



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:11 AM UTC

PDB ID : 1R4N / pdb\_00001r4n  
Title : APPBP1-UBA3-NEDD8, an E1-ubiquitin-like protein complex with ATP  
Authors : Walden, H.; Podgorski, M.S.; Holton, J.M.; Schulman, B.A.  
Deposited on : 2003-10-07  
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| 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                                                             |

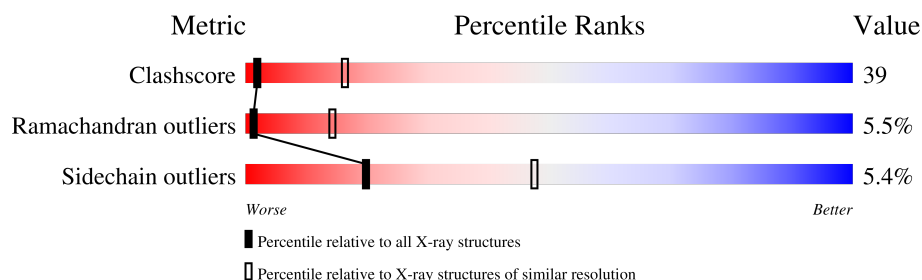
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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                      | 1827 (3.70-3.50)                                      |
| Ramachandran outliers | 187476                      | 1773 (3.70-3.50)                                      |
| Sidechain outliers    | 187428                      | 1772 (3.70-3.50)                                      |

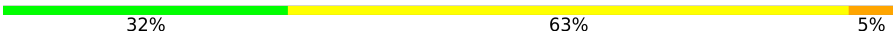
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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     | 529    |                  |
| 1   | C     | 529    |                  |
| 1   | E     | 529    |                  |
| 1   | G     | 529    |                  |
| 2   | B     | 431    |                  |
| 2   | D     | 431    |                  |
| 2   | F     | 431    |                  |
| 2   | H     | 431    |                  |

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| Mol | Chain | Length | Quality of chain                                                                              |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 3   | I     | 76     |  33% 63% 5% |
| 3   | J     | 76     |  33% 62% 5% |
| 3   | K     | 76     |  37% 58% 5% |
| 3   | L     | 76     |  32% 63% 5% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | ATP  | H     | 8   | -         | -        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31744 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 amyloid beta precursor protein-binding protein 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 516      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4105  | 2602 | 699 | 789 | 15 |         |         |       |
| 1   | C     | 516      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4105  | 2602 | 699 | 789 | 15 |         |         |       |
| 1   | E     | 516      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4105  | 2602 | 699 | 789 | 15 |         |         |       |
| 1   | G     | 516      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4105  | 2602 | 699 | 789 | 15 |         |         |       |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | ?       | -        | ASN    | deletion | UNP Q13564 |
| A     | ?       | -        | GLU    | deletion | UNP Q13564 |
| A     | ?       | -        | ASN    | deletion | UNP Q13564 |
| A     | ?       | -        | GLY    | deletion | UNP Q13564 |
| A     | ?       | -        | ALA    | deletion | UNP Q13564 |
| C     | ?       | -        | ASN    | deletion | UNP Q13564 |
| C     | ?       | -        | GLU    | deletion | UNP Q13564 |
| C     | ?       | -        | ASN    | deletion | UNP Q13564 |
| C     | ?       | -        | GLY    | deletion | UNP Q13564 |
| C     | ?       | -        | ALA    | deletion | UNP Q13564 |
| E     | ?       | -        | ASN    | deletion | UNP Q13564 |
| E     | ?       | -        | GLU    | deletion | UNP Q13564 |
| E     | ?       | -        | ASN    | deletion | UNP Q13564 |
| E     | ?       | -        | GLY    | deletion | UNP Q13564 |
| E     | ?       | -        | ALA    | deletion | UNP Q13564 |
| G     | ?       | -        | ASN    | deletion | UNP Q13564 |
| G     | ?       | -        | GLU    | deletion | UNP Q13564 |
| G     | ?       | -        | ASN    | deletion | UNP Q13564 |
| G     | ?       | -        | GLY    | deletion | UNP Q13564 |
| G     | ?       | -        | ALA    | deletion | UNP Q13564 |

- Molecule 2 is a protein called ubiquitin-activating enzyme E1C.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 418      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3199  | 2038 | 549 | 595 | 17 |         |         |       |
| 2   | D     | 418      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3199  | 2038 | 549 | 595 | 17 |         |         |       |
| 2   | F     | 418      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3199  | 2038 | 549 | 595 | 17 |         |         |       |
| 2   | H     | 418      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3199  | 2038 | 549 | 595 | 17 |         |         |       |

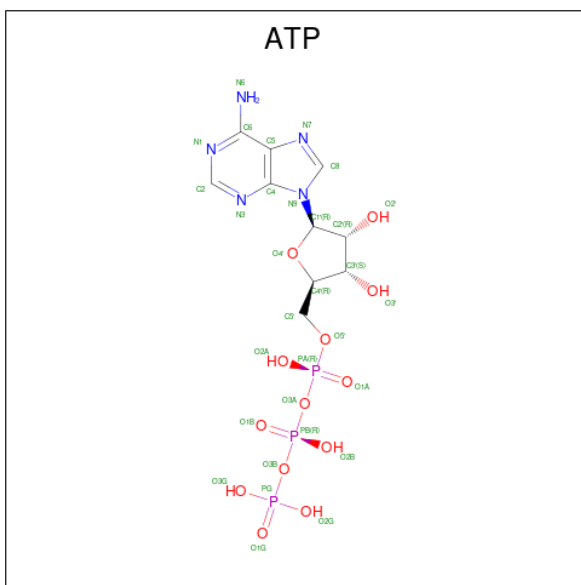
There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | 150     | ALA      | CYS    | engineered mutation | UNP Q8TBC4 |
| D     | 150     | ALA      | CYS    | engineered mutation | UNP Q8TBC4 |
| F     | 150     | ALA      | CYS    | engineered mutation | UNP Q8TBC4 |
| H     | 150     | ALA      | CYS    | engineered mutation | UNP Q8TBC4 |

- Molecule 3 is a protein called Ubiquitin-like protein NEDD8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | I     | 76       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 600   | 378 | 104 | 116 | 2 |         |         |       |
| 3   | J     | 76       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 600   | 378 | 104 | 116 | 2 |         |         |       |
| 3   | K     | 76       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 600   | 378 | 104 | 116 | 2 |         |         |       |
| 3   | L     | 76       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 600   | 378 | 104 | 116 | 2 |         |         |       |

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 4   | B     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       | 0       |
| 4   | D     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       | 0       |
| 4   | F     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       | 0       |
| 4   | H     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       | 0       |

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

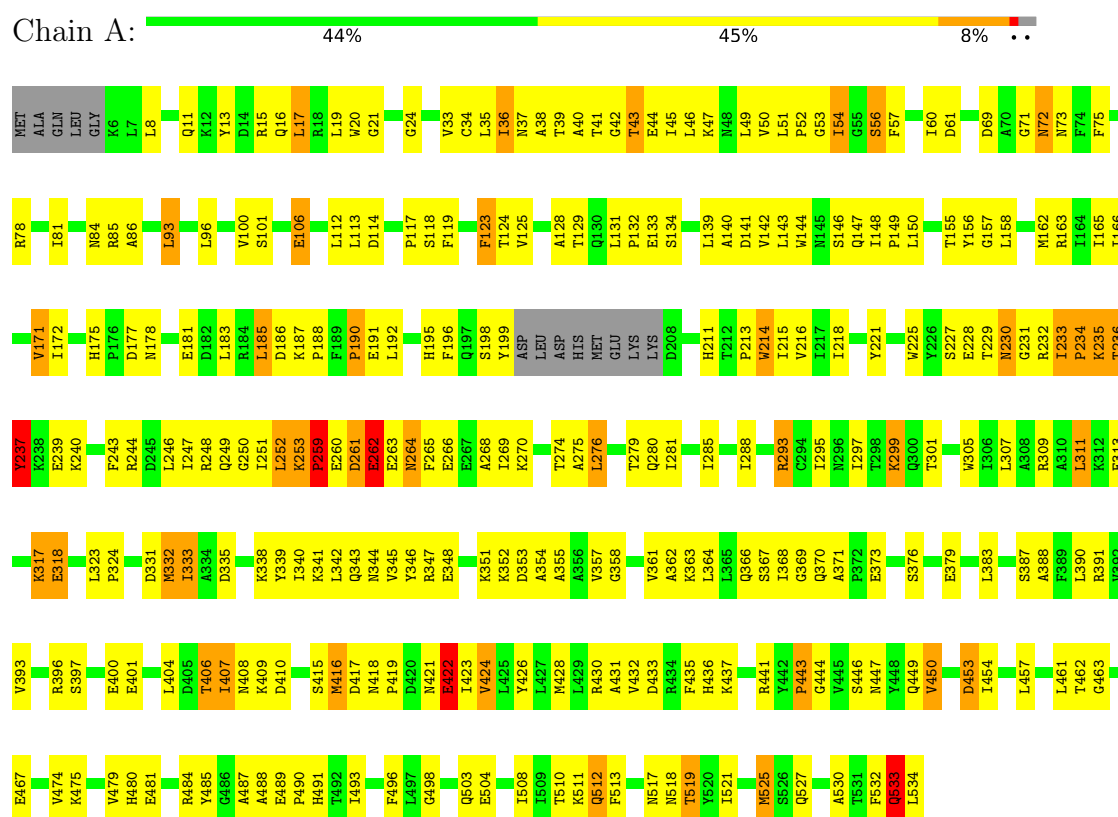
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5   | J     | 1        | Total Zn<br>1 1 | 0       | 0       |
| 5   | F     | 1        | Total Zn<br>1 1 | 0       | 0       |
| 5   | H     | 2        | Total Zn<br>2 2 | 0       | 0       |

### 3 Residue-property plots

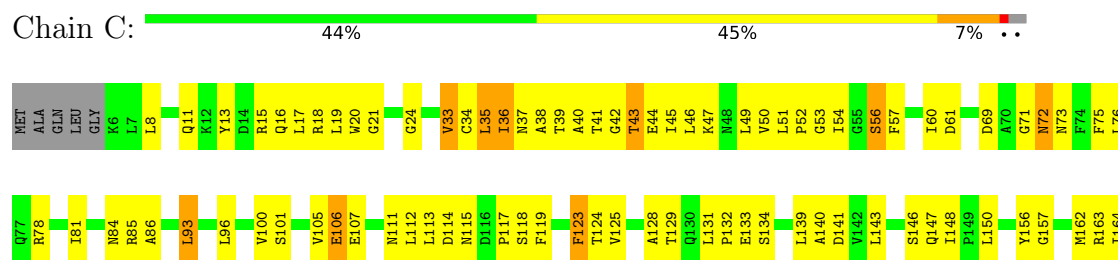
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

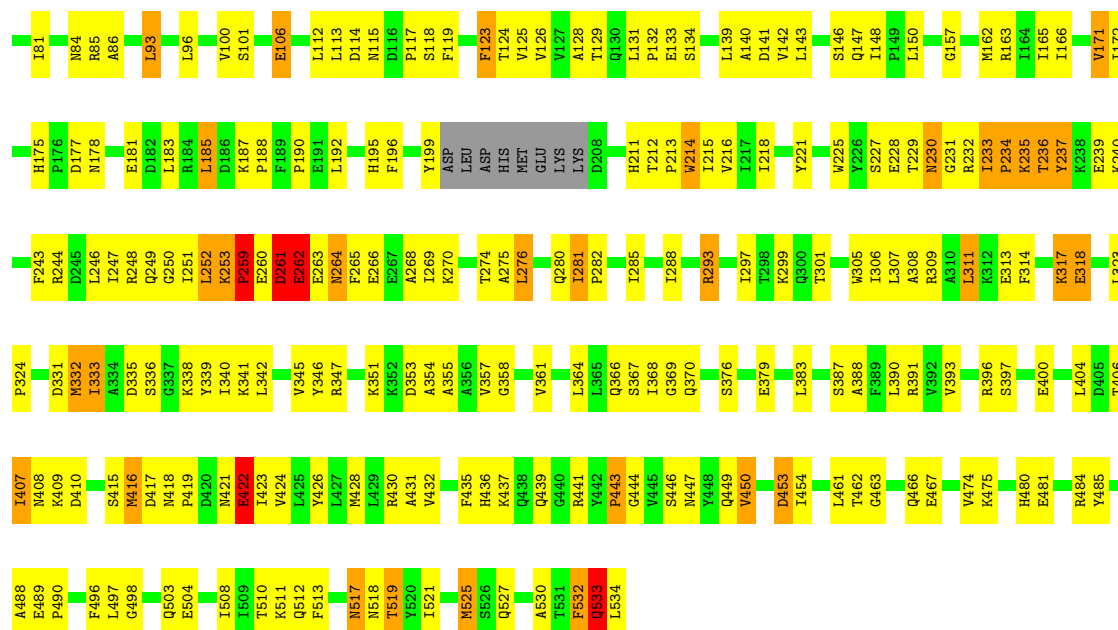
- Molecule 1: amyloid beta precursor protein-binding protein 1



- Molecule 1: amyloid beta precursor protein-binding protein 1

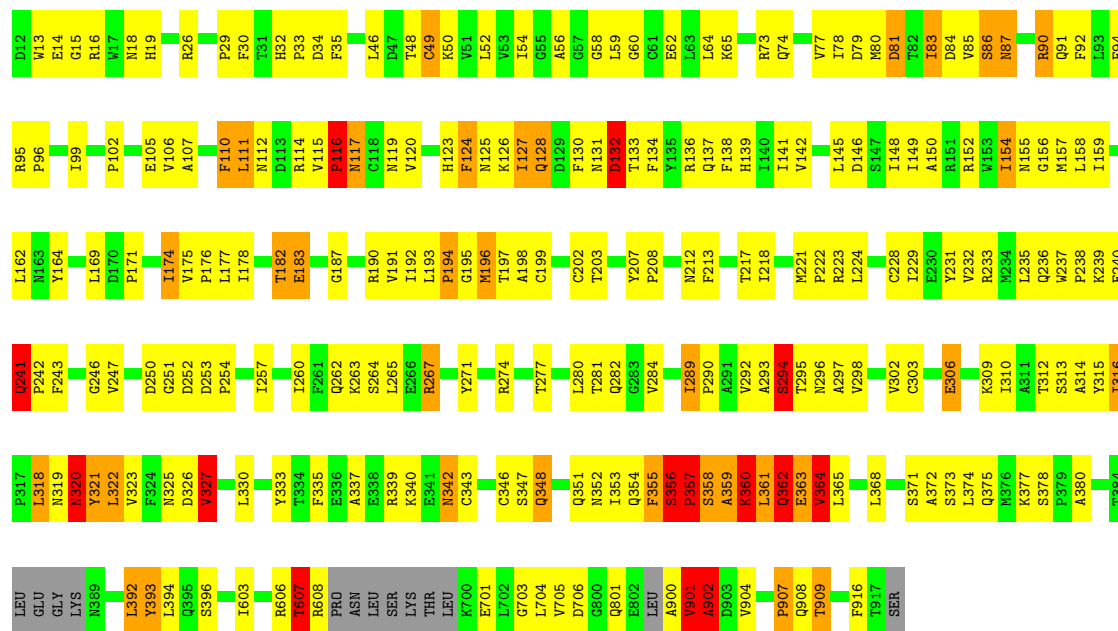






• Molecule 2: ubiquitin-activating enzyme E1C

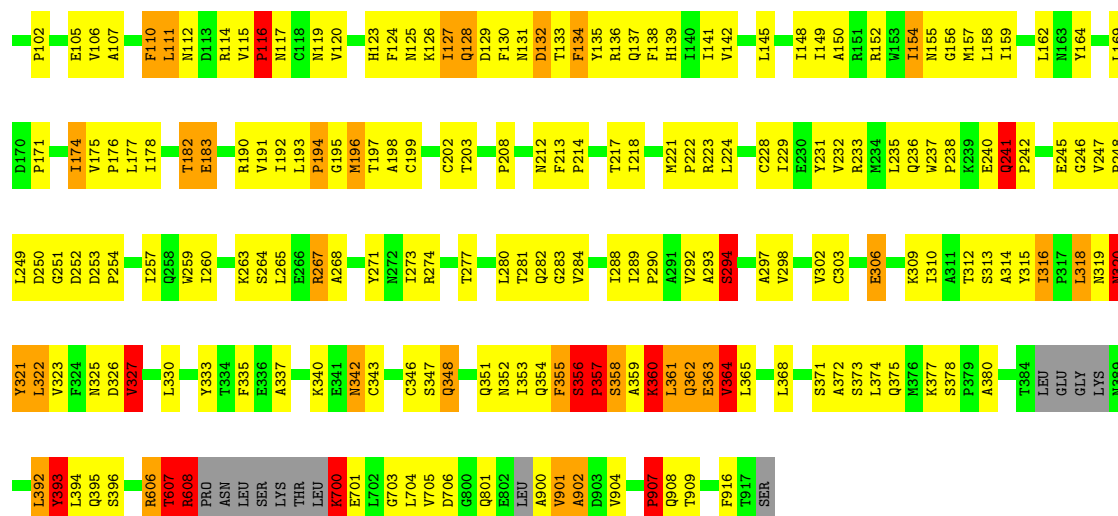
Chain B: 41% 44% 8% . .



• Molecule 2: ubiquitin-activating enzyme E1C

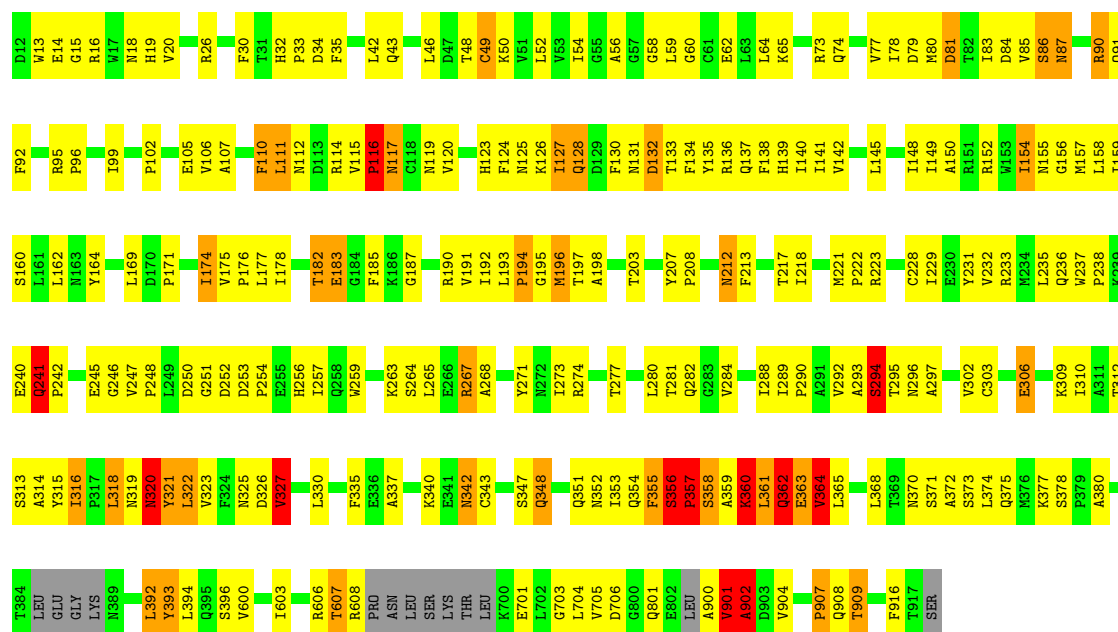
Chain D: 41% 45% 8% . .





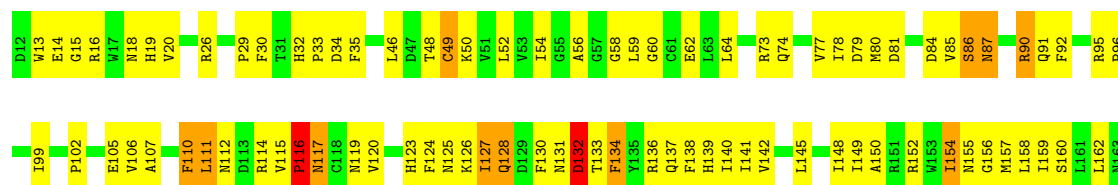
• Molecule 2: ubiquitin-activating enzyme E1C

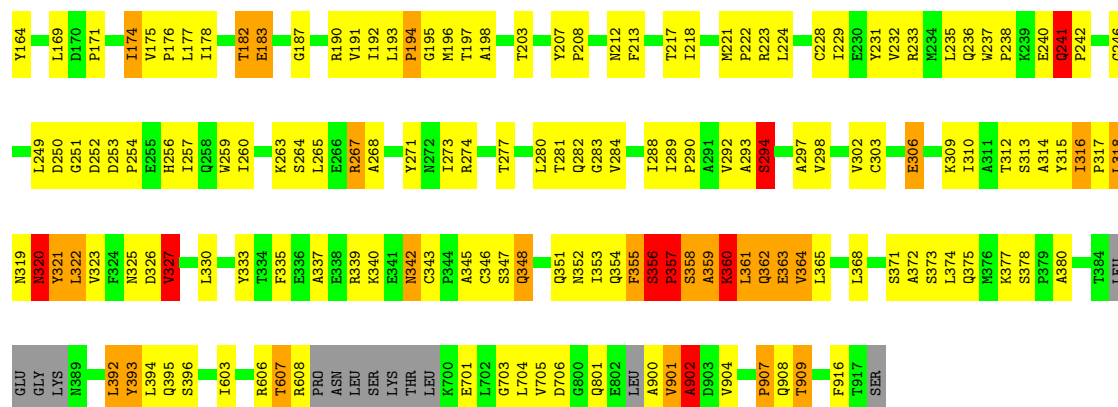
Chain F: 41% 45% 8% . .



• Molecule 2: ubiquitin-activating enzyme E1C

Chain H: 41% 45% 8% . .

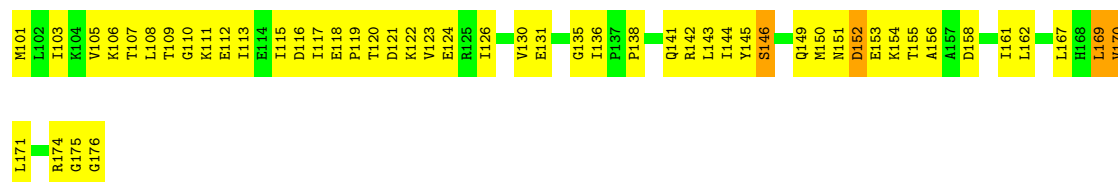




• Molecule 3: Ubiquitin-like protein NEDD8



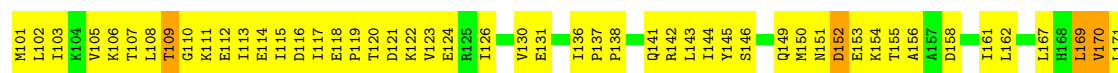
• Molecule 3: Ubiquitin-like protein NEDD8



• Molecule 3: Ubiquitin-like protein NEDD8



• Molecule 3: Ubiquitin-like protein NEDD8



|      |      |      |      |      |
|------|------|------|------|------|
| A172 | L173 | R174 | G175 | G176 |
|------|------|------|------|------|

## 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 21                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 135.00Å 197.90Å 211.00Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 50.00 – 3.60                                    | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (50.00-3.60)                    | Depositor |
| $R_{merge}$                                              | 0.09                                            | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | CNS                                             | Depositor |
| R, $R_{free}$                                            | 0.251 , 0.290                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 31744                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 85.0                                            | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.71         | 5/4185 (0.1%)   | 1.17        | 43/5661 (0.8%)   |
| 1   | C     | 0.71         | 7/4185 (0.2%)   | 1.20        | 46/5661 (0.8%)   |
| 1   | E     | 0.75         | 5/4185 (0.1%)   | 1.17        | 38/5661 (0.7%)   |
| 1   | G     | 0.71         | 8/4185 (0.2%)   | 1.20        | 38/5661 (0.7%)   |
| 2   | B     | 0.68         | 3/3268 (0.1%)   | 1.19        | 33/4447 (0.7%)   |
| 2   | D     | 1.16         | 10/3269 (0.3%)  | 1.23        | 33/4450 (0.7%)   |
| 2   | F     | 0.63         | 3/3268 (0.1%)   | 1.17        | 30/4447 (0.7%)   |
| 2   | H     | 0.62         | 1/3268 (0.0%)   | 1.15        | 28/4447 (0.6%)   |
| 3   | I     | 0.47         | 0/605           | 1.01        | 2/808 (0.2%)     |
| 3   | J     | 0.41         | 0/605           | 1.00        | 3/808 (0.4%)     |
| 3   | K     | 0.44         | 0/605           | 1.00        | 3/808 (0.4%)     |
| 3   | L     | 0.43         | 0/605           | 1.01        | 3/808 (0.4%)     |
| All | All   | 0.74         | 42/32233 (0.1%) | 1.17        | 300/43667 (0.7%) |

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                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | G     | 0                   | 1                   |
| 2   | B     | 0                   | 1                   |
| 2   | D     | 0                   | 2                   |
| 2   | F     | 0                   | 1                   |
| 2   | H     | 0                   | 1                   |
| All | All   | 0                   | 8                   |

All (42) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | D     | 700 | LYS  | N-CA   | 26.02  | 1.79        | 1.46     |
| 2   | D     | 608 | ARG  | CA-C   | 22.40  | 1.82        | 1.52     |
| 2   | D     | 608 | ARG  | N-CA   | 20.93  | 1.73        | 1.46     |
| 2   | D     | 700 | LYS  | CA-C   | 20.63  | 1.80        | 1.52     |
| 1   | E     | 253 | LYS  | CA-C   | 19.82  | 1.77        | 1.53     |
| 2   | D     | 608 | ARG  | C-N    | 19.72  | 1.61        | 1.33     |
| 2   | D     | 700 | LYS  | C-N    | 19.55  | 1.61        | 1.33     |
| 1   | C     | 253 | LYS  | CA-C   | 18.92  | 1.76        | 1.52     |
| 1   | C     | 259 | PRO  | N-CA   | 18.60  | 1.71        | 1.47     |
| 1   | A     | 259 | PRO  | N-CA   | 18.53  | 1.71        | 1.47     |
| 1   | A     | 253 | LYS  | CA-C   | 18.39  | 1.76        | 1.52     |
| 1   | E     | 259 | PRO  | N-CA   | 16.64  | 1.68        | 1.47     |
| 1   | G     | 259 | PRO  | N-CA   | 16.18  | 1.68        | 1.47     |
| 1   | G     | 253 | LYS  | CA-C   | 16.15  | 1.73        | 1.52     |
| 2   | D     | 607 | THR  | C-N    | 15.97  | 1.56        | 1.33     |
| 2   | B     | 392 | LEU  | CG-CD2 | -14.83 | 1.03        | 1.52     |
| 2   | D     | 607 | THR  | CA-C   | 13.20  | 1.70        | 1.52     |
| 1   | C     | 259 | PRO  | C-N    | -8.61  | 1.21        | 1.33     |
| 1   | G     | 259 | PRO  | C-N    | -8.15  | 1.22        | 1.33     |
| 1   | A     | 253 | LYS  | C-N    | 8.06   | 1.52        | 1.33     |
| 1   | A     | 253 | LYS  | CA-CB  | 8.03   | 1.66        | 1.53     |
| 1   | G     | 253 | LYS  | CA-CB  | 8.00   | 1.66        | 1.53     |
| 1   | C     | 253 | LYS  | CA-CB  | 7.83   | 1.65        | 1.53     |
| 1   | E     | 253 | LYS  | C-N    | 7.67   | 1.51        | 1.33     |
| 1   | G     | 252 | LEU  | C-N    | -7.50  | 1.18        | 1.33     |
| 1   | A     | 252 | LEU  | C-N    | -7.38  | 1.18        | 1.33     |
| 1   | E     | 253 | LYS  | CA-CB  | 7.04   | 1.64        | 1.53     |
| 1   | C     | 252 | LEU  | C-N    | -7.03  | 1.19        | 1.33     |
| 2   | F     | 392 | LEU  | CG-CD2 | -6.45  | 1.31        | 1.52     |
| 2   | D     | 392 | LEU  | CG-CD2 | -6.44  | 1.31        | 1.52     |
| 1   | E     | 252 | LEU  | C-N    | -6.15  | 1.23        | 1.33     |
| 2   | H     | 392 | LEU  | CG-CD2 | -6.07  | 1.32        | 1.52     |
| 1   | G     | 253 | LYS  | C-N    | 6.00   | 1.47        | 1.33     |
| 2   | B     | 901 | VAL  | C-N    | 5.88   | 1.42        | 1.33     |
| 2   | F     | 607 | THR  | C-N    | 5.88   | 1.41        | 1.33     |
| 1   | C     | 253 | LYS  | C-N    | 5.61   | 1.47        | 1.33     |
| 2   | D     | 606 | ARG  | C-N    | -5.23  | 1.26        | 1.33     |
| 2   | F     | 901 | VAL  | C-N    | 5.20   | 1.41        | 1.33     |
| 1   | G     | 259 | PRO  | CA-CB  | -5.13  | 1.46        | 1.53     |
| 1   | G     | 236 | THR  | CA-CB  | 5.12   | 1.61        | 1.52     |
| 2   | B     | 289 | ILE  | CA-CB  | -5.09  | 1.49        | 1.54     |
| 1   | C     | 253 | LYS  | N-CA   | -5.08  | 1.39        | 1.46     |

All (300) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | C     | 253 | LYS  | CA-C-N     | 24.74  | 150.77      | 119.84   |
| 1   | C     | 253 | LYS  | C-N-CA     | 24.74  | 150.77      | 119.84   |
| 1   | G     | 253 | LYS  | CA-C-N     | 24.70  | 150.72      | 119.84   |
| 1   | G     | 253 | LYS  | C-N-CA     | 24.70  | 150.72      | 119.84   |
| 1   | A     | 253 | LYS  | CA-C-N     | 22.37  | 147.80      | 119.84   |
| 1   | A     | 253 | LYS  | C-N-CA     | 22.37  | 147.80      | 119.84   |
| 1   | E     | 253 | LYS  | CA-C-N     | 20.15  | 145.03      | 119.84   |
| 1   | E     | 253 | LYS  | C-N-CA     | 20.15  | 145.03      | 119.84   |
| 2   | B     | 392 | LEU  | CB-CG-CD2  | -18.10 | 56.40       | 110.70   |
| 2   | D     | 700 | LYS  | N-CA-C     | 15.21  | 143.21      | 110.80   |
| 1   | C     | 259 | PRO  | CA-N-CD    | -14.68 | 91.45       | 112.00   |
| 2   | D     | 902 | ALA  | N-CA-C     | -14.16 | 91.89       | 110.43   |
| 1   | E     | 253 | LYS  | CB-CA-C    | 13.49  | 129.97      | 109.60   |
| 2   | D     | 608 | ARG  | N-CA-C     | 12.87  | 138.21      | 110.80   |
| 2   | B     | 392 | LEU  | CD1-CG-CD2 | -12.74 | 82.78       | 110.80   |
| 1   | E     | 259 | PRO  | CA-N-CD    | -12.55 | 94.43       | 112.00   |
| 2   | D     | 362 | GLN  | N-CA-C     | -12.31 | 97.96       | 113.23   |
| 2   | B     | 362 | GLN  | N-CA-C     | -12.18 | 98.12       | 113.23   |
| 2   | F     | 362 | GLN  | N-CA-C     | -12.13 | 98.19       | 113.23   |
| 2   | H     | 362 | GLN  | N-CA-C     | -11.50 | 98.97       | 113.23   |
| 1   | A     | 253 | LYS  | CB-CA-C    | 11.47  | 132.77      | 110.17   |
| 2   | H     | 356 | SER  | CA-C-N     | 11.06  | 133.66      | 119.84   |
| 2   | H     | 356 | SER  | C-N-CA     | 11.06  | 133.66      | 119.84   |
| 1   | G     | 259 | PRO  | CA-N-CD    | -10.60 | 97.17       | 112.00   |
| 2   | F     | 356 | SER  | CA-C-N     | 10.47  | 132.93      | 119.84   |
| 2   | F     | 356 | SER  | C-N-CA     | 10.47  | 132.93      | 119.84   |
| 2   | D     | 356 | SER  | CA-C-N     | 10.46  | 132.91      | 119.84   |
| 2   | D     | 356 | SER  | C-N-CA     | 10.46  | 132.91      | 119.84   |
| 2   | F     | 607 | THR  | CA-C-N     | 10.22  | 140.10      | 121.70   |
| 2   | F     | 607 | THR  | C-N-CA     | 10.22  | 140.10      | 121.70   |
| 2   | B     | 356 | SER  | CA-C-N     | 10.18  | 132.56      | 119.84   |
| 2   | B     | 356 | SER  | C-N-CA     | 10.18  | 132.56      | 119.84   |
| 1   | A     | 259 | PRO  | CA-N-CD    | -10.13 | 97.82       | 112.00   |
| 1   | C     | 259 | PRO  | CA-CB-CG   | -9.86  | 85.76       | 104.50   |
| 1   | E     | 259 | PRO  | CA-CB-CG   | -9.50  | 86.45       | 104.50   |
| 1   | G     | 259 | PRO  | CA-CB-CG   | -9.43  | 86.59       | 104.50   |
| 1   | A     | 235 | LYS  | N-CA-C     | -9.39  | 98.13       | 110.53   |
| 1   | G     | 259 | PRO  | N-CA-C     | 9.31   | 131.65      | 112.47   |
| 1   | E     | 235 | LYS  | N-CA-C     | -9.24  | 98.33       | 110.53   |
| 1   | C     | 259 | PRO  | N-CA-C     | 9.01   | 131.03      | 112.47   |
| 2   | D     | 606 | ARG  | CA-C-N     | -8.85  | 104.63      | 121.54   |
| 2   | D     | 606 | ARG  | C-N-CA     | -8.85  | 104.63      | 121.54   |
| 1   | C     | 235 | LYS  | N-CA-C     | -8.79  | 98.93       | 110.53   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | G     | 252 | LEU  | CA-C-N    | -8.52 | 101.00      | 121.80   |
| 1   | G     | 252 | LEU  | C-N-CA    | -8.52 | 101.00      | 121.80   |
| 2   | B     | 392 | LEU  | CB-CG-CD1 | 8.50  | 136.20      | 110.70   |
| 1   | A     | 259 | PRO  | CA-CB-CG  | -8.43 | 88.49       | 104.50   |
| 1   | C     | 253 | LYS  | CB-CA-C   | 8.31  | 126.54      | 110.17   |
| 1   | E     | 252 | LEU  | CA-C-N    | -8.25 | 106.68      | 121.69   |
| 1   | E     | 252 | LEU  | C-N-CA    | -8.25 | 106.68      | 121.69   |
| 2   | F     | 902 | ALA  | N-CA-C    | -8.19 | 93.35       | 110.80   |
| 1   | G     | 253 | LYS  | CB-CA-C   | 8.14  | 126.22      | 110.17   |
| 1   | C     | 252 | LEU  | CA-C-N    | -8.11 | 102.02      | 121.80   |
| 1   | C     | 252 | LEU  | C-N-CA    | -8.11 | 102.02      | 121.80   |
| 1   | E     | 532 | PHE  | N-CA-C    | 8.09  | 123.61      | 108.65   |
| 1   | G     | 236 | THR  | N-CA-C    | 8.00  | 123.93      | 107.37   |
| 1   | G     | 235 | LYS  | N-CA-C    | -7.89 | 100.11      | 110.53   |
| 1   | A     | 263 | GLU  | N-CA-C    | -7.83 | 102.06      | 111.69   |
| 1   | A     | 259 | PRO  | N-CA-C    | 7.82  | 128.57      | 112.47   |
| 1   | G     | 263 | GLU  | N-CA-C    | -7.80 | 102.10      | 111.69   |
| 1   | C     | 263 | GLU  | N-CA-C    | -7.35 | 102.66      | 111.69   |
| 2   | B     | 354 | GLN  | CA-C-N    | -7.27 | 113.04      | 122.79   |
| 2   | B     | 354 | GLN  | C-N-CA    | -7.27 | 113.04      | 122.79   |
| 1   | E     | 263 | GLU  | N-CA-C    | -7.22 | 102.81      | 111.69   |
| 1   | A     | 301 | THR  | CA-C-N    | 7.17  | 127.13      | 120.03   |
| 1   | A     | 301 | THR  | C-N-CA    | 7.17  | 127.13      | 120.03   |
| 1   | G     | 235 | LYS  | CA-C-N    | -7.10 | 111.19      | 122.76   |
| 1   | G     | 235 | LYS  | C-N-CA    | -7.10 | 111.19      | 122.76   |
| 2   | D     | 354 | GLN  | CA-C-N    | -7.10 | 112.20      | 122.06   |
| 2   | D     | 354 | GLN  | C-N-CA    | -7.10 | 112.20      | 122.06   |
| 2   | H     | 360 | LYS  | N-CA-C    | 7.05  | 125.82      | 110.80   |
| 1   | A     | 236 | THR  | N-CA-C    | 7.03  | 121.92      | 107.37   |
| 1   | G     | 301 | THR  | CA-C-N    | 7.02  | 126.98      | 120.03   |
| 1   | G     | 301 | THR  | C-N-CA    | 7.02  | 126.98      | 120.03   |
| 2   | F     | 354 | GLN  | CA-C-N    | -7.01 | 113.39      | 122.79   |
| 2   | F     | 354 | GLN  | C-N-CA    | -7.01 | 113.39      | 122.79   |
| 2   | H     | 354 | GLN  | CA-C-N    | -7.00 | 113.41      | 122.79   |
| 2   | H     | 354 | GLN  | C-N-CA    | -7.00 | 113.41      | 122.79   |
| 2   | H     | 87  | ASN  | N-CA-C    | -6.95 | 105.08      | 113.97   |
| 2   | D     | 608 | ARG  | CA-C-N    | 6.89  | 134.70      | 121.54   |
| 2   | D     | 608 | ARG  | C-N-CA    | 6.89  | 134.70      | 121.54   |
| 2   | F     | 138 | PHE  | N-CA-C    | 6.89  | 120.68      | 110.48   |
| 2   | F     | 49  | CYS  | N-CA-C    | 6.85  | 119.01      | 109.15   |
| 2   | H     | 907 | PRO  | N-CA-CB   | 6.82  | 110.41      | 103.25   |
| 2   | D     | 360 | LYS  | N-CA-C    | 6.79  | 125.27      | 110.80   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | H     | 607 | THR  | CA-C-N  | 6.79  | 133.92      | 121.70   |
| 2   | H     | 607 | THR  | C-N-CA  | 6.79  | 133.92      | 121.70   |
| 1   | C     | 301 | THR  | CA-C-N  | 6.79  | 126.75      | 120.03   |
| 1   | C     | 301 | THR  | C-N-CA  | 6.79  | 126.75      | 120.03   |
| 2   | H     | 902 | ALA  | N-CA-C  | -6.78 | 96.36       | 110.80   |
| 2   | F     | 360 | LYS  | N-CA-C  | 6.76  | 125.19      | 110.80   |
| 2   | B     | 360 | LYS  | N-CA-C  | 6.75  | 125.19      | 110.80   |
| 2   | D     | 49  | CYS  | N-CA-C  | 6.74  | 118.86      | 109.15   |
| 1   | A     | 533 | GLN  | N-CA-C  | 6.68  | 125.03      | 110.80   |
| 2   | F     | 907 | PRO  | N-CA-CB | 6.66  | 110.25      | 103.25   |
| 1   | E     | 259 | PRO  | CA-C-N  | -6.65 | 108.83      | 121.54   |
| 1   | E     | 259 | PRO  | C-N-CA  | -6.65 | 108.83      | 121.54   |
| 2   | D     | 907 | PRO  | N-CA-CB | 6.65  | 110.23      | 103.25   |
| 2   | B     | 902 | ALA  | N-CA-C  | -6.64 | 96.65       | 110.80   |
| 2   | H     | 49  | CYS  | N-CA-C  | 6.64  | 119.25      | 108.63   |
| 2   | D     | 87  | ASN  | N-CA-C  | -6.63 | 105.72      | 113.88   |
| 2   | D     | 327 | VAL  | N-CA-C  | 6.63  | 117.32      | 110.36   |
| 1   | E     | 533 | GLN  | N-CA-C  | 6.62  | 124.91      | 110.80   |
| 1   | E     | 259 | PRO  | N-CA-C  | 6.61  | 126.09      | 112.47   |
| 2   | H     | 327 | VAL  | N-CA-C  | 6.60  | 117.29      | 110.36   |
| 1   | A     | 281 | ILE  | CA-C-N  | 6.54  | 126.89      | 119.83   |
| 1   | A     | 281 | ILE  | C-N-CA  | 6.54  | 126.89      | 119.83   |
| 2   | F     | 364 | VAL  | N-CA-C  | -6.51 | 107.15      | 113.53   |
| 1   | A     | 252 | LEU  | CA-C-N  | -6.48 | 106.00      | 121.80   |
| 1   | A     | 252 | LEU  | C-N-CA  | -6.48 | 106.00      | 121.80   |
| 1   | G     | 533 | GLN  | N-CA-C  | 6.46  | 124.57      | 110.80   |
| 2   | B     | 907 | PRO  | N-CA-CB | 6.46  | 110.03      | 103.25   |
| 1   | E     | 236 | THR  | N-CA-C  | 6.46  | 120.73      | 107.37   |
| 2   | B     | 327 | VAL  | N-CA-C  | 6.42  | 117.11      | 110.36   |
| 2   | B     | 364 | VAL  | N-CA-C  | -6.42 | 107.24      | 113.53   |
| 1   | C     | 235 | LYS  | CA-C-N  | -6.41 | 112.32      | 122.76   |
| 1   | C     | 235 | LYS  | C-N-CA  | -6.41 | 112.32      | 122.76   |
| 2   | H     | 14  | GLU  | N-CA-C  | 6.40  | 119.50      | 109.96   |
| 1   | C     | 236 | THR  | N-CA-C  | 6.36  | 120.54      | 107.37   |
| 1   | E     | 235 | LYS  | CA-C-N  | -6.34 | 112.42      | 122.76   |
| 1   | E     | 235 | LYS  | C-N-CA  | -6.34 | 112.42      | 122.76   |
| 1   | E     | 301 | THR  | CA-C-N  | 6.34  | 126.31      | 120.03   |
| 1   | E     | 301 | THR  | C-N-CA  | 6.34  | 126.31      | 120.03   |
| 1   | C     | 253 | LYS  | CA-C-O  | -6.29 | 111.54      | 120.16   |
| 2   | F     | 14  | GLU  | N-CA-C  | 6.26  | 119.29      | 109.96   |
| 2   | F     | 87  | ASN  | N-CA-C  | -6.26 | 105.95      | 113.97   |
| 1   | A     | 235 | LYS  | CA-C-N  | -6.25 | 112.57      | 122.76   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 235 | LYS  | C-N-CA   | -6.25 | 112.57      | 122.76   |
| 2   | H     | 138 | PHE  | N-CA-C   | 6.25  | 119.73      | 110.48   |
| 2   | B     | 49  | CYS  | N-CA-C   | 6.25  | 118.63      | 108.63   |
| 1   | C     | 281 | ILE  | CA-C-N   | 6.25  | 126.58      | 119.83   |
| 1   | C     | 281 | ILE  | C-N-CA   | 6.25  | 126.58      | 119.83   |
| 2   | D     | 361 | LEU  | N-CA-C   | 6.25  | 120.94      | 112.88   |
| 1   | G     | 511 | LYS  | N-CA-C   | -6.24 | 103.05      | 111.54   |
| 2   | D     | 14  | GLU  | N-CA-C   | 6.24  | 119.26      | 109.96   |
| 1   | C     | 453 | ASP  | N-CA-C   | 6.23  | 118.07      | 111.28   |
| 2   | B     | 392 | LEU  | CA-CB-CG | 6.20  | 138.01      | 116.30   |
| 2   | F     | 327 | VAL  | N-CA-C   | 6.18  | 116.85      | 110.36   |
| 2   | H     | 361 | LEU  | N-CA-C   | 6.17  | 120.84      | 112.88   |
| 1   | C     | 165 | ILE  | N-CA-C   | 6.17  | 115.73      | 106.42   |
| 1   | G     | 165 | ILE  | N-CA-C   | 6.17  | 115.73      | 106.42   |
| 1   | A     | 453 | ASP  | N-CA-C   | 6.16  | 118.00      | 111.28   |
| 1   | A     | 511 | LYS  | N-CA-C   | -6.16 | 103.17      | 111.54   |
| 2   | B     | 14  | GLU  | N-CA-C   | 6.15  | 119.12      | 109.96   |
| 1   | C     | 511 | LYS  | N-CA-C   | -6.11 | 103.23      | 111.54   |
| 2   | B     | 115 | VAL  | CA-C-N   | 6.09  | 127.45      | 119.84   |
| 2   | B     | 115 | VAL  | C-N-CA   | 6.09  | 127.45      | 119.84   |
| 2   | B     | 138 | PHE  | N-CA-C   | 6.05  | 119.43      | 110.48   |
| 3   | L     | 169 | LEU  | N-CA-C   | -6.03 | 100.67      | 110.20   |
| 1   | A     | 259 | PRO  | N-CA-CB  | -6.03 | 96.92       | 103.25   |
| 2   | B     | 361 | LEU  | N-CA-C   | 6.02  | 120.65      | 112.88   |
| 1   | A     | 165 | ILE  | N-CA-C   | 6.02  | 115.51      | 106.42   |
| 1   | E     | 511 | LYS  | N-CA-C   | -6.02 | 103.35      | 111.54   |
| 1   | A     | 253 | LYS  | N-CA-CB  | -6.01 | 99.67       | 110.37   |
| 1   | C     | 533 | GLN  | N-CA-C   | 5.99  | 123.56      | 110.80   |
| 1   | G     | 93  | LEU  | N-CA-C   | -5.99 | 104.75      | 111.28   |
| 1   | E     | 519 | THR  | N-CA-C   | 5.99  | 123.55      | 110.80   |
| 1   | C     | 253 | LYS  | C-N-CD   | -5.98 | 100.49      | 125.00   |
| 1   | A     | 24  | GLY  | N-CA-C   | -5.98 | 105.56      | 112.50   |
| 2   | B     | 87  | ASN  | N-CA-C   | -5.98 | 106.32      | 113.97   |
| 1   | C     | 253 | LYS  | O-C-N    | -5.96 | 114.47      | 121.32   |
| 1   | G     | 185 | LEU  | N-CA-C   | -5.96 | 105.10      | 112.90   |
| 2   | H     | 115 | VAL  | CA-C-N   | 5.95  | 127.28      | 119.84   |
| 2   | H     | 115 | VAL  | C-N-CA   | 5.95  | 127.28      | 119.84   |
| 2   | D     | 607 | THR  | O-C-N    | -5.94 | 114.69      | 122.59   |
| 1   | C     | 253 | LYS  | N-CA-CB  | -5.93 | 99.81       | 110.37   |
| 1   | G     | 517 | ASN  | N-CA-C   | 5.93  | 118.19      | 108.52   |
| 2   | F     | 361 | LEU  | N-CA-C   | 5.93  | 120.53      | 112.88   |
| 2   | H     | 48  | THR  | N-CA-C   | 5.92  | 120.65      | 112.90   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | H     | 117 | ASN  | N-CA-C | 5.91  | 119.24      | 112.57   |
| 1   | G     | 519 | THR  | N-CA-C | 5.90  | 123.37      | 110.80   |
| 1   | G     | 453 | ASP  | N-CA-C | 5.90  | 117.71      | 111.28   |
| 2   | D     | 364 | VAL  | N-CA-C | -5.90 | 107.75      | 113.53   |
| 1   | C     | 24  | GLY  | N-CA-C | -5.89 | 105.66      | 112.50   |
| 2   | D     | 92  | PHE  | N-CA-C | 5.87  | 119.97      | 112.34   |
| 2   | D     | 138 | PHE  | N-CA-C | 5.87  | 119.17      | 110.48   |
| 3   | I     | 174 | ARG  | N-CA-C | 5.87  | 118.56      | 111.40   |
| 2   | H     | 92  | PHE  | N-CA-C | 5.86  | 119.96      | 112.34   |
| 2   | F     | 48  | THR  | N-CA-C | 5.85  | 120.57      | 112.90   |
| 3   | K     | 169 | LEU  | N-CA-C | -5.85 | 100.96      | 110.20   |
| 1   | C     | 93  | LEU  | N-CA-C | -5.83 | 104.93      | 111.28   |
| 1   | C     | 519 | THR  | N-CA-C | 5.83  | 123.22      | 110.80   |
| 1   | C     | 461 | LEU  | N-CA-C | -5.81 | 104.85      | 111.07   |
| 2   | B     | 241 | GLN  | CA-C-N | 5.79  | 127.08      | 119.84   |
| 2   | B     | 241 | GLN  | C-N-CA | 5.79  | 127.08      | 119.84   |
| 3   | J     | 169 | LEU  | N-CA-C | -5.79 | 101.06      | 110.20   |
| 1   | A     | 532 | PHE  | N-CA-C | 5.78  | 123.10      | 110.80   |
| 2   | F     | 92  | PHE  | N-CA-C | 5.78  | 119.85      | 112.34   |
| 2   | F     | 241 | GLN  | CA-C-N | 5.78  | 127.06      | 119.84   |
| 2   | F     | 241 | GLN  | C-N-CA | 5.78  | 127.06      | 119.84   |
| 3   | I     | 169 | LEU  | N-CA-C | -5.77 | 101.09      | 110.20   |
| 1   | E     | 185 | LEU  | N-CA-C | -5.70 | 105.43      | 112.90   |
| 1   | A     | 259 | PRO  | CA-C-N | -5.68 | 110.69      | 121.54   |
| 1   | A     | 259 | PRO  | C-N-CA | -5.68 | 110.69      | 121.54   |
| 2   | D     | 48  | THR  | N-CA-C | 5.68  | 120.34      | 112.90   |
| 1   | G     | 532 | PHE  | N-CA-C | 5.68  | 122.90      | 110.80   |
| 2   | B     | 48  | THR  | N-CA-C | 5.68  | 120.34      | 112.90   |
| 1   | E     | 453 | ASP  | N-CA-C | 5.67  | 117.46      | 111.28   |
| 2   | H     | 241 | GLN  | CA-C-N | 5.67  | 126.92      | 119.84   |
| 2   | H     | 241 | GLN  | C-N-CA | 5.67  | 126.92      | 119.84   |
| 2   | D     | 241 | GLN  | CA-C-N | 5.66  | 126.91      | 119.84   |
| 2   | D     | 241 | GLN  | C-N-CA | 5.66  | 126.91      | 119.84   |
| 1   | A     | 461 | LEU  | N-CA-C | -5.66 | 105.02      | 111.07   |
| 2   | H     | 359 | ALA  | N-CA-C | -5.64 | 101.50      | 109.96   |
| 2   | F     | 115 | VAL  | CA-C-N | 5.64  | 126.89      | 119.84   |
| 2   | F     | 115 | VAL  | C-N-CA | 5.64  | 126.89      | 119.84   |
| 3   | L     | 174 | ARG  | N-CA-C | 5.63  | 118.27      | 111.40   |
| 1   | A     | 519 | THR  | N-CA-C | 5.62  | 122.78      | 110.80   |
| 1   | A     | 123 | PHE  | N-CA-C | 5.62  | 118.84      | 110.52   |
| 1   | A     | 521 | ILE  | N-CA-C | 5.61  | 116.07      | 107.77   |
| 1   | G     | 123 | PHE  | N-CA-C | 5.61  | 119.23      | 110.32   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | L     | 109 | THR  | N-CA-C  | -5.57 | 104.12      | 112.54   |
| 1   | C     | 259 | PRO  | CA-C-N  | -5.56 | 110.93      | 121.54   |
| 1   | C     | 259 | PRO  | C-N-CA  | -5.56 | 110.93      | 121.54   |
| 1   | A     | 93  | LEU  | N-CA-C  | -5.54 | 105.24      | 111.28   |
| 2   | D     | 115 | VAL  | CA-C-N  | 5.53  | 126.76      | 119.84   |
| 2   | D     | 115 | VAL  | C-N-CA  | 5.53  | 126.76      | 119.84   |
| 1   | A     | 185 | LEU  | N-CA-C  | -5.53 | 105.66      | 112.90   |
| 1   | E     | 93  | LEU  | N-CA-C  | -5.53 | 105.25      | 111.28   |
| 2   | D     | 700 | LYS  | N-CA-CB | -5.52 | 101.16      | 110.49   |
| 1   | A     | 424 | VAL  | N-CA-C  | -5.51 | 104.49      | 110.23   |
| 1   | G     | 281 | ILE  | CA-C-N  | 5.51  | 125.78      | 119.83   |
| 1   | G     | 281 | ILE  | C-N-CA  | 5.51  | 125.78      | 119.83   |
| 2   | B     | 320 | ASN  | N-CA-C  | 5.50  | 122.53      | 110.80   |
| 1   | A     | 187 | LYS  | CA-C-N  | 5.49  | 125.49      | 119.89   |
| 1   | A     | 187 | LYS  | C-N-CA  | 5.49  | 125.49      | 119.89   |
| 2   | F     | 81  | ASP  | N-CA-C  | 5.49  | 118.55      | 110.59   |
| 1   | G     | 253 | LYS  | O-C-N   | -5.46 | 115.04      | 121.32   |
| 2   | B     | 83  | ILE  | N-CA-C  | 5.44  | 116.43      | 109.30   |
| 1   | A     | 410 | ASP  | N-CA-C  | -5.43 | 105.28      | 111.14   |
| 2   | B     | 909 | THR  | N-CA-C  | -5.43 | 104.60      | 111.11   |
| 1   | C     | 123 | PHE  | N-CA-C  | 5.42  | 118.55      | 110.52   |
| 1   | C     | 521 | ILE  | N-CA-C  | 5.42  | 115.80      | 107.77   |
| 1   | A     | 252 | LEU  | N-CA-C  | 5.42  | 122.35      | 110.80   |
| 3   | K     | 109 | THR  | N-CA-C  | -5.42 | 104.36      | 112.54   |
| 2   | B     | 92  | PHE  | N-CA-C  | 5.40  | 119.36      | 112.34   |
| 1   | C     | 424 | VAL  | N-CA-C  | -5.39 | 104.62      | 110.23   |
| 1   | C     | 185 | LEU  | N-CA-C  | -5.39 | 105.84      | 112.90   |
| 2   | F     | 83  | ILE  | N-CA-C  | 5.39  | 116.36      | 109.30   |
| 2   | F     | 320 | ASN  | N-CA-C  | 5.39  | 122.28      | 110.80   |
| 2   | D     | 320 | ASN  | N-CA-C  | 5.38  | 122.26      | 110.80   |
| 1   | G     | 521 | ILE  | N-CA-C  | 5.38  | 115.73      | 107.77   |
| 2   | H     | 320 | ASN  | N-CA-C  | 5.38  | 122.25      | 110.80   |
| 1   | C     | 517 | ASN  | N-CA-C  | 5.37  | 117.28      | 108.52   |
| 1   | E     | 461 | LEU  | N-CA-C  | -5.37 | 105.32      | 111.07   |
| 1   | G     | 252 | LEU  | N-CA-C  | 5.37  | 122.24      | 110.80   |
| 1   | E     | 252 | LEU  | N-CA-C  | 5.36  | 122.22      | 110.80   |
| 2   | D     | 83  | ILE  | N-CA-C  | 5.35  | 116.31      | 109.30   |
| 3   | K     | 174 | ARG  | N-CA-C  | 5.35  | 117.93      | 111.40   |
| 1   | G     | 261 | ASP  | N-CA-C  | -5.35 | 99.41       | 110.80   |
| 1   | G     | 253 | LYS  | N-CA-CB | -5.34 | 100.87      | 110.37   |
| 1   | A     | 17  | LEU  | N-CA-C  | -5.33 | 106.28      | 112.89   |
| 1   | C     | 532 | PHE  | N-CA-C  | 5.32  | 122.14      | 110.80   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | H     | 607 | THR  | N-CA-C | -5.31 | 99.49       | 110.80   |
| 2   | D     | 134 | PHE  | N-CA-C | 5.30  | 116.74      | 111.07   |
| 1   | G     | 187 | LYS  | CA-C-N | 5.27  | 125.26      | 119.89   |
| 1   | G     | 187 | LYS  | C-N-CA | 5.27  | 125.26      | 119.89   |
| 1   | E     | 187 | LYS  | CA-C-N | 5.25  | 125.24      | 119.89   |
| 1   | E     | 187 | LYS  | C-N-CA | 5.25  | 125.24      | 119.89   |
| 1   | E     | 517 | ASN  | N-CA-C | 5.24  | 117.06      | 108.52   |
| 2   | F     | 607 | THR  | O-C-N  | 5.24  | 129.55      | 122.59   |
| 1   | E     | 123 | PHE  | N-CA-C | 5.23  | 118.26      | 110.52   |
| 3   | J     | 174 | ARG  | N-CA-C | 5.22  | 117.77      | 111.40   |
| 1   | E     | 521 | ILE  | N-CA-C | 5.20  | 115.47      | 107.77   |
| 1   | C     | 261 | ASP  | N-CA-C | -5.19 | 99.74       | 110.80   |
| 2   | F     | 117 | ASN  | N-CA-C | 5.19  | 118.44      | 112.57   |
| 2   | F     | 909 | THR  | N-CA-C | -5.19 | 104.88      | 111.11   |
| 1   | A     | 295 | ILE  | N-CA-C | 5.19  | 115.85      | 110.82   |
| 1   | C     | 410 | ASP  | N-CA-C | -5.18 | 105.54      | 111.14   |
| 1   | E     | 261 | ASP  | N-CA-C | -5.17 | 99.79       | 110.80   |
| 1   | G     | 461 | LEU  | N-CA-C | -5.17 | 105.54      | 111.07   |
| 1   | C     | 252 | LEU  | N-CA-C | 5.17  | 121.80      | 110.80   |
| 3   | J     | 175 | GLY  | N-CA-C | 5.16  | 119.17      | 112.25   |
| 2   | D     | 81  | ASP  | N-CA-C | 5.16  | 118.06      | 110.59   |
| 2   | B     | 607 | THR  | CA-C-N | 5.15  | 130.97      | 121.70   |
| 2   | B     | 607 | THR  | C-N-CA | 5.15  | 130.97      | 121.70   |
| 1   | C     | 33  | VAL  | N-CA-C | 5.13  | 116.67      | 108.87   |
| 1   | A     | 299 | LYS  | N-CA-C | -5.12 | 106.13      | 112.38   |
| 2   | B     | 81  | ASP  | N-CA-C | 5.12  | 118.01      | 110.59   |
| 1   | E     | 410 | ASP  | N-CA-C | -5.12 | 105.61      | 111.14   |
| 1   | A     | 512 | GLN  | N-CA-C | 5.11  | 120.36      | 113.72   |
| 2   | H     | 909 | THR  | N-CA-C | -5.10 | 104.80      | 111.02   |
| 2   | B     | 117 | ASN  | N-CA-C | 5.09  | 118.33      | 112.57   |
| 1   | E     | 253 | LYS  | CA-C-O | -5.07 | 115.18      | 119.59   |
| 1   | G     | 253 | LYS  | C-N-CD | -5.06 | 104.26      | 125.00   |
| 1   | C     | 115 | ASN  | N-CA-C | 5.05  | 119.07      | 113.01   |
| 1   | G     | 115 | ASN  | N-CA-C | 5.05  | 119.07      | 113.01   |
| 2   | F     | 356 | SER  | N-CA-C | 5.04  | 120.95      | 109.81   |
| 2   | H     | 134 | PHE  | N-CA-C | 5.04  | 116.46      | 111.07   |
| 1   | E     | 288 | ILE  | N-CA-C | -5.03 | 105.80      | 110.53   |
| 1   | A     | 406 | THR  | N-CA-C | 5.03  | 119.47      | 113.23   |
| 1   | E     | 281 | ILE  | CA-C-N | 5.03  | 125.26      | 119.83   |
| 1   | E     | 281 | ILE  | C-N-CA | 5.03  | 125.26      | 119.83   |
| 1   | C     | 187 | LYS  | CA-C-N | 5.02  | 125.01      | 119.89   |
| 1   | C     | 187 | LYS  | C-N-CA | 5.02  | 125.01      | 119.89   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 410 | ASP  | N-CA-C | -5.02 | 105.72      | 111.14   |
| 2   | B     | 359 | ALA  | N-CA-C | -5.02 | 102.44      | 109.96   |
| 1   | E     | 424 | VAL  | N-CA-C | -5.01 | 105.01      | 110.23   |
| 1   | C     | 233 | ILE  | CA-C-N | 5.01  | 124.62      | 119.56   |
| 1   | C     | 233 | ILE  | C-N-CA | 5.01  | 124.62      | 119.56   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 259 | PRO  | Peptide   |
| 2   | B     | 355 | PHE  | Sidechain |
| 1   | C     | 259 | PRO  | Peptide   |
| 2   | D     | 355 | PHE  | Sidechain |
| 2   | D     | 393 | TYR  | Sidechain |
| 2   | F     | 355 | PHE  | Sidechain |
| 1   | G     | 259 | PRO  | Peptide   |
| 2   | H     | 355 | PHE  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4105  | 0        | 4063     | 300     | 0            |
| 1   | C     | 4105  | 0        | 4063     | 289     | 0            |
| 1   | E     | 4105  | 0        | 4063     | 301     | 0            |
| 1   | G     | 4105  | 0        | 4063     | 283     | 0            |
| 2   | B     | 3199  | 0        | 3066     | 286     | 0            |
| 2   | D     | 3199  | 0        | 3067     | 288     | 0            |
| 2   | F     | 3199  | 0        | 3062     | 280     | 0            |
| 2   | H     | 3199  | 0        | 3062     | 283     | 0            |
| 3   | I     | 600   | 0        | 635      | 61      | 0            |
| 3   | J     | 600   | 0        | 635      | 62      | 0            |
| 3   | K     | 600   | 0        | 635      | 65      | 0            |
| 3   | L     | 600   | 0        | 635      | 67      | 0            |
| 4   | B     | 31    | 0        | 12       | 3       | 0            |
| 4   | D     | 31    | 0        | 12       | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | F     | 31    | 0        | 11       | 7       | 0            |
| 4   | H     | 31    | 0        | 12       | 11      | 0            |
| 5   | F     | 1     | 0        | 0        | 0       | 0            |
| 5   | H     | 2     | 0        | 0        | 0       | 0            |
| 5   | J     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 31744 | 0        | 31096    | 2441    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (2441) 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:253:LYS:CA   | 1:A:253:LYS:C    | 1.76                     | 1.59              |
| 1:C:253:LYS:CA   | 1:C:253:LYS:C    | 1.76                     | 1.58              |
| 2:D:700:LYS:CA   | 2:D:700:LYS:C    | 1.80                     | 1.53              |
| 1:E:253:LYS:C    | 1:E:253:LYS:CA   | 1.77                     | 1.52              |
| 2:D:608:ARG:CA   | 2:D:608:ARG:C    | 1.82                     | 1.49              |
| 2:D:608:ARG:CA   | 2:D:608:ARG:N    | 1.73                     | 1.47              |
| 2:D:700:LYS:CA   | 2:D:700:LYS:N    | 1.79                     | 1.43              |
| 1:C:259:PRO:N    | 1:C:259:PRO:CA   | 1.71                     | 1.40              |
| 1:E:259:PRO:N    | 1:E:259:PRO:CA   | 1.68                     | 1.30              |
| 1:G:259:PRO:N    | 1:G:259:PRO:CA   | 1.68                     | 1.30              |
| 1:A:259:PRO:N    | 1:A:259:PRO:CA   | 1.71                     | 1.28              |
| 2:B:361:LEU:HD11 | 2:B:704:LEU:HA   | 1.32                     | 1.12              |
| 2:B:274:ARG:HH22 | 1:E:107:GLU:HA   | 0.99                     | 1.11              |
| 2:F:361:LEU:HD11 | 2:F:704:LEU:HA   | 1.34                     | 1.09              |
| 2:H:380:ALA:HB2  | 2:H:394:LEU:HD13 | 1.31                     | 1.09              |
| 2:D:361:LEU:HD11 | 2:D:704:LEU:HA   | 1.31                     | 1.09              |
| 2:H:361:LEU:HD11 | 2:H:704:LEU:HA   | 1.29                     | 1.09              |
| 2:D:380:ALA:HB2  | 2:D:394:LEU:HD13 | 1.35                     | 1.08              |
| 2:B:262:GLN:NE2  | 1:E:67:GLY:H     | 1.49                     | 1.07              |
| 1:A:396:ARG:HG3  | 1:A:534:LEU:HD11 | 1.36                     | 1.07              |
| 2:B:380:ALA:HB2  | 2:B:394:LEU:HD13 | 1.35                     | 1.05              |
| 2:F:380:ALA:HB2  | 2:F:394:LEU:HD13 | 1.37                     | 1.05              |
| 2:B:274:ARG:NH2  | 1:E:107:GLU:HA   | 1.73                     | 1.04              |
| 1:A:252:LEU:O    | 1:A:253:LYS:C    | 2.00                     | 1.04              |
| 1:A:344:ASN:ND2  | 1:E:111:ASN:HD22 | 1.57                     | 1.02              |
| 3:K:150:MET:HE1  | 3:K:167:LEU:HD22 | 1.36                     | 1.02              |
| 1:G:396:ARG:HG3  | 1:G:534:LEU:HD11 | 1.39                     | 1.02              |
| 3:L:150:MET:HE1  | 3:L:167:LEU:HD22 | 1.39                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:262:GLN:HE22 | 1:E:67:GLY:N     | 1.59                     | 1.01              |
| 2:B:606:ARG:C    | 2:B:608:ARG:H    | 1.68                     | 1.01              |
| 1:E:396:ARG:HG3  | 1:E:534:LEU:HD11 | 1.39                     | 1.01              |
| 1:E:518:ASN:ND2  | 1:E:533:GLN:HG3  | 1.77                     | 1.00              |
| 3:I:150:MET:HE1  | 3:I:167:LEU:HD22 | 1.41                     | 1.00              |
| 3:J:150:MET:HE1  | 3:J:167:LEU:HD22 | 1.41                     | 0.99              |
| 1:G:518:ASN:ND2  | 1:G:533:GLN:HG3  | 1.78                     | 0.98              |
| 2:B:128:GLN:H    | 2:B:128:GLN:NE2  | 1.59                     | 0.98              |
| 2:H:128:GLN:H    | 2:H:128:GLN:NE2  | 1.61                     | 0.97              |
| 2:B:128:GLN:HE21 | 2:B:128:GLN:N    | 1.59                     | 0.97              |
| 2:F:58:GLY:H     | 2:F:91:GLN:HG2   | 1.29                     | 0.97              |
| 2:F:229:ILE:HD13 | 2:F:281:THR:HA   | 1.45                     | 0.97              |
| 1:C:396:ARG:HG3  | 1:C:534:LEU:HD11 | 1.41                     | 0.97              |
| 1:G:252:LEU:O    | 1:G:253:LYS:C    | 2.04                     | 0.97              |
| 2:F:128:GLN:H    | 2:F:128:GLN:NE2  | 1.63                     | 0.97              |
| 2:H:128:GLN:HE21 | 2:H:128:GLN:N    | 1.61                     | 0.96              |
| 2:D:58:GLY:H     | 2:D:91:GLN:HG2   | 1.31                     | 0.96              |
| 2:D:128:GLN:H    | 2:D:128:GLN:NE2  | 1.63                     | 0.95              |
| 2:F:128:GLN:HE21 | 2:F:128:GLN:N    | 1.64                     | 0.95              |
| 2:D:229:ILE:HD13 | 2:D:281:THR:HA   | 1.48                     | 0.95              |
| 2:D:128:GLN:HE21 | 2:D:128:GLN:N    | 1.65                     | 0.94              |
| 1:A:344:ASN:ND2  | 1:E:111:ASN:ND2  | 2.15                     | 0.94              |
| 1:E:253:LYS:O    | 1:E:260:GLU:CG   | 2.16                     | 0.94              |
| 1:C:252:LEU:O    | 1:C:253:LYS:C    | 2.12                     | 0.93              |
| 1:E:252:LEU:O    | 1:E:253:LYS:C    | 2.12                     | 0.93              |
| 1:C:518:ASN:ND2  | 1:C:533:GLN:HG3  | 1.82                     | 0.93              |
| 2:B:606:ARG:O    | 2:B:608:ARG:N    | 2.02                     | 0.92              |
| 2:F:323:VAL:HG21 | 3:K:170:VAL:HG22 | 1.48                     | 0.92              |
| 1:A:253:LYS:O    | 1:A:260:GLU:CG   | 2.18                     | 0.92              |
| 2:H:229:ILE:HD13 | 2:H:281:THR:HA   | 1.50                     | 0.91              |
| 2:D:208:PRO:HG3  | 3:J:171:LEU:HD11 | 1.53                     | 0.90              |
| 1:A:285:ILE:HD11 | 1:A:388:ALA:HA   | 1.53                     | 0.90              |
| 1:G:285:ILE:HD11 | 1:G:388:ALA:HA   | 1.54                     | 0.90              |
| 2:B:229:ILE:HD13 | 2:B:281:THR:HA   | 1.50                     | 0.90              |
| 2:B:267:ARG:HG2  | 2:B:267:ARG:HH11 | 1.37                     | 0.90              |
| 1:A:518:ASN:ND2  | 1:A:533:GLN:HG3  | 1.87                     | 0.89              |
| 2:H:58:GLY:H     | 2:H:91:GLN:HG2   | 1.37                     | 0.89              |
| 3:I:138:PRO:HA   | 3:I:141:GLN:HE21 | 1.38                     | 0.89              |
| 3:L:138:PRO:HA   | 3:L:141:GLN:HE21 | 1.38                     | 0.89              |
| 2:B:274:ARG:HH22 | 1:E:107:GLU:CA   | 1.84                     | 0.88              |
| 1:C:309:ARG:HG3  | 1:C:364:LEU:HD21 | 1.56                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:307:LEU:HB3  | 1:E:383:LEU:HD22 | 1.56                     | 0.88              |
| 2:B:58:GLY:H     | 2:B:91:GLN:HG2   | 1.39                     | 0.87              |
| 2:H:323:VAL:HG21 | 3:L:170:VAL:HG22 | 1.57                     | 0.87              |
| 1:E:285:ILE:HD11 | 1:E:388:ALA:HA   | 1.57                     | 0.86              |
| 2:F:901:VAL:C    | 2:F:902:ALA:O    | 2.08                     | 0.86              |
| 2:D:267:ARG:HG2  | 2:D:267:ARG:HH11 | 1.39                     | 0.86              |
| 2:D:361:LEU:CD1  | 2:D:704:LEU:HA   | 2.06                     | 0.86              |
| 2:H:208:PRO:HG3  | 3:L:171:LEU:HD11 | 1.55                     | 0.86              |
| 2:H:380:ALA:HB2  | 2:H:394:LEU:CD1  | 2.06                     | 0.86              |
| 1:A:309:ARG:HG3  | 1:A:364:LEU:HD21 | 1.56                     | 0.86              |
| 2:H:267:ARG:HG2  | 2:H:267:ARG:HH11 | 1.38                     | 0.86              |
| 2:H:322:LEU:HD12 | 2:H:323:VAL:N    | 1.91                     | 0.86              |
| 1:E:232:ARG:HB3  | 1:E:234:PRO:HD3  | 1.57                     | 0.85              |
| 2:F:208:PRO:HG3  | 3:K:171:LEU:HD11 | 1.58                     | 0.85              |
| 2:B:208:PRO:HG3  | 3:I:171:LEU:HD11 | 1.58                     | 0.85              |
| 1:A:253:LYS:C    | 1:A:253:LYS:HA   | 2.01                     | 0.85              |
| 3:K:138:PRO:HA   | 3:K:141:GLN:HE21 | 1.41                     | 0.85              |
| 1:G:232:ARG:HB3  | 1:G:234:PRO:HD3  | 1.56                     | 0.85              |
| 1:A:232:ARG:HB3  | 1:A:234:PRO:HD3  | 1.56                     | 0.85              |
| 1:E:61:ASP:HB3   | 1:E:86:ALA:HB2   | 1.56                     | 0.85              |
| 1:E:307:LEU:HB3  | 1:E:383:LEU:CD2  | 2.07                     | 0.85              |
| 2:F:316:ILE:HD12 | 2:F:316:ILE:H    | 1.41                     | 0.85              |
| 1:A:344:ASN:HD21 | 1:E:111:ASN:HD22 | 1.22                     | 0.84              |
| 1:C:285:ILE:HD11 | 1:C:388:ALA:HA   | 1.57                     | 0.84              |
| 2:D:316:ILE:H    | 2:D:316:ILE:HD12 | 1.40                     | 0.84              |
| 1:G:309:ARG:HG3  | 1:G:364:LEU:HD21 | 1.57                     | 0.84              |
| 1:C:232:ARG:HB3  | 1:C:234:PRO:HD3  | 1.58                     | 0.84              |
| 1:G:61:ASP:HB3   | 1:G:86:ALA:HB2   | 1.59                     | 0.84              |
| 2:H:361:LEU:CD1  | 2:H:704:LEU:HA   | 2.07                     | 0.84              |
| 1:C:236:THR:O    | 1:C:237:TYR:HB2  | 1.76                     | 0.84              |
| 1:E:309:ARG:HG3  | 1:E:364:LEU:HD21 | 1.57                     | 0.84              |
| 3:I:155:THR:HG22 | 3:I:158:ASP:OD2  | 1.78                     | 0.84              |
| 2:F:267:ARG:HG2  | 2:F:267:ARG:HH11 | 1.41                     | 0.83              |
| 3:J:138:PRO:HA   | 3:J:141:GLN:HE21 | 1.41                     | 0.83              |
| 1:A:61:ASP:HB3   | 1:A:86:ALA:HB2   | 1.58                     | 0.83              |
| 1:C:307:LEU:HB3  | 1:C:383:LEU:HD22 | 1.57                     | 0.83              |
| 2:B:361:LEU:CD1  | 2:B:704:LEU:HA   | 2.07                     | 0.83              |
| 2:H:606:ARG:O    | 2:H:608:ARG:N    | 2.09                     | 0.83              |
| 1:C:253:LYS:C    | 1:C:253:LYS:HA   | 2.00                     | 0.82              |
| 2:B:316:ILE:H    | 2:B:316:ILE:HD12 | 1.43                     | 0.82              |
| 1:C:61:ASP:HB3   | 1:C:86:ALA:HB2   | 1.60                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:307:LEU:HB3  | 1:A:383:LEU:HD22 | 1.60                     | 0.82              |
| 2:F:361:LEU:CD1  | 2:F:704:LEU:HA   | 2.09                     | 0.82              |
| 1:E:253:LYS:C    | 1:E:253:LYS:HA   | 2.04                     | 0.82              |
| 2:B:74:GLN:HE22  | 2:B:119:ASN:HD22 | 1.28                     | 0.81              |
| 1:C:253:LYS:O    | 1:C:260:GLU:OE2  | 1.98                     | 0.81              |
| 2:B:323:VAL:HG21 | 3:I:170:VAL:HG22 | 1.61                     | 0.81              |
| 2:H:316:ILE:H    | 2:H:316:ILE:HD12 | 1.44                     | 0.81              |
| 2:D:323:VAL:HG21 | 3:J:170:VAL:HG22 | 1.63                     | 0.81              |
| 2:H:361:LEU:HD11 | 2:H:704:LEU:CA   | 2.11                     | 0.81              |
| 2:B:368:LEU:HA   | 2:B:374:LEU:HD12 | 1.63                     | 0.81              |
| 1:C:307:LEU:HB3  | 1:C:383:LEU:CD2  | 2.10                     | 0.81              |
| 1:G:307:LEU:HB3  | 1:G:383:LEU:CD2  | 2.11                     | 0.81              |
| 1:C:56:SER:HB3   | 1:C:101:SER:OG   | 1.80                     | 0.80              |
| 1:E:236:THR:O    | 1:E:237:TYR:HB2  | 1.79                     | 0.80              |
| 1:G:421:ASN:O    | 1:G:424:VAL:HG23 | 1.81                     | 0.80              |
| 2:D:380:ALA:HB2  | 2:D:394:LEU:CD1  | 2.10                     | 0.80              |
| 1:A:307:LEU:HB3  | 1:A:383:LEU:CD2  | 2.12                     | 0.80              |
| 2:D:325:ASN:ND2  | 2:D:327:VAL:HG22 | 1.97                     | 0.80              |
| 2:D:322:LEU:HD12 | 2:D:323:VAL:N    | 1.97                     | 0.80              |
| 2:D:700:LYS:C    | 2:D:700:LYS:HA   | 2.05                     | 0.80              |
| 1:A:236:THR:O    | 1:A:237:TYR:HB2  | 1.81                     | 0.80              |
| 2:D:361:LEU:HD11 | 2:D:704:LEU:CA   | 2.12                     | 0.79              |
| 2:H:901:VAL:C    | 2:H:902:ALA:O    | 2.17                     | 0.79              |
| 1:A:533:GLN:O    | 1:A:534:LEU:HG   | 1.81                     | 0.79              |
| 2:B:606:ARG:C    | 2:B:608:ARG:N    | 2.39                     | 0.79              |
| 2:F:380:ALA:HB2  | 2:F:394:LEU:CD1  | 2.13                     | 0.79              |
| 2:H:325:ASN:ND2  | 2:H:327:VAL:HG22 | 1.97                     | 0.79              |
| 2:B:380:ALA:HB2  | 2:B:394:LEU:CD1  | 2.12                     | 0.79              |
| 1:G:533:GLN:O    | 1:G:534:LEU:HG   | 1.82                     | 0.79              |
| 2:F:368:LEU:HA   | 2:F:374:LEU:HD12 | 1.64                     | 0.79              |
| 1:A:344:ASN:HD22 | 1:E:111:ASN:ND2  | 1.79                     | 0.79              |
| 1:E:533:GLN:O    | 1:E:534:LEU:HG   | 1.82                     | 0.79              |
| 2:F:701:GLU:HA   | 2:F:704:LEU:CB   | 2.13                     | 0.79              |
| 3:K:123:VAL:HB   | 3:K:152:ASP:HA   | 1.65                     | 0.79              |
| 1:G:307:LEU:HB3  | 1:G:383:LEU:HD22 | 1.64                     | 0.79              |
| 1:A:56:SER:HB3   | 1:A:101:SER:OG   | 1.83                     | 0.78              |
| 2:H:368:LEU:HA   | 2:H:374:LEU:HD12 | 1.64                     | 0.78              |
| 2:D:368:LEU:HA   | 2:D:374:LEU:HD12 | 1.64                     | 0.78              |
| 2:B:901:VAL:C    | 2:B:902:ALA:O    | 2.22                     | 0.78              |
| 2:F:322:LEU:HD12 | 2:F:323:VAL:N    | 1.98                     | 0.78              |
| 3:J:123:VAL:HB   | 3:J:152:ASP:HA   | 1.66                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:155:THR:HG22 | 3:J:158:ASP:OD2  | 1.81                     | 0.78              |
| 3:K:155:THR:HG22 | 3:K:158:ASP:OD2  | 1.83                     | 0.78              |
| 2:H:325:ASN:HD21 | 2:H:327:VAL:HG22 | 1.49                     | 0.77              |
| 3:L:155:THR:HG22 | 3:L:158:ASP:OD2  | 1.84                     | 0.77              |
| 1:C:213:PRO:HB3  | 1:C:332:MET:HE3  | 1.66                     | 0.77              |
| 2:D:74:GLN:HE22  | 2:D:119:ASN:HD22 | 1.29                     | 0.77              |
| 2:F:81:ASP:HB2   | 4:F:7:ATP:O2'    | 1.85                     | 0.77              |
| 3:I:123:VAL:HB   | 3:I:152:ASP:HA   | 1.66                     | 0.77              |
| 3:K:155:THR:HG23 | 3:K:158:ASP:H    | 1.50                     | 0.77              |
| 3:I:124:GLU:HB2  | 3:I:152:ASP:O    | 1.84                     | 0.77              |
| 2:D:700:LYS:C    | 2:D:700:LYS:CB   | 2.58                     | 0.77              |
| 1:A:213:PRO:HB3  | 1:A:332:MET:HE3  | 1.67                     | 0.76              |
| 3:J:124:GLU:HB2  | 3:J:152:ASP:O    | 1.85                     | 0.76              |
| 2:D:608:ARG:C    | 2:D:608:ARG:HA   | 2.08                     | 0.76              |
| 1:E:421:ASN:O    | 1:E:424:VAL:HG23 | 1.85                     | 0.76              |
| 1:G:56:SER:HB3   | 1:G:101:SER:OG   | 1.84                     | 0.76              |
| 2:B:361:LEU:HD11 | 2:B:704:LEU:CA   | 2.13                     | 0.76              |
| 3:I:155:THR:HG23 | 3:I:158:ASP:H    | 1.49                     | 0.76              |
| 2:B:81:ASP:HB2   | 4:B:5:ATP:O2'    | 1.84                     | 0.76              |
| 1:C:421:ASN:O    | 1:C:424:VAL:HG23 | 1.85                     | 0.76              |
| 1:G:213:PRO:HB3  | 1:G:332:MET:HE3  | 1.67                     | 0.76              |
| 2:H:701:GLU:HA   | 2:H:704:LEU:CB   | 2.16                     | 0.76              |
| 3:L:155:THR:HG23 | 3:L:158:ASP:H    | 1.50                     | 0.76              |
| 1:G:307:LEU:HD13 | 1:G:383:LEU:HD22 | 1.68                     | 0.76              |
| 1:G:393:VAL:HG13 | 1:G:517:ASN:HD22 | 1.50                     | 0.76              |
| 2:H:606:ARG:C    | 2:H:608:ARG:N    | 2.43                     | 0.76              |
| 1:A:252:LEU:C    | 1:A:253:LYS:C    | 2.53                     | 0.76              |
| 2:B:262:GLN:HE22 | 1:E:67:GLY:H     | 0.79                     | 0.76              |
| 3:L:123:VAL:HB   | 3:L:152:ASP:HA   | 1.68                     | 0.76              |
| 1:A:233:ILE:N    | 1:A:234:PRO:CD   | 2.49                     | 0.75              |
| 2:D:325:ASN:HD21 | 2:D:327:VAL:HG22 | 1.48                     | 0.75              |
| 1:G:51:LEU:HB2   | 1:G:52:PRO:HD3   | 1.68                     | 0.75              |
| 2:H:64:LEU:HB3   | 2:H:111:LEU:CD1  | 2.16                     | 0.75              |
| 2:F:325:ASN:ND2  | 2:F:327:VAL:HG22 | 2.00                     | 0.75              |
| 1:C:51:LEU:HB2   | 1:C:52:PRO:HD3   | 1.68                     | 0.75              |
| 1:E:56:SER:HB3   | 1:E:101:SER:OG   | 1.85                     | 0.75              |
| 1:E:233:ILE:N    | 1:E:234:PRO:CD   | 2.49                     | 0.75              |
| 1:G:233:ILE:N    | 1:G:234:PRO:CD   | 2.50                     | 0.75              |
| 2:F:74:GLN:HE22  | 2:F:119:ASN:HD22 | 1.32                     | 0.75              |
| 2:D:64:LEU:HB3   | 2:D:111:LEU:CD1  | 2.17                     | 0.75              |
| 2:H:380:ALA:CB   | 2:H:394:LEU:HD13 | 2.13                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:606:ARG:C    | 2:H:608:ARG:H    | 1.95                     | 0.75              |
| 1:C:163:ARG:HG2  | 1:C:163:ARG:HH11 | 1.52                     | 0.75              |
| 3:J:155:THR:HG23 | 3:J:158:ASP:H    | 1.51                     | 0.74              |
| 2:F:64:LEU:HB3   | 2:F:111:LEU:CD1  | 2.17                     | 0.74              |
| 1:A:348:GLU:HG3  | 1:E:115:ASN:CG   | 2.12                     | 0.74              |
| 1:E:253:LYS:O    | 1:E:260:GLU:HG2  | 1.87                     | 0.74              |
| 1:A:396:ARG:CG   | 1:A:534:LEU:HD11 | 2.17                     | 0.74              |
| 1:A:51:LEU:HB2   | 1:A:52:PRO:HD3   | 1.70                     | 0.74              |
| 1:A:253:LYS:O    | 1:A:260:GLU:HG3  | 1.85                     | 0.74              |
| 2:D:701:GLU:HA   | 2:D:704:LEU:CB   | 2.17                     | 0.74              |
| 1:E:163:ARG:HH11 | 1:E:163:ARG:HG2  | 1.50                     | 0.74              |
| 1:A:348:GLU:HG3  | 1:E:115:ASN:ND2  | 2.03                     | 0.74              |
| 1:A:351:LYS:O    | 1:A:354:ALA:HB3  | 1.88                     | 0.74              |
| 2:B:325:ASN:ND2  | 2:B:327:VAL:HG22 | 2.02                     | 0.74              |
| 1:C:393:VAL:HG13 | 1:C:517:ASN:HD22 | 1.53                     | 0.74              |
| 1:E:213:PRO:HB3  | 1:E:332:MET:HE3  | 1.69                     | 0.74              |
| 1:G:163:ARG:HG2  | 1:G:163:ARG:HH11 | 1.51                     | 0.74              |
| 1:G:34:CYS:HB2   | 1:G:123:PHE:CD2  | 2.23                     | 0.74              |
| 1:A:421:ASN:O    | 1:A:424:VAL:HG23 | 1.86                     | 0.73              |
| 2:B:322:LEU:HD12 | 2:B:323:VAL:N    | 2.03                     | 0.73              |
| 1:E:351:LYS:O    | 1:E:354:ALA:HB3  | 1.87                     | 0.73              |
| 2:B:701:GLU:HA   | 2:B:704:LEU:CB   | 2.17                     | 0.73              |
| 1:C:233:ILE:N    | 1:C:234:PRO:CD   | 2.50                     | 0.73              |
| 2:F:325:ASN:HD21 | 2:F:327:VAL:HG22 | 1.54                     | 0.73              |
| 2:H:74:GLN:HE22  | 2:H:119:ASN:HD22 | 1.34                     | 0.73              |
| 2:H:318:LEU:HD21 | 2:H:321:TYR:H    | 1.54                     | 0.73              |
| 2:D:84:ASP:H     | 2:D:87:ASN:ND2   | 1.86                     | 0.73              |
| 3:K:124:GLU:HB2  | 3:K:152:ASP:O    | 1.86                     | 0.73              |
| 2:B:237:TRP:HB3  | 2:B:238:PRO:HD3  | 1.71                     | 0.73              |
| 1:G:45:ILE:HG12  | 1:G:498:GLY:HA2  | 1.70                     | 0.73              |
| 3:L:124:GLU:HB2  | 3:L:152:ASP:O    | 1.87                     | 0.73              |
| 1:E:143:LEU:CD1  | 1:E:150:LEU:HD13 | 2.19                     | 0.72              |
| 1:E:396:ARG:CG   | 1:E:534:LEU:HD11 | 2.19                     | 0.72              |
| 1:A:163:ARG:HG2  | 1:A:163:ARG:HH11 | 1.54                     | 0.72              |
| 1:A:533:GLN:HG3  | 1:A:533:GLN:O    | 1.87                     | 0.72              |
| 2:B:361:LEU:HA   | 2:B:364:VAL:HG22 | 1.71                     | 0.72              |
| 2:F:361:LEU:HD11 | 2:F:704:LEU:CA   | 2.16                     | 0.72              |
| 1:C:533:GLN:HG3  | 1:C:533:GLN:O    | 1.88                     | 0.72              |
| 2:H:158:LEU:HD22 | 2:H:175:VAL:HB   | 1.70                     | 0.72              |
| 1:E:34:CYS:HB2   | 1:E:123:PHE:CD2  | 2.24                     | 0.72              |
| 2:F:84:ASP:H     | 2:F:87:ASN:ND2   | 1.87                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:396:ARG:CG   | 1:G:534:LEU:HD11 | 2.19                     | 0.72              |
| 3:L:123:VAL:HG11 | 3:L:150:MET:HB3  | 1.72                     | 0.72              |
| 1:C:351:LYS:O    | 1:C:354:ALA:HB3  | 1.90                     | 0.72              |
| 2:H:32:HIS:ND1   | 2:H:33:PRO:HD2   | 2.05                     | 0.72              |
| 1:C:533:GLN:O    | 1:C:534:LEU:HG   | 1.90                     | 0.71              |
| 3:J:101:MET:HB3  | 3:J:117:ILE:O    | 1.90                     | 0.71              |
| 1:G:351:LYS:O    | 1:G:354:ALA:HB3  | 1.89                     | 0.71              |
| 1:E:49:LEU:C     | 1:E:52:PRO:HD2   | 2.15                     | 0.71              |
| 2:H:84:ASP:H     | 2:H:87:ASN:ND2   | 1.88                     | 0.71              |
| 1:A:143:LEU:CD1  | 1:A:150:LEU:HD13 | 2.20                     | 0.71              |
| 2:F:171:PRO:O    | 2:F:174:ILE:HG13 | 1.91                     | 0.71              |
| 2:H:357:PRO:O    | 2:H:358:SER:HB3  | 1.89                     | 0.71              |
| 2:D:237:TRP:HB3  | 2:D:238:PRO:HD3  | 1.72                     | 0.71              |
| 2:D:608:ARG:N    | 2:D:608:ARG:CB   | 2.54                     | 0.71              |
| 3:J:106:LYS:HA   | 3:J:112:GLU:HA   | 1.73                     | 0.71              |
| 2:B:361:LEU:O    | 2:B:364:VAL:HG23 | 1.91                     | 0.71              |
| 2:D:318:LEU:HD21 | 2:D:321:TYR:H    | 1.56                     | 0.71              |
| 2:F:901:VAL:O    | 2:F:902:ALA:O    | 2.07                     | 0.71              |
| 2:B:325:ASN:HD21 | 2:B:327:VAL:HG22 | 1.56                     | 0.71              |
| 2:D:158:LEU:HD22 | 2:D:175:VAL:HB   | 1.73                     | 0.71              |
| 1:G:533:GLN:HG3  | 1:G:533:GLN:O    | 1.89                     | 0.71              |
| 2:H:361:LEU:O    | 2:H:364:VAL:HG23 | 1.90                     | 0.71              |
| 1:C:34:CYS:HB2   | 1:C:123:PHE:CD2  | 2.26                     | 0.70              |
| 1:C:264:ASN:HD22 | 1:C:264:ASN:N    | 1.89                     | 0.70              |
| 1:G:236:THR:O    | 1:G:237:TYR:HB2  | 1.90                     | 0.70              |
| 1:G:422:GLU:HG3  | 1:G:530:ALA:HB3  | 1.73                     | 0.70              |
| 2:D:342:ASN:HD22 | 2:D:342:ASN:H    | 1.38                     | 0.70              |
| 1:G:143:LEU:CD1  | 1:G:150:LEU:HD13 | 2.21                     | 0.70              |
| 1:A:49:LEU:C     | 1:A:52:PRO:HD2   | 2.16                     | 0.70              |
| 2:B:84:ASP:H     | 2:B:87:ASN:ND2   | 1.89                     | 0.70              |
| 1:E:45:ILE:HG12  | 1:E:498:GLY:HA2  | 1.74                     | 0.70              |
| 3:I:123:VAL:HG11 | 3:I:150:MET:HB3  | 1.72                     | 0.70              |
| 1:E:51:LEU:HB2   | 1:E:52:PRO:HD3   | 1.74                     | 0.70              |
| 2:F:158:LEU:HD22 | 2:F:175:VAL:HB   | 1.72                     | 0.70              |
| 2:F:606:ARG:O    | 2:F:608:ARG:N    | 2.22                     | 0.70              |
| 2:H:237:TRP:HB3  | 2:H:238:PRO:HD3  | 1.74                     | 0.70              |
| 2:D:608:ARG:C    | 2:D:608:ARG:CB   | 2.64                     | 0.70              |
| 1:C:236:THR:O    | 1:C:237:TYR:CB   | 2.39                     | 0.70              |
| 1:A:285:ILE:CD1  | 1:A:388:ALA:HA   | 2.22                     | 0.70              |
| 2:B:318:LEU:HD21 | 2:B:321:TYR:H    | 1.56                     | 0.70              |
| 2:D:361:LEU:HA   | 2:D:364:VAL:HG22 | 1.73                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:237:TRP:CE3  | 2:H:242:PRO:HG2  | 2.27                     | 0.70              |
| 1:C:422:GLU:HG3  | 1:C:530:ALA:HB3  | 1.73                     | 0.69              |
| 2:F:342:ASN:HD22 | 2:F:342:ASN:H    | 1.39                     | 0.69              |
| 1:E:533:GLN:HG3  | 1:E:533:GLN:O    | 1.90                     | 0.69              |
| 2:F:237:TRP:HB3  | 2:F:238:PRO:HD3  | 1.72                     | 0.69              |
| 3:K:106:LYS:HA   | 3:K:112:GLU:HA   | 1.74                     | 0.69              |
| 2:B:32:HIS:ND1   | 2:B:33:PRO:HD2   | 2.07                     | 0.69              |
| 2:F:606:ARG:C    | 2:F:608:ARG:H    | 1.99                     | 0.69              |
| 1:C:45:ILE:HG12  | 1:C:498:GLY:HA2  | 1.72                     | 0.69              |
| 2:F:32:HIS:ND1   | 2:F:33:PRO:HD2   | 2.08                     | 0.69              |
| 3:K:105:VAL:HG11 | 3:K:130:VAL:HG22 | 1.74                     | 0.69              |
| 1:G:49:LEU:C     | 1:G:52:PRO:HD2   | 2.17                     | 0.69              |
| 1:A:393:VAL:HG13 | 1:A:517:ASN:HD22 | 1.56                     | 0.69              |
| 2:B:64:LEU:HB3   | 2:B:111:LEU:CD1  | 2.21                     | 0.69              |
| 3:L:106:LYS:HA   | 3:L:112:GLU:HA   | 1.74                     | 0.69              |
| 2:B:157:MET:HA   | 2:B:157:MET:HE3  | 1.74                     | 0.69              |
| 2:B:262:GLN:NE2  | 1:E:67:GLY:N     | 2.29                     | 0.69              |
| 1:C:49:LEU:C     | 1:C:52:PRO:HD2   | 2.18                     | 0.69              |
| 2:D:361:LEU:O    | 2:D:364:VAL:HG23 | 1.92                     | 0.69              |
| 1:E:422:GLU:HG3  | 1:E:530:ALA:HB3  | 1.74                     | 0.69              |
| 2:F:318:LEU:HD21 | 2:F:321:TYR:H    | 1.56                     | 0.69              |
| 2:F:361:LEU:HA   | 2:F:364:VAL:HG22 | 1.73                     | 0.69              |
| 1:A:45:ILE:HG12  | 1:A:498:GLY:HA2  | 1.75                     | 0.69              |
| 2:B:158:LEU:HD22 | 2:B:175:VAL:HB   | 1.74                     | 0.69              |
| 1:G:264:ASN:N    | 1:G:264:ASN:HD22 | 1.88                     | 0.69              |
| 1:A:366:GLN:C    | 1:A:368:ILE:H    | 2.01                     | 0.69              |
| 2:D:237:TRP:CE3  | 2:D:242:PRO:HG2  | 2.28                     | 0.69              |
| 2:D:360:LYS:C    | 2:D:361:LEU:HD23 | 2.18                     | 0.69              |
| 3:I:101:MET:HB3  | 3:I:117:ILE:O    | 1.93                     | 0.68              |
| 1:E:393:VAL:HG13 | 1:E:517:ASN:HD22 | 1.58                     | 0.68              |
| 1:A:264:ASN:HD22 | 1:A:264:ASN:N    | 1.88                     | 0.68              |
| 3:L:101:MET:HB3  | 3:L:117:ILE:O    | 1.92                     | 0.68              |
| 1:A:162:MET:HE1  | 2:B:330:LEU:HD11 | 1.76                     | 0.68              |
| 2:D:128:GLN:H    | 2:D:128:GLN:HE21 | 0.80                     | 0.68              |
| 2:B:342:ASN:H    | 2:B:342:ASN:HD22 | 1.41                     | 0.68              |
| 2:F:380:ALA:CB   | 2:F:394:LEU:HD13 | 2.21                     | 0.68              |
| 3:K:123:VAL:HG11 | 3:K:150:MET:HB3  | 1.76                     | 0.68              |
| 2:H:380:ALA:HB1  | 2:H:394:LEU:HB2  | 1.75                     | 0.68              |
| 1:A:236:THR:O    | 1:A:237:TYR:CB   | 2.42                     | 0.68              |
| 2:F:237:TRP:CE3  | 2:F:242:PRO:HG2  | 2.28                     | 0.68              |
| 1:G:162:MET:HE1  | 2:H:330:LEU:HD11 | 1.74                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:253:LYS:O    | 1:G:260:GLU:OE2  | 2.11                     | 0.68              |
| 1:E:366:GLN:C    | 1:E:368:ILE:H    | 2.01                     | 0.68              |
| 1:G:211:HIS:HB3  | 1:G:335:ASP:HB2  | 1.75                     | 0.68              |
| 3:L:105:VAL:HG11 | 3:L:130:VAL:HG22 | 1.76                     | 0.68              |
| 1:E:72:ASN:HD22  | 1:E:72:ASN:C     | 2.00                     | 0.68              |
| 1:C:72:ASN:C     | 1:C:72:ASN:HD22  | 2.02                     | 0.68              |
| 2:D:380:ALA:CB   | 2:D:394:LEU:HD13 | 2.19                     | 0.68              |
| 2:D:700:LYS:N    | 2:D:700:LYS:CB   | 2.57                     | 0.68              |
| 1:E:264:ASN:HD22 | 1:E:264:ASN:N    | 1.89                     | 0.68              |
| 2:F:360:LYS:C    | 2:F:361:LEU:HD23 | 2.18                     | 0.68              |
| 2:H:357:PRO:O    | 2:H:358:SER:CB   | 2.42                     | 0.68              |
| 1:A:34:CYS:HB2   | 1:A:123:PHE:CD2  | 2.28                     | 0.67              |
| 1:A:396:ARG:HG3  | 1:A:534:LEU:CD1  | 2.19                     | 0.67              |
| 1:A:422:GLU:HG3  | 1:A:530:ALA:HB3  | 1.74                     | 0.67              |
| 1:C:285:ILE:CD1  | 1:C:388:ALA:HA   | 2.24                     | 0.67              |
| 1:E:211:HIS:HB3  | 1:E:335:ASP:HB2  | 1.77                     | 0.67              |
| 1:G:72:ASN:C     | 1:G:72:ASN:HD22  | 1.99                     | 0.67              |
| 1:G:262:GLU:HB3  | 1:G:265:PHE:HB2  | 1.76                     | 0.67              |
| 2:F:361:LEU:O    | 2:F:364:VAL:HG23 | 1.94                     | 0.67              |
| 3:I:106:LYS:HA   | 3:I:112:GLU:HA   | 1.74                     | 0.67              |
| 2:D:348:GLN:HE21 | 2:D:348:GLN:C    | 2.02                     | 0.67              |
| 3:K:101:MET:HB3  | 3:K:117:ILE:O    | 1.93                     | 0.67              |
| 2:H:348:GLN:HE21 | 2:H:348:GLN:C    | 2.02                     | 0.67              |
| 2:D:157:MET:HA   | 2:D:157:MET:HE3  | 1.76                     | 0.67              |
| 1:A:264:ASN:HD22 | 1:A:264:ASN:H    | 1.43                     | 0.67              |
| 1:C:211:HIS:HB3  | 1:C:335:ASP:HB2  | 1.75                     | 0.67              |
| 1:A:260:GLU:C    | 1:A:261:ASP:OD1  | 2.38                     | 0.67              |
| 2:B:360:LYS:C    | 2:B:361:LEU:HD23 | 2.20                     | 0.67              |
| 1:C:213:PRO:HB3  | 1:C:332:MET:CE   | 2.24                     | 0.67              |
| 2:D:164:TYR:HE2  | 2:D:169:LEU:HB2  | 1.59                     | 0.67              |
| 2:F:154:ILE:HD13 | 2:F:154:ILE:O    | 1.95                     | 0.67              |
| 2:F:192:ILE:HG22 | 2:F:194:PRO:HD3  | 1.75                     | 0.67              |
| 1:G:75:PHE:CE2   | 1:G:96:LEU:HD11  | 2.30                     | 0.67              |
| 1:A:232:ARG:C    | 1:A:234:PRO:HD3  | 2.20                     | 0.67              |
| 2:F:157:MET:HA   | 2:F:157:MET:HE3  | 1.76                     | 0.67              |
| 2:H:251:GLY:O    | 2:H:257:ILE:HD11 | 1.95                     | 0.67              |
| 2:H:361:LEU:HA   | 2:H:364:VAL:HG22 | 1.77                     | 0.67              |
| 2:D:32:HIS:ND1   | 2:D:33:PRO:HD2   | 2.09                     | 0.67              |
| 2:D:213:PHE:HB2  | 2:D:218:ILE:HD11 | 1.77                     | 0.67              |
| 3:J:105:VAL:HG11 | 3:J:130:VAL:HG22 | 1.76                     | 0.67              |
| 1:G:260:GLU:C    | 1:G:261:ASP:OD1  | 2.37                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:348:GLN:C    | 2:B:348:GLN:HE21 | 2.02                     | 0.66              |
| 1:E:285:ILE:CD1  | 1:E:388:ALA:HA   | 2.23                     | 0.66              |
| 2:F:606:ARG:C    | 2:F:608:ARG:N    | 2.51                     | 0.66              |
| 2:H:64:LEU:HB3   | 2:H:111:LEU:HD13 | 1.76                     | 0.66              |
| 2:H:360:LYS:C    | 2:H:361:LEU:HD23 | 2.20                     | 0.66              |
| 1:A:376:SER:OG   | 1:A:379:GLU:HG3  | 1.95                     | 0.66              |
| 2:B:202:CYS:HG   | 2:B:343:CYS:HG   | 1.42                     | 0.66              |
| 2:D:192:ILE:HG22 | 2:D:194:PRO:HD3  | 1.78                     | 0.66              |
| 1:E:376:SER:OG   | 1:E:379:GLU:HG3  | 1.95                     | 0.66              |
| 2:H:164:TYR:HE2  | 2:H:169:LEU:HB2  | 1.58                     | 0.66              |
| 2:H:342:ASN:H    | 2:H:342:ASN:HD22 | 1.42                     | 0.66              |
| 1:C:390:LEU:O    | 1:C:391:ARG:HG2  | 1.96                     | 0.66              |
| 2:F:64:LEU:HB3   | 2:F:111:LEU:HD13 | 1.76                     | 0.66              |
| 1:A:213:PRO:HB3  | 1:A:332:MET:CE   | 2.24                     | 0.66              |
| 1:E:262:GLU:HB3  | 1:E:265:PHE:HB2  | 1.76                     | 0.66              |
| 1:C:260:GLU:C    | 1:C:261:ASP:OD1  | 2.39                     | 0.66              |
| 1:G:232:ARG:C    | 1:G:234:PRO:HD3  | 2.20                     | 0.66              |
| 1:E:307:LEU:HD13 | 1:E:383:LEU:HD22 | 1.78                     | 0.66              |
| 1:A:397:SER:OG   | 1:A:400:GLU:HG3  | 1.95                     | 0.66              |
| 1:C:396:ARG:CG   | 1:C:534:LEU:HD11 | 2.22                     | 0.65              |
| 1:E:397:SER:OG   | 1:E:400:GLU:HG3  | 1.96                     | 0.65              |
| 2:H:359:ALA:HB1  | 2:H:363:GLU:OE1  | 1.97                     | 0.65              |
| 1:C:214:TRP:CD1  | 1:C:214:TRP:C    | 2.74                     | 0.65              |
| 1:E:390:LEU:O    | 1:E:391:ARG:HG2  | 1.96                     | 0.65              |
| 1:G:213:PRO:HB3  | 1:G:332:MET:CE   | 2.25                     | 0.65              |
| 1:G:390:LEU:O    | 1:G:391:ARG:HG2  | 1.95                     | 0.65              |
| 1:G:397:SER:OG   | 1:G:400:GLU:HG3  | 1.97                     | 0.65              |
| 2:H:213:PHE:HB2  | 2:H:218:ILE:HD11 | 1.77                     | 0.65              |
| 2:H:217:THR:HA   | 2:H:221:MET:HG2  | 1.77                     | 0.65              |
| 1:A:72:ASN:C     | 1:A:72:ASN:HD22  | 2.02                     | 0.65              |
| 2:B:164:TYR:HE2  | 2:B:169:LEU:HB2  | 1.61                     | 0.65              |
| 1:A:211:HIS:HB3  | 1:A:335:ASP:HB2  | 1.77                     | 0.65              |
| 2:B:154:ILE:O    | 2:B:154:ILE:HD13 | 1.97                     | 0.65              |
| 1:C:143:LEU:CD1  | 1:C:150:LEU:HD13 | 2.26                     | 0.65              |
| 1:C:366:GLN:C    | 1:C:368:ILE:H    | 2.02                     | 0.65              |
| 1:E:264:ASN:HD22 | 1:E:264:ASN:H    | 1.44                     | 0.65              |
| 1:A:262:GLU:HB3  | 1:A:265:PHE:HB2  | 1.79                     | 0.65              |
| 2:B:110:PHE:HD2  | 2:B:110:PHE:C    | 2.04                     | 0.65              |
| 3:J:123:VAL:HG11 | 3:J:150:MET:HB3  | 1.77                     | 0.65              |
| 1:E:232:ARG:C    | 1:E:234:PRO:HD3  | 2.21                     | 0.65              |
| 2:H:157:MET:HE3  | 2:H:157:MET:HA   | 1.77                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:171:PRO:O    | 2:H:174:ILE:HG13 | 1.97                     | 0.65              |
| 2:B:217:THR:HG21 | 2:B:223:ARG:HH22 | 1.60                     | 0.65              |
| 1:C:36:ILE:HG22  | 1:C:37:ASN:N     | 2.10                     | 0.65              |
| 1:G:264:ASN:HD22 | 1:G:264:ASN:H    | 1.43                     | 0.65              |
| 1:G:447:ASN:ND2  | 2:H:26:ARG:HE    | 1.95                     | 0.65              |
| 2:B:213:PHE:HB2  | 2:B:218:ILE:HD11 | 1.78                     | 0.65              |
| 2:B:251:GLY:O    | 2:B:257:ILE:HD11 | 1.97                     | 0.65              |
| 1:C:232:ARG:C    | 1:C:234:PRO:HD3  | 2.21                     | 0.65              |
| 2:D:154:ILE:O    | 2:D:154:ILE:HD13 | 1.96                     | 0.65              |
| 2:D:171:PRO:O    | 2:D:174:ILE:HG13 | 1.97                     | 0.65              |
| 1:E:36:ILE:HG22  | 1:E:37:ASN:N     | 2.10                     | 0.65              |
| 1:E:262:GLU:OE1  | 1:E:262:GLU:HA   | 1.97                     | 0.65              |
| 1:G:214:TRP:CD1  | 1:G:214:TRP:C    | 2.75                     | 0.65              |
| 1:G:366:GLN:C    | 1:G:368:ILE:H    | 2.03                     | 0.65              |
| 1:A:266:GLU:HA   | 1:A:269:ILE:HD12 | 1.79                     | 0.65              |
| 2:B:356:SER:HB2  | 2:B:359:ALA:HB3  | 1.79                     | 0.65              |
| 2:F:703:GLY:HA2  | 2:F:706:ASP:CB   | 2.26                     | 0.65              |
| 2:B:237:TRP:CE3  | 2:B:242:PRO:HG2  | 2.32                     | 0.65              |
| 1:A:488:ALA:O    | 1:A:490:PRO:HD3  | 1.97                     | 0.64              |
| 2:F:213:PHE:HB2  | 2:F:218:ILE:HD11 | 1.79                     | 0.64              |
| 2:D:356:SER:HB2  | 2:D:359:ALA:HB3  | 1.80                     | 0.64              |
| 1:E:36:ILE:HB    | 1:E:128:ALA:HA   | 1.79                     | 0.64              |
| 1:C:262:GLU:HB3  | 1:C:265:PHE:HB2  | 1.78                     | 0.64              |
| 1:C:307:LEU:HD13 | 1:C:383:LEU:HD22 | 1.80                     | 0.64              |
| 1:E:213:PRO:HB3  | 1:E:332:MET:CE   | 2.27                     | 0.64              |
| 2:F:159:ILE:HG23 | 2:F:162:LEU:HD12 | 1.78                     | 0.64              |
| 1:A:261:ASP:O    | 1:A:262:GLU:CB   | 2.45                     | 0.64              |
| 2:B:361:LEU:HA   | 2:B:364:VAL:CG2  | 2.27                     | 0.64              |
| 2:B:380:ALA:HB1  | 2:B:394:LEU:HB2  | 1.79                     | 0.64              |
| 2:D:608:ARG:N    | 2:D:608:ARG:HA   | 2.02                     | 0.64              |
| 2:F:348:GLN:HE21 | 2:F:348:GLN:C    | 2.05                     | 0.64              |
| 2:F:380:ALA:HB1  | 2:F:394:LEU:HB2  | 1.79                     | 0.64              |
| 1:A:307:LEU:HD13 | 1:A:383:LEU:HD22 | 1.78                     | 0.64              |
| 2:B:703:GLY:HA2  | 2:B:706:ASP:CB   | 2.28                     | 0.64              |
| 1:C:75:PHE:CE2   | 1:C:96:LEU:HD11  | 2.32                     | 0.64              |
| 2:D:217:THR:HA   | 2:D:221:MET:HG2  | 1.78                     | 0.64              |
| 2:F:356:SER:HB2  | 2:F:359:ALA:HB3  | 1.79                     | 0.64              |
| 1:G:396:ARG:HG3  | 1:G:534:LEU:CD1  | 2.22                     | 0.64              |
| 2:B:171:PRO:O    | 2:B:174:ILE:HG13 | 1.97                     | 0.64              |
| 3:I:105:VAL:HG11 | 3:I:130:VAL:HG22 | 1.78                     | 0.64              |
| 1:C:33:VAL:HG23  | 1:C:54:ILE:HD11  | 1.80                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:54:ILE:HD13  | 2:D:127:ILE:HG21 | 1.80                     | 0.64              |
| 1:E:260:GLU:C    | 1:E:261:ASP:OD1  | 2.39                     | 0.64              |
| 2:H:154:ILE:O    | 2:H:154:ILE:HD13 | 1.98                     | 0.64              |
| 2:H:322:LEU:HD12 | 2:H:322:LEU:C    | 2.23                     | 0.64              |
| 2:H:703:GLY:HA2  | 2:H:706:ASP:CB   | 2.28                     | 0.64              |
| 1:A:36:ILE:HG22  | 1:A:37:ASN:N     | 2.11                     | 0.64              |
| 1:A:46:LEU:HD23  | 1:A:93:LEU:HD13  | 1.79                     | 0.64              |
| 1:A:527:GLN:OE1  | 2:B:302:VAL:HG13 | 1.97                     | 0.64              |
| 1:G:285:ILE:CD1  | 1:G:388:ALA:HA   | 2.24                     | 0.64              |
| 1:G:533:GLN:O    | 1:G:534:LEU:CG   | 2.45                     | 0.64              |
| 2:B:192:ILE:HG22 | 2:B:194:PRO:HD3  | 1.79                     | 0.64              |
| 1:C:251:ILE:HG23 | 1:C:262:GLU:HG2  | 1.80                     | 0.64              |
| 1:C:264:ASN:HD22 | 1:C:264:ASN:H    | 1.44                     | 0.64              |
| 1:E:214:TRP:CD1  | 1:E:214:TRP:C    | 2.76                     | 0.64              |
| 2:B:217:THR:HA   | 2:B:221:MET:HG2  | 1.80                     | 0.63              |
| 1:E:229:THR:O    | 1:E:230:ASN:HB2  | 1.98                     | 0.63              |
| 1:E:251:ILE:HG23 | 1:E:262:GLU:HG2  | 1.79                     | 0.63              |
| 2:F:164:TYR:HE2  | 2:F:169:LEU:HB2  | 1.62                     | 0.63              |
| 3:K:107:THR:CG2  | 3:K:111:LYS:H    | 2.11                     | 0.63              |
| 2:H:110:PHE:HD2  | 2:H:110:PHE:C    | 2.06                     | 0.63              |
| 2:B:145:LEU:HD13 | 2:B:150:ALA:HB1  | 1.80                     | 0.63              |
| 1:C:488:ALA:O    | 1:C:490:PRO:HD3  | 1.97                     | 0.63              |
| 2:D:267:ARG:HG2  | 2:D:267:ARG:NH1  | 2.13                     | 0.63              |
| 2:D:361:LEU:HA   | 2:D:364:VAL:CG2  | 2.28                     | 0.63              |
| 1:E:396:ARG:HG3  | 1:E:534:LEU:CD1  | 2.22                     | 0.63              |
| 1:A:262:GLU:OE1  | 1:A:262:GLU:HA   | 1.98                     | 0.63              |
| 1:C:446:SER:HB2  | 1:C:449:GLN:HG3  | 1.79                     | 0.63              |
| 1:C:450:VAL:O    | 1:C:454:ILE:HG13 | 1.98                     | 0.63              |
| 2:D:64:LEU:HB3   | 2:D:111:LEU:HD13 | 1.79                     | 0.63              |
| 3:L:107:THR:CG2  | 3:L:111:LYS:H    | 2.12                     | 0.63              |
| 1:G:72:ASN:C     | 1:G:72:ASN:ND2   | 2.53                     | 0.63              |
| 1:G:262:GLU:OE1  | 1:G:262:GLU:HA   | 1.98                     | 0.63              |
| 1:A:533:GLN:O    | 1:A:534:LEU:CG   | 2.46                     | 0.63              |
| 2:B:351:GLN:HE21 | 2:B:351:GLN:HA   | 1.64                     | 0.63              |
| 3:I:107:THR:CG2  | 3:I:111:LYS:H    | 2.12                     | 0.63              |
| 1:C:447:ASN:HD22 | 2:D:26:ARG:HH21  | 1.45                     | 0.63              |
| 1:E:253:LYS:O    | 1:E:260:GLU:OE2  | 2.16                     | 0.63              |
| 1:G:376:SER:OG   | 1:G:379:GLU:HG3  | 1.98                     | 0.63              |
| 1:G:450:VAL:O    | 1:G:454:ILE:HG13 | 1.97                     | 0.63              |
| 2:B:110:PHE:C    | 2:B:110:PHE:CD2  | 2.76                     | 0.63              |
| 1:C:261:ASP:O    | 1:C:262:GLU:HB2  | 1.98                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:74:GLN:NE2   | 2:D:119:ASN:HD22 | 1.96                     | 0.63              |
| 2:H:318:LEU:HD21 | 2:H:321:TYR:N    | 2.12                     | 0.63              |
| 3:L:138:PRO:HA   | 3:L:141:GLN:NE2  | 2.10                     | 0.63              |
| 1:A:261:ASP:O    | 1:A:262:GLU:HB2  | 1.98                     | 0.63              |
| 3:I:138:PRO:HA   | 3:I:141:GLN:NE2  | 2.10                     | 0.63              |
| 1:E:72:ASN:C     | 1:E:72:ASN:ND2   | 2.54                     | 0.63              |
| 1:E:253:LYS:O    | 1:E:260:GLU:HG3  | 1.97                     | 0.63              |
| 1:E:488:ALA:O    | 1:E:490:PRO:HD3  | 1.99                     | 0.63              |
| 2:F:217:THR:HA   | 2:F:221:MET:HG2  | 1.79                     | 0.63              |
| 3:I:107:THR:HA   | 3:I:169:LEU:HD12 | 1.81                     | 0.63              |
| 2:D:217:THR:HG21 | 2:D:223:ARG:HH22 | 1.64                     | 0.63              |
| 1:E:75:PHE:CE2   | 1:E:96:LEU:HD11  | 2.34                     | 0.63              |
| 1:A:214:TRP:C    | 1:A:214:TRP:CD1  | 2.76                     | 0.63              |
| 1:A:229:THR:O    | 1:A:230:ASN:HB2  | 1.98                     | 0.63              |
| 3:I:107:THR:HG22 | 3:I:111:LYS:H    | 1.64                     | 0.63              |
| 1:C:259:PRO:C    | 1:C:260:GLU:HG2  | 2.22                     | 0.63              |
| 1:C:261:ASP:O    | 1:C:262:GLU:CB   | 2.47                     | 0.63              |
| 1:E:49:LEU:O     | 1:E:52:PRO:HD2   | 1.98                     | 0.63              |
| 3:K:138:PRO:HA   | 3:K:141:GLN:NE2  | 2.12                     | 0.63              |
| 1:G:488:ALA:O    | 1:G:490:PRO:HD3  | 1.99                     | 0.63              |
| 1:E:61:ASP:CB    | 1:E:86:ALA:HB2   | 2.26                     | 0.62              |
| 2:F:251:GLY:O    | 2:F:257:ILE:HD11 | 1.99                     | 0.62              |
| 2:F:359:ALA:HB1  | 2:F:363:GLU:OE1  | 1.99                     | 0.62              |
| 2:B:74:GLN:NE2   | 2:B:119:ASN:HD22 | 1.96                     | 0.62              |
| 1:C:448:TYR:HE2  | 2:H:240:GLU:OE2  | 1.82                     | 0.62              |
| 2:D:703:GLY:HA2  | 2:D:706:ASP:CB   | 2.30                     | 0.62              |
| 2:F:361:LEU:HA   | 2:F:364:VAL:CG2  | 2.29                     | 0.62              |
| 1:G:229:THR:O    | 1:G:230:ASN:HB2  | 1.98                     | 0.62              |
| 3:J:107:THR:CG2  | 3:J:111:LYS:H    | 2.12                     | 0.62              |
| 2:H:351:GLN:HA   | 2:H:351:GLN:HE21 | 1.65                     | 0.62              |
| 1:A:36:ILE:HB    | 1:A:128:ALA:HA   | 1.82                     | 0.62              |
| 1:A:61:ASP:CB    | 1:A:86:ALA:HB2   | 2.29                     | 0.62              |
| 1:E:447:ASN:ND2  | 2:F:26:ARG:HE    | 1.95                     | 0.62              |
| 3:J:156:ALA:HA   | 3:J:161:ILE:HD12 | 1.80                     | 0.62              |
| 1:E:518:ASN:HD22 | 1:E:533:GLN:HG3  | 1.63                     | 0.62              |
| 1:A:72:ASN:C     | 1:A:72:ASN:ND2   | 2.56                     | 0.62              |
| 3:I:156:ALA:HA   | 3:I:161:ILE:HD12 | 1.80                     | 0.62              |
| 1:C:36:ILE:HB    | 1:C:128:ALA:HA   | 1.81                     | 0.62              |
| 1:E:259:PRO:C    | 1:E:260:GLU:HG2  | 2.23                     | 0.62              |
| 1:G:36:ILE:HB    | 1:G:128:ALA:HA   | 1.82                     | 0.62              |
| 1:C:252:LEU:C    | 1:C:253:LYS:C    | 2.67                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:145:LEU:HD13 | 2:D:150:ALA:HB1  | 1.81                     | 0.62              |
| 1:E:233:ILE:N    | 1:E:234:PRO:HD3  | 2.14                     | 0.62              |
| 1:E:236:THR:O    | 1:E:237:TYR:CB   | 2.42                     | 0.62              |
| 1:E:446:SER:HB2  | 1:E:449:GLN:HG3  | 1.80                     | 0.62              |
| 2:H:110:PHE:C    | 2:H:110:PHE:CD2  | 2.78                     | 0.62              |
| 2:D:80:MET:HG2   | 4:D:6:ATP:C2     | 2.34                     | 0.62              |
| 2:D:110:PHE:HD2  | 2:D:110:PHE:C    | 2.07                     | 0.62              |
| 1:G:36:ILE:HG22  | 1:G:37:ASN:N     | 2.15                     | 0.62              |
| 1:G:260:GLU:CB   | 1:G:261:ASP:OD1  | 2.48                     | 0.62              |
| 1:A:233:ILE:N    | 1:A:234:PRO:HD3  | 2.15                     | 0.62              |
| 2:B:365:LEU:HD22 | 2:B:393:TYR:OH   | 1.99                     | 0.62              |
| 1:C:229:THR:O    | 1:C:230:ASN:HB2  | 1.98                     | 0.62              |
| 1:C:266:GLU:HA   | 1:C:269:ILE:HD12 | 1.81                     | 0.62              |
| 1:G:253:LYS:O    | 1:G:260:GLU:CG   | 2.48                     | 0.62              |
| 2:H:102:PRO:HB2  | 2:H:105:GLU:HB2  | 1.82                     | 0.62              |
| 1:A:253:LYS:O    | 1:A:260:GLU:HG2  | 1.97                     | 0.61              |
| 1:A:260:GLU:CB   | 1:A:261:ASP:OD1  | 2.48                     | 0.61              |
| 1:A:390:LEU:O    | 1:A:391:ARG:HG2  | 2.00                     | 0.61              |
| 1:A:510:THR:HB   | 1:A:512:GLN:HG3  | 1.81                     | 0.61              |
| 2:B:318:LEU:HD21 | 2:B:321:TYR:N    | 2.15                     | 0.61              |
| 1:C:72:ASN:C     | 1:C:72:ASN:ND2   | 2.56                     | 0.61              |
| 1:E:533:GLN:O    | 1:E:534:LEU:CG   | 2.47                     | 0.61              |
| 2:B:87:ASN:HB3   | 2:B:91:GLN:CD    | 2.25                     | 0.61              |
| 1:C:376:SER:OG   | 1:C:379:GLU:HG3  | 1.99                     | 0.61              |
| 2:D:318:LEU:HD21 | 2:D:321:TYR:N    | 2.15                     | 0.61              |
| 2:D:380:ALA:HB1  | 2:D:394:LEU:HB2  | 1.81                     | 0.61              |
| 1:E:162:MET:HE1  | 2:F:330:LEU:HD11 | 1.82                     | 0.61              |
| 3:K:156:ALA:HA   | 3:K:161:ILE:HD12 | 1.80                     | 0.61              |
| 1:G:46:LEU:HD23  | 1:G:93:LEU:HD13  | 1.81                     | 0.61              |
| 2:H:178:ILE:HD11 | 2:H:310:ILE:HD12 | 1.82                     | 0.61              |
| 1:C:262:GLU:OE1  | 1:C:262:GLU:HA   | 1.98                     | 0.61              |
| 1:C:347:ARG:HH22 | 2:D:274:ARG:HH11 | 1.46                     | 0.61              |
| 2:D:252:ASP:O    | 2:D:254:PRO:HD3  | 2.01                     | 0.61              |
| 3:L:107:THR:HG22 | 3:L:111:LYS:H    | 1.65                     | 0.61              |
| 3:K:107:THR:HG22 | 3:K:111:LYS:H    | 1.65                     | 0.61              |
| 2:D:110:PHE:C    | 2:D:110:PHE:CD2  | 2.79                     | 0.61              |
| 1:G:61:ASP:CB    | 1:G:86:ALA:HB2   | 2.29                     | 0.61              |
| 1:G:266:GLU:HA   | 1:G:269:ILE:HD12 | 1.81                     | 0.61              |
| 2:H:217:THR:HG21 | 2:H:223:ARG:HH22 | 1.64                     | 0.61              |
| 2:B:380:ALA:CB   | 2:B:394:LEU:HD13 | 2.20                     | 0.61              |
| 2:F:110:PHE:HD2  | 2:F:110:PHE:C    | 2.08                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:54:ILE:HD13  | 2:H:127:ILE:HG21 | 1.83                     | 0.61              |
| 2:H:901:VAL:O    | 2:H:902:ALA:O    | 2.18                     | 0.61              |
| 2:B:359:ALA:HB1  | 2:B:363:GLU:OE1  | 2.01                     | 0.61              |
| 3:I:138:PRO:CA   | 3:I:141:GLN:HE21 | 2.13                     | 0.61              |
| 2:F:351:GLN:HA   | 2:F:351:GLN:HE21 | 1.66                     | 0.61              |
| 3:K:107:THR:HA   | 3:K:169:LEU:HD12 | 1.82                     | 0.61              |
| 3:L:107:THR:HA   | 3:L:169:LEU:HD12 | 1.81                     | 0.61              |
| 1:A:75:PHE:CE2   | 1:A:96:LEU:HD11  | 2.36                     | 0.61              |
| 1:C:428:MET:O    | 1:C:431:ALA:HB3  | 2.01                     | 0.61              |
| 2:F:102:PRO:HB2  | 2:F:105:GLU:HB2  | 1.83                     | 0.61              |
| 2:F:318:LEU:HD21 | 2:F:321:TYR:N    | 2.15                     | 0.61              |
| 2:F:394:LEU:CG   | 2:F:396:SER:HB3  | 2.31                     | 0.61              |
| 1:G:38:ALA:O     | 1:G:85:ARG:HD3   | 2.00                     | 0.61              |
| 1:G:49:LEU:O     | 1:G:52:PRO:HD2   | 2.00                     | 0.61              |
| 1:C:309:ARG:CG   | 1:C:364:LEU:HD21 | 2.31                     | 0.60              |
| 2:B:54:ILE:HD13  | 2:B:127:ILE:HG21 | 1.82                     | 0.60              |
| 3:K:118:GLU:O    | 3:K:120:THR:N    | 2.29                     | 0.60              |
| 2:H:145:LEU:HD13 | 2:H:150:ALA:HB1  | 1.81                     | 0.60              |
| 3:L:156:ALA:HA   | 3:L:161:ILE:HD12 | 1.82                     | 0.60              |
| 2:B:252:ASP:O    | 2:B:254:PRO:HD3  | 2.02                     | 0.60              |
| 2:D:64:LEU:HD21  | 2:D:77:VAL:HG22  | 1.83                     | 0.60              |
| 2:D:257:ILE:HD13 | 2:D:282:GLN:HG2  | 1.82                     | 0.60              |
| 2:D:335:PHE:HE1  | 2:D:337:ALA:HB2  | 1.65                     | 0.60              |
| 3:J:138:PRO:HA   | 3:J:141:GLN:NE2  | 2.13                     | 0.60              |
| 1:E:252:LEU:C    | 1:E:253:LYS:C    | 2.69                     | 0.60              |
| 3:K:141:GLN:O    | 3:K:142:ARG:HD3  | 2.02                     | 0.60              |
| 1:G:446:SER:HB2  | 1:G:449:GLN:HG3  | 1.83                     | 0.60              |
| 1:C:260:GLU:CB   | 1:C:261:ASP:OD1  | 2.50                     | 0.60              |
| 1:C:397:SER:OG   | 1:C:400:GLU:HG3  | 2.01                     | 0.60              |
| 1:C:49:LEU:O     | 1:C:52:PRO:HD2   | 2.01                     | 0.60              |
| 1:E:347:ARG:HH22 | 2:F:274:ARG:HH11 | 1.48                     | 0.60              |
| 1:G:428:MET:O    | 1:G:431:ALA:HB3  | 2.01                     | 0.60              |
| 2:H:394:LEU:CG   | 2:H:396:SER:HB3  | 2.31                     | 0.60              |
| 2:D:102:PRO:HB2  | 2:D:105:GLU:HB2  | 1.83                     | 0.60              |
| 2:D:322:LEU:HD12 | 2:D:322:LEU:C    | 2.27                     | 0.60              |
| 2:D:359:ALA:HB1  | 2:D:363:GLU:OE1  | 2.02                     | 0.60              |
| 2:F:217:THR:HG21 | 2:F:223:ARG:HH22 | 1.66                     | 0.60              |
| 1:G:518:ASN:HD22 | 1:G:533:GLN:HG3  | 1.66                     | 0.60              |
| 3:J:107:THR:HA   | 3:J:169:LEU:HD12 | 1.83                     | 0.60              |
| 2:B:267:ARG:HG2  | 2:B:267:ARG:NH1  | 2.12                     | 0.60              |
| 2:F:74:GLN:NE2   | 2:F:119:ASN:HD22 | 1.99                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:192:ILE:HG22 | 2:H:194:PRO:HD3  | 1.82                     | 0.60              |
| 2:B:64:LEU:HB3   | 2:B:111:LEU:HD13 | 1.82                     | 0.60              |
| 1:G:8:LEU:HD12   | 1:G:11:GLN:OE1   | 2.01                     | 0.60              |
| 2:H:54:ILE:CD1   | 2:H:154:ILE:HG13 | 2.32                     | 0.60              |
| 1:C:481:GLU:OE1  | 1:C:481:GLU:HA   | 2.02                     | 0.60              |
| 2:F:394:LEU:HD21 | 2:F:396:SER:HB3  | 1.82                     | 0.60              |
| 1:A:49:LEU:O     | 1:A:52:PRO:HD2   | 2.01                     | 0.59              |
| 2:B:229:ILE:HA   | 2:B:264:SER:OG   | 2.02                     | 0.59              |
| 3:I:118:GLU:O    | 3:I:120:THR:N    | 2.30                     | 0.59              |
| 2:D:240:GLU:O    | 2:D:241:GLN:C    | 2.45                     | 0.59              |
| 1:G:261:ASP:OD1  | 1:G:261:ASP:N    | 2.35                     | 0.59              |
| 2:H:81:ASP:HB2   | 4:H:8:ATP:O2'    | 2.02                     | 0.59              |
| 3:L:138:PRO:CA   | 3:L:141:GLN:HE21 | 2.13                     | 0.59              |
| 1:A:16:GLN:NE2   | 1:A:20:TRP:HZ2   | 2.01                     | 0.59              |
| 1:C:162:MET:HE1  | 2:D:330:LEU:HD11 | 1.84                     | 0.59              |
| 1:E:13:TYR:O     | 1:E:17:LEU:HG    | 2.01                     | 0.59              |
| 1:G:422:GLU:HG3  | 1:G:530:ALA:CB   | 2.31                     | 0.59              |
| 1:A:309:ARG:CG   | 1:A:364:LEU:HD21 | 2.30                     | 0.59              |
| 2:B:394:LEU:CG   | 2:B:396:SER:HB3  | 2.32                     | 0.59              |
| 1:C:233:ILE:N    | 1:C:234:PRO:HD3  | 2.16                     | 0.59              |
| 1:E:450:VAL:O    | 1:E:454:ILE:HG13 | 2.01                     | 0.59              |
| 1:C:46:LEU:HD23  | 1:C:93:LEU:HD13  | 1.84                     | 0.59              |
| 2:D:251:GLY:O    | 2:D:257:ILE:HD11 | 2.02                     | 0.59              |
| 3:J:107:THR:HG22 | 3:J:111:LYS:H    | 1.67                     | 0.59              |
| 1:E:407:ILE:O    | 1:E:407:ILE:HG23 | 2.02                     | 0.59              |
| 1:G:233:ILE:N    | 1:G:234:PRO:HD3  | 2.16                     | 0.59              |
| 2:H:240:GLU:O    | 2:H:241:GLN:C    | 2.45                     | 0.59              |
| 2:H:356:SER:HB2  | 2:H:359:ALA:HB3  | 1.84                     | 0.59              |
| 1:C:34:CYS:HB2   | 1:C:123:PHE:CE2  | 2.38                     | 0.59              |
| 1:C:61:ASP:CB    | 1:C:86:ALA:HB2   | 2.30                     | 0.59              |
| 1:C:510:THR:HB   | 1:C:512:GLN:HG3  | 1.83                     | 0.59              |
| 2:D:351:GLN:HE21 | 2:D:351:GLN:HA   | 1.67                     | 0.59              |
| 2:D:394:LEU:CG   | 2:D:396:SER:HB3  | 2.33                     | 0.59              |
| 1:G:518:ASN:ND2  | 1:G:533:GLN:CG   | 2.62                     | 0.59              |
| 2:H:229:ILE:HA   | 2:H:264:SER:OG   | 2.01                     | 0.59              |
| 2:B:178:ILE:HD11 | 2:B:310:ILE:HD12 | 1.84                     | 0.59              |
| 3:I:170:VAL:HG13 | 3:I:171:LEU:N    | 2.16                     | 0.59              |
| 1:G:261:ASP:O    | 1:G:262:GLU:CB   | 2.51                     | 0.59              |
| 2:D:56:ALA:HA    | 2:D:60:GLY:HA3   | 1.83                     | 0.59              |
| 2:F:277:THR:HG23 | 2:F:280:LEU:H    | 1.68                     | 0.59              |
| 2:H:87:ASN:HB3   | 2:H:91:GLN:CD    | 2.27                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:243:PHE:O    | 1:A:246:LEU:HB3  | 2.02                     | 0.59              |
| 1:A:261:ASP:OD1  | 1:A:261:ASP:N    | 2.35                     | 0.59              |
| 1:A:450:VAL:O    | 1:A:454:ILE:HG13 | 2.01                     | 0.59              |
| 2:B:64:LEU:HD21  | 2:B:77:VAL:HG22  | 1.84                     | 0.59              |
| 1:C:243:PHE:O    | 1:C:246:LEU:HB3  | 2.03                     | 0.59              |
| 1:C:422:GLU:HG3  | 1:C:530:ALA:CB   | 2.32                     | 0.59              |
| 2:F:335:PHE:HE1  | 2:F:337:ALA:HB2  | 1.67                     | 0.59              |
| 2:H:159:ILE:HG23 | 2:H:162:LEU:HD12 | 1.83                     | 0.59              |
| 2:B:357:PRO:O    | 2:B:358:SER:CB   | 2.51                     | 0.59              |
| 1:C:396:ARG:HG3  | 1:C:534:LEU:CD1  | 2.24                     | 0.59              |
| 1:E:447:ASN:HD22 | 2:F:26:ARG:HH21  | 1.50                     | 0.59              |
| 2:F:54:ILE:HD13  | 2:F:127:ILE:HG21 | 1.85                     | 0.59              |
| 3:L:117:ILE:CD1  | 3:L:126:ILE:HG23 | 2.32                     | 0.59              |
| 1:E:366:GLN:O    | 1:E:368:ILE:N    | 2.36                     | 0.59              |
| 1:G:236:THR:O    | 1:G:237:TYR:CB   | 2.49                     | 0.59              |
| 1:G:347:ARG:HH22 | 2:H:274:ARG:HH11 | 1.50                     | 0.59              |
| 1:A:248:ARG:C    | 1:A:250:GLY:H    | 2.11                     | 0.58              |
| 1:A:259:PRO:C    | 1:A:260:GLU:HG2  | 2.27                     | 0.58              |
| 2:F:80:MET:HE2   | 2:F:126:LYS:HB3  | 1.84                     | 0.58              |
| 2:F:110:PHE:C    | 2:F:110:PHE:CD2  | 2.80                     | 0.58              |
| 2:B:152:ARG:O    | 2:B:155:ASN:HB3  | 2.04                     | 0.58              |
| 1:C:8:LEU:HD12   | 1:C:11:GLN:OE1   | 2.03                     | 0.58              |
| 2:F:357:PRO:O    | 2:F:358:SER:CB   | 2.51                     | 0.58              |
| 2:H:64:LEU:HD21  | 2:H:77:VAL:HG22  | 1.86                     | 0.58              |
| 3:L:141:GLN:O    | 3:L:142:ARG:HD3  | 2.03                     | 0.58              |
| 2:B:240:GLU:O    | 2:B:241:GLN:C    | 2.46                     | 0.58              |
| 2:H:74:GLN:NE2   | 2:H:119:ASN:HD22 | 2.00                     | 0.58              |
| 1:C:214:TRP:CE3  | 1:C:332:MET:HB3  | 2.39                     | 0.58              |
| 2:D:700:LYS:N    | 2:D:700:LYS:HA   | 2.04                     | 0.58              |
| 2:F:87:ASN:HB3   | 2:F:91:GLN:CD    | 2.29                     | 0.58              |
| 2:H:128:GLN:HE22 | 4:H:8:ATP:HN62   | 1.51                     | 0.58              |
| 1:A:33:VAL:HG23  | 1:A:54:ILE:HD11  | 1.84                     | 0.58              |
| 1:A:446:SER:HB2  | 1:A:449:GLN:HG3  | 1.84                     | 0.58              |
| 1:G:307:LEU:HB3  | 1:G:383:LEU:HD21 | 1.85                     | 0.58              |
| 2:B:102:PRO:HB2  | 2:B:105:GLU:HB2  | 1.85                     | 0.58              |
| 1:C:211:HIS:NE2  | 2:D:221:MET:HE1  | 2.18                     | 0.58              |
| 1:C:248:ARG:C    | 1:C:250:GLY:H    | 2.12                     | 0.58              |
| 1:G:332:MET:HG2  | 1:G:339:TYR:HE1  | 1.68                     | 0.58              |
| 1:G:527:GLN:OE1  | 2:H:302:VAL:HG13 | 2.04                     | 0.58              |
| 1:A:422:GLU:HG3  | 1:A:530:ALA:CB   | 2.34                     | 0.58              |
| 3:I:141:GLN:O    | 3:I:142:ARG:HD3  | 2.04                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:178:ILE:HD11 | 2:D:310:ILE:HD12 | 1.85                     | 0.58              |
| 1:E:199:TYR:CD2  | 1:E:216:VAL:HG11 | 2.39                     | 0.58              |
| 2:B:56:ALA:HA    | 2:B:60:GLY:HA3   | 1.86                     | 0.58              |
| 1:E:266:GLU:HA   | 1:E:269:ILE:HD12 | 1.84                     | 0.58              |
| 1:E:341:LYS:O    | 1:E:345:VAL:HG23 | 2.04                     | 0.58              |
| 2:F:54:ILE:CD1   | 2:F:154:ILE:HG13 | 2.33                     | 0.58              |
| 2:F:240:GLU:O    | 2:F:241:GLN:C    | 2.46                     | 0.58              |
| 3:K:138:PRO:CA   | 3:K:141:GLN:HE21 | 2.15                     | 0.58              |
| 2:H:80:MET:HG2   | 4:H:8:ATP:C4     | 2.39                     | 0.58              |
| 2:H:361:LEU:HA   | 2:H:364:VAL:CG2  | 2.32                     | 0.58              |
| 2:B:277:THR:HG23 | 2:B:280:LEU:H    | 1.69                     | 0.58              |
| 1:C:199:TYR:CD2  | 1:C:216:VAL:HG11 | 2.39                     | 0.58              |
| 2:D:229:ILE:HA   | 2:D:264:SER:OG   | 2.03                     | 0.58              |
| 2:D:901:VAL:C    | 2:D:902:ALA:O    | 2.40                     | 0.58              |
| 1:E:422:GLU:HG3  | 1:E:530:ALA:CB   | 2.33                     | 0.58              |
| 3:K:117:ILE:CD1  | 3:K:126:ILE:HG23 | 2.34                     | 0.58              |
| 1:G:481:GLU:OE1  | 1:G:481:GLU:HA   | 2.04                     | 0.57              |
| 3:J:118:GLU:O    | 3:J:120:THR:N    | 2.31                     | 0.57              |
| 1:E:261:ASP:OD1  | 1:E:261:ASP:N    | 2.36                     | 0.57              |
| 3:K:170:VAL:HG13 | 3:K:171:LEU:N    | 2.18                     | 0.57              |
| 1:A:8:LEU:HD12   | 1:A:11:GLN:OE1   | 2.04                     | 0.57              |
| 1:C:341:LYS:O    | 1:C:345:VAL:HG23 | 2.04                     | 0.57              |
| 1:C:533:GLN:O    | 1:C:534:LEU:CG   | 2.52                     | 0.57              |
| 2:F:56:ALA:N     | 2:F:79:ASP:OD1   | 2.38                     | 0.57              |
| 1:A:199:TYR:CD2  | 1:A:216:VAL:HG11 | 2.40                     | 0.57              |
| 1:E:16:GLN:NE2   | 1:E:20:TRP:HZ2   | 2.02                     | 0.57              |
| 1:E:260:GLU:CB   | 1:E:261:ASP:OD1  | 2.52                     | 0.57              |
| 2:F:64:LEU:HD21  | 2:F:77:VAL:HG22  | 1.86                     | 0.57              |
| 1:A:297:ILE:HD11 | 1:A:309:ARG:HG2  | 1.87                     | 0.57              |
| 2:B:13:TRP:HZ3   | 2:B:116:PRO:HG2  | 1.69                     | 0.57              |
| 1:E:46:LEU:HD23  | 1:E:93:LEU:HD13  | 1.85                     | 0.57              |
| 1:G:16:GLN:NE2   | 1:G:20:TRP:HZ2   | 2.03                     | 0.57              |
| 2:H:365:LEU:HD22 | 2:H:393:TYR:OH   | 2.05                     | 0.57              |
| 3:L:118:GLU:O    | 3:L:120:THR:N    | 2.30                     | 0.57              |
| 1:E:307:LEU:CB   | 1:E:383:LEU:HD22 | 2.33                     | 0.57              |
| 2:F:229:ILE:HA   | 2:F:264:SER:OG   | 2.03                     | 0.57              |
| 2:F:365:LEU:HD22 | 2:F:393:TYR:OH   | 2.04                     | 0.57              |
| 2:H:152:ARG:O    | 2:H:155:ASN:HB3  | 2.04                     | 0.57              |
| 1:E:8:LEU:HD12   | 1:E:11:GLN:OE1   | 2.03                     | 0.57              |
| 2:F:145:LEU:HD13 | 2:F:150:ALA:HB1  | 1.85                     | 0.57              |
| 2:H:277:THR:HG23 | 2:H:280:LEU:H    | 1.69                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:335:PHE:HE1  | 2:H:337:ALA:HB2  | 1.70                     | 0.57              |
| 1:A:366:GLN:O    | 1:A:368:ILE:N    | 2.38                     | 0.57              |
| 1:C:261:ASP:OD1  | 1:C:261:ASP:N    | 2.37                     | 0.57              |
| 1:E:248:ARG:C    | 1:E:250:GLY:H    | 2.11                     | 0.57              |
| 1:G:33:VAL:HG23  | 1:G:54:ILE:HD11  | 1.87                     | 0.57              |
| 1:G:251:ILE:HG23 | 1:G:262:GLU:HG2  | 1.85                     | 0.57              |
| 2:B:257:ILE:HD13 | 2:B:282:GLN:HG2  | 1.87                     | 0.57              |
| 2:B:335:PHE:HE1  | 2:B:337:ALA:HB2  | 1.69                     | 0.57              |
| 1:E:307:LEU:HB3  | 1:E:383:LEU:HD21 | 1.86                     | 0.57              |
| 1:G:259:PRO:C    | 1:G:260:GLU:HG2  | 2.28                     | 0.57              |
| 1:A:251:ILE:HG23 | 1:A:262:GLU:HG2  | 1.85                     | 0.57              |
| 1:C:84:ASN:OD1   | 1:C:106:GLU:HG2  | 2.05                     | 0.57              |
| 2:D:46:LEU:O     | 2:D:73:ARG:HB2   | 2.05                     | 0.57              |
| 2:D:54:ILE:CD1   | 2:D:154:ILE:HG13 | 2.35                     | 0.57              |
| 2:D:58:GLY:N     | 2:D:91:GLN:HG2   | 2.12                     | 0.57              |
| 1:E:481:GLU:OE1  | 1:E:481:GLU:HA   | 2.05                     | 0.57              |
| 2:F:152:ARG:O    | 2:F:155:ASN:HB3  | 2.05                     | 0.57              |
| 1:G:13:TYR:O     | 1:G:17:LEU:HG    | 2.04                     | 0.57              |
| 1:G:199:TYR:CD2  | 1:G:216:VAL:HG11 | 2.40                     | 0.57              |
| 1:A:347:ARG:HH22 | 2:B:274:ARG:HH11 | 1.52                     | 0.56              |
| 1:E:407:ILE:HD12 | 1:E:409:LYS:HB3  | 1.86                     | 0.56              |
| 1:E:510:THR:HB   | 1:E:512:GLN:HG3  | 1.87                     | 0.56              |
| 1:G:84:ASN:OD1   | 1:G:106:GLU:HG2  | 2.04                     | 0.56              |
| 2:H:371:SER:C    | 2:H:373:SER:H    | 2.13                     | 0.56              |
| 1:A:332:MET:HG2  | 1:A:339:TYR:HE1  | 1.70                     | 0.56              |
| 1:A:341:LYS:O    | 1:A:345:VAL:HG23 | 2.06                     | 0.56              |
| 1:C:342:LEU:HD11 | 1:C:346:TYR:HE1  | 1.69                     | 0.56              |
| 2:D:87:ASN:HB3   | 2:D:91:GLN:CD    | 2.30                     | 0.56              |
| 1:G:214:TRP:CE3  | 1:G:332:MET:HB3  | 2.40                     | 0.56              |
| 2:H:56:ALA:HA    | 2:H:60:GLY:HA3   | 1.86                     | 0.56              |
| 2:B:80:MET:HE2   | 2:B:126:LYS:HB3  | 1.87                     | 0.56              |
| 2:B:267:ARG:HH11 | 2:B:267:ARG:CG   | 2.16                     | 0.56              |
| 3:J:141:GLN:O    | 3:J:142:ARG:HD3  | 2.05                     | 0.56              |
| 1:E:243:PHE:O    | 1:E:246:LEU:HB3  | 2.04                     | 0.56              |
| 1:E:407:ILE:O    | 1:E:409:LYS:N    | 2.38                     | 0.56              |
| 2:F:901:VAL:O    | 2:F:902:ALA:C    | 2.44                     | 0.56              |
| 2:H:335:PHE:CZ   | 3:L:144:ILE:HD13 | 2.40                     | 0.56              |
| 1:A:13:TYR:O     | 1:A:17:LEU:HG    | 2.04                     | 0.56              |
| 1:A:84:ASN:OD1   | 1:A:106:GLU:HG2  | 2.05                     | 0.56              |
| 1:A:253:LYS:C    | 1:A:253:LYS:N    | 2.57                     | 0.56              |
| 2:D:394:LEU:HG   | 2:D:396:SER:H    | 1.71                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:38:ALA:O     | 1:E:85:ARG:HD3   | 2.05                     | 0.56              |
| 2:F:257:ILE:HD13 | 2:F:282:GLN:HG2  | 1.88                     | 0.56              |
| 1:G:407:ILE:O    | 1:G:409:LYS:N    | 2.38                     | 0.56              |
| 2:D:357:PRO:O    | 2:D:358:SER:HB3  | 2.05                     | 0.56              |
| 2:D:606:ARG:O    | 2:D:607:THR:C    | 2.46                     | 0.56              |
| 1:E:34:CYS:HB2   | 1:E:123:PHE:CE2  | 2.40                     | 0.56              |
| 1:E:261:ASP:O    | 1:E:262:GLU:HB2  | 2.05                     | 0.56              |
| 2:F:357:PRO:O    | 2:F:358:SER:HB3  | 2.03                     | 0.56              |
| 1:G:185:LEU:O    | 1:G:188:PRO:HD3  | 2.05                     | 0.56              |
| 2:H:252:ASP:O    | 2:H:254:PRO:HD3  | 2.05                     | 0.56              |
| 2:D:394:LEU:HD21 | 2:D:396:SER:HB3  | 1.88                     | 0.56              |
| 3:J:117:ILE:CD1  | 3:J:126:ILE:HG23 | 2.35                     | 0.56              |
| 1:G:407:ILE:HD12 | 1:G:409:LYS:HB3  | 1.87                     | 0.56              |
| 2:B:357:PRO:O    | 2:B:358:SER:HB3  | 2.05                     | 0.56              |
| 2:D:277:THR:HG23 | 2:D:280:LEU:H    | 1.69                     | 0.56              |
| 1:E:214:TRP:CE3  | 1:E:332:MET:HB3  | 2.40                     | 0.56              |
| 1:E:261:ASP:O    | 1:E:262:GLU:CB   | 2.54                     | 0.56              |
| 2:F:394:LEU:HG   | 2:F:396:SER:H    | 1.71                     | 0.56              |
| 1:G:510:THR:HB   | 1:G:512:GLN:HG3  | 1.88                     | 0.56              |
| 2:H:267:ARG:HG2  | 2:H:267:ARG:NH1  | 2.13                     | 0.56              |
| 2:H:901:VAL:O    | 2:H:902:ALA:C    | 2.47                     | 0.56              |
| 1:C:39:THR:O     | 1:C:43:THR:HB    | 2.06                     | 0.56              |
| 2:D:365:LEU:HD22 | 2:D:393:TYR:OH   | 2.06                     | 0.56              |
| 1:E:50:VAL:HG13  | 1:E:100:VAL:HG21 | 1.88                     | 0.56              |
| 1:G:407:ILE:O    | 1:G:407:ILE:HG23 | 2.06                     | 0.56              |
| 2:H:80:MET:HE2   | 2:H:126:LYS:HB3  | 1.87                     | 0.56              |
| 1:A:235:LYS:HB2  | 1:A:239:GLU:OE1  | 2.06                     | 0.56              |
| 2:B:54:ILE:CD1   | 2:B:154:ILE:HG13 | 2.36                     | 0.56              |
| 2:B:64:LEU:HD11  | 2:B:77:VAL:HG21  | 1.88                     | 0.56              |
| 2:D:80:MET:HE2   | 2:D:126:LYS:HB3  | 1.88                     | 0.56              |
| 1:E:342:LEU:HD11 | 1:E:346:TYR:HE1  | 1.71                     | 0.56              |
| 1:G:243:PHE:O    | 1:G:246:LEU:HB3  | 2.04                     | 0.56              |
| 2:D:343:CYS:SG   | 2:D:346:CYS:SG   | 3.04                     | 0.56              |
| 2:F:335:PHE:CZ   | 3:K:144:ILE:HD13 | 2.41                     | 0.56              |
| 1:G:248:ARG:C    | 1:G:250:GLY:H    | 2.13                     | 0.56              |
| 1:E:84:ASN:C     | 1:E:84:ASN:ND2   | 2.64                     | 0.55              |
| 2:D:357:PRO:O    | 2:D:358:SER:CB   | 2.54                     | 0.55              |
| 1:E:33:VAL:HG23  | 1:E:54:ILE:HD11  | 1.88                     | 0.55              |
| 1:E:309:ARG:CG   | 1:E:364:LEU:HD21 | 2.31                     | 0.55              |
| 2:F:64:LEU:HD11  | 2:F:77:VAL:HG21  | 1.88                     | 0.55              |
| 1:G:309:ARG:CG   | 1:G:364:LEU:HD21 | 2.33                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:394:LEU:HG   | 2:H:396:SER:H    | 1.71                     | 0.55              |
| 2:B:16:ARG:NH2   | 2:B:116:PRO:HB2  | 2.21                     | 0.55              |
| 2:D:335:PHE:HE2  | 3:J:170:VAL:HG21 | 1.71                     | 0.55              |
| 3:J:170:VAL:HG13 | 3:J:171:LEU:N    | 2.20                     | 0.55              |
| 1:A:481:GLU:HA   | 1:A:481:GLU:OE1  | 2.06                     | 0.55              |
| 1:E:332:MET:HG2  | 1:E:339:TYR:HE1  | 1.71                     | 0.55              |
| 2:F:178:ILE:N    | 2:F:178:ILE:HD12 | 2.21                     | 0.55              |
| 1:G:261:ASP:O    | 1:G:262:GLU:HB2  | 2.06                     | 0.55              |
| 1:G:533:GLN:O    | 1:G:534:LEU:CB   | 2.55                     | 0.55              |
| 2:B:159:ILE:HG23 | 2:B:162:LEU:HD12 | 1.87                     | 0.55              |
| 1:C:229:THR:HG22 | 1:C:231:GLY:H    | 1.72                     | 0.55              |
| 1:C:297:ILE:HD11 | 1:C:309:ARG:HG2  | 1.89                     | 0.55              |
| 2:D:64:LEU:HD11  | 2:D:77:VAL:HG21  | 1.88                     | 0.55              |
| 1:E:518:ASN:ND2  | 1:E:533:GLN:CG   | 2.61                     | 0.55              |
| 2:F:322:LEU:HD12 | 2:F:322:LEU:C    | 2.31                     | 0.55              |
| 1:G:341:LYS:O    | 1:G:345:VAL:HG23 | 2.06                     | 0.55              |
| 1:G:407:ILE:C    | 1:G:407:ILE:HD13 | 2.31                     | 0.55              |
| 2:H:351:GLN:HA   | 2:H:351:GLN:NE2  | 2.22                     | 0.55              |
| 1:A:235:LYS:HB2  | 1:A:239:GLU:CD   | 2.31                     | 0.55              |
| 1:E:46:LEU:HD21  | 1:E:57:PHE:CD1   | 2.41                     | 0.55              |
| 1:E:84:ASN:OD1   | 1:E:106:GLU:HG2  | 2.06                     | 0.55              |
| 1:E:428:MET:O    | 1:E:431:ALA:HB3  | 2.07                     | 0.55              |
| 3:K:117:ILE:HD13 | 3:K:126:ILE:HG12 | 1.89                     | 0.55              |
| 1:A:229:THR:HG22 | 1:A:231:GLY:N    | 2.22                     | 0.55              |
| 1:A:407:ILE:HG23 | 1:A:407:ILE:O    | 2.07                     | 0.55              |
| 2:B:164:TYR:CE2  | 2:B:169:LEU:HD13 | 2.41                     | 0.55              |
| 3:I:117:ILE:CD1  | 3:I:126:ILE:HG23 | 2.37                     | 0.55              |
| 1:C:16:GLN:NE2   | 1:C:20:TRP:HZ2   | 2.05                     | 0.55              |
| 3:J:138:PRO:CA   | 3:J:141:GLN:HE21 | 2.16                     | 0.55              |
| 2:F:252:ASP:O    | 2:F:254:PRO:HD3  | 2.06                     | 0.55              |
| 1:G:117:PRO:C    | 1:G:119:PHE:H    | 2.15                     | 0.55              |
| 2:B:394:LEU:HG   | 2:B:396:SER:H    | 1.72                     | 0.55              |
| 1:C:407:ILE:HG23 | 1:C:407:ILE:O    | 2.07                     | 0.55              |
| 1:C:422:GLU:CD   | 1:C:422:GLU:H    | 2.14                     | 0.55              |
| 2:D:152:ARG:O    | 2:D:155:ASN:HB3  | 2.06                     | 0.55              |
| 2:D:325:ASN:HD22 | 2:D:326:ASP:N    | 2.04                     | 0.55              |
| 1:A:229:THR:O    | 1:A:230:ASN:CB   | 2.55                     | 0.55              |
| 1:A:407:ILE:C    | 1:A:407:ILE:HD13 | 2.31                     | 0.55              |
| 1:C:235:LYS:HB2  | 1:C:239:GLU:OE1  | 2.07                     | 0.55              |
| 1:E:133:GLU:O    | 1:E:134:SER:C    | 2.50                     | 0.55              |
| 1:G:342:LEU:HD11 | 1:G:346:TYR:HE1  | 1.72                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:380:ALA:CB   | 2:H:394:LEU:HB2  | 2.37                     | 0.55              |
| 2:B:351:GLN:HA   | 2:B:351:GLN:NE2  | 2.21                     | 0.54              |
| 1:C:41:THR:O     | 1:C:45:ILE:HG13  | 2.07                     | 0.54              |
| 1:C:353:ASP:O    | 1:C:357:VAL:HG23 | 2.07                     | 0.54              |
| 2:D:237:TRP:CD2  | 2:D:242:PRO:HG2  | 2.41                     | 0.54              |
| 1:E:407:ILE:HD13 | 1:E:407:ILE:C    | 2.31                     | 0.54              |
| 2:F:237:TRP:CD2  | 2:F:242:PRO:HG2  | 2.42                     | 0.54              |
| 1:G:229:THR:HG22 | 1:G:231:GLY:H    | 1.73                     | 0.54              |
| 2:B:356:SER:CB   | 2:B:359:ALA:HB3  | 2.38                     | 0.54              |
| 2:D:371:SER:C    | 2:D:373:SER:H    | 2.15                     | 0.54              |
| 2:F:56:ALA:HA    | 2:F:60:GLY:HA3   | 1.88                     | 0.54              |
| 2:F:178:ILE:HD11 | 2:F:310:ILE:HD12 | 1.89                     | 0.54              |
| 2:F:325:ASN:HD22 | 2:F:326:ASP:N    | 2.05                     | 0.54              |
| 2:B:85:VAL:HG13  | 2:B:86:SER:N     | 2.22                     | 0.54              |
| 2:B:394:LEU:HD21 | 2:B:396:SER:HB3  | 1.89                     | 0.54              |
| 3:K:103:ILE:CD1  | 3:K:115:ILE:HB   | 2.37                     | 0.54              |
| 2:H:162:LEU:HD21 | 2:H:174:ILE:HG23 | 1.89                     | 0.54              |
| 2:H:237:TRP:CD2  | 2:H:242:PRO:HG2  | 2.41                     | 0.54              |
| 1:A:60:ILE:HD11  | 1:A:119:PHE:HE2  | 1.73                     | 0.54              |
| 1:A:214:TRP:CE3  | 1:A:332:MET:HB3  | 2.42                     | 0.54              |
| 1:A:229:THR:HG22 | 1:A:231:GLY:H    | 1.71                     | 0.54              |
| 2:B:131:ASN:O    | 2:B:132:ASP:C    | 2.50                     | 0.54              |
| 1:C:232:ARG:CB   | 1:C:234:PRO:HD3  | 2.35                     | 0.54              |
| 1:C:366:GLN:O    | 1:C:368:ILE:N    | 2.40                     | 0.54              |
| 2:D:13:TRP:HZ3   | 2:D:116:PRO:HG2  | 1.72                     | 0.54              |
| 1:G:297:ILE:HD11 | 1:G:309:ARG:HG2  | 1.90                     | 0.54              |
| 1:A:317:LYS:HB3  | 1:A:318:GLU:OE1  | 2.08                     | 0.54              |
| 1:C:185:LEU:O    | 1:C:188:PRO:HD3  | 2.06                     | 0.54              |
| 1:C:518:ASN:HD22 | 1:C:533:GLN:HG3  | 1.71                     | 0.54              |
| 2:D:64:LEU:HD21  | 2:D:77:VAL:CG2   | 2.37                     | 0.54              |
| 2:D:159:ILE:HG23 | 2:D:162:LEU:HD12 | 1.89                     | 0.54              |
| 1:E:185:LEU:O    | 1:E:188:PRO:HD3  | 2.07                     | 0.54              |
| 1:E:229:THR:HG22 | 1:E:231:GLY:H    | 1.72                     | 0.54              |
| 2:H:131:ASN:O    | 2:H:132:ASP:C    | 2.50                     | 0.54              |
| 2:H:325:ASN:HD22 | 2:H:326:ASP:N    | 2.05                     | 0.54              |
| 1:A:221:TYR:OH   | 1:A:250:GLY:HA3  | 2.07                     | 0.54              |
| 2:B:371:SER:C    | 2:B:373:SER:H    | 2.16                     | 0.54              |
| 1:C:221:TYR:OH   | 1:C:250:GLY:HA3  | 2.07                     | 0.54              |
| 2:D:81:ASP:HB2   | 4:D:6:ATP:O2'    | 2.08                     | 0.54              |
| 1:E:416:MET:C    | 1:E:418:ASN:H    | 2.16                     | 0.54              |
| 2:F:195:GLY:O    | 2:F:196:MET:HG3  | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:232:VAL:HG11 | 2:F:263:LYS:HB2  | 1.88                     | 0.54              |
| 1:A:447:ASN:ND2  | 2:B:26:ARG:HE    | 2.04                     | 0.54              |
| 2:B:56:ALA:N     | 2:B:79:ASP:OD1   | 2.40                     | 0.54              |
| 1:C:253:LYS:O    | 1:C:260:GLU:CG   | 2.55                     | 0.54              |
| 1:E:84:ASN:C     | 1:E:84:ASN:HD22  | 2.14                     | 0.54              |
| 2:F:164:TYR:CE2  | 2:F:169:LEU:HD13 | 2.43                     | 0.54              |
| 1:G:211:HIS:NE2  | 2:H:221:MET:HE1  | 2.23                     | 0.54              |
| 1:G:426:TYR:CZ   | 1:G:430:ARG:HD3  | 2.43                     | 0.54              |
| 1:A:133:GLU:O    | 1:A:134:SER:C    | 2.51                     | 0.54              |
| 1:C:332:MET:HG2  | 1:C:339:TYR:HE1  | 1.73                     | 0.54              |
| 1:C:407:ILE:HD13 | 1:C:407:ILE:C    | 2.33                     | 0.54              |
| 2:D:351:GLN:HA   | 2:D:351:GLN:NE2  | 2.23                     | 0.54              |
| 1:E:235:LYS:HB2  | 1:E:239:GLU:OE1  | 2.08                     | 0.54              |
| 2:F:58:GLY:N     | 2:F:91:GLN:HG2   | 2.11                     | 0.54              |
| 2:F:351:GLN:HA   | 2:F:351:GLN:NE2  | 2.22                     | 0.54              |
| 2:B:87:ASN:HB3   | 2:B:91:GLN:NE2   | 2.23                     | 0.54              |
| 2:B:217:THR:CG2  | 2:B:223:ARG:HH22 | 2.21                     | 0.54              |
| 2:D:178:ILE:HD12 | 2:D:178:ILE:N    | 2.23                     | 0.54              |
| 1:E:16:GLN:CB    | 2:F:292:VAL:HG12 | 2.38                     | 0.54              |
| 2:F:316:ILE:H    | 2:F:316:ILE:CD1  | 2.08                     | 0.54              |
| 1:G:34:CYS:HB2   | 1:G:123:PHE:CE2  | 2.42                     | 0.54              |
| 1:G:366:GLN:O    | 1:G:368:ILE:N    | 2.41                     | 0.54              |
| 1:A:232:ARG:CB   | 1:A:234:PRO:HD3  | 2.33                     | 0.53              |
| 2:B:322:LEU:HD12 | 2:B:322:LEU:C    | 2.33                     | 0.53              |
| 1:C:293:ARG:HG2  | 1:C:305:TRP:CD1  | 2.43                     | 0.53              |
| 2:D:164:TYR:CE2  | 2:D:169:LEU:HD13 | 2.44                     | 0.53              |
| 1:E:253:LYS:O    | 1:E:260:GLU:CD   | 2.51                     | 0.53              |
| 2:F:162:LEU:HD21 | 2:F:174:ILE:HG23 | 1.90                     | 0.53              |
| 1:G:336:SER:OG   | 2:H:271:TYR:HD2  | 1.91                     | 0.53              |
| 2:H:13:TRP:HZ3   | 2:H:116:PRO:HG2  | 1.73                     | 0.53              |
| 1:A:533:GLN:O    | 1:A:534:LEU:CB   | 2.56                     | 0.53              |
| 3:I:101:MET:SD   | 3:I:162:LEU:HA   | 2.48                     | 0.53              |
| 3:I:103:ILE:HD11 | 3:I:115:ILE:HB   | 1.90                     | 0.53              |
| 3:I:155:THR:O    | 3:I:158:ASP:HB2  | 2.09                     | 0.53              |
| 1:C:13:TYR:O     | 1:C:17:LEU:HG    | 2.08                     | 0.53              |
| 1:C:229:THR:HG22 | 1:C:231:GLY:N    | 2.23                     | 0.53              |
| 3:J:143:LEU:HB3  | 3:J:150:MET:HE2  | 1.88                     | 0.53              |
| 1:G:133:GLU:O    | 1:G:134:SER:C    | 2.52                     | 0.53              |
| 2:H:371:SER:O    | 2:H:373:SER:N    | 2.41                     | 0.53              |
| 3:L:103:ILE:CD1  | 3:L:115:ILE:HB   | 2.38                     | 0.53              |
| 1:A:407:ILE:O    | 1:A:409:LYS:N    | 2.40                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:178:ILE:HD12 | 2:B:178:ILE:N    | 2.23                     | 0.53              |
| 2:B:380:ALA:CB   | 2:B:394:LEU:HB2  | 2.38                     | 0.53              |
| 1:C:407:ILE:HD12 | 1:C:409:LYS:HB3  | 1.89                     | 0.53              |
| 2:D:131:ASN:O    | 2:D:132:ASP:C    | 2.51                     | 0.53              |
| 2:F:87:ASN:HB3   | 2:F:91:GLN:NE2   | 2.23                     | 0.53              |
| 3:K:143:LEU:HB3  | 3:K:150:MET:HE2  | 1.89                     | 0.53              |
| 2:H:58:GLY:N     | 2:H:91:GLN:HG2   | 2.17                     | 0.53              |
| 1:A:407:ILE:HD12 | 1:A:409:LYS:HB3  | 1.91                     | 0.53              |
| 3:I:143:LEU:HB3  | 3:I:150:MET:HE2  | 1.90                     | 0.53              |
| 2:D:195:GLY:O    | 2:D:196:MET:HG3  | 2.09                     | 0.53              |
| 1:E:366:GLN:C    | 1:E:368:ILE:N    | 2.66                     | 0.53              |
| 2:F:13:TRP:HZ3   | 2:F:116:PRO:HG2  | 1.74                     | 0.53              |
| 2:F:371:SER:C    | 2:F:373:SER:H    | 2.16                     | 0.53              |
| 1:C:133:GLU:O    | 1:C:134:SER:C    | 2.51                     | 0.53              |
| 1:C:307:LEU:HB3  | 1:C:383:LEU:HD21 | 1.90                     | 0.53              |
| 2:D:356:SER:CB   | 2:D:359:ALA:HB3  | 2.39                     | 0.53              |
| 1:E:422:GLU:H    | 1:E:422:GLU:CD   | 2.16                     | 0.53              |
| 2:F:128:GLN:H    | 2:F:128:GLN:HE21 | 0.79                     | 0.53              |
| 2:H:158:LEU:CD1  | 2:H:177:LEU:HB2  | 2.38                     | 0.53              |
| 2:H:320:ASN:O    | 2:H:321:TYR:HB2  | 2.09                     | 0.53              |
| 1:A:34:CYS:HB2   | 1:A:123:PHE:CE2  | 2.43                     | 0.53              |
| 1:E:181:GLU:OE1  | 1:E:181:GLU:HA   | 2.08                     | 0.53              |
| 1:G:50:VAL:HG13  | 1:G:100:VAL:HG21 | 1.91                     | 0.53              |
| 3:L:170:VAL:HG13 | 3:L:171:LEU:N    | 2.22                     | 0.53              |
| 1:A:260:GLU:HB3  | 1:A:261:ASP:OD1  | 2.09                     | 0.53              |
| 2:B:46:LEU:O     | 2:B:73:ARG:HB2   | 2.08                     | 0.53              |
| 1:E:229:THR:HG22 | 1:E:231:GLY:N    | 2.24                     | 0.53              |
| 2:H:111:LEU:O    | 2:H:111:LEU:HD23 | 2.08                     | 0.53              |
| 1:A:474:VAL:O    | 1:A:475:LYS:C    | 2.51                     | 0.53              |
| 2:B:197:THR:HG22 | 2:B:198:ALA:N    | 2.23                     | 0.53              |
| 2:B:901:VAL:O    | 2:B:902:ALA:O    | 2.26                     | 0.53              |
| 3:I:103:ILE:HD12 | 3:I:103:ILE:O    | 2.09                     | 0.53              |
| 1:E:297:ILE:HD11 | 1:E:309:ARG:HG2  | 1.91                     | 0.53              |
| 1:E:357:VAL:O    | 1:E:361:VAL:HG23 | 2.08                     | 0.53              |
| 2:F:356:SER:CB   | 2:F:359:ALA:HB3  | 2.38                     | 0.53              |
| 3:K:101:MET:SD   | 3:K:162:LEU:HA   | 2.49                     | 0.53              |
| 1:A:496:PHE:CE1  | 2:B:298:VAL:HG13 | 2.43                     | 0.53              |
| 2:B:90:ARG:NH2   | 4:B:5:ATP:O2G    | 2.42                     | 0.53              |
| 2:B:213:PHE:CB   | 2:B:218:ILE:HD11 | 2.39                     | 0.53              |
| 3:K:103:ILE:HD11 | 3:K:115:ILE:HB   | 1.90                     | 0.53              |
| 2:H:62:GLU:HG2   | 2:H:297:ALA:HA   | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:394:LEU:HD21 | 2:H:396:SER:HB3  | 1.89                     | 0.53              |
| 2:H:908:GLN:O    | 2:H:909:THR:C    | 2.52                     | 0.53              |
| 1:A:342:LEU:HD11 | 1:A:346:TYR:HE1  | 1.74                     | 0.53              |
| 1:A:428:MET:O    | 1:A:431:ALA:HB3  | 2.08                     | 0.53              |
| 1:C:229:THR:O    | 1:C:230:ASN:CB   | 2.57                     | 0.53              |
| 2:D:199:CYS:HG   | 2:D:202:CYS:HG   | 1.53                     | 0.53              |
| 2:H:164:TYR:CE2  | 2:H:169:LEU:HD13 | 2.44                     | 0.53              |
| 2:H:164:TYR:CE2  | 2:H:169:LEU:HB2  | 2.42                     | 0.53              |
| 2:H:257:ILE:HD13 | 2:H:282:GLN:HG2  | 1.91                     | 0.53              |
| 2:H:360:LYS:N    | 2:H:363:GLU:OE1  | 2.42                     | 0.53              |
| 1:A:422:GLU:CD   | 1:A:422:GLU:H    | 2.17                     | 0.52              |
| 3:I:117:ILE:HD13 | 3:I:126:ILE:HG12 | 1.91                     | 0.52              |
| 1:C:177:ASP:O    | 1:C:178:ASN:HB2  | 2.09                     | 0.52              |
| 1:C:251:ILE:HG23 | 1:C:262:GLU:CG   | 2.39                     | 0.52              |
| 1:C:307:LEU:CB   | 1:C:383:LEU:HD22 | 2.34                     | 0.52              |
| 3:J:108:LEU:HG   | 3:J:108:LEU:O    | 2.10                     | 0.52              |
| 1:E:229:THR:O    | 1:E:230:ASN:CB   | 2.56                     | 0.52              |
| 1:G:84:ASN:ND2   | 1:G:84:ASN:C     | 2.67                     | 0.52              |
| 1:G:221:TYR:OH   | 1:G:250:GLY:HA3  | 2.08                     | 0.52              |
| 3:L:103:ILE:HD11 | 3:L:115:ILE:HB   | 1.90                     | 0.52              |
| 2:B:162:LEU:HD21 | 2:B:174:ILE:HG23 | 1.91                     | 0.52              |
| 1:C:117:PRO:C    | 1:C:119:PHE:H    | 2.16                     | 0.52              |
| 1:G:229:THR:O    | 1:G:230:ASN:CB   | 2.57                     | 0.52              |
| 1:A:518:ASN:HD22 | 1:A:533:GLN:HG3  | 1.73                     | 0.52              |
| 2:B:111:LEU:O    | 2:B:111:LEU:HD23 | 2.09                     | 0.52              |
| 1:C:18:ARG:NH2   | 2:D:288:ILE:HD12 | 2.23                     | 0.52              |
| 1:C:527:GLN:OE1  | 2:D:302:VAL:HG13 | 2.10                     | 0.52              |
| 3:L:155:THR:O    | 3:L:158:ASP:HB2  | 2.08                     | 0.52              |
| 1:A:15:ARG:HG3   | 1:A:15:ARG:HH11  | 1.74                     | 0.52              |
| 1:C:235:LYS:HB2  | 1:C:239:GLU:CD   | 2.34                     | 0.52              |
| 1:C:481:GLU:OE2  | 1:C:525:MET:HE3  | 2.09                     | 0.52              |
| 3:J:117:ILE:HD13 | 3:J:126:ILE:HG12 | 1.91                     | 0.52              |
| 1:E:39:THR:O     | 1:E:43:THR:HB    | 2.09                     | 0.52              |
| 1:G:19:LEU:HD21  | 2:H:290:PRO:HB2  | 1.92                     | 0.52              |
| 1:G:34:CYS:HB2   | 1:G:123:PHE:CG   | 2.43                     | 0.52              |
| 2:H:127:ILE:HG13 | 2:H:128:GLN:NE2  | 2.24                     | 0.52              |
| 1:A:47:LYS:HD3   | 1:A:51:LEU:HD11  | 1.91                     | 0.52              |
| 2:B:335:PHE:HE2  | 3:I:170:VAL:HG21 | 1.75                     | 0.52              |
| 2:B:361:LEU:CG   | 2:B:704:LEU:HA   | 2.40                     | 0.52              |
| 3:I:107:THR:HG23 | 3:I:109:THR:H    | 1.74                     | 0.52              |
| 1:C:309:ARG:HD2  | 1:C:313:GLU:HG2  | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:197:THR:HG22 | 2:D:198:ALA:N    | 2.24                     | 0.52              |
| 1:E:117:PRO:C    | 1:E:119:PHE:H    | 2.16                     | 0.52              |
| 2:F:111:LEU:O    | 2:F:111:LEU:HD23 | 2.09                     | 0.52              |
| 2:F:158:LEU:CD1  | 2:F:177:LEU:HB2  | 2.40                     | 0.52              |
| 2:F:393:TYR:HB3  | 2:F:606:ARG:CB   | 2.39                     | 0.52              |
| 1:G:47:LYS:HD3   | 1:G:51:LEU:HD11  | 1.91                     | 0.52              |
| 3:L:108:LEU:HG   | 3:L:108:LEU:O    | 2.09                     | 0.52              |
| 2:B:901:VAL:O    | 2:B:902:ALA:C    | 2.51                     | 0.52              |
| 3:I:108:LEU:HG   | 3:I:108:LEU:O    | 2.08                     | 0.52              |
| 1:C:60:ILE:HD11  | 1:C:119:PHE:HE2  | 1.75                     | 0.52              |
| 1:G:229:THR:HG22 | 1:G:231:GLY:N    | 2.25                     | 0.52              |
| 1:G:232:ARG:CB   | 1:G:234:PRO:HD3  | 2.33                     | 0.52              |
| 2:H:127:ILE:HG12 | 4:H:8:ATP:HN62   | 1.73                     | 0.52              |
| 4:H:8:ATP:O1A    | 4:H:8:ATP:O2B    | 2.28                     | 0.52              |
| 1:A:185:LEU:O    | 1:A:188:PRO:HD3  | 2.09                     | 0.52              |
| 2:B:195:GLY:O    | 2:B:196:MET:HG3  | 2.09                     | 0.52              |
| 1:C:407:ILE:O    | 1:C:409:LYS:N    | 2.41                     | 0.52              |
| 1:E:235:LYS:HB2  | 1:E:239:GLU:CD   | 2.33                     | 0.52              |
| 1:E:489:GLU:O    | 1:E:489:GLU:HG2  | 2.10                     | 0.52              |
| 2:F:136:ARG:HG2  | 2:F:136:ARG:HH11 | 1.75                     | 0.52              |
| 3:K:108:LEU:O    | 3:K:108:LEU:HG   | 2.09                     | 0.52              |
| 1:G:244:ARG:HD3  | 1:G:269:ILE:CG2  | 2.39                     | 0.52              |
| 1:A:192:LEU:HG   | 1:A:196:PHE:CE1  | 2.45                     | 0.52              |
| 1:E:533:GLN:O    | 1:E:534:LEU:CB   | 2.58                     | 0.52              |
| 2:F:197:THR:HG22 | 2:F:198:ALA:N    | 2.24                     | 0.52              |
| 2:H:54:ILE:HD12  | 2:H:154:ILE:HG13 | 1.92                     | 0.52              |
| 2:H:64:LEU:HD11  | 2:H:77:VAL:HG21  | 1.91                     | 0.52              |
| 3:L:143:LEU:HB3  | 3:L:150:MET:HE2  | 1.90                     | 0.52              |
| 2:B:342:ASN:HD22 | 2:B:342:ASN:N    | 2.02                     | 0.52              |
| 1:C:489:GLU:HG2  | 1:C:489:GLU:O    | 2.10                     | 0.52              |
| 2:D:606:ARG:O    | 2:D:608:ARG:N    | 2.43                     | 0.52              |
| 1:E:481:GLU:OE2  | 1:E:525:MET:HE3  | 2.10                     | 0.52              |
| 2:H:213:PHE:CB   | 2:H:218:ILE:HD11 | 2.40                     | 0.52              |
| 2:H:394:LEU:HG   | 2:H:396:SER:HB3  | 1.92                     | 0.52              |
| 2:B:239:LYS:HG2  | 1:E:448:TYR:CZ   | 2.45                     | 0.52              |
| 1:C:47:LYS:HD3   | 1:C:51:LEU:HD11  | 1.91                     | 0.52              |
| 1:C:50:VAL:HG13  | 1:C:100:VAL:HG21 | 1.92                     | 0.52              |
| 1:E:309:ARG:HD2  | 1:E:313:GLU:HG2  | 1.93                     | 0.52              |
| 2:H:603:ILE:O    | 2:H:607:THR:N    | 2.43                     | 0.52              |
| 1:A:261:ASP:O    | 1:A:262:GLU:HG2  | 2.10                     | 0.51              |
| 1:A:293:ARG:HG2  | 1:A:305:TRP:CD1  | 2.45                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:307:LEU:HB3  | 1:A:383:LEU:HD21 | 1.91                     | 0.51              |
| 2:D:908:GLN:O    | 2:D:909:THR:C    | 2.51                     | 0.51              |
| 2:F:394:LEU:CD2  | 2:F:396:SER:HB3  | 2.40                     | 0.51              |
| 4:F:7:ATP:H3'    | 4:F:7:ATP:O1B    | 2.10                     | 0.51              |
| 1:G:422:GLU:H    | 1:G:422:GLU:CD   | 2.17                     | 0.51              |
| 2:H:80:MET:HG2   | 4:H:8:ATP:N3     | 2.25                     | 0.51              |
| 2:B:158:LEU:CD1  | 2:B:177:LEU:HB2  | 2.40                     | 0.51              |
| 3:I:155:THR:HG22 | 3:I:158:ASP:CG   | 2.35                     | 0.51              |
| 2:D:361:LEU:CG   | 2:D:704:LEU:HA   | 2.39                     | 0.51              |
| 2:D:371:SER:O    | 2:D:373:SER:N    | 2.43                     | 0.51              |
| 2:F:900:ALA:O    | 2:F:901:VAL:CB   | 2.58                     | 0.51              |
| 3:K:155:THR:O    | 3:K:158:ASP:HB2  | 2.10                     | 0.51              |
| 2:H:46:LEU:O     | 2:H:73:ARG:HB2   | 2.10                     | 0.51              |
| 2:H:393:TYR:HB3  | 2:H:606:ARG:CB   | 2.40                     | 0.51              |
| 1:A:117:PRO:C    | 1:A:119:PHE:H    | 2.19                     | 0.51              |
| 2:D:342:ASN:HD22 | 2:D:342:ASN:N    | 2.01                     | 0.51              |
| 2:F:15:GLY:HA2   | 2:F:18:ASN:OD1   | 2.10                     | 0.51              |
| 1:G:41:THR:O     | 1:G:45:ILE:HG13  | 2.11                     | 0.51              |
| 1:A:236:THR:O    | 1:A:237:TYR:CD1  | 2.64                     | 0.51              |
| 3:I:103:ILE:CD1  | 3:I:115:ILE:HB   | 2.40                     | 0.51              |
| 2:D:342:ASN:H    | 2:D:342:ASN:ND2  | 2.07                     | 0.51              |
| 3:J:103:ILE:CD1  | 3:J:115:ILE:HB   | 2.41                     | 0.51              |
| 1:E:244:ARG:HD3  | 1:E:269:ILE:CG2  | 2.40                     | 0.51              |
| 2:F:16:ARG:NH2   | 2:F:116:PRO:HB2  | 2.24                     | 0.51              |
| 1:G:235:LYS:HB2  | 1:G:239:GLU:CD   | 2.34                     | 0.51              |
| 1:G:416:MET:C    | 1:G:418:ASN:H    | 2.19                     | 0.51              |
| 2:B:237:TRP:CD2  | 2:B:242:PRO:HG2  | 2.45                     | 0.51              |
| 1:E:15:ARG:NH1   | 4:F:7:ATP:O1G    | 2.44                     | 0.51              |
| 2:F:342:ASN:HD22 | 2:F:342:ASN:N    | 2.01                     | 0.51              |
| 2:F:603:ILE:O    | 2:F:607:THR:N    | 2.43                     | 0.51              |
| 1:G:317:LYS:HB3  | 1:G:318:GLU:OE1  | 2.10                     | 0.51              |
| 1:A:309:ARG:HD2  | 1:A:313:GLU:HG2  | 1.93                     | 0.51              |
| 2:B:393:TYR:HB3  | 2:B:606:ARG:CB   | 2.41                     | 0.51              |
| 1:G:16:GLN:CB    | 2:H:292:VAL:HG12 | 2.41                     | 0.51              |
| 2:H:56:ALA:N     | 2:H:79:ASP:OD1   | 2.43                     | 0.51              |
| 2:H:87:ASN:HB3   | 2:H:91:GLN:NE2   | 2.26                     | 0.51              |
| 2:H:197:THR:HG21 | 2:H:320:ASN:HB3  | 1.93                     | 0.51              |
| 1:A:236:THR:O    | 1:A:237:TYR:HD1  | 1.92                     | 0.51              |
| 1:A:416:MET:C    | 1:A:418:ASN:H    | 2.19                     | 0.51              |
| 2:B:15:GLY:HA2   | 2:B:18:ASN:OD1   | 2.11                     | 0.51              |
| 1:C:15:ARG:HH11  | 1:C:15:ARG:HG3   | 1.76                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:259:PRO:CA   | 1:C:260:GLU:HG2  | 2.40                     | 0.51              |
| 1:E:474:VAL:O    | 1:E:475:LYS:C    | 2.52                     | 0.51              |
| 2:F:908:GLN:O    | 2:F:909:THR:C    | 2.54                     | 0.51              |
| 3:K:117:ILE:HD11 | 3:K:126:ILE:HG23 | 1.92                     | 0.51              |
| 3:K:150:MET:CE   | 3:K:167:LEU:HD13 | 2.41                     | 0.51              |
| 1:G:366:GLN:C    | 1:G:368:ILE:N    | 2.69                     | 0.51              |
| 2:B:316:ILE:H    | 2:B:316:ILE:CD1  | 2.10                     | 0.51              |
| 2:D:16:ARG:NH2   | 2:D:116:PRO:HB2  | 2.25                     | 0.51              |
| 2:F:13:TRP:CD1   | 2:F:13:TRP:C     | 2.88                     | 0.51              |
| 2:F:46:LEU:O     | 2:F:73:ARG:HB2   | 2.11                     | 0.51              |
| 1:G:84:ASN:C     | 1:G:84:ASN:HD22  | 2.17                     | 0.51              |
| 1:G:112:LEU:C    | 1:G:114:ASP:N    | 2.68                     | 0.51              |
| 1:G:481:GLU:OE2  | 1:G:525:MET:HE3  | 2.11                     | 0.51              |
| 2:H:90:ARG:HH11  | 2:H:90:ARG:HG2   | 1.74                     | 0.51              |
| 2:H:96:PRO:O     | 2:H:99:ILE:HG13  | 2.11                     | 0.51              |
| 2:H:178:ILE:N    | 2:H:178:ILE:HD12 | 2.25                     | 0.51              |
| 2:B:59:LEU:HD12  | 3:I:176:GLY:CA   | 2.41                     | 0.51              |
| 3:I:150:MET:CE   | 3:I:167:LEU:HD13 | 2.41                     | 0.51              |
| 1:C:166:ILE:HD11 | 1:C:508:ILE:HD13 | 1.93                     | 0.51              |
| 1:C:416:MET:C    | 1:C:418:ASN:H    | 2.18                     | 0.51              |
| 2:D:111:LEU:HD23 | 2:D:111:LEU:O    | 2.10                     | 0.51              |
| 2:F:193:LEU:O    | 2:F:194:PRO:C    | 2.54                     | 0.51              |
| 2:F:380:ALA:CB   | 2:F:394:LEU:HB2  | 2.40                     | 0.51              |
| 1:G:260:GLU:HB3  | 1:G:261:ASP:OD1  | 2.10                     | 0.51              |
| 2:H:232:VAL:HG11 | 2:H:263:LYS:HB2  | 1.93                     | 0.51              |
| 3:L:107:THR:HG22 | 3:L:111:LYS:N    | 2.26                     | 0.51              |
| 3:L:117:ILE:HD11 | 3:L:126:ILE:HG23 | 1.92                     | 0.51              |
| 1:C:244:ARG:HD3  | 1:C:269:ILE:CG2  | 2.41                     | 0.51              |
| 2:D:54:ILE:HD12  | 2:D:154:ILE:HG13 | 1.93                     | 0.51              |
| 3:J:155:THR:O    | 3:J:158:ASP:HB2  | 2.11                     | 0.51              |
| 1:E:232:ARG:CB   | 1:E:234:PRO:HD3  | 2.34                     | 0.51              |
| 1:E:317:LYS:HB3  | 1:E:318:GLU:OE1  | 2.11                     | 0.51              |
| 2:F:320:ASN:O    | 2:F:321:TYR:HB2  | 2.11                     | 0.51              |
| 3:K:107:THR:HG22 | 3:K:111:LYS:N    | 2.26                     | 0.51              |
| 1:C:140:ALA:HA   | 1:C:150:LEU:HD22 | 1.93                     | 0.50              |
| 2:F:360:LYS:N    | 2:F:363:GLU:OE1  | 2.44                     | 0.50              |
| 1:A:19:LEU:HD21  | 2:B:290:PRO:HB2  | 1.93                     | 0.50              |
| 2:D:178:ILE:HG21 | 2:D:303:CYS:HB3  | 1.93                     | 0.50              |
| 1:E:163:ARG:HG2  | 1:E:163:ARG:NH1  | 2.24                     | 0.50              |
| 1:G:163:ARG:HG2  | 1:G:163:ARG:NH1  | 2.24                     | 0.50              |
| 2:H:197:THR:HG22 | 2:H:198:ALA:N    | 2.25                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:181:GLU:OE1  | 1:A:181:GLU:HA   | 2.10                     | 0.50              |
| 1:A:489:GLU:H    | 2:B:19:HIS:CD2   | 2.29                     | 0.50              |
| 2:B:320:ASN:O    | 2:B:321:TYR:HB2  | 2.12                     | 0.50              |
| 1:C:236:THR:O    | 1:C:237:TYR:CD1  | 2.65                     | 0.50              |
| 1:C:317:LYS:HB3  | 1:C:318:GLU:OE1  | 2.11                     | 0.50              |
| 1:C:447:ASN:ND2  | 2:D:26:ARG:HE    | 2.09                     | 0.50              |
| 2:F:371:SER:O    | 2:F:373:SER:N    | 2.44                     | 0.50              |
| 1:G:489:GLU:O    | 1:G:489:GLU:HG2  | 2.12                     | 0.50              |
| 3:L:105:VAL:HG13 | 3:L:105:VAL:O    | 2.11                     | 0.50              |
| 2:B:136:ARG:HG2  | 2:B:136:ARG:HH11 | 1.76                     | 0.50              |
| 2:D:15:GLY:HA2   | 2:D:18:ASN:OD1   | 2.10                     | 0.50              |
| 2:D:33:PRO:C     | 2:D:35:PHE:H     | 2.18                     | 0.50              |
| 2:D:213:PHE:CB   | 2:D:218:ILE:HD11 | 2.40                     | 0.50              |
| 2:F:361:LEU:CG   | 2:F:704:LEU:HA   | 2.40                     | 0.50              |
| 3:K:107:THR:HG23 | 3:K:109:THR:H    | 1.76                     | 0.50              |
| 1:G:47:LYS:O     | 1:G:51:LEU:HD12  | 2.11                     | 0.50              |
| 1:G:140:ALA:HA   | 1:G:150:LEU:HD22 | 1.94                     | 0.50              |
| 1:G:309:ARG:HD2  | 1:G:313:GLU:HG2  | 1.94                     | 0.50              |
| 2:H:49:CYS:HA    | 2:H:139:HIS:CD2  | 2.46                     | 0.50              |
| 2:H:217:THR:CG2  | 2:H:223:ARG:HH22 | 2.24                     | 0.50              |
| 1:A:396:ARG:HH11 | 1:A:533:GLN:NE2  | 2.10                     | 0.50              |
| 1:C:163:ARG:HG2  | 1:C:163:ARG:NH1  | 2.25                     | 0.50              |
| 2:D:56:ALA:N     | 2:D:79:ASP:OD1   | 2.44                     | 0.50              |
| 3:J:105:VAL:HG13 | 3:J:105:VAL:O    | 2.11                     | 0.50              |
| 1:E:527:GLN:OE1  | 2:F:302:VAL:HG13 | 2.11                     | 0.50              |
| 1:G:60:ILE:HD11  | 1:G:119:PHE:HE2  | 1.76                     | 0.50              |
| 2:H:191:VAL:H    | 2:H:320:ASN:HA   | 1.77                     | 0.50              |
| 2:B:62:GLU:HG2   | 2:B:297:ALA:HA   | 1.93                     | 0.50              |
| 1:C:84:ASN:HD22  | 1:C:84:ASN:C     | 2.19                     | 0.50              |
| 2:D:377:LYS:O    | 2:D:378:SER:C    | 2.54                     | 0.50              |
| 1:E:47:LYS:HD3   | 1:E:51:LEU:HD11  | 1.93                     | 0.50              |
| 1:G:47:LYS:C     | 1:G:47:LYS:HD2   | 2.37                     | 0.50              |
| 1:G:157:GLY:HA3  | 1:G:485:TYR:CG   | 2.46                     | 0.50              |
| 1:G:353:ASP:O    | 1:G:357:VAL:HG23 | 2.11                     | 0.50              |
| 2:D:62:GLU:HG2   | 2:D:297:ALA:HA   | 1.94                     | 0.50              |
| 2:D:335:PHE:CE2  | 3:J:170:VAL:HG21 | 2.47                     | 0.50              |
| 2:F:85:VAL:HG13  | 2:F:86:SER:N     | 2.27                     | 0.50              |
| 1:G:488:ALA:C    | 1:G:490:PRO:HD3  | 2.36                     | 0.50              |
| 2:H:235:LEU:O    | 2:H:238:PRO:HD2  | 2.12                     | 0.50              |
| 2:H:342:ASN:HD22 | 2:H:342:ASN:N    | 2.03                     | 0.50              |
| 1:A:227:SER:C    | 1:A:229:THR:H    | 2.20                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:64:LEU:HD21  | 2:B:77:VAL:CG2   | 2.42                     | 0.50              |
| 1:C:128:ALA:HB1  | 1:C:131:LEU:HD11 | 1.93                     | 0.50              |
| 2:D:217:THR:CG2  | 2:D:223:ARG:HH22 | 2.25                     | 0.50              |
| 1:E:112:LEU:C    | 1:E:114:ASP:N    | 2.68                     | 0.50              |
| 1:E:244:ARG:HD3  | 1:E:269:ILE:HG23 | 1.93                     | 0.50              |
| 2:F:126:LYS:HA   | 4:F:7:ATP:C2     | 2.47                     | 0.50              |
| 2:F:342:ASN:H    | 2:F:342:ASN:ND2  | 2.07                     | 0.50              |
| 1:G:244:ARG:HD3  | 1:G:269:ILE:HG23 | 1.93                     | 0.50              |
| 1:A:140:ALA:HA   | 1:A:150:LEU:HD22 | 1.94                     | 0.50              |
| 1:A:166:ILE:HD11 | 1:A:508:ILE:HD13 | 1.94                     | 0.50              |
| 1:A:447:ASN:HD22 | 2:B:26:ARG:HH21  | 1.60                     | 0.50              |
| 2:B:164:TYR:CE2  | 2:B:169:LEU:HB2  | 2.45                     | 0.50              |
| 2:B:199:CYS:HG   | 2:B:343:CYS:HG   | 1.59                     | 0.50              |
| 2:B:371:SER:O    | 2:B:373:SER:N    | 2.45                     | 0.50              |
| 1:C:474:VAL:O    | 1:C:475:LYS:C    | 2.55                     | 0.50              |
| 3:K:105:VAL:O    | 3:K:105:VAL:HG13 | 2.12                     | 0.50              |
| 1:G:39:THR:O     | 1:G:43:THR:HB    | 2.12                     | 0.50              |
| 1:G:46:LEU:HD21  | 1:G:57:PHE:CD1   | 2.47                     | 0.50              |
| 2:H:33:PRO:C     | 2:H:35:PHE:H     | 2.20                     | 0.50              |
| 2:H:377:LYS:O    | 2:H:378:SER:C    | 2.54                     | 0.50              |
| 1:A:37:ASN:HB2   | 1:A:129:THR:O    | 2.12                     | 0.49              |
| 1:A:489:GLU:HG2  | 1:A:489:GLU:O    | 2.12                     | 0.49              |
| 1:C:50:VAL:HA    | 1:C:54:ILE:HG22  | 1.94                     | 0.49              |
| 3:J:103:ILE:HD11 | 3:J:115:ILE:HB   | 1.93                     | 0.49              |
| 1:E:221:TYR:OH   | 1:E:250:GLY:HA3  | 2.11                     | 0.49              |
| 2:F:377:LYS:O    | 2:F:378:SER:C    | 2.55                     | 0.49              |
| 3:K:150:MET:HE1  | 3:K:167:LEU:CD2  | 2.26                     | 0.49              |
| 1:G:474:VAL:O    | 1:G:475:LYS:C    | 2.54                     | 0.49              |
| 2:H:15:GLY:HA2   | 2:H:18:ASN:OD1   | 2.11                     | 0.49              |
| 3:I:107:THR:HG22 | 3:I:111:LYS:N    | 2.26                     | 0.49              |
| 1:C:489:GLU:H    | 2:D:19:HIS:CD2   | 2.30                     | 0.49              |
| 2:D:360:LYS:N    | 2:D:363:GLU:OE1  | 2.45                     | 0.49              |
| 3:J:155:THR:HG22 | 3:J:158:ASP:CG   | 2.37                     | 0.49              |
| 1:E:251:ILE:HG23 | 1:E:262:GLU:CG   | 2.42                     | 0.49              |
| 2:F:267:ARG:HG2  | 2:F:267:ARG:NH1  | 2.15                     | 0.49              |
| 1:G:15:ARG:HH11  | 1:G:15:ARG:HG3   | 1.77                     | 0.49              |
| 2:H:195:GLY:O    | 2:H:196:MET:HG3  | 2.12                     | 0.49              |
| 1:A:481:GLU:OE2  | 1:A:525:MET:HE3  | 2.12                     | 0.49              |
| 2:B:380:ALA:O    | 2:B:904:VAL:HA   | 2.12                     | 0.49              |
| 1:C:236:THR:O    | 1:C:237:TYR:HD1  | 1.95                     | 0.49              |
| 2:D:85:VAL:HG13  | 2:D:86:SER:N     | 2.27                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:192:LEU:O    | 1:E:195:HIS:HB3  | 2.11                     | 0.49              |
| 2:F:213:PHE:CB   | 2:F:218:ILE:HD11 | 2.42                     | 0.49              |
| 3:K:161:ILE:O    | 3:K:162:LEU:HD23 | 2.12                     | 0.49              |
| 1:G:37:ASN:HB2   | 1:G:129:THR:O    | 2.12                     | 0.49              |
| 1:G:78:ARG:O     | 1:G:81:ILE:HG13  | 2.12                     | 0.49              |
| 1:G:227:SER:C    | 1:G:229:THR:H    | 2.21                     | 0.49              |
| 1:G:251:ILE:HG23 | 1:G:262:GLU:CG   | 2.42                     | 0.49              |
| 1:G:261:ASP:O    | 1:G:262:GLU:HG2  | 2.12                     | 0.49              |
| 1:A:39:THR:O     | 1:A:43:THR:HB    | 2.11                     | 0.49              |
| 2:B:73:ARG:HD3   | 2:B:117:ASN:O    | 2.12                     | 0.49              |
| 2:B:360:LYS:N    | 2:B:363:GLU:OE1  | 2.46                     | 0.49              |
| 2:B:908:GLN:O    | 2:B:909:THR:C    | 2.52                     | 0.49              |
| 2:D:162:LEU:HD21 | 2:D:174:ILE:HG23 | 1.94                     | 0.49              |
| 2:D:393:TYR:HB3  | 2:D:606:ARG:CB   | 2.42                     | 0.49              |
| 1:E:211:HIS:NE2  | 2:F:221:MET:HE1  | 2.26                     | 0.49              |
| 1:E:353:ASP:O    | 1:E:357:VAL:HG23 | 2.12                     | 0.49              |
| 1:E:503:GLN:OE1  | 1:E:503:GLN:HA   | 2.12                     | 0.49              |
| 2:F:235:LEU:O    | 2:F:238:PRO:HD2  | 2.12                     | 0.49              |
| 1:G:192:LEU:O    | 1:G:195:HIS:HB3  | 2.11                     | 0.49              |
| 1:A:41:THR:O     | 1:A:45:ILE:HG13  | 2.12                     | 0.49              |
| 2:B:49:CYS:HA    | 2:B:139:HIS:CD2  | 2.47                     | 0.49              |
| 1:C:38:ALA:O     | 1:C:85:ARG:HD3   | 2.11                     | 0.49              |
| 1:C:192:LEU:O    | 1:C:195:HIS:HB3  | 2.12                     | 0.49              |
| 1:C:253:LYS:CA   | 1:C:253:LYS:O    | 2.49                     | 0.49              |
| 1:C:533:GLN:O    | 1:C:534:LEU:CB   | 2.60                     | 0.49              |
| 2:D:123:HIS:O    | 2:D:125:ASN:N    | 2.46                     | 0.49              |
| 2:D:164:TYR:CE2  | 2:D:169:LEU:HB2  | 2.44                     | 0.49              |
| 2:D:232:VAL:HG11 | 2:D:263:LYS:HB2  | 1.95                     | 0.49              |
| 2:F:80:MET:HG2   | 4:F:7:ATP:C4     | 2.47                     | 0.49              |
| 2:H:139:HIS:O    | 2:H:176:PRO:HD2  | 2.13                     | 0.49              |
| 2:H:178:ILE:HG21 | 2:H:303:CYS:HB3  | 1.94                     | 0.49              |
| 1:C:34:CYS:HB2   | 1:C:123:PHE:CG   | 2.47                     | 0.49              |
| 1:C:84:ASN:C     | 1:C:84:ASN:ND2   | 2.69                     | 0.49              |
| 1:C:181:GLU:OE1  | 1:C:181:GLU:HA   | 2.13                     | 0.49              |
| 2:D:191:VAL:H    | 2:D:320:ASN:HA   | 1.77                     | 0.49              |
| 3:J:106:LYS:HG3  | 3:J:112:GLU:HB2  | 1.94                     | 0.49              |
| 1:E:34:CYS:HB2   | 1:E:123:PHE:CG   | 2.47                     | 0.49              |
| 1:E:112:LEU:C    | 1:E:114:ASP:H    | 2.20                     | 0.49              |
| 1:E:143:LEU:HD22 | 1:E:148:ILE:HG21 | 1.94                     | 0.49              |
| 1:E:444:GLY:HA2  | 1:E:449:GLN:HB2  | 1.95                     | 0.49              |
| 2:F:128:GLN:HE22 | 4:F:7:ATP:HN62   | 1.60                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:155:THR:HG22 | 3:K:158:ASP:CG   | 2.37                     | 0.49              |
| 1:A:192:LEU:O    | 1:A:195:HIS:HB3  | 2.12                     | 0.49              |
| 1:A:211:HIS:NE2  | 2:B:221:MET:HE1  | 2.27                     | 0.49              |
| 2:B:33:PRO:C     | 2:B:35:PHE:H     | 2.21                     | 0.49              |
| 2:B:156:GLY:O    | 2:B:157:MET:C    | 2.55                     | 0.49              |
| 2:B:199:CYS:SG   | 2:B:346:CYS:SG   | 3.10                     | 0.49              |
| 2:D:335:PHE:C    | 2:D:335:PHE:CD1  | 2.91                     | 0.49              |
| 1:E:293:ARG:HG2  | 1:E:305:TRP:CD1  | 2.48                     | 0.49              |
| 2:F:54:ILE:HD12  | 2:F:154:ILE:HG13 | 1.94                     | 0.49              |
| 2:F:62:GLU:HG2   | 2:F:297:ALA:HA   | 1.93                     | 0.49              |
| 2:F:394:LEU:HD11 | 2:F:396:SER:CB   | 2.43                     | 0.49              |
| 2:H:112:ASN:HD21 | 2:H:120:VAL:HB   | 1.77                     | 0.49              |
| 3:L:150:MET:CE   | 3:L:167:LEU:HD13 | 2.43                     | 0.49              |
| 1:A:488:ALA:C    | 1:A:490:PRO:HD3  | 2.38                     | 0.49              |
| 2:B:74:GLN:NE2   | 2:B:74:GLN:HA    | 2.28                     | 0.49              |
| 2:B:190:ARG:NH2  | 2:B:203:THR:OG1  | 2.45                     | 0.49              |
| 2:D:380:ALA:O    | 2:D:904:VAL:HA   | 2.13                     | 0.49              |
| 1:E:60:ILE:HD11  | 1:E:119:PHE:HE2  | 1.76                     | 0.49              |
| 2:F:33:PRO:C     | 2:F:35:PHE:H     | 2.20                     | 0.49              |
| 2:F:380:ALA:O    | 2:F:904:VAL:HA   | 2.13                     | 0.49              |
| 1:G:112:LEU:C    | 1:G:114:ASP:H    | 2.19                     | 0.49              |
| 2:H:241:GLN:HE21 | 2:H:246:GLY:H    | 1.61                     | 0.49              |
| 3:L:106:LYS:HG2  | 3:L:110:GLY:HA2  | 1.95                     | 0.49              |
| 1:A:244:ARG:HD3  | 1:A:269:ILE:CG2  | 2.42                     | 0.49              |
| 2:B:78:ILE:O     | 2:B:79:ASP:HB2   | 2.12                     | 0.49              |
| 2:B:132:ASP:O    | 2:B:133:THR:C    | 2.56                     | 0.49              |
| 2:B:235:LEU:O    | 2:B:238:PRO:HD2  | 2.11                     | 0.49              |
| 3:I:145:TYR:O    | 3:I:146:SER:C    | 2.55                     | 0.49              |
| 1:C:260:GLU:HB3  | 1:C:261:ASP:OD1  | 2.12                     | 0.49              |
| 1:C:430:ARG:NH1  | 1:C:430:ARG:HB3  | 2.28                     | 0.49              |
| 1:C:488:ALA:C    | 1:C:490:PRO:HD3  | 2.38                     | 0.49              |
| 2:D:141:ILE:HD12 | 2:D:158:LEU:HD11 | 1.93                     | 0.49              |
| 2:D:380:ALA:CB   | 2:D:394:LEU:HB2  | 2.42                     | 0.49              |
| 1:E:50:VAL:HA    | 1:E:54:ILE:HG22  | 1.94                     | 0.49              |
| 2:F:131:ASN:O    | 2:F:132:ASP:C    | 2.55                     | 0.49              |
| 2:F:190:ARG:NH2  | 2:F:203:THR:OG1  | 2.46                     | 0.49              |
| 1:G:166:ILE:HD11 | 1:G:508:ILE:HD13 | 1.93                     | 0.49              |
| 2:H:380:ALA:O    | 2:H:904:VAL:HA   | 2.12                     | 0.49              |
| 2:H:900:ALA:O    | 2:H:901:VAL:CB   | 2.61                     | 0.49              |
| 3:L:155:THR:HG22 | 3:L:158:ASP:CG   | 2.37                     | 0.49              |
| 1:A:112:LEU:C    | 1:A:114:ASP:H    | 2.21                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:58:GLY:N     | 2:B:91:GLN:HG2   | 2.19                     | 0.49              |
| 2:D:49:CYS:HA    | 2:D:139:HIS:CD2  | 2.48                     | 0.49              |
| 2:F:49:CYS:HA    | 2:F:139:HIS:CD2  | 2.48                     | 0.49              |
| 2:F:191:VAL:H    | 2:F:320:ASN:HA   | 1.78                     | 0.49              |
| 1:A:430:ARG:HB3  | 1:A:430:ARG:NH1  | 2.28                     | 0.48              |
| 2:B:236:GLN:HE22 | 2:B:263:LYS:HB3  | 1.78                     | 0.48              |
| 1:C:227:SER:C    | 1:C:229:THR:H    | 2.22                     | 0.48              |
| 1:C:252:LEU:O    | 1:C:259:PRO:N    | 2.46                     | 0.48              |
| 3:L:117:ILE:HD13 | 3:L:126:ILE:HG12 | 1.94                     | 0.48              |
| 2:B:335:PHE:CE2  | 3:I:170:VAL:HG21 | 2.48                     | 0.48              |
| 3:I:105:VAL:HG21 | 3:I:143:LEU:HD21 | 1.94                     | 0.48              |
| 1:C:18:ARG:CZ    | 2:D:288:ILE:HD12 | 2.42                     | 0.48              |
| 1:C:336:SER:OG   | 2:D:271:TYR:HD2  | 1.94                     | 0.48              |
| 2:D:241:GLN:NE2  | 2:D:246:GLY:H    | 2.11                     | 0.48              |
| 1:G:50:VAL:HA    | 1:G:54:ILE:HG22  | 1.94                     | 0.48              |
| 1:G:181:GLU:OE1  | 1:G:181:GLU:HA   | 2.13                     | 0.48              |
| 2:H:112:ASN:ND2  | 2:H:120:VAL:HB   | 2.28                     | 0.48              |
| 1:A:78:ARG:O     | 1:A:81:ILE:HG13  | 2.13                     | 0.48              |
| 1:C:112:LEU:C    | 1:C:114:ASP:H    | 2.20                     | 0.48              |
| 1:E:47:LYS:HD2   | 1:E:47:LYS:C     | 2.37                     | 0.48              |
| 1:E:177:ASP:O    | 1:E:178:ASN:HB2  | 2.13                     | 0.48              |
| 2:F:156:GLY:O    | 2:F:157:MET:C    | 2.54                     | 0.48              |
| 2:F:164:TYR:CE2  | 2:F:169:LEU:HB2  | 2.47                     | 0.48              |
| 2:F:183:GLU:HG3  | 2:F:289:ILE:CG2  | 2.43                     | 0.48              |
| 1:G:192:LEU:HG   | 1:G:196:PHE:CE1  | 2.48                     | 0.48              |
| 1:G:252:LEU:O    | 1:G:259:PRO:N    | 2.44                     | 0.48              |
| 2:H:355:PHE:O    | 2:H:356:SER:CB   | 2.61                     | 0.48              |
| 1:A:112:LEU:C    | 1:A:114:ASP:N    | 2.70                     | 0.48              |
| 1:A:244:ARG:HD3  | 1:A:269:ILE:HG23 | 1.95                     | 0.48              |
| 3:I:123:VAL:HA   | 3:I:126:ILE:HD12 | 1.95                     | 0.48              |
| 2:D:78:ILE:O     | 2:D:79:ASP:HB2   | 2.13                     | 0.48              |
| 2:D:320:ASN:O    | 2:D:321:TYR:HB2  | 2.13                     | 0.48              |
| 2:D:900:ALA:O    | 2:D:901:VAL:CB   | 2.61                     | 0.48              |
| 3:J:117:ILE:HD11 | 3:J:126:ILE:HG23 | 1.94                     | 0.48              |
| 1:E:15:ARG:HH11  | 1:E:15:ARG:HG3   | 1.79                     | 0.48              |
| 2:F:217:THR:CG2  | 2:F:223:ARG:HH22 | 2.27                     | 0.48              |
| 2:F:241:GLN:HE21 | 2:F:246:GLY:H    | 1.61                     | 0.48              |
| 1:G:264:ASN:N    | 1:G:264:ASN:ND2  | 2.61                     | 0.48              |
| 2:H:78:ILE:O     | 2:H:79:ASP:HB2   | 2.12                     | 0.48              |
| 3:L:101:MET:SD   | 3:L:162:LEU:HA   | 2.53                     | 0.48              |
| 1:A:50:VAL:HA    | 1:A:54:ILE:HG22  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:244:ARG:O    | 1:A:247:ILE:N    | 2.46                     | 0.48              |
| 1:A:261:ASP:O    | 1:A:262:GLU:CG   | 2.62                     | 0.48              |
| 1:A:307:LEU:CB   | 1:A:383:LEU:HD22 | 2.38                     | 0.48              |
| 2:H:85:VAL:HG13  | 2:H:86:SER:N     | 2.28                     | 0.48              |
| 2:H:232:VAL:O    | 2:H:232:VAL:HG12 | 2.12                     | 0.48              |
| 2:D:335:PHE:CZ   | 3:J:144:ILE:HD13 | 2.48                     | 0.48              |
| 3:J:107:THR:HG22 | 3:J:111:LYS:N    | 2.28                     | 0.48              |
| 2:F:80:MET:HE2   | 2:F:126:LYS:CB   | 2.43                     | 0.48              |
| 1:G:235:LYS:HB2  | 1:G:239:GLU:OE1  | 2.14                     | 0.48              |
| 1:A:177:ASP:O    | 1:A:178:ASN:HB2  | 2.13                     | 0.48              |
| 1:E:140:ALA:HA   | 1:E:150:LEU:HD22 | 1.96                     | 0.48              |
| 2:H:355:PHE:O    | 2:H:356:SER:OG   | 2.24                     | 0.48              |
| 1:A:157:GLY:HA3  | 1:A:485:TYR:CG   | 2.49                     | 0.48              |
| 2:B:30:PHE:N     | 2:B:30:PHE:CD1   | 2.82                     | 0.48              |
| 2:B:197:THR:CG2  | 2:B:198:ALA:N    | 2.77                     | 0.48              |
| 1:C:157:GLY:HA3  | 1:C:485:TYR:CG   | 2.49                     | 0.48              |
| 3:K:106:LYS:HG2  | 3:K:110:GLY:HA2  | 1.95                     | 0.48              |
| 2:H:32:HIS:CE1   | 2:H:33:PRO:HD2   | 2.48                     | 0.48              |
| 1:A:251:ILE:HG23 | 1:A:262:GLU:CG   | 2.44                     | 0.48              |
| 2:B:139:HIS:O    | 2:B:176:PRO:HD2  | 2.13                     | 0.48              |
| 2:B:377:LYS:O    | 2:B:378:SER:C    | 2.56                     | 0.48              |
| 1:C:112:LEU:C    | 1:C:114:ASP:N    | 2.70                     | 0.48              |
| 1:C:177:ASP:O    | 1:C:178:ASN:CB   | 2.61                     | 0.48              |
| 2:D:199:CYS:SG   | 2:D:346:CYS:SG   | 3.10                     | 0.48              |
| 2:D:394:LEU:CD2  | 2:D:396:SER:HB3  | 2.44                     | 0.48              |
| 1:E:335:ASP:HB3  | 1:E:338:LYS:HB2  | 1.96                     | 0.48              |
| 2:F:124:PHE:CD1  | 2:F:124:PHE:C    | 2.92                     | 0.48              |
| 1:G:236:THR:O    | 1:G:237:TYR:HD1  | 1.97                     | 0.48              |
| 3:L:107:THR:HG23 | 3:L:109:THR:H    | 1.78                     | 0.48              |
| 1:A:426:TYR:CZ   | 1:A:430:ARG:HD3  | 2.49                     | 0.48              |
| 2:B:191:VAL:H    | 2:B:320:ASN:HA   | 1.79                     | 0.48              |
| 1:C:35:LEU:HD23  | 1:C:46:LEU:HD22  | 1.95                     | 0.48              |
| 1:C:47:LYS:HD2   | 1:C:47:LYS:C     | 2.38                     | 0.48              |
| 2:D:87:ASN:HB3   | 2:D:91:GLN:NE2   | 2.29                     | 0.48              |
| 2:D:197:THR:HG21 | 2:D:320:ASN:HB3  | 1.96                     | 0.48              |
| 1:G:124:THR:HG22 | 1:G:125:VAL:HG23 | 1.96                     | 0.48              |
| 2:H:361:LEU:CG   | 2:H:704:LEU:HA   | 2.44                     | 0.48              |
| 1:A:34:CYS:HB2   | 1:A:123:PHE:CG   | 2.48                     | 0.47              |
| 1:A:221:TYR:CD2  | 1:A:247:ILE:HA   | 2.49                     | 0.47              |
| 2:B:312:THR:O    | 2:B:313:SER:HB2  | 2.14                     | 0.47              |
| 1:C:37:ASN:HB2   | 1:C:129:THR:O    | 2.13                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:106:LYS:HG2  | 3:J:110:GLY:HA2  | 1.96                     | 0.47              |
| 1:E:53:GLY:O     | 1:E:54:ILE:C     | 2.57                     | 0.47              |
| 1:E:489:GLU:H    | 2:F:19:HIS:CD2   | 2.32                     | 0.47              |
| 2:F:64:LEU:HD21  | 2:F:77:VAL:CG2   | 2.43                     | 0.47              |
| 3:K:103:ILE:HD12 | 3:K:103:ILE:O    | 2.14                     | 0.47              |
| 1:G:307:LEU:CD1  | 1:G:383:LEU:HD22 | 2.42                     | 0.47              |
| 1:A:84:ASN:C     | 1:A:84:ASN:HD22  | 2.22                     | 0.47              |
| 1:A:84:ASN:C     | 1:A:84:ASN:ND2   | 2.71                     | 0.47              |
| 2:B:13:TRP:CZ3   | 2:B:116:PRO:HG2  | 2.48                     | 0.47              |
| 2:B:325:ASN:HD22 | 2:B:326:ASP:N    | 2.12                     | 0.47              |
| 2:B:394:LEU:HG   | 2:B:396:SER:HB3  | 1.95                     | 0.47              |
| 1:C:244:ARG:HD3  | 1:C:269:ILE:HG23 | 1.95                     | 0.47              |
| 1:C:340:ILE:HD11 | 2:D:273:ILE:HG12 | 1.95                     | 0.47              |
| 2:D:30:PHE:N     | 2:D:30:PHE:CD1   | 2.82                     | 0.47              |
| 2:D:236:GLN:HE22 | 2:D:263:LYS:HB3  | 1.79                     | 0.47              |
| 3:J:101:MET:SD   | 3:J:162:LEU:HA   | 2.54                     | 0.47              |
| 1:E:227:SER:C    | 1:E:229:THR:H    | 2.23                     | 0.47              |
| 1:G:84:ASN:O     | 1:G:85:ARG:C     | 2.56                     | 0.47              |
| 1:A:285:ILE:HD11 | 1:A:388:ALA:CA   | 2.36                     | 0.47              |
| 2:B:356:SER:HA   | 2:B:357:PRO:HD3  | 1.55                     | 0.47              |
| 3:I:117:ILE:HD11 | 3:I:126:ILE:HG23 | 1.96                     | 0.47              |
| 1:C:16:GLN:CB    | 2:D:292:VAL:HG12 | 2.43                     | 0.47              |
| 2:D:112:ASN:ND2  | 2:D:120:VAL:HB   | 2.29                     | 0.47              |
| 2:D:136:ARG:HH11 | 2:D:136:ARG:HG2  | 1.79                     | 0.47              |
| 2:D:190:ARG:NH2  | 2:D:203:THR:OG1  | 2.47                     | 0.47              |
| 1:E:124:THR:HG22 | 1:E:125:VAL:HG23 | 1.96                     | 0.47              |
| 2:F:112:ASN:ND2  | 2:F:120:VAL:HB   | 2.28                     | 0.47              |
| 2:F:112:ASN:HD21 | 2:F:120:VAL:HB   | 1.79                     | 0.47              |
| 2:F:394:LEU:HD11 | 2:F:396:SER:HB3  | 1.97                     | 0.47              |
| 3:K:145:TYR:O    | 3:K:146:SER:C    | 2.58                     | 0.47              |
| 2:H:73:ARG:HD3   | 2:H:117:ASN:O    | 2.13                     | 0.47              |
| 3:L:106:LYS:HG3  | 3:L:112:GLU:HB2  | 1.96                     | 0.47              |
| 1:A:53:GLY:O     | 1:A:54:ILE:C     | 2.57                     | 0.47              |
| 1:A:503:GLN:OE1  | 1:A:503:GLN:HA   | 2.14                     | 0.47              |
| 2:B:124:PHE:HD1  | 2:B:124:PHE:C    | 2.22                     | 0.47              |
| 1:C:78:ARG:O     | 1:C:81:ILE:HG13  | 2.14                     | 0.47              |
| 1:C:415:SER:C    | 1:C:417:ASP:H    | 2.22                     | 0.47              |
| 1:C:496:PHE:CE1  | 2:D:298:VAL:HG13 | 2.50                     | 0.47              |
| 2:F:73:ARG:HD3   | 2:F:117:ASN:O    | 2.14                     | 0.47              |
| 1:G:236:THR:O    | 1:G:237:TYR:CD1  | 2.67                     | 0.47              |
| 1:G:462:THR:O    | 1:G:463:GLY:C    | 2.57                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:394:LEU:CD2  | 2:H:396:SER:HB3  | 2.44                     | 0.47              |
| 2:B:351:GLN:HB3  | 2:B:916:PHE:CB   | 2.44                     | 0.47              |
| 1:C:84:ASN:O     | 1:C:85:ARG:C     | 2.57                     | 0.47              |
| 2:F:132:ASP:O    | 2:F:133:THR:C    | 2.58                     | 0.47              |
| 1:G:211:HIS:O    | 1:G:338:LYS:HD2  | 2.15                     | 0.47              |
| 1:G:415:SER:C    | 1:G:417:ASP:H    | 2.22                     | 0.47              |
| 2:H:267:ARG:HH11 | 2:H:267:ARG:CG   | 2.17                     | 0.47              |
| 2:H:335:PHE:CD1  | 2:H:335:PHE:C    | 2.93                     | 0.47              |
| 2:B:162:LEU:HD22 | 2:B:169:LEU:HD11 | 1.97                     | 0.47              |
| 2:D:162:LEU:HD22 | 2:D:169:LEU:HD11 | 1.96                     | 0.47              |
| 2:D:193:LEU:O    | 2:D:194:PRO:C    | 2.58                     | 0.47              |
| 1:E:78:ARG:O     | 1:E:81:ILE:HG13  | 2.14                     | 0.47              |
| 1:E:157:GLY:HA3  | 1:E:485:TYR:CG   | 2.49                     | 0.47              |
| 1:E:426:TYR:CZ   | 1:E:430:ARG:HD3  | 2.49                     | 0.47              |
| 3:K:106:LYS:HG3  | 3:K:112:GLU:HB2  | 1.97                     | 0.47              |
| 1:G:307:LEU:CB   | 1:G:383:LEU:HD22 | 2.39                     | 0.47              |
| 1:A:128:ALA:HB1  | 1:A:131:LEU:HD11 | 1.96                     | 0.47              |
| 1:A:262:GLU:OE1  | 1:A:262:GLU:CA   | 2.63                     | 0.47              |
| 1:A:264:ASN:N    | 1:A:264:ASN:ND2  | 2.60                     | 0.47              |
| 1:A:415:SER:C    | 1:A:417:ASP:H    | 2.23                     | 0.47              |
| 2:B:293:ALA:O    | 2:B:294:SER:C    | 2.57                     | 0.47              |
| 2:B:394:LEU:HD11 | 2:B:396:SER:HB3  | 1.96                     | 0.47              |
| 3:I:106:LYS:HG3  | 3:I:112:GLU:HB2  | 1.97                     | 0.47              |
| 2:D:241:GLN:HE21 | 2:D:246:GLY:H    | 1.61                     | 0.47              |
| 1:E:45:ILE:CG1   | 1:E:498:GLY:HA2  | 2.44                     | 0.47              |
| 1:E:84:ASN:O     | 1:E:85:ARG:C     | 2.58                     | 0.47              |
| 2:F:78:ILE:O     | 2:F:79:ASP:HB2   | 2.15                     | 0.47              |
| 2:F:241:GLN:NE2  | 2:F:246:GLY:H    | 2.12                     | 0.47              |
| 2:F:312:THR:O    | 2:F:313:SER:HB2  | 2.14                     | 0.47              |
| 2:F:335:PHE:CD1  | 2:F:335:PHE:C    | 2.93                     | 0.47              |
| 2:F:392:LEU:HA   | 2:F:392:LEU:HD23 | 1.45                     | 0.47              |
| 3:K:105:VAL:HG11 | 3:K:130:VAL:CG2  | 2.41                     | 0.47              |
| 1:G:225:TRP:CE2  | 1:G:233:ILE:HG12 | 2.50                     | 0.47              |
| 1:G:489:GLU:H    | 2:H:19:HIS:CD2   | 2.33                     | 0.47              |
| 2:H:124:PHE:CD1  | 2:H:124:PHE:C    | 2.92                     | 0.47              |
| 2:H:124:PHE:C    | 2:H:124:PHE:HD1  | 2.22                     | 0.47              |
| 2:H:241:GLN:NE2  | 2:H:246:GLY:H    | 2.12                     | 0.47              |
| 1:A:143:LEU:HD22 | 1:A:148:ILE:HG21 | 1.96                     | 0.47              |
| 2:B:394:LEU:HD11 | 2:B:396:SER:CB   | 2.45                     | 0.47              |
| 2:D:139:HIS:O    | 2:D:176:PRO:HD2  | 2.14                     | 0.47              |
| 2:D:361:LEU:HD23 | 2:D:361:LEU:N    | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:30:PHE:CD1   | 2:F:30:PHE:N     | 2.83                     | 0.47              |
| 2:F:351:GLN:HB3  | 2:F:916:PHE:CB   | 2.45                     | 0.47              |
| 1:G:331:ASP:HB2  | 2:H:224:LEU:HD11 | 1.96                     | 0.47              |
| 1:G:447:ASN:HD22 | 2:H:26:ARG:HH21  | 1.61                     | 0.47              |
| 2:H:52:LEU:HD11  | 2:H:78:ILE:HG13  | 1.96                     | 0.47              |
| 2:H:314:ALA:O    | 2:H:315:TYR:CD1  | 2.67                     | 0.47              |
| 1:A:265:PHE:O    | 1:A:269:ILE:HG13 | 2.15                     | 0.47              |
| 2:B:146:ASP:HB3  | 4:B:5:ATP:H5'2   | 1.97                     | 0.47              |
| 2:B:148:ILE:O    | 2:B:149:ILE:C    | 2.58                     | 0.47              |
| 3:I:105:VAL:O    | 3:I:105:VAL:HG13 | 2.15                     | 0.47              |
| 3:I:106:LYS:HG2  | 3:I:110:GLY:HA2  | 1.96                     | 0.47              |
| 1:E:396:ARG:HH11 | 1:E:533:GLN:NE2  | 2.13                     | 0.47              |
| 2:F:394:LEU:HG   | 2:F:396:SER:HB3  | 1.96                     | 0.47              |
| 3:K:123:VAL:HA   | 3:K:126:ILE:HD12 | 1.97                     | 0.47              |
| 1:G:415:SER:O    | 1:G:417:ASP:N    | 2.48                     | 0.47              |
| 2:H:132:ASP:O    | 2:H:133:THR:C    | 2.58                     | 0.47              |
| 2:H:342:ASN:H    | 2:H:342:ASN:ND2  | 2.10                     | 0.47              |
| 3:L:113:ILE:HD11 | 3:L:130:VAL:HG13 | 1.97                     | 0.47              |
| 3:L:145:TYR:O    | 3:L:146:SER:C    | 2.58                     | 0.47              |
| 1:A:163:ARG:HG2  | 1:A:163:ARG:NH1  | 2.26                     | 0.47              |
| 1:A:211:HIS:O    | 1:A:338:LYS:HD2  | 2.15                     | 0.47              |
| 2:B:13:TRP:CD1   | 2:B:13:TRP:C     | 2.93                     | 0.47              |
| 2:B:193:LEU:O    | 2:B:194:PRO:C    | 2.57                     | 0.47              |
| 1:C:221:TYR:CD2  | 1:C:247:ILE:HA   | 2.50                     | 0.47              |
| 1:C:225:TRP:CE2  | 1:C:233:ILE:HG12 | 2.50                     | 0.47              |
| 1:C:357:VAL:O    | 1:C:361:VAL:HG23 | 2.14                     | 0.47              |
| 2:F:197:THR:HG21 | 2:F:320:ASN:HB3  | 1.96                     | 0.47              |
| 1:G:177:ASP:O    | 1:G:178:ASN:HB2  | 2.15                     | 0.47              |
| 1:G:218:ILE:HD11 | 1:G:268:ALA:O    | 2.14                     | 0.47              |
| 2:H:64:LEU:HD21  | 2:H:77:VAL:CG2   | 2.44                     | 0.47              |
| 2:H:190:ARG:NH2  | 2:H:203:THR:OG1  | 2.48                     | 0.47              |
| 2:H:356:SER:CB   | 2:H:359:ALA:HB3  | 2.45                     | 0.47              |
| 1:A:47:LYS:HD2   | 1:A:47:LYS:C     | 2.40                     | 0.46              |
| 1:A:84:ASN:O     | 1:A:85:ARG:C     | 2.58                     | 0.46              |
| 2:B:394:LEU:CD2  | 2:B:396:SER:HB3  | 2.45                     | 0.46              |
| 2:D:229:ILE:HG21 | 2:D:284:VAL:HB   | 1.96                     | 0.46              |
| 3:J:105:VAL:HG21 | 3:J:143:LEU:HD21 | 1.97                     | 0.46              |
| 1:G:335:ASP:HB3  | 1:G:338:LYS:HB2  | 1.97                     | 0.46              |
| 2:H:16:ARG:NH2   | 2:H:116:PRO:HB2  | 2.30                     | 0.46              |
| 2:H:126:LYS:HA   | 4:H:8:ATP:C2     | 2.50                     | 0.46              |
| 2:H:158:LEU:HD12 | 2:H:177:LEU:HB2  | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:351:GLN:HB3  | 2:H:916:PHE:CB   | 2.45                     | 0.46              |
| 3:L:103:ILE:HD12 | 3:L:103:ILE:O    | 2.15                     | 0.46              |
| 1:A:124:THR:HG22 | 1:A:125:VAL:HG23 | 1.97                     | 0.46              |
| 2:B:178:ILE:HG21 | 2:B:303:CYS:HB3  | 1.97                     | 0.46              |
| 2:B:236:GLN:NE2  | 2:B:263:LYS:HB3  | 2.30                     | 0.46              |
| 2:B:703:GLY:C    | 2:B:705:VAL:H    | 2.23                     | 0.46              |
| 2:D:158:LEU:CD1  | 2:D:177:LEU:HB2  | 2.44                     | 0.46              |
| 2:D:232:VAL:O    | 2:D:232:VAL:HG12 | 2.14                     | 0.46              |
| 1:E:441:ARG:HH21 | 1:E:453:ASP:CG   | 2.23                     | 0.46              |
| 2:F:212:ASN:HD22 | 2:F:212:ASN:HA   | 1.59                     | 0.46              |
| 2:F:236:GLN:HE22 | 2:F:263:LYS:HB3  | 1.79                     | 0.46              |
| 3:L:105:VAL:HG21 | 3:L:143:LEU:HD21 | 1.96                     | 0.46              |
| 1:A:33:VAL:CG2   | 1:A:54:ILE:HD11  | 2.46                     | 0.46              |
| 1:A:421:ASN:O    | 1:A:423:ILE:N    | 2.48                     | 0.46              |
| 2:B:54:ILE:HD12  | 2:B:154:ILE:HG13 | 1.98                     | 0.46              |
| 2:B:112:ASN:ND2  | 2:B:120:VAL:HB   | 2.30                     | 0.46              |
| 2:D:13:TRP:CZ3   | 2:D:116:PRO:HG2  | 2.49                     | 0.46              |
| 2:D:80:MET:HG2   | 4:D:6:ATP:N3     | 2.29                     | 0.46              |
| 2:D:335:PHE:CE1  | 2:D:337:ALA:HB2  | 2.49                     | 0.46              |
| 2:F:124:PHE:C    | 2:F:124:PHE:HD1  | 2.22                     | 0.46              |
| 3:K:105:VAL:HG21 | 3:K:143:LEU:HD21 | 1.97                     | 0.46              |
| 1:G:221:TYR:CD2  | 1:G:247:ILE:HA   | 2.50                     | 0.46              |
| 1:G:444:GLY:HA2  | 1:G:449:GLN:HB2  | 1.98                     | 0.46              |
| 2:B:124:PHE:C    | 2:B:124:PHE:CD1  | 2.92                     | 0.46              |
| 3:I:105:VAL:HG11 | 3:I:130:VAL:CG2  | 2.44                     | 0.46              |
| 1:C:239:GLU:O    | 1:C:240:LYS:C    | 2.59                     | 0.46              |
| 1:C:299:LYS:HA   | 1:C:368:ILE:CG2  | 2.46                     | 0.46              |
| 1:C:396:ARG:HH11 | 1:C:533:GLN:NE2  | 2.12                     | 0.46              |
| 2:D:73:ARG:HD3   | 2:D:117:ASN:O    | 2.15                     | 0.46              |
| 2:D:197:THR:CG2  | 2:D:198:ALA:N    | 2.78                     | 0.46              |
| 3:J:107:THR:HG23 | 3:J:109:THR:H    | 1.79                     | 0.46              |
| 1:E:262:GLU:OE1  | 1:E:262:GLU:CA   | 2.64                     | 0.46              |
| 1:G:435:PHE:C    | 1:G:435:PHE:CD2  | 2.94                     | 0.46              |
| 1:A:143:LEU:HD13 | 1:A:150:LEU:HD13 | 1.96                     | 0.46              |
| 1:A:253:LYS:O    | 1:A:260:GLU:CD   | 2.59                     | 0.46              |
| 1:A:355:ALA:O    | 1:A:358:GLY:N    | 2.48                     | 0.46              |
| 1:A:357:VAL:O    | 1:A:361:VAL:HG23 | 2.16                     | 0.46              |
| 2:B:158:LEU:HD12 | 2:B:177:LEU:HB2  | 1.98                     | 0.46              |
| 1:C:175:HIS:HD2  | 1:C:512:GLN:O    | 1.99                     | 0.46              |
| 1:C:253:LYS:O    | 1:C:260:GLU:CD   | 2.58                     | 0.46              |
| 2:D:112:ASN:HD21 | 2:D:120:VAL:HB   | 1.80                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:128:ALA:HB1  | 1:E:131:LEU:HD11 | 1.98                     | 0.46              |
| 1:E:143:LEU:HD13 | 1:E:150:LEU:HD13 | 1.95                     | 0.46              |
| 2:F:340:LYS:HB3  | 2:F:342:ASN:ND2  | 2.30                     | 0.46              |
| 2:B:229:ILE:HD12 | 2:B:284:VAL:HG21 | 1.97                     | 0.46              |
| 2:B:232:VAL:HG11 | 2:B:263:LYS:HB2  | 1.97                     | 0.46              |
| 1:C:15:ARG:HD3   | 1:C:15:ARG:HA    | 1.82                     | 0.46              |
| 1:C:47:LYS:O     | 1:C:51:LEU:HD12  | 2.16                     | 0.46              |
| 1:E:211:HIS:O    | 1:E:338:LYS:HD2  | 2.15                     | 0.46              |
| 1:E:288:ILE:HG23 | 1:E:305:TRP:CZ3  | 2.51                     | 0.46              |
| 1:E:488:ALA:C    | 1:E:490:PRO:HD3  | 2.40                     | 0.46              |
| 2:F:182:THR:CG2  | 2:F:183:GLU:N    | 2.77                     | 0.46              |
| 1:G:140:ALA:HA   | 1:G:150:LEU:CD2  | 2.45                     | 0.46              |
| 2:H:30:PHE:N     | 2:H:30:PHE:CD1   | 2.83                     | 0.46              |
| 2:H:340:LYS:HB3  | 2:H:342:ASN:ND2  | 2.30                     | 0.46              |
| 1:A:335:ASP:HB3  | 1:A:338:LYS:HB2  | 1.98                     | 0.46              |
| 1:A:462:THR:O    | 1:A:463:GLY:C    | 2.59                     | 0.46              |
| 2:B:127:ILE:HG13 | 2:B:128:GLN:NE2  | 2.30                     | 0.46              |
| 2:B:900:ALA:O    | 2:B:901:VAL:CB   | 2.64                     | 0.46              |
| 1:C:19:LEU:HD21  | 2:D:290:PRO:HB2  | 1.98                     | 0.46              |
| 1:C:40:ALA:HB3   | 1:C:489:GLU:CD   | 2.41                     | 0.46              |
| 3:J:103:ILE:HD12 | 3:J:103:ILE:O    | 2.16                     | 0.46              |
| 3:J:161:ILE:O    | 3:J:162:LEU:HD23 | 2.15                     | 0.46              |
| 2:H:371:SER:C    | 2:H:373:SER:N    | 2.74                     | 0.46              |
| 1:A:15:ARG:HA    | 1:A:15:ARG:HD3   | 1.84                     | 0.46              |
| 3:I:103:ILE:HD12 | 3:I:103:ILE:C    | 2.40                     | 0.46              |
| 1:C:33:VAL:CG2   | 1:C:54:ILE:HD11  | 2.44                     | 0.46              |
| 2:D:236:GLN:NE2  | 2:D:263:LYS:HB3  | 2.31                     | 0.46              |
| 2:D:394:LEU:HD11 | 2:D:396:SER:CB   | 2.46                     | 0.46              |
| 1:E:215:ILE:HD12 | 1:E:342:LEU:HD21 | 1.98                     | 0.46              |
| 1:E:218:ILE:HD11 | 1:E:268:ALA:O    | 2.15                     | 0.46              |
| 1:E:221:TYR:CD2  | 1:E:247:ILE:HA   | 2.51                     | 0.46              |
| 1:E:244:ARG:O    | 1:E:247:ILE:N    | 2.48                     | 0.46              |
| 1:E:259:PRO:C    | 1:E:260:GLU:CG   | 2.88                     | 0.46              |
| 1:E:336:SER:OG   | 2:F:271:TYR:HD2  | 1.99                     | 0.46              |
| 1:E:430:ARG:NH1  | 1:E:430:ARG:HB3  | 2.30                     | 0.46              |
| 2:F:197:THR:CG2  | 2:F:198:ALA:N    | 2.78                     | 0.46              |
| 2:H:148:ILE:O    | 2:H:149:ILE:C    | 2.59                     | 0.46              |
| 2:H:222:PRO:HD2  | 2:H:271:TYR:CD2  | 2.50                     | 0.46              |
| 3:L:123:VAL:HA   | 3:L:126:ILE:HD12 | 1.97                     | 0.46              |
| 1:A:38:ALA:O     | 1:A:85:ARG:HD3   | 2.16                     | 0.46              |
| 1:A:139:LEU:C    | 1:A:141:ASP:H    | 2.24                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:335:PHE:CD1  | 2:B:335:PHE:C    | 2.94                     | 0.46              |
| 1:C:96:LEU:HD23  | 2:D:95:ARG:HH21  | 1.79                     | 0.46              |
| 1:C:426:TYR:CZ   | 1:C:430:ARG:HD3  | 2.51                     | 0.46              |
| 2:F:74:GLN:NE2   | 2:F:74:GLN:HA    | 2.31                     | 0.46              |
| 2:F:123:HIS:O    | 2:F:125:ASN:N    | 2.47                     | 0.46              |
| 2:F:267:ARG:HH11 | 2:F:267:ARG:CG   | 2.19                     | 0.46              |
| 3:L:105:VAL:HG11 | 3:L:130:VAL:CG2  | 2.43                     | 0.46              |
| 2:B:49:CYS:HA    | 2:B:139:HIS:HD2  | 1.80                     | 0.46              |
| 2:B:262:GLN:NE2  | 1:E:66:SER:OG    | 2.49                     | 0.46              |
| 3:J:107:THR:OG1  | 3:J:108:LEU:N    | 2.49                     | 0.46              |
| 2:F:703:GLY:C    | 2:F:705:VAL:H    | 2.23                     | 0.46              |
| 2:H:271:TYR:N    | 2:H:271:TYR:CD1  | 2.84                     | 0.46              |
| 2:B:112:ASN:HD21 | 2:B:120:VAL:HB   | 1.81                     | 0.45              |
| 2:B:335:PHE:CZ   | 3:I:144:ILE:HD13 | 2.51                     | 0.45              |
| 1:C:218:ILE:HD11 | 1:C:268:ALA:O    | 2.15                     | 0.45              |
| 1:C:265:PHE:O    | 1:C:269:ILE:HG13 | 2.16                     | 0.45              |
| 2:D:13:TRP:CD1   | 2:D:13:TRP:C     | 2.94                     | 0.45              |
| 2:F:32:HIS:CE1   | 2:F:33:PRO:HD2   | 2.51                     | 0.45              |
| 1:G:128:ALA:HB1  | 1:G:131:LEU:HD11 | 1.97                     | 0.45              |
| 2:H:127:ILE:CG1  | 2:H:128:GLN:NE2  | 2.79                     | 0.45              |
| 3:I:161:ILE:O    | 3:I:162:LEU:HD23 | 2.15                     | 0.45              |
| 1:C:140:ALA:HA   | 1:C:150:LEU:CD2  | 2.46                     | 0.45              |
| 1:C:369:GLY:O    | 1:C:370:GLN:C    | 2.59                     | 0.45              |
| 1:C:462:THR:O    | 1:C:463:GLY:C    | 2.59                     | 0.45              |
| 2:D:74:GLN:NE2   | 2:D:74:GLN:HA    | 2.30                     | 0.45              |
| 2:D:183:GLU:HG3  | 2:D:289:ILE:CG2  | 2.46                     | 0.45              |
| 3:J:145:TYR:O    | 3:J:146:SER:C    | 2.59                     | 0.45              |
| 1:E:41:THR:O     | 1:E:45:ILE:HG13  | 2.16                     | 0.45              |
| 1:E:84:ASN:HD22  | 1:E:85:ARG:N     | 2.13                     | 0.45              |
| 1:E:192:LEU:HG   | 1:E:196:PHE:CE1  | 2.50                     | 0.45              |
| 1:E:369:GLY:O    | 1:E:370:GLN:C    | 2.59                     | 0.45              |
| 3:K:115:ILE:HG22 | 3:K:116:ASP:N    | 2.32                     | 0.45              |
| 3:K:151:ASN:C    | 3:K:153:GLU:H    | 2.24                     | 0.45              |
| 2:H:236:GLN:HE22 | 2:H:263:LYS:HB3  | 1.80                     | 0.45              |
| 1:A:232:ARG:C    | 1:A:233:ILE:HG13 | 2.42                     | 0.45              |
| 1:A:311:LEU:HD12 | 1:A:311:LEU:HA   | 1.82                     | 0.45              |
| 1:C:61:ASP:OD2   | 1:C:85:ARG:HD2   | 2.17                     | 0.45              |
| 1:C:518:ASN:ND2  | 1:C:533:GLN:CG   | 2.69                     | 0.45              |
| 2:D:124:PHE:C    | 2:D:124:PHE:HD1  | 2.25                     | 0.45              |
| 3:J:105:VAL:HG11 | 3:J:130:VAL:CG2  | 2.44                     | 0.45              |
| 1:E:37:ASN:HB2   | 1:E:129:THR:O    | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:299:LYS:HA   | 1:E:368:ILE:CG2  | 2.46                     | 0.45              |
| 1:E:512:GLN:C    | 1:E:513:PHE:CD1  | 2.95                     | 0.45              |
| 1:G:47:LYS:CD    | 1:G:51:LEU:HD11  | 2.46                     | 0.45              |
| 1:G:215:ILE:HD12 | 1:G:342:LEU:HD21 | 1.99                     | 0.45              |
| 1:G:233:ILE:HG22 | 1:G:233:ILE:O    | 2.16                     | 0.45              |
| 1:G:262:GLU:OE1  | 1:G:262:GLU:CA   | 2.64                     | 0.45              |
| 1:G:333:ILE:HA   | 2:H:223:ARG:HH21 | 1.81                     | 0.45              |
| 2:H:74:GLN:NE2   | 2:H:74:GLN:HA    | 2.31                     | 0.45              |
| 2:H:232:VAL:HA   | 2:H:236:GLN:HB3  | 1.99                     | 0.45              |
| 1:A:46:LEU:HD21  | 1:A:57:PHE:CD1   | 2.52                     | 0.45              |
| 1:A:404:LEU:HD21 | 1:A:467:GLU:O    | 2.16                     | 0.45              |
| 1:C:42:GLY:HA2   | 1:C:129:THR:HG21 | 1.99                     | 0.45              |
| 1:C:186:ASP:OD2  | 1:C:279:THR:HB   | 2.16                     | 0.45              |
| 1:C:366:GLN:C    | 1:C:368:ILE:N    | 2.68                     | 0.45              |
| 1:C:444:GLY:HA2  | 1:C:449:GLN:HB2  | 1.98                     | 0.45              |
| 1:C:481:GLU:O    | 1:C:484:ARG:HB3  | 2.16                     | 0.45              |
| 2:D:312:THR:O    | 2:D:313:SER:HB2  | 2.16                     | 0.45              |
| 3:J:150:MET:CE   | 3:J:167:LEU:HD13 | 2.46                     | 0.45              |
| 1:E:232:ARG:C    | 1:E:233:ILE:HG13 | 2.41                     | 0.45              |
| 2:F:136:ARG:HG2  | 2:F:136:ARG:NH1  | 2.31                     | 0.45              |
| 2:F:314:ALA:O    | 2:F:315:TYR:CD1  | 2.69                     | 0.45              |
| 2:F:361:LEU:HD23 | 2:F:361:LEU:N    | 2.29                     | 0.45              |
| 1:G:53:GLY:O     | 1:G:54:ILE:C     | 2.59                     | 0.45              |
| 1:A:332:MET:HE2  | 1:A:342:LEU:HD23 | 1.99                     | 0.45              |
| 1:A:415:SER:O    | 1:A:417:ASP:N    | 2.50                     | 0.45              |
| 2:B:32:HIS:CE1   | 2:B:33:PRO:HD2   | 2.51                     | 0.45              |
| 2:B:102:PRO:HB3  | 2:B:124:PHE:CD2  | 2.52                     | 0.45              |
| 2:B:232:VAL:O    | 2:B:232:VAL:HG12 | 2.14                     | 0.45              |
| 1:E:75:PHE:O     | 1:E:76:LEU:HD23  | 2.16                     | 0.45              |
| 1:E:233:ILE:O    | 1:E:233:ILE:HG22 | 2.17                     | 0.45              |
| 1:E:239:GLU:O    | 1:E:240:LYS:C    | 2.59                     | 0.45              |
| 1:E:274:THR:O    | 1:E:276:LEU:N    | 2.50                     | 0.45              |
| 1:G:15:ARG:HA    | 1:G:15:ARG:HD3   | 1.83                     | 0.45              |
| 1:G:143:LEU:HD22 | 1:G:148:ILE:HG21 | 1.99                     | 0.45              |
| 1:G:232:ARG:C    | 1:G:233:ILE:HG13 | 2.42                     | 0.45              |
| 1:G:239:GLU:O    | 1:G:240:LYS:C    | 2.59                     | 0.45              |
| 1:A:47:LYS:CD    | 1:A:51:LEU:HD11  | 2.46                     | 0.45              |
| 1:A:143:LEU:HD22 | 1:A:148:ILE:CG2  | 2.47                     | 0.45              |
| 1:A:253:LYS:HA   | 1:A:259:PRO:CD   | 2.47                     | 0.45              |
| 2:B:136:ARG:HG2  | 2:B:136:ARG:NH1  | 2.32                     | 0.45              |
| 2:D:49:CYS:HA    | 2:D:139:HIS:HD2  | 1.82                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:394:LEU:HG   | 2:D:396:SER:HB3  | 1.97                     | 0.45              |
| 3:J:113:ILE:HD11 | 3:J:130:VAL:HG13 | 1.98                     | 0.45              |
| 2:F:158:LEU:HD12 | 2:F:177:LEU:HB2  | 1.99                     | 0.45              |
| 2:F:229:ILE:HD12 | 2:F:284:VAL:HG21 | 1.98                     | 0.45              |
| 1:G:288:ILE:HG23 | 1:G:305:TRP:CZ3  | 2.52                     | 0.45              |
| 2:H:228:CYS:O    | 2:H:231:TYR:HB3  | 2.17                     | 0.45              |
| 2:H:293:ALA:O    | 2:H:294:SER:C    | 2.59                     | 0.45              |
| 2:H:392:LEU:HD23 | 2:H:392:LEU:HA   | 1.50                     | 0.45              |
| 1:A:37:ASN:HD22  | 1:A:37:ASN:HA    | 1.62                     | 0.45              |
| 1:C:262:GLU:OE1  | 1:C:262:GLU:CA   | 2.65                     | 0.45              |
| 2:D:342:ASN:N    | 2:D:342:ASN:ND2  | 2.63                     | 0.45              |
| 2:D:703:GLY:C    | 2:D:705:VAL:H    | 2.23                     | 0.45              |
| 1:E:143:LEU:HD22 | 1:E:148:ILE:CG2  | 2.46                     | 0.45              |
| 1:E:177:ASP:O    | 1:E:178:ASN:CB   | 2.65                     | 0.45              |
| 2:F:90:ARG:HG2   | 2:F:90:ARG:HH11  | 1.81                     | 0.45              |
| 2:F:95:ARG:HD3   | 2:F:95:ARG:HA    | 1.67                     | 0.45              |
| 2:F:182:THR:O    | 2:F:183:GLU:HB2  | 2.16                     | 0.45              |
| 2:F:232:VAL:HA   | 2:F:236:GLN:HB3  | 1.99                     | 0.45              |
| 2:F:235:LEU:C    | 2:F:238:PRO:HD2  | 2.42                     | 0.45              |
| 2:H:162:LEU:HD22 | 2:H:169:LEU:HD11 | 1.98                     | 0.45              |
| 2:H:236:GLN:NE2  | 2:H:263:LYS:HB3  | 2.32                     | 0.45              |
| 2:H:335:PHE:CZ   | 3:L:144:ILE:CD1  | 2.99                     | 0.45              |
| 1:A:139:LEU:C    | 1:A:141:ASP:N    | 2.75                     | 0.45              |
| 1:A:177:ASP:O    | 1:A:178:ASN:CB   | 2.65                     | 0.45              |
| 1:A:518:ASN:ND2  | 1:A:534:LEU:HD12 | 2.32                     | 0.45              |
| 2:B:183:GLU:HG3  | 2:B:289:ILE:CG2  | 2.47                     | 0.45              |
| 2:B:229:ILE:HG21 | 2:B:284:VAL:HB   | 1.99                     | 0.45              |
| 2:B:342:ASN:H    | 2:B:342:ASN:ND2  | 2.09                     | 0.45              |
| 1:C:259:PRO:N    | 1:C:260:GLU:HG2  | 2.32                     | 0.45              |
| 1:C:274:THR:O    | 1:C:276:LEU:N    | 2.49                     | 0.45              |
| 1:C:288:ILE:HG23 | 1:C:305:TRP:CZ3  | 2.52                     | 0.45              |
| 1:C:518:ASN:ND2  | 1:C:534:LEU:HD12 | 2.32                     | 0.45              |
| 2:D:90:ARG:HG2   | 2:D:90:ARG:HH11  | 1.80                     | 0.45              |
| 1:E:18:ARG:NH2   | 2:F:288:ILE:HD12 | 2.31                     | 0.45              |
| 1:E:285:ILE:HD11 | 1:E:387:SER:O    | 2.17                     | 0.45              |
| 1:E:340:ILE:O    | 1:E:341:LYS:C    | 2.60                     | 0.45              |
| 1:E:504:GLU:O    | 1:E:508:ILE:HG13 | 2.17                     | 0.45              |
| 2:F:356:SER:HA   | 2:F:357:PRO:HD3  | 1.52                     | 0.45              |
| 2:H:136:ARG:HG2  | 2:H:136:ARG:HH11 | 1.82                     | 0.45              |
| 3:L:161:ILE:O    | 3:L:162:LEU:HD23 | 2.17                     | 0.45              |
| 1:A:491:HIS:NE2  | 2:B:65:LYS:NZ    | 2.62                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:265:PHE:O    | 1:E:269:ILE:HG13 | 2.17                     | 0.45              |
| 2:F:110:PHE:HE2  | 2:F:114:ARG:HB2  | 1.82                     | 0.45              |
| 1:G:18:ARG:NH2   | 2:H:288:ILE:HD12 | 2.32                     | 0.45              |
| 1:G:293:ARG:HG2  | 1:G:305:TRP:CD1  | 2.52                     | 0.45              |
| 1:G:396:ARG:HH11 | 1:G:533:GLN:NE2  | 2.15                     | 0.45              |
| 2:H:13:TRP:CD1   | 2:H:13:TRP:C     | 2.95                     | 0.45              |
| 2:H:182:THR:O    | 2:H:183:GLU:HB2  | 2.16                     | 0.45              |
| 2:H:229:ILE:HG21 | 2:H:284:VAL:HB   | 1.99                     | 0.45              |
| 1:A:233:ILE:O    | 1:A:233:ILE:HG22 | 2.17                     | 0.45              |
| 1:A:353:ASP:O    | 1:A:357:VAL:HG23 | 2.17                     | 0.45              |
| 2:B:306:GLU:OE2  | 2:B:309:LYS:HD2  | 2.17                     | 0.45              |
| 1:C:335:ASP:HB3  | 1:C:338:LYS:HB2  | 1.99                     | 0.45              |
| 1:C:355:ALA:O    | 1:C:358:GLY:N    | 2.49                     | 0.45              |
| 2:D:199:CYS:HG   | 2:D:346:CYS:HG   | 1.60                     | 0.45              |
| 2:D:340:LYS:HB3  | 2:D:342:ASN:ND2  | 2.32                     | 0.45              |
| 2:D:351:GLN:HB3  | 2:D:916:PHE:CB   | 2.47                     | 0.45              |
| 3:J:107:THR:CG2  | 3:J:111:LYS:HB3  | 2.47                     | 0.45              |
| 2:F:183:GLU:HG3  | 2:F:289:ILE:HG21 | 1.99                     | 0.45              |
| 2:F:236:GLN:NE2  | 2:F:263:LYS:HB3  | 2.31                     | 0.45              |
| 2:F:293:ALA:O    | 2:F:294:SER:C    | 2.59                     | 0.45              |
| 1:G:369:GLY:O    | 1:G:370:GLN:C    | 2.60                     | 0.45              |
| 2:H:356:SER:HA   | 2:H:357:PRO:HD3  | 1.55                     | 0.45              |
| 1:A:16:GLN:CB    | 2:B:292:VAL:HG12 | 2.47                     | 0.44              |
| 1:A:225:TRP:CE2  | 1:A:233:ILE:HG12 | 2.52                     | 0.44              |
| 1:C:211:HIS:O    | 1:C:338:LYS:HD2  | 2.16                     | 0.44              |
| 1:C:447:ASN:ND2  | 2:D:26:ARG:HH21  | 2.12                     | 0.44              |
| 2:D:127:ILE:HG13 | 2:D:128:GLN:NE2  | 2.33                     | 0.44              |
| 2:D:236:GLN:HE22 | 2:D:263:LYS:HD2  | 1.82                     | 0.44              |
| 2:D:371:SER:C    | 2:D:373:SER:N    | 2.75                     | 0.44              |
| 1:E:42:GLY:HA2   | 1:E:129:THR:HG21 | 1.99                     | 0.44              |
| 2:F:80:MET:HB3   | 2:F:126:LYS:HB3  | 1.98                     | 0.44              |
| 2:F:232:VAL:O    | 2:F:232:VAL:HG12 | 2.16                     | 0.44              |
| 1:G:432:VAL:HG13 | 1:G:443:PRO:CD   | 2.46                     | 0.44              |
| 2:H:80:MET:HE3   | 4:H:8:ATP:C6     | 2.52                     | 0.44              |
| 1:A:218:ILE:HD11 | 1:A:268:ALA:O    | 2.17                     | 0.44              |
| 1:A:288:ILE:HG23 | 1:A:305:TRP:CZ3  | 2.52                     | 0.44              |
| 2:B:703:GLY:C    | 2:B:705:VAL:N    | 2.75                     | 0.44              |
| 2:D:394:LEU:HD11 | 2:D:396:SER:HB3  | 1.98                     | 0.44              |
| 2:D:607:THR:O    | 2:D:608:ARG:CB   | 2.65                     | 0.44              |
| 2:F:335:PHE:HE2  | 3:K:170:VAL:HG21 | 1.81                     | 0.44              |
| 2:F:360:LYS:H    | 2:F:360:LYS:HG3  | 1.61                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:42:GLY:HA2   | 1:G:129:THR:HG21 | 2.00                     | 0.44              |
| 1:G:421:ASN:O    | 1:G:423:ILE:N    | 2.50                     | 0.44              |
| 2:H:80:MET:HE2   | 2:H:126:LYS:CB   | 2.47                     | 0.44              |
| 2:H:197:THR:CG2  | 2:H:198:ALA:N    | 2.79                     | 0.44              |
| 2:H:283:GLY:HA2  | 2:H:288:ILE:HG13 | 1.98                     | 0.44              |
| 2:H:312:THR:O    | 2:H:313:SER:HB2  | 2.16                     | 0.44              |
| 1:A:43:THR:HG22  | 1:A:44:GLU:N     | 2.33                     | 0.44              |
| 1:A:432:VAL:HG13 | 1:A:443:PRO:CD   | 2.47                     | 0.44              |
| 2:B:361:LEU:HD23 | 2:B:361:LEU:N    | 2.31                     | 0.44              |
| 1:C:143:LEU:HD22 | 1:C:148:ILE:HG21 | 1.99                     | 0.44              |
| 1:C:331:ASP:HB2  | 2:D:224:LEU:HD11 | 1.99                     | 0.44              |
| 2:D:132:ASP:O    | 2:D:133:THR:C    | 2.60                     | 0.44              |
| 2:D:314:ALA:O    | 2:D:315:TYR:CD1  | 2.70                     | 0.44              |
| 2:D:703:GLY:C    | 2:D:705:VAL:N    | 2.76                     | 0.44              |
| 3:J:151:ASN:C    | 3:J:153:GLU:H    | 2.25                     | 0.44              |
| 1:E:133:GLU:HG3  | 1:E:433:ASP:HB3  | 1.99                     | 0.44              |
| 1:E:415:SER:C    | 1:E:417:ASP:H    | 2.24                     | 0.44              |
| 2:F:187:GLY:CA   | 3:K:173:LEU:CD1  | 2.95                     | 0.44              |
| 2:F:268:ALA:HB1  | 2:F:273:ILE:O    | 2.16                     | 0.44              |
| 1:G:281:ILE:HA   | 1:G:282:PRO:HD3  | 1.84                     | 0.44              |
| 1:G:357:VAL:O    | 1:G:361:VAL:HG23 | 2.16                     | 0.44              |
| 1:G:436:HIS:O    | 1:G:437:LYS:C    | 2.59                     | 0.44              |
| 1:A:132:PRO:O    | 1:A:133:GLU:C    | 2.61                     | 0.44              |
| 2:B:124:PHE:CD1  | 2:B:124:PHE:O    | 2.70                     | 0.44              |
| 2:B:197:THR:HG21 | 2:B:320:ASN:HB3  | 1.99                     | 0.44              |
| 2:B:235:LEU:C    | 2:B:238:PRO:HD2  | 2.42                     | 0.44              |
| 1:C:156:TYR:CE1  | 1:C:487:ALA:HA   | 2.53                     | 0.44              |
| 1:C:233:ILE:O    | 1:C:233:ILE:HG22 | 2.17                     | 0.44              |
| 3:J:123:VAL:HA   | 3:J:126:ILE:HD12 | 1.98                     | 0.44              |
| 1:E:462:THR:O    | 1:E:463:GLY:C    | 2.57                     | 0.44              |
| 1:G:139:LEU:C    | 1:G:141:ASP:N    | 2.76                     | 0.44              |
| 2:H:112:ASN:OD1  | 2:H:120:VAL:N    | 2.46                     | 0.44              |
| 2:H:394:LEU:HD11 | 2:H:396:SER:HB3  | 2.00                     | 0.44              |
| 2:D:192:ILE:HG22 | 2:D:194:PRO:CD   | 2.47                     | 0.44              |
| 2:D:321:TYR:CD2  | 2:D:322:LEU:N    | 2.86                     | 0.44              |
| 1:E:415:SER:O    | 1:E:417:ASP:N    | 2.50                     | 0.44              |
| 2:F:13:TRP:CZ3   | 2:F:116:PRO:HG2  | 2.52                     | 0.44              |
| 2:H:13:TRP:CZ3   | 2:H:116:PRO:HG2  | 2.51                     | 0.44              |
| 2:H:50:LYS:H     | 2:H:139:HIS:CD2  | 2.35                     | 0.44              |
| 2:H:236:GLN:HE22 | 2:H:263:LYS:HD2  | 1.82                     | 0.44              |
| 2:H:703:GLY:C    | 2:H:705:VAL:N    | 2.76                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:115:ILE:HG22 | 3:L:116:ASP:N    | 2.33                     | 0.44              |
| 1:A:61:ASP:OD2   | 1:A:85:ARG:HD2   | 2.17                     | 0.44              |
| 1:A:131:LEU:HA   | 1:A:132:PRO:HD3  | 1.86                     | 0.44              |
| 2:B:314:ALA:O    | 2:B:315:TYR:CD1  | 2.71                     | 0.44              |
| 1:C:43:THR:HG22  | 1:C:44:GLU:N     | 2.31                     | 0.44              |
| 1:C:512:GLN:C    | 1:C:513:PHE:CD1  | 2.96                     | 0.44              |
| 2:D:78:ILE:HD11  | 2:D:134:PHE:HE2  | 1.83                     | 0.44              |
| 2:F:187:GLY:HA2  | 3:K:173:LEU:CD1  | 2.47                     | 0.44              |
| 1:G:393:VAL:HG13 | 1:G:517:ASN:ND2  | 2.28                     | 0.44              |
| 2:H:123:HIS:O    | 2:H:125:ASN:N    | 2.49                     | 0.44              |
| 2:H:156:GLY:O    | 2:H:157:MET:C    | 2.59                     | 0.44              |
| 1:A:299:LYS:HA   | 1:A:368:ILE:CG2  | 2.47                     | 0.44              |
| 1:A:444:GLY:HA2  | 1:A:449:GLN:HB2  | 1.98                     | 0.44              |
| 1:A:481:GLU:O    | 1:A:484:ARG:HB3  | 2.18                     | 0.44              |
| 2:B:131:ASN:HD22 | 2:D:131:ASN:HB3  | 1.83                     | 0.44              |
| 1:C:53:GLY:O     | 1:C:54:ILE:C     | 2.60                     | 0.44              |
| 1:C:139:LEU:C    | 1:C:141:ASP:H    | 2.24                     | 0.44              |
| 2:D:80:MET:HB3   | 2:D:126:LYS:HB3  | 1.98                     | 0.44              |
| 2:D:343:CYS:O    | 2:D:347:SER:HB3  | 2.18                     | 0.44              |
| 2:F:343:CYS:O    | 2:F:347:SER:HB3  | 2.18                     | 0.44              |
| 2:F:351:GLN:O    | 2:F:353:ILE:N    | 2.51                     | 0.44              |
| 1:G:38:ALA:C     | 1:G:85:ARG:HD3   | 2.43                     | 0.44              |
| 1:G:332:MET:HE2  | 1:G:342:LEU:HD23 | 1.99                     | 0.44              |
| 2:H:80:MET:HG2   | 4:H:8:ATP:C2     | 2.52                     | 0.44              |
| 2:H:229:ILE:HD12 | 2:H:284:VAL:HG21 | 1.99                     | 0.44              |
| 2:H:268:ALA:HB1  | 2:H:273:ILE:O    | 2.18                     | 0.44              |
| 1:A:42:GLY:HA2   | 1:A:129:THR:HG21 | 1.99                     | 0.44              |
| 1:A:480:HIS:HB2  | 2:B:29:PRO:HG2   | 1.99                     | 0.44              |
| 2:B:106:VAL:O    | 2:B:107:ALA:C    | 2.61                     | 0.44              |
| 2:B:335:PHE:CE1  | 2:B:337:ALA:HB2  | 2.51                     | 0.44              |
| 1:C:39:THR:HB    | 1:C:489:GLU:OE1  | 2.17                     | 0.44              |
| 1:C:532:PHE:HB3  | 1:C:533:GLN:H    | 1.37                     | 0.44              |
| 2:D:293:ALA:O    | 2:D:294:SER:C    | 2.59                     | 0.44              |
| 1:E:266:GLU:HG3  | 1:E:270:LYS:HE3  | 2.00                     | 0.44              |
| 2:F:50:LYS:H     | 2:F:139:HIS:CD2  | 2.36                     | 0.44              |
| 2:F:192:ILE:HG22 | 2:F:194:PRO:CD   | 2.43                     | 0.44              |
| 3:K:113:ILE:HD11 | 3:K:130:VAL:HG13 | 1.99                     | 0.44              |
| 3:K:155:THR:O    | 3:K:158:ASP:N    | 2.51                     | 0.44              |
| 2:H:141:ILE:HD12 | 2:H:158:LEU:HD11 | 2.00                     | 0.44              |
| 2:H:250:ASP:H    | 2:H:256:HIS:CE1  | 2.36                     | 0.44              |
| 2:B:123:HIS:O    | 2:B:125:ASN:N    | 2.49                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:250:ASP:OD2  | 2:B:253:ASP:HB2  | 2.17                     | 0.44              |
| 1:C:131:LEU:HA   | 1:C:132:PRO:HD3  | 1.85                     | 0.44              |
| 1:C:441:ARG:HH21 | 1:C:453:ASP:CG   | 2.25                     | 0.44              |
| 2:D:156:GLY:O    | 2:D:157:MET:C    | 2.60                     | 0.44              |
| 2:D:353:ILE:HG23 | 2:D:355:PHE:HE1  | 1.82                     | 0.44              |
| 1:E:421:ASN:O    | 1:E:423:ILE:N    | 2.50                     | 0.44              |
| 1:E:447:ASN:ND2  | 2:F:26:ARG:HH21  | 2.14                     | 0.44              |
| 2:F:52:LEU:HD11  | 2:F:78:ILE:HG13  | 1.98                     | 0.44              |
| 2:F:106:VAL:O    | 2:F:107:ALA:C    | 2.60                     | 0.44              |
| 3:K:131:GLU:CD   | 3:K:138:PRO:HD3  | 2.43                     | 0.44              |
| 1:G:35:LEU:HD23  | 1:G:46:LEU:HD22  | 2.00                     | 0.44              |
| 1:G:69:ASP:C     | 1:G:71:GLY:N     | 2.76                     | 0.44              |
| 1:G:261:ASP:O    | 1:G:262:GLU:CG   | 2.66                     | 0.44              |
| 2:H:110:PHE:HE2  | 2:H:114:ARG:HB2  | 1.83                     | 0.44              |
| 2:H:306:GLU:OE2  | 2:H:309:LYS:HD2  | 2.18                     | 0.44              |
| 3:L:155:THR:O    | 3:L:158:ASP:N    | 2.51                     | 0.44              |
| 1:A:504:GLU:O    | 1:A:508:ILE:HG13 | 2.18                     | 0.43              |
| 2:B:80:MET:HE2   | 2:B:126:LYS:CB   | 2.48                     | 0.43              |
| 3:J:115:ILE:HG22 | 3:J:116:ASP:N    | 2.33                     | 0.43              |
| 1:E:47:LYS:HD2   | 1:E:51:LEU:HD12  | 2.00                     | 0.43              |
| 1:E:190:PRO:O    | 1:E:191:GLU:C    | 2.61                     | 0.43              |
| 1:E:481:GLU:O    | 1:E:484:ARG:N    | 2.51                     | 0.43              |
| 3:K:107:THR:CG2  | 3:K:111:LYS:HB3  | 2.48                     | 0.43              |
| 3:K:107:THR:OG1  | 3:K:108:LEU:N    | 2.51                     | 0.43              |
| 1:G:497:LEU:HD12 | 1:G:497:LEU:HA   | 1.87                     | 0.43              |
| 2:H:187:GLY:CA   | 3:L:173:LEU:CD1  | 2.96                     | 0.43              |
| 1:A:518:ASN:ND2  | 1:A:533:GLN:CG   | 2.71                     | 0.43              |
| 2:B:16:ARG:HH22  | 2:B:116:PRO:HB2  | 1.83                     | 0.43              |
| 2:B:127:ILE:CG1  | 2:B:128:GLN:NE2  | 2.81                     | 0.43              |
| 2:B:236:GLN:HE22 | 2:B:263:LYS:HD2  | 1.83                     | 0.43              |
| 2:B:371:SER:C    | 2:B:373:SER:N    | 2.76                     | 0.43              |
| 3:I:151:ASN:C    | 3:I:153:GLU:H    | 2.26                     | 0.43              |
| 1:C:139:LEU:C    | 1:C:141:ASP:N    | 2.75                     | 0.43              |
| 1:C:340:ILE:O    | 1:C:341:LYS:C    | 2.61                     | 0.43              |
| 1:E:35:LEU:HD12  | 1:E:36:ILE:N     | 2.33                     | 0.43              |
| 1:E:146:SER:O    | 1:E:147:GLN:HB2  | 2.17                     | 0.43              |
| 2:F:228:CYS:O    | 2:F:231:TYR:HB3  | 2.19                     | 0.43              |
| 2:F:236:GLN:HE22 | 2:F:263:LYS:HD2  | 1.83                     | 0.43              |
| 1:G:47:LYS:HD2   | 1:G:51:LEU:HD12  | 2.00                     | 0.43              |
| 1:G:323:LEU:HB3  | 1:G:324:PRO:CD   | 2.48                     | 0.43              |
| 1:G:323:LEU:HD22 | 1:G:387:SER:HB2  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:512:GLN:C    | 1:G:513:PHE:CD1  | 2.97                     | 0.43              |
| 1:G:532:PHE:HB3  | 1:G:533:GLN:H    | 1.37                     | 0.43              |
| 2:H:242:PRO:HG3  | 2:H:259:TRP:CH2  | 2.53                     | 0.43              |
| 2:H:361:LEU:HD23 | 2:H:361:LEU:N    | 2.31                     | 0.43              |
| 2:H:703:GLY:C    | 2:H:705:VAL:H    | 2.24                     | 0.43              |
| 2:B:78:ILE:HD11  | 2:B:134:PHE:HE2  | 1.83                     | 0.43              |
| 2:B:80:MET:HB3   | 2:B:126:LYS:HB3  | 2.00                     | 0.43              |
| 2:B:134:PHE:O    | 2:B:137:GLN:HG3  | 2.17                     | 0.43              |
| 1:C:47:LYS:CD    | 1:C:51:LEU:HD11  | 2.48                     | 0.43              |
| 1:C:281:ILE:HA   | 1:C:282:PRO:HD3  | 1.85                     | 0.43              |
| 1:C:432:VAL:HG13 | 1:C:443:PRO:CD   | 2.48                     | 0.43              |
| 1:C:466:GLN:O    | 1:C:467:GLU:C    | 2.61                     | 0.43              |
| 1:C:503:GLN:OE1  | 1:C:503:GLN:HA   | 2.18                     | 0.43              |
| 2:D:124:PHE:C    | 2:D:124:PHE:CD1  | 2.95                     | 0.43              |
| 1:E:19:LEU:HD13  | 2:F:185:PHE:CE1  | 2.54                     | 0.43              |
| 2:F:148:ILE:O    | 2:F:149:ILE:C    | 2.62                     | 0.43              |
| 2:F:232:VAL:HG21 | 2:F:263:LYS:C    | 2.44                     | 0.43              |
| 2:F:335:PHE:CZ   | 3:K:144:ILE:CD1  | 3.01                     | 0.43              |
| 1:G:340:ILE:HD11 | 2:H:273:ILE:HG12 | 2.00                     | 0.43              |
| 2:H:49:CYS:HA    | 2:H:139:HIS:HD2  | 1.81                     | 0.43              |
| 1:A:50:VAL:HG13  | 1:A:100:VAL:HG21 | 2.00                     | 0.43              |
| 1:A:133:GLU:HG3  | 1:A:433:ASP:HB3  | 2.00                     | 0.43              |
| 1:A:215:ILE:O    | 1:A:216:VAL:C    | 2.60                     | 0.43              |
| 1:A:512:GLN:C    | 1:A:513:PHE:CD1  | 2.96                     | 0.43              |
| 2:B:50:LYS:H     | 2:B:139:HIS:CD2  | 2.36                     | 0.43              |
| 1:C:192:LEU:HG   | 1:C:196:PHE:CE1  | 2.52                     | 0.43              |
| 1:C:415:SER:O    | 1:C:417:ASP:N    | 2.50                     | 0.43              |
| 2:D:333:TYR:CZ   | 2:D:335:PHE:HB3  | 2.54                     | 0.43              |
| 2:F:49:CYS:HA    | 2:F:139:HIS:HD2  | 1.81                     | 0.43              |
| 2:F:178:ILE:HG21 | 2:F:303:CYS:HB3  | 1.99                     | 0.43              |
| 1:G:139:LEU:C    | 1:G:141:ASP:H    | 2.25                     | 0.43              |
| 1:G:221:TYR:O    | 1:G:243:PHE:HE1  | 2.01                     | 0.43              |
| 1:G:333:ILE:HA   | 2:H:223:ARG:NH2  | 2.34                     | 0.43              |
| 1:G:430:ARG:HB3  | 1:G:430:ARG:NH1  | 2.32                     | 0.43              |
| 2:H:335:PHE:HE2  | 3:L:170:VAL:HG21 | 1.83                     | 0.43              |
| 2:H:335:PHE:CE1  | 2:H:337:ALA:HB2  | 2.52                     | 0.43              |
| 1:A:190:PRO:O    | 1:A:191:GLU:C    | 2.61                     | 0.43              |
| 1:A:340:ILE:O    | 1:A:341:LYS:C    | 2.60                     | 0.43              |
| 1:A:340:ILE:O    | 1:A:343:GLN:N    | 2.51                     | 0.43              |
| 2:B:231:TYR:C    | 2:B:233:ARG:N    | 2.76                     | 0.43              |
| 2:B:333:TYR:CZ   | 2:B:335:PHE:HB3  | 2.54                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:236:THR:HG23 | 1:C:240:LYS:HE3  | 2.01                     | 0.43              |
| 1:C:332:MET:HE2  | 1:C:342:LEU:HD23 | 1.99                     | 0.43              |
| 1:C:421:ASN:O    | 1:C:423:ILE:N    | 2.51                     | 0.43              |
| 1:E:225:TRP:CE2  | 1:E:233:ILE:HG12 | 2.54                     | 0.43              |
| 1:E:236:THR:O    | 1:E:237:TYR:HD1  | 2.02                     | 0.43              |
| 1:E:285:ILE:HD11 | 1:E:388:ALA:CA   | 2.39                     | 0.43              |
| 2:F:139:HIS:O    | 2:F:176:PRO:HD2  | 2.18                     | 0.43              |
| 3:K:103:ILE:HD11 | 3:K:117:ILE:HD12 | 2.01                     | 0.43              |
| 1:G:183:LEU:HD22 | 1:G:215:ILE:HD11 | 2.00                     | 0.43              |
| 1:G:265:PHE:O    | 1:G:269:ILE:HG13 | 2.19                     | 0.43              |
| 1:G:518:ASN:ND2  | 1:G:534:LEU:HD12 | 2.33                     | 0.43              |
| 3:L:107:THR:CG2  | 3:L:111:LYS:HB3  | 2.48                     | 0.43              |
| 1:A:113:LEU:HD22 | 1:A:142:VAL:HG21 | 2.01                     | 0.43              |
| 1:A:253:LYS:O    | 1:A:260:GLU:OE2  | 2.36                     | 0.43              |
| 1:C:132:PRO:O    | 1:C:133:GLU:C    | 2.60                     | 0.43              |
| 1:C:190:PRO:O    | 1:C:191:GLU:C    | 2.61                     | 0.43              |
| 2:D:148:ILE:O    | 2:D:149:ILE:C    | 2.62                     | 0.43              |
| 1:E:69:ASP:C     | 1:E:71:GLY:N     | 2.75                     | 0.43              |
| 2:F:157:MET:HE3  | 2:F:160:SER:OG   | 2.18                     | 0.43              |
| 2:F:182:THR:HG23 | 2:F:183:GLU:N    | 2.33                     | 0.43              |
| 2:F:231:TYR:C    | 2:F:233:ARG:H    | 2.27                     | 0.43              |
| 2:F:267:ARG:NH1  | 2:F:267:ARG:CG   | 2.80                     | 0.43              |
| 1:G:146:SER:O    | 1:G:147:GLN:HB2  | 2.17                     | 0.43              |
| 1:G:177:ASP:O    | 1:G:178:ASN:CB   | 2.67                     | 0.43              |
| 1:G:244:ARG:O    | 1:G:247:ILE:N    | 2.51                     | 0.43              |
| 2:H:395:GLN:H    | 2:H:395:GLN:HG3  | 1.67                     | 0.43              |
| 2:B:351:GLN:HE21 | 2:B:351:GLN:CA   | 2.26                     | 0.43              |
| 1:C:96:LEU:HD23  | 2:D:95:ARG:NH2   | 2.33                     | 0.43              |
| 1:C:124:THR:HG22 | 1:C:125:VAL:HG23 | 2.01                     | 0.43              |
| 1:C:266:GLU:HG3  | 1:C:270:LYS:HE3  | 2.00                     | 0.43              |
| 2:D:32:HIS:CE1   | 2:D:33:PRO:HD2   | 2.54                     | 0.43              |
| 2:D:271:TYR:CD1  | 2:D:271:TYR:N    | 2.85                     | 0.43              |
| 2:F:335:PHE:CE1  | 2:F:337:ALA:HB2  | 2.51                     | 0.43              |
| 1:G:75:PHE:CZ    | 1:G:96:LEU:HD11  | 2.53                     | 0.43              |
| 1:G:504:GLU:O    | 1:G:508:ILE:HG13 | 2.19                     | 0.43              |
| 2:H:193:LEU:O    | 2:H:194:PRO:C    | 2.60                     | 0.43              |
| 1:A:362:ALA:O    | 1:A:363:LYS:C    | 2.61                     | 0.43              |
| 3:I:115:ILE:HG22 | 3:I:116:ASP:N    | 2.33                     | 0.43              |
| 1:C:107:GLU:OE2  | 1:G:351:LYS:NZ   | 2.51                     | 0.43              |
| 1:C:133:GLU:HG3  | 1:C:433:ASP:HB3  | 2.01                     | 0.43              |
| 1:C:139:LEU:HG   | 1:C:143:LEU:HD12 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:47:LYS:CD    | 1:E:51:LEU:HD11  | 2.48                     | 0.43              |
| 1:E:117:PRO:C    | 1:E:119:PHE:N    | 2.77                     | 0.43              |
| 1:E:166:ILE:HD11 | 1:E:508:ILE:HD13 | 2.00                     | 0.43              |
| 1:E:175:HIS:HD2  | 1:E:512:GLN:O    | 2.02                     | 0.43              |
| 1:E:186:ASP:OD2  | 1:E:279:THR:HB   | 2.19                     | 0.43              |
| 1:E:215:ILE:O    | 1:E:216:VAL:C    | 2.60                     | 0.43              |
| 1:E:264:ASN:ND2  | 1:E:265:PHE:H    | 2.16                     | 0.43              |
| 1:G:215:ILE:O    | 1:G:216:VAL:C    | 2.61                     | 0.43              |
| 1:G:266:GLU:HG3  | 1:G:270:LYS:HE3  | 2.01                     | 0.43              |
| 1:G:285:ILE:HD11 | 1:G:388:ALA:CA   | 2.38                     | 0.43              |
| 1:G:466:GLN:O    | 1:G:467:GLU:C    | 2.61                     | 0.43              |
| 2:H:267:ARG:NH1  | 2:H:267:ARG:CG   | 2.78                     | 0.43              |
| 1:A:47:LYS:HD2   | 1:A:51:LEU:HD12  | 2.00                     | 0.43              |
| 1:C:128:ALA:HB1  | 1:C:131:LEU:CD1  | 2.49                     | 0.43              |
| 1:C:232:ARG:C    | 1:C:233:ILE:HG13 | 2.43                     | 0.43              |
| 1:C:261:ASP:O    | 1:C:262:GLU:HG2  | 2.18                     | 0.43              |
| 2:D:178:ILE:CG2  | 2:D:303:CYS:HB3  | 2.49                     | 0.43              |
| 1:E:518:ASN:ND2  | 1:E:534:LEU:HD12 | 2.34                     | 0.43              |
| 1:G:496:PHE:CE1  | 2:H:298:VAL:HG13 | 2.53                     | 0.43              |
| 2:H:178:ILE:CG2  | 2:H:303:CYS:HB3  | 2.49                     | 0.43              |
| 2:H:235:LEU:C    | 2:H:238:PRO:HD2  | 2.44                     | 0.43              |
| 1:A:172:ILE:HA   | 1:A:390:LEU:HD23 | 2.01                     | 0.43              |
| 2:B:207:TYR:HA   | 2:B:208:PRO:HD3  | 1.90                     | 0.43              |
| 3:I:113:ILE:HD11 | 3:I:130:VAL:HG13 | 2.01                     | 0.43              |
| 1:C:163:ARG:HH11 | 1:C:163:ARG:CG   | 2.25                     | 0.43              |
| 1:C:215:ILE:HD12 | 1:C:342:LEU:HD21 | 2.01                     | 0.43              |
| 2:D:126:LYS:HA   | 4:D:6:ATP:C2     | 2.54                     | 0.43              |
| 2:D:235:LEU:O    | 2:D:238:PRO:HD2  | 2.18                     | 0.43              |
| 3:J:149:GLN:HG3  | 3:J:149:GLN:O    | 2.19                     | 0.43              |
| 3:K:118:GLU:O    | 3:K:121:ASP:OD1  | 2.37                     | 0.43              |
| 1:G:40:ALA:HB3   | 1:G:489:GLU:CD   | 2.44                     | 0.43              |
| 1:G:43:THR:HG22  | 1:G:44:GLU:N     | 2.33                     | 0.43              |
| 2:H:164:TYR:HD2  | 2:H:169:LEU:HA   | 1.84                     | 0.43              |
| 2:H:314:ALA:O    | 2:H:315:TYR:CG   | 2.72                     | 0.43              |
| 2:H:320:ASN:O    | 2:H:321:TYR:CB   | 2.67                     | 0.43              |
| 2:B:182:THR:O    | 2:B:183:GLU:HB2  | 2.18                     | 0.42              |
| 1:C:35:LEU:HD12  | 1:C:36:ILE:N     | 2.34                     | 0.42              |
| 1:C:56:SER:HB3   | 1:C:101:SER:HG   | 1.80                     | 0.42              |
| 1:C:497:LEU:HD12 | 1:C:497:LEU:HA   | 1.91                     | 0.42              |
| 2:D:130:PHE:CG   | 2:D:134:PHE:CD2  | 3.07                     | 0.42              |
| 2:D:228:CYS:O    | 2:D:231:TYR:HB3  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:229:ILE:HD12 | 2:D:284:VAL:HG21 | 2.00                     | 0.42              |
| 2:D:306:GLU:OE2  | 2:D:309:LYS:HD2  | 2.19                     | 0.42              |
| 2:D:395:GLN:H    | 2:D:395:GLN:HG3  | 1.69                     | 0.42              |
| 1:E:16:GLN:HB2   | 2:F:292:VAL:HG12 | 2.00                     | 0.42              |
| 1:E:305:TRP:O    | 1:E:308:ALA:HB3  | 2.19                     | 0.42              |
| 2:F:187:GLY:HA2  | 3:K:173:LEU:HD12 | 2.01                     | 0.42              |
| 2:F:250:ASP:OD2  | 2:F:253:ASP:HB2  | 2.19                     | 0.42              |
| 2:H:228:CYS:SG   | 2:H:268:ALA:HA   | 2.59                     | 0.42              |
| 1:A:16:GLN:NE2   | 1:A:20:TRP:CZ2   | 2.85                     | 0.42              |
| 1:A:248:ARG:C    | 1:A:250:GLY:N    | 2.77                     | 0.42              |
| 1:A:401:GLU:HG3  | 1:A:533:GLN:HE22 | 1.85                     | 0.42              |
| 1:A:517:ASN:OD1  | 1:A:534:LEU:HB2  | 2.18                     | 0.42              |
| 2:B:182:THR:CG2  | 2:B:183:GLU:N    | 2.81                     | 0.42              |
| 2:B:232:VAL:HA   | 2:B:236:GLN:HB3  | 2.00                     | 0.42              |
| 2:B:241:GLN:NE2  | 2:B:246:GLY:H    | 2.17                     | 0.42              |
| 2:B:271:TYR:N    | 2:B:271:TYR:CD1  | 2.87                     | 0.42              |
| 3:I:131:GLU:CD   | 3:I:138:PRO:HD3  | 2.44                     | 0.42              |
| 1:C:46:LEU:HD21  | 1:C:57:PHE:CD1   | 2.54                     | 0.42              |
| 1:C:244:ARG:O    | 1:C:247:ILE:N    | 2.50                     | 0.42              |
| 1:C:520:TYR:CG   | 2:D:330:LEU:HD12 | 2.54                     | 0.42              |
| 2:D:54:ILE:HG22  | 2:D:145:LEU:HD21 | 2.01                     | 0.42              |
| 2:D:232:VAL:HA   | 2:D:236:GLN:HB3  | 2.01                     | 0.42              |
| 2:D:242:PRO:HG3  | 2:D:259:TRP:CH2  | 2.54                     | 0.42              |
| 2:D:250:ASP:OD2  | 2:D:253:ASP:HB2  | 2.19                     | 0.42              |
| 1:E:96:LEU:HD23  | 2:F:95:ARG:HH21  | 1.84                     | 0.42              |
| 1:E:260:GLU:HB3  | 1:E:261:ASP:OD1  | 2.19                     | 0.42              |
| 1:E:355:ALA:O    | 1:E:358:GLY:N    | 2.52                     | 0.42              |
| 1:E:435:PHE:CD2  | 1:E:435:PHE:C    | 2.97                     | 0.42              |
| 2:F:59:LEU:O     | 2:F:60:GLY:C     | 2.61                     | 0.42              |
| 2:F:207:TYR:HA   | 2:F:208:PRO:HD3  | 1.90                     | 0.42              |
| 2:F:347:SER:O    | 2:F:348:GLN:C    | 2.62                     | 0.42              |
| 3:L:151:ASN:C    | 3:L:153:GLU:H    | 2.26                     | 0.42              |
| 1:A:183:LEU:HD22 | 1:A:215:ILE:HD11 | 2.01                     | 0.42              |
| 1:C:72:ASN:HD22  | 1:C:73:ASN:N     | 2.17                     | 0.42              |
| 2:D:149:ILE:O    | 2:D:150:ALA:C    | 2.63                     | 0.42              |
| 2:D:222:PRO:HD2  | 2:D:271:TYR:CD2  | 2.54                     | 0.42              |
| 3:J:111:LYS:O    | 3:J:112:GLU:HB3  | 2.18                     | 0.42              |
| 3:J:131:GLU:CD   | 3:J:138:PRO:HD3  | 2.45                     | 0.42              |
| 3:J:136:ILE:HG22 | 3:J:141:GLN:HG2  | 2.01                     | 0.42              |
| 1:E:132:PRO:O    | 1:E:133:GLU:C    | 2.61                     | 0.42              |
| 1:E:236:THR:O    | 1:E:237:TYR:CD1  | 2.71                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:141:ILE:HD12 | 2:F:158:LEU:HD11 | 2.02                     | 0.42              |
| 1:G:47:LYS:HD2   | 1:G:51:LEU:CD1   | 2.49                     | 0.42              |
| 1:G:299:LYS:HA   | 1:G:368:ILE:CG2  | 2.49                     | 0.42              |
| 1:G:311:LEU:O    | 1:G:314:PHE:HB3  | 2.19                     | 0.42              |
| 1:G:441:ARG:HH21 | 1:G:453:ASP:CG   | 2.27                     | 0.42              |
| 1:G:503:GLN:OE1  | 1:G:503:GLN:HA   | 2.19                     | 0.42              |
| 2:H:353:ILE:HG23 | 2:H:355:PHE:HE1  | 1.84                     | 0.42              |
| 2:H:360:LYS:H    | 2:H:360:LYS:HG3  | 1.65                     | 0.42              |
| 1:A:239:GLU:O    | 1:A:240:LYS:C    | 2.61                     | 0.42              |
| 1:A:435:PHE:C    | 1:A:435:PHE:CD2  | 2.97                     | 0.42              |
| 2:B:222:PRO:HD2  | 2:B:271:TYR:CD2  | 2.54                     | 0.42              |
| 2:B:351:GLN:O    | 2:B:353:ILE:N    | 2.52                     | 0.42              |
| 3:I:107:THR:OG1  | 3:I:108:LEU:N    | 2.52                     | 0.42              |
| 2:D:136:ARG:HG2  | 2:D:136:ARG:NH1  | 2.34                     | 0.42              |
| 2:D:232:VAL:HG12 | 2:D:260:ILE:HG23 | 2.01                     | 0.42              |
| 1:E:72:ASN:HD22  | 1:E:73:ASN:N     | 2.17                     | 0.42              |
| 1:E:436:HIS:O    | 1:E:437:LYS:C    | 2.61                     | 0.42              |
| 1:E:491:HIS:NE2  | 2:F:65:LYS:NZ    | 2.64                     | 0.42              |
| 2:F:222:PRO:HD2  | 2:F:271:TYR:CD2  | 2.54                     | 0.42              |
| 2:F:314:ALA:O    | 2:F:315:TYR:CG   | 2.73                     | 0.42              |
| 1:G:72:ASN:HD22  | 1:G:73:ASN:N     | 2.18                     | 0.42              |
| 2:H:106:VAL:O    | 2:H:107:ALA:C    | 2.61                     | 0.42              |
| 1:A:47:LYS:O     | 1:A:51:LEU:HD12  | 2.19                     | 0.42              |
| 1:A:69:ASP:C     | 1:A:71:GLY:N     | 2.76                     | 0.42              |
| 1:A:266:GLU:HG3  | 1:A:270:LYS:HE3  | 2.00                     | 0.42              |
| 1:A:274:THR:O    | 1:A:276:LEU:N    | 2.52                     | 0.42              |
| 2:B:228:CYS:O    | 2:B:231:TYR:HB3  | 2.19                     | 0.42              |
| 2:B:342:ASN:N    | 2:B:342:ASN:ND2  | 2.64                     | 0.42              |
| 3:I:107:THR:CG2  | 3:I:111:LYS:HB3  | 2.50                     | 0.42              |
| 1:C:189:PHE:CE1  | 1:C:192:LEU:HB2  | 2.55                     | 0.42              |
| 1:C:371:ALA:O    | 1:C:374:SER:N    | 2.48                     | 0.42              |
| 2:D:52:LEU:HD11  | 2:D:78:ILE:HG13  | 2.01                     | 0.42              |
| 2:D:80:MET:HE2   | 2:D:126:LYS:CB   | 2.49                     | 0.42              |
| 2:D:355:PHE:O    | 2:D:356:SER:CB   | 2.68                     | 0.42              |
| 2:D:356:SER:HA   | 2:D:357:PRO:HD3  | 1.53                     | 0.42              |
| 1:E:61:ASP:OD2   | 1:E:85:ARG:HD2   | 2.19                     | 0.42              |
| 2:F:124:PHE:CD1  | 2:F:124:PHE:O    | 2.72                     | 0.42              |
| 2:F:353:ILE:HG23 | 2:F:355:PHE:HE1  | 1.84                     | 0.42              |
| 1:G:132:PRO:O    | 1:G:133:GLU:C    | 2.63                     | 0.42              |
| 1:G:259:PRO:CA   | 1:G:260:GLU:HG2  | 2.50                     | 0.42              |
| 1:G:355:ALA:O    | 1:G:358:GLY:N    | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:404:LEU:HD21 | 1:G:467:GLU:O    | 2.19                     | 0.42              |
| 2:H:183:GLU:HG3  | 2:H:289:ILE:CG2  | 2.50                     | 0.42              |
| 2:H:249:LEU:CD1  | 2:H:260:ILE:HD11 | 2.49                     | 0.42              |
| 2:H:343:CYS:O    | 2:H:347:SER:HB3  | 2.19                     | 0.42              |
| 4:H:8:ATP:H3'    | 4:H:8:ATP:O1B    | 2.18                     | 0.42              |
| 1:A:195:HIS:O    | 1:A:198:SER:HB3  | 2.20                     | 0.42              |
| 2:B:241:GLN:HE21 | 2:B:246:GLY:H    | 1.67                     | 0.42              |
| 2:B:353:ILE:HG23 | 2:B:355:PHE:HE1  | 1.84                     | 0.42              |
| 1:C:517:ASN:OD1  | 1:C:534:LEU:HB2  | 2.20                     | 0.42              |
| 2:D:18:ASN:C     | 2:D:20:VAL:H     | 2.27                     | 0.42              |
| 2:D:84:ASP:OD1   | 2:D:84:ASP:C     | 2.63                     | 0.42              |
| 2:D:392:LEU:HA   | 2:D:392:LEU:HD23 | 1.46                     | 0.42              |
| 1:E:111:ASN:OD1  | 1:E:111:ASN:O    | 2.37                     | 0.42              |
| 1:E:317:LYS:HG2  | 1:E:318:GLU:N    | 2.35                     | 0.42              |
| 1:E:332:MET:HE2  | 1:E:342:LEU:HD23 | 2.01                     | 0.42              |
| 1:E:371:ALA:C    | 1:E:373:GLU:H    | 2.27                     | 0.42              |
| 2:F:703:GLY:C    | 2:F:705:VAL:N    | 2.75                     | 0.42              |
| 1:G:39:THR:HB    | 1:G:489:GLU:OE1  | 2.19                     | 0.42              |
| 2:H:102:PRO:HB3  | 2:H:124:PHE:CD2  | 2.55                     | 0.42              |
| 2:H:351:GLN:HE21 | 2:H:351:GLN:CA   | 2.27                     | 0.42              |
| 1:A:47:LYS:HD2   | 1:A:51:LEU:CD1   | 2.49                     | 0.42              |
| 1:A:146:SER:O    | 1:A:147:GLN:HB2  | 2.19                     | 0.42              |
| 1:A:261:ASP:HB2  | 1:A:262:GLU:H    | 1.66                     | 0.42              |
| 1:A:331:ASP:OD1  | 2:B:223:ARG:HD2  | 2.19                     | 0.42              |
| 2:B:74:GLN:HA    | 2:B:74:GLN:HE21  | 1.84                     | 0.42              |
| 2:B:130:PHE:CG   | 2:B:134:PHE:CD2  | 3.08                     | 0.42              |
| 2:B:183:GLU:HG3  | 2:B:289:ILE:HG21 | 2.02                     | 0.42              |
| 2:B:243:PHE:O    | 2:B:247:VAL:HG21 | 2.19                     | 0.42              |
| 1:C:47:LYS:HD2   | 1:C:51:LEU:HD12  | 2.02                     | 0.42              |
| 1:C:435:PHE:C    | 1:C:435:PHE:CD2  | 2.98                     | 0.42              |
| 1:C:436:HIS:O    | 1:C:437:LYS:C    | 2.62                     | 0.42              |
| 1:C:504:GLU:HG3  | 1:C:516:PHE:CE2  | 2.55                     | 0.42              |
| 2:D:351:GLN:O    | 2:D:353:ILE:N    | 2.53                     | 0.42              |
| 1:E:47:LYS:HD2   | 1:E:51:LEU:CD1   | 2.50                     | 0.42              |
| 1:E:281:ILE:HA   | 1:E:282:PRO:HD3  | 1.85                     | 0.42              |
| 2:F:96:PRO:O     | 2:F:99:ILE:HG13  | 2.20                     | 0.42              |
| 2:F:127:ILE:HG13 | 2:F:128:GLN:NE2  | 2.34                     | 0.42              |
| 2:F:355:PHE:O    | 2:F:356:SER:CB   | 2.67                     | 0.42              |
| 1:G:84:ASN:HD22  | 1:G:85:ARG:N     | 2.16                     | 0.42              |
| 1:G:143:LEU:HD13 | 1:G:150:LEU:HD13 | 2.00                     | 0.42              |
| 1:G:253:LYS:O    | 1:G:260:GLU:CD   | 2.62                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:525:MET:HE2  | 2:H:30:PHE:CG    | 2.54                     | 0.42              |
| 1:A:175:HIS:HD2  | 1:A:512:GLN:O    | 2.02                     | 0.42              |
| 1:A:323:LEU:HD22 | 1:A:387:SER:HB2  | 2.01                     | 0.42              |
| 2:B:158:LEU:HD23 | 2:B:158:LEU:HA   | 1.79                     | 0.42              |
| 1:C:75:PHE:O     | 1:C:76:LEU:HD23  | 2.20                     | 0.42              |
| 1:C:221:TYR:O    | 1:C:243:PHE:HE1  | 2.03                     | 0.42              |
| 1:C:248:ARG:C    | 1:C:250:GLY:N    | 2.77                     | 0.42              |
| 1:C:504:GLU:O    | 1:C:508:ILE:HG13 | 2.20                     | 0.42              |
| 2:D:74:GLN:HA    | 2:D:74:GLN:HE21  | 1.85                     | 0.42              |
| 2:D:164:TYR:HD2  | 2:D:169:LEU:HA   | 1.84                     | 0.42              |
| 1:E:19:LEU:HD21  | 2:F:290:PRO:HB2  | 2.01                     | 0.42              |
| 1:E:40:ALA:HB3   | 1:E:489:GLU:CD   | 2.45                     | 0.42              |
| 1:E:144:TRP:CZ3  | 1:E:397:SER:HA   | 2.55                     | 0.42              |
| 2:F:130:PHE:CG   | 2:F:134:PHE:CD2  | 3.07                     | 0.42              |
| 3:K:103:ILE:HD12 | 3:K:103:ILE:C    | 2.44                     | 0.42              |
| 1:G:163:ARG:NH1  | 1:G:163:ARG:CG   | 2.82                     | 0.42              |
| 1:G:274:THR:O    | 1:G:276:LEU:N    | 2.53                     | 0.42              |
| 1:G:305:TRP:O    | 1:G:308:ALA:HB3  | 2.19                     | 0.42              |
| 2:H:347:SER:O    | 2:H:348:GLN:C    | 2.62                     | 0.42              |
| 3:L:150:MET:CE   | 3:L:167:LEU:HD22 | 2.29                     | 0.42              |
| 1:A:35:LEU:HD23  | 1:A:46:LEU:HD22  | 2.01                     | 0.42              |
| 1:A:39:THR:HB    | 1:A:489:GLU:OE1  | 2.19                     | 0.42              |
| 2:B:131:ASN:HB3  | 2:D:131:ASN:HD22 | 1.85                     | 0.42              |
| 2:B:149:ILE:O    | 2:B:150:ALA:C    | 2.62                     | 0.42              |
| 2:B:232:VAL:HG21 | 2:B:263:LYS:C    | 2.45                     | 0.42              |
| 1:C:51:LEU:C     | 1:C:53:GLY:H     | 2.28                     | 0.42              |
| 3:J:122:LYS:HA   | 3:J:154:LYS:O    | 2.20                     | 0.42              |
| 1:E:38:ALA:C     | 1:E:85:ARG:HD3   | 2.45                     | 0.42              |
| 1:E:51:LEU:C     | 1:E:53:GLY:H     | 2.28                     | 0.42              |
| 2:F:140:ILE:HG22 | 2:F:141:ILE:N    | 2.35                     | 0.42              |
| 1:G:18:ARG:CZ    | 2:H:288:ILE:HD12 | 2.49                     | 0.42              |
| 1:G:143:LEU:HD22 | 1:G:148:ILE:CG2  | 2.50                     | 0.42              |
| 2:H:321:TYR:CD2  | 2:H:322:LEU:N    | 2.87                     | 0.42              |
| 1:A:46:LEU:HD12  | 1:A:46:LEU:HA    | 1.94                     | 0.42              |
| 1:A:140:ALA:HA   | 1:A:150:LEU:CD2  | 2.49                     | 0.42              |
| 1:A:323:LEU:HB3  | 1:A:324:PRO:CD   | 2.50                     | 0.42              |
| 1:A:348:GLU:OE2  | 1:E:107:GLU:OE1  | 2.38                     | 0.42              |
| 2:B:232:VAL:HG21 | 2:B:264:SER:N    | 2.35                     | 0.42              |
| 2:B:274:ARG:NH1  | 1:E:106:GLU:O    | 2.53                     | 0.42              |
| 1:C:404:LEU:HD21 | 1:C:467:GLU:O    | 2.20                     | 0.42              |
| 2:D:50:LYS:H     | 2:D:139:HIS:CD2  | 2.38                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:54:ILE:HG12  | 1:E:55:GLY:N     | 2.35                     | 0.42              |
| 1:E:140:ALA:HA   | 1:E:150:LEU:CD2  | 2.49                     | 0.42              |
| 2:F:84:ASP:OD1   | 2:F:84:ASP:C     | 2.63                     | 0.42              |
| 2:F:250:ASP:H    | 2:F:256:HIS:CE1  | 2.38                     | 0.42              |
| 2:F:370:ASN:O    | 2:F:371:SER:C    | 2.62                     | 0.42              |
| 1:G:264:ASN:ND2  | 1:G:265:PHE:H    | 2.17                     | 0.42              |
| 2:H:80:MET:HB3   | 2:H:126:LYS:HB3  | 2.02                     | 0.42              |
| 1:A:347:ARG:HH22 | 2:B:274:ARG:NH1  | 2.17                     | 0.41              |
| 1:A:366:GLN:C    | 1:A:368:ILE:N    | 2.67                     | 0.41              |
| 2:B:59:LEU:O     | 2:B:60:GLY:C     | 2.63                     | 0.41              |
| 2:B:347:SER:O    | 2:B:348:GLN:C    | 2.62                     | 0.41              |
| 2:B:394:LEU:CD1  | 2:B:396:SER:HB3  | 2.50                     | 0.41              |
| 1:C:113:LEU:HD11 | 1:C:139:LEU:HB2  | 2.02                     | 0.41              |
| 1:C:215:ILE:O    | 1:C:216:VAL:C    | 2.63                     | 0.41              |
| 2:D:110:PHE:HE2  | 2:D:114:ARG:HB2  | 1.85                     | 0.41              |
| 2:D:182:THR:HG23 | 2:D:183:GLU:N    | 2.34                     | 0.41              |
| 1:E:139:LEU:C    | 1:E:141:ASP:H    | 2.28                     | 0.41              |
| 1:E:432:VAL:HG13 | 1:E:443:PRO:CD   | 2.49                     | 0.41              |
| 2:F:231:TYR:C    | 2:F:233:ARG:N    | 2.75                     | 0.41              |
| 1:G:33:VAL:CG2   | 1:G:54:ILE:HD11  | 2.49                     | 0.41              |
| 1:G:96:LEU:HD23  | 2:H:95:ARG:HH21  | 1.84                     | 0.41              |
| 1:G:480:HIS:HB2  | 2:H:29:PRO:HG2   | 2.02                     | 0.41              |
| 2:H:362:GLN:H    | 2:H:362:GLN:HG3  | 1.49                     | 0.41              |
| 3:L:103:ILE:HD11 | 3:L:117:ILE:HD12 | 2.01                     | 0.41              |
| 1:A:171:VAL:HG13 | 1:A:391:ARG:O    | 2.20                     | 0.41              |
| 1:A:186:ASP:OD2  | 1:A:279:THR:HB   | 2.19                     | 0.41              |
| 3:I:111:LYS:O    | 3:I:112:GLU:HB3  | 2.21                     | 0.41              |
| 1:C:19:LEU:HD23  | 1:C:19:LEU:HA    | 1.90                     | 0.41              |
| 1:C:362:ALA:O    | 1:C:363:LYS:C    | 2.63                     | 0.41              |
| 2:D:80:MET:HE3   | 4:D:6:ATP:C6     | 2.55                     | 0.41              |
| 1:E:47:LYS:O     | 1:E:51:LEU:HD12  | 2.20                     | 0.41              |
| 1:E:260:GLU:HB2  | 1:E:261:ASP:OD1  | 2.20                     | 0.41              |
| 3:K:150:MET:HE3  | 3:K:167:LEU:HD13 | 2.02                     | 0.41              |
| 1:G:175:HIS:HD2  | 1:G:512:GLN:O    | 2.03                     | 0.41              |
| 2:H:250:ASP:OD2  | 2:H:253:ASP:HB2  | 2.20                     | 0.41              |
| 3:L:131:GLU:CD   | 3:L:138:PRO:HD3  | 2.45                     | 0.41              |
| 3:L:144:ILE:HD12 | 3:L:170:VAL:HG11 | 2.02                     | 0.41              |
| 3:L:149:GLN:HG3  | 3:L:149:GLN:O    | 2.20                     | 0.41              |
| 2:B:340:LYS:HB3  | 2:B:342:ASN:ND2  | 2.34                     | 0.41              |
| 2:B:343:CYS:O    | 2:B:347:SER:HB3  | 2.19                     | 0.41              |
| 1:C:213:PRO:CB   | 1:C:332:MET:HE3  | 2.45                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:493:ILE:O    | 1:C:494:ALA:C    | 2.63                     | 0.41              |
| 2:D:182:THR:CG2  | 2:D:183:GLU:N    | 2.79                     | 0.41              |
| 3:J:103:ILE:HD11 | 3:J:117:ILE:HD12 | 2.02                     | 0.41              |
| 1:E:441:ARG:HH11 | 1:E:441:ARG:HG2  | 1.85                     | 0.41              |
| 2:F:187:GLY:CA   | 3:K:173:LEU:HD12 | 2.51                     | 0.41              |
| 2:F:245:GLU:C    | 2:F:247:VAL:H    | 2.28                     | 0.41              |
| 3:K:122:LYS:HA   | 3:K:154:LYS:O    | 2.19                     | 0.41              |
| 1:G:61:ASP:OD2   | 1:G:85:ARG:HD2   | 2.20                     | 0.41              |
| 2:H:124:PHE:CD1  | 2:H:124:PHE:O    | 2.73                     | 0.41              |
| 2:H:126:LYS:HA   | 4:H:8:ATP:N1     | 2.35                     | 0.41              |
| 2:H:187:GLY:C    | 3:L:173:LEU:HD12 | 2.45                     | 0.41              |
| 3:L:122:LYS:HA   | 3:L:154:LYS:O    | 2.20                     | 0.41              |
| 1:A:317:LYS:HG2  | 1:A:318:GLU:N    | 2.36                     | 0.41              |
| 1:A:333:ILE:HA   | 2:B:223:ARG:HH21 | 1.85                     | 0.41              |
| 1:A:481:GLU:O    | 1:A:484:ARG:N    | 2.53                     | 0.41              |
| 2:B:95:ARG:HD3   | 2:B:95:ARG:HA    | 1.66                     | 0.41              |
| 2:B:96:PRO:O     | 2:B:99:ILE:HG13  | 2.20                     | 0.41              |
| 2:B:231:TYR:C    | 2:B:233:ARG:H    | 2.28                     | 0.41              |
| 2:B:355:PHE:O    | 2:B:356:SER:CB   | 2.68                     | 0.41              |
| 2:D:158:LEU:HD12 | 2:D:177:LEU:HB2  | 2.01                     | 0.41              |
| 2:D:231:TYR:C    | 2:D:233:ARG:H    | 2.27                     | 0.41              |
| 1:E:36:ILE:HD13  | 1:E:36:ILE:HA    | 1.92                     | 0.41              |
| 1:E:139:LEU:C    | 1:E:141:ASP:N    | 2.79                     | 0.41              |
| 1:E:143:LEU:HD12 | 1:E:150:LEU:HD13 | 1.97                     | 0.41              |
| 1:E:248:ARG:C    | 1:E:250:GLY:N    | 2.77                     | 0.41              |
| 1:E:323:LEU:HB3  | 1:E:324:PRO:CD   | 2.50                     | 0.41              |
| 2:F:130:PHE:HB2  | 2:F:135:TYR:CE1  | 2.56                     | 0.41              |
| 2:F:174:ILE:HG23 | 2:F:194:PRO:O    | 2.20                     | 0.41              |
| 2:F:316:ILE:HD12 | 2:F:316:ILE:N    | 2.23                     | 0.41              |
| 2:F:394:LEU:C    | 2:F:396:SER:H    | 2.29                     | 0.41              |
| 2:H:333:TYR:CZ   | 2:H:335:PHE:HB3  | 2.56                     | 0.41              |
| 2:H:351:GLN:O    | 2:H:353:ILE:N    | 2.53                     | 0.41              |
| 1:A:40:ALA:HB3   | 1:A:489:GLU:CD   | 2.46                     | 0.41              |
| 1:A:112:LEU:HD23 | 1:A:112:LEU:HA   | 1.87                     | 0.41              |
| 1:A:213:PRO:CB   | 1:A:332:MET:HE3  | 2.46                     | 0.41              |
| 2:B:394:LEU:C    | 2:B:396:SER:H    | 2.29                     | 0.41              |
| 2:B:603:ILE:O    | 2:B:607:THR:N    | 2.53                     | 0.41              |
| 3:I:122:LYS:HA   | 3:I:154:LYS:O    | 2.20                     | 0.41              |
| 1:C:69:ASP:C     | 1:C:71:GLY:N     | 2.77                     | 0.41              |
| 1:C:84:ASN:HD22  | 1:C:85:ARG:N     | 2.18                     | 0.41              |
| 1:C:220:LYS:HD2  | 1:C:220:LYS:HA   | 1.94                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:106:VAL:O    | 2:D:107:ALA:C    | 2.63                     | 0.41              |
| 2:D:231:TYR:C    | 2:D:233:ARG:N    | 2.76                     | 0.41              |
| 2:D:283:GLY:HA2  | 2:D:288:ILE:HG13 | 2.03                     | 0.41              |
| 1:E:66:SER:O     | 1:E:69:ASP:HB2   | 2.20                     | 0.41              |
| 1:E:311:LEU:HD12 | 1:E:311:LEU:HA   | 1.81                     | 0.41              |
| 1:E:404:LEU:HD21 | 1:E:467:GLU:O    | 2.21                     | 0.41              |
| 2:F:271:TYR:CD1  | 2:F:271:TYR:N    | 2.88                     | 0.41              |
| 2:F:306:GLU:OE2  | 2:F:309:LYS:HD2  | 2.20                     | 0.41              |
| 3:K:149:GLN:HG3  | 3:K:149:GLN:O    | 2.21                     | 0.41              |
| 2:H:394:LEU:HD11 | 2:H:396:SER:CB   | 2.49                     | 0.41              |
| 1:A:156:TYR:CE1  | 1:A:487:ALA:HA   | 2.56                     | 0.41              |
| 2:B:187:GLY:C    | 3:I:173:LEU:HD12 | 2.46                     | 0.41              |
| 3:I:102:LEU:HD21 | 3:I:114:GLU:CD   | 2.45                     | 0.41              |
| 1:C:307:LEU:CD1  | 1:C:383:LEU:HD22 | 2.50                     | 0.41              |
| 1:C:371:ALA:C    | 1:C:373:GLU:H    | 2.28                     | 0.41              |
| 2:D:347:SER:O    | 2:D:348:GLN:C    | 2.63                     | 0.41              |
| 2:F:42:LEU:O     | 2:F:43:GLN:C     | 2.64                     | 0.41              |
| 2:F:102:PRO:HB3  | 2:F:124:PHE:CD2  | 2.56                     | 0.41              |
| 2:F:134:PHE:O    | 2:F:137:GLN:HG3  | 2.20                     | 0.41              |
| 2:F:320:ASN:O    | 2:F:321:TYR:CB   | 2.68                     | 0.41              |
| 1:G:117:PRO:C    | 1:G:119:PHE:N    | 2.75                     | 0.41              |
| 1:G:253:LYS:O    | 1:G:260:GLU:HG2  | 2.20                     | 0.41              |
| 2:H:309:LYS:O    | 2:H:313:SER:N    | 2.39                     | 0.41              |
| 1:A:139:LEU:HG   | 1:A:143:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:259:PRO:C    | 1:A:260:GLU:CG   | 2.93                     | 0.41              |
| 3:I:118:GLU:O    | 3:I:121:ASP:OD1  | 2.38                     | 0.41              |
| 1:C:61:ASP:CG    | 1:C:85:ARG:HD2   | 2.46                     | 0.41              |
| 1:C:164:ILE:HD13 | 1:C:515:ILE:HD12 | 2.02                     | 0.41              |
| 2:D:59:LEU:HD12  | 3:J:176:GLY:CA   | 2.50                     | 0.41              |
| 2:D:82:THR:O     | 2:D:82:THR:HG23  | 2.20                     | 0.41              |
| 2:D:130:PHE:HB2  | 2:D:135:TYR:CE1  | 2.56                     | 0.41              |
| 2:D:157:MET:HE3  | 2:D:157:MET:CA   | 2.49                     | 0.41              |
| 2:D:182:THR:O    | 2:D:183:GLU:HB2  | 2.20                     | 0.41              |
| 1:E:16:GLN:NE2   | 1:E:20:TRP:CZ2   | 2.86                     | 0.41              |
| 1:E:158:LEU:HA   | 1:E:158:LEU:HD23 | 1.82                     | 0.41              |
| 1:E:163:ARG:NH1  | 1:E:163:ARG:CG   | 2.83                     | 0.41              |
| 1:E:323:LEU:HD22 | 1:E:387:SER:HB2  | 2.03                     | 0.41              |
| 2:F:33:PRO:O     | 2:F:35:PHE:N     | 2.54                     | 0.41              |
| 2:F:351:GLN:HE21 | 2:F:351:GLN:CA   | 2.28                     | 0.41              |
| 1:G:75:PHE:O     | 1:G:76:LEU:HD23  | 2.21                     | 0.41              |
| 1:G:141:ASP:O    | 1:G:142:VAL:C    | 2.63                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:187:GLY:CA   | 3:L:173:LEU:HD12 | 2.50                     | 0.41              |
| 2:H:249:LEU:HD11 | 2:H:260:ILE:HD11 | 2.03                     | 0.41              |
| 3:L:136:ILE:O    | 3:L:137:PRO:C    | 2.62                     | 0.41              |
| 1:A:61:ASP:CG    | 1:A:85:ARG:HD2   | 2.45                     | 0.41              |
| 1:A:259:PRO:CA   | 1:A:260:GLU:HG2  | 2.51                     | 0.41              |
| 2:B:124:PHE:HD1  | 2:B:124:PHE:O    | 2.04                     | 0.41              |
| 1:C:264:ASN:ND2  | 1:C:265:PHE:H    | 2.18                     | 0.41              |
| 1:C:311:LEU:O    | 1:C:314:PHE:HB3  | 2.21                     | 0.41              |
| 1:E:466:GLN:O    | 1:E:467:GLU:C    | 2.64                     | 0.41              |
| 2:F:247:VAL:HA   | 2:F:248:PRO:HD3  | 1.81                     | 0.41              |
| 1:G:45:ILE:CG1   | 1:G:498:GLY:HA2  | 2.43                     | 0.41              |
| 1:G:117:PRO:O    | 1:G:119:PHE:N    | 2.53                     | 0.41              |
| 1:G:157:GLY:HA3  | 1:G:485:TYR:CD1  | 2.55                     | 0.41              |
| 1:A:51:LEU:C     | 1:A:53:GLY:H     | 2.29                     | 0.41              |
| 1:A:141:ASP:O    | 1:A:142:VAL:C    | 2.64                     | 0.41              |
| 1:A:155:THR:HG23 | 1:A:493:ILE:CG2  | 2.51                     | 0.41              |
| 1:A:236:THR:HG23 | 1:A:240:LYS:HE3  | 2.03                     | 0.41              |
| 1:A:371:ALA:C    | 1:A:373:GLU:H    | 2.29                     | 0.41              |
| 1:A:441:ARG:HH21 | 1:A:453:ASP:CG   | 2.29                     | 0.41              |
| 2:B:74:GLN:HE22  | 2:B:119:ASN:ND2  | 2.08                     | 0.41              |
| 2:B:84:ASP:OD1   | 2:B:84:ASP:C     | 2.64                     | 0.41              |
| 2:B:110:PHE:HE2  | 2:B:114:ARG:HB2  | 1.85                     | 0.41              |
| 2:B:127:ILE:HG13 | 2:B:128:GLN:N    | 2.36                     | 0.41              |
| 2:B:232:VAL:HG12 | 2:B:260:ILE:HG23 | 2.03                     | 0.41              |
| 2:B:274:ARG:NH2  | 1:E:108:SER:N    | 2.69                     | 0.41              |
| 2:B:320:ASN:O    | 2:B:321:TYR:CB   | 2.68                     | 0.41              |
| 2:B:339:ARG:NH2  | 2:B:346:CYS:O    | 2.54                     | 0.41              |
| 3:I:149:GLN:O    | 3:I:149:GLN:HG3  | 2.21                     | 0.41              |
| 1:C:37:ASN:HD22  | 1:C:37:ASN:HA    | 1.60                     | 0.41              |
| 1:C:146:SER:O    | 1:C:147:GLN:HB2  | 2.21                     | 0.41              |
| 2:D:158:LEU:HA   | 2:D:158:LEU:HD23 | 1.85                     | 0.41              |
| 2:D:202:CYS:SG   | 2:D:343:CYS:SG   | 3.02                     | 0.41              |
| 2:D:268:ALA:HB1  | 2:D:273:ILE:O    | 2.20                     | 0.41              |
| 2:D:361:LEU:CA   | 2:D:364:VAL:CG2  | 2.99                     | 0.41              |
| 3:J:103:ILE:HD12 | 3:J:103:ILE:C    | 2.45                     | 0.41              |
| 1:E:111:ASN:OD1  | 1:E:111:ASN:C    | 2.64                     | 0.41              |
| 1:E:225:TRP:CD1  | 1:E:225:TRP:O    | 2.74                     | 0.41              |
| 1:E:261:ASP:HB2  | 1:E:262:GLU:H    | 1.64                     | 0.41              |
| 1:E:371:ALA:O    | 1:E:374:SER:N    | 2.51                     | 0.41              |
| 1:E:532:PHE:HB3  | 1:E:533:GLN:H    | 1.40                     | 0.41              |
| 2:F:232:VAL:HG21 | 2:F:264:SER:N    | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:392:LEU:O    | 2:F:393:TYR:O    | 2.39                     | 0.41              |
| 2:F:394:LEU:CD1  | 2:F:396:SER:HB3  | 2.51                     | 0.41              |
| 3:K:111:LYS:O    | 3:K:112:GLU:HB3  | 2.20                     | 0.41              |
| 1:G:16:GLN:HB2   | 2:H:292:VAL:HG12 | 2.03                     | 0.41              |
| 1:G:34:CYS:HB3   | 1:G:126:VAL:HG22 | 2.02                     | 0.41              |
| 1:G:311:LEU:HD12 | 1:G:311:LEU:HA   | 1.87                     | 0.41              |
| 1:G:435:PHE:CZ   | 1:G:439:GLN:HG3  | 2.56                     | 0.41              |
| 1:G:481:GLU:O    | 1:G:484:ARG:N    | 2.54                     | 0.41              |
| 2:H:182:THR:CG2  | 2:H:183:GLU:N    | 2.81                     | 0.41              |
| 2:B:126:LYS:O    | 2:B:127:ILE:C    | 2.63                     | 0.41              |
| 2:D:127:ILE:CG1  | 2:D:128:GLN:NE2  | 2.84                     | 0.41              |
| 2:D:127:ILE:C    | 2:D:129:ASP:H    | 2.29                     | 0.41              |
| 2:D:392:LEU:O    | 2:D:393:TYR:O    | 2.39                     | 0.41              |
| 1:E:15:ARG:HA    | 1:E:15:ARG:HD3   | 1.81                     | 0.41              |
| 1:E:362:ALA:O    | 1:E:363:LYS:C    | 2.64                     | 0.41              |
| 2:F:164:TYR:HD2  | 2:F:169:LEU:HA   | 1.86                     | 0.41              |
| 2:F:253:ASP:O    | 2:F:254:PRO:C    | 2.64                     | 0.41              |
| 2:F:396:SER:O    | 2:F:600:VAL:N    | 2.54                     | 0.41              |
| 1:G:172:ILE:HA   | 1:G:390:LEU:HD23 | 2.02                     | 0.41              |
| 2:H:231:TYR:C    | 2:H:233:ARG:H    | 2.29                     | 0.41              |
| 1:A:36:ILE:HD13  | 1:A:36:ILE:HA    | 1.91                     | 0.40              |
| 1:A:331:ASP:HB2  | 2:B:224:LEU:HD11 | 2.02                     | 0.40              |
| 2:B:218:ILE:O    | 2:B:218:ILE:HG22 | 2.21                     | 0.40              |
| 2:B:237:TRP:O    | 2:B:242:PRO:HD3  | 2.21                     | 0.40              |
| 2:B:267:ARG:NH1  | 2:B:267:ARG:CG   | 2.77                     | 0.40              |
| 2:B:295:THR:O    | 2:B:296:ASN:C    | 2.63                     | 0.40              |
| 2:B:335:PHE:CZ   | 3:I:144:ILE:CD1  | 3.04                     | 0.40              |
| 1:C:111:ASN:OD1  | 1:C:111:ASN:O    | 2.39                     | 0.40              |
| 1:C:143:LEU:HD13 | 1:C:150:LEU:HD13 | 1.99                     | 0.40              |
| 1:C:457:LEU:HD23 | 1:C:479:VAL:HG12 | 2.02                     | 0.40              |
| 2:D:85:VAL:C     | 2:D:87:ASN:H     | 2.29                     | 0.40              |
| 2:D:102:PRO:HB3  | 2:D:124:PHE:CD2  | 2.56                     | 0.40              |
| 2:D:134:PHE:O    | 2:D:137:GLN:HG3  | 2.21                     | 0.40              |
| 2:D:249:LEU:CD1  | 2:D:260:ILE:HD11 | 2.51                     | 0.40              |
| 1:E:117:PRO:O    | 1:E:119:PHE:N    | 2.54                     | 0.40              |
| 1:E:221:TYR:O    | 1:E:243:PHE:HE1  | 2.04                     | 0.40              |
| 2:F:371:SER:C    | 2:F:373:SER:N    | 2.76                     | 0.40              |
| 1:G:113:LEU:HD23 | 1:G:113:LEU:HA   | 1.87                     | 0.40              |
| 1:G:317:LYS:HG2  | 1:G:318:GLU:N    | 2.37                     | 0.40              |
| 2:H:207:TYR:HA   | 2:H:208:PRO:HD3  | 1.90                     | 0.40              |
| 2:H:392:LEU:O    | 2:H:393:TYR:O    | 2.39                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:102:LEU:HD21 | 3:L:114:GLU:CD   | 2.46                     | 0.40              |
| 1:A:148:ILE:HA   | 1:A:149:PRO:HD3  | 1.95                     | 0.40              |
| 1:A:352:LYS:C    | 1:A:354:ALA:N    | 2.77                     | 0.40              |
| 1:A:352:LYS:O    | 1:A:353:ASP:C    | 2.62                     | 0.40              |
| 1:A:493:ILE:HD13 | 1:A:493:ILE:HA   | 1.91                     | 0.40              |
| 2:B:164:TYR:HD2  | 2:B:169:LEU:HA   | 1.85                     | 0.40              |
| 1:C:143:LEU:HD22 | 1:C:148:ILE:CG2  | 2.50                     | 0.40              |
| 1:C:261:ASP:O    | 1:C:262:GLU:CG   | 2.69                     | 0.40              |
| 2:D:126:LYS:O    | 2:D:127:ILE:C    | 2.64                     | 0.40              |
| 3:J:155:THR:O    | 3:J:158:ASP:N    | 2.54                     | 0.40              |
| 2:F:84:ASP:H     | 2:F:87:ASN:HD22  | 1.67                     | 0.40              |
| 2:F:362:GLN:H    | 2:F:362:GLN:HG3  | 1.48                     | 0.40              |
| 1:G:340:ILE:O    | 1:G:341:LYS:C    | 2.61                     | 0.40              |
| 1:G:517:ASN:OD1  | 1:G:534:LEU:HB2  | 2.22                     | 0.40              |
| 2:H:134:PHE:O    | 2:H:137:GLN:HG3  | 2.20                     | 0.40              |
| 2:H:187:GLY:HA2  | 3:L:173:LEU:CD1  | 2.51                     | 0.40              |
| 2:H:316:ILE:HA   | 2:H:317:PRO:HD3  | 1.95                     | 0.40              |
| 2:H:606:ARG:O    | 2:H:608:ARG:C    | 2.65                     | 0.40              |
| 3:L:111:LYS:O    | 3:L:112:GLU:HB3  | 2.21                     | 0.40              |
| 1:A:45:ILE:CG1   | 1:A:498:GLY:HA2  | 2.49                     | 0.40              |
| 1:A:215:ILE:HD12 | 1:A:342:LEU:HD21 | 2.03                     | 0.40              |
| 2:B:83:ILE:HD13  | 2:B:94:PHE:CG    | 2.57                     | 0.40              |
| 2:B:141:ILE:HD12 | 2:B:158:LEU:HD11 | 2.03                     | 0.40              |
| 2:B:362:GLN:H    | 2:B:362:GLN:HG3  | 1.50                     | 0.40              |
| 2:D:245:GLU:C    | 2:D:247:VAL:H    | 2.29                     | 0.40              |
| 2:D:247:VAL:HA   | 2:D:248:PRO:HD3  | 1.80                     | 0.40              |
| 2:D:907:PRO:C    | 2:D:909:THR:H    | 2.29                     | 0.40              |
| 3:J:118:GLU:O    | 3:J:121:ASP:OD1  | 2.39                     | 0.40              |
| 1:E:113:LEU:HD23 | 1:E:113:LEU:HA   | 1.90                     | 0.40              |
| 1:E:507:LYS:HG2  | 1:E:513:PHE:HB2  | 2.02                     | 0.40              |
| 1:E:517:ASN:OD1  | 1:E:534:LEU:HB2  | 2.21                     | 0.40              |
| 1:G:212:THR:O    | 1:G:213:PRO:C    | 2.64                     | 0.40              |
| 1:G:481:GLU:O    | 1:G:484:ARG:HB3  | 2.21                     | 0.40              |
| 2:H:95:ARG:HD3   | 2:H:95:ARG:HA    | 1.67                     | 0.40              |
| 2:H:130:PHE:CG   | 2:H:134:PHE:CD2  | 3.08                     | 0.40              |
| 2:H:140:ILE:HG22 | 2:H:141:ILE:N    | 2.36                     | 0.40              |
| 3:L:107:THR:OG1  | 3:L:108:LEU:N    | 2.54                     | 0.40              |
| 1:A:84:ASN:HD22  | 1:A:85:ARG:N     | 2.19                     | 0.40              |
| 1:A:225:TRP:O    | 1:A:225:TRP:CD1  | 2.75                     | 0.40              |
| 1:A:436:HIS:O    | 1:A:437:LYS:C    | 2.61                     | 0.40              |
| 1:A:457:LEU:HD23 | 1:A:479:VAL:CG1  | 2.52                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:52:LEU:HD11  | 2:B:78:ILE:HG13  | 2.02                     | 0.40              |
| 2:B:253:ASP:O    | 2:B:254:PRO:C    | 2.63                     | 0.40              |
| 1:C:105:VAL:HG12 | 1:C:107:GLU:H    | 1.86                     | 0.40              |
| 2:D:33:PRO:O     | 2:D:35:PHE:N     | 2.53                     | 0.40              |
| 2:D:213:PHE:HA   | 2:D:214:PRO:HD3  | 1.98                     | 0.40              |
| 2:D:357:PRO:O    | 2:D:357:PRO:CG   | 2.69                     | 0.40              |
| 1:E:359:ASN:HD22 | 1:E:359:ASN:HA   | 1.69                     | 0.40              |
| 2:F:18:ASN:C     | 2:F:20:VAL:H     | 2.29                     | 0.40              |
| 2:F:229:ILE:HG21 | 2:F:284:VAL:HB   | 2.04                     | 0.40              |
| 1:G:416:MET:SD   | 1:G:423:ILE:HG23 | 2.61                     | 0.40              |
| 2:H:18:ASN:C     | 2:H:20:VAL:H     | 2.30                     | 0.40              |
| 2:H:339:ARG:NH2  | 2:H:346:CYS:O    | 2.54                     | 0.40              |
| 3:L:103:ILE:HD12 | 3:L:103:ILE:C    | 2.46                     | 0.40              |
| 1:A:72:ASN:HD22  | 1:A:73:ASN:N     | 2.19                     | 0.40              |
| 1:A:128:ALA:HB1  | 1:A:131:LEU:CD1  | 2.52                     | 0.40              |
| 1:A:144:TRP:CZ3  | 1:A:397:SER:HA   | 2.56                     | 0.40              |
| 1:A:158:LEU:HD23 | 1:A:158:LEU:HA   | 1.87                     | 0.40              |
| 1:A:252:LEU:O    | 1:A:259:PRO:N    | 2.54                     | 0.40              |
| 1:A:369:GLY:O    | 1:A:370:GLN:C    | 2.63                     | 0.40              |
| 1:C:45:ILE:CG1   | 1:C:498:GLY:HA2  | 2.48                     | 0.40              |
| 1:C:180:LEU:HD23 | 3:J:135:GLY:CA   | 2.52                     | 0.40              |
| 1:E:264:ASN:N    | 1:E:264:ASN:ND2  | 2.61                     | 0.40              |
| 2:F:80:MET:HE3   | 4:F:7:ATP:C6     | 2.57                     | 0.40              |
| 2:F:141:ILE:HD12 | 2:F:158:LEU:HD21 | 2.04                     | 0.40              |
| 2:F:242:PRO:HG3  | 2:F:259:TRP:CH2  | 2.56                     | 0.40              |
| 2:F:295:THR:O    | 2:F:296:ASN:C    | 2.65                     | 0.40              |
| 1:G:16:GLN:NE2   | 1:G:20:TRP:CZ2   | 2.86                     | 0.40              |
| 1:G:171:VAL:HG13 | 1:G:391:ARG:O    | 2.21                     | 0.40              |
| 1:G:264:ASN:H    | 1:G:264:ASN:ND2  | 2.14                     | 0.40              |
| 2:H:59:LEU:O     | 2:H:60:GLY:C     | 2.62                     | 0.40              |
| 2:H:136:ARG:HG2  | 2:H:136:ARG:NH1  | 2.37                     | 0.40              |
| 2:H:157:MET:HE3  | 2:H:160:SER:OG   | 2.21                     | 0.40              |
| 2:H:316:ILE:H    | 2:H:316:ILE:CD1  | 2.12                     | 0.40              |
| 2:H:343:CYS:C    | 2:H:345:ALA:N    | 2.77                     | 0.40              |
| 3:L:118:GLU:O    | 3:L:121:ASP:OD1  | 2.39                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 512/529 (97%)   | 418 (82%)  | 66 (13%)  | 28 (6%)  | 1           | 14 |
| 1   | C     | 512/529 (97%)   | 418 (82%)  | 67 (13%)  | 27 (5%)  | 1           | 14 |
| 1   | E     | 512/529 (97%)   | 416 (81%)  | 70 (14%)  | 26 (5%)  | 1           | 15 |
| 1   | G     | 512/529 (97%)   | 412 (80%)  | 72 (14%)  | 28 (6%)  | 1           | 14 |
| 2   | B     | 408/431 (95%)   | 310 (76%)  | 73 (18%)  | 25 (6%)  | 1           | 13 |
| 2   | D     | 410/431 (95%)   | 307 (75%)  | 76 (18%)  | 27 (7%)  | 1           | 12 |
| 2   | F     | 408/431 (95%)   | 309 (76%)  | 75 (18%)  | 24 (6%)  | 1           | 13 |
| 2   | H     | 408/431 (95%)   | 308 (76%)  | 77 (19%)  | 23 (6%)  | 1           | 14 |
| 3   | I     | 74/76 (97%)     | 65 (88%)   | 7 (10%)   | 2 (3%)   | 4           | 27 |
| 3   | J     | 74/76 (97%)     | 65 (88%)   | 6 (8%)    | 3 (4%)   | 2           | 19 |
| 3   | K     | 74/76 (97%)     | 66 (89%)   | 6 (8%)    | 2 (3%)   | 4           | 27 |
| 3   | L     | 74/76 (97%)     | 66 (89%)   | 6 (8%)    | 2 (3%)   | 4           | 27 |
| All | All   | 3978/4144 (96%) | 3160 (79%) | 601 (15%) | 217 (6%) | 1           | 14 |

All (217) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 233 | ILE  |
| 1   | A     | 259 | PRO  |
| 1   | A     | 262 | GLU  |
| 1   | A     | 275 | ALA  |
| 1   | A     | 533 | GLN  |
| 2   | B     | 116 | PRO  |
| 2   | B     | 356 | SER  |
| 2   | B     | 357 | PRO  |
| 2   | B     | 393 | TYR  |
| 2   | B     | 901 | VAL  |
| 1   | C     | 36  | ILE  |
| 1   | C     | 233 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 259 | PRO  |
| 1   | C     | 262 | GLU  |
| 1   | C     | 275 | ALA  |
| 1   | C     | 533 | GLN  |
| 2   | D     | 116 | PRO  |
| 2   | D     | 356 | SER  |
| 2   | D     | 357 | PRO  |
| 2   | D     | 393 | TYR  |
| 2   | D     | 607 | THR  |
| 2   | D     | 608 | ARG  |
| 2   | D     | 700 | LYS  |
| 2   | D     | 901 | VAL  |
| 1   | E     | 233 | ILE  |
| 1   | E     | 259 | PRO  |
| 1   | E     | 262 | GLU  |
| 1   | E     | 275 | ALA  |
| 1   | E     | 533 | GLN  |
| 2   | F     | 116 | PRO  |
| 2   | F     | 356 | SER  |
| 2   | F     | 357 | PRO  |
| 2   | F     | 393 | TYR  |
| 2   | F     | 901 | VAL  |
| 2   | F     | 902 | ALA  |
| 1   | G     | 233 | ILE  |
| 1   | G     | 259 | PRO  |
| 1   | G     | 262 | GLU  |
| 1   | G     | 275 | ALA  |
| 1   | G     | 533 | GLN  |
| 2   | H     | 116 | PRO  |
| 2   | H     | 356 | SER  |
| 2   | H     | 357 | PRO  |
| 2   | H     | 393 | TYR  |
| 2   | H     | 901 | VAL  |
| 2   | H     | 902 | ALA  |
| 1   | A     | 21  | GLY  |
| 1   | A     | 36  | ILE  |
| 1   | A     | 237 | TYR  |
| 1   | A     | 317 | LYS  |
| 1   | A     | 367 | SER  |
| 1   | A     | 408 | ASN  |
| 1   | A     | 416 | MET  |
| 1   | A     | 422 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 34  | ASP  |
| 2   | B     | 127 | ILE  |
| 2   | B     | 132 | ASP  |
| 2   | B     | 183 | GLU  |
| 2   | B     | 294 | SER  |
| 2   | B     | 320 | ASN  |
| 2   | B     | 352 | ASN  |
| 2   | B     | 358 | SER  |
| 2   | B     | 372 | ALA  |
| 2   | B     | 902 | ALA  |
| 3   | I     | 152 | ASP  |
| 1   | C     | 21  | GLY  |
| 1   | C     | 237 | TYR  |
| 1   | C     | 317 | LYS  |
| 1   | C     | 367 | SER  |
| 1   | C     | 408 | ASN  |
| 1   | C     | 416 | MET  |
| 1   | C     | 422 | GLU  |
| 2   | D     | 34  | ASP  |
| 2   | D     | 127 | ILE  |
| 2   | D     | 132 | ASP  |
| 2   | D     | 183 | GLU  |
| 2   | D     | 294 | SER  |
| 2   | D     | 320 | ASN  |
| 2   | D     | 352 | ASN  |
| 2   | D     | 358 | SER  |
| 2   | D     | 372 | ALA  |
| 3   | J     | 152 | ASP  |
| 1   | E     | 21  | GLY  |
| 1   | E     | 36  | ILE  |
| 1   | E     | 237 | TYR  |
| 1   | E     | 276 | LEU  |
| 1   | E     | 367 | SER  |
| 1   | E     | 408 | ASN  |
| 1   | E     | 416 | MET  |
| 1   | E     | 422 | GLU  |
| 2   | F     | 34  | ASP  |
| 2   | F     | 127 | ILE  |
| 2   | F     | 132 | ASP  |
| 2   | F     | 183 | GLU  |
| 2   | F     | 294 | SER  |
| 2   | F     | 320 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 352 | ASN  |
| 2   | F     | 358 | SER  |
| 2   | F     | 372 | ALA  |
| 3   | K     | 152 | ASP  |
| 1   | G     | 21  | GLY  |
| 1   | G     | 36  | ILE  |
| 1   | G     | 237 | TYR  |
| 1   | G     | 276 | LEU  |
| 1   | G     | 367 | SER  |
| 1   | G     | 408 | ASN  |
| 1   | G     | 416 | MET  |
| 1   | G     | 422 | GLU  |
| 2   | H     | 34  | ASP  |
| 2   | H     | 127 | ILE  |
| 2   | H     | 183 | GLU  |
| 2   | H     | 294 | SER  |
| 2   | H     | 320 | ASN  |
| 2   | H     | 352 | ASN  |
| 2   | H     | 358 | SER  |
| 2   | H     | 372 | ALA  |
| 3   | L     | 152 | ASP  |
| 1   | A     | 118 | SER  |
| 1   | A     | 228 | GLU  |
| 1   | A     | 249 | GLN  |
| 1   | A     | 276 | LEU  |
| 1   | A     | 318 | GLU  |
| 2   | B     | 86  | SER  |
| 2   | B     | 360 | LYS  |
| 2   | B     | 607 | THR  |
| 1   | C     | 118 | SER  |
| 1   | C     | 190 | PRO  |
| 1   | C     | 228 | GLU  |
| 1   | C     | 249 | GLN  |
| 1   | C     | 276 | LEU  |
| 1   | C     | 318 | GLU  |
| 2   | D     | 86  | SER  |
| 2   | D     | 360 | LYS  |
| 2   | D     | 375 | GLN  |
| 1   | E     | 118 | SER  |
| 1   | E     | 190 | PRO  |
| 1   | E     | 228 | GLU  |
| 1   | E     | 249 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 317 | LYS  |
| 1   | E     | 318 | GLU  |
| 2   | F     | 86  | SER  |
| 2   | F     | 360 | LYS  |
| 2   | F     | 801 | GLN  |
| 1   | G     | 118 | SER  |
| 1   | G     | 190 | PRO  |
| 1   | G     | 228 | GLU  |
| 1   | G     | 249 | GLN  |
| 1   | G     | 317 | LYS  |
| 1   | G     | 318 | GLU  |
| 2   | H     | 86  | SER  |
| 2   | H     | 132 | ASP  |
| 2   | H     | 360 | LYS  |
| 2   | H     | 801 | GLN  |
| 1   | A     | 106 | GLU  |
| 1   | A     | 190 | PRO  |
| 1   | A     | 230 | ASN  |
| 1   | A     | 450 | VAL  |
| 2   | B     | 90  | ARG  |
| 2   | B     | 241 | GLN  |
| 2   | B     | 801 | GLN  |
| 2   | B     | 907 | PRO  |
| 3   | I     | 119 | PRO  |
| 1   | C     | 106 | GLU  |
| 1   | C     | 450 | VAL  |
| 2   | D     | 801 | GLN  |
| 2   | D     | 907 | PRO  |
| 3   | J     | 119 | PRO  |
| 1   | E     | 106 | GLU  |
| 1   | E     | 450 | VAL  |
| 2   | F     | 375 | GLN  |
| 2   | F     | 907 | PRO  |
| 3   | K     | 119 | PRO  |
| 2   | H     | 375 | GLN  |
| 2   | H     | 907 | PRO  |
| 3   | L     | 119 | PRO  |
| 1   | A     | 280 | GLN  |
| 1   | C     | 230 | ASN  |
| 1   | C     | 280 | GLN  |
| 1   | C     | 519 | THR  |
| 2   | D     | 88  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 90  | ARG  |
| 2   | D     | 241 | GLN  |
| 1   | E     | 230 | ASN  |
| 1   | E     | 280 | GLN  |
| 2   | F     | 90  | ARG  |
| 2   | F     | 241 | GLN  |
| 1   | G     | 106 | GLU  |
| 1   | G     | 280 | GLN  |
| 1   | G     | 519 | THR  |
| 2   | H     | 90  | ARG  |
| 2   | H     | 241 | GLN  |
| 1   | A     | 443 | PRO  |
| 1   | A     | 519 | THR  |
| 2   | B     | 196 | MET  |
| 2   | B     | 375 | GLN  |
| 2   | D     | 194 | PRO  |
| 2   | D     | 196 | MET  |
| 3   | J     | 146 | SER  |
| 1   | E     | 419 | PRO  |
| 2   | F     | 194 | PRO  |
| 2   | F     | 196 | MET  |
| 1   | G     | 230 | ASN  |
| 1   | G     | 419 | PRO  |
| 1   | G     | 450 | VAL  |
| 1   | A     | 419 | PRO  |
| 2   | B     | 194 | PRO  |
| 1   | C     | 419 | PRO  |
| 1   | C     | 443 | PRO  |
| 1   | G     | 54  | ILE  |
| 2   | H     | 194 | PRO  |
| 1   | A     | 54  | ILE  |
| 1   | A     | 333 | ILE  |
| 1   | E     | 54  | ILE  |
| 1   | E     | 443 | PRO  |
| 1   | G     | 443 | PRO  |
| 1   | C     | 372 | PRO  |
| 1   | G     | 333 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 450/461 (98%)   | 432 (96%)  | 18 (4%)  | 28          | 54 |
| 1   | C     | 450/461 (98%)   | 430 (96%)  | 20 (4%)  | 25          | 52 |
| 1   | E     | 450/461 (98%)   | 429 (95%)  | 21 (5%)  | 23          | 50 |
| 1   | G     | 450/461 (98%)   | 432 (96%)  | 18 (4%)  | 28          | 54 |
| 2   | B     | 334/379 (88%)   | 306 (92%)  | 28 (8%)  | 10          | 35 |
| 2   | D     | 334/379 (88%)   | 308 (92%)  | 26 (8%)  | 11          | 38 |
| 2   | F     | 334/379 (88%)   | 309 (92%)  | 25 (8%)  | 12          | 39 |
| 2   | H     | 334/379 (88%)   | 309 (92%)  | 25 (8%)  | 12          | 39 |
| 3   | I     | 66/66 (100%)    | 65 (98%)   | 1 (2%)   | 57          | 70 |
| 3   | J     | 66/66 (100%)    | 65 (98%)   | 1 (2%)   | 57          | 70 |
| 3   | K     | 66/66 (100%)    | 65 (98%)   | 1 (2%)   | 57          | 70 |
| 3   | L     | 66/66 (100%)    | 65 (98%)   | 1 (2%)   | 57          | 70 |
| All | All   | 3400/3624 (94%) | 3215 (95%) | 185 (5%) | 20          | 47 |

All (185) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 43  | THR  |
| 1   | A     | 56  | SER  |
| 1   | A     | 72  | ASN  |
| 1   | A     | 171 | VAL  |
| 1   | A     | 214 | TRP  |
| 1   | A     | 234 | PRO  |
| 1   | A     | 237 | TYR  |
| 1   | A     | 259 | PRO  |
| 1   | A     | 261 | ASP  |
| 1   | A     | 262 | GLU  |
| 1   | A     | 264 | ASN  |
| 1   | A     | 293 | ARG  |
| 1   | A     | 311 | LEU  |
| 1   | A     | 332 | MET  |
| 1   | A     | 406 | THR  |
| 1   | A     | 407 | ILE  |
| 1   | A     | 422 | GLU  |
| 1   | A     | 525 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 110 | PHE  |
| 2   | B     | 111 | LEU  |
| 2   | B     | 116 | PRO  |
| 2   | B     | 124 | PHE  |
| 2   | B     | 128 | GLN  |
| 2   | B     | 132 | ASP  |
| 2   | B     | 142 | VAL  |
| 2   | B     | 154 | ILE  |
| 2   | B     | 174 | ILE  |
| 2   | B     | 182 | THR  |
| 2   | B     | 212 | ASN  |
| 2   | B     | 265 | LEU  |
| 2   | B     | 267 | ARG  |
| 2   | B     | 294 | SER  |
| 2   | B     | 306 | GLU  |
| 2   | B     | 316 | ILE  |
| 2   | B     | 318 | LEU  |
| 2   | B     | 319 | ASN  |
| 2   | B     | 321 | TYR  |
| 2   | B     | 322 | LEU  |
| 2   | B     | 327 | VAL  |
| 2   | B     | 342 | ASN  |
| 2   | B     | 348 | GLN  |
| 2   | B     | 357 | PRO  |
| 2   | B     | 362 | GLN  |
| 2   | B     | 363 | GLU  |
| 2   | B     | 364 | VAL  |
| 2   | B     | 392 | LEU  |
| 3   | I     | 170 | VAL  |
| 1   | C     | 35  | LEU  |
| 1   | C     | 43  | THR  |
| 1   | C     | 56  | SER  |
| 1   | C     | 72  | ASN  |
| 1   | C     | 171 | VAL  |
| 1   | C     | 214 | TRP  |
| 1   | C     | 234 | PRO  |
| 1   | C     | 237 | TYR  |
| 1   | C     | 259 | PRO  |
| 1   | C     | 261 | ASP  |
| 1   | C     | 262 | GLU  |
| 1   | C     | 264 | ASN  |
| 1   | C     | 293 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 311 | LEU  |
| 1   | C     | 332 | MET  |
| 1   | C     | 406 | THR  |
| 1   | C     | 407 | ILE  |
| 1   | C     | 410 | ASP  |
| 1   | C     | 422 | GLU  |
| 1   | C     | 525 | MET  |
| 2   | D     | 49  | CYS  |
| 2   | D     | 110 | PHE  |
| 2   | D     | 111 | LEU  |
| 2   | D     | 116 | PRO  |
| 2   | D     | 128 | GLN  |
| 2   | D     | 142 | VAL  |
| 2   | D     | 154 | ILE  |
| 2   | D     | 174 | ILE  |
| 2   | D     | 182 | THR  |
| 2   | D     | 212 | ASN  |
| 2   | D     | 265 | LEU  |
| 2   | D     | 267 | ARG  |
| 2   | D     | 294 | SER  |
| 2   | D     | 306 | GLU  |
| 2   | D     | 316 | ILE  |
| 2   | D     | 318 | LEU  |
| 2   | D     | 319 | ASN  |
| 2   | D     | 321 | TYR  |
| 2   | D     | 322 | LEU  |
| 2   | D     | 327 | VAL  |
| 2   | D     | 342 | ASN  |
| 2   | D     | 348 | GLN  |
| 2   | D     | 357 | PRO  |
| 2   | D     | 362 | GLN  |
| 2   | D     | 363 | GLU  |
| 2   | D     | 364 | VAL  |
| 3   | J     | 170 | VAL  |
| 1   | E     | 43  | THR  |
| 1   | E     | 56  | SER  |
| 1   | E     | 72  | ASN  |
| 1   | E     | 171 | VAL  |
| 1   | E     | 214 | TRP  |
| 1   | E     | 234 | PRO  |
| 1   | E     | 237 | TYR  |
| 1   | E     | 259 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 261 | ASP  |
| 1   | E     | 262 | GLU  |
| 1   | E     | 264 | ASN  |
| 1   | E     | 293 | ARG  |
| 1   | E     | 301 | THR  |
| 1   | E     | 306 | ILE  |
| 1   | E     | 311 | LEU  |
| 1   | E     | 332 | MET  |
| 1   | E     | 364 | LEU  |
| 1   | E     | 406 | THR  |
| 1   | E     | 407 | ILE  |
| 1   | E     | 422 | GLU  |
| 1   | E     | 525 | MET  |
| 2   | F     | 110 | PHE  |
| 2   | F     | 111 | LEU  |
| 2   | F     | 116 | PRO  |
| 2   | F     | 128 | GLN  |
| 2   | F     | 142 | VAL  |
| 2   | F     | 154 | ILE  |
| 2   | F     | 174 | ILE  |
| 2   | F     | 182 | THR  |
| 2   | F     | 212 | ASN  |
| 2   | F     | 265 | LEU  |
| 2   | F     | 267 | ARG  |
| 2   | F     | 294 | SER  |
| 2   | F     | 306 | GLU  |
| 2   | F     | 316 | ILE  |
| 2   | F     | 318 | LEU  |
| 2   | F     | 319 | ASN  |
| 2   | F     | 321 | TYR  |
| 2   | F     | 322 | LEU  |
| 2   | F     | 327 | VAL  |
| 2   | F     | 342 | ASN  |
| 2   | F     | 348 | GLN  |
| 2   | F     | 357 | PRO  |
| 2   | F     | 362 | GLN  |
| 2   | F     | 363 | GLU  |
| 2   | F     | 364 | VAL  |
| 3   | K     | 170 | VAL  |
| 1   | G     | 43  | THR  |
| 1   | G     | 56  | SER  |
| 1   | G     | 72  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 171 | VAL  |
| 1   | G     | 214 | TRP  |
| 1   | G     | 234 | PRO  |
| 1   | G     | 259 | PRO  |
| 1   | G     | 261 | ASP  |
| 1   | G     | 262 | GLU  |
| 1   | G     | 264 | ASN  |
| 1   | G     | 293 | ARG  |
| 1   | G     | 306 | ILE  |
| 1   | G     | 311 | LEU  |
| 1   | G     | 332 | MET  |
| 1   | G     | 406 | THR  |
| 1   | G     | 407 | ILE  |
| 1   | G     | 422 | GLU  |
| 1   | G     | 525 | MET  |
| 2   | H     | 110 | PHE  |
| 2   | H     | 111 | LEU  |
| 2   | H     | 116 | PRO  |
| 2   | H     | 128 | GLN  |
| 2   | H     | 132 | ASP  |
| 2   | H     | 142 | VAL  |
| 2   | H     | 154 | ILE  |
| 2   | H     | 174 | ILE  |
| 2   | H     | 182 | THR  |
| 2   | H     | 212 | ASN  |
| 2   | H     | 265 | LEU  |
| 2   | H     | 267 | ARG  |
| 2   | H     | 294 | SER  |
| 2   | H     | 306 | GLU  |
| 2   | H     | 316 | ILE  |
| 2   | H     | 318 | LEU  |
| 2   | H     | 319 | ASN  |
| 2   | H     | 321 | TYR  |
| 2   | H     | 322 | LEU  |
| 2   | H     | 327 | VAL  |
| 2   | H     | 342 | ASN  |
| 2   | H     | 348 | GLN  |
| 2   | H     | 357 | PRO  |
| 2   | H     | 363 | GLU  |
| 2   | H     | 364 | VAL  |
| 3   | L     | 170 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 37  | ASN  |
| 1   | A     | 72  | ASN  |
| 1   | A     | 77  | GLN  |
| 1   | A     | 178 | ASN  |
| 1   | A     | 195 | HIS  |
| 1   | A     | 197 | GLN  |
| 1   | A     | 264 | ASN  |
| 1   | A     | 271 | ASN  |
| 1   | A     | 277 | ASN  |
| 1   | A     | 320 | GLN  |
| 1   | A     | 344 | ASN  |
| 1   | A     | 359 | ASN  |
| 1   | A     | 366 | GLN  |
| 1   | A     | 418 | ASN  |
| 1   | A     | 439 | GLN  |
| 1   | A     | 447 | ASN  |
| 1   | A     | 533 | GLN  |
| 2   | B     | 19  | HIS  |
| 2   | B     | 74  | GLN  |
| 2   | B     | 87  | ASN  |
| 2   | B     | 119 | ASN  |
| 2   | B     | 125 | ASN  |
| 2   | B     | 128 | GLN  |
| 2   | B     | 131 | ASN  |
| 2   | B     | 139 | HIS  |
| 2   | B     | 212 | ASN  |
| 2   | B     | 236 | GLN  |
| 2   | B     | 262 | GLN  |
| 2   | B     | 270 | GLN  |
| 2   | B     | 325 | ASN  |
| 2   | B     | 342 | ASN  |
| 2   | B     | 348 | GLN  |
| 2   | B     | 351 | GLN  |
| 3   | I     | 141 | GLN  |
| 3   | I     | 168 | HIS  |
| 1   | C     | 37  | ASN  |
| 1   | C     | 72  | ASN  |
| 1   | C     | 77  | GLN  |
| 1   | C     | 178 | ASN  |
| 1   | C     | 195 | HIS  |
| 1   | C     | 197 | GLN  |
| 1   | C     | 230 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 264 | ASN  |
| 1   | C     | 271 | ASN  |
| 1   | C     | 277 | ASN  |
| 1   | C     | 320 | GLN  |
| 1   | C     | 344 | ASN  |
| 1   | C     | 359 | ASN  |
| 1   | C     | 366 | GLN  |
| 1   | C     | 418 | ASN  |
| 1   | C     | 439 | GLN  |
| 1   | C     | 447 | ASN  |
| 1   | C     | 517 | ASN  |
| 1   | C     | 533 | GLN  |
| 2   | D     | 19  | HIS  |
| 2   | D     | 74  | GLN  |
| 2   | D     | 87  | ASN  |
| 2   | D     | 119 | ASN  |
| 2   | D     | 125 | ASN  |
| 2   | D     | 128 | GLN  |
| 2   | D     | 131 | ASN  |
| 2   | D     | 139 | HIS  |
| 2   | D     | 212 | ASN  |
| 2   | D     | 236 | GLN  |
| 2   | D     | 325 | ASN  |
| 2   | D     | 342 | ASN  |
| 2   | D     | 348 | GLN  |
| 2   | D     | 351 | GLN  |
| 3   | J     | 141 | GLN  |
| 3   | J     | 168 | HIS  |
| 1   | E     | 37  | ASN  |
| 1   | E     | 72  | ASN  |
| 1   | E     | 77  | GLN  |
| 1   | E     | 178 | ASN  |
| 1   | E     | 195 | HIS  |
| 1   | E     | 197 | GLN  |
| 1   | E     | 230 | ASN  |
| 1   | E     | 264 | ASN  |
| 1   | E     | 271 | ASN  |
| 1   | E     | 277 | ASN  |
| 1   | E     | 320 | GLN  |
| 1   | E     | 359 | ASN  |
| 1   | E     | 366 | GLN  |
| 1   | E     | 418 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 436 | HIS  |
| 1   | E     | 439 | GLN  |
| 1   | E     | 447 | ASN  |
| 1   | E     | 533 | GLN  |
| 2   | F     | 19  | HIS  |
| 2   | F     | 74  | GLN  |
| 2   | F     | 87  | ASN  |
| 2   | F     | 119 | ASN  |
| 2   | F     | 125 | ASN  |
| 2   | F     | 128 | GLN  |
| 2   | F     | 139 | HIS  |
| 2   | F     | 212 | ASN  |
| 2   | F     | 236 | GLN  |
| 2   | F     | 325 | ASN  |
| 2   | F     | 342 | ASN  |
| 2   | F     | 348 | GLN  |
| 2   | F     | 351 | GLN  |
| 3   | K     | 141 | GLN  |
| 1   | G     | 37  | ASN  |
| 1   | G     | 72  | ASN  |
| 1   | G     | 77  | GLN  |
| 1   | G     | 178 | ASN  |
| 1   | G     | 195 | HIS  |
| 1   | G     | 197 | GLN  |
| 1   | G     | 230 | ASN  |
| 1   | G     | 264 | ASN  |
| 1   | G     | 271 | ASN  |
| 1   | G     | 277 | ASN  |
| 1   | G     | 320 | GLN  |
| 1   | G     | 344 | ASN  |
| 1   | G     | 359 | ASN  |
| 1   | G     | 366 | GLN  |
| 1   | G     | 418 | ASN  |
| 1   | G     | 439 | GLN  |
| 1   | G     | 447 | ASN  |
| 1   | G     | 533 | GLN  |
| 2   | H     | 19  | HIS  |
| 2   | H     | 74  | GLN  |
| 2   | H     | 87  | ASN  |
| 2   | H     | 119 | ASN  |
| 2   | H     | 125 | ASN  |
| 2   | H     | 128 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 139 | HIS  |
| 2   | H     | 212 | ASN  |
| 2   | H     | 236 | GLN  |
| 2   | H     | 325 | ASN  |
| 2   | H     | 342 | ASN  |
| 2   | H     | 348 | GLN  |
| 2   | H     | 351 | GLN  |
| 3   | L     | 141 | GLN  |
| 3   | L     | 168 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 4   | ATP  | H     | 8   | -    | 32,33,33     | 1.44 | 4 (12%)     | 48,52,52    | 2.88 | 18 (37%)    |
| 4   | ATP  | D     | 6   | -    | 32,33,33     | 2.57 | 5 (15%)     | 48,52,52    | 2.66 | 17 (35%)    |
| 4   | ATP  | B     | 5   | -    | 32,33,33     | 2.67 | 6 (18%)     | 48,52,52    | 2.77 | 17 (35%)    |
| 4   | ATP  | F     | 7   | -    | 32,33,33     | 1.70 | 6 (18%)     | 48,52,52    | 2.78 | 18 (37%)    |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 4   | ATP  | H     | 8   | -    | -       | 11/22/38/38 | 0/3/3/3 |
| 4   | ATP  | D     | 6   | -    | -       | 10/22/38/38 | 0/3/3/3 |
| 4   | ATP  | B     | 5   | -    | -       | 10/22/38/38 | 0/3/3/3 |
| 4   | ATP  | F     | 7   | -    | -       | 6/22/38/38  | 0/3/3/3 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | B     | 5   | ATP  | PB-O3A  | 11.26 | 1.71        | 1.59     |
| 4   | D     | 6   | ATP  | PB-O3A  | 10.47 | 1.70        | 1.59     |
| 4   | D     | 6   | ATP  | PA-O3A  | 8.44  | 1.68        | 1.59     |
| 4   | B     | 5   | ATP  | PA-O3A  | 6.97  | 1.67        | 1.59     |
| 4   | F     | 7   | ATP  | PB-O3A  | 6.08  | 1.66        | 1.59     |
| 4   | H     | 8   | ATP  | PB-O3A  | 5.08  | 1.65        | 1.59     |
| 4   | B     | 5   | ATP  | C2-N3   | 3.51  | 1.40        | 1.33     |
| 4   | F     | 7   | ATP  | PA-O3A  | 3.17  | 1.62        | 1.59     |
| 4   | F     | 7   | ATP  | C5-N7   | -3.04 | 1.33        | 1.39     |
| 4   | H     | 8   | ATP  | C5-N7   | -3.02 | 1.33        | 1.39     |
| 4   | B     | 5   | ATP  | C5-N7   | -2.80 | 1.34        | 1.39     |
| 4   | D     | 6   | ATP  | C5-N7   | -2.59 | 1.34        | 1.39     |
| 4   | F     | 7   | ATP  | C2-N3   | 2.58  | 1.38        | 1.33     |
| 4   | F     | 7   | ATP  | O2'-C2' | -2.47 | 1.36        | 1.43     |
| 4   | D     | 6   | ATP  | C2-N3   | 2.41  | 1.38        | 1.33     |
| 4   | B     | 5   | ATP  | C2-N1   | 2.39  | 1.38        | 1.33     |
| 4   | H     | 8   | ATP  | O2'-C2' | -2.32 | 1.37        | 1.43     |
| 4   | D     | 6   | ATP  | O2'-C2' | -2.17 | 1.37        | 1.43     |
| 4   | H     | 8   | ATP  | C2-N3   | 2.06  | 1.37        | 1.33     |
| 4   | F     | 7   | ATP  | PB-O3B  | -2.06 | 1.57        | 1.59     |
| 4   | B     | 5   | ATP  | O2'-C2' | -2.00 | 1.38        | 1.43     |

All (70) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 4   | H     | 8   | ATP  | O3A-PB-O1B | -11.63 | 75.73       | 110.70   |
| 4   | F     | 7   | ATP  | O3A-PB-O1B | -10.58 | 78.88       | 110.70   |
| 4   | B     | 5   | ATP  | O3A-PB-O1B | -10.46 | 79.24       | 110.70   |
| 4   | D     | 6   | ATP  | O3A-PB-O1B | -9.78  | 81.27       | 110.70   |
| 4   | H     | 8   | ATP  | O2B-PB-O3A | -7.25  | 87.68       | 107.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | B     | 5   | ATP  | O2B-PB-O3A  | -7.12 | 88.02       | 107.27   |
| 4   | D     | 6   | ATP  | O2B-PB-O3A  | -6.93 | 88.54       | 107.27   |
| 4   | F     | 7   | ATP  | O2B-PB-O3A  | -6.46 | 89.80       | 107.27   |
| 4   | F     | 7   | ATP  | N3-C2-N1    | -6.01 | 119.48      | 128.58   |
| 4   | F     | 7   | ATP  | C5-N7-C8    | 5.76  | 112.50      | 103.45   |
| 4   | B     | 5   | ATP  | N3-C2-N1    | -5.51 | 120.23      | 128.58   |
| 4   | H     | 8   | ATP  | N3-C2-N1    | -5.49 | 120.26      | 128.58   |
| 4   | D     | 6   | ATP  | C5-N7-C8    | 5.21  | 111.64      | 103.45   |
| 4   | H     | 8   | ATP  | C5-N7-C8    | 5.19  | 111.61      | 103.45   |
| 4   | D     | 6   | ATP  | N3-C2-N1    | -5.18 | 120.74      | 128.58   |
| 4   | B     | 5   | ATP  | C5-N7-C8    | 5.09  | 111.45      | 103.45   |
| 4   | F     | 7   | ATP  | N9-C8-N7    | -5.07 | 106.74      | 113.94   |
| 4   | H     | 8   | ATP  | N9-C8-N7    | -4.91 | 106.97      | 113.94   |
| 4   | D     | 6   | ATP  | N9-C8-N7    | -4.59 | 107.43      | 113.94   |
| 4   | F     | 7   | ATP  | C4-C5-N7    | -4.32 | 105.64      | 110.58   |
| 4   | D     | 6   | ATP  | C4-C5-N7    | -4.19 | 105.79      | 110.58   |
| 4   | B     | 5   | ATP  | C4-C5-N7    | -4.15 | 105.84      | 110.58   |
| 4   | H     | 8   | ATP  | O2B-PB-O3B  | 4.00  | 118.09      | 107.27   |
| 4   | B     | 5   | ATP  | O2B-PB-O3B  | 3.87  | 117.75      | 107.27   |
| 4   | B     | 5   | ATP  | N9-C8-N7    | -3.84 | 108.49      | 113.94   |
| 4   | H     | 8   | ATP  | C4-C5-N7    | -3.79 | 106.25      | 110.58   |
| 4   | B     | 5   | ATP  | O4'-C1'-N9  | -3.71 | 100.97      | 108.09   |
| 4   | D     | 6   | ATP  | O2B-PB-O3B  | 3.55  | 116.88      | 107.27   |
| 4   | B     | 5   | ATP  | O2B-PB-O1B  | 3.52  | 128.84      | 112.44   |
| 4   | D     | 6   | ATP  | C5-C4-N3    | -3.52 | 121.87      | 126.72   |
| 4   | F     | 7   | ATP  | C5-C4-N3    | -3.52 | 121.87      | 126.72   |
| 4   | F     | 7   | ATP  | O2B-PB-O3B  | 3.48  | 116.67      | 107.27   |
| 4   | H     | 8   | ATP  | O2B-PB-O1B  | 3.38  | 128.17      | 112.44   |
| 4   | B     | 5   | ATP  | C5-C4-N3    | -3.32 | 122.14      | 126.72   |
| 4   | H     | 8   | ATP  | C5-C4-N3    | -3.32 | 122.14      | 126.72   |
| 4   | D     | 6   | ATP  | O2B-PB-O1B  | 3.21  | 127.36      | 112.44   |
| 4   | F     | 7   | ATP  | C2-N3-C4    | 3.09  | 119.37      | 111.83   |
| 4   | H     | 8   | ATP  | O4'-C1'-N9  | -3.03 | 102.27      | 108.09   |
| 4   | B     | 5   | ATP  | C2-N3-C4    | 2.93  | 118.98      | 111.83   |
| 4   | F     | 7   | ATP  | O4'-C1'-N9  | -2.84 | 102.62      | 108.09   |
| 4   | H     | 8   | ATP  | C2-N3-C4    | 2.83  | 118.75      | 111.83   |
| 4   | D     | 6   | ATP  | C2-N3-C4    | 2.82  | 118.71      | 111.83   |
| 4   | F     | 7   | ATP  | O2B-PB-O1B  | 2.77  | 125.35      | 112.44   |
| 4   | H     | 8   | ATP  | C2'-C1'-N9  | 2.76  | 120.16      | 113.30   |
| 4   | B     | 5   | ATP  | O2'-C2'-C3' | 2.71  | 120.49      | 111.82   |
| 4   | B     | 5   | ATP  | N3-C4-N9    | 2.39  | 131.24      | 127.17   |
| 4   | F     | 7   | ATP  | C2'-C1'-N9  | 2.38  | 119.23      | 113.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | B     | 5   | ATP  | C1'-N9-C8   | -2.37 | 121.83      | 127.09   |
| 4   | H     | 8   | ATP  | C4-N9-C8    | 2.37  | 108.22      | 105.74   |
| 4   | D     | 6   | ATP  | O2G-PG-O3B  | 2.34  | 112.49      | 104.64   |
| 4   | D     | 6   | ATP  | O4'-C1'-N9  | -2.34 | 103.60      | 108.09   |
| 4   | D     | 6   | ATP  | N3-C4-N9    | 2.34  | 131.14      | 127.17   |
| 4   | H     | 8   | ATP  | O2G-PG-O3B  | 2.32  | 112.42      | 104.64   |
| 4   | F     | 7   | ATP  | N3-C4-N9    | 2.32  | 131.11      | 127.17   |
| 4   | D     | 6   | ATP  | C4-N9-C8    | 2.31  | 108.16      | 105.74   |
| 4   | F     | 7   | ATP  | C6-C5-N7    | 2.29  | 136.51      | 132.09   |
| 4   | H     | 8   | ATP  | N6-C6-N1    | -2.29 | 113.27      | 118.38   |
| 4   | B     | 5   | ATP  | O3'-C3'-C4' | -2.27 | 104.57      | 111.08   |
| 4   | F     | 7   | ATP  | C4-N9-C8    | 2.24  | 108.09      | 105.74   |
| 4   | D     | 6   | ATP  | O2'-C2'-C3' | 2.21  | 118.92      | 111.82   |
| 4   | H     | 8   | ATP  | C6-C5-N7    | 2.21  | 136.35      | 132.09   |
| 4   | H     | 8   | ATP  | N3-C4-N9    | 2.20  | 130.91      | 127.17   |
| 4   | D     | 6   | ATP  | C6-C5-N7    | 2.19  | 136.32      | 132.09   |
| 4   | D     | 6   | ATP  | C2'-C1'-N9  | 2.16  | 118.68      | 113.30   |
| 4   | B     | 5   | ATP  | C2'-C1'-N9  | 2.13  | 118.60      | 113.30   |
| 4   | B     | 5   | ATP  | O2G-PG-O3B  | 2.02  | 111.41      | 104.64   |
| 4   | F     | 7   | ATP  | N6-C6-N1    | -2.02 | 113.88      | 118.38   |
| 4   | F     | 7   | ATP  | O2'-C2'-C3' | 2.01  | 118.26      | 111.82   |
| 4   | F     | 7   | ATP  | O2G-PG-O3B  | 2.01  | 111.37      | 104.64   |
| 4   | H     | 8   | ATP  | O2'-C2'-C3' | 2.00  | 118.23      | 111.82   |

There are no chirality outliers.

All (37) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | D     | 6   | ATP  | C5'-O5'-PA-O1A  |
| 4   | D     | 6   | ATP  | C5'-O5'-PA-O2A  |
| 4   | D     | 6   | ATP  | C5'-O5'-PA-O3A  |
| 4   | F     | 7   | ATP  | C5'-O5'-PA-O2A  |
| 4   | F     | 7   | ATP  | C5'-O5'-PA-O3A  |
| 4   | H     | 8   | ATP  | PB-O3B-PG-O2G   |
| 4   | H     | 8   | ATP  | C5'-O5'-PA-O2A  |
| 4   | B     | 5   | ATP  | O4'-C4'-C5'-O5' |
| 4   | B     | 5   | ATP  | C3'-C4'-C5'-O5' |
| 4   | F     | 7   | ATP  | O4'-C4'-C5'-O5' |
| 4   | D     | 6   | ATP  | O4'-C4'-C5'-O5' |
| 4   | F     | 7   | ATP  | C3'-C4'-C5'-O5' |
| 4   | B     | 5   | ATP  | PA-O3A-PB-O2B   |
| 4   | D     | 6   | ATP  | PA-O3A-PB-O2B   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | F     | 7   | ATP  | PA-O3A-PB-O2B   |
| 4   | H     | 8   | ATP  | PA-O3A-PB-O2B   |
| 4   | H     | 8   | ATP  | PB-O3A-PA-O1A   |
| 4   | B     | 5   | ATP  | C5'-O5'-PA-O1A  |
| 4   | B     | 5   | ATP  | C5'-O5'-PA-O2A  |
| 4   | B     | 5   | ATP  | C5'-O5'-PA-O3A  |
| 4   | H     | 8   | ATP  | C5'-O5'-PA-O1A  |
| 4   | H     | 8   | ATP  | C5'-O5'-PA-O3A  |
| 4   | H     | 8   | ATP  | O4'-C4'-C5'-O5' |
| 4   | D     | 6   | ATP  | C3'-C4'-C5'-O5' |
| 4   | H     | 8   | ATP  | C3'-C4'-C5'-O5' |
| 4   | D     | 6   | ATP  | PB-O3A-PA-O1A   |
| 4   | B     | 5   | ATP  | C4'-C5'-O5'-PA  |
| 4   | H     | 8   | ATP  | PB-O3B-PG-O3G   |
| 4   | B     | 5   | ATP  | PA-O3A-PB-O1B   |
| 4   | B     | 5   | ATP  | PB-O3A-PA-O1A   |
| 4   | D     | 6   | ATP  | PG-O3B-PB-O2B   |
| 4   | D     | 6   | ATP  | PA-O3A-PB-O1B   |
| 4   | F     | 7   | ATP  | PA-O3A-PB-O1B   |
| 4   | H     | 8   | ATP  | PA-O3A-PB-O1B   |
| 4   | B     | 5   | ATP  | PB-O3A-PA-O2A   |
| 4   | D     | 6   | ATP  | PB-O3A-PA-O2A   |
| 4   | H     | 8   | ATP  | PB-O3A-PA-O2A   |

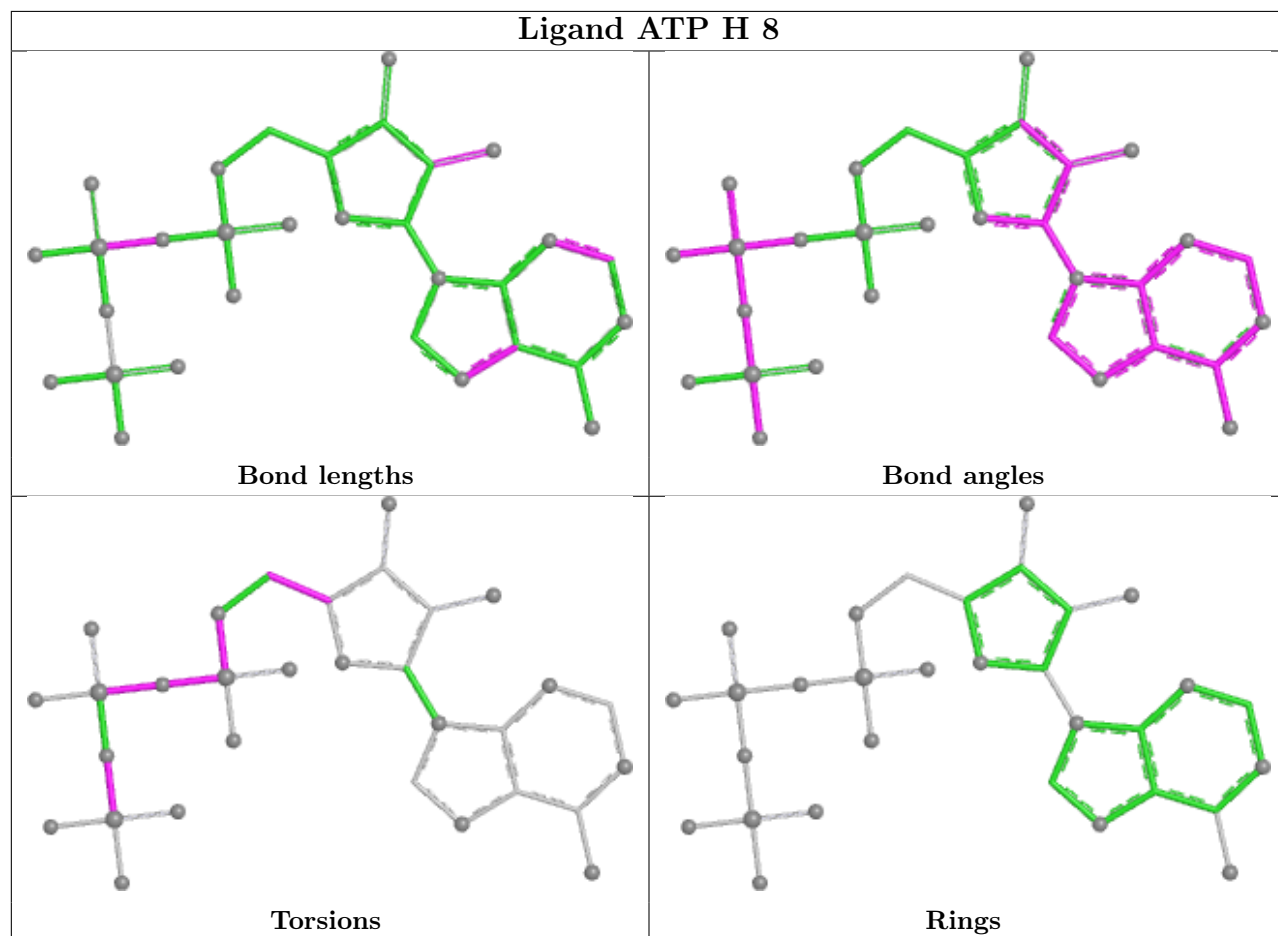
There are no ring outliers.

4 monomers are involved in 26 short contacts:

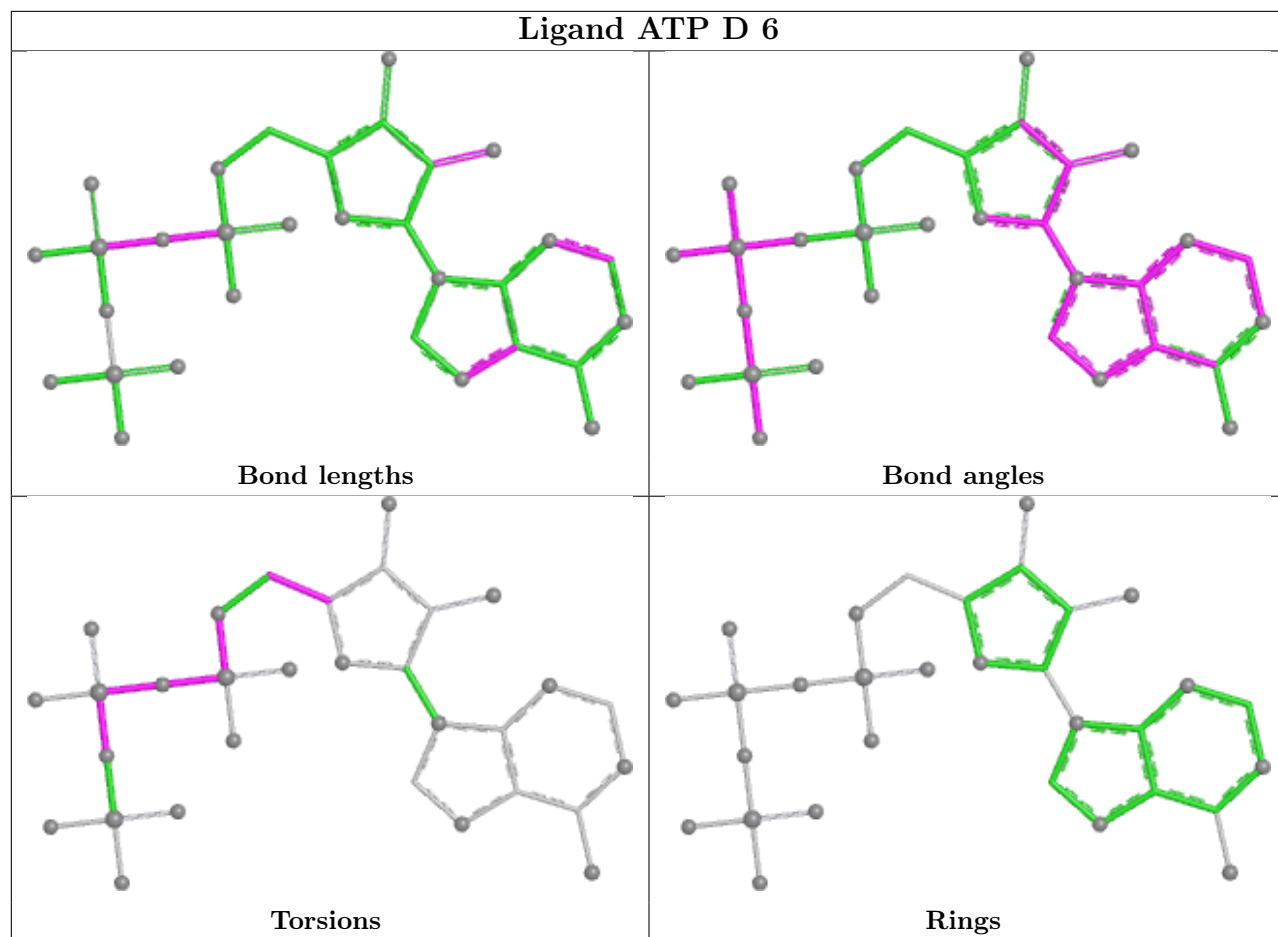
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | H     | 8   | ATP  | 11      | 0            |
| 4   | D     | 6   | ATP  | 5       | 0            |
| 4   | B     | 5   | ATP  | 3       | 0            |
| 4   | F     | 7   | ATP  | 7       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

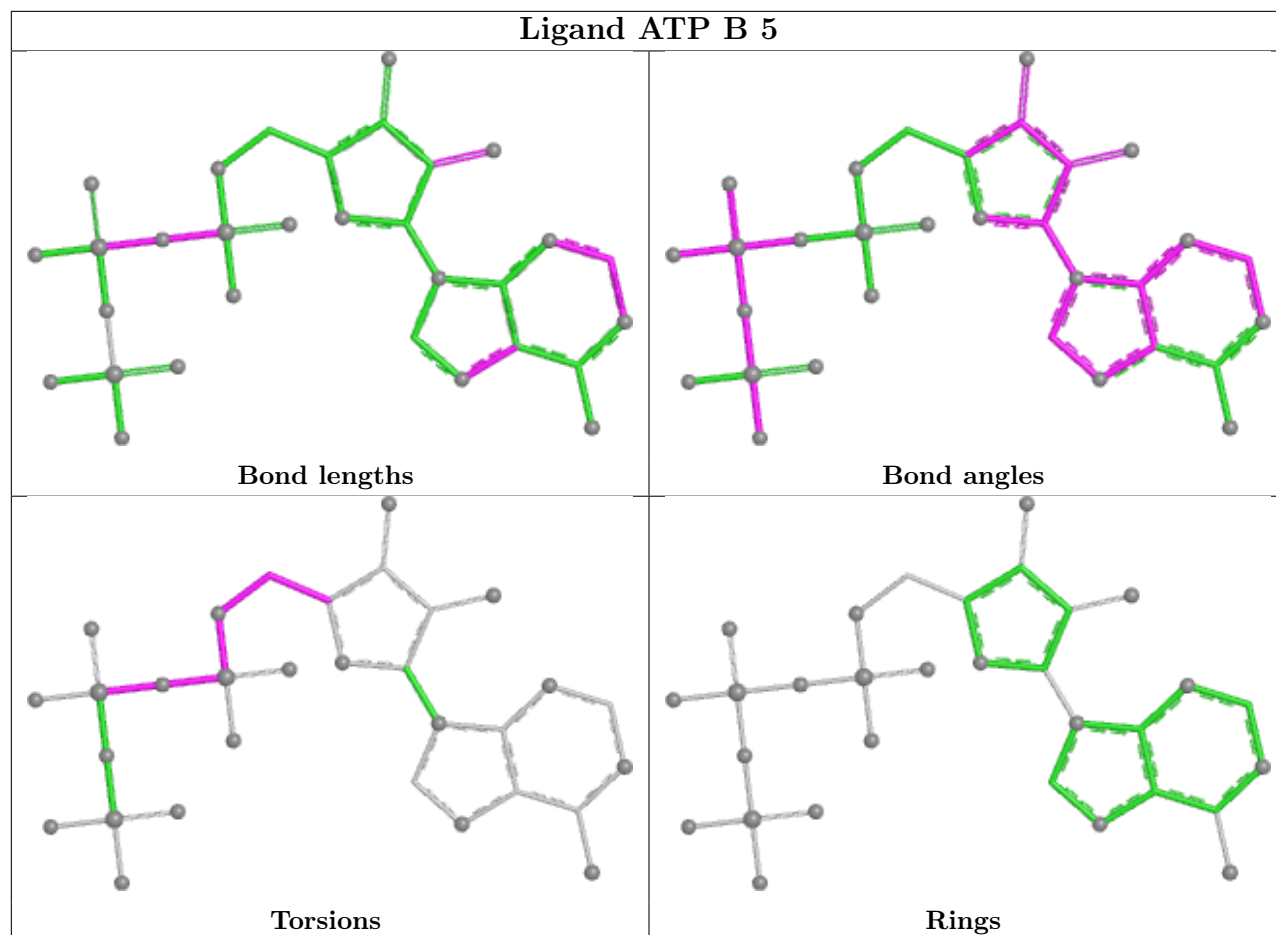
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

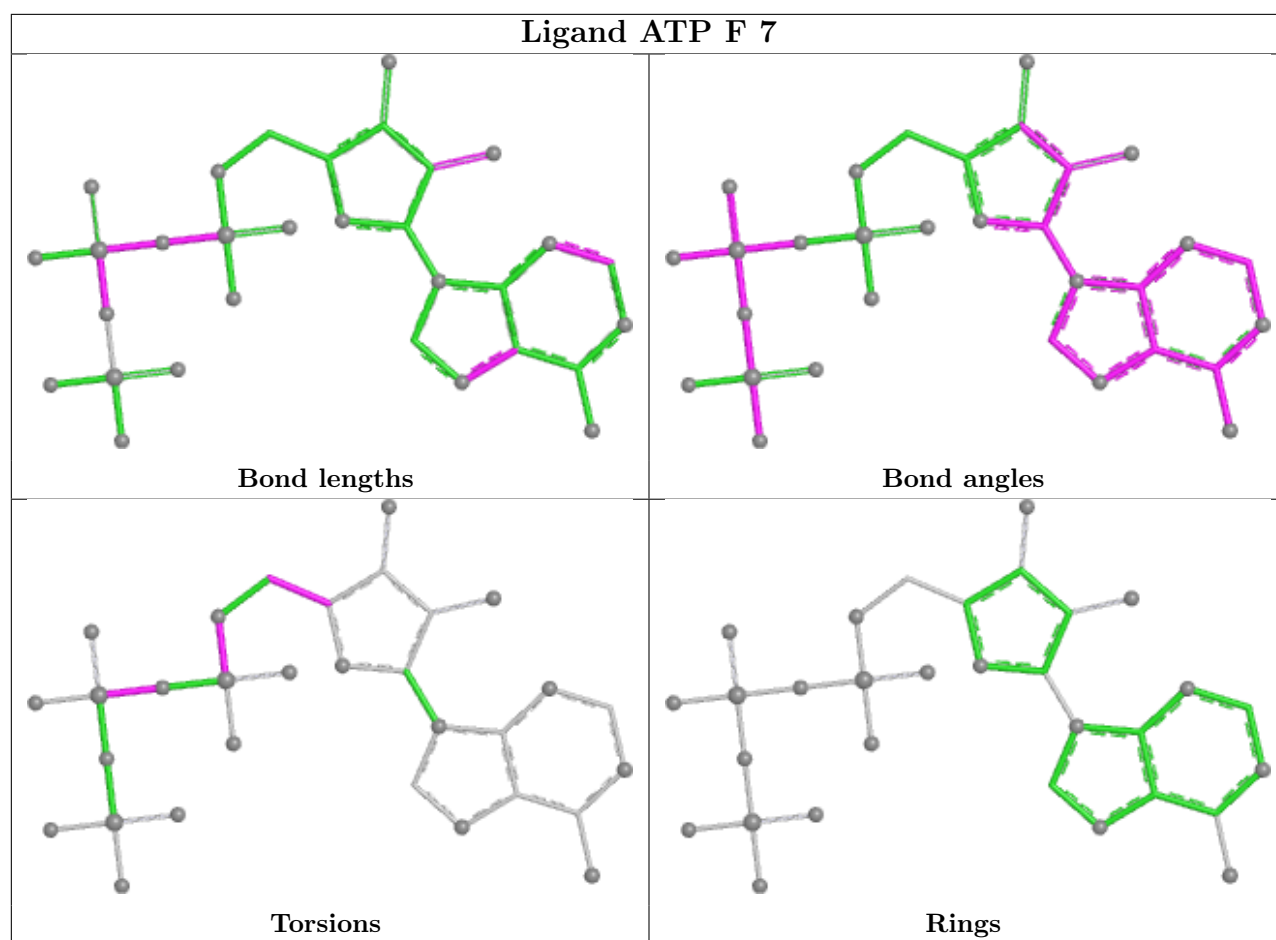


## Ligand ATP D 6



## Ligand ATP B 5





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | D     | 2                |
| 2   | B     | 1                |
| 2   | H     | 1                |
| 2   | F     | 1                |
| 1   | C     | 1                |
| 1   | A     | 1                |
| 1   | G     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 396:SER   | C      | 600:VAL   | N      | 2.96         |
| 1     | D     | 396:SER   | C      | 600:VAL   | N      | 2.96         |
| 1     | H     | 396:SER   | C      | 600:VAL   | N      | 2.96         |
| 1     | F     | 396:SER   | C      | 600:VAL   | N      | 2.95         |
| 1     | D     | 700:LYS   | C      | 701:GLU   | N      | 1.61         |
| 1     | C     | 252:LEU   | C      | 253:LYS   | N      | 1.19         |
| 1     | A     | 252:LEU   | C      | 253:LYS   | N      | 1.18         |
| 1     | G     | 252:LEU   | C      | 253:LYS   | N      | 1.18         |

## 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.