430:LEU:HD12  | 2:B:442:LEU:HD21  | 1.93                     | 0.50              |
| 1:A:256:PRO:O     | 1:A:257:VAL:C     | 2.54                     | 0.50              |
| 1:A:360:LEU:HD22  | 1:A:408:VAL:HA    | 1.94                     | 0.50              |
| 2:B:595:PHE:HB3   | 2:B:674:GLY:O     | 2.12                     | 0.50              |
| 2:B:765:VAL:HG23  | 2:B:772:TYR:C     | 2.36                     | 0.50              |
| 4:D:2131:THR:H    | 4:D:2134:GLU:CB   | 2.20                     | 0.50              |
| 2:B:716:VAL:HG22  | 2:B:719:MET:HE2   | 1.93                     | 0.49              |
| 1:A:21:TRP:O      | 1:A:24:LEU:N      | 2.44                     | 0.49              |
| 1:A:119:TYR:O     | 1:A:120:THR:C     | 2.54                     | 0.49              |
| 1:A:234:SER:CB    | 1:A:235:GLN:HE21  | 2.24                     | 0.49              |
| 1:A:248:SER:CB    | 1:A:299:HIS:HE2   | 2.26                     | 0.49              |
| 1:A:296:ILE:HG21  | 1:A:325:LEU:C     | 2.37                     | 0.49              |
| 2:B:690:THR:HG23  | 2:B:691:GLU:N     | 2.27                     | 0.49              |
| 4:D:2131:THR:OG1  | 4:D:2134:GLU:HB2  | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:3129:LEU:HA   | 5:E:3132:VAL:CG2  | 2.41                     | 0.49              |
| 1:A:205:VAL:O     | 1:A:206:GLN:C     | 2.53                     | 0.49              |
| 2:B:476:HIS:N     | 2:B:476:HIS:HD2   | 2.08                     | 0.49              |
| 4:D:2018:VAL:HG23 | 4:D:2019:GLU:N    | 2.19                     | 0.49              |
| 1:A:108:GLU:O     | 1:A:109:ASP:CB    | 2.60                     | 0.49              |
| 4:D:2085:ILE:H    | 4:D:2085:ILE:CD1  | 2.24                     | 0.49              |
| 1:A:402:PHE:C     | 1:A:404:ASN:N     | 2.71                     | 0.49              |
| 2:B:442:LEU:HD23  | 2:B:484:ALA:CB    | 2.43                     | 0.49              |
| 4:D:2051:LYS:HE3  | 4:D:2092:PHE:CZ   | 2.48                     | 0.49              |
| 1:A:181:ASN:O     | 1:A:182:ALA:C     | 2.56                     | 0.49              |
| 2:B:583:TYR:C     | 2:B:585:LEU:H     | 2.20                     | 0.49              |
| 5:E:3125:CYS:O    | 5:E:3126:LEU:C    | 2.55                     | 0.49              |
| 1:A:204:VAL:O     | 1:A:207:SER:N     | 2.45                     | 0.49              |
| 1:A:227:VAL:CA    | 1:A:230:GLU:HG2   | 2.40                     | 0.49              |
| 1:A:286:GLU:O     | 1:A:287:LEU:C     | 2.56                     | 0.49              |
| 1:A:297:GLU:C     | 1:A:299:HIS:N     | 2.70                     | 0.49              |
| 2:B:608:MET:CE    | 3:C:1024:VAL:HG13 | 2.42                     | 0.49              |
| 4:D:2118:VAL:CG1  | 4:D:2119:THR:H    | 2.25                     | 0.49              |
| 1:A:107:GLY:HA3   | 1:A:118:PHE:CE2   | 2.47                     | 0.49              |
| 1:A:126:TYR:O     | 1:A:130:SER:OG    | 2.24                     | 0.49              |
| 1:A:260:TYR:O     | 1:A:264:ALA:N     | 2.42                     | 0.49              |
| 2:B:453:PHE:C     | 2:B:455:TYR:N     | 2.71                     | 0.49              |
| 3:C:1020:LYS:O    | 3:C:1021:ARG:HB2  | 2.13                     | 0.49              |
| 4:D:2131:THR:O    | 4:D:2135:ILE:N    | 2.45                     | 0.49              |
| 4:D:2037:ASP:O    | 4:D:2038:PRO:C    | 2.52                     | 0.48              |
| 1:A:97:LYS:O      | 1:A:101:THR:HG23  | 2.13                     | 0.48              |
| 1:A:147:ARG:HH22  | 5:E:3146:GLU:CG   | 2.21                     | 0.48              |
| 1:A:186:LEU:HD11  | 1:A:200:LEU:HD12  | 1.95                     | 0.48              |
| 1:A:226:THR:O     | 1:A:230:GLU:N     | 2.44                     | 0.48              |
| 2:B:694:GLN:O     | 2:B:695:GLU:C     | 2.56                     | 0.48              |
| 4:D:2055:TRP:CG   | 4:D:2115:LEU:HD12 | 2.48                     | 0.48              |
| 1:A:92:LEU:HD12   | 1:A:159:ILE:HD11  | 1.95                     | 0.48              |
| 4:D:2046:ALA:O    | 4:D:2047:ALA:C    | 2.56                     | 0.48              |
| 4:D:2119:THR:OG1  | 4:D:2120:CYS:N    | 2.46                     | 0.48              |
| 1:A:43:MET:CE     | 4:D:2036:MET:HE1  | 2.43                     | 0.48              |
| 1:A:268:LEU:HD11  | 1:A:296:ILE:HD11  | 1.95                     | 0.48              |
| 2:B:458:ASP:HB3   | 2:B:460:ASP:OD1   | 2.13                     | 0.48              |
| 2:B:691:GLU:O     | 2:B:695:GLU:HB2   | 2.14                     | 0.48              |
| 1:A:352:ILE:CD1   | 1:A:406:ASN:HB3   | 2.33                     | 0.48              |
| 4:D:2008:SER:OG   | 4:D:2049:LEU:CD1  | 2.61                     | 0.48              |
| 4:D:2097:GLN:O    | 4:D:2100:LEU:N    | 2.47                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:427:ASP:OD1   | 2:B:431:LYS:HG3   | 2.14                     | 0.48              |
| 2:B:573:ARG:C     | 2:B:574:HIS:CG    | 2.90                     | 0.48              |
| 2:B:717:ARG:HA    | 2:B:720:LYS:CE    | 2.44                     | 0.48              |
| 2:B:739:SER:C     | 2:B:741:ARG:N     | 2.72                     | 0.48              |
| 4:D:2133:GLU:HA   | 4:D:2136:ARG:NE   | 2.27                     | 0.48              |
| 1:A:189:LYS:HB3   | 1:A:193:GLY:HA2   | 1.95                     | 0.48              |
| 1:A:404:ASN:C     | 1:A:405:ASN:CG    | 2.80                     | 0.48              |
| 2:B:571:ALA:HB2   | 2:B:577:ARG:HH21  | 1.67                     | 0.48              |
| 5:E:3117:LEU:CD2  | 5:E:3142:LEU:HD13 | 2.43                     | 0.48              |
| 1:A:371:LEU:HD22  | 2:B:448:GLN:NE2   | 2.28                     | 0.48              |
| 2:B:712:GLN:OE1   | 2:B:756:LEU:CD2   | 2.59                     | 0.48              |
| 1:A:257:VAL:O     | 1:A:260:TYR:CB    | 2.54                     | 0.48              |
| 2:B:708:LYS:O     | 2:B:709:LEU:C     | 2.56                     | 0.48              |
| 1:A:306:GLU:O     | 1:A:307:PHE:C     | 2.56                     | 0.48              |
| 1:A:362:ASP:OD1   | 1:A:362:ASP:O     | 2.32                     | 0.48              |
| 1:A:371:LEU:O     | 1:A:372:ASP:C     | 2.57                     | 0.48              |
| 2:B:508:PHE:C     | 2:B:511:ILE:HG22  | 2.39                     | 0.47              |
| 2:B:611:LEU:CD2   | 2:B:648:LEU:HD23  | 2.44                     | 0.47              |
| 2:B:620:TYR:CE1   | 2:B:624:GLN:OE1   | 2.65                     | 0.47              |
| 4:D:2004:ILE:CG1  | 4:D:2031:LEU:HD11 | 2.43                     | 0.47              |
| 1:A:322:MET:C     | 1:A:324:ASN:N     | 2.70                     | 0.47              |
| 2:B:482:ASP:HB3   | 2:B:508:PHE:HZ    | 1.79                     | 0.47              |
| 2:B:652:GLU:HG3   | 2:B:668:LEU:HB2   | 1.96                     | 0.47              |
| 2:B:725:LEU:HD12  | 2:B:725:LEU:C     | 2.38                     | 0.47              |
| 4:D:2052:VAL:HG12 | 4:D:2056:CYS:SG   | 2.54                     | 0.47              |
| 1:A:204:VAL:O     | 1:A:205:VAL:C     | 2.58                     | 0.47              |
| 2:B:450:MET:C     | 2:B:453:PHE:H     | 2.22                     | 0.47              |
| 1:A:249:THR:O     | 1:A:250:GLU:C     | 2.55                     | 0.47              |
| 1:A:257:VAL:CG1   | 1:A:258:THR:H     | 2.26                     | 0.47              |
| 2:B:688:MET:H     | 2:B:688:MET:HG3   | 1.32                     | 0.47              |
| 4:D:2008:SER:OG   | 4:D:2049:LEU:HD12 | 2.14                     | 0.47              |
| 4:D:2037:ASP:CB   | 4:D:2038:PRO:CD   | 2.91                     | 0.47              |
| 2:B:450:MET:O     | 2:B:453:PHE:N     | 2.44                     | 0.47              |
| 2:B:587:LYS:HB3   | 2:B:603:ALA:O     | 2.15                     | 0.47              |
| 2:B:671:LEU:HD22  | 2:B:672:TYR:H     | 1.77                     | 0.47              |
| 4:D:2037:ASP:O    | 4:D:2039:VAL:N    | 2.47                     | 0.47              |
| 2:B:514:SER:O     | 2:B:517:LEU:HB3   | 2.15                     | 0.47              |
| 1:A:86:LEU:HD23   | 1:A:87:GLU:CD     | 2.40                     | 0.47              |
| 1:A:207:SER:OG    | 1:A:211:LEU:HD22  | 2.14                     | 0.47              |
| 1:A:296:ILE:HA    | 1:A:303:PHE:HE2   | 1.79                     | 0.47              |
| 1:A:345:HIS:CE1   | 1:A:401:ARG:O     | 2.68                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:525:LEU:HD12  | 2:B:529:GLU:HB3  | 1.97                     | 0.47              |
| 2:B:540:LEU:HD22  | 2:B:545:TRP:CH2  | 2.49                     | 0.47              |
| 2:B:571:ALA:HA    | 2:B:577:ARG:CZ   | 2.44                     | 0.47              |
| 2:B:574:HIS:O     | 2:B:577:ARG:CG   | 2.63                     | 0.47              |
| 2:B:672:TYR:O     | 2:B:673:LEU:C    | 2.57                     | 0.47              |
| 2:B:756:LEU:HB3   | 2:B:761:TYR:HB2  | 1.96                     | 0.47              |
| 4:D:2049:LEU:HD23 | 4:D:2053:ILE:H   | 1.80                     | 0.47              |
| 5:E:3120:ILE:C    | 5:E:3122:SER:H   | 2.22                     | 0.47              |
| 1:A:261:MET:O     | 1:A:265:GLU:N    | 2.41                     | 0.47              |
| 2:B:491:LYS:H     | 2:B:491:LYS:CD   | 2.24                     | 0.47              |
| 2:B:671:LEU:HD12  | 3:C:1020:LYS:HE2 | 1.95                     | 0.47              |
| 2:B:697:GLU:HG3   | 2:B:698:THR:N    | 2.29                     | 0.47              |
| 2:B:765:VAL:HB    | 2:B:771:THR:CB   | 2.44                     | 0.47              |
| 5:E:3136:CYS:O    | 5:E:3137:LYS:C   | 2.57                     | 0.47              |
| 1:A:257:VAL:O     | 1:A:260:TYR:N    | 2.43                     | 0.47              |
| 1:A:292:GLU:OE1   | 1:A:328:ARG:HB3  | 2.15                     | 0.47              |
| 1:A:303:PHE:HB3   | 1:A:322:MET:HE2  | 1.96                     | 0.47              |
| 1:A:326:VAL:O     | 1:A:329:ILE:N    | 2.36                     | 0.47              |
| 1:A:326:VAL:C     | 1:A:328:ARG:N    | 2.72                     | 0.47              |
| 2:B:553:PHE:CZ    | 2:B:629:THR:HB   | 2.43                     | 0.47              |
| 2:B:765:VAL:HB    | 2:B:771:THR:HB   | 1.96                     | 0.47              |
| 1:A:120:THR:O     | 1:A:123:TRP:HB3  | 2.15                     | 0.47              |
| 1:A:233:GLU:HG3   | 1:A:283:THR:HG23 | 1.96                     | 0.47              |
| 2:B:422:LEU:CD2   | 2:B:449:VAL:HG13 | 2.45                     | 0.47              |
| 2:B:432:LYS:HB2   | 2:B:478:ASN:OD1  | 2.15                     | 0.47              |
| 1:A:160:TYR:OH    | 1:A:210:GLU:OE2  | 2.23                     | 0.46              |
| 2:B:611:LEU:HD21  | 2:B:648:LEU:HD23 | 1.97                     | 0.46              |
| 2:B:642:ILE:HD11  | 2:B:687:PRO:C    | 2.39                     | 0.46              |
| 2:B:716:VAL:O     | 2:B:719:MET:N    | 2.48                     | 0.46              |
| 2:B:723:LYS:HA    | 2:B:774:TYR:HE2  | 1.71                     | 0.46              |
| 2:B:734:VAL:O     | 2:B:738:LEU:HB3  | 2.15                     | 0.46              |
| 1:A:215:GLU:O     | 1:A:216:ASP:O    | 2.33                     | 0.46              |
| 2:B:421:LEU:O     | 2:B:424:ARG:N    | 2.45                     | 0.46              |
| 2:B:471:ALA:O     | 2:B:475:VAL:HG23 | 2.16                     | 0.46              |
| 2:B:607:GLN:HA    | 2:B:610:ILE:HD11 | 1.97                     | 0.46              |
| 4:D:2016:VAL:HG21 | 4:D:2053:ILE:CD1 | 2.45                     | 0.46              |
| 1:A:129:SER:O     | 1:A:132:VAL:HG12 | 2.14                     | 0.46              |
| 1:A:173:ARG:HB3   | 1:A:174:PRO:CD   | 2.45                     | 0.46              |
| 1:A:280:HIS:CE1   | 1:A:282:SER:HG   | 2.30                     | 0.46              |
| 1:A:310:LEU:O     | 1:A:313:ALA:C    | 2.58                     | 0.46              |
| 2:B:671:LEU:HD12  | 3:C:1020:LYS:CE  | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:2025:VAL:CG2 | 4:D:2111:ASP:HB3 | 2.45                     | 0.46              |
| 4:D:2049:LEU:O   | 4:D:2053:ILE:N   | 2.45                     | 0.46              |
| 1:A:147:ARG:NH2  | 5:E:3146:GLU:HG2 | 2.24                     | 0.46              |
| 1:A:322:MET:C    | 1:A:324:ASN:H    | 2.24                     | 0.46              |
| 1:A:409:THR:O    | 1:A:410:LYS:C    | 2.58                     | 0.46              |
| 2:B:432:LYS:HB2  | 2:B:478:ASN:CG   | 2.41                     | 0.46              |
| 2:B:537:ILE:HG12 | 2:B:538:GLN:N    | 2.30                     | 0.46              |
| 2:B:540:LEU:HD13 | 2:B:545:TRP:CE3  | 2.51                     | 0.46              |
| 4:D:2101:PHE:O   | 4:D:2102:GLU:CA  | 2.61                     | 0.46              |
| 1:A:95:PHE:C     | 1:A:95:PHE:CD2   | 2.92                     | 0.46              |
| 1:A:180:THR:HG23 | 1:A:232:PHE:HD1  | 1.80                     | 0.46              |
| 2:B:485:GLU:C    | 2:B:487:SER:N    | 2.73                     | 0.46              |
| 1:A:167:TRP:HD1  | 1:A:211:LEU:HD21 | 1.80                     | 0.46              |
| 1:A:364:LYS:HG3  | 2:B:425:TYR:CE2  | 2.51                     | 0.46              |
| 2:B:765:VAL:HB   | 2:B:771:THR:OG1  | 2.16                     | 0.46              |
| 1:A:401:ARG:HG3  | 1:A:401:ARG:NH1  | 2.26                     | 0.46              |
| 2:B:534:ASP:CB   | 3:C:1026:LYS:HG3 | 2.39                     | 0.46              |
| 2:B:756:LEU:HB3  | 2:B:761:TYR:CB   | 2.45                     | 0.46              |
| 3:C:1024:VAL:O   | 3:C:1025:LYS:C   | 2.58                     | 0.46              |
| 5:E:3136:CYS:SG  | 5:E:3139:TRP:CD1 | 3.08                     | 0.46              |
| 1:A:371:LEU:CD1  | 2:B:448:GLN:HB3  | 2.45                     | 0.46              |
| 2:B:540:LEU:HD13 | 2:B:545:TRP:CD2  | 2.51                     | 0.46              |
| 1:A:104:LEU:HD13 | 1:A:108:GLU:CD   | 2.41                     | 0.46              |
| 1:A:280:HIS:CE1  | 1:A:282:SER:H    | 2.34                     | 0.46              |
| 1:A:368:GLN:O    | 1:A:369:THR:C    | 2.59                     | 0.46              |
| 2:B:632:LYS:HB3  | 2:B:635:ILE:CG2  | 2.46                     | 0.46              |
| 2:B:672:TYR:O    | 2:B:674:GLY:N    | 2.48                     | 0.46              |
| 2:B:704:GLU:OE1  | 2:B:704:GLU:HA   | 2.16                     | 0.46              |
| 1:A:260:TYR:O    | 1:A:263:LYS:N    | 2.49                     | 0.46              |
| 1:A:281:GLU:C    | 1:A:283:THR:N    | 2.73                     | 0.46              |
| 1:A:333:LEU:O    | 1:A:335:GLU:N    | 2.48                     | 0.46              |
| 2:B:648:LEU:C    | 2:B:649:LEU:HD12 | 2.41                     | 0.46              |
| 2:B:683:ASN:O    | 2:B:684:ILE:HG23 | 2.16                     | 0.46              |
| 1:A:140:LEU:HG   | 1:A:144:TRP:HD1  | 1.81                     | 0.45              |
| 1:A:164:LEU:O    | 1:A:165:VAL:C    | 2.59                     | 0.45              |
| 1:A:173:ARG:CB   | 1:A:174:PRO:HD3  | 2.46                     | 0.45              |
| 1:A:294:VAL:HG12 | 1:A:295:LEU:CG   | 2.46                     | 0.45              |
| 2:B:553:PHE:HZ   | 2:B:609:ALA:HB2  | 1.81                     | 0.45              |
| 2:B:730:LEU:HD11 | 2:B:734:VAL:CG2  | 2.46                     | 0.45              |
| 1:A:135:GLY:O    | 1:A:137:CYS:N    | 2.49                     | 0.45              |
| 1:A:230:GLU:HG3  | 1:A:231:SER:N    | 2.31                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:541:SER:H    | 2:B:545:TRP:CD1  | 2.32                     | 0.45              |
| 2:B:629:THR:OG1  | 2:B:631:ILE:HG13 | 2.15                     | 0.45              |
| 1:A:362:ASP:OD1  | 1:A:362:ASP:C    | 2.60                     | 0.45              |
| 2:B:716:VAL:HG22 | 2:B:719:MET:CE   | 2.47                     | 0.45              |
| 4:D:2098:GLY:O   | 4:D:2102:GLU:HG3 | 2.17                     | 0.45              |
| 1:A:229:LYS:HG3  | 1:A:233:GLU:OE1  | 2.17                     | 0.45              |
| 2:B:460:ASP:OD2  | 2:B:703:ILE:HD11 | 2.16                     | 0.45              |
| 2:B:524:HIS:O    | 2:B:527:ASN:N    | 2.48                     | 0.45              |
| 2:B:612:LEU:C    | 2:B:614:TYR:H    | 2.24                     | 0.45              |
| 1:A:26:ALA:O     | 1:A:30:GLN:HG3   | 2.15                     | 0.45              |
| 1:A:166:THR:C    | 1:A:168:ARG:N    | 2.71                     | 0.45              |
| 1:A:345:HIS:CE1  | 1:A:401:ARG:HG2  | 2.51                     | 0.45              |
| 2:B:537:ILE:CG1  | 2:B:538:GLN:N    | 2.79                     | 0.45              |
| 2:B:578:LYS:C    | 2:B:579:LEU:HG   | 2.42                     | 0.45              |
| 2:B:620:TYR:HD2  | 2:B:624:GLN:HG2  | 1.65                     | 0.45              |
| 2:B:703:ILE:HG23 | 2:B:704:GLU:N    | 2.32                     | 0.45              |
| 1:A:232:PHE:CZ   | 1:A:236:PHE:HB2  | 2.51                     | 0.45              |
| 1:A:242:ARG:HG3  | 1:A:242:ARG:NH1  | 2.30                     | 0.45              |
| 1:A:340:LEU:O    | 1:A:340:LEU:HD12 | 2.16                     | 0.45              |
| 2:B:652:GLU:OE1  | 2:B:652:GLU:N    | 2.37                     | 0.45              |
| 2:B:668:LEU:N    | 2:B:668:LEU:CD1  | 2.80                     | 0.45              |
| 2:B:751:LYS:HZ1  | 2:B:755:ILE:HD11 | 1.80                     | 0.45              |
| 1:A:127:ARG:O    | 1:A:130:SER:HB2  | 2.16                     | 0.45              |
| 1:A:316:ASN:CG   | 1:A:380:LEU:HD13 | 2.41                     | 0.45              |
| 1:A:326:VAL:O    | 1:A:327:SER:C    | 2.59                     | 0.45              |
| 1:A:402:PHE:C    | 1:A:404:ASN:H    | 2.24                     | 0.45              |
| 2:B:426:CYS:O    | 2:B:427:ASP:C    | 2.59                     | 0.45              |
| 2:B:648:LEU:O    | 2:B:672:TYR:N    | 2.41                     | 0.45              |
| 1:A:296:ILE:O    | 1:A:303:PHE:CE2  | 2.70                     | 0.45              |
| 1:A:312:ASP:C    | 1:A:313:ALA:O    | 2.57                     | 0.45              |
| 1:A:318:ASP:O    | 1:A:319:LEU:C    | 2.60                     | 0.45              |
| 1:A:371:LEU:O    | 1:A:374:HIS:HB3  | 2.16                     | 0.45              |
| 2:B:442:LEU:CD2  | 2:B:484:ALA:HB1  | 2.47                     | 0.45              |
| 2:B:584:GLN:HB2  | 2:B:585:LEU:HD12 | 1.98                     | 0.45              |
| 2:B:649:LEU:HD12 | 2:B:649:LEU:N    | 2.31                     | 0.45              |
| 2:B:758:GLU:O    | 2:B:758:GLU:HG2  | 2.16                     | 0.45              |
| 4:D:2022:LYS:HA  | 4:D:2028:LYS:HG3 | 1.97                     | 0.45              |
| 1:A:41:ARG:O     | 1:A:42:TYR:C     | 2.60                     | 0.45              |
| 1:A:86:LEU:O     | 1:A:87:GLU:C     | 2.58                     | 0.45              |
| 1:A:154:LYS:N    | 1:A:154:LYS:CD   | 2.79                     | 0.45              |
| 1:A:175:LEU:O    | 1:A:176:ASN:C    | 2.60                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:195:THR:O     | 1:A:195:THR:CG2   | 2.61                     | 0.45              |
| 1:A:286:GLU:HA    | 1:A:289:ARG:HB2   | 1.99                     | 0.45              |
| 1:A:342:THR:HG22  | 1:A:346:ASN:ND2   | 2.32                     | 0.45              |
| 1:A:364:LYS:O     | 1:A:365:MET:C     | 2.59                     | 0.45              |
| 2:B:652:GLU:CG    | 2:B:668:LEU:HB2   | 2.46                     | 0.45              |
| 2:B:714:ALA:HB1   | 2:B:738:LEU:HD22  | 1.99                     | 0.45              |
| 4:D:2044:VAL:O    | 4:D:2044:VAL:HG12 | 2.16                     | 0.45              |
| 4:D:2099:THR:O    | 4:D:2103:LEU:HG   | 2.16                     | 0.45              |
| 1:A:162:LEU:C     | 1:A:162:LEU:HD23  | 2.42                     | 0.45              |
| 1:A:212:GLY:O     | 1:A:214:ASN:OD1   | 2.35                     | 0.45              |
| 2:B:423:ALA:HA    | 2:B:462:PHE:HE1   | 1.82                     | 0.45              |
| 2:B:522:LYS:NZ    | 2:B:522:LYS:CB    | 2.80                     | 0.45              |
| 2:B:632:LYS:HB3   | 2:B:635:ILE:HG22  | 1.98                     | 0.45              |
| 1:A:127:ARG:NE    | 1:A:210:GLU:OE1   | 2.49                     | 0.44              |
| 2:B:475:VAL:HG21  | 2:B:547:PHE:CE2   | 2.52                     | 0.44              |
| 2:B:751:LYS:HE2   | 2:B:751:LYS:O     | 2.17                     | 0.44              |
| 4:D:2116:LEU:O    | 4:D:2119:THR:OG1  | 2.35                     | 0.44              |
| 4:D:2122:THR:C    | 4:D:2124:ALA:N    | 2.75                     | 0.44              |
| 1:A:97:LYS:HD2    | 1:A:101:THR:HG21  | 1.99                     | 0.44              |
| 1:A:135:GLY:O     | 1:A:136:ILE:C     | 2.59                     | 0.44              |
| 1:A:286:GLU:HG3   | 1:A:289:ARG:CZ    | 2.46                     | 0.44              |
| 1:A:368:GLN:O     | 1:A:371:LEU:N     | 2.45                     | 0.44              |
| 2:B:540:LEU:HB3   | 2:B:545:TRP:CE2   | 2.52                     | 0.44              |
| 1:A:54:THR:O      | 1:A:54:THR:HG22   | 2.17                     | 0.44              |
| 1:A:87:GLU:O      | 1:A:88:LEU:C      | 2.59                     | 0.44              |
| 1:A:135:GLY:C     | 1:A:137:CYS:H     | 2.24                     | 0.44              |
| 1:A:145:VAL:HG13  | 1:A:157:TYR:HD2   | 1.81                     | 0.44              |
| 1:A:287:LEU:HD23  | 1:A:287:LEU:O     | 2.17                     | 0.44              |
| 2:B:464:LYS:NZ    | 2:B:702:ASN:O     | 2.50                     | 0.44              |
| 2:B:513:VAL:CG1   | 2:B:514:SER:N     | 2.81                     | 0.44              |
| 1:A:173:ARG:CB    | 1:A:174:PRO:CD    | 2.93                     | 0.44              |
| 1:A:186:LEU:HD11  | 1:A:197:ASN:CG    | 2.42                     | 0.44              |
| 1:A:232:PHE:C     | 1:A:232:PHE:CD2   | 2.94                     | 0.44              |
| 2:B:431:LYS:O     | 2:B:432:LYS:C     | 2.60                     | 0.44              |
| 2:B:475:VAL:HG12  | 2:B:476:HIS:HD2   | 1.82                     | 0.44              |
| 2:B:590:LEU:O     | 2:B:600:THR:HA    | 2.18                     | 0.44              |
| 2:B:756:LEU:CB    | 2:B:761:TYR:HB2   | 2.47                     | 0.44              |
| 4:D:2104:ILE:HG22 | 5:E:3116:LEU:HD13 | 2.00                     | 0.44              |
| 1:A:21:TRP:CD1    | 1:A:91:ARG:HD3    | 2.53                     | 0.44              |
| 1:A:227:VAL:O     | 1:A:230:GLU:N     | 2.51                     | 0.44              |
| 1:A:227:VAL:O     | 1:A:229:LYS:N     | 2.51                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:248:SER:O    | 1:A:251:PHE:HB3  | 2.18                     | 0.44              |
| 1:A:366:TYR:O    | 1:A:367:VAL:C    | 2.60                     | 0.44              |
| 1:A:399:CYS:HA   | 1:A:402:PHE:CE2  | 2.53                     | 0.44              |
| 2:B:475:VAL:HG12 | 2:B:476:HIS:CD2  | 2.52                     | 0.44              |
| 2:B:655:ASN:O    | 2:B:656:ALA:HB2  | 2.16                     | 0.44              |
| 2:B:712:GLN:O    | 2:B:761:TYR:CE2  | 2.71                     | 0.44              |
| 4:D:2018:VAL:C   | 4:D:2020:ILE:H   | 2.26                     | 0.44              |
| 4:D:2046:ALA:C   | 4:D:2048:ILE:N   | 2.74                     | 0.44              |
| 1:A:24:LEU:CD1   | 1:A:28:ILE:HD11  | 2.48                     | 0.44              |
| 2:B:545:TRP:CD1  | 2:B:545:TRP:N    | 2.86                     | 0.44              |
| 2:B:619:ALA:HB1  | 2:B:670:LYS:HA   | 2.00                     | 0.44              |
| 2:B:620:TYR:CZ   | 2:B:624:GLN:CD   | 2.96                     | 0.44              |
| 1:A:335:GLU:O    | 1:A:339:LEU:N    | 2.40                     | 0.44              |
| 1:A:360:LEU:HB2  | 1:A:408:VAL:HG13 | 1.99                     | 0.44              |
| 2:B:430:LEU:N    | 2:B:430:LEU:HD22 | 2.32                     | 0.44              |
| 2:B:507:MET:HG2  | 2:B:545:TRP:CE2  | 2.53                     | 0.44              |
| 2:B:641:GLN:HA   | 2:B:644:LEU:CD1  | 2.40                     | 0.44              |
| 1:A:257:VAL:HG13 | 1:A:258:THR:N    | 2.28                     | 0.44              |
| 2:B:511:ILE:HD11 | 2:B:538:GLN:HE21 | 1.83                     | 0.44              |
| 4:D:2059:HIS:CD2 | 4:D:2062:ASP:OD2 | 2.71                     | 0.44              |
| 5:E:3130:LEU:O   | 5:E:3133:SER:HB3 | 2.18                     | 0.44              |
| 1:A:167:TRP:CD1  | 1:A:211:LEU:HD21 | 2.53                     | 0.43              |
| 2:B:506:ARG:HA   | 2:B:509:GLN:HE21 | 1.83                     | 0.43              |
| 4:D:2018:VAL:C   | 4:D:2020:ILE:N   | 2.75                     | 0.43              |
| 4:D:2101:PHE:O   | 4:D:2102:GLU:HA  | 2.17                     | 0.43              |
| 1:A:28:ILE:C     | 1:A:31:VAL:HG12  | 2.43                     | 0.43              |
| 2:B:458:ASP:C    | 2:B:460:ASP:N    | 2.73                     | 0.43              |
| 2:B:542:SER:CB   | 3:C:1032:LEU:HB3 | 2.48                     | 0.43              |
| 2:B:633:MET:O    | 2:B:633:MET:CG   | 2.63                     | 0.43              |
| 2:B:703:ILE:CG2  | 2:B:704:GLU:N    | 2.80                     | 0.43              |
| 2:B:450:MET:HE2  | 2:B:491:LYS:C    | 2.43                     | 0.43              |
| 2:B:481:SER:O    | 2:B:484:ALA:HB3  | 2.18                     | 0.43              |
| 2:B:631:ILE:HB   | 2:B:636:LEU:CD1  | 2.48                     | 0.43              |
| 1:A:27:GLY:HA3   | 1:A:45:LEU:HD21  | 2.00                     | 0.43              |
| 1:A:243:PHE:CD1  | 1:A:243:PHE:C    | 2.96                     | 0.43              |
| 2:B:464:LYS:O    | 2:B:465:PHE:C    | 2.61                     | 0.43              |
| 2:B:689:LYS:HE2  | 2:B:689:LYS:CA   | 2.46                     | 0.43              |
| 1:A:169:ASP:OD1  | 1:A:169:ASP:C    | 2.61                     | 0.43              |
| 1:A:170:CYS:O    | 1:A:170:CYS:SG   | 2.77                     | 0.43              |
| 1:A:228:TYR:O    | 1:A:232:PHE:HB3  | 2.18                     | 0.43              |
| 1:A:380:LEU:HD12 | 1:A:384:ALA:HB2  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:171:LEU:O    | 1:A:173:ARG:N     | 2.52                     | 0.43              |
| 2:B:450:MET:HG3  | 2:B:491:LYS:HB3   | 1.99                     | 0.43              |
| 2:B:590:LEU:HD21 | 2:B:608:MET:SD    | 2.58                     | 0.43              |
| 2:B:638:GLN:CD   | 2:B:688:MET:CE    | 2.83                     | 0.43              |
| 2:B:730:LEU:HD11 | 2:B:734:VAL:HG23  | 2.01                     | 0.43              |
| 1:A:235:GLN:O    | 1:A:238:ALA:HB3   | 2.19                     | 0.43              |
| 1:A:299:HIS:C    | 1:A:301:GLU:N     | 2.75                     | 0.43              |
| 4:D:2010:ASP:OD2 | 4:D:2010:ASP:N    | 2.52                     | 0.43              |
| 1:A:227:VAL:C    | 1:A:229:LYS:N     | 2.75                     | 0.43              |
| 1:A:321:ARG:CG   | 1:A:321:ARG:NH1   | 2.80                     | 0.43              |
| 2:B:553:PHE:CZ   | 2:B:609:ALA:HB2   | 2.53                     | 0.43              |
| 2:B:559:LEU:C    | 2:B:561:ARG:N     | 2.77                     | 0.43              |
| 1:A:192:ASN:O    | 1:A:193:GLY:O     | 2.36                     | 0.43              |
| 1:A:297:GLU:C    | 1:A:299:HIS:H     | 2.27                     | 0.43              |
| 1:A:297:GLU:HA   | 1:A:300:LEU:CB    | 2.48                     | 0.43              |
| 1:A:388:ASP:OD1  | 1:A:390:GLY:N     | 2.47                     | 0.43              |
| 2:B:540:LEU:HB3  | 2:B:545:TRP:CD1   | 2.53                     | 0.43              |
| 2:B:541:SER:N    | 2:B:545:TRP:NE1   | 2.51                     | 0.43              |
| 1:A:38:ALA:O     | 1:A:40:SER:N      | 2.51                     | 0.43              |
| 1:A:107:GLY:CA   | 1:A:110:LEU:CD1   | 2.86                     | 0.43              |
| 1:A:273:ARG:O    | 1:A:277:VAL:HG23  | 2.18                     | 0.43              |
| 1:A:287:LEU:HD23 | 1:A:291:CYS:SG    | 2.58                     | 0.43              |
| 1:A:293:GLN:HG2  | 1:A:298:LYS:HE3   | 2.00                     | 0.43              |
| 1:A:386:ASN:C    | 1:A:386:ASN:HD22  | 2.26                     | 0.43              |
| 2:B:430:LEU:CD1  | 2:B:442:LEU:HD21  | 2.49                     | 0.43              |
| 2:B:432:LYS:HD2  | 2:B:480:ALA:CA    | 2.48                     | 0.43              |
| 2:B:745:ARG:HB3  | 2:B:747:PRO:HD2   | 2.00                     | 0.43              |
| 4:D:2131:THR:HB  | 4:D:2132:PRO:CD   | 2.48                     | 0.43              |
| 1:A:110:LEU:CD1  | 1:A:118:PHE:CD2   | 3.02                     | 0.42              |
| 1:A:197:ASN:O    | 1:A:198:THR:C     | 2.61                     | 0.42              |
| 2:B:590:LEU:HB2  | 2:B:601:LEU:CB    | 2.47                     | 0.42              |
| 2:B:608:MET:HE1  | 3:C:1024:VAL:HG13 | 2.00                     | 0.42              |
| 2:B:711:ILE:HB   | 2:B:712:GLN:HE21  | 1.84                     | 0.42              |
| 1:A:116:LEU:HD21 | 1:A:182:ALA:HB3   | 2.00                     | 0.42              |
| 1:A:208:TYR:CD1  | 1:A:232:PHE:HB2   | 2.54                     | 0.42              |
| 1:A:310:LEU:O    | 1:A:313:ALA:N     | 2.52                     | 0.42              |
| 1:A:396:ASP:O    | 1:A:397:LYS:C     | 2.60                     | 0.42              |
| 2:B:438:GLU:O    | 2:B:439:GLU:C     | 2.62                     | 0.42              |
| 2:B:505:GLN:O    | 2:B:506:ARG:C     | 2.61                     | 0.42              |
| 2:B:668:LEU:O    | 2:B:669:ILE:HD12  | 2.19                     | 0.42              |
| 4:D:2024:SER:CA  | 4:D:2112:ILE:HG12 | 2.45                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:2114:GLY:O    | 4:D:2115:LEU:C    | 2.61                     | 0.42              |
| 5:E:3126:LEU:N    | 5:E:3127:PRO:HD2  | 2.34                     | 0.42              |
| 5:E:3132:VAL:HG23 | 5:E:3133:SER:N    | 2.34                     | 0.42              |
| 1:A:19:GLN:O      | 1:A:23:ASP:CG     | 2.62                     | 0.42              |
| 1:A:32:TYR:HE2    | 1:A:126:TYR:CE1   | 2.37                     | 0.42              |
| 1:A:121:GLN:HB2   | 1:A:121:GLN:HE21  | 1.61                     | 0.42              |
| 1:A:381:VAL:HG21  | 1:A:395:LEU:HD12  | 2.00                     | 0.42              |
| 1:A:409:THR:HG23  | 2:B:415:SER:CA    | 2.16                     | 0.42              |
| 2:B:541:SER:O     | 2:B:542:SER:C     | 2.61                     | 0.42              |
| 2:B:545:TRP:C     | 2:B:547:PHE:H     | 2.27                     | 0.42              |
| 2:B:712:GLN:OE1   | 2:B:756:LEU:HD11  | 2.20                     | 0.42              |
| 2:B:738:LEU:O     | 2:B:740:SER:N     | 2.52                     | 0.42              |
| 4:D:2119:THR:O    | 4:D:2122:THR:N    | 2.53                     | 0.42              |
| 1:A:197:ASN:CG    | 1:A:200:LEU:CD1   | 2.72                     | 0.42              |
| 1:A:304:HIS:ND1   | 1:A:335:GLU:HB3   | 2.33                     | 0.42              |
| 1:A:330:GLN:O     | 1:A:330:GLN:HG3   | 2.19                     | 0.42              |
| 1:A:343:HIS:CD2   | 1:A:347:GLN:HG3   | 2.55                     | 0.42              |
| 2:B:468:LYS:CE    | 2:B:699:THR:HB    | 2.49                     | 0.42              |
| 2:B:607:GLN:O     | 2:B:608:MET:C     | 2.62                     | 0.42              |
| 4:D:2017:ASP:O    | 4:D:2020:ILE:HB   | 2.18                     | 0.42              |
| 4:D:2114:GLY:O    | 4:D:2117:ASP:HB2  | 2.19                     | 0.42              |
| 1:A:162:LEU:C     | 1:A:162:LEU:CD2   | 2.92                     | 0.42              |
| 2:B:617:GLU:O     | 2:B:618:ASP:O     | 2.38                     | 0.42              |
| 1:A:37:MET:HG2    | 1:A:42:TYR:CE1    | 2.54                     | 0.42              |
| 1:A:323:TYR:CG    | 1:A:385:PHE:HA    | 2.55                     | 0.42              |
| 2:B:620:TYR:CD2   | 2:B:624:GLN:OE1   | 2.72                     | 0.42              |
| 2:B:734:VAL:HG12  | 2:B:734:VAL:O     | 2.19                     | 0.42              |
| 4:D:2006:LEU:O    | 4:D:2008:SER:N    | 2.53                     | 0.42              |
| 4:D:2043:ASN:HB2  | 4:D:2109:TYR:CZ   | 2.54                     | 0.42              |
| 1:A:162:LEU:O     | 1:A:163:ALA:C     | 2.63                     | 0.42              |
| 1:A:287:LEU:HD21  | 1:A:291:CYS:SG    | 2.60                     | 0.42              |
| 2:B:466:TYR:CZ    | 2:B:488:MET:HE3   | 2.55                     | 0.42              |
| 2:B:728:GLN:HA    | 2:B:728:GLN:NE2   | 2.33                     | 0.42              |
| 1:A:191:ARG:O     | 1:A:193:GLY:N     | 2.51                     | 0.42              |
| 1:A:261:MET:O     | 1:A:264:ALA:HB3   | 2.19                     | 0.42              |
| 1:A:297:GLU:HG3   | 1:A:298:LYS:N     | 2.34                     | 0.42              |
| 1:A:323:TYR:CD2   | 1:A:323:TYR:C     | 2.97                     | 0.42              |
| 2:B:619:ALA:HB1   | 2:B:670:LYS:CA    | 2.50                     | 0.42              |
| 2:B:675:TYR:C     | 2:B:676:LYS:HE3   | 2.44                     | 0.42              |
| 2:B:746:VAL:HG22  | 2:B:747:PRO:HD3   | 2.02                     | 0.42              |
| 4:D:2016:VAL:CG2  | 4:D:2053:ILE:HD11 | 2.50                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:26:ALA:O      | 1:A:29:GLN:HB3    | 2.20                     | 0.42              |
| 1:A:134:ASN:OD1   | 1:A:159:ILE:HG22  | 2.19                     | 0.42              |
| 1:A:366:TYR:O     | 1:A:370:VAL:HG23  | 2.20                     | 0.42              |
| 2:B:432:LYS:HA    | 2:B:480:ALA:H     | 1.84                     | 0.42              |
| 5:E:3136:CYS:HG   | 5:E:3139:TRP:CD1  | 2.38                     | 0.42              |
| 1:A:124:GLU:O     | 1:A:125:ASP:C     | 2.61                     | 0.42              |
| 1:A:360:LEU:C     | 1:A:362:ASP:N     | 2.78                     | 0.42              |
| 1:A:370:VAL:HG13  | 1:A:402:PHE:CE1   | 2.55                     | 0.42              |
| 2:B:738:LEU:C     | 2:B:740:SER:N     | 2.77                     | 0.42              |
| 4:D:2026:THR:HB   | 4:D:2110:LEU:CA   | 2.50                     | 0.42              |
| 1:A:39:LYS:HG2    | 4:D:2036:MET:CB   | 2.44                     | 0.41              |
| 1:A:167:TRP:O     | 1:A:170:CYS:HB3   | 2.19                     | 0.41              |
| 1:A:286:GLU:O     | 1:A:289:ARG:HB2   | 2.19                     | 0.41              |
| 1:A:315:LYS:HD3   | 1:A:318:ASP:OD2   | 2.20                     | 0.41              |
| 1:A:357:GLU:H     | 1:A:359:ALA:H     | 1.68                     | 0.41              |
| 4:D:2054:GLN:O    | 4:D:2057:THR:HB   | 2.20                     | 0.41              |
| 1:A:84:VAL:HG23   | 1:A:84:VAL:O      | 2.20                     | 0.41              |
| 1:A:88:LEU:HD12   | 1:A:88:LEU:O      | 2.20                     | 0.41              |
| 1:A:129:SER:CA    | 1:A:132:VAL:HG12  | 2.50                     | 0.41              |
| 1:A:244:TYR:HE2   | 1:A:267:ARG:CG    | 2.32                     | 0.41              |
| 1:A:307:PHE:HD1   | 1:A:322:MET:SD    | 2.43                     | 0.41              |
| 2:B:416:SER:C     | 2:B:419:PRO:HD2   | 2.44                     | 0.41              |
| 2:B:489:ILE:N     | 2:B:489:ILE:HD13  | 2.35                     | 0.41              |
| 2:B:622:VAL:HB    | 2:B:665:PRO:HA    | 2.02                     | 0.41              |
| 4:D:2022:LYS:CB   | 4:D:2028:LYS:HG3  | 2.50                     | 0.41              |
| 1:A:168:ARG:HH12  | 1:A:215:GLU:CG    | 2.32                     | 0.41              |
| 1:A:306:GLU:OE1   | 1:A:309:ASN:ND2   | 2.47                     | 0.41              |
| 2:B:714:ALA:HB1   | 2:B:738:LEU:HD21  | 2.01                     | 0.41              |
| 4:D:2124:ALA:HB1  | 5:E:3124:LEU:HD21 | 2.02                     | 0.41              |
| 4:D:2130:LYS:O    | 5:E:3131:LYS:HD2  | 2.21                     | 0.41              |
| 5:E:3116:LEU:O    | 5:E:3119:GLY:N    | 2.39                     | 0.41              |
| 1:A:303:PHE:CB    | 1:A:322:MET:HE2   | 2.51                     | 0.41              |
| 2:B:571:ALA:HB2   | 2:B:577:ARG:HH22  | 1.77                     | 0.41              |
| 2:B:650:VAL:O     | 2:B:670:LYS:HD3   | 2.20                     | 0.41              |
| 2:B:723:LYS:CB    | 2:B:774:TYR:CE2   | 2.97                     | 0.41              |
| 5:E:3109:TRP:HB2  | 5:E:3110:ASP:H    | 1.66                     | 0.41              |
| 1:A:250:GLU:C     | 1:A:250:GLU:CD    | 2.88                     | 0.41              |
| 1:A:386:ASN:ND2   | 1:A:386:ASN:C     | 2.79                     | 0.41              |
| 2:B:489:ILE:O     | 2:B:493:LYS:HG3   | 2.20                     | 0.41              |
| 4:D:2053:ILE:HG23 | 4:D:2054:GLN:N    | 2.36                     | 0.41              |
| 4:D:2126:MET:O    | 4:D:2127:ILE:HD13 | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:89:TYR:CD1    | 1:A:89:TYR:C      | 2.98                     | 0.41              |
| 2:B:422:LEU:HD22  | 2:B:449:VAL:HG13  | 2.02                     | 0.41              |
| 2:B:432:LYS:H     | 2:B:478:ASN:C     | 2.28                     | 0.41              |
| 2:B:477:GLN:O     | 2:B:477:GLN:CG    | 2.47                     | 0.41              |
| 2:B:537:ILE:HG13  | 3:C:1030:VAL:CA   | 2.50                     | 0.41              |
| 2:B:583:TYR:C     | 2:B:585:LEU:N     | 2.76                     | 0.41              |
| 2:B:707:ARG:NH1   | 2:B:742:PHE:CB    | 2.82                     | 0.41              |
| 2:B:718:ILE:C     | 2:B:720:LYS:H     | 2.28                     | 0.41              |
| 1:A:104:LEU:HD13  | 1:A:108:GLU:OE1   | 2.21                     | 0.41              |
| 1:A:297:GLU:CG    | 1:A:298:LYS:N     | 2.83                     | 0.41              |
| 1:A:341:GLU:HG3   | 1:A:398:ALA:HB2   | 2.03                     | 0.41              |
| 2:B:513:VAL:O     | 2:B:517:LEU:N     | 2.52                     | 0.41              |
| 2:B:545:TRP:HE3   | 2:B:547:PHE:HE2   | 1.69                     | 0.41              |
| 2:B:691:GLU:HA    | 2:B:694:GLN:HB2   | 2.02                     | 0.41              |
| 1:A:96:LEU:HD22   | 1:A:162:LEU:HD22  | 2.03                     | 0.41              |
| 1:A:126:TYR:C     | 1:A:128:PHE:N     | 2.70                     | 0.41              |
| 1:A:197:ASN:O     | 1:A:201:ILE:N     | 2.49                     | 0.41              |
| 1:A:310:LEU:O     | 1:A:311:LEU:C     | 2.63                     | 0.41              |
| 1:A:404:ASN:CG    | 2:B:457:GLU:HB2   | 2.46                     | 0.41              |
| 2:B:421:LEU:C     | 2:B:423:ALA:N     | 2.79                     | 0.41              |
| 2:B:762:LEU:CD2   | 2:B:772:TYR:HB3   | 2.50                     | 0.41              |
| 1:A:86:LEU:O      | 1:A:89:TYR:N      | 2.54                     | 0.41              |
| 1:A:196:ILE:O     | 1:A:196:ILE:HG22  | 2.20                     | 0.41              |
| 1:A:316:ASN:O     | 1:A:319:LEU:HB3   | 2.20                     | 0.41              |
| 1:A:401:ARG:O     | 1:A:401:ARG:HG2   | 2.21                     | 0.41              |
| 2:B:414:SER:HB3   | 2:B:417:LYS:HB2   | 2.01                     | 0.41              |
| 2:B:431:LYS:CA    | 2:B:479:SER:HA    | 2.46                     | 0.41              |
| 2:B:436:ASN:OD1   | 2:B:437:PRO:N     | 2.54                     | 0.41              |
| 2:B:581:TRP:HA    | 3:C:1031:ALA:HB2  | 2.03                     | 0.41              |
| 2:B:657:ASN:C     | 2:B:659:ASP:N     | 2.79                     | 0.41              |
| 2:B:671:LEU:HD22  | 2:B:671:LEU:C     | 2.46                     | 0.41              |
| 4:D:2110:LEU:HD12 | 4:D:2112:ILE:HD11 | 2.02                     | 0.41              |
| 1:A:50:TYR:HD1    | 1:A:51:ASN:HD22   | 1.69                     | 0.41              |
| 1:A:250:GLU:HG3   | 1:A:251:PHE:N     | 2.36                     | 0.41              |
| 1:A:343:HIS:CD2   | 1:A:347:GLN:CG    | 3.04                     | 0.41              |
| 2:B:590:LEU:HD23  | 3:C:1024:VAL:HA   | 2.03                     | 0.41              |
| 2:B:746:VAL:HG23  | 2:B:747:PRO:CD    | 2.51                     | 0.41              |
| 3:C:1021:ARG:HG3  | 3:C:1022:PHE:N    | 2.35                     | 0.41              |
| 4:D:2049:LEU:HD22 | 4:D:2053:ILE:HB   | 2.01                     | 0.41              |
| 4:D:2085:ILE:HG13 | 4:D:2121:LYS:HE3  | 2.03                     | 0.41              |
| 5:E:3144:SER:O    | 5:E:3145:ASP:C    | 2.60                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:37:MET:HG2    | 1:A:42:TYR:HE1   | 1.85                     | 0.40              |
| 1:A:39:LYS:CG     | 4:D:2036:MET:HG2 | 2.51                     | 0.40              |
| 1:A:43:MET:HE2    | 4:D:2036:MET:HE1 | 2.03                     | 0.40              |
| 1:A:335:GLU:HG3   | 1:A:339:LEU:HD22 | 2.03                     | 0.40              |
| 1:A:367:VAL:HG13  | 2:B:422:LEU:HD23 | 2.02                     | 0.40              |
| 2:B:451:VAL:HG12  | 2:B:452:VAL:N    | 2.36                     | 0.40              |
| 2:B:553:PHE:HE1   | 2:B:631:ILE:CG1  | 2.09                     | 0.40              |
| 2:B:644:LEU:HA    | 2:B:649:LEU:O    | 2.20                     | 0.40              |
| 4:D:2004:ILE:HD11 | 4:D:2039:VAL:CG2 | 2.51                     | 0.40              |
| 4:D:2034:LEU:O    | 4:D:2034:LEU:HG  | 2.21                     | 0.40              |
| 1:A:111:MET:O     | 1:A:115:VAL:CG1  | 2.69                     | 0.40              |
| 1:A:186:LEU:HD22  | 1:A:197:ASN:HB2  | 2.03                     | 0.40              |
| 1:A:251:PHE:CE2   | 1:A:255:ASN:CB   | 3.04                     | 0.40              |
| 2:B:425:TYR:O     | 2:B:428:SER:HB3  | 2.21                     | 0.40              |
| 1:A:45:LEU:HB3    | 1:A:136:ILE:CG2  | 2.52                     | 0.40              |
| 1:A:209:VAL:O     | 1:A:212:GLY:HA3  | 2.22                     | 0.40              |
| 2:B:637:ALA:CB    | 2:B:663:LEU:HD12 | 2.26                     | 0.40              |
| 2:B:669:ILE:HD12  | 2:B:669:ILE:N    | 2.36                     | 0.40              |
| 2:B:723:LYS:HA    | 2:B:774:TYR:CD2  | 2.55                     | 0.40              |
| 4:D:2004:ILE:HG13 | 4:D:2005:LYS:N   | 2.36                     | 0.40              |
| 4:D:2022:LYS:CA   | 4:D:2028:LYS:HG3 | 2.51                     | 0.40              |
| 1:A:124:GLU:O     | 1:A:126:TYR:N    | 2.54                     | 0.40              |
| 1:A:162:LEU:O     | 1:A:166:THR:N    | 2.38                     | 0.40              |
| 1:A:316:ASN:OD1   | 1:A:380:LEU:HD13 | 2.21                     | 0.40              |
| 1:A:399:CYS:C     | 1:A:401:ARG:H    | 2.29                     | 0.40              |
| 2:B:524:HIS:O     | 2:B:529:GLU:OE1  | 2.39                     | 0.40              |
| 2:B:633:MET:O     | 2:B:633:MET:HG2  | 2.21                     | 0.40              |
| 2:B:691:GLU:HA    | 2:B:694:GLN:CG   | 2.51                     | 0.40              |
| 4:D:2051:LYS:HA   | 4:D:2054:GLN:OE1 | 2.20                     | 0.40              |
| 4:D:2097:GLN:O    | 4:D:2098:GLY:C   | 2.63                     | 0.40              |
| 1:A:268:LEU:HD13  | 1:A:328:ARG:NH2  | 2.37                     | 0.40              |
| 2:B:500:TYR:HB3   | 2:B:504:LEU:HD12 | 2.03                     | 0.40              |
| 2:B:681:ARG:NH1   | 2:B:681:ARG:HG2  | 2.36                     | 0.40              |
| 2:B:709:LEU:HD23  | 2:B:709:LEU:HA   | 1.95                     | 0.40              |
| 4:D:2024:SER:OG   | 4:D:2110:LEU:CB  | 2.66                     | 0.40              |

All (4) 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:A:199:ARG:NH2 | 1:A:305:THR:OG1[3_546] | 1.76                     | 0.44              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 2:B:597:ASN:OD1 | 2:B:659:ASP:OD2[3_547] | 2.00                     | 0.20              |
| 2:B:572:SER:O   | 3:C:1061:ALA:CB[1_545] | 2.04                     | 0.16              |
| 2:B:660:GLU:OE1 | 2:B:676:LYS:CB[3_557]  | 2.04                     | 0.16              |

## 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     | 350/396 (88%)  | 236 (67%) | 92 (26%)  | 22 (6%)  | 1           | 6 |
| 2   | B     | 364/366 (100%) | 261 (72%) | 75 (21%)  | 28 (8%)  | 1           | 4 |
| 3   | C     | 86/90 (96%)    | 44 (51%)  | 24 (28%)  | 18 (21%) | 0           | 0 |
| 4   | D     | 114/133 (86%)  | 68 (60%)  | 31 (27%)  | 15 (13%) | 0           | 1 |
| 5   | E     | 39/41 (95%)    | 26 (67%)  | 9 (23%)   | 4 (10%)  | 0           | 2 |
| All | All   | 953/1026 (93%) | 635 (67%) | 231 (24%) | 87 (9%)  | 0           | 3 |

All (87) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 83  | PHE  |
| 1   | A     | 174 | PRO  |
| 1   | A     | 176 | ASN  |
| 1   | A     | 192 | ASN  |
| 1   | A     | 193 | GLY  |
| 2   | B     | 431 | LYS  |
| 2   | B     | 454 | LYS  |
| 2   | B     | 527 | ASN  |
| 2   | B     | 536 | SER  |
| 2   | B     | 557 | SER  |
| 2   | B     | 594 | CYS  |
| 2   | B     | 618 | ASP  |
| 2   | B     | 622 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 661  | VAL  |
| 2   | B     | 688  | MET  |
| 2   | B     | 731  | LEU  |
| 3   | C     | 1088 | LEU  |
| 3   | C     | 1104 | GLN  |
| 4   | D     | 2015 | GLU  |
| 4   | D     | 2018 | VAL  |
| 4   | D     | 2037 | ASP  |
| 4   | D     | 2038 | PRO  |
| 5   | E     | 3147 | SER  |
| 1   | A     | 212  | GLY  |
| 1   | A     | 227  | VAL  |
| 1   | A     | 298  | LYS  |
| 1   | A     | 327  | SER  |
| 1   | A     | 331  | ASP  |
| 1   | A     | 334  | GLY  |
| 2   | B     | 459  | LYS  |
| 2   | B     | 601  | LEU  |
| 2   | B     | 658  | VAL  |
| 2   | B     | 673  | LEU  |
| 2   | B     | 680  | LEU  |
| 2   | B     | 684  | ILE  |
| 2   | B     | 738  | LEU  |
| 2   | B     | 739  | SER  |
| 3   | C     | 1098 | ASN  |
| 4   | D     | 2007 | GLN  |
| 4   | D     | 2019 | GLU  |
| 4   | D     | 2114 | GLY  |
| 4   | D     | 2126 | MET  |
| 5   | E     | 3137 | LYS  |
| 1   | A     | 86   | LEU  |
| 1   | A     | 315  | LYS  |
| 1   | A     | 317  | GLU  |
| 1   | A     | 405  | ASN  |
| 2   | B     | 439  | GLU  |
| 2   | B     | 504  | LEU  |
| 2   | B     | 713  | ALA  |
| 3   | C     | 1021 | ARG  |
| 3   | C     | 1047 | ASN  |
| 3   | C     | 1076 | ASN  |
| 3   | C     | 1078 | ALA  |
| 3   | C     | 1089 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 531  | LEU  |
| 2   | B     | 546  | PRO  |
| 2   | B     | 556  | PRO  |
| 2   | B     | 567  | THR  |
| 2   | B     | 751  | LYS  |
| 3   | C     | 1080 | HIS  |
| 3   | C     | 1105 | LYS  |
| 4   | D     | 2060 | LYS  |
| 1   | A     | 103  | LEU  |
| 1   | A     | 169  | ASP  |
| 1   | A     | 173  | ARG  |
| 2   | B     | 656  | ALA  |
| 3   | C     | 1054 | ILE  |
| 3   | C     | 1069 | THR  |
| 3   | C     | 1099 | ARG  |
| 3   | C     | 1103 | PHE  |
| 4   | D     | 2030 | MET  |
| 4   | D     | 2035 | GLY  |
| 4   | D     | 2039 | VAL  |
| 4   | D     | 2052 | VAL  |
| 5   | E     | 3110 | ASP  |
| 1   | A     | 39   | LYS  |
| 1   | A     | 84   | VAL  |
| 1   | A     | 85   | GLY  |
| 1   | A     | 258  | THR  |
| 3   | C     | 1090 | THR  |
| 3   | C     | 1091 | ARG  |
| 4   | D     | 2113 | LYS  |
| 3   | C     | 1024 | VAL  |
| 3   | C     | 1038 | VAL  |
| 4   | D     | 2132 | PRO  |
| 5   | E     | 3126 | LEU  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |    |
|-----|-------|----------------|-----------|-----------|-------------|----|
| 1   | A     | 321/347 (92%)  | 271 (84%) | 50 (16%)  | 2           | 12 |
| 2   | B     | 338/338 (100%) | 299 (88%) | 39 (12%)  | 5           | 23 |
| 3   | C     | 78/79 (99%)    | 71 (91%)  | 7 (9%)    | 9           | 33 |
| 4   | D     | 105/122 (86%)  | 101 (96%) | 4 (4%)    | 29          | 60 |
| 5   | E     | 37/38 (97%)    | 33 (89%)  | 4 (11%)   | 6           | 25 |
| All | All   | 879/924 (95%)  | 775 (88%) | 104 (12%) | 5           | 21 |

All (104) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 24  | LEU  |
| 1   | A     | 25  | ARG  |
| 1   | A     | 33  | THR  |
| 1   | A     | 37  | MET  |
| 1   | A     | 39  | LYS  |
| 1   | A     | 86  | LEU  |
| 1   | A     | 103 | LEU  |
| 1   | A     | 104 | LEU  |
| 1   | A     | 121 | GLN  |
| 1   | A     | 124 | GLU  |
| 1   | A     | 125 | ASP  |
| 1   | A     | 137 | CYS  |
| 1   | A     | 140 | LEU  |
| 1   | A     | 142 | ARG  |
| 1   | A     | 144 | TRP  |
| 1   | A     | 159 | ILE  |
| 1   | A     | 162 | LEU  |
| 1   | A     | 168 | ARG  |
| 1   | A     | 171 | LEU  |
| 1   | A     | 175 | LEU  |
| 1   | A     | 184 | LEU  |
| 1   | A     | 186 | LEU  |
| 1   | A     | 191 | ARG  |
| 1   | A     | 196 | ILE  |
| 1   | A     | 211 | LEU  |
| 1   | A     | 235 | GLN  |
| 1   | A     | 237 | LEU  |
| 1   | A     | 245 | THR  |
| 1   | A     | 249 | THR  |
| 1   | A     | 250 | GLU  |
| 1   | A     | 252 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 256 | PRO  |
| 1   | A     | 257 | VAL  |
| 1   | A     | 258 | THR  |
| 1   | A     | 259 | GLU  |
| 1   | A     | 281 | GLU  |
| 1   | A     | 284 | GLN  |
| 1   | A     | 294 | VAL  |
| 1   | A     | 300 | LEU  |
| 1   | A     | 302 | ILE  |
| 1   | A     | 311 | LEU  |
| 1   | A     | 321 | ARG  |
| 1   | A     | 328 | ARG  |
| 1   | A     | 339 | LEU  |
| 1   | A     | 349 | LEU  |
| 1   | A     | 352 | ILE  |
| 1   | A     | 355 | CYS  |
| 1   | A     | 363 | PRO  |
| 1   | A     | 368 | GLN  |
| 1   | A     | 371 | LEU  |
| 2   | B     | 413 | GLN  |
| 2   | B     | 422 | LEU  |
| 2   | B     | 437 | PRO  |
| 2   | B     | 451 | VAL  |
| 2   | B     | 456 | ILE  |
| 2   | B     | 476 | HIS  |
| 2   | B     | 477 | GLN  |
| 2   | B     | 488 | MET  |
| 2   | B     | 489 | ILE  |
| 2   | B     | 522 | LYS  |
| 2   | B     | 549 | GLN  |
| 2   | B     | 550 | SER  |
| 2   | B     | 559 | LEU  |
| 2   | B     | 564 | GLN  |
| 2   | B     | 566 | PHE  |
| 2   | B     | 577 | ARG  |
| 2   | B     | 579 | LEU  |
| 2   | B     | 580 | THR  |
| 2   | B     | 591 | VAL  |
| 2   | B     | 600 | THR  |
| 2   | B     | 610 | ILE  |
| 2   | B     | 617 | GLU  |
| 2   | B     | 620 | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 621  | THR  |
| 2   | B     | 634  | ASP  |
| 2   | B     | 636  | LEU  |
| 2   | B     | 658  | VAL  |
| 2   | B     | 668  | LEU  |
| 2   | B     | 670  | LYS  |
| 2   | B     | 671  | LEU  |
| 2   | B     | 676  | LYS  |
| 2   | B     | 684  | ILE  |
| 2   | B     | 688  | MET  |
| 2   | B     | 689  | LYS  |
| 2   | B     | 708  | LYS  |
| 2   | B     | 749  | ILE  |
| 2   | B     | 751  | LYS  |
| 2   | B     | 756  | LEU  |
| 2   | B     | 758  | GLU  |
| 3   | C     | 1019 | LYS  |
| 3   | C     | 1033 | TRP  |
| 3   | C     | 1035 | TRP  |
| 3   | C     | 1037 | ILE  |
| 3   | C     | 1057 | GLN  |
| 3   | C     | 1097 | ASP  |
| 3   | C     | 1100 | GLU  |
| 4   | D     | 2019 | GLU  |
| 4   | D     | 2026 | THR  |
| 4   | D     | 2031 | LEU  |
| 4   | D     | 2039 | VAL  |
| 5   | E     | 3113 | PRO  |
| 5   | E     | 3115 | GLU  |
| 5   | E     | 3126 | LEU  |
| 5   | E     | 3146 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 30  | GLN  |
| 1   | A     | 48  | HIS  |
| 1   | A     | 51  | ASN  |
| 1   | A     | 82  | GLN  |
| 1   | A     | 102 | ASN  |
| 1   | A     | 121 | GLN  |
| 1   | A     | 141 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 214  | ASN  |
| 1   | A     | 235  | GLN  |
| 1   | A     | 276  | GLN  |
| 1   | A     | 284  | GLN  |
| 1   | A     | 293  | GLN  |
| 1   | A     | 316  | ASN  |
| 1   | A     | 324  | ASN  |
| 1   | A     | 346  | ASN  |
| 1   | A     | 368  | GLN  |
| 1   | A     | 378  | ASN  |
| 1   | A     | 386  | ASN  |
| 1   | A     | 387  | ASN  |
| 2   | B     | 448  | GLN  |
| 2   | B     | 463  | GLN  |
| 2   | B     | 476  | HIS  |
| 2   | B     | 477  | GLN  |
| 2   | B     | 509  | GLN  |
| 2   | B     | 574  | HIS  |
| 2   | B     | 602  | GLN  |
| 2   | B     | 607  | GLN  |
| 2   | B     | 615  | ASN  |
| 2   | B     | 630  | GLN  |
| 2   | B     | 657  | ASN  |
| 2   | B     | 677  | ASN  |
| 2   | B     | 692  | GLN  |
| 2   | B     | 696  | GLN  |
| 2   | B     | 728  | GLN  |
| 2   | B     | 737  | GLN  |
| 4   | D     | 2023 | GLN  |
| 4   | D     | 2043 | ASN  |
| 4   | D     | 2059 | HIS  |
| 4   | D     | 2090 | GLN  |
| 4   | D     | 2097 | GLN  |
| 4   | D     | 2125 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.