



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 11:20 PM EDT

PDB ID : 1KQM / pdb\_00001kqm  
Title : SCALLOP MYOSIN S1-AMPPNP IN THE ACTIN-DETACHED CONFORMATION  
Authors : Himmel, D.M.; Gourinath, S.; Reshetnikova, L.; Shen, Y.; Szent-Gyorgyi, G.; Cohen, C.  
Deposited on : 2002-01-07  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

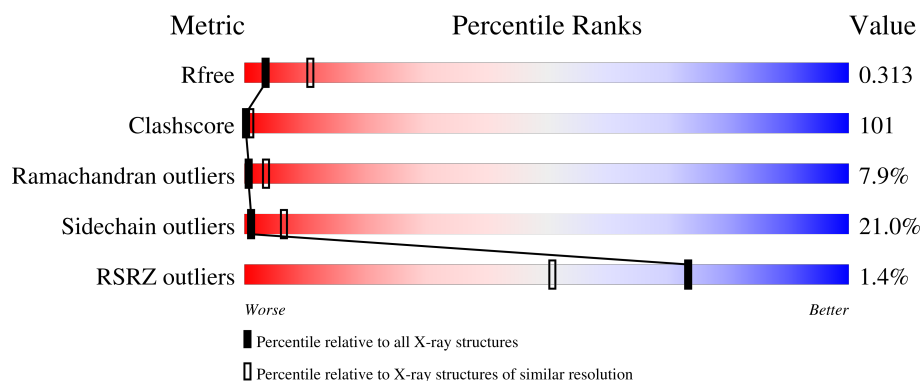
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 835    |                  |
| 2   | B     | 156    |                  |
| 3   | C     | 156    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5   | ANP  | A     | 999 | -         | -        | X       | -                |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8276 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 MYOSIN heavy chain.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 777      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 5964  | 3781 | 1028 | 1120 | 35 |         |         |       |

- Molecule 2 is a protein called MYOSIN REGULATORY LIGHT CHAIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1097  | 691 | 176 | 223 | 7 |         |         |       |

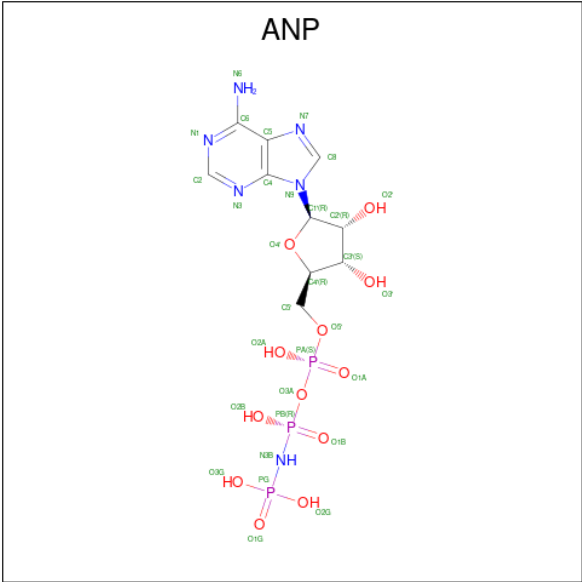
- Molecule 3 is a protein called MYOSIN ESSENTIAL LIGHT CHAIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | C     | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1174  | 744 | 183 | 240 | 7 |         |         |       |

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | B     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

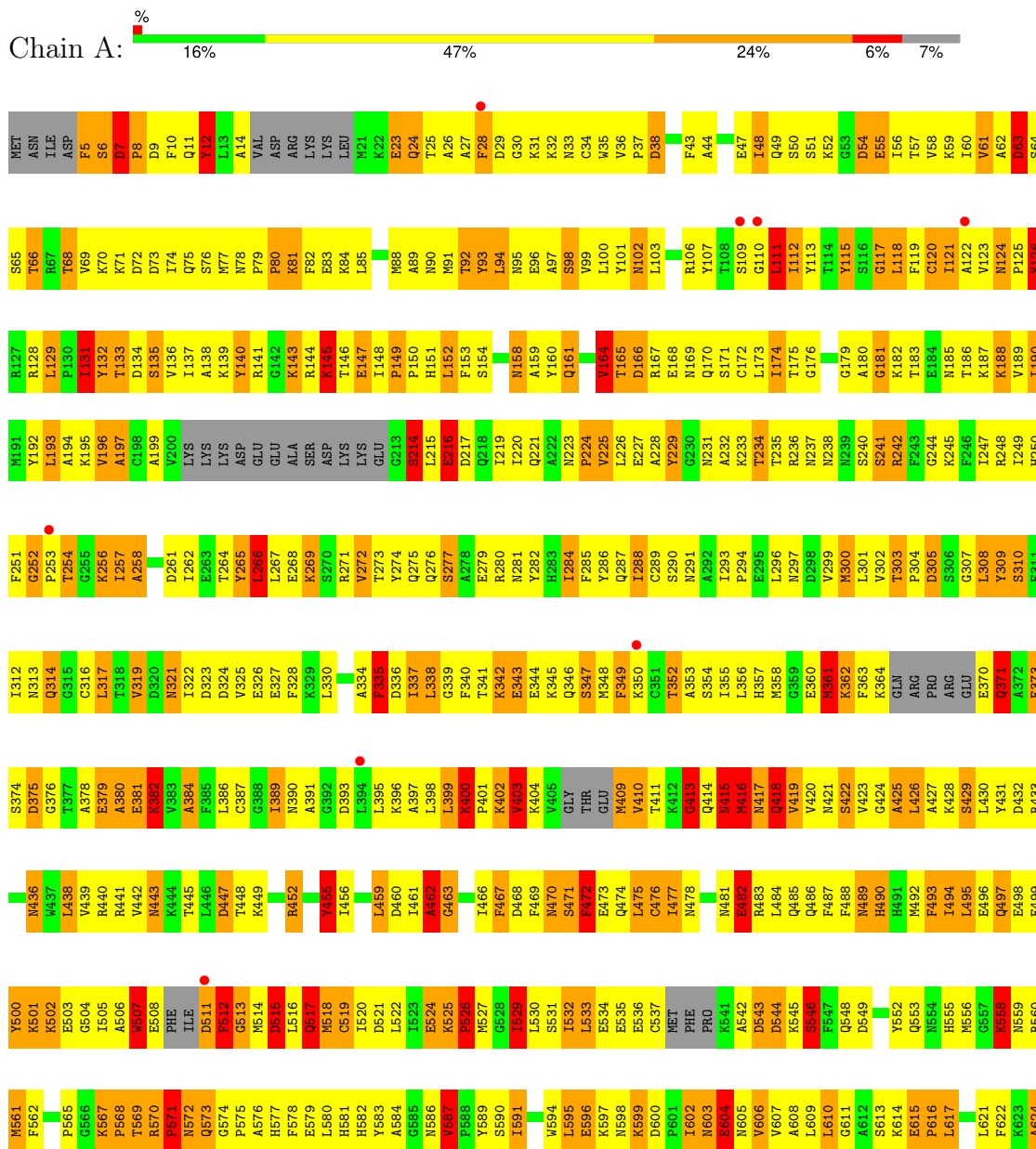
- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

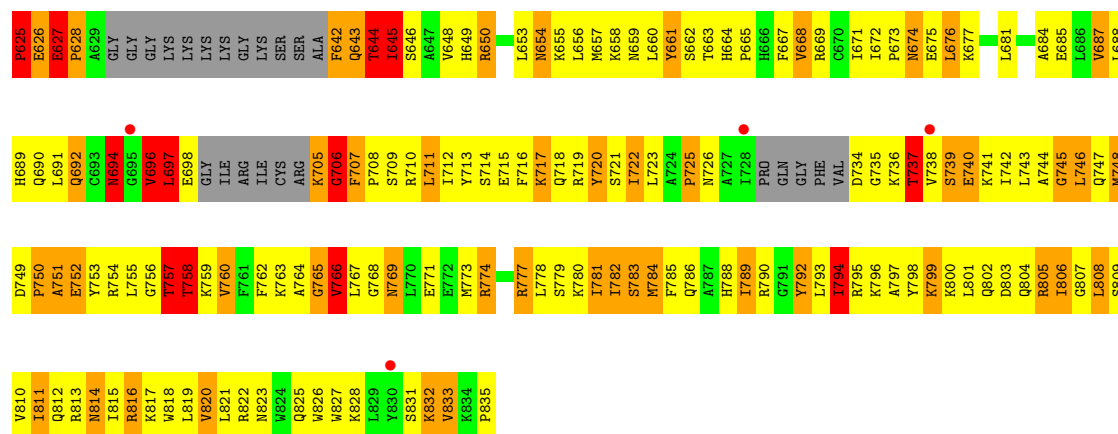


### 3 Residue-property plots

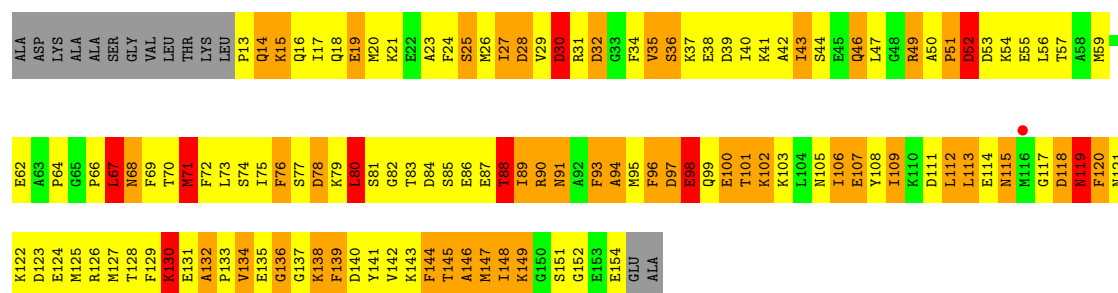
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: MYOSIN heavy chain

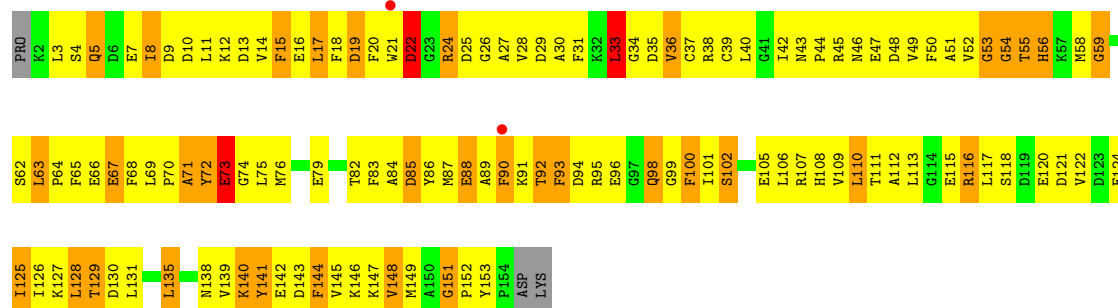
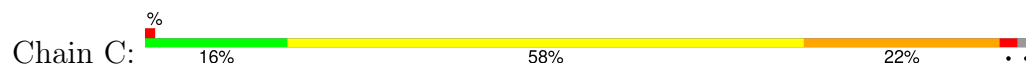




### • Molecule 2: MYOSIN REGULATORY LIGHT CHAIN



### • Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 52.40Å 58.64Å 148.87Å<br>81.64° 82.39° 87.43°               | Depositor        |
| Resolution (Å)                                                          | 39.81 – 3.00<br>39.81 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 73.1 (39.81-3.00)<br>82.9 (39.81-3.00)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.08                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.54 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 0.9                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.277 , 0.316<br>0.279 , 0.313                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1543 reflections (4.96%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 70.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.525                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 66.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 8276                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 77.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, CA, MG

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

| Mol | Chain | Bond lengths |               | Bond angles |                  |
|-----|-------|--------------|---------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 1.03         | 8/6074 (0.1%) | 1.80        | 212/8217 (2.6%)  |
| 2   | B     | 0.95         | 0/1114        | 1.62        | 31/1494 (2.1%)   |
| 3   | C     | 0.84         | 0/1198        | 1.26        | 16/1619 (1.0%)   |
| All | All   | 0.99         | 8/8386 (0.1%) | 1.71        | 259/11330 (2.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 158 | ASN  | C-N   | 7.76  | 1.44        | 1.34     |
| 1   | A     | 625 | PRO  | CA-C  | -7.38 | 1.42        | 1.52     |
| 1   | A     | 696 | VAL  | CA-C  | 5.80  | 1.59        | 1.52     |
| 1   | A     | 7   | ASP  | CA-C  | -5.53 | 1.50        | 1.53     |
| 1   | A     | 172 | CYS  | N-CA  | -5.51 | 1.40        | 1.46     |
| 1   | A     | 7   | ASP  | N-CA  | -5.40 | 1.41        | 1.46     |
| 1   | A     | 472 | PHE  | N-CA  | -5.13 | 1.40        | 1.46     |
| 1   | A     | 696 | VAL  | N-CA  | 5.07  | 1.51        | 1.46     |

All (259) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 626 | GLU  | N-CA-C | -15.91 | 91.61       | 111.02   |
| 1   | A     | 643 | GLN  | N-CA-C | 15.32  | 135.11      | 107.99   |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 24  | GLN  | N-CA-C  | -15.25 | 93.20       | 112.72   |
| 1   | A     | 402 | LYS  | N-CA-C  | 15.14  | 133.83      | 110.36   |
| 1   | A     | 751 | ALA  | N-CA-C  | -14.77 | 94.69       | 111.82   |
| 1   | A     | 644 | THR  | N-CA-C  | -13.72 | 87.04       | 109.40   |
| 1   | A     | 63  | ASP  | N-CA-C  | -13.19 | 96.81       | 113.43   |
| 1   | A     | 399 | LEU  | N-CA-C  | -13.04 | 94.41       | 111.24   |
| 1   | A     | 525 | LYS  | CA-C-N  | 12.90  | 135.97      | 119.84   |
| 1   | A     | 525 | LYS  | C-N-CA  | 12.90  | 135.97      | 119.84   |
| 1   | A     | 252 | GLY  | CA-C-N  | -12.76 | 104.67      | 119.47   |
| 1   | A     | 252 | GLY  | C-N-CA  | -12.76 | 104.67      | 119.47   |
| 1   | A     | 66  | THR  | N-CA-C  | 12.70  | 126.74      | 110.24   |
| 1   | A     | 567 | LYS  | CA-C-N  | 12.22  | 135.18      | 121.00   |
| 1   | A     | 567 | LYS  | C-N-CA  | 12.22  | 135.18      | 121.00   |
| 1   | A     | 544 | ASP  | N-CA-C  | 11.91  | 125.74      | 111.33   |
| 1   | A     | 568 | PRO  | N-CA-C  | -11.60 | 101.12      | 114.92   |
| 1   | A     | 26  | ALA  | N-CA-C  | -11.56 | 87.67       | 108.48   |
| 2   | B     | 71  | MET  | N-CA-C  | -11.16 | 99.39       | 113.23   |
| 1   | A     | 737 | THR  | N-CA-C  | -10.97 | 100.21      | 112.72   |
| 1   | A     | 500 | TYR  | N-CA-C  | -10.75 | 97.00       | 113.02   |
| 1   | A     | 820 | VAL  | N-CA-C  | -10.50 | 103.32      | 111.62   |
| 2   | B     | 67  | LEU  | N-CA-C  | 10.26  | 132.65      | 110.80   |
| 1   | A     | 558 | LYS  | N-CA-C  | 10.09  | 123.98      | 112.57   |
| 1   | A     | 25  | THR  | N-CA-C  | 10.03  | 126.11      | 109.06   |
| 1   | A     | 542 | ALA  | N-CA-C  | 10.00  | 123.55      | 109.15   |
| 1   | A     | 574 | GLY  | CA-C-N  | 9.98   | 130.61      | 119.93   |
| 1   | A     | 574 | GLY  | C-N-CA  | 9.98   | 130.61      | 119.93   |
| 1   | A     | 573 | GLN  | N-CA-C  | 9.89   | 123.39      | 110.43   |
| 1   | A     | 707 | PHE  | CA-C-N  | 9.29   | 129.66      | 119.90   |
| 1   | A     | 707 | PHE  | C-N-CA  | 9.29   | 129.66      | 119.90   |
| 1   | A     | 145 | LYS  | N-CA-C  | 9.23   | 123.56      | 111.75   |
| 1   | A     | 572 | ASN  | N-CA-C  | -9.22  | 101.96      | 113.02   |
| 2   | B     | 115 | ASN  | CA-C-N  | 9.18   | 136.88      | 122.74   |
| 2   | B     | 115 | ASN  | C-N-CA  | 9.18   | 136.88      | 122.74   |
| 1   | A     | 6   | SER  | CA-C-N  | 9.16   | 131.89      | 123.10   |
| 1   | A     | 6   | SER  | C-N-CA  | 9.16   | 131.89      | 123.10   |
| 1   | A     | 706 | GLY  | N-CA-C  | 9.09   | 134.73      | 113.18   |
| 1   | A     | 254 | THR  | CB-CA-C | -9.06  | 99.31       | 111.82   |
| 1   | A     | 266 | LEU  | N-CA-C  | 9.05   | 123.88      | 111.39   |
| 1   | A     | 418 | GLN  | N-CA-C  | -8.95  | 101.42      | 111.71   |
| 3   | C     | 90  | PHE  | N-CA-C  | -8.86  | 102.01      | 113.17   |
| 1   | A     | 161 | GLN  | N-CA-C  | -8.82  | 100.66      | 111.33   |
| 1   | A     | 546 | SER  | N-CA-C  | -8.81  | 101.68      | 111.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 512 | PHE  | N-CA-C  | -8.80 | 102.08      | 113.17   |
| 1   | A     | 833 | VAL  | N-CA-C  | 8.76  | 127.55      | 109.34   |
| 3   | C     | 17  | LEU  | N-CA-C  | -8.72 | 103.15      | 113.88   |
| 1   | A     | 519 | CYS  | N-CA-C  | -8.70 | 100.22      | 112.13   |
| 1   | A     | 515 | ASP  | N-CA-C  | -8.56 | 103.02      | 113.97   |
| 1   | A     | 833 | VAL  | CB-CA-C | -8.48 | 97.39       | 111.29   |
| 2   | B     | 25  | SER  | N-CA-C  | -8.48 | 101.73      | 110.97   |
| 1   | A     | 309 | TYR  | N-CA-C  | -8.38 | 97.44       | 110.42   |
| 1   | A     | 779 | SER  | N-CA-C  | -8.38 | 101.39      | 111.69   |
| 1   | A     | 642 | PHE  | CA-C-N  | 8.32  | 134.93      | 123.11   |
| 1   | A     | 642 | PHE  | C-N-CA  | 8.32  | 134.93      | 123.11   |
| 1   | A     | 303 | THR  | N-CA-C  | -8.29 | 97.15       | 109.42   |
| 1   | A     | 749 | ASP  | CA-C-N  | 8.29  | 129.28      | 120.83   |
| 1   | A     | 749 | ASP  | C-N-CA  | 8.29  | 129.28      | 120.83   |
| 1   | A     | 380 | ALA  | N-CA-C  | -8.26 | 101.60      | 112.34   |
| 1   | A     | 214 | SER  | N-CA-C  | -8.24 | 93.25       | 110.80   |
| 1   | A     | 750 | PRO  | N-CA-C  | 8.22  | 123.23      | 114.68   |
| 1   | A     | 254 | THR  | N-CA-C  | 8.17  | 124.28      | 107.37   |
| 1   | A     | 27  | ALA  | N-CA-C  | 8.05  | 121.42      | 109.59   |
| 1   | A     | 628 | PRO  | N-CA-C  | 8.04  | 129.04      | 112.47   |
| 1   | A     | 342 | LYS  | N-CA-C  | -8.00 | 102.64      | 111.36   |
| 2   | B     | 89  | ILE  | N-CA-C  | -7.98 | 105.44      | 111.90   |
| 2   | B     | 15  | LYS  | N-CA-C  | -7.93 | 102.58      | 111.71   |
| 1   | A     | 489 | ASN  | N-CA-C  | -7.91 | 103.63      | 113.28   |
| 1   | A     | 832 | LYS  | N-CA-C  | -7.88 | 101.80      | 111.33   |
| 1   | A     | 624 | ALA  | N-CA-C  | -7.87 | 98.59       | 110.01   |
| 1   | A     | 73  | ASP  | N-CA-C  | -7.87 | 103.81      | 113.41   |
| 2   | B     | 32  | ASP  | N-CA-C  | -7.86 | 103.48      | 113.23   |
| 1   | A     | 382 | LYS  | N-CA-C  | 7.82  | 122.50      | 112.34   |
| 1   | A     | 575 | PRO  | N-CA-C  | 7.76  | 123.90      | 111.26   |
| 1   | A     | 132 | TYR  | N-CA-C  | 7.59  | 123.47      | 113.30   |
| 1   | A     | 472 | PHE  | CA-C-N  | -7.52 | 110.20      | 120.28   |
| 1   | A     | 472 | PHE  | C-N-CA  | -7.52 | 110.20      | 120.28   |
| 1   | A     | 495 | LEU  | N-CA-C  | -7.50 | 104.10      | 113.18   |
| 1   | A     | 513 | GLY  | N-CA-C  | -7.47 | 95.47       | 113.18   |
| 1   | A     | 447 | ASP  | N-CA-C  | 7.46  | 123.34      | 113.20   |
| 1   | A     | 533 | LEU  | N-CA-C  | -7.45 | 102.65      | 112.34   |
| 1   | A     | 507 | TRP  | N-CA-C  | -7.42 | 99.26       | 109.95   |
| 1   | A     | 258 | ALA  | N-CA-C  | -7.40 | 104.78      | 113.88   |
| 1   | A     | 676 | LEU  | N-CA-C  | 7.35  | 122.27      | 113.16   |
| 2   | B     | 19  | GLU  | N-CA-C  | -7.35 | 103.20      | 111.14   |
| 1   | A     | 650 | ARG  | N-CA-C  | -7.32 | 103.31      | 111.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 413 | GLY  | N-CA-C  | 7.28  | 130.44      | 113.18   |
| 2   | B     | 118 | ASP  | N-CA-C  | -7.24 | 95.25       | 107.99   |
| 1   | A     | 379 | GLU  | N-CA-C  | -7.17 | 103.15      | 112.68   |
| 3   | C     | 67  | GLU  | N-CA-C  | -7.16 | 104.53      | 113.55   |
| 1   | A     | 25  | THR  | CA-C-N  | 7.14  | 134.31      | 121.89   |
| 1   | A     | 25  | THR  | C-N-CA  | 7.14  | 134.31      | 121.89   |
| 3   | C     | 63  | LEU  | CA-C-N  | 7.14  | 128.76      | 119.84   |
| 3   | C     | 63  | LEU  | C-N-CA  | 7.14  | 128.76      | 119.84   |
| 1   | A     | 317 | LEU  | N-CA-C  | -7.08 | 105.17      | 114.31   |
| 1   | A     | 697 | LEU  | N-CA-C  | 7.08  | 119.46      | 110.33   |
| 1   | A     | 79  | PRO  | CA-C-N  | 7.07  | 128.68      | 119.84   |
| 1   | A     | 79  | PRO  | C-N-CA  | 7.07  | 128.68      | 119.84   |
| 1   | A     | 750 | PRO  | CA-C-N  | -7.07 | 109.57      | 120.31   |
| 1   | A     | 750 | PRO  | C-N-CA  | -7.07 | 109.57      | 120.31   |
| 1   | A     | 415 | ASN  | N-CA-C  | 7.06  | 120.08      | 110.55   |
| 2   | B     | 93  | PHE  | N-CA-C  | -7.02 | 100.16      | 111.04   |
| 1   | A     | 734 | ASP  | N-CA-C  | 6.97  | 130.51      | 111.00   |
| 1   | A     | 606 | VAL  | N-CA-C  | -6.96 | 102.69      | 110.62   |
| 1   | A     | 587 | VAL  | CA-C-N  | 6.96  | 128.54      | 119.84   |
| 1   | A     | 587 | VAL  | C-N-CA  | 6.96  | 128.54      | 119.84   |
| 1   | A     | 571 | PRO  | N-CA-C  | 6.95  | 126.78      | 112.47   |
| 1   | A     | 65  | SER  | N-CA-C  | 6.94  | 119.73      | 108.34   |
| 2   | B     | 152 | GLY  | N-CA-C  | -6.93 | 97.79       | 111.31   |
| 1   | A     | 796 | LYS  | N-CA-C  | -6.92 | 103.94      | 112.38   |
| 1   | A     | 628 | PRO  | CB-CA-C | -6.90 | 100.18      | 111.56   |
| 2   | B     | 134 | VAL  | N-CA-C  | 6.87  | 117.89      | 109.30   |
| 1   | A     | 532 | ILE  | N-CA-C  | 6.87  | 117.47      | 111.56   |
| 1   | A     | 574 | GLY  | N-CA-C  | 6.71  | 126.03      | 112.34   |
| 1   | A     | 694 | ASN  | N-CA-C  | 6.70  | 121.31      | 112.13   |
| 1   | A     | 199 | ALA  | N-CA-C  | 6.67  | 120.48      | 110.14   |
| 2   | B     | 132 | ALA  | CA-C-N  | 6.66  | 128.16      | 119.84   |
| 2   | B     | 132 | ALA  | C-N-CA  | 6.66  | 128.16      | 119.84   |
| 3   | C     | 19  | ASP  | N-CA-C  | -6.61 | 103.75      | 112.34   |
| 2   | B     | 144 | PHE  | N-CA-C  | -6.59 | 104.50      | 112.54   |
| 3   | C     | 16  | GLU  | N-CA-C  | -6.58 | 105.32      | 113.15   |
| 1   | A     | 129 | LEU  | CA-C-N  | 6.57  | 126.26      | 119.82   |
| 1   | A     | 129 | LEU  | C-N-CA  | 6.57  | 126.26      | 119.82   |
| 1   | A     | 477 | ILE  | N-CA-C  | -6.53 | 103.96      | 110.62   |
| 3   | C     | 151 | GLY  | N-CA-C  | 6.52  | 125.63      | 112.34   |
| 1   | A     | 65  | SER  | CA-C-N  | 6.44  | 130.28      | 120.82   |
| 1   | A     | 65  | SER  | C-N-CA  | 6.44  | 130.28      | 120.82   |
| 1   | A     | 511 | ASP  | CA-C-N  | 6.41  | 133.12      | 122.54   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 511 | ASP  | C-N-CA  | 6.41  | 133.12      | 122.54   |
| 1   | A     | 833 | VAL  | O-C-N   | -6.40 | 114.57      | 122.57   |
| 1   | A     | 517 | GLN  | N-CA-C  | -6.39 | 105.44      | 113.18   |
| 1   | A     | 23  | GLU  | CA-C-N  | 6.38  | 133.95      | 122.46   |
| 1   | A     | 23  | GLU  | C-N-CA  | 6.38  | 133.95      | 122.46   |
| 1   | A     | 422 | SER  | N-CA-C  | -6.38 | 105.43      | 113.72   |
| 1   | A     | 126 | TYR  | N-CA-C  | 6.35  | 120.75      | 113.19   |
| 3   | C     | 13  | ASP  | N-CA-C  | 6.34  | 118.19      | 111.28   |
| 2   | B     | 148 | ILE  | N-CA-C  | -6.32 | 103.15      | 111.05   |
| 1   | A     | 627 | GLU  | CA-C-N  | 6.31  | 127.73      | 119.84   |
| 1   | A     | 627 | GLU  | C-N-CA  | 6.31  | 127.73      | 119.84   |
| 1   | A     | 462 | ALA  | N-CA-C  | 6.30  | 124.22      | 110.80   |
| 1   | A     | 516 | LEU  | N-CA-C  | -6.28 | 104.35      | 111.07   |
| 3   | C     | 8   | ILE  | N-CA-C  | -6.26 | 104.81      | 112.76   |
| 1   | A     | 725 | PRO  | N-CA-C  | 6.26  | 124.71      | 113.70   |
| 1   | A     | 758 | THR  | CB-CA-C | 6.23  | 121.22      | 110.01   |
| 1   | A     | 400 | LYS  | CA-C-N  | 6.21  | 127.07      | 120.11   |
| 1   | A     | 400 | LYS  | C-N-CA  | 6.21  | 127.07      | 120.11   |
| 1   | A     | 494 | ILE  | CA-C-N  | -6.21 | 109.47      | 121.58   |
| 1   | A     | 494 | ILE  | C-N-CA  | -6.21 | 109.47      | 121.58   |
| 1   | A     | 149 | PRO  | CA-C-N  | 6.20  | 127.59      | 119.84   |
| 1   | A     | 149 | PRO  | C-N-CA  | 6.20  | 127.59      | 119.84   |
| 1   | A     | 501 | LYS  | N-CA-C  | -6.20 | 97.60       | 110.80   |
| 1   | A     | 720 | TYR  | N-CA-C  | 6.20  | 120.46      | 113.02   |
| 1   | A     | 269 | LYS  | N-CA-C  | -6.19 | 104.08      | 111.69   |
| 1   | A     | 371 | GLN  | N-CA-C  | -6.18 | 103.42      | 113.19   |
| 1   | A     | 570 | ARG  | N-CA-C  | -6.17 | 101.98      | 109.57   |
| 1   | A     | 167 | ARG  | N-CA-C  | 6.17  | 120.19      | 111.92   |
| 1   | A     | 497 | GLN  | N-CA-C  | -6.17 | 105.81      | 113.15   |
| 1   | A     | 748 | MET  | N-CA-C  | 6.13  | 120.26      | 109.96   |
| 1   | A     | 749 | ASP  | N-CA-C  | -6.12 | 97.29       | 109.60   |
| 1   | A     | 737 | THR  | CA-C-N  | -6.12 | 110.95      | 121.97   |
| 1   | A     | 737 | THR  | C-N-CA  | -6.12 | 110.95      | 121.97   |
| 1   | A     | 759 | LYS  | N-CA-C  | 6.11  | 118.70      | 109.41   |
| 1   | A     | 7   | ASP  | CA-C-N  | -6.09 | 112.22      | 119.84   |
| 1   | A     | 7   | ASP  | C-N-CA  | -6.09 | 112.22      | 119.84   |
| 1   | A     | 256 | LYS  | N-CA-C  | -6.09 | 100.34      | 109.96   |
| 1   | A     | 319 | VAL  | N-CA-C  | -6.08 | 98.99       | 107.80   |
| 1   | A     | 164 | VAL  | CB-CA-C | -6.06 | 101.35      | 111.29   |
| 1   | A     | 308 | LEU  | N-CA-C  | 6.04  | 120.50      | 111.81   |
| 1   | A     | 674 | ASN  | N-CA-C  | 6.04  | 117.42      | 108.60   |
| 2   | B     | 52  | ASP  | N-CA-C  | -5.98 | 101.15      | 110.42   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 471 | SER  | N-CA-CB | 5.95  | 119.64      | 109.10   |
| 1   | A     | 782 | ILE  | N-CA-C  | -5.95 | 105.92      | 111.45   |
| 1   | A     | 596 | GLU  | N-CA-C  | -5.95 | 105.69      | 113.12   |
| 1   | A     | 111 | LEU  | N-CA-C  | -5.93 | 100.13      | 109.50   |
| 1   | A     | 455 | TYR  | N-CA-C  | 5.92  | 118.40      | 109.23   |
| 1   | A     | 757 | THR  | CA-C-N  | -5.92 | 111.67      | 122.38   |
| 1   | A     | 757 | THR  | C-N-CA  | -5.92 | 111.67      | 122.38   |
| 3   | C     | 22  | ASP  | N-CA-C  | -5.89 | 98.24       | 110.80   |
| 1   | A     | 471 | SER  | CB-CA-C | -5.89 | 103.88      | 113.37   |
| 1   | A     | 524 | GLU  | N-CA-C  | 5.89  | 119.72      | 112.54   |
| 1   | A     | 740 | GLU  | N-CA-C  | -5.88 | 104.22      | 111.75   |
| 1   | A     | 362 | LYS  | N-CA-C  | 5.85  | 118.09      | 110.43   |
| 1   | A     | 225 | VAL  | N-CA-C  | 5.82  | 115.89      | 110.42   |
| 1   | A     | 425 | ALA  | N-CA-C  | -5.81 | 104.14      | 111.11   |
| 1   | A     | 707 | PHE  | N-CA-C  | 5.81  | 117.28      | 110.31   |
| 1   | A     | 381 | GLU  | N-CA-C  | -5.80 | 104.86      | 111.07   |
| 2   | B     | 138 | LYS  | N-CA-C  | 5.80  | 117.74      | 108.41   |
| 1   | A     | 92  | THR  | N-CA-C  | -5.77 | 103.73      | 112.04   |
| 1   | A     | 28  | PHE  | N-CA-C  | -5.74 | 100.34      | 109.59   |
| 1   | A     | 625 | PRO  | N-CA-C  | 5.72  | 124.26      | 112.47   |
| 1   | A     | 305 | ASP  | CA-C-N  | 5.72  | 128.21      | 120.38   |
| 1   | A     | 305 | ASP  | C-N-CA  | 5.72  | 128.21      | 120.38   |
| 1   | A     | 506 | ALA  | N-CA-C  | -5.64 | 99.70       | 108.90   |
| 1   | A     | 384 | ALA  | N-CA-C  | 5.61  | 117.20      | 111.14   |
| 1   | A     | 569 | THR  | CA-C-N  | -5.61 | 112.81      | 120.83   |
| 1   | A     | 569 | THR  | C-N-CA  | -5.61 | 112.81      | 120.83   |
| 2   | B     | 91  | ASN  | N-CA-C  | -5.57 | 108.27      | 114.62   |
| 1   | A     | 443 | ASN  | N-CA-C  | -5.56 | 105.32      | 111.71   |
| 1   | A     | 140 | TYR  | N-CA-C  | 5.55  | 119.73      | 112.13   |
| 1   | A     | 303 | THR  | CA-C-N  | 5.54  | 126.77      | 119.84   |
| 1   | A     | 303 | THR  | C-N-CA  | 5.54  | 126.77      | 119.84   |
| 1   | A     | 98  | SER  | N-CA-C  | -5.53 | 105.57      | 112.93   |
| 1   | A     | 197 | ALA  | N-CA-C  | 5.52  | 117.89      | 108.90   |
| 1   | A     | 463 | GLY  | CA-C-O  | -5.52 | 117.22      | 122.13   |
| 3   | C     | 51  | ALA  | N-CA-C  | -5.51 | 104.14      | 111.24   |
| 1   | A     | 799 | LYS  | N-CA-C  | -5.48 | 104.33      | 111.02   |
| 1   | A     | 216 | GLU  | N-CA-C  | -5.47 | 104.96      | 111.03   |
| 2   | B     | 38  | GLU  | N-CA-C  | -5.46 | 106.70      | 113.19   |
| 1   | A     | 705 | LYS  | CA-C-O  | -5.43 | 111.56      | 120.80   |
| 1   | A     | 692 | GLN  | CA-C-N  | -5.41 | 114.03      | 122.37   |
| 1   | A     | 692 | GLN  | C-N-CA  | -5.41 | 114.03      | 122.37   |
| 1   | A     | 416 | MET  | N-CA-C  | 5.41  | 122.32      | 110.80   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 472 | PHE  | CA-CB-CG | -5.41 | 108.39      | 113.80   |
| 1   | A     | 518 | MET  | N-CA-C   | -5.39 | 106.47      | 113.16   |
| 1   | A     | 527 | MET  | N-CA-C   | -5.38 | 104.28      | 111.87   |
| 1   | A     | 482 | GLU  | N-CA-C   | -5.37 | 104.67      | 111.11   |
| 2   | B     | 27  | ILE  | N-CA-C   | 5.37  | 116.74      | 110.62   |
| 1   | A     | 265 | TYR  | N-CA-C   | 5.36  | 117.16      | 108.26   |
| 1   | A     | 117 | GLY  | N-CA-C   | -5.34 | 102.28      | 111.47   |
| 1   | A     | 310 | SER  | N-CA-C   | 5.30  | 120.22      | 113.55   |
| 3   | C     | 88  | GLU  | N-CA-C   | -5.29 | 106.67      | 113.02   |
| 1   | A     | 472 | PHE  | N-CA-CB  | 5.28  | 118.38      | 109.78   |
| 1   | A     | 711 | LEU  | N-CA-C   | 5.26  | 116.95      | 108.32   |
| 1   | A     | 493 | PHE  | N-CA-C   | -5.26 | 105.02      | 111.75   |
| 1   | A     | 7   | ASP  | N-CA-C   | 5.25  | 123.26      | 112.40   |
| 1   | A     | 93  | TYR  | N-CA-C   | 5.23  | 121.95      | 110.80   |
| 1   | A     | 124 | ASN  | CA-C-N   | 5.23  | 126.38      | 119.84   |
| 1   | A     | 124 | ASN  | C-N-CA   | 5.23  | 126.38      | 119.84   |
| 1   | A     | 419 | VAL  | N-CA-C   | -5.23 | 104.86      | 110.36   |
| 1   | A     | 490 | HIS  | N-CA-C   | -5.23 | 105.69      | 111.71   |
| 1   | A     | 409 | MET  | CB-CG-SD | 5.22  | 128.36      | 112.70   |
| 2   | B     | 88  | THR  | N-CA-C   | -5.22 | 106.69      | 113.16   |
| 1   | A     | 500 | TYR  | CA-C-O   | 5.20  | 125.00      | 119.34   |
| 1   | A     | 38  | ASP  | N-CA-C   | -5.19 | 102.78      | 110.46   |
| 3   | C     | 73  | GLU  | N-CA-C   | 5.17  | 117.32      | 111.11   |
| 2   | B     | 66  | PRO  | CA-C-N   | 5.17  | 131.41      | 121.54   |
| 2   | B     | 66  | PRO  | C-N-CA   | 5.17  | 131.41      | 121.54   |
| 1   | A     | 642 | PHE  | N-CA-C   | 5.16  | 125.46      | 111.00   |
| 1   | A     | 181 | GLY  | CA-C-N   | -5.16 | 113.62      | 120.79   |
| 1   | A     | 181 | GLY  | C-N-CA   | -5.16 | 113.62      | 120.79   |
| 1   | A     | 403 | VAL  | N-CA-C   | 5.15  | 114.81      | 108.53   |
| 3   | C     | 65  | PHE  | N-CA-C   | 5.15  | 116.74      | 111.03   |
| 1   | A     | 338 | LEU  | N-CA-C   | -5.14 | 106.79      | 113.16   |
| 2   | B     | 30  | ASP  | N-CA-C   | -5.13 | 105.18      | 111.75   |
| 1   | A     | 229 | TYR  | N-CA-C   | 5.13  | 117.54      | 111.33   |
| 1   | A     | 661 | TYR  | N-CA-C   | -5.13 | 106.97      | 113.18   |
| 2   | B     | 28  | ASP  | CA-C-N   | -5.13 | 114.06      | 121.65   |
| 2   | B     | 28  | ASP  | C-N-CA   | -5.13 | 114.06      | 121.65   |
| 1   | A     | 6   | SER  | N-CA-C   | 5.12  | 116.97      | 109.24   |
| 1   | A     | 12  | TYR  | N-CA-C   | -5.11 | 105.34      | 112.03   |
| 1   | A     | 645 | ILE  | N-CA-C   | 5.09  | 119.92      | 109.34   |
| 2   | B     | 101 | THR  | N-CA-C   | -5.08 | 107.11      | 113.72   |
| 1   | A     | 124 | ASN  | N-CA-C   | 5.08  | 121.03      | 109.81   |
| 1   | A     | 54  | ASP  | N-CA-C   | -5.07 | 104.74      | 112.04   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 502 | LYS  | N-CA-C | 5.07  | 117.19      | 111.11   |
| 1   | A     | 135 | SER  | N-CA-C | -5.06 | 105.03      | 111.11   |
| 2   | B     | 97  | ASP  | N-CA-C | -5.06 | 104.36      | 110.44   |
| 2   | B     | 127 | MET  | N-CA-C | -5.05 | 106.63      | 112.89   |
| 3   | C     | 93  | PHE  | N-CA-C | -5.00 | 106.34      | 114.09   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 126 | TYR  | Sidechain |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5964  | 0        | 5725     | 1232    | 1            |
| 2   | B     | 1097  | 0        | 1040     | 232     | 0            |
| 3   | C     | 1174  | 0        | 1061     | 233     | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 31    | 0        | 13       | 15      | 0            |
| 6   | C     | 1     | 0        | 0        | 0       | 0            |
| 7   | A     | 5     | 0        | 0        | 5       | 0            |
| 7   | B     | 1     | 0        | 0        | 1       | 0            |
| 7   | C     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 8276  | 0        | 7839     | 1621    | 1            |

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 101.

All (1621) 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:472:PHE:HE1 | 1:A:476:CYS:SG | 1.25                     | 1.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:398:LEU:CA   | 1:A:401:PRO:HG2  | 1.36                     | 1.53              |
| 1:A:398:LEU:N    | 1:A:401:PRO:CG   | 1.78                     | 1.46              |
| 1:A:472:PHE:CE1  | 1:A:476:CYS:SG   | 2.11                     | 1.43              |
| 1:A:397:ALA:C    | 1:A:401:PRO:CG   | 1.94                     | 1.39              |
| 1:A:397:ALA:C    | 1:A:401:PRO:HG2  | 1.50                     | 1.35              |
| 1:A:398:LEU:N    | 1:A:401:PRO:HG2  | 1.02                     | 1.34              |
| 1:A:395:LEU:O    | 1:A:399:LEU:HG   | 1.29                     | 1.25              |
| 1:A:472:PHE:HD1  | 1:A:472:PHE:C    | 1.35                     | 1.24              |
| 1:A:237:ASN:ND2  | 5:A:999:ANP:H5'2 | 1.54                     | 1.23              |
| 1:A:472:PHE:HD1  | 1:A:472:PHE:O    | 1.18                     | 1.22              |
| 1:A:397:ALA:O    | 1:A:401:PRO:HB2  | 1.33                     | 1.22              |
| 1:A:197:ALA:HB2  | 1:A:256:LYS:CB   | 1.69                     | 1.21              |
| 1:A:403:VAL:C    | 1:A:409:MET:HG3  | 1.66                     | 1.20              |
| 1:A:833:VAL:O    | 1:A:833:VAL:CG1  | 1.85                     | 1.19              |
| 1:A:471:SER:OG   | 1:A:594:TRP:CZ2  | 1.97                     | 1.18              |
| 1:A:743:LEU:HA   | 1:A:748:MET:HE1  | 1.23                     | 1.17              |
| 1:A:14:ALA:HB2   | 1:A:149:PRO:CB   | 1.74                     | 1.17              |
| 1:A:694:ASN:HD22 | 1:A:694:ASN:N    | 1.37                     | 1.17              |
| 1:A:397:ALA:C    | 1:A:401:PRO:CB   | 2.18                     | 1.16              |
| 1:A:397:ALA:O    | 1:A:398:LEU:HG   | 1.47                     | 1.13              |
| 1:A:694:ASN:H    | 1:A:694:ASN:ND2  | 1.36                     | 1.13              |
| 1:A:472:PHE:C    | 1:A:472:PHE:CD1  | 2.11                     | 1.12              |
| 1:A:363:PHE:HA   | 1:A:373:GLU:O    | 1.51                     | 1.11              |
| 1:A:418:GLN:O    | 1:A:422:SER:N    | 1.82                     | 1.11              |
| 1:A:402:LYS:N    | 1:A:411:THR:HG23 | 1.65                     | 1.11              |
| 1:A:398:LEU:CA   | 1:A:401:PRO:CG   | 2.22                     | 1.10              |
| 1:A:257:ILE:HD12 | 1:A:257:ILE:H    | 0.97                     | 1.09              |
| 1:A:529:ILE:HG12 | 1:A:530:LEU:N    | 1.56                     | 1.09              |
| 1:A:707:PHE:HB3  | 1:A:708:PRO:HD2  | 1.25                     | 1.09              |
| 1:A:141:ARG:NH1  | 1:A:196:VAL:HB   | 1.67                     | 1.08              |
| 2:B:44:SER:OG    | 2:B:50:ALA:HA    | 1.53                     | 1.08              |
| 2:B:114:GLU:HB2  | 2:B:125:MET:HE2  | 1.28                     | 1.08              |
| 1:A:697:LEU:HD12 | 1:A:697:LEU:H    | 1.13                     | 1.08              |
| 1:A:400:LYS:HA   | 1:A:414:GLN:HB2  | 1.15                     | 1.08              |
| 1:A:197:ALA:CB   | 1:A:256:LYS:CB   | 2.31                     | 1.08              |
| 1:A:257:ILE:HD12 | 1:A:257:ILE:N    | 1.59                     | 1.07              |
| 1:A:100:LEU:HD22 | 1:A:688:LEU:HD21 | 1.29                     | 1.07              |
| 1:A:123:VAL:HG12 | 1:A:673:PRO:HG3  | 1.28                     | 1.07              |
| 1:A:296:LEU:HD22 | 1:A:299:VAL:HG11 | 1.37                     | 1.07              |
| 1:A:417:ASN:HD22 | 1:A:417:ASN:N    | 1.47                     | 1.07              |
| 1:A:461:ILE:CD1  | 1:A:462:ALA:H    | 1.67                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:472:PHE:O    | 1:A:472:PHE:CD1  | 2.06                     | 1.07              |
| 1:A:416:MET:HG3  | 1:A:416:MET:O    | 1.53                     | 1.06              |
| 1:A:598:ASN:ND2  | 1:A:644:THR:HB   | 1.68                     | 1.06              |
| 1:A:400:LYS:N    | 1:A:401:PRO:HD3  | 1.72                     | 1.05              |
| 1:A:713:TYR:HE2  | 1:A:757:THR:O    | 1.37                     | 1.05              |
| 1:A:223:ASN:HB2  | 1:A:224:PRO:HD3  | 1.35                     | 1.04              |
| 1:A:598:ASN:ND2  | 1:A:644:THR:CB   | 2.19                     | 1.04              |
| 1:A:751:ALA:HA   | 1:A:754:ARG:HH12 | 1.17                     | 1.04              |
| 1:A:400:LYS:N    | 1:A:401:PRO:CD   | 2.19                     | 1.04              |
| 1:A:95:ASN:O     | 1:A:99:VAL:HG23  | 1.57                     | 1.03              |
| 1:A:284:ILE:HD12 | 1:A:285:PHE:H    | 1.18                     | 1.02              |
| 1:A:461:ILE:HD12 | 1:A:462:ALA:H    | 1.19                     | 1.02              |
| 1:A:353:ALA:HA   | 1:A:356:LEU:HD12 | 1.42                     | 1.01              |
| 1:A:598:ASN:HD21 | 1:A:644:THR:CB   | 1.71                     | 1.00              |
| 2:B:119:ASN:HD22 | 2:B:119:ASN:N    | 1.51                     | 1.00              |
| 1:A:48:ILE:HG23  | 1:A:58:VAL:HG12  | 1.38                     | 1.00              |
| 1:A:398:LEU:HA   | 1:A:401:PRO:HG2  | 1.39                     | 1.00              |
| 1:A:511:ASP:CA   | 1:A:514:MET:HB2  | 1.91                     | 1.00              |
| 1:A:14:ALA:CB    | 1:A:149:PRO:HG3  | 1.92                     | 1.00              |
| 1:A:511:ASP:N    | 1:A:514:MET:HB2  | 1.77                     | 0.99              |
| 1:A:396:LYS:O    | 1:A:401:PRO:HG3  | 1.60                     | 0.99              |
| 1:A:14:ALA:HB2   | 1:A:149:PRO:CG   | 1.91                     | 0.99              |
| 1:A:417:ASN:H    | 1:A:417:ASN:ND2  | 1.54                     | 0.99              |
| 1:A:131:ILE:HG13 | 1:A:132:TYR:CE1  | 1.98                     | 0.98              |
| 1:A:237:ASN:HD21 | 5:A:999:ANP:H5'2 | 1.25                     | 0.98              |
| 1:A:384:ALA:HB2  | 1:A:391:ALA:HB2  | 1.47                     | 0.97              |
| 1:A:399:LEU:N    | 1:A:401:PRO:CD   | 2.28                     | 0.97              |
| 1:A:512:PHE:O    | 1:A:706:GLY:HA3  | 1.62                     | 0.97              |
| 3:C:98:GLN:HE21  | 3:C:98:GLN:HA    | 1.28                     | 0.97              |
| 3:C:135:LEU:HD12 | 3:C:135:LEU:H    | 1.30                     | 0.97              |
| 1:A:515:ASP:OD2  | 1:A:515:ASP:N    | 1.96                     | 0.97              |
| 1:A:805:ARG:HA   | 3:C:21:TRP:CZ2   | 2.00                     | 0.96              |
| 1:A:257:ILE:H    | 1:A:257:ILE:CD1  | 1.64                     | 0.96              |
| 1:A:82:PHE:CZ    | 1:A:91:MET:HA    | 2.00                     | 0.96              |
| 1:A:753:TYR:O    | 1:A:754:ARG:HD3  | 1.64                     | 0.96              |
| 1:A:833:VAL:O    | 1:A:835:PRO:HD3  | 1.63                     | 0.96              |
| 1:A:395:LEU:O    | 1:A:399:LEU:CG   | 2.12                     | 0.96              |
| 2:B:119:ASN:H    | 2:B:119:ASN:ND2  | 1.52                     | 0.96              |
| 1:A:293:ILE:HD11 | 1:A:296:LEU:HD12 | 1.48                     | 0.96              |
| 1:A:183:THR:HB   | 5:A:999:ANP:O1A  | 1.67                     | 0.95              |
| 1:A:257:ILE:N    | 1:A:257:ILE:CD1  | 2.25                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:284:ILE:HA   | 1:A:287:GLN:OE1  | 1.67                     | 0.94              |
| 1:A:397:ALA:O    | 1:A:401:PRO:CB   | 2.11                     | 0.94              |
| 1:A:420:VAL:O    | 1:A:423:VAL:HG12 | 1.65                     | 0.94              |
| 1:A:400:LYS:H    | 1:A:401:PRO:HD3  | 1.27                     | 0.94              |
| 2:B:142:VAL:HG12 | 2:B:143:LYS:NZ   | 1.82                     | 0.94              |
| 2:B:143:LYS:HD3  | 2:B:146:ALA:HB3  | 1.50                     | 0.94              |
| 1:A:555:HIS:HD2  | 1:A:558:LYS:HE3  | 1.29                     | 0.94              |
| 1:A:398:LEU:C    | 1:A:401:PRO:HD2  | 1.92                     | 0.93              |
| 1:A:530:LEU:O    | 1:A:534:GLU:HG3  | 1.68                     | 0.93              |
| 1:A:471:SER:OG   | 1:A:472:PHE:N    | 1.89                     | 0.93              |
| 1:A:11:GLN:HG2   | 1:A:12:TYR:HE1   | 1.32                     | 0.93              |
| 2:B:93:PHE:CD2   | 2:B:141:TYR:HB2  | 2.03                     | 0.93              |
| 3:C:42:ILE:HG22  | 3:C:44:PRO:HD3   | 1.51                     | 0.93              |
| 1:A:364:LYS:CB   | 1:A:373:GLU:HG2  | 1.98                     | 0.92              |
| 1:A:370:GLU:C    | 1:A:371:GLN:HE21 | 1.77                     | 0.92              |
| 1:A:390:ASN:HD22 | 1:A:393:ASP:H    | 1.14                     | 0.92              |
| 1:A:403:VAL:O    | 1:A:409:MET:HG3  | 1.67                     | 0.92              |
| 2:B:114:GLU:HB2  | 2:B:125:MET:CE   | 2.00                     | 0.92              |
| 1:A:812:GLN:NE2  | 2:B:118:ASP:O    | 2.02                     | 0.92              |
| 1:A:555:HIS:CD2  | 1:A:558:LYS:HE3  | 2.03                     | 0.92              |
| 1:A:237:ASN:ND2  | 5:A:999:ANP:O2A  | 2.01                     | 0.92              |
| 1:A:400:LYS:HA   | 1:A:414:GLN:CB   | 2.00                     | 0.91              |
| 1:A:529:ILE:HG12 | 1:A:530:LEU:H    | 1.29                     | 0.91              |
| 2:B:118:ASP:OD2  | 3:C:24:ARG:NH2   | 2.02                     | 0.91              |
| 1:A:397:ALA:O    | 1:A:398:LEU:CG   | 2.19                     | 0.91              |
| 2:B:86:GLU:HG3   | 2:B:149:LYS:HD3  | 1.52                     | 0.91              |
| 1:A:468:ASP:HB3  | 1:A:573:GLN:HA   | 1.51                     | 0.90              |
| 1:A:395:LEU:CD2  | 1:A:399:LEU:HD21 | 2.02                     | 0.90              |
| 1:A:397:ALA:CB   | 1:A:609:LEU:HD11 | 2.00                     | 0.90              |
| 1:A:488:PHE:CE1  | 1:A:489:ASN:OD1  | 2.25                     | 0.90              |
| 1:A:742:ILE:O    | 1:A:746:LEU:HD12 | 1.71                     | 0.90              |
| 2:B:28:ASP:OD2   | 2:B:31:ARG:HA    | 1.70                     | 0.90              |
| 1:A:470:ASN:N    | 1:A:470:ASN:HD22 | 1.70                     | 0.89              |
| 1:A:126:TYR:CE1  | 1:A:677:LYS:HA   | 2.07                     | 0.89              |
| 1:A:833:VAL:O    | 1:A:833:VAL:HG12 | 1.10                     | 0.89              |
| 1:A:397:ALA:C    | 1:A:401:PRO:HB2  | 1.89                     | 0.89              |
| 1:A:743:LEU:CA   | 1:A:748:MET:HE1  | 2.02                     | 0.89              |
| 1:A:395:LEU:HD23 | 1:A:399:LEU:HD21 | 1.51                     | 0.89              |
| 1:A:461:ILE:CG1  | 1:A:462:ALA:H    | 1.84                     | 0.89              |
| 3:C:69:LEU:HB3   | 3:C:70:PRO:HD3   | 1.53                     | 0.89              |
| 1:A:384:ALA:HA   | 1:A:389:ILE:HD12 | 1.53                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:398:LEU:N    | 1:A:401:PRO:HG3  | 1.87                     | 0.89              |
| 2:B:25:SER:OG    | 2:B:26:MET:N     | 1.98                     | 0.88              |
| 2:B:142:VAL:HG12 | 2:B:143:LYS:HZ3  | 1.37                     | 0.88              |
| 1:A:404:LYS:HA   | 1:A:409:MET:HA   | 1.56                     | 0.88              |
| 1:A:720:TYR:HB3  | 1:A:723:LEU:HD12 | 1.53                     | 0.88              |
| 1:A:512:PHE:N    | 1:A:512:PHE:CD2  | 2.40                     | 0.88              |
| 1:A:713:TYR:CE2  | 1:A:757:THR:O    | 2.26                     | 0.88              |
| 1:A:712:ILE:HD12 | 1:A:714:SER:HB3  | 1.55                     | 0.88              |
| 2:B:53:ASP:HA    | 2:B:56:LEU:HD12  | 1.55                     | 0.88              |
| 3:C:90:PHE:HB3   | 3:C:141:TYR:CE1  | 2.09                     | 0.88              |
| 1:A:296:LEU:O    | 1:A:299:VAL:HG12 | 1.73                     | 0.87              |
| 1:A:607:VAL:O    | 1:A:611:GLY:N    | 2.06                     | 0.87              |
| 1:A:488:PHE:CD1  | 1:A:489:ASN:OD1  | 2.28                     | 0.87              |
| 1:A:402:LYS:CB   | 1:A:411:THR:OG1  | 2.23                     | 0.87              |
| 1:A:115:TYR:CE1  | 1:A:150:PRO:HB3  | 2.09                     | 0.86              |
| 1:A:403:VAL:C    | 1:A:409:MET:CG   | 2.47                     | 0.86              |
| 1:A:475:LEU:HD23 | 1:A:475:LEU:C    | 2.00                     | 0.86              |
| 1:A:795:ARG:HD2  | 3:C:38:ARG:O     | 1.75                     | 0.86              |
| 1:A:234:THR:HG22 | 1:A:236:ARG:H    | 1.41                     | 0.85              |
| 1:A:293:ILE:O    | 1:A:293:ILE:HG13 | 1.75                     | 0.85              |
| 2:B:80:LEU:H     | 2:B:80:LEU:HD23  | 1.39                     | 0.85              |
| 1:A:397:ALA:HB3  | 1:A:609:LEU:HD11 | 1.59                     | 0.85              |
| 1:A:757:THR:OG1  | 1:A:758:THR:N    | 2.08                     | 0.85              |
| 2:B:15:LYS:O     | 2:B:19:GLU:N     | 2.09                     | 0.85              |
| 2:B:85:SER:HB2   | 2:B:88:THR:CG2   | 2.05                     | 0.85              |
| 1:A:398:LEU:HD11 | 1:A:605:ASN:HB3  | 1.59                     | 0.85              |
| 1:A:461:ILE:HD12 | 1:A:462:ALA:N    | 1.92                     | 0.85              |
| 1:A:166:ASP:OD1  | 1:A:166:ASP:C    | 2.19                     | 0.85              |
| 1:A:111:LEU:C    | 1:A:112:ILE:HD12 | 2.00                     | 0.85              |
| 1:A:14:ALA:CB    | 1:A:149:PRO:CB   | 2.55                     | 0.84              |
| 1:A:364:LYS:H    | 1:A:373:GLU:HB3  | 1.42                     | 0.84              |
| 1:A:735:GLY:O    | 1:A:738:VAL:HG23 | 1.76                     | 0.84              |
| 1:A:300:MET:HB2  | 1:A:302:VAL:HG22 | 1.60                     | 0.84              |
| 1:A:389:ILE:HD12 | 1:A:389:ILE:O    | 1.78                     | 0.84              |
| 1:A:598:ASN:HD22 | 1:A:644:THR:HB   | 1.35                     | 0.84              |
| 1:A:778:LEU:HD11 | 3:C:89:ALA:HB1   | 1.58                     | 0.84              |
| 1:A:14:ALA:HB2   | 1:A:149:PRO:HB3  | 1.56                     | 0.84              |
| 1:A:361:MET:O    | 1:A:363:PHE:CE1  | 2.30                     | 0.84              |
| 1:A:552:TYR:HA   | 1:A:556:MET:CB   | 2.06                     | 0.84              |
| 1:A:242:ARG:O    | 1:A:267:LEU:HA   | 1.77                     | 0.84              |
| 1:A:286:TYR:HE2  | 1:A:317:LEU:HA   | 1.40                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:313:ASN:HB2  | 1:A:317:LEU:HD21 | 1.59                     | 0.84              |
| 1:A:805:ARG:CA   | 3:C:21:TRP:HZ2   | 1.89                     | 0.84              |
| 3:C:98:GLN:HA    | 3:C:98:GLN:NE2   | 1.93                     | 0.84              |
| 1:A:512:PHE:O    | 1:A:706:GLY:CA   | 2.26                     | 0.84              |
| 1:A:707:PHE:HB3  | 1:A:708:PRO:CD   | 2.07                     | 0.84              |
| 2:B:145:THR:HG22 | 2:B:146:ALA:N    | 1.92                     | 0.84              |
| 2:B:80:LEU:HD23  | 2:B:80:LEU:N     | 1.93                     | 0.83              |
| 1:A:763:LYS:O    | 1:A:766:VAL:CG2  | 2.26                     | 0.83              |
| 1:A:511:ASP:HA   | 1:A:514:MET:HB2  | 1.59                     | 0.83              |
| 1:A:533:LEU:O    | 1:A:537:CYS:SG   | 2.36                     | 0.83              |
| 1:A:697:LEU:H    | 1:A:697:LEU:CD1  | 1.89                     | 0.83              |
| 3:C:4:SER:OG     | 3:C:7:GLU:HG3    | 1.79                     | 0.83              |
| 1:A:82:PHE:HZ    | 1:A:91:MET:HA    | 1.40                     | 0.82              |
| 1:A:833:VAL:HG22 | 2:B:47:LEU:CD1   | 2.09                     | 0.82              |
| 1:A:530:LEU:HD21 | 1:A:650:ARG:NE   | 1.95                     | 0.82              |
| 1:A:145:LYS:NZ   | 1:A:158:ASN:OD1  | 2.12                     | 0.82              |
| 1:A:124:ASN:O    | 1:A:673:PRO:HG2  | 1.79                     | 0.82              |
| 1:A:284:ILE:CD1  | 1:A:285:PHE:H    | 1.93                     | 0.82              |
| 2:B:24:PHE:HD1   | 2:B:24:PHE:O     | 1.63                     | 0.82              |
| 2:B:135:GLU:HG3  | 2:B:136:GLY:H    | 1.43                     | 0.82              |
| 1:A:11:GLN:C     | 1:A:12:TYR:CD1   | 2.58                     | 0.82              |
| 1:A:697:LEU:HD12 | 1:A:697:LEU:N    | 1.95                     | 0.82              |
| 1:A:507:TRP:HE3  | 1:A:508:GLU:H    | 1.28                     | 0.81              |
| 1:A:722:ILE:HD11 | 1:A:781:ILE:HD12 | 1.63                     | 0.81              |
| 2:B:109:ILE:O    | 2:B:112:LEU:HB2  | 1.80                     | 0.81              |
| 1:A:11:GLN:HB3   | 1:A:12:TYR:CD1   | 2.15                     | 0.81              |
| 2:B:111:ASP:O    | 2:B:115:ASN:ND2  | 2.14                     | 0.81              |
| 1:A:269:LYS:NZ   | 1:A:600:ASP:OD2  | 2.13                     | 0.81              |
| 1:A:242:ARG:NH1  | 1:A:268:GLU:OE1  | 2.13                     | 0.81              |
| 1:A:14:ALA:CB    | 1:A:149:PRO:HB3  | 2.10                     | 0.81              |
| 1:A:174:ILE:HG23 | 1:A:668:VAL:HB   | 1.63                     | 0.81              |
| 2:B:35:VAL:C     | 2:B:67:LEU:HD23  | 2.06                     | 0.81              |
| 2:B:106:ILE:HG22 | 2:B:137:GLY:O    | 1.81                     | 0.80              |
| 1:A:232:ALA:HB1  | 1:A:271:ARG:NH1  | 1.96                     | 0.80              |
| 1:A:14:ALA:CB    | 1:A:149:PRO:CG   | 2.56                     | 0.80              |
| 1:A:78:ASN:ND2   | 1:A:91:MET:HE3   | 1.97                     | 0.80              |
| 1:A:570:ARG:CB   | 1:A:573:GLN:CB   | 2.60                     | 0.80              |
| 1:A:778:LEU:O    | 1:A:782:ILE:HG13 | 1.81                     | 0.80              |
| 1:A:286:TYR:OH   | 1:A:312:ILE:O    | 1.99                     | 0.80              |
| 1:A:287:GLN:HE21 | 1:A:328:PHE:HA   | 1.46                     | 0.80              |
| 1:A:398:LEU:HA   | 1:A:401:PRO:CG   | 2.02                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:807:GLY:HA3  | 2:B:95:MET:HE3   | 1.64                     | 0.80              |
| 2:B:121:ASN:ND2  | 2:B:124:GLU:HG3  | 1.97                     | 0.80              |
| 1:A:59:LYS:HA    | 1:A:66:THR:HG22  | 1.63                     | 0.79              |
| 1:A:521:ASP:HB3  | 1:A:525:LYS:HD3  | 1.63                     | 0.79              |
| 1:A:738:VAL:HG12 | 1:A:738:VAL:O    | 1.80                     | 0.79              |
| 1:A:402:LYS:CB   | 1:A:411:THR:CB   | 2.60                     | 0.79              |
| 1:A:364:LYS:N    | 1:A:373:GLU:HB3  | 1.98                     | 0.79              |
| 1:A:115:TYR:OH   | 1:A:150:PRO:HA   | 1.82                     | 0.79              |
| 1:A:269:LYS:NZ   | 1:A:600:ASP:CG   | 2.41                     | 0.79              |
| 1:A:751:ALA:HA   | 1:A:754:ARG:NH1  | 1.96                     | 0.79              |
| 3:C:131:LEU:HD13 | 3:C:144:PHE:HD1  | 1.48                     | 0.79              |
| 1:A:175:THR:HG22 | 1:A:176:GLY:N    | 1.97                     | 0.79              |
| 1:A:598:ASN:HA   | 1:A:645:ILE:HD12 | 1.63                     | 0.79              |
| 1:A:404:LYS:N    | 1:A:409:MET:HG3  | 1.98                     | 0.79              |
| 1:A:60:ILE:HG21  | 1:A:63:ASP:HB3   | 1.65                     | 0.78              |
| 1:A:512:PHE:O    | 1:A:706:GLY:N    | 2.14                     | 0.78              |
| 1:A:808:LEU:C    | 1:A:808:LEU:HD23 | 2.08                     | 0.78              |
| 2:B:114:GLU:CB   | 2:B:125:MET:HE2  | 2.12                     | 0.78              |
| 1:A:83:GLU:HG2   | 1:A:84:LYS:N     | 1.98                     | 0.78              |
| 1:A:402:LYS:CB   | 1:A:411:THR:CA   | 2.61                     | 0.78              |
| 1:A:402:LYS:CB   | 1:A:411:THR:HA   | 2.13                     | 0.78              |
| 2:B:113:LEU:O    | 2:B:120:PHE:HB2  | 1.83                     | 0.78              |
| 1:A:805:ARG:CA   | 3:C:21:TRP:CZ2   | 2.66                     | 0.78              |
| 1:A:11:GLN:HB3   | 1:A:12:TYR:HD1   | 1.49                     | 0.78              |
| 1:A:133:THR:HG1  | 1:A:135:SER:HG   | 1.28                     | 0.78              |
| 1:A:559:ASN:HD22 | 1:A:560:ARG:N    | 1.81                     | 0.78              |
| 1:A:361:MET:O    | 1:A:363:PHE:HE1  | 1.66                     | 0.78              |
| 2:B:118:ASP:CG   | 3:C:24:ARG:HH21  | 1.91                     | 0.78              |
| 1:A:684:ALA:O    | 1:A:687:VAL:HG23 | 1.83                     | 0.78              |
| 1:A:363:PHE:CA   | 1:A:373:GLU:O    | 2.31                     | 0.78              |
| 1:A:240:SER:OG   | 5:A:999:ANP:O2G  | 2.02                     | 0.77              |
| 1:A:751:ALA:CA   | 1:A:754:ARG:HH12 | 1.97                     | 0.77              |
| 1:A:399:LEU:N    | 1:A:401:PRO:HD2  | 1.97                     | 0.77              |
| 1:A:360:GLU:O    | 1:A:362:LYS:HD2  | 1.84                     | 0.77              |
| 1:A:396:LYS:C    | 1:A:401:PRO:HG3  | 2.08                     | 0.77              |
| 1:A:808:LEU:HD21 | 1:A:812:GLN:OE1  | 1.84                     | 0.77              |
| 1:A:833:VAL:HG12 | 1:A:835:PRO:HD3  | 1.67                     | 0.77              |
| 1:A:384:ALA:HB2  | 1:A:391:ALA:CB   | 2.14                     | 0.77              |
| 1:A:624:ALA:HB1  | 1:A:628:PRO:HG3  | 1.66                     | 0.77              |
| 1:A:223:ASN:HB2  | 1:A:224:PRO:CD   | 2.11                     | 0.77              |
| 2:B:89:ILE:C     | 2:B:91:ASN:H     | 1.93                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:64:PRO:HG2   | 3:C:66:GLU:OE2   | 1.84                     | 0.77              |
| 1:A:49:GLN:HB2   | 1:A:57:THR:HG22  | 1.67                     | 0.77              |
| 1:A:100:LEU:HD22 | 1:A:688:LEU:CD2  | 2.12                     | 0.76              |
| 2:B:147:MET:HE3  | 2:B:151:SER:H    | 1.50                     | 0.76              |
| 1:A:403:VAL:O    | 1:A:410:VAL:O    | 2.03                     | 0.76              |
| 1:A:532:ILE:HA   | 1:A:535:GLU:HG2  | 1.66                     | 0.76              |
| 3:C:144:PHE:O    | 3:C:148:VAL:HG12 | 1.84                     | 0.76              |
| 1:A:410:VAL:CG1  | 1:A:411:THR:N    | 2.48                     | 0.76              |
| 1:A:565:PRO:HA   | 1:A:579:GLU:HG3  | 1.68                     | 0.76              |
| 1:A:798:TYR:OH   | 3:C:14:VAL:HG12  | 1.85                     | 0.76              |
| 1:A:505:ILE:HD12 | 1:A:505:ILE:O    | 1.85                     | 0.76              |
| 3:C:98:GLN:HE21  | 3:C:98:GLN:CA    | 1.96                     | 0.76              |
| 1:A:466:ILE:HG23 | 1:A:587:VAL:HG12 | 1.68                     | 0.76              |
| 1:A:503:GLU:O    | 1:A:505:ILE:HG13 | 1.86                     | 0.76              |
| 2:B:145:THR:CG2  | 2:B:146:ALA:N    | 2.46                     | 0.76              |
| 1:A:85:LEU:HB3   | 1:A:102:ASN:HD21 | 1.49                     | 0.76              |
| 1:A:461:ILE:CG1  | 1:A:462:ALA:N    | 2.48                     | 0.76              |
| 1:A:296:LEU:HD22 | 1:A:299:VAL:CG1  | 2.15                     | 0.76              |
| 1:A:100:LEU:CD2  | 1:A:688:LEU:HD21 | 2.14                     | 0.76              |
| 1:A:256:LYS:CB   | 1:A:257:ILE:HD12 | 2.16                     | 0.76              |
| 1:A:447:ASP:OD2  | 1:A:449:LYS:NZ   | 2.19                     | 0.76              |
| 3:C:40:LEU:HB3   | 3:C:72:TYR:OH    | 1.85                     | 0.76              |
| 1:A:88:MET:HE3   | 1:A:102:ASN:HB3  | 1.68                     | 0.75              |
| 1:A:233:LYS:HD2  | 1:A:238:ASN:HA   | 1.66                     | 0.75              |
| 1:A:459:LEU:HD22 | 1:A:461:ILE:HG22 | 1.68                     | 0.75              |
| 1:A:806:ILE:HG22 | 1:A:807:GLY:H    | 1.51                     | 0.75              |
| 1:A:398:LEU:C    | 1:A:401:PRO:CD   | 2.59                     | 0.75              |
| 1:A:280:ARG:HH11 | 1:A:319:VAL:HG13 | 1.51                     | 0.75              |
| 1:A:790:ARG:HH21 | 3:C:117:LEU:HD23 | 1.52                     | 0.75              |
| 1:A:642:PHE:CG   | 1:A:643:GLN:N    | 2.54                     | 0.75              |
| 3:C:42:ILE:HG22  | 3:C:43:ASN:N     | 2.01                     | 0.75              |
| 1:A:60:ILE:CG2   | 1:A:63:ASP:HB3   | 2.16                     | 0.75              |
| 1:A:521:ASP:O    | 1:A:525:LYS:HG2  | 1.87                     | 0.75              |
| 1:A:767:LEU:O    | 1:A:767:LEU:HD12 | 1.87                     | 0.75              |
| 1:A:237:ASN:HD21 | 5:A:999:ANP:C5'  | 1.98                     | 0.75              |
| 1:A:358:MET:C    | 1:A:360:GLU:H    | 1.93                     | 0.75              |
| 1:A:398:LEU:CA   | 1:A:401:PRO:CD   | 2.65                     | 0.75              |
| 1:A:226:LEU:CD2  | 1:A:439:VAL:HG22 | 2.16                     | 0.75              |
| 1:A:148:ILE:HD12 | 1:A:149:PRO:HD2  | 1.69                     | 0.74              |
| 1:A:397:ALA:C    | 1:A:401:PRO:HG3  | 2.12                     | 0.74              |
| 1:A:376:GLY:C    | 1:A:378:ALA:H    | 1.91                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:32:ASP:OD2   | 7:B:503:HOH:O    | 2.05                     | 0.74              |
| 3:C:33:LEU:O     | 3:C:36:VAL:HG13  | 1.87                     | 0.74              |
| 1:A:11:GLN:C     | 1:A:12:TYR:HD1   | 1.95                     | 0.74              |
| 1:A:398:LEU:HD13 | 1:A:606:VAL:N    | 2.01                     | 0.74              |
| 1:A:642:PHE:CD1  | 1:A:643:GLN:N    | 2.53                     | 0.74              |
| 1:A:415:ASN:ND2  | 1:A:417:ASN:HD21 | 1.85                     | 0.74              |
| 1:A:433:ARG:HH21 | 1:A:602:ILE:CD1  | 2.00                     | 0.74              |
| 1:A:615:GLU:OE1  | 1:A:616:PRO:HD2  | 1.86                     | 0.74              |
| 1:A:112:ILE:HG23 | 1:A:123:VAL:O    | 1.88                     | 0.74              |
| 2:B:143:LYS:HD3  | 2:B:146:ALA:CB   | 2.18                     | 0.74              |
| 1:A:493:PHE:O    | 1:A:497:GLN:HG3  | 1.87                     | 0.74              |
| 1:A:52:LYS:O     | 1:A:52:LYS:HG2   | 1.87                     | 0.73              |
| 2:B:106:ILE:HD12 | 2:B:106:ILE:O    | 1.88                     | 0.73              |
| 2:B:117:GLY:O    | 2:B:119:ASN:ND2  | 2.21                     | 0.73              |
| 3:C:101:ILE:O    | 3:C:139:VAL:HG22 | 1.87                     | 0.73              |
| 1:A:95:ASN:OD1   | 1:A:95:ASN:C     | 2.31                     | 0.73              |
| 1:A:390:ASN:HD22 | 1:A:393:ASP:N    | 1.86                     | 0.73              |
| 3:C:90:PHE:HB3   | 3:C:141:TYR:CD1  | 2.23                     | 0.73              |
| 1:A:559:ASN:HD22 | 1:A:560:ARG:H    | 1.36                     | 0.73              |
| 1:A:403:VAL:O    | 1:A:409:MET:CG   | 2.34                     | 0.73              |
| 1:A:326:GLU:OE1  | 1:A:326:GLU:HA   | 1.89                     | 0.73              |
| 1:A:626:GLU:C    | 1:A:627:GLU:HG3  | 2.11                     | 0.73              |
| 2:B:85:SER:HB2   | 2:B:88:THR:HG22  | 1.70                     | 0.73              |
| 1:A:398:LEU:CB   | 1:A:606:VAL:HG22 | 2.19                     | 0.73              |
| 1:A:515:ASP:HA   | 1:A:518:MET:HB3  | 1.71                     | 0.73              |
| 1:A:29:ASP:OD1   | 1:A:30:GLY:N     | 2.21                     | 0.73              |
| 1:A:386:LEU:HD21 | 7:A:1000:HOH:O   | 1.87                     | 0.73              |
| 1:A:499:GLU:HA   | 1:A:502:LYS:HB3  | 1.70                     | 0.73              |
| 1:A:590:SER:O    | 1:A:594:TRP:CZ2  | 2.42                     | 0.73              |
| 1:A:751:ALA:O    | 1:A:754:ARG:CZ   | 2.36                     | 0.73              |
| 1:A:765:GLY:O    | 1:A:769:ASN:ND2  | 2.22                     | 0.73              |
| 1:A:482:GLU:OE2  | 1:A:582:HIS:HA   | 1.89                     | 0.72              |
| 3:C:122:VAL:O    | 3:C:126:ILE:HG13 | 1.88                     | 0.72              |
| 1:A:530:LEU:HG   | 1:A:650:ARG:HH21 | 1.55                     | 0.72              |
| 1:A:707:PHE:CB   | 1:A:708:PRO:HD2  | 2.10                     | 0.72              |
| 1:A:349:PHE:H    | 1:A:349:PHE:HD2  | 1.34                     | 0.72              |
| 1:A:537:CYS:HB2  | 1:A:595:LEU:HD21 | 1.69                     | 0.72              |
| 1:A:28:PHE:CE1   | 1:A:29:ASP:O     | 2.42                     | 0.72              |
| 1:A:300:MET:O    | 1:A:302:VAL:HG13 | 1.90                     | 0.72              |
| 1:A:399:LEU:N    | 1:A:401:PRO:HD3  | 2.05                     | 0.72              |
| 1:A:403:VAL:O    | 1:A:410:VAL:N    | 2.22                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:415:ASN:CG   | 1:A:417:ASN:ND2  | 2.48                     | 0.72              |
| 1:A:350:LYS:HE2  | 1:A:386:LEU:HA   | 1.72                     | 0.72              |
| 1:A:189:VAL:O    | 1:A:193:LEU:HG   | 1.90                     | 0.72              |
| 1:A:447:ASP:OD1  | 1:A:447:ASP:O    | 2.07                     | 0.72              |
| 3:C:83:PHE:N     | 3:C:149:MET:HE1  | 2.05                     | 0.71              |
| 1:A:234:THR:HG22 | 1:A:236:ARG:N    | 2.05                     | 0.71              |
| 1:A:379:GLU:O    | 1:A:382:LYS:HB2  | 1.90                     | 0.71              |
| 1:A:486:GLN:NE2  | 1:A:517:GLN:HG2  | 2.03                     | 0.71              |
| 3:C:45:ARG:O     | 3:C:48:ASP:HB2   | 1.90                     | 0.71              |
| 1:A:362:LYS:C    | 1:A:363:PHE:CD1  | 2.68                     | 0.71              |
| 2:B:145:THR:HG22 | 2:B:146:ALA:H    | 1.53                     | 0.71              |
| 1:A:81:LYS:HE2   | 1:A:81:LYS:N     | 2.04                     | 0.71              |
| 1:A:784:MET:HE1  | 3:C:79:GLU:HG2   | 1.71                     | 0.71              |
| 1:A:598:ASN:HD21 | 1:A:644:THR:CA   | 2.03                     | 0.71              |
| 1:A:511:ASP:N    | 1:A:514:MET:CB   | 2.54                     | 0.71              |
| 1:A:402:LYS:CA   | 1:A:411:THR:HG23 | 2.21                     | 0.71              |
| 1:A:809:SER:O    | 1:A:813:ARG:HB2  | 1.90                     | 0.71              |
| 1:A:71:LYS:HA    | 1:A:74:ILE:HD12  | 1.73                     | 0.71              |
| 1:A:23:GLU:O     | 1:A:81:LYS:NZ    | 2.24                     | 0.70              |
| 1:A:817:LYS:C    | 1:A:819:LEU:H    | 1.98                     | 0.70              |
| 3:C:109:VAL:HA   | 3:C:113:LEU:HD13 | 1.73                     | 0.70              |
| 1:A:580:LEU:HD23 | 1:A:581:HIS:N    | 2.06                     | 0.70              |
| 1:A:183:THR:OG1  | 7:A:1003:HOH:O   | 2.09                     | 0.70              |
| 1:A:232:ALA:HB1  | 1:A:271:ARG:HH11 | 1.53                     | 0.70              |
| 1:A:379:GLU:HA   | 1:A:382:LYS:HE3  | 1.72                     | 0.70              |
| 1:A:529:ILE:CG1  | 1:A:530:LEU:N    | 2.45                     | 0.70              |
| 2:B:64:PRO:HD2   | 2:B:71:MET:SD    | 2.31                     | 0.70              |
| 1:A:436:ASN:HB3  | 1:A:440:ARG:HH22 | 1.56                     | 0.70              |
| 1:A:250:HIS:O    | 1:A:257:ILE:HG22 | 1.92                     | 0.69              |
| 3:C:7:GLU:HA     | 3:C:10:ASP:OD2   | 1.92                     | 0.69              |
| 1:A:80:PRO:C     | 1:A:82:PHE:H     | 2.00                     | 0.69              |
| 1:A:806:ILE:CG2  | 1:A:807:GLY:N    | 2.55                     | 0.69              |
| 1:A:33:ASN:OD1   | 1:A:47:GLU:HG2   | 1.92                     | 0.69              |
| 1:A:131:ILE:HG13 | 1:A:132:TYR:CZ   | 2.27                     | 0.69              |
| 1:A:400:LYS:CA   | 1:A:414:GLN:HB2  | 2.09                     | 0.69              |
| 1:A:441:ARG:HH12 | 1:A:445:THR:HG23 | 1.57                     | 0.69              |
| 1:A:241:SER:OG   | 7:A:1003:HOH:O   | 2.11                     | 0.69              |
| 2:B:138:LYS:H    | 2:B:138:LYS:HD2  | 1.56                     | 0.69              |
| 1:A:390:ASN:ND2  | 1:A:393:ASP:H    | 1.89                     | 0.69              |
| 1:A:11:GLN:HG2   | 1:A:12:TYR:CE1   | 2.22                     | 0.69              |
| 1:A:266:LEU:HD23 | 1:A:266:LEU:N    | 2.07                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:398:LEU:HD11 | 1:A:605:ASN:CB   | 2.23                     | 0.69              |
| 2:B:44:SER:HG    | 2:B:50:ALA:HA    | 1.57                     | 0.69              |
| 1:A:350:LYS:HE2  | 1:A:386:LEU:O    | 1.93                     | 0.69              |
| 1:A:357:HIS:O    | 1:A:360:GLU:HB2  | 1.92                     | 0.69              |
| 1:A:537:CYS:HB2  | 1:A:595:LEU:CD2  | 2.23                     | 0.69              |
| 1:A:805:ARG:HA   | 3:C:21:TRP:CH2   | 2.28                     | 0.69              |
| 2:B:93:PHE:O     | 2:B:95:MET:N     | 2.26                     | 0.69              |
| 1:A:244:GLY:N    | 1:A:265:TYR:O    | 2.26                     | 0.68              |
| 1:A:266:LEU:HD11 | 1:A:649:HIS:CD2  | 2.28                     | 0.68              |
| 1:A:495:LEU:HD12 | 1:A:498:GLU:CB   | 2.23                     | 0.68              |
| 1:A:537:CYS:CA   | 1:A:595:LEU:HD21 | 2.23                     | 0.68              |
| 1:A:403:VAL:HG23 | 1:A:604:GLU:HB2  | 1.75                     | 0.68              |
| 1:A:532:ILE:C    | 1:A:534:GLU:N    | 2.49                     | 0.68              |
| 1:A:438:LEU:O    | 1:A:442:VAL:HG23 | 1.92                     | 0.68              |
| 1:A:788:HIS:NE2  | 3:C:149:MET:HA   | 2.08                     | 0.68              |
| 1:A:795:ARG:HG3  | 3:C:39:CYS:HA    | 1.75                     | 0.68              |
| 1:A:826:TRP:HZ2  | 2:B:59:MET:O     | 1.76                     | 0.68              |
| 1:A:169:ASN:CB   | 1:A:663:THR:HG22 | 2.24                     | 0.68              |
| 1:A:507:TRP:HH2  | 1:A:763:LYS:CE   | 2.06                     | 0.68              |
| 2:B:145:THR:C    | 2:B:147:MET:N    | 2.48                     | 0.68              |
| 3:C:143:ASP:O    | 3:C:146:LYS:N    | 2.16                     | 0.68              |
| 1:A:197:ALA:HB1  | 1:A:256:LYS:CB   | 2.22                     | 0.68              |
| 1:A:398:LEU:HA   | 1:A:401:PRO:CD   | 2.22                     | 0.68              |
| 3:C:30:ALA:HB3   | 3:C:55:THR:HB    | 1.75                     | 0.68              |
| 1:A:169:ASN:HB3  | 1:A:663:THR:HG22 | 1.74                     | 0.68              |
| 1:A:763:LYS:N    | 1:A:766:VAL:HG21 | 2.09                     | 0.68              |
| 1:A:112:ILE:HD12 | 1:A:112:ILE:N    | 2.09                     | 0.67              |
| 1:A:269:LYS:NZ   | 1:A:600:ASP:OD1  | 2.27                     | 0.67              |
| 1:A:415:ASN:OD1  | 1:A:416:MET:N    | 2.27                     | 0.67              |
| 1:A:717:LYS:O    | 1:A:719:ARG:N    | 2.27                     | 0.67              |
| 1:A:769:ASN:HD22 | 1:A:769:ASN:N    | 1.90                     | 0.67              |
| 1:A:815:ILE:HD11 | 2:B:144:PHE:HE2  | 1.57                     | 0.67              |
| 3:C:107:ARG:O    | 3:C:110:LEU:HD12 | 1.94                     | 0.67              |
| 1:A:753:TYR:C    | 1:A:754:ARG:HD3  | 2.19                     | 0.67              |
| 1:A:763:LYS:O    | 1:A:766:VAL:HG23 | 1.94                     | 0.67              |
| 3:C:8:ILE:O      | 3:C:12:LYS:HG3   | 1.94                     | 0.67              |
| 1:A:269:LYS:HZ2  | 1:A:600:ASP:CG   | 2.02                     | 0.67              |
| 1:A:433:ARG:NH2  | 1:A:602:ILE:CD1  | 2.57                     | 0.67              |
| 1:A:813:ARG:NH2  | 2:B:84:ASP:OD2   | 2.26                     | 0.67              |
| 2:B:27:ILE:HG22  | 2:B:35:VAL:HG11  | 1.75                     | 0.67              |
| 1:A:321:ASN:N    | 1:A:321:ASN:HD22 | 1.92                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:370:GLU:O    | 1:A:371:GLN:NE2  | 2.26                     | 0.67              |
| 1:A:799:LYS:HA   | 1:A:802:GLN:HE21 | 1.58                     | 0.67              |
| 1:A:398:LEU:CA   | 1:A:401:PRO:HD2  | 2.24                     | 0.67              |
| 1:A:763:LYS:C    | 1:A:766:VAL:CG2  | 2.66                     | 0.67              |
| 1:A:54:ASP:HB3   | 1:A:70:LYS:CD    | 2.24                     | 0.67              |
| 1:A:266:LEU:HD11 | 1:A:649:HIS:NE2  | 2.10                     | 0.67              |
| 1:A:397:ALA:O    | 1:A:398:LEU:CD1  | 2.43                     | 0.67              |
| 1:A:466:ILE:HG23 | 1:A:587:VAL:CG1  | 2.25                     | 0.67              |
| 3:C:90:PHE:HB3   | 3:C:141:TYR:HE1  | 1.60                     | 0.67              |
| 1:A:299:VAL:HG13 | 1:A:300:MET:HG2  | 1.77                     | 0.67              |
| 1:A:774:ARG:HG3  | 1:A:774:ARG:HH11 | 1.60                     | 0.67              |
| 1:A:395:LEU:C    | 1:A:399:LEU:HG   | 2.18                     | 0.66              |
| 1:A:555:HIS:CD2  | 1:A:558:LYS:CE   | 2.76                     | 0.66              |
| 1:A:488:PHE:HE1  | 1:A:489:ASN:OD1  | 1.75                     | 0.66              |
| 1:A:819:LEU:HD23 | 1:A:822:ARG:HH21 | 1.60                     | 0.66              |
| 1:A:5:PHE:N      | 1:A:5:PHE:CD2    | 2.63                     | 0.66              |
| 1:A:422:SER:O    | 1:A:425:ALA:HB3  | 1.95                     | 0.66              |
| 1:A:475:LEU:C    | 1:A:475:LEU:CD2  | 2.68                     | 0.66              |
| 1:A:271:ARG:NH2  | 1:A:279:GLU:HG2  | 2.10                     | 0.66              |
| 1:A:798:TYR:O    | 1:A:802:GLN:HG3  | 1.95                     | 0.66              |
| 1:A:11:GLN:CG    | 1:A:12:TYR:HE1   | 2.07                     | 0.66              |
| 1:A:215:LEU:HD12 | 1:A:215:LEU:O    | 1.96                     | 0.66              |
| 1:A:237:ASN:CG   | 5:A:999:ANP:H5'2 | 2.20                     | 0.66              |
| 1:A:441:ARG:NH1  | 1:A:445:THR:HG23 | 2.11                     | 0.66              |
| 1:A:743:LEU:C    | 1:A:748:MET:SD   | 2.79                     | 0.66              |
| 2:B:53:ASP:CG    | 2:B:54:LYS:H     | 2.04                     | 0.66              |
| 1:A:691:LEU:HA   | 1:A:694:ASN:HD21 | 1.61                     | 0.66              |
| 1:A:410:VAL:HG13 | 1:A:411:THR:H    | 1.60                     | 0.66              |
| 1:A:469:PHE:C    | 1:A:470:ASN:HD22 | 2.04                     | 0.66              |
| 1:A:607:VAL:O    | 1:A:610:LEU:N    | 2.28                     | 0.66              |
| 3:C:71:ALA:O     | 3:C:72:TYR:C     | 2.37                     | 0.66              |
| 3:C:99:GLY:C     | 3:C:100:PHE:HD2  | 2.04                     | 0.66              |
| 1:A:112:ILE:O    | 1:A:122:ALA:HA   | 1.95                     | 0.65              |
| 1:A:461:ILE:HG13 | 1:A:462:ALA:N    | 2.11                     | 0.65              |
| 1:A:792:TYR:HE1  | 3:C:128:LEU:HD13 | 1.61                     | 0.65              |
| 1:A:806:ILE:HG22 | 1:A:807:GLY:N    | 2.10                     | 0.65              |
| 2:B:143:LYS:HA   | 2:B:146:ALA:HB3  | 1.77                     | 0.65              |
| 1:A:440:ARG:NH1  | 1:A:440:ARG:HB2  | 2.10                     | 0.65              |
| 1:A:532:ILE:HG12 | 1:A:535:GLU:OE2  | 1.95                     | 0.65              |
| 1:A:252:GLY:O    | 1:A:253:PRO:C    | 2.33                     | 0.65              |
| 1:A:402:LYS:CB   | 1:A:411:THR:HG23 | 2.27                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:284:ILE:O    | 1:A:287:GLN:HG2  | 1.95                     | 0.65              |
| 1:A:402:LYS:CB   | 1:A:410:VAL:O    | 2.45                     | 0.65              |
| 2:B:24:PHE:O     | 2:B:24:PHE:CD1   | 2.49                     | 0.65              |
| 1:A:341:THR:HB   | 1:A:343:GLU:HG2  | 1.79                     | 0.65              |
| 2:B:43:ILE:HD12  | 2:B:46:GLN:HB3   | 1.79                     | 0.65              |
| 1:A:343:GLU:O    | 1:A:347:SER:OG   | 2.15                     | 0.65              |
| 1:A:569:THR:O    | 1:A:570:ARG:C    | 2.39                     | 0.65              |
| 1:A:166:ASP:OD1  | 1:A:166:ASP:O    | 2.15                     | 0.65              |
| 1:A:175:THR:HG22 | 1:A:176:GLY:H    | 1.60                     | 0.65              |
| 1:A:175:THR:CG2  | 1:A:176:GLY:N    | 2.60                     | 0.65              |
| 1:A:235:THR:N    | 1:A:279:GLU:OE1  | 2.24                     | 0.64              |
| 1:A:254:THR:O    | 1:A:254:THR:HG23 | 1.96                     | 0.64              |
| 1:A:537:CYS:O    | 1:A:595:LEU:HD21 | 1.97                     | 0.64              |
| 1:A:54:ASP:HB3   | 1:A:70:LYS:HD3   | 1.78                     | 0.64              |
| 1:A:415:ASN:ND2  | 1:A:417:ASN:ND2  | 2.45                     | 0.64              |
| 1:A:531:SER:O    | 1:A:535:GLU:HB3  | 1.96                     | 0.64              |
| 1:A:694:ASN:N    | 1:A:694:ASN:ND2  | 2.10                     | 0.64              |
| 1:A:722:ILE:HD12 | 1:A:778:LEU:HD13 | 1.78                     | 0.64              |
| 1:A:818:TRP:CD1  | 2:B:148:ILE:O    | 2.51                     | 0.64              |
| 1:A:415:ASN:CG   | 1:A:417:ASN:HD21 | 2.04                     | 0.64              |
| 3:C:42:ILE:CG2   | 3:C:44:PRO:HD3   | 2.24                     | 0.64              |
| 1:A:175:THR:CG2  | 1:A:176:GLY:H    | 2.11                     | 0.64              |
| 1:A:190:ILE:HD13 | 1:A:247:ILE:HD13 | 1.80                     | 0.64              |
| 1:A:341:THR:CB   | 1:A:343:GLU:HG2  | 2.28                     | 0.64              |
| 1:A:488:PHE:CD1  | 1:A:488:PHE:C    | 2.76                     | 0.64              |
| 2:B:98:GLU:H     | 2:B:98:GLU:CD    | 2.04                     | 0.64              |
| 1:A:80:PRO:O     | 1:A:82:PHE:N     | 2.31                     | 0.64              |
| 1:A:717:LYS:C    | 1:A:719:ARG:H    | 2.06                     | 0.64              |
| 1:A:806:ILE:HG22 | 2:B:95:MET:HE1   | 1.79                     | 0.64              |
| 2:B:40:ILE:O     | 2:B:42:ALA:N     | 2.30                     | 0.64              |
| 1:A:244:GLY:O    | 1:A:265:TYR:N    | 2.31                     | 0.64              |
| 1:A:507:TRP:CH2  | 1:A:763:LYS:HE2  | 2.32                     | 0.64              |
| 1:A:229:TYR:OH   | 1:A:348:MET:HE3  | 1.97                     | 0.64              |
| 1:A:170:GLN:OE1  | 1:A:664:HIS:HB3  | 1.97                     | 0.64              |
| 1:A:308:LEU:N    | 7:A:1004:HOH:O   | 2.31                     | 0.64              |
| 1:A:471:SER:OG   | 1:A:594:TRP:CE2  | 2.51                     | 0.64              |
| 1:A:471:SER:OG   | 1:A:594:TRP:HZ2  | 1.55                     | 0.64              |
| 1:A:507:TRP:CH2  | 1:A:763:LYS:CE   | 2.81                     | 0.64              |
| 1:A:417:ASN:ND2  | 1:A:418:GLN:H    | 1.95                     | 0.63              |
| 1:A:514:MET:HE3  | 1:A:514:MET:HA   | 1.80                     | 0.63              |
| 2:B:145:THR:C    | 2:B:147:MET:H    | 2.05                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:124:ASN:C    | 1:A:124:ASN:OD1  | 2.40                     | 0.63              |
| 1:A:266:LEU:HD23 | 1:A:266:LEU:H    | 1.62                     | 0.63              |
| 1:A:799:LYS:HA   | 1:A:802:GLN:NE2  | 2.13                     | 0.63              |
| 1:A:438:LEU:C    | 1:A:438:LEU:CD2  | 2.71                     | 0.63              |
| 1:A:778:LEU:HD11 | 3:C:89:ALA:CB    | 2.29                     | 0.63              |
| 1:A:833:VAL:HG22 | 2:B:47:LEU:HD12  | 1.80                     | 0.63              |
| 3:C:15:PHE:CD1   | 3:C:15:PHE:C     | 2.76                     | 0.63              |
| 1:A:384:ALA:HA   | 1:A:389:ILE:CD1  | 2.27                     | 0.63              |
| 1:A:404:LYS:CB   | 1:A:409:MET:HE2  | 2.28                     | 0.63              |
| 1:A:822:ARG:HA   | 1:A:827:TRP:HD1  | 1.62                     | 0.63              |
| 2:B:49:ARG:HD3   | 2:B:50:ALA:N     | 2.13                     | 0.63              |
| 3:C:9:ASP:C      | 3:C:11:LEU:H     | 2.05                     | 0.63              |
| 1:A:398:LEU:HA   | 1:A:401:PRO:HD2  | 1.80                     | 0.63              |
| 3:C:18:PHE:C     | 3:C:20:PHE:N     | 2.51                     | 0.63              |
| 1:A:286:TYR:CE2  | 1:A:317:LEU:HA   | 2.29                     | 0.63              |
| 1:A:617:LEU:O    | 1:A:621:LEU:HG   | 1.97                     | 0.63              |
| 1:A:743:LEU:O    | 1:A:748:MET:SD   | 2.57                     | 0.63              |
| 1:A:805:ARG:CB   | 3:C:21:TRP:HZ2   | 2.10                     | 0.63              |
| 1:A:807:GLY:H    | 2:B:95:MET:HE1   | 1.61                     | 0.63              |
| 2:B:90:ARG:HB2   | 2:B:145:THR:HG21 | 1.79                     | 0.63              |
| 1:A:475:LEU:HD23 | 1:A:475:LEU:O    | 1.97                     | 0.63              |
| 1:A:744:ALA:C    | 1:A:746:LEU:H    | 2.07                     | 0.63              |
| 2:B:29:VAL:O     | 2:B:30:ASP:C     | 2.42                     | 0.63              |
| 3:C:63:LEU:HD22  | 3:C:67:GLU:OE2   | 1.99                     | 0.63              |
| 3:C:140:LYS:HE2  | 3:C:140:LYS:O    | 1.99                     | 0.63              |
| 1:A:245:LYS:O    | 1:A:459:LEU:HD23 | 1.99                     | 0.63              |
| 1:A:364:LYS:CB   | 1:A:373:GLU:CG   | 2.75                     | 0.63              |
| 2:B:28:ASP:OD2   | 2:B:31:ARG:CA    | 2.46                     | 0.62              |
| 2:B:135:GLU:HA   | 2:B:135:GLU:OE2  | 1.99                     | 0.62              |
| 1:A:384:ALA:HB2  | 1:A:391:ALA:N    | 2.14                     | 0.62              |
| 1:A:455:TYR:OH   | 1:A:659:ASN:HB3  | 1.99                     | 0.62              |
| 1:A:490:HIS:O    | 1:A:494:ILE:HG12 | 1.99                     | 0.62              |
| 3:C:18:PHE:C     | 3:C:20:PHE:H     | 2.05                     | 0.62              |
| 1:A:286:TYR:CZ   | 1:A:312:ILE:O    | 2.51                     | 0.62              |
| 1:A:397:ALA:HB1  | 1:A:605:ASN:ND2  | 2.14                     | 0.62              |
| 1:A:126:TYR:CD1  | 1:A:677:LYS:HA   | 2.33                     | 0.62              |
| 1:A:293:ILE:O    | 1:A:293:ILE:CG1  | 2.46                     | 0.62              |
| 1:A:440:ARG:HB2  | 1:A:440:ARG:HH11 | 1.65                     | 0.62              |
| 1:A:722:ILE:HG12 | 1:A:722:ILE:O    | 1.96                     | 0.62              |
| 1:A:735:GLY:C    | 1:A:737:THR:H    | 2.06                     | 0.62              |
| 2:B:30:ASP:OD2   | 2:B:39:ASP:OD2   | 2.17                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:107:GLU:O    | 2:B:111:ASP:HB2  | 2.00                     | 0.62              |
| 2:B:108:TYR:O    | 2:B:111:ASP:HB3  | 1.99                     | 0.62              |
| 3:C:42:ILE:CG2   | 3:C:43:ASN:N     | 2.61                     | 0.62              |
| 3:C:83:PHE:HA    | 3:C:149:MET:HE1  | 1.80                     | 0.62              |
| 1:A:78:ASN:HD21  | 1:A:91:MET:HE3   | 1.63                     | 0.62              |
| 1:A:152:LEU:HD12 | 1:A:152:LEU:O    | 1.98                     | 0.62              |
| 1:A:486:GLN:HE22 | 1:A:517:GLN:HG2  | 1.63                     | 0.62              |
| 1:A:594:TRP:HA   | 1:A:597:LYS:HB3  | 1.80                     | 0.62              |
| 1:A:792:TYR:CD1  | 1:A:792:TYR:C    | 2.78                     | 0.62              |
| 1:A:403:VAL:HG13 | 1:A:404:LYS:N    | 2.15                     | 0.62              |
| 1:A:404:LYS:HA   | 1:A:409:MET:HG3  | 1.80                     | 0.62              |
| 3:C:84:ALA:O     | 3:C:87:MET:N     | 2.30                     | 0.62              |
| 1:A:293:ILE:CD1  | 1:A:296:LEU:HD12 | 2.27                     | 0.62              |
| 1:A:537:CYS:CB   | 1:A:595:LEU:HD21 | 2.30                     | 0.62              |
| 1:A:387:CYS:HB2  | 1:A:389:ILE:HG13 | 1.81                     | 0.62              |
| 1:A:403:VAL:HG22 | 1:A:404:LYS:H    | 1.63                     | 0.62              |
| 1:A:410:VAL:HG12 | 1:A:411:THR:N    | 2.15                     | 0.62              |
| 1:A:398:LEU:HD22 | 1:A:606:VAL:HG23 | 1.81                     | 0.62              |
| 1:A:397:ALA:HB3  | 1:A:609:LEU:CD1  | 2.29                     | 0.62              |
| 1:A:669:ARG:NH1  | 1:A:694:ASN:HB2  | 2.15                     | 0.62              |
| 1:A:805:ARG:HB2  | 3:C:21:TRP:HZ2   | 1.65                     | 0.62              |
| 1:A:426:LEU:HG   | 1:A:427:ALA:N    | 2.15                     | 0.61              |
| 2:B:36:SER:N     | 2:B:39:ASP:HB3   | 2.15                     | 0.61              |
| 1:A:164:VAL:HG12 | 1:A:165:THR:N    | 2.14                     | 0.61              |
| 1:A:275:GLN:HB2  | 1:A:314:GLN:HB2  | 1.81                     | 0.61              |
| 2:B:145:THR:HA   | 2:B:148:ILE:HG22 | 1.81                     | 0.61              |
| 3:C:135:LEU:HD12 | 3:C:135:LEU:N    | 2.08                     | 0.61              |
| 3:C:33:LEU:C     | 3:C:33:LEU:HD23  | 2.25                     | 0.61              |
| 1:A:404:LYS:CA   | 1:A:409:MET:HG3  | 2.29                     | 0.61              |
| 1:A:604:GLU:O    | 1:A:607:VAL:HB   | 2.00                     | 0.61              |
| 1:A:744:ALA:O    | 1:A:746:LEU:N    | 2.28                     | 0.61              |
| 1:A:8:PRO:HG2    | 1:A:9:ASP:H      | 1.65                     | 0.61              |
| 1:A:190:ILE:HD11 | 1:A:247:ILE:HG21 | 1.81                     | 0.61              |
| 1:A:296:LEU:CA   | 1:A:299:VAL:HG12 | 2.29                     | 0.61              |
| 3:C:36:VAL:HG21  | 3:C:68:PHE:CZ    | 2.35                     | 0.61              |
| 1:A:738:VAL:O    | 1:A:738:VAL:CG1  | 2.48                     | 0.61              |
| 1:A:376:GLY:C    | 1:A:378:ALA:N    | 2.59                     | 0.61              |
| 1:A:384:ALA:CB   | 1:A:391:ALA:H    | 2.13                     | 0.61              |
| 1:A:429:SER:O    | 1:A:433:ARG:HG3  | 2.00                     | 0.61              |
| 3:C:36:VAL:HG11  | 3:C:68:PHE:HZ    | 1.64                     | 0.61              |
| 3:C:131:LEU:HD13 | 3:C:144:PHE:CD1  | 2.33                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:169:ASN:HB2  | 1:A:662:SER:O    | 2.00                     | 0.61              |
| 1:A:441:ARG:HH12 | 1:A:445:THR:CG2  | 2.12                     | 0.61              |
| 3:C:86:TYR:HB3   | 3:C:145:VAL:HG11 | 1.83                     | 0.61              |
| 1:A:217:ASP:O    | 1:A:221:GLN:HG2  | 2.00                     | 0.61              |
| 1:A:766:VAL:C    | 1:A:768:GLY:H    | 2.09                     | 0.61              |
| 1:A:801:LEU:HD21 | 3:C:21:TRP:NE1   | 2.16                     | 0.61              |
| 1:A:488:PHE:HD1  | 1:A:489:ASN:CG   | 2.09                     | 0.60              |
| 1:A:488:PHE:HD1  | 1:A:489:ASN:OD1  | 1.81                     | 0.60              |
| 1:A:232:ALA:CB   | 1:A:271:ARG:NH1  | 2.64                     | 0.60              |
| 1:A:313:ASN:CB   | 1:A:317:LEU:HD21 | 2.31                     | 0.60              |
| 1:A:354:SER:O    | 1:A:358:MET:HG2  | 2.01                     | 0.60              |
| 1:A:404:LYS:HA   | 1:A:409:MET:CA   | 2.30                     | 0.60              |
| 2:B:29:VAL:C     | 2:B:31:ARG:N     | 2.55                     | 0.60              |
| 1:A:14:ALA:HB3   | 1:A:149:PRO:HG3  | 1.78                     | 0.60              |
| 1:A:801:LEU:HD22 | 3:C:17:LEU:HD11  | 1.82                     | 0.60              |
| 2:B:27:ILE:CG2   | 2:B:35:VAL:HG11  | 2.31                     | 0.60              |
| 3:C:40:LEU:HD12  | 3:C:72:TYR:CE1   | 2.36                     | 0.60              |
| 1:A:535:GLU:CG   | 1:A:536:GLU:N    | 2.64                     | 0.60              |
| 1:A:571:PRO:C    | 1:A:573:GLN:H    | 2.09                     | 0.60              |
| 2:B:24:PHE:HE2   | 2:B:69:PHE:HA    | 1.66                     | 0.60              |
| 2:B:35:VAL:O     | 2:B:67:LEU:HD23  | 2.01                     | 0.60              |
| 2:B:40:ILE:C     | 2:B:42:ALA:H     | 2.10                     | 0.60              |
| 2:B:142:VAL:CG1  | 2:B:143:LYS:HZ3  | 2.13                     | 0.60              |
| 1:A:323:ASP:OD1  | 1:A:325:VAL:HG22 | 2.00                     | 0.60              |
| 1:A:425:ALA:O    | 1:A:429:SER:HB3  | 2.01                     | 0.60              |
| 3:C:94:ASP:OD1   | 3:C:99:GLY:N     | 2.34                     | 0.60              |
| 3:C:108:HIS:ND1  | 3:C:112:ALA:HB3  | 2.16                     | 0.60              |
| 1:A:245:LYS:HB2  | 7:A:1002:HOH:O   | 2.01                     | 0.60              |
| 1:A:358:MET:HE1  | 1:A:426:LEU:HD11 | 1.83                     | 0.60              |
| 1:A:399:LEU:H    | 1:A:401:PRO:CD   | 2.09                     | 0.60              |
| 1:A:537:CYS:HA   | 1:A:595:LEU:HD11 | 1.84                     | 0.60              |
| 1:A:398:LEU:HD11 | 1:A:605:ASN:ND2  | 2.17                     | 0.60              |
| 1:A:353:ALA:CA   | 1:A:356:LEU:HD12 | 2.27                     | 0.60              |
| 1:A:143:LYS:HE3  | 1:A:143:LYS:HA   | 1.83                     | 0.60              |
| 1:A:469:PHE:C    | 1:A:470:ASN:ND2  | 2.60                     | 0.60              |
| 1:A:598:ASN:ND2  | 1:A:644:THR:OG1  | 2.32                     | 0.60              |
| 1:A:137:ILE:HG12 | 1:A:153:PHE:CE2  | 2.37                     | 0.60              |
| 1:A:275:GLN:NE2  | 1:A:281:ASN:HD22 | 2.00                     | 0.60              |
| 1:A:361:MET:O    | 1:A:363:PHE:CD1  | 2.55                     | 0.60              |
| 1:A:397:ALA:CA   | 1:A:401:PRO:CB   | 2.79                     | 0.60              |
| 1:A:423:VAL:HG13 | 1:A:424:GLY:N    | 2.17                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:535:GLU:CG   | 1:A:536:GLU:H    | 2.14                     | 0.60              |
| 1:A:691:LEU:C    | 1:A:694:ASN:HD21 | 2.10                     | 0.60              |
| 1:A:751:ALA:CA   | 1:A:754:ARG:NH1  | 2.60                     | 0.60              |
| 2:B:79:LYS:C     | 2:B:81:SER:H     | 2.09                     | 0.60              |
| 1:A:160:TYR:O    | 1:A:161:GLN:C    | 2.44                     | 0.59              |
| 1:A:534:GLU:CD   | 1:A:650:ARG:HH22 | 2.10                     | 0.59              |
| 3:C:3:LEU:HB2    | 3:C:7:GLU:OE1    | 2.02                     | 0.59              |
| 3:C:107:ARG:HD3  | 3:C:122:VAL:HG11 | 1.83                     | 0.59              |
| 1:A:141:ARG:HH12 | 1:A:196:VAL:HB   | 1.60                     | 0.59              |
| 1:A:274:TYR:CD1  | 1:A:275:GLN:N    | 2.70                     | 0.59              |
| 1:A:325:VAL:HG23 | 1:A:326:GLU:N    | 2.17                     | 0.59              |
| 1:A:342:LYS:HG2  | 1:A:346:GLN:HE21 | 1.66                     | 0.59              |
| 1:A:400:LYS:N    | 1:A:401:PRO:HD2  | 2.12                     | 0.59              |
| 1:A:512:PHE:C    | 1:A:706:GLY:HA3  | 2.26                     | 0.59              |
| 1:A:814:ASN:N    | 1:A:814:ASN:HD22 | 2.00                     | 0.59              |
| 1:A:471:SER:HG   | 1:A:594:TRP:HZ2  | 0.72                     | 0.59              |
| 2:B:68:ASN:N     | 2:B:68:ASN:HD22  | 2.00                     | 0.59              |
| 1:A:792:TYR:CD1  | 1:A:792:TYR:O    | 2.55                     | 0.59              |
| 3:C:42:ILE:HG22  | 3:C:44:PRO:CD    | 2.27                     | 0.59              |
| 3:C:64:PRO:CG    | 3:C:66:GLU:OE2   | 2.50                     | 0.59              |
| 3:C:101:ILE:O    | 3:C:139:VAL:CG2  | 2.50                     | 0.59              |
| 1:A:789:ILE:HG23 | 3:C:125:ILE:HG12 | 1.85                     | 0.59              |
| 1:A:477:ILE:O    | 1:A:481:ASN:ND2  | 2.35                     | 0.59              |
| 3:C:17:LEU:O     | 3:C:21:TRP:CD1   | 2.55                     | 0.59              |
| 1:A:24:GLN:HA    | 1:A:81:LYS:HD2   | 1.85                     | 0.59              |
| 1:A:296:LEU:C    | 1:A:299:VAL:HG12 | 2.27                     | 0.59              |
| 1:A:55:GLU:O     | 1:A:56:ILE:HD13  | 2.03                     | 0.59              |
| 1:A:233:LYS:O    | 1:A:279:GLU:HG3  | 2.03                     | 0.59              |
| 1:A:517:GLN:O    | 1:A:517:GLN:NE2  | 2.36                     | 0.58              |
| 1:A:720:TYR:OH   | 1:A:771:GLU:HG2  | 2.03                     | 0.58              |
| 3:C:17:LEU:CD1   | 3:C:21:TRP:HE1   | 2.16                     | 0.58              |
| 1:A:496:GLU:OE2  | 1:A:710:ARG:NH2  | 2.37                     | 0.58              |
| 1:A:777:ARG:NH1  | 1:A:780:LYS:HD3  | 2.17                     | 0.58              |
| 2:B:24:PHE:HA    | 2:B:27:ILE:HD12  | 1.84                     | 0.58              |
| 1:A:240:SER:CB   | 5:A:999:ANP:O2G  | 2.51                     | 0.58              |
| 1:A:532:ILE:C    | 1:A:534:GLU:H    | 2.12                     | 0.58              |
| 3:C:28:VAL:HG22  | 3:C:29:ASP:H     | 1.69                     | 0.58              |
| 1:A:28:PHE:CD1   | 1:A:29:ASP:O     | 2.57                     | 0.58              |
| 1:A:158:ASN:HA   | 1:A:161:GLN:HB2  | 1.84                     | 0.58              |
| 1:A:739:SER:O    | 1:A:740:GLU:C    | 2.45                     | 0.58              |
| 1:A:801:LEU:O    | 1:A:801:LEU:HD23 | 2.02                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:37:CYS:O     | 3:C:42:ILE:HB    | 2.03                     | 0.58              |
| 3:C:83:PHE:CA    | 3:C:149:MET:HE1  | 2.33                     | 0.58              |
| 1:A:343:GLU:CD   | 1:A:343:GLU:H    | 2.11                     | 0.58              |
| 1:A:674:ASN:ND2  | 1:A:681:LEU:HB3  | 2.18                     | 0.58              |
| 1:A:766:VAL:C    | 1:A:768:GLY:N    | 2.56                     | 0.58              |
| 2:B:44:SER:OG    | 2:B:50:ALA:CA    | 2.42                     | 0.58              |
| 2:B:89:ILE:C     | 2:B:91:ASN:N     | 2.57                     | 0.58              |
| 3:C:3:LEU:H      | 3:C:3:LEU:HD23   | 1.68                     | 0.58              |
| 1:A:288:ILE:HD12 | 1:A:352:THR:CG2  | 2.34                     | 0.58              |
| 1:A:455:TYR:CD1  | 1:A:455:TYR:C    | 2.82                     | 0.58              |
| 1:A:799:LYS:CA   | 1:A:802:GLN:HE21 | 2.17                     | 0.58              |
| 2:B:67:LEU:N     | 2:B:67:LEU:CD1   | 2.66                     | 0.58              |
| 3:C:28:VAL:HG22  | 3:C:29:ASP:N     | 2.18                     | 0.58              |
| 3:C:145:VAL:O    | 3:C:149:MET:HB2  | 2.04                     | 0.58              |
| 1:A:78:ASN:OD1   | 1:A:92:THR:HB    | 2.03                     | 0.58              |
| 1:A:145:LYS:HB2  | 1:A:145:LYS:HZ3  | 1.68                     | 0.58              |
| 1:A:166:ASP:OD1  | 1:A:168:GLU:HG2  | 2.04                     | 0.58              |
| 1:A:459:LEU:HD22 | 1:A:461:ILE:CG2  | 2.34                     | 0.58              |
| 1:A:598:ASN:ND2  | 1:A:644:THR:CA   | 2.63                     | 0.58              |
| 1:A:769:ASN:HD22 | 1:A:769:ASN:H    | 1.50                     | 0.58              |
| 1:A:515:ASP:HA   | 1:A:518:MET:CB   | 2.34                     | 0.58              |
| 1:A:808:LEU:HD23 | 1:A:809:SER:N    | 2.17                     | 0.58              |
| 2:B:90:ARG:O     | 2:B:90:ARG:HG2   | 2.04                     | 0.58              |
| 1:A:94:LEU:HD12  | 1:A:94:LEU:O     | 2.03                     | 0.58              |
| 1:A:379:GLU:O    | 1:A:382:LYS:CB   | 2.52                     | 0.58              |
| 1:A:720:TYR:HB3  | 1:A:723:LEU:CD1  | 2.30                     | 0.58              |
| 2:B:87:GLU:OE1   | 2:B:87:GLU:HA    | 2.03                     | 0.58              |
| 1:A:121:ILE:O    | 1:A:121:ILE:HG22 | 2.04                     | 0.57              |
| 1:A:221:GLN:O    | 1:A:224:PRO:HD2  | 2.04                     | 0.57              |
| 1:A:225:VAL:HG11 | 1:A:438:LEU:HD21 | 1.86                     | 0.57              |
| 1:A:384:ALA:HB2  | 1:A:391:ALA:H    | 1.68                     | 0.57              |
| 1:A:396:LYS:O    | 1:A:401:PRO:CG   | 2.45                     | 0.57              |
| 1:A:398:LEU:HD13 | 1:A:606:VAL:CA   | 2.33                     | 0.57              |
| 1:A:410:VAL:CG1  | 1:A:411:THR:H    | 2.16                     | 0.57              |
| 1:A:642:PHE:CZ   | 1:A:643:GLN:O    | 2.57                     | 0.57              |
| 1:A:719:ARG:HH21 | 1:A:771:GLU:CD   | 2.12                     | 0.57              |
| 1:A:739:SER:C    | 1:A:741:LYS:N    | 2.58                     | 0.57              |
| 2:B:121:ASN:HD21 | 2:B:124:GLU:HG3  | 1.66                     | 0.57              |
| 3:C:15:PHE:C     | 3:C:15:PHE:HD1   | 2.12                     | 0.57              |
| 1:A:287:GLN:HE21 | 1:A:328:PHE:CA   | 2.16                     | 0.57              |
| 1:A:515:ASP:OD1  | 1:A:560:ARG:NH2  | 2.38                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:580:LEU:HD23 | 1:A:581:HIS:H    | 1.68                     | 0.57              |
| 1:A:582:HIS:C    | 1:A:584:ALA:H    | 2.12                     | 0.57              |
| 1:A:789:ILE:HG12 | 3:C:148:VAL:HG21 | 1.85                     | 0.57              |
| 1:A:313:ASN:OD1  | 1:A:313:ASN:O    | 2.22                     | 0.57              |
| 2:B:145:THR:O    | 2:B:147:MET:N    | 2.37                     | 0.57              |
| 3:C:109:VAL:O    | 3:C:113:LEU:HD13 | 2.04                     | 0.57              |
| 1:A:56:ILE:HB    | 1:A:69:VAL:HG23  | 1.87                     | 0.57              |
| 2:B:111:ASP:OD1  | 2:B:115:ASN:ND2  | 2.36                     | 0.57              |
| 1:A:596:GLU:HG3  | 1:A:597:LYS:N    | 2.20                     | 0.57              |
| 1:A:725:PRO:HG2  | 3:C:85:ASP:OD1   | 2.05                     | 0.57              |
| 2:B:105:ASN:HB3  | 2:B:108:TYR:HB2  | 1.85                     | 0.57              |
| 3:C:84:ALA:O     | 3:C:85:ASP:C     | 2.48                     | 0.57              |
| 3:C:99:GLY:C     | 3:C:141:TYR:HE2  | 2.13                     | 0.57              |
| 1:A:88:MET:HE1   | 1:A:99:VAL:HA    | 1.85                     | 0.57              |
| 1:A:174:ILE:HG23 | 1:A:668:VAL:CB   | 2.34                     | 0.57              |
| 1:A:517:GLN:NE2  | 1:A:521:ASP:OD2  | 2.37                     | 0.57              |
| 2:B:139:PHE:CD1  | 2:B:139:PHE:C    | 2.82                     | 0.57              |
| 1:A:36:VAL:CG1   | 1:A:37:PRO:HD2   | 2.35                     | 0.57              |
| 1:A:363:PHE:HE2  | 1:A:399:LEU:HD22 | 1.69                     | 0.57              |
| 1:A:696:VAL:HG13 | 1:A:697:LEU:N    | 2.19                     | 0.57              |
| 1:A:774:ARG:HG3  | 1:A:774:ARG:NH1  | 2.17                     | 0.57              |
| 1:A:805:ARG:HB2  | 3:C:21:TRP:CZ2   | 2.39                     | 0.57              |
| 1:A:124:ASN:HB2  | 1:A:180:ALA:O    | 2.04                     | 0.57              |
| 1:A:133:THR:OG1  | 1:A:135:SER:OG   | 2.12                     | 0.57              |
| 1:A:833:VAL:CG2  | 2:B:47:LEU:HD12  | 2.35                     | 0.57              |
| 2:B:121:ASN:O    | 2:B:124:GLU:HB2  | 2.04                     | 0.57              |
| 1:A:287:GLN:NE2  | 1:A:328:PHE:HA   | 2.18                     | 0.57              |
| 1:A:395:LEU:HD22 | 1:A:399:LEU:HD11 | 1.87                     | 0.57              |
| 3:C:7:GLU:C      | 3:C:9:ASP:N      | 2.62                     | 0.57              |
| 1:A:336:ASP:C    | 1:A:338:LEU:H    | 2.13                     | 0.57              |
| 1:A:416:MET:O    | 1:A:420:VAL:HG23 | 2.04                     | 0.57              |
| 1:A:537:CYS:HB2  | 1:A:595:LEU:CG   | 2.34                     | 0.57              |
| 2:B:27:ILE:HG22  | 2:B:35:VAL:CG1   | 2.34                     | 0.57              |
| 2:B:126:ARG:O    | 2:B:130:LYS:HB2  | 2.04                     | 0.57              |
| 3:C:3:LEU:HD11   | 3:C:8:ILE:HD13   | 1.86                     | 0.57              |
| 1:A:88:MET:HE3   | 1:A:102:ASN:CB   | 2.33                     | 0.56              |
| 1:A:801:LEU:HD23 | 1:A:801:LEU:C    | 2.30                     | 0.56              |
| 1:A:11:GLN:CG    | 1:A:12:TYR:CE1   | 2.84                     | 0.56              |
| 1:A:113:TYR:HA   | 1:A:121:ILE:O    | 2.05                     | 0.56              |
| 1:A:183:THR:OG1  | 5:A:999:ANP:O2B  | 2.23                     | 0.56              |
| 1:A:345:LYS:O    | 1:A:349:PHE:CE2  | 2.58                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:423:VAL:CG1  | 1:A:424:GLY:N    | 2.68                     | 0.56              |
| 1:A:507:TRP:HH2  | 1:A:763:LYS:HE3  | 1.68                     | 0.56              |
| 1:A:532:ILE:O    | 1:A:535:GLU:N    | 2.38                     | 0.56              |
| 1:A:398:LEU:HB2  | 1:A:606:VAL:HG22 | 1.86                     | 0.56              |
| 1:A:517:GLN:O    | 1:A:521:ASP:HB2  | 2.05                     | 0.56              |
| 1:A:817:LYS:HA   | 1:A:820:VAL:HG23 | 1.87                     | 0.56              |
| 1:A:11:GLN:CB    | 1:A:12:TYR:CD1   | 2.88                     | 0.56              |
| 1:A:397:ALA:C    | 1:A:398:LEU:HG   | 2.28                     | 0.56              |
| 1:A:397:ALA:HA   | 1:A:401:PRO:HB3  | 1.87                     | 0.56              |
| 1:A:472:PHE:O    | 1:A:473:GLU:C    | 2.45                     | 0.56              |
| 1:A:535:GLU:HG3  | 1:A:536:GLU:N    | 2.20                     | 0.56              |
| 1:A:671:ILE:O    | 1:A:673:PRO:HD3  | 2.04                     | 0.56              |
| 1:A:14:ALA:HB2   | 1:A:149:PRO:HB2  | 1.79                     | 0.56              |
| 1:A:78:ASN:HD21  | 1:A:93:TYR:H     | 1.54                     | 0.56              |
| 1:A:225:VAL:HG12 | 1:A:438:LEU:HD11 | 1.88                     | 0.56              |
| 1:A:696:VAL:CG1  | 1:A:697:LEU:N    | 2.68                     | 0.56              |
| 1:A:113:TYR:CE1  | 1:A:152:LEU:HB2  | 2.41                     | 0.56              |
| 1:A:226:LEU:HD22 | 1:A:439:VAL:HG22 | 1.84                     | 0.56              |
| 3:C:135:LEU:H    | 3:C:135:LEU:CD1  | 2.08                     | 0.56              |
| 1:A:617:LEU:HD22 | 1:A:621:LEU:HD11 | 1.88                     | 0.56              |
| 3:C:72:TYR:O     | 3:C:76:MET:HB2   | 2.06                     | 0.56              |
| 1:A:299:VAL:CG1  | 1:A:300:MET:HG2  | 2.36                     | 0.56              |
| 1:A:353:ALA:HA   | 1:A:356:LEU:CD1  | 2.28                     | 0.56              |
| 1:A:515:ASP:CA   | 1:A:518:MET:HB3  | 2.35                     | 0.56              |
| 1:A:603:ASN:O    | 1:A:606:VAL:HG23 | 2.06                     | 0.56              |
| 1:A:674:ASN:CG   | 1:A:681:LEU:HD23 | 2.31                     | 0.56              |
| 1:A:735:GLY:O    | 1:A:738:VAL:N    | 2.39                     | 0.56              |
| 1:A:819:LEU:HD23 | 1:A:822:ARG:NH2  | 2.20                     | 0.56              |
| 1:A:310:SER:HA   | 1:A:313:ASN:ND2  | 2.20                     | 0.56              |
| 1:A:565:PRO:CA   | 1:A:579:GLU:HG3  | 2.36                     | 0.56              |
| 2:B:14:GLN:OE1   | 2:B:18:GLN:HG3   | 2.06                     | 0.56              |
| 1:A:124:ASN:HD21 | 1:A:126:TYR:HE2  | 1.54                     | 0.55              |
| 1:A:362:LYS:O    | 1:A:363:PHE:CD1  | 2.58                     | 0.55              |
| 1:A:397:ALA:HB1  | 1:A:609:LEU:HD11 | 1.88                     | 0.55              |
| 1:A:672:ILE:HG23 | 1:A:672:ILE:O    | 2.06                     | 0.55              |
| 2:B:85:SER:CB    | 2:B:88:THR:CG2   | 2.83                     | 0.55              |
| 1:A:669:ARG:HH11 | 1:A:694:ASN:HB2  | 1.71                     | 0.55              |
| 1:A:821:LEU:HD11 | 1:A:827:TRP:CD2  | 2.42                     | 0.55              |
| 1:A:240:SER:HA   | 5:A:999:ANP:O2G  | 2.06                     | 0.55              |
| 1:A:296:LEU:CD2  | 1:A:299:VAL:HG11 | 2.24                     | 0.55              |
| 1:A:415:ASN:O    | 1:A:419:VAL:HG23 | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:461:ILE:HG13 | 1:A:462:ALA:H    | 1.66                     | 0.55              |
| 1:A:598:ASN:CA   | 1:A:645:ILE:HD12 | 2.36                     | 0.55              |
| 1:A:657:MET:HA   | 1:A:660:LEU:HD12 | 1.89                     | 0.55              |
| 1:A:75:GLN:HE21  | 1:A:95:ASN:HB2   | 1.72                     | 0.55              |
| 1:A:288:ILE:CD1  | 1:A:352:THR:CG2  | 2.84                     | 0.55              |
| 1:A:296:LEU:O    | 1:A:297:ASN:C    | 2.47                     | 0.55              |
| 1:A:477:ILE:HD12 | 1:A:477:ILE:N    | 2.22                     | 0.55              |
| 1:A:556:MET:C    | 1:A:558:LYS:H    | 2.14                     | 0.55              |
| 1:A:795:ARG:CG   | 3:C:39:CYS:HA    | 2.36                     | 0.55              |
| 1:A:428:LYS:C    | 1:A:430:LEU:H    | 2.15                     | 0.55              |
| 3:C:73:GLU:O     | 3:C:76:MET:HB3   | 2.06                     | 0.55              |
| 1:A:190:ILE:CD1  | 1:A:247:ILE:HD13 | 2.36                     | 0.55              |
| 1:A:280:ARG:NH1  | 1:A:319:VAL:HG13 | 2.18                     | 0.55              |
| 1:A:417:ASN:N    | 1:A:417:ASN:ND2  | 2.21                     | 0.55              |
| 3:C:87:MET:CE    | 3:C:142:GLU:HG2  | 2.37                     | 0.55              |
| 3:C:92:THR:C     | 3:C:93:PHE:HD1   | 2.14                     | 0.55              |
| 1:A:244:GLY:O    | 1:A:264:THR:HA   | 2.07                     | 0.55              |
| 1:A:280:ARG:NH2  | 1:A:286:TYR:HB2  | 2.22                     | 0.55              |
| 1:A:807:GLY:O    | 1:A:810:VAL:HB   | 2.06                     | 0.55              |
| 2:B:44:SER:C     | 2:B:46:GLN:H     | 2.14                     | 0.55              |
| 1:A:141:ARG:HH11 | 1:A:196:VAL:HB   | 1.66                     | 0.55              |
| 1:A:481:ASN:O    | 1:A:484:LEU:HB2  | 2.07                     | 0.55              |
| 1:A:537:CYS:C    | 1:A:595:LEU:HD21 | 2.31                     | 0.55              |
| 1:A:763:LYS:C    | 1:A:766:VAL:HG22 | 2.31                     | 0.55              |
| 2:B:24:PHE:CE2   | 2:B:69:PHE:HA    | 2.42                     | 0.55              |
| 2:B:124:GLU:O    | 2:B:128:THR:OG1  | 2.16                     | 0.55              |
| 1:A:833:VAL:HG22 | 2:B:47:LEU:HD11  | 1.86                     | 0.55              |
| 1:A:129:LEU:HB2  | 1:A:131:ILE:HD11 | 1.89                     | 0.54              |
| 1:A:168:GLU:O    | 1:A:170:GLN:NE2  | 2.36                     | 0.54              |
| 1:A:321:ASN:N    | 1:A:321:ASN:ND2  | 2.54                     | 0.54              |
| 1:A:349:PHE:N    | 1:A:349:PHE:CD2  | 2.72                     | 0.54              |
| 1:A:402:LYS:CB   | 1:A:411:THR:CG2  | 2.84                     | 0.54              |
| 1:A:425:ALA:O    | 1:A:429:SER:CB   | 2.55                     | 0.54              |
| 2:B:35:VAL:O     | 2:B:67:LEU:CD2   | 2.55                     | 0.54              |
| 3:C:9:ASP:C      | 3:C:11:LEU:N     | 2.63                     | 0.54              |
| 1:A:717:LYS:C    | 1:A:719:ARG:N    | 2.64                     | 0.54              |
| 1:A:819:LEU:CD2  | 1:A:822:ARG:NH2  | 2.70                     | 0.54              |
| 1:A:190:ILE:HG23 | 1:A:249:ILE:CD1  | 2.36                     | 0.54              |
| 1:A:321:ASN:HD22 | 1:A:321:ASN:H    | 1.53                     | 0.54              |
| 1:A:746:LEU:O    | 1:A:747:GLN:HB2  | 2.08                     | 0.54              |
| 1:A:785:PHE:HE1  | 3:C:148:VAL:HG11 | 1.72                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:794:ILE:HD13 | 3:C:35:ASP:HA    | 1.88                     | 0.54              |
| 2:B:32:ASP:OD1   | 2:B:34:PHE:N     | 2.39                     | 0.54              |
| 2:B:71:MET:HE3   | 2:B:71:MET:HA    | 1.89                     | 0.54              |
| 3:C:92:THR:C     | 3:C:93:PHE:CD1   | 2.86                     | 0.54              |
| 1:A:103:LEU:CD2  | 1:A:121:ILE:HG21 | 2.37                     | 0.54              |
| 1:A:447:ASP:OD1  | 1:A:449:LYS:HD2  | 2.07                     | 0.54              |
| 1:A:751:ALA:O    | 1:A:754:ARG:NH1  | 2.40                     | 0.54              |
| 1:A:417:ASN:HD22 | 1:A:417:ASN:H    | 0.70                     | 0.54              |
| 1:A:626:GLU:C    | 1:A:627:GLU:CG   | 2.79                     | 0.54              |
| 1:A:789:ILE:HG23 | 3:C:125:ILE:CD1  | 2.38                     | 0.54              |
| 1:A:136:VAL:HA   | 1:A:139:LYS:HD2  | 1.90                     | 0.54              |
| 2:B:14:GLN:OE1   | 2:B:14:GLN:C     | 2.51                     | 0.54              |
| 3:C:28:VAL:O     | 3:C:62:SER:HA    | 2.08                     | 0.54              |
| 1:A:9:ASP:CG     | 1:A:139:LYS:NZ   | 2.66                     | 0.54              |
| 1:A:389:ILE:HG23 | 1:A:613:SER:OG   | 2.08                     | 0.54              |
| 2:B:14:GLN:C     | 2:B:14:GLN:CD    | 2.76                     | 0.54              |
| 1:A:110:GLY:C    | 1:A:111:LEU:HD23 | 2.32                     | 0.54              |
| 1:A:120:CYS:O    | 1:A:669:ARG:HB2  | 2.07                     | 0.54              |
| 1:A:190:ILE:HG23 | 1:A:249:ILE:HD11 | 1.90                     | 0.54              |
| 1:A:605:ASN:O    | 1:A:609:LEU:HG   | 2.08                     | 0.54              |
| 1:A:762:PHE:HB3  | 1:A:766:VAL:HG21 | 1.90                     | 0.54              |
| 1:A:795:ARG:C    | 1:A:797:ALA:N    | 2.62                     | 0.54              |
| 2:B:106:ILE:O    | 2:B:106:ILE:CD1  | 2.56                     | 0.54              |
| 3:C:31:PHE:CA    | 3:C:55:THR:HG22  | 2.37                     | 0.54              |
| 3:C:99:GLY:C     | 3:C:100:PHE:CD2  | 2.84                     | 0.54              |
| 1:A:11:GLN:CB    | 1:A:12:TYR:HD1   | 2.20                     | 0.54              |
| 1:A:395:LEU:HD22 | 1:A:399:LEU:HD21 | 1.86                     | 0.54              |
| 1:A:401:PRO:C    | 1:A:411:THR:HG23 | 2.31                     | 0.54              |
| 1:A:144:ARG:O    | 1:A:147:GLU:HG3  | 2.08                     | 0.54              |
| 1:A:185:ASN:O    | 1:A:189:VAL:HG23 | 2.08                     | 0.54              |
| 1:A:226:LEU:HD21 | 1:A:439:VAL:HG22 | 1.90                     | 0.54              |
| 1:A:650:ARG:HH11 | 1:A:650:ARG:HB3  | 1.73                     | 0.54              |
| 1:A:792:TYR:C    | 1:A:792:TYR:HD1  | 2.14                     | 0.54              |
| 1:A:794:ILE:CD1  | 3:C:35:ASP:HA    | 2.38                     | 0.54              |
| 1:A:124:ASN:ND2  | 1:A:126:TYR:CE2  | 2.75                     | 0.53              |
| 1:A:258:ALA:O    | 1:A:448:THR:HG23 | 2.08                     | 0.53              |
| 1:A:486:GLN:O    | 1:A:490:HIS:HB2  | 2.08                     | 0.53              |
| 1:A:556:MET:C    | 1:A:558:LYS:N    | 2.66                     | 0.53              |
| 1:A:790:ARG:HH21 | 3:C:117:LEU:CD2  | 2.19                     | 0.53              |
| 1:A:269:LYS:O    | 1:A:428:LYS:HD2  | 2.08                     | 0.53              |
| 1:A:284:ILE:HD12 | 1:A:285:PHE:N    | 2.04                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:355:ILE:HA   | 1:A:358:MET:CG   | 2.39                     | 0.53              |
| 2:B:145:THR:O    | 2:B:148:ILE:HG22 | 2.08                     | 0.53              |
| 1:A:511:ASP:CB   | 1:A:512:PHE:HD2  | 2.21                     | 0.53              |
| 3:C:95:ARG:CZ    | 3:C:96:GLU:HG2   | 2.37                     | 0.53              |
| 1:A:399:LEU:H    | 1:A:401:PRO:HD3  | 1.71                     | 0.53              |
| 1:A:467:PHE:C    | 1:A:469:PHE:H    | 2.15                     | 0.53              |
| 1:A:499:GLU:HA   | 1:A:502:LYS:CB   | 2.38                     | 0.53              |
| 1:A:603:ASN:H    | 1:A:603:ASN:HD22 | 1.55                     | 0.53              |
| 1:A:826:TRP:HB3  | 2:B:76:PHE:HE1   | 1.74                     | 0.53              |
| 1:A:605:ASN:HA   | 1:A:608:ALA:HB3  | 1.90                     | 0.53              |
| 2:B:55:GLU:O     | 2:B:59:MET:HG3   | 2.08                     | 0.53              |
| 3:C:128:LEU:C    | 3:C:130:ASP:H    | 2.16                     | 0.53              |
| 1:A:101:TYR:O    | 1:A:102:ASN:C    | 2.51                     | 0.53              |
| 1:A:234:THR:CG2  | 1:A:236:ARG:H    | 2.19                     | 0.53              |
| 1:A:515:ASP:O    | 1:A:518:MET:HB3  | 2.09                     | 0.53              |
| 1:A:691:LEU:CA   | 1:A:694:ASN:HD21 | 2.22                     | 0.53              |
| 2:B:86:GLU:CG    | 2:B:149:LYS:HD3  | 2.30                     | 0.53              |
| 1:A:256:LYS:CB   | 1:A:257:ILE:CD1  | 2.87                     | 0.53              |
| 1:A:284:ILE:O    | 1:A:287:GLN:N    | 2.40                     | 0.53              |
| 1:A:579:GLU:O    | 1:A:580:LEU:HB2  | 2.09                     | 0.53              |
| 2:B:34:PHE:HA    | 2:B:67:LEU:O     | 2.08                     | 0.53              |
| 2:B:40:ILE:C     | 2:B:42:ALA:N     | 2.67                     | 0.53              |
| 3:C:42:ILE:CG2   | 3:C:43:ASN:H     | 2.21                     | 0.53              |
| 1:A:120:CYS:HB3  | 1:A:668:VAL:HG13 | 1.91                     | 0.53              |
| 1:A:240:SER:CA   | 5:A:999:ANP:O2G  | 2.57                     | 0.53              |
| 1:A:537:CYS:HB2  | 1:A:595:LEU:HG   | 1.91                     | 0.53              |
| 1:A:805:ARG:CB   | 3:C:21:TRP:CZ2   | 2.92                     | 0.53              |
| 1:A:5:PHE:N      | 1:A:5:PHE:HD2    | 2.08                     | 0.53              |
| 1:A:138:ALA:C    | 1:A:140:TYR:H    | 2.16                     | 0.53              |
| 1:A:364:LYS:CA   | 1:A:373:GLU:HB3  | 2.39                     | 0.53              |
| 3:C:82:THR:C     | 3:C:149:MET:HE1  | 2.33                     | 0.53              |
| 1:A:179:GLY:H    | 5:A:999:ANP:HNB1 | 1.57                     | 0.52              |
| 1:A:256:LYS:C    | 1:A:257:ILE:HD12 | 2.29                     | 0.52              |
| 1:A:416:MET:O    | 1:A:416:MET:CG   | 2.40                     | 0.52              |
| 1:A:530:LEU:HD11 | 1:A:650:ARG:NH2  | 2.23                     | 0.52              |
| 1:A:719:ARG:O    | 1:A:774:ARG:NH1  | 2.42                     | 0.52              |
| 2:B:16:GLN:O     | 2:B:20:MET:CG    | 2.57                     | 0.52              |
| 3:C:36:VAL:HG11  | 3:C:68:PHE:CZ    | 2.44                     | 0.52              |
| 3:C:74:GLY:C     | 3:C:76:MET:H     | 2.16                     | 0.52              |
| 1:A:106:ARG:HB3  | 1:A:111:LEU:HD12 | 1.91                     | 0.52              |
| 1:A:428:LYS:C    | 1:A:430:LEU:N    | 2.66                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:507:TRP:CZ3  | 1:A:763:LYS:HE2  | 2.45                     | 0.52              |
| 1:A:594:TRP:HA   | 1:A:597:LYS:CB   | 2.39                     | 0.52              |
| 1:A:598:ASN:OD1  | 1:A:645:ILE:HB   | 2.09                     | 0.52              |
| 1:A:492:MET:O    | 1:A:495:LEU:N    | 2.42                     | 0.52              |
| 1:A:530:LEU:HD21 | 1:A:650:ARG:HE   | 1.72                     | 0.52              |
| 3:C:17:LEU:O     | 3:C:20:PHE:HB3   | 2.09                     | 0.52              |
| 3:C:140:LYS:HE2  | 3:C:143:ASP:H    | 1.73                     | 0.52              |
| 1:A:190:ILE:HA   | 1:A:193:LEU:HD12 | 1.90                     | 0.52              |
| 1:A:336:ASP:C    | 1:A:338:LEU:N    | 2.66                     | 0.52              |
| 1:A:778:LEU:O    | 1:A:782:ILE:CG1  | 2.56                     | 0.52              |
| 2:B:53:ASP:CG    | 2:B:54:LYS:N     | 2.68                     | 0.52              |
| 2:B:97:ASP:OD2   | 2:B:100:GLU:HA   | 2.09                     | 0.52              |
| 2:B:147:MET:CE   | 2:B:151:SER:OG   | 2.57                     | 0.52              |
| 3:C:36:VAL:HG21  | 3:C:68:PHE:HZ    | 1.74                     | 0.52              |
| 3:C:113:LEU:HD12 | 3:C:113:LEU:N    | 2.25                     | 0.52              |
| 3:C:122:VAL:HA   | 3:C:125:ILE:CG2  | 2.39                     | 0.52              |
| 1:A:705:LYS:O    | 1:A:707:PHE:N    | 2.43                     | 0.52              |
| 3:C:31:PHE:N     | 3:C:55:THR:HG22  | 2.24                     | 0.52              |
| 1:A:400:LYS:CB   | 1:A:414:GLN:N    | 2.73                     | 0.52              |
| 1:A:556:MET:O    | 1:A:558:LYS:N    | 2.38                     | 0.52              |
| 1:A:707:PHE:CB   | 1:A:708:PRO:CD   | 2.80                     | 0.52              |
| 1:A:786:GLN:OE1  | 3:C:115:GLU:N    | 2.39                     | 0.52              |
| 3:C:33:LEU:C     | 3:C:33:LEU:CD2   | 2.82                     | 0.52              |
| 1:A:233:LYS:HA   | 1:A:238:ASN:C    | 2.35                     | 0.52              |
| 1:A:764:ALA:O    | 1:A:766:VAL:N    | 2.42                     | 0.52              |
| 2:B:136:GLY:C    | 2:B:138:LYS:HD2  | 2.34                     | 0.52              |
| 1:A:515:ASP:C    | 1:A:518:MET:H    | 2.18                     | 0.52              |
| 1:A:60:ILE:O     | 1:A:64:SER:HA    | 2.10                     | 0.52              |
| 1:A:586:ASN:O    | 1:A:587:VAL:HG13 | 2.10                     | 0.52              |
| 1:A:676:LEU:HD12 | 1:A:681:LEU:HD22 | 1.91                     | 0.52              |
| 2:B:14:GLN:O     | 2:B:18:GLN:HG3   | 2.09                     | 0.52              |
| 1:A:31:LYS:HD3   | 1:A:31:LYS:N     | 2.24                     | 0.52              |
| 1:A:192:TYR:C    | 1:A:194:ALA:N    | 2.67                     | 0.52              |
| 1:A:231:ASN:O    | 1:A:282:TYR:HD2  | 1.92                     | 0.52              |
| 1:A:492:MET:O    | 1:A:496:GLU:N    | 2.40                     | 0.52              |
| 3:C:7:GLU:C      | 3:C:9:ASP:H      | 2.15                     | 0.52              |
| 1:A:14:ALA:HB1   | 1:A:149:PRO:HB3  | 1.92                     | 0.51              |
| 1:A:300:MET:CB   | 1:A:302:VAL:HG22 | 2.37                     | 0.51              |
| 1:A:744:ALA:C    | 1:A:746:LEU:N    | 2.67                     | 0.51              |
| 1:A:764:ALA:C    | 1:A:766:VAL:H    | 2.18                     | 0.51              |
| 1:A:807:GLY:HA3  | 2:B:95:MET:CE    | 2.37                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:822:ARG:HA   | 1:A:827:TRP:CD1  | 2.45                     | 0.51              |
| 2:B:67:LEU:N     | 2:B:67:LEU:HD13  | 2.24                     | 0.51              |
| 3:C:69:LEU:C     | 3:C:71:ALA:H     | 2.18                     | 0.51              |
| 1:A:71:LYS:HA    | 1:A:74:ILE:CD1   | 2.38                     | 0.51              |
| 1:A:143:LYS:HD3  | 1:A:147:GLU:OE2  | 2.10                     | 0.51              |
| 1:A:363:PHE:CE2  | 1:A:399:LEU:HD22 | 2.45                     | 0.51              |
| 1:A:387:CYS:HB2  | 1:A:389:ILE:CG1  | 2.40                     | 0.51              |
| 1:A:399:LEU:C    | 1:A:401:PRO:HD2  | 2.35                     | 0.51              |
| 1:A:399:LEU:C    | 1:A:401:PRO:CD   | 2.83                     | 0.51              |
| 1:A:487:PHE:HD1  | 1:A:661:TYR:CE1  | 2.27                     | 0.51              |
| 3:C:141:TYR:O    | 3:C:142:GLU:C    | 2.52                     | 0.51              |
| 1:A:341:THR:OG1  | 1:A:343:GLU:HG2  | 2.09                     | 0.51              |
| 1:A:815:ILE:C    | 1:A:817:LYS:H    | 2.17                     | 0.51              |
| 2:B:52:ASP:N     | 2:B:55:GLU:OE2   | 2.41                     | 0.51              |
| 2:B:72:PHE:C     | 2:B:74:SER:N     | 2.68                     | 0.51              |
| 3:C:140:LYS:CE   | 3:C:143:ASP:H    | 2.24                     | 0.51              |
| 1:A:223:ASN:O    | 1:A:224:PRO:C    | 2.54                     | 0.51              |
| 1:A:345:LYS:O    | 1:A:349:PHE:CD2  | 2.63                     | 0.51              |
| 1:A:512:PHE:N    | 1:A:512:PHE:HD2  | 2.01                     | 0.51              |
| 3:C:95:ARG:HD2   | 3:C:95:ARG:C     | 2.35                     | 0.51              |
| 3:C:95:ARG:NE    | 3:C:96:GLU:HG2   | 2.26                     | 0.51              |
| 3:C:122:VAL:HA   | 3:C:125:ILE:HG22 | 1.93                     | 0.51              |
| 1:A:192:TYR:O    | 1:A:194:ALA:N    | 2.43                     | 0.51              |
| 1:A:395:LEU:O    | 1:A:399:LEU:CD1  | 2.59                     | 0.51              |
| 1:A:399:LEU:N    | 1:A:401:PRO:CG   | 2.73                     | 0.51              |
| 1:A:743:LEU:HA   | 1:A:748:MET:CE   | 2.17                     | 0.51              |
| 1:A:355:ILE:HA   | 1:A:358:MET:HG2  | 1.93                     | 0.51              |
| 1:A:379:GLU:C    | 1:A:381:GLU:N    | 2.65                     | 0.51              |
| 1:A:543:ASP:O    | 1:A:546:SER:OG   | 2.28                     | 0.51              |
| 1:A:625:PRO:O    | 1:A:626:GLU:C    | 2.51                     | 0.51              |
| 2:B:121:ASN:CG   | 2:B:124:GLU:HG3  | 2.35                     | 0.51              |
| 3:C:3:LEU:HD12   | 3:C:7:GLU:HB3    | 1.91                     | 0.51              |
| 1:A:766:VAL:O    | 1:A:768:GLY:N    | 2.44                     | 0.51              |
| 1:A:817:LYS:C    | 1:A:819:LEU:N    | 2.62                     | 0.51              |
| 1:A:398:LEU:HD11 | 1:A:605:ASN:HD22 | 1.74                     | 0.51              |
| 1:A:438:LEU:O    | 1:A:438:LEU:HD23 | 2.11                     | 0.51              |
| 2:B:68:ASN:N     | 2:B:68:ASN:ND2   | 2.58                     | 0.51              |
| 3:C:4:SER:O      | 3:C:7:GLU:HB2    | 2.11                     | 0.51              |
| 3:C:87:MET:C     | 3:C:89:ALA:H     | 2.19                     | 0.51              |
| 1:A:11:GLN:HB3   | 1:A:12:TYR:CE1   | 2.45                     | 0.51              |
| 1:A:229:TYR:CZ   | 1:A:348:MET:HE3  | 2.46                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:492:MET:C    | 1:A:494:ILE:N    | 2.68                     | 0.51              |
| 1:A:784:MET:HE1  | 3:C:79:GLU:CG    | 2.41                     | 0.51              |
| 1:A:821:LEU:HD12 | 1:A:821:LEU:O    | 2.11                     | 0.51              |
| 1:A:140:TYR:HE2  | 1:A:154:SER:HG   | 1.58                     | 0.50              |
| 1:A:653:LEU:O    | 1:A:654:ASN:C    | 2.53                     | 0.50              |
| 1:A:103:LEU:HD22 | 1:A:121:ILE:HG21 | 1.92                     | 0.50              |
| 1:A:488:PHE:CE1  | 1:A:492:MET:HG3  | 2.46                     | 0.50              |
| 2:B:67:LEU:HD13  | 2:B:67:LEU:H     | 1.77                     | 0.50              |
| 1:A:50:SER:OG    | 1:A:57:THR:HB    | 2.10                     | 0.50              |
| 1:A:61:VAL:HG12  | 1:A:62:ALA:N     | 2.24                     | 0.50              |
| 1:A:93:TYR:O     | 1:A:98:SER:OG    | 2.29                     | 0.50              |
| 1:A:663:THR:O    | 1:A:665:PRO:HD3  | 2.12                     | 0.50              |
| 2:B:97:ASP:O     | 2:B:97:ASP:CG    | 2.55                     | 0.50              |
| 1:A:145:LYS:NZ   | 1:A:145:LYS:HB2  | 2.27                     | 0.50              |
| 1:A:272:VAL:HA   | 1:A:281:ASN:HD21 | 1.76                     | 0.50              |
| 1:A:833:VAL:CG1  | 1:A:835:PRO:HD3  | 2.39                     | 0.50              |
| 1:A:36:VAL:HG13  | 1:A:37:PRO:HD2   | 1.93                     | 0.50              |
| 1:A:433:ARG:NH2  | 1:A:602:ILE:HD12 | 2.26                     | 0.50              |
| 1:A:511:ASP:N    | 1:A:514:MET:SD   | 2.85                     | 0.50              |
| 1:A:582:HIS:O    | 1:A:584:ALA:N    | 2.40                     | 0.50              |
| 1:A:814:ASN:N    | 1:A:814:ASN:ND2  | 2.60                     | 0.50              |
| 3:C:86:TYR:HB3   | 3:C:145:VAL:CG1  | 2.42                     | 0.50              |
| 1:A:12:TYR:CD1   | 1:A:12:TYR:N     | 2.79                     | 0.50              |
| 1:A:43:PHE:CD2   | 1:A:97:ALA:HB2   | 2.47                     | 0.50              |
| 1:A:234:THR:O    | 1:A:235:THR:C    | 2.54                     | 0.50              |
| 1:A:423:VAL:O    | 1:A:426:LEU:HD23 | 2.12                     | 0.50              |
| 1:A:811:ILE:HD13 | 2:B:93:PHE:CD1   | 2.46                     | 0.50              |
| 2:B:29:VAL:O     | 2:B:31:ARG:HG3   | 2.12                     | 0.50              |
| 2:B:36:SER:O     | 2:B:39:ASP:HB3   | 2.12                     | 0.50              |
| 1:A:112:ILE:N    | 1:A:112:ILE:CD1  | 2.74                     | 0.50              |
| 1:A:187:LYS:C    | 1:A:189:VAL:N    | 2.68                     | 0.50              |
| 2:B:21:LYS:C     | 2:B:23:ALA:N     | 2.70                     | 0.50              |
| 1:A:146:THR:O    | 1:A:146:THR:HG22 | 2.11                     | 0.50              |
| 1:A:216:GLU:O    | 1:A:219:ILE:HG22 | 2.12                     | 0.50              |
| 1:A:384:ALA:HB2  | 1:A:391:ALA:CA   | 2.41                     | 0.50              |
| 1:A:390:ASN:ND2  | 1:A:393:ASP:OD1  | 2.45                     | 0.50              |
| 1:A:602:ILE:HB   | 1:A:607:VAL:CG2  | 2.42                     | 0.50              |
| 1:A:719:ARG:C    | 1:A:774:ARG:HH12 | 2.20                     | 0.50              |
| 2:B:15:LYS:HE3   | 2:B:19:GLU:OE2   | 2.12                     | 0.50              |
| 3:C:31:PHE:HB2   | 3:C:55:THR:HG22  | 1.94                     | 0.50              |
| 3:C:67:GLU:O     | 3:C:70:PRO:HD2   | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:530:LEU:HD11 | 1:A:646:SER:OG   | 2.12                     | 0.49              |
| 1:A:89:ALA:HB2   | 1:A:117:GLY:N    | 2.26                     | 0.49              |
| 1:A:384:ALA:CB   | 1:A:391:ALA:HB2  | 2.32                     | 0.49              |
| 1:A:522:LEU:HD21 | 1:A:562:PHE:CB   | 2.42                     | 0.49              |
| 1:A:577:HIS:N    | 1:A:589:TYR:O    | 2.37                     | 0.49              |
| 2:B:119:ASN:C    | 2:B:120:PHE:O    | 2.53                     | 0.49              |
| 3:C:53:GLY:O     | 3:C:54:GLY:O     | 2.30                     | 0.49              |
| 3:C:67:GLU:C     | 3:C:69:LEU:H     | 2.19                     | 0.49              |
| 1:A:71:LYS:HG2   | 1:A:71:LYS:O     | 2.12                     | 0.49              |
| 1:A:187:LYS:O    | 1:A:189:VAL:N    | 2.45                     | 0.49              |
| 1:A:722:ILE:CD1  | 1:A:778:LEU:HD13 | 2.43                     | 0.49              |
| 1:A:216:GLU:N    | 1:A:216:GLU:CD   | 2.70                     | 0.49              |
| 1:A:397:ALA:HB1  | 1:A:605:ASN:HD21 | 1.78                     | 0.49              |
| 1:A:288:ILE:CD1  | 1:A:352:THR:HG21 | 2.42                     | 0.49              |
| 1:A:358:MET:C    | 1:A:360:GLU:N    | 2.58                     | 0.49              |
| 2:B:68:ASN:HD22  | 2:B:68:ASN:H     | 1.60                     | 0.49              |
| 2:B:102:LYS:O    | 2:B:103:LYS:HG3  | 2.12                     | 0.49              |
| 3:C:63:LEU:HD13  | 3:C:67:GLU:CB    | 2.43                     | 0.49              |
| 3:C:69:LEU:HB3   | 3:C:70:PRO:CD    | 2.34                     | 0.49              |
| 1:A:24:GLN:HA    | 1:A:81:LYS:CE    | 2.43                     | 0.49              |
| 1:A:31:LYS:HD3   | 1:A:31:LYS:H     | 1.77                     | 0.49              |
| 1:A:309:TYR:O    | 1:A:313:ASN:ND2  | 2.45                     | 0.49              |
| 1:A:789:ILE:CG2  | 3:C:125:ILE:HG12 | 2.42                     | 0.49              |
| 2:B:29:VAL:O     | 2:B:31:ARG:N     | 2.46                     | 0.49              |
| 2:B:56:LEU:O     | 2:B:59:MET:HB2   | 2.13                     | 0.49              |
| 3:C:86:TYR:N     | 3:C:86:TYR:CD1   | 2.80                     | 0.49              |
| 1:A:63:ASP:C     | 1:A:63:ASP:OD1   | 2.55                     | 0.49              |
| 1:A:397:ALA:C    | 1:A:398:LEU:CG   | 2.83                     | 0.49              |
| 1:A:468:ASP:HB3  | 1:A:573:GLN:CA   | 2.33                     | 0.49              |
| 1:A:688:LEU:O    | 1:A:689:HIS:C    | 2.56                     | 0.49              |
| 2:B:97:ASP:CG    | 2:B:101:THR:H    | 2.21                     | 0.49              |
| 1:A:336:ASP:O    | 1:A:338:LEU:N    | 2.46                     | 0.49              |
| 1:A:507:TRP:CH2  | 1:A:763:LYS:HE3  | 2.47                     | 0.49              |
| 2:B:81:SER:O     | 2:B:83:THR:N     | 2.43                     | 0.49              |
| 3:C:19:ASP:OD2   | 3:C:26:GLY:HA2   | 2.13                     | 0.49              |
| 3:C:36:VAL:CG2   | 3:C:37:CYS:N     | 2.75                     | 0.49              |
| 1:A:137:ILE:HG12 | 1:A:153:PHE:CZ   | 2.47                     | 0.49              |
| 1:A:379:GLU:O    | 1:A:382:LYS:N    | 2.46                     | 0.49              |
| 1:A:402:LYS:N    | 1:A:411:THR:CG2  | 2.57                     | 0.49              |
| 1:A:438:LEU:C    | 1:A:438:LEU:HD23 | 2.38                     | 0.49              |
| 1:A:525:LYS:HA   | 1:A:526:PRO:HD3  | 1.68                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:187:LYS:HD2  | 1:A:227:GLU:OE2  | 2.13                     | 0.49              |
| 1:A:268:GLU:O    | 1:A:282:TYR:OH   | 2.30                     | 0.49              |
| 1:A:284:ILE:HA   | 1:A:287:GLN:CD   | 2.36                     | 0.49              |
| 1:A:380:ALA:HB1  | 1:A:395:LEU:HD11 | 1.94                     | 0.49              |
| 1:A:808:LEU:HD13 | 3:C:21:TRP:CZ3   | 2.48                     | 0.49              |
| 2:B:80:LEU:N     | 2:B:80:LEU:CD2   | 2.65                     | 0.49              |
| 3:C:28:VAL:O     | 3:C:62:SER:CA    | 2.61                     | 0.49              |
| 3:C:107:ARG:O    | 3:C:111:THR:HG23 | 2.13                     | 0.49              |
| 3:C:143:ASP:O    | 3:C:145:VAL:N    | 2.46                     | 0.49              |
| 1:A:505:ILE:HG23 | 1:A:756:GLY:HA2  | 1.93                     | 0.48              |
| 1:A:521:ASP:OD1  | 1:A:525:LYS:HB3  | 2.13                     | 0.48              |
| 2:B:96:PHE:CD1   | 2:B:96:PHE:N     | 2.81                     | 0.48              |
| 1:A:76:SER:HB3   | 1:A:93:TYR:CE1   | 2.48                     | 0.48              |
| 1:A:335:PHE:O    | 1:A:340:PHE:HB2  | 2.14                     | 0.48              |
| 1:A:535:GLU:HG2  | 1:A:536:GLU:H    | 1.78                     | 0.48              |
| 1:A:594:TRP:C    | 1:A:596:GLU:N    | 2.70                     | 0.48              |
| 1:A:831:SER:O    | 1:A:832:LYS:C    | 2.56                     | 0.48              |
| 2:B:135:GLU:HG3  | 2:B:136:GLY:N    | 2.22                     | 0.48              |
| 3:C:28:VAL:O     | 3:C:63:LEU:N     | 2.41                     | 0.48              |
| 1:A:225:VAL:CG1  | 1:A:438:LEU:HD11 | 2.43                     | 0.48              |
| 1:A:607:VAL:O    | 1:A:608:ALA:C    | 2.55                     | 0.48              |
| 1:A:610:LEU:O    | 1:A:611:GLY:C    | 2.54                     | 0.48              |
| 2:B:35:VAL:H     | 2:B:67:LEU:HB3   | 1.77                     | 0.48              |
| 2:B:118:ASP:CG   | 3:C:24:ARG:NH2   | 2.64                     | 0.48              |
| 3:C:36:VAL:HG22  | 3:C:37:CYS:N     | 2.28                     | 0.48              |
| 1:A:83:GLU:HG3   | 1:A:101:TYR:HE2  | 1.78                     | 0.48              |
| 1:A:94:LEU:O     | 1:A:94:LEU:CG    | 2.61                     | 0.48              |
| 1:A:120:CYS:CB   | 1:A:668:VAL:HA   | 2.44                     | 0.48              |
| 1:A:276:GLN:O    | 1:A:277:SER:C    | 2.56                     | 0.48              |
| 1:A:646:SER:C    | 1:A:648:VAL:N    | 2.69                     | 0.48              |
| 1:A:783:SER:CB   | 3:C:115:GLU:HG3  | 2.44                     | 0.48              |
| 2:B:102:LYS:HD2  | 2:B:102:LYS:N    | 2.29                     | 0.48              |
| 3:C:15:PHE:CD1   | 3:C:15:PHE:O     | 2.66                     | 0.48              |
| 1:A:159:ALA:O    | 1:A:170:GLN:HG3  | 2.13                     | 0.48              |
| 1:A:418:GLN:O    | 1:A:421:ASN:C    | 2.53                     | 0.48              |
| 1:A:748:MET:O    | 1:A:748:MET:HG2  | 2.12                     | 0.48              |
| 1:A:801:LEU:C    | 1:A:801:LEU:CD2  | 2.87                     | 0.48              |
| 2:B:37:LYS:C     | 2:B:39:ASP:H     | 2.19                     | 0.48              |
| 3:C:124:GLU:O    | 3:C:127:LYS:N    | 2.46                     | 0.48              |
| 1:A:93:TYR:O     | 1:A:95:ASN:N     | 2.47                     | 0.48              |
| 1:A:289:CYS:O    | 1:A:304:PRO:O    | 2.30                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:397:ALA:HA   | 1:A:401:PRO:CB   | 2.42                     | 0.48              |
| 1:A:598:ASN:HD21 | 1:A:644:THR:C    | 2.22                     | 0.48              |
| 1:A:792:TYR:O    | 1:A:792:TYR:HD1  | 1.95                     | 0.48              |
| 1:A:342:LYS:HE2  | 1:A:346:GLN:NE2  | 2.29                     | 0.48              |
| 1:A:413:GLY:O    | 1:A:414:GLN:C    | 2.55                     | 0.48              |
| 2:B:16:GLN:O     | 2:B:20:MET:HG2   | 2.14                     | 0.48              |
| 3:C:69:LEU:C     | 3:C:71:ALA:N     | 2.71                     | 0.48              |
| 1:A:138:ALA:C    | 1:A:140:TYR:N    | 2.71                     | 0.48              |
| 1:A:515:ASP:HB3  | 1:A:560:ARG:NH2  | 2.28                     | 0.48              |
| 1:A:519:CYS:O    | 1:A:520:ILE:C    | 2.57                     | 0.48              |
| 1:A:743:LEU:CA   | 1:A:748:MET:CE   | 2.85                     | 0.48              |
| 1:A:794:ILE:HG23 | 1:A:794:ILE:O    | 2.13                     | 0.48              |
| 2:B:13:PRO:O     | 2:B:17:ILE:HG12  | 2.14                     | 0.48              |
| 2:B:142:VAL:O    | 2:B:145:THR:HG22 | 2.14                     | 0.48              |
| 1:A:140:TYR:O    | 1:A:141:ARG:C    | 2.55                     | 0.48              |
| 1:A:397:ALA:C    | 1:A:398:LEU:HD12 | 2.39                     | 0.48              |
| 1:A:140:TYR:CE2  | 1:A:154:SER:OG   | 2.67                     | 0.48              |
| 1:A:143:LYS:HE3  | 1:A:143:LYS:CA   | 2.44                     | 0.48              |
| 1:A:532:ILE:HA   | 1:A:535:GLU:CG   | 2.41                     | 0.48              |
| 1:A:735:GLY:C    | 1:A:737:THR:N    | 2.72                     | 0.48              |
| 1:A:737:THR:C    | 1:A:739:SER:H    | 2.22                     | 0.48              |
| 2:B:62:GLU:O     | 2:B:75:ILE:HG21  | 2.14                     | 0.48              |
| 1:A:89:ALA:HB2   | 1:A:117:GLY:H    | 1.79                     | 0.47              |
| 1:A:275:GLN:NE2  | 1:A:281:ASN:ND2  | 2.61                     | 0.47              |
| 3:C:47:GLU:O     | 3:C:50:PHE:HB2   | 2.13                     | 0.47              |
| 1:A:82:PHE:CE2   | 1:A:90:ASN:O     | 2.67                     | 0.47              |
| 1:A:719:ARG:NE   | 1:A:771:GLU:OE2  | 2.43                     | 0.47              |
| 2:B:53:ASP:O     | 2:B:56:LEU:HB2   | 2.14                     | 0.47              |
| 2:B:140:ASP:OD2  | 2:B:142:VAL:HB   | 2.13                     | 0.47              |
| 3:C:105:GLU:O    | 3:C:109:VAL:HG23 | 2.14                     | 0.47              |
| 1:A:428:LYS:O    | 1:A:430:LEU:N    | 2.47                     | 0.47              |
| 1:A:505:ILE:HD12 | 1:A:505:ILE:C    | 2.40                     | 0.47              |
| 1:A:576:ALA:HB1  | 1:A:589:TYR:O    | 2.15                     | 0.47              |
| 1:A:672:ILE:O    | 1:A:673:PRO:C    | 2.57                     | 0.47              |
| 1:A:743:LEU:O    | 1:A:746:LEU:HB2  | 2.14                     | 0.47              |
| 1:A:819:LEU:CD2  | 1:A:822:ARG:HH21 | 2.24                     | 0.47              |
| 1:A:192:TYR:O    | 1:A:193:LEU:C    | 2.58                     | 0.47              |
| 1:A:248:ARG:HB2  | 1:A:261:ASP:OD2  | 2.14                     | 0.47              |
| 1:A:723:LEU:HD21 | 1:A:773:MET:HB3  | 1.95                     | 0.47              |
| 3:C:90:PHE:CB    | 3:C:141:TYR:CE1  | 2.91                     | 0.47              |
| 1:A:672:ILE:HG22 | 1:A:690:GLN:NE2  | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:794:ILE:HD13 | 3:C:35:ASP:CA    | 2.44                     | 0.47              |
| 1:A:826:TRP:CZ2  | 2:B:59:MET:HB3   | 2.50                     | 0.47              |
| 3:C:108:HIS:ND1  | 3:C:112:ALA:CB   | 2.76                     | 0.47              |
| 1:A:696:VAL:HG13 | 1:A:697:LEU:H    | 1.79                     | 0.47              |
| 3:C:90:PHE:CB    | 3:C:141:TYR:HE1  | 2.27                     | 0.47              |
| 1:A:120:CYS:HB3  | 1:A:668:VAL:HA   | 1.97                     | 0.47              |
| 1:A:140:TYR:HE2  | 1:A:154:SER:OG   | 1.98                     | 0.47              |
| 1:A:214:SER:O    | 1:A:217:ASP:N    | 2.47                     | 0.47              |
| 1:A:403:VAL:HG13 | 1:A:404:LYS:O    | 2.14                     | 0.47              |
| 1:A:430:LEU:HD12 | 1:A:622:PHE:CE2  | 2.50                     | 0.47              |
| 1:A:511:ASP:CB   | 1:A:512:PHE:CD2  | 2.97                     | 0.47              |
| 1:A:598:ASN:HD22 | 1:A:599:LYS:HD3  | 1.80                     | 0.47              |
| 1:A:750:PRO:O    | 1:A:751:ALA:C    | 2.54                     | 0.47              |
| 1:A:802:GLN:HG2  | 3:C:17:LEU:HD22  | 1.96                     | 0.47              |
| 1:A:816:ARG:NH2  | 2:B:120:PHE:CD1  | 2.82                     | 0.47              |
| 1:A:826:TRP:HB3  | 2:B:76:PHE:CE1   | 2.50                     | 0.47              |
| 3:C:17:LEU:HD11  | 3:C:21:TRP:HE1   | 1.79                     | 0.47              |
| 3:C:49:VAL:HA    | 3:C:52:VAL:CG2   | 2.45                     | 0.47              |
| 3:C:143:ASP:O    | 3:C:144:PHE:C    | 2.56                     | 0.47              |
| 1:A:135:SER:O    | 1:A:139:LYS:HG3  | 2.14                     | 0.47              |
| 1:A:266:LEU:HD11 | 1:A:649:HIS:CE1  | 2.50                     | 0.47              |
| 1:A:382:LYS:HB2  | 1:A:382:LYS:HE3  | 1.63                     | 0.47              |
| 1:A:475:LEU:O    | 1:A:478:ASN:HB2  | 2.15                     | 0.47              |
| 3:C:28:VAL:O     | 3:C:62:SER:HB2   | 2.15                     | 0.47              |
| 3:C:141:TYR:H    | 3:C:141:TYR:HD2  | 1.61                     | 0.47              |
| 1:A:48:ILE:HG23  | 1:A:58:VAL:CG1   | 2.27                     | 0.47              |
| 1:A:128:ARG:HH12 | 1:A:188:LYS:NZ   | 2.13                     | 0.47              |
| 1:A:237:ASN:ND2  | 5:A:999:ANP:PA   | 2.87                     | 0.47              |
| 1:A:473:GLU:O    | 1:A:477:ILE:HD13 | 2.15                     | 0.47              |
| 1:A:520:ILE:O    | 1:A:524:GLU:HG2  | 2.15                     | 0.47              |
| 1:A:795:ARG:CD   | 3:C:38:ARG:O     | 2.56                     | 0.47              |
| 2:B:89:ILE:O     | 2:B:91:ASN:N     | 2.48                     | 0.47              |
| 3:C:86:TYR:N     | 3:C:86:TYR:HD1   | 2.13                     | 0.47              |
| 1:A:68:THR:O     | 1:A:69:VAL:HG13  | 2.15                     | 0.47              |
| 1:A:173:LEU:HD21 | 1:A:660:LEU:HD21 | 1.96                     | 0.47              |
| 1:A:251:PHE:C    | 1:A:258:ALA:HB2  | 2.39                     | 0.47              |
| 1:A:415:ASN:OD1  | 1:A:415:ASN:C    | 2.57                     | 0.47              |
| 1:A:716:PHE:CE1  | 1:A:720:TYR:HD2  | 2.33                     | 0.47              |
| 2:B:122:LYS:O    | 2:B:123:ASP:C    | 2.57                     | 0.47              |
| 2:B:141:TYR:O    | 2:B:145:THR:HB   | 2.15                     | 0.47              |
| 3:C:128:LEU:C    | 3:C:130:ASP:N    | 2.73                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:288:ILE:CD1  | 1:A:352:THR:HG22 | 2.44                     | 0.46              |
| 2:B:68:ASN:ND2   | 2:B:68:ASN:H     | 2.13                     | 0.46              |
| 1:A:737:THR:C    | 1:A:739:SER:N    | 2.71                     | 0.46              |
| 1:A:783:SER:HA   | 1:A:786:GLN:OE1  | 2.15                     | 0.46              |
| 1:A:828:LYS:O    | 1:A:832:LYS:N    | 2.43                     | 0.46              |
| 1:A:118:LEU:C    | 1:A:119:PHE:CD1  | 2.93                     | 0.46              |
| 1:A:169:ASN:HB2  | 1:A:663:THR:HG22 | 1.94                     | 0.46              |
| 1:A:236:ARG:O    | 1:A:677:LYS:HE3  | 2.16                     | 0.46              |
| 1:A:325:VAL:HG23 | 1:A:326:GLU:H    | 1.80                     | 0.46              |
| 1:A:397:ALA:CA   | 1:A:401:PRO:CG   | 2.85                     | 0.46              |
| 1:A:604:GLU:CD   | 1:A:604:GLU:N    | 2.72                     | 0.46              |
| 1:A:604:GLU:N    | 1:A:604:GLU:OE2  | 2.49                     | 0.46              |
| 1:A:685:GLU:H    | 1:A:685:GLU:CD   | 2.22                     | 0.46              |
| 3:C:17:LEU:HD12  | 3:C:21:TRP:HE1   | 1.79                     | 0.46              |
| 3:C:18:PHE:O     | 3:C:19:ASP:C     | 2.56                     | 0.46              |
| 3:C:67:GLU:C     | 3:C:69:LEU:N     | 2.73                     | 0.46              |
| 1:A:24:GLN:HA    | 1:A:81:LYS:HE3   | 1.98                     | 0.46              |
| 1:A:95:ASN:OD1   | 1:A:98:SER:N     | 2.47                     | 0.46              |
| 1:A:296:LEU:HA   | 1:A:299:VAL:HG12 | 1.98                     | 0.46              |
| 1:A:505:ILE:CG2  | 1:A:756:GLY:HA2  | 2.45                     | 0.46              |
| 1:A:818:TRP:NE1  | 2:B:148:ILE:O    | 2.49                     | 0.46              |
| 2:B:105:ASN:O    | 2:B:108:TYR:N    | 2.37                     | 0.46              |
| 1:A:294:PRO:HA   | 1:A:297:ASN:ND2  | 2.30                     | 0.46              |
| 1:A:362:LYS:C    | 1:A:363:PHE:HD1  | 2.19                     | 0.46              |
| 1:A:447:ASP:O    | 1:A:447:ASP:CG   | 2.57                     | 0.46              |
| 1:A:653:LEU:O    | 1:A:656:LEU:HB3  | 2.15                     | 0.46              |
| 2:B:21:LYS:O     | 2:B:24:PHE:N     | 2.47                     | 0.46              |
| 3:C:87:MET:HE1   | 3:C:142:GLU:HG2  | 1.97                     | 0.46              |
| 1:A:24:GLN:HA    | 1:A:81:LYS:CD    | 2.46                     | 0.46              |
| 1:A:214:SER:C    | 1:A:216:GLU:N    | 2.73                     | 0.46              |
| 1:A:430:LEU:O    | 1:A:433:ARG:N    | 2.48                     | 0.46              |
| 1:A:488:PHE:CD1  | 1:A:489:ASN:N    | 2.84                     | 0.46              |
| 1:A:644:THR:O    | 1:A:646:SER:N    | 2.48                     | 0.46              |
| 1:A:713:TYR:CE1  | 1:A:760:VAL:HG22 | 2.50                     | 0.46              |
| 2:B:139:PHE:C    | 2:B:139:PHE:HD1  | 2.22                     | 0.46              |
| 3:C:120:GLU:O    | 3:C:121:ASP:C    | 2.57                     | 0.46              |
| 1:A:54:ASP:CB    | 1:A:70:LYS:NZ    | 2.79                     | 0.46              |
| 1:A:229:TYR:HA   | 1:A:284:ILE:CG1  | 2.46                     | 0.46              |
| 1:A:514:MET:N    | 1:A:515:ASP:OD2  | 2.49                     | 0.46              |
| 1:A:794:ILE:HG23 | 3:C:39:CYS:SG    | 2.55                     | 0.46              |
| 1:A:816:ARG:NH2  | 2:B:120:PHE:HD1  | 2.13                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:140:TYR:CE2  | 1:A:151:HIS:HB3  | 2.51                     | 0.46              |
| 1:A:143:LYS:HA   | 1:A:143:LYS:CE   | 2.43                     | 0.46              |
| 1:A:237:ASN:ND2  | 5:A:999:ANP:C5'  | 2.47                     | 0.46              |
| 1:A:336:ASP:O    | 1:A:339:GLY:N    | 2.44                     | 0.46              |
| 1:A:789:ILE:HG23 | 3:C:125:ILE:CG1  | 2.45                     | 0.46              |
| 1:A:7:ASP:O      | 1:A:7:ASP:CG     | 2.59                     | 0.46              |
| 1:A:271:ARG:HH22 | 1:A:279:GLU:CG   | 2.29                     | 0.46              |
| 1:A:398:LEU:HD11 | 1:A:605:ASN:CG   | 2.41                     | 0.46              |
| 1:A:496:GLU:C    | 1:A:498:GLU:H    | 2.24                     | 0.46              |
| 1:A:785:PHE:CE1  | 3:C:148:VAL:HG11 | 2.51                     | 0.46              |
| 3:C:8:ILE:O      | 3:C:12:LYS:HE3   | 2.16                     | 0.46              |
| 1:A:131:ILE:HG13 | 1:A:132:TYR:CD1  | 2.47                     | 0.46              |
| 1:A:443:ASN:O    | 1:A:447:ASP:HB2  | 2.16                     | 0.46              |
| 1:A:521:ASP:O    | 1:A:522:LEU:C    | 2.59                     | 0.46              |
| 1:A:570:ARG:C    | 1:A:573:GLN:CB   | 2.88                     | 0.46              |
| 1:A:785:PHE:O    | 1:A:789:ILE:HG13 | 2.15                     | 0.46              |
| 2:B:80:LEU:H     | 2:B:80:LEU:CD2   | 2.09                     | 0.46              |
| 3:C:93:PHE:CE2   | 3:C:109:VAL:HG13 | 2.50                     | 0.46              |
| 1:A:106:ARG:CB   | 1:A:111:LEU:HD12 | 2.47                     | 0.45              |
| 1:A:430:LEU:C    | 1:A:432:ASP:N    | 2.69                     | 0.45              |
| 1:A:750:PRO:C    | 1:A:752:GLU:N    | 2.66                     | 0.45              |
| 1:A:751:ALA:C    | 1:A:754:ARG:NH1  | 2.74                     | 0.45              |
| 1:A:808:LEU:C    | 1:A:808:LEU:CD2  | 2.79                     | 0.45              |
| 2:B:99:GLN:O     | 2:B:99:GLN:CG    | 2.64                     | 0.45              |
| 1:A:236:ARG:NH2  | 1:A:672:ILE:HD13 | 2.29                     | 0.45              |
| 1:A:387:CYS:CB   | 1:A:389:ILE:HG13 | 2.46                     | 0.45              |
| 1:A:415:ASN:O    | 1:A:419:VAL:CG2  | 2.64                     | 0.45              |
| 1:A:447:ASP:CG   | 1:A:449:LYS:NZ   | 2.73                     | 0.45              |
| 1:A:470:ASN:N    | 1:A:470:ASN:ND2  | 2.38                     | 0.45              |
| 2:B:37:LYS:CE    | 2:B:57:THR:HG23  | 2.46                     | 0.45              |
| 2:B:139:PHE:HE1  | 2:B:141:TYR:HA   | 1.80                     | 0.45              |
| 1:A:232:ALA:CB   | 1:A:271:ARG:HH11 | 2.22                     | 0.45              |
| 1:A:271:ARG:HH22 | 1:A:279:GLU:HG2  | 1.78                     | 0.45              |
| 1:A:398:LEU:HB3  | 1:A:606:VAL:HG22 | 1.98                     | 0.45              |
| 1:A:833:VAL:CG2  | 2:B:47:LEU:CD1   | 2.89                     | 0.45              |
| 2:B:108:TYR:CD1  | 2:B:108:TYR:C    | 2.95                     | 0.45              |
| 2:B:109:ILE:HA   | 2:B:112:LEU:HD12 | 1.98                     | 0.45              |
| 3:C:63:LEU:HD13  | 3:C:67:GLU:HB3   | 1.99                     | 0.45              |
| 1:A:125:PRO:O    | 1:A:125:PRO:HG2  | 2.16                     | 0.45              |
| 1:A:477:ILE:HD12 | 1:A:477:ILE:H    | 1.81                     | 0.45              |
| 1:A:8:PRO:HG2    | 1:A:9:ASP:N      | 2.29                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:285:PHE:HE2  | 1:A:431:TYR:CE2  | 2.35                     | 0.45              |
| 1:A:398:LEU:C    | 1:A:401:PRO:CG   | 2.83                     | 0.45              |
| 1:A:473:GLU:O    | 1:A:477:ILE:CD1  | 2.64                     | 0.45              |
| 1:A:603:ASN:HB2  | 1:A:606:VAL:CG2  | 2.46                     | 0.45              |
| 1:A:781:ILE:HG21 | 3:C:89:ALA:HB2   | 1.97                     | 0.45              |
| 1:A:815:ILE:C    | 1:A:817:LYS:N    | 2.75                     | 0.45              |
| 1:A:323:ASP:OD1  | 1:A:323:ASP:C    | 2.59                     | 0.45              |
| 1:A:337:ILE:H    | 1:A:337:ILE:HG13 | 1.53                     | 0.45              |
| 1:A:615:GLU:O    | 1:A:616:PRO:C    | 2.60                     | 0.45              |
| 1:A:818:TRP:O    | 1:A:818:TRP:CG   | 2.70                     | 0.45              |
| 1:A:123:VAL:CG1  | 1:A:673:PRO:HG3  | 2.21                     | 0.45              |
| 1:A:355:ILE:O    | 1:A:356:LEU:C    | 2.58                     | 0.45              |
| 1:A:415:ASN:OD1  | 1:A:417:ASN:ND2  | 2.50                     | 0.45              |
| 1:A:467:PHE:HE1  | 1:A:474:GLN:HB3  | 1.82                     | 0.45              |
| 1:A:470:ASN:O    | 1:A:589:TYR:HA   | 2.17                     | 0.45              |
| 1:A:545:LYS:O    | 1:A:546:SER:C    | 2.56                     | 0.45              |
| 1:A:136:VAL:O    | 1:A:137:ILE:C    | 2.59                     | 0.45              |
| 1:A:185:ASN:O    | 1:A:186:THR:C    | 2.58                     | 0.45              |
| 1:A:187:LYS:O    | 1:A:188:LYS:C    | 2.60                     | 0.45              |
| 1:A:578:PHE:O    | 1:A:589:TYR:N    | 2.49                     | 0.45              |
| 1:A:788:HIS:HD2  | 3:C:148:VAL:HG22 | 1.82                     | 0.45              |
| 1:A:799:LYS:O    | 1:A:800:LYS:C    | 2.60                     | 0.45              |
| 2:B:71:MET:O     | 2:B:71:MET:HG3   | 2.17                     | 0.45              |
| 2:B:105:ASN:O    | 2:B:108:TYR:HB3  | 2.16                     | 0.45              |
| 2:B:142:VAL:CG1  | 2:B:143:LYS:NZ   | 2.67                     | 0.45              |
| 3:C:18:PHE:O     | 3:C:20:PHE:N     | 2.49                     | 0.45              |
| 3:C:22:ASP:OD1   | 3:C:22:ASP:O     | 2.35                     | 0.45              |
| 1:A:140:TYR:CZ   | 1:A:148:ILE:HG12 | 2.52                     | 0.45              |
| 1:A:455:TYR:C    | 1:A:455:TYR:HD1  | 2.24                     | 0.45              |
| 2:B:143:LYS:C    | 2:B:145:THR:N    | 2.73                     | 0.45              |
| 1:A:300:MET:O    | 1:A:301:LEU:HB2  | 2.17                     | 0.45              |
| 1:A:389:ILE:O    | 1:A:389:ILE:CD1  | 2.56                     | 0.45              |
| 2:B:36:SER:C     | 2:B:39:ASP:H     | 2.25                     | 0.45              |
| 2:B:136:GLY:HA3  | 2:B:138:LYS:NZ   | 2.32                     | 0.45              |
| 3:C:108:HIS:O    | 3:C:112:ALA:HB3  | 2.18                     | 0.45              |
| 1:A:94:LEU:O     | 1:A:94:LEU:CD1   | 2.64                     | 0.44              |
| 1:A:241:SER:O    | 1:A:242:ARG:HG2  | 2.18                     | 0.44              |
| 1:A:344:GLU:HA   | 1:A:347:SER:OG   | 2.18                     | 0.44              |
| 1:A:350:LYS:HE2  | 1:A:386:LEU:CA   | 2.45                     | 0.44              |
| 1:A:400:LYS:CB   | 1:A:413:GLY:C    | 2.90                     | 0.44              |
| 1:A:463:GLY:O    | 1:A:477:ILE:HG22 | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:483:ARG:NH1  | 1:A:657:MET:HG3  | 2.32                     | 0.44              |
| 1:A:483:ARG:HH12 | 1:A:657:MET:HG3  | 1.82                     | 0.44              |
| 1:A:515:ASP:C    | 1:A:518:MET:HB3  | 2.42                     | 0.44              |
| 1:A:530:LEU:HG   | 1:A:650:ARG:NH2  | 2.28                     | 0.44              |
| 2:B:135:GLU:O    | 2:B:137:GLY:N    | 2.48                     | 0.44              |
| 1:A:530:LEU:CD1  | 1:A:650:ARG:NH2  | 2.79                     | 0.44              |
| 1:A:169:ASN:O    | 1:A:663:THR:HA   | 2.18                     | 0.44              |
| 1:A:518:MET:O    | 1:A:518:MET:HG2  | 2.16                     | 0.44              |
| 1:A:549:ASP:O    | 1:A:553:GLN:HG2  | 2.17                     | 0.44              |
| 1:A:676:LEU:HD12 | 1:A:681:LEU:CD2  | 2.47                     | 0.44              |
| 1:A:735:GLY:O    | 1:A:737:THR:N    | 2.50                     | 0.44              |
| 1:A:28:PHE:CZ    | 1:A:29:ASP:O     | 2.71                     | 0.44              |
| 1:A:534:GLU:OE1  | 1:A:650:ARG:NH2  | 2.39                     | 0.44              |
| 1:A:626:GLU:O    | 1:A:627:GLU:CG   | 2.65                     | 0.44              |
| 1:A:657:MET:O    | 1:A:658:LYS:C    | 2.60                     | 0.44              |
| 1:A:785:PHE:O    | 1:A:785:PHE:CG   | 2.71                     | 0.44              |
| 2:B:51:PRO:HB2   | 2:B:55:GLU:OE2   | 2.17                     | 0.44              |
| 2:B:142:VAL:HG12 | 2:B:143:LYS:HZ2  | 1.73                     | 0.44              |
| 3:C:141:TYR:N    | 3:C:141:TYR:CD2  | 2.86                     | 0.44              |
| 1:A:38:ASP:HB2   | 1:A:44:ALA:HB2   | 1.99                     | 0.44              |
| 1:A:534:GLU:O    | 1:A:537:CYS:SG   | 2.76                     | 0.44              |
| 1:A:545:LYS:C    | 1:A:548:GLN:H    | 2.26                     | 0.44              |
| 1:A:713:TYR:C    | 1:A:715:GLU:N    | 2.73                     | 0.44              |
| 2:B:72:PHE:O     | 2:B:74:SER:N     | 2.50                     | 0.44              |
| 2:B:145:THR:O    | 2:B:146:ALA:C    | 2.61                     | 0.44              |
| 3:C:31:PHE:CD1   | 3:C:56:HIS:O     | 2.70                     | 0.44              |
| 3:C:102:SER:HA   | 3:C:138:ASN:HA   | 2.00                     | 0.44              |
| 1:A:182:LYS:O    | 1:A:186:THR:OG1  | 2.34                     | 0.44              |
| 1:A:228:ALA:HB1  | 1:A:284:ILE:HG23 | 2.00                     | 0.44              |
| 1:A:284:ILE:O    | 1:A:285:PHE:C    | 2.61                     | 0.44              |
| 1:A:400:LYS:HA   | 1:A:414:GLN:CA   | 2.46                     | 0.44              |
| 1:A:712:ILE:CD1  | 1:A:714:SER:HB3  | 2.36                     | 0.44              |
| 2:B:55:GLU:O     | 2:B:56:LEU:C     | 2.60                     | 0.44              |
| 1:A:56:ILE:O     | 1:A:69:VAL:HG22  | 2.17                     | 0.44              |
| 1:A:80:PRO:O     | 1:A:83:GLU:N     | 2.49                     | 0.44              |
| 1:A:258:ALA:O    | 1:A:448:THR:CG2  | 2.66                     | 0.44              |
| 1:A:341:THR:HB   | 1:A:343:GLU:OE2  | 2.17                     | 0.44              |
| 1:A:398:LEU:HD13 | 1:A:606:VAL:HA   | 1.99                     | 0.44              |
| 3:C:115:GLU:O    | 3:C:116:ARG:C    | 2.61                     | 0.44              |
| 3:C:122:VAL:CA   | 3:C:125:ILE:HG22 | 2.48                     | 0.44              |
| 3:C:129:THR:HB   | 3:C:147:LYS:HD3  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:334:ALA:O    | 1:A:336:ASP:N    | 2.50                     | 0.44              |
| 1:A:404:LYS:HA   | 1:A:409:MET:CB   | 2.48                     | 0.44              |
| 1:A:495:LEU:HG   | 1:A:495:LEU:O    | 2.17                     | 0.44              |
| 1:A:500:TYR:HA   | 1:A:505:ILE:CD1  | 2.47                     | 0.44              |
| 1:A:530:LEU:C    | 1:A:532:ILE:H    | 2.26                     | 0.44              |
| 2:B:36:SER:N     | 2:B:39:ASP:CB    | 2.80                     | 0.44              |
| 2:B:90:ARG:HH12  | 2:B:143:LYS:NZ   | 2.16                     | 0.44              |
| 2:B:100:GLU:CA   | 2:B:102:LYS:HE3  | 2.47                     | 0.44              |
| 3:C:100:PHE:CD2  | 3:C:100:PHE:N    | 2.85                     | 0.44              |
| 1:A:94:LEU:O     | 1:A:94:LEU:HG    | 2.18                     | 0.44              |
| 1:A:603:ASN:HB2  | 1:A:606:VAL:HG21 | 2.00                     | 0.44              |
| 2:B:37:LYS:HE3   | 2:B:57:THR:HG23  | 2.00                     | 0.44              |
| 2:B:93:PHE:O     | 2:B:94:ALA:C     | 2.60                     | 0.44              |
| 1:A:8:PRO:HD2    | 1:A:10:PHE:CD2   | 2.53                     | 0.43              |
| 1:A:8:PRO:CG     | 1:A:9:ASP:H      | 2.31                     | 0.43              |
| 1:A:32:LYS:NZ    | 3:C:95:ARG:HH22  | 2.16                     | 0.43              |
| 1:A:384:ALA:CB   | 1:A:391:ALA:N    | 2.76                     | 0.43              |
| 1:A:577:HIS:HD2  | 1:A:591:ILE:H    | 1.65                     | 0.43              |
| 2:B:20:MET:HE1   | 2:B:76:PHE:HD2   | 1.82                     | 0.43              |
| 1:A:780:LYS:O    | 1:A:782:ILE:N    | 2.51                     | 0.43              |
| 2:B:37:LYS:C     | 2:B:39:ASP:N     | 2.75                     | 0.43              |
| 3:C:109:VAL:O    | 3:C:113:LEU:HB2  | 2.18                     | 0.43              |
| 3:C:128:LEU:O    | 3:C:130:ASP:N    | 2.51                     | 0.43              |
| 1:A:280:ARG:HD3  | 1:A:319:VAL:CG1  | 2.48                     | 0.43              |
| 1:A:511:ASP:HA   | 1:A:514:MET:CB   | 2.40                     | 0.43              |
| 1:A:806:ILE:HD12 | 1:A:806:ILE:HA   | 1.78                     | 0.43              |
| 1:A:815:ILE:O    | 1:A:817:LYS:N    | 2.51                     | 0.43              |
| 2:B:97:ASP:O     | 2:B:98:GLU:C     | 2.61                     | 0.43              |
| 3:C:10:ASP:O     | 3:C:40:LEU:HD21  | 2.18                     | 0.43              |
| 1:A:229:TYR:HA   | 1:A:284:ILE:HG12 | 1.99                     | 0.43              |
| 1:A:284:ILE:CD1  | 1:A:285:PHE:N    | 2.72                     | 0.43              |
| 1:A:656:LEU:HD11 | 1:A:660:LEU:HD11 | 1.99                     | 0.43              |
| 1:A:786:GLN:NE2  | 3:C:110:LEU:O    | 2.51                     | 0.43              |
| 3:C:42:ILE:HG22  | 3:C:43:ASN:H     | 1.75                     | 0.43              |
| 1:A:120:CYS:CB   | 1:A:668:VAL:HG13 | 2.48                     | 0.43              |
| 1:A:499:GLU:HA   | 1:A:502:LYS:H    | 1.83                     | 0.43              |
| 3:C:36:VAL:HG21  | 3:C:68:PHE:CE2   | 2.53                     | 0.43              |
| 3:C:100:PHE:HD2  | 3:C:100:PHE:N    | 2.16                     | 0.43              |
| 3:C:106:LEU:CA   | 3:C:109:VAL:HG23 | 2.48                     | 0.43              |
| 1:A:598:ASN:ND2  | 1:A:598:ASN:O    | 2.52                     | 0.43              |
| 1:A:54:ASP:CG    | 1:A:70:LYS:HZ2   | 2.27                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:82:PHE:HE1   | 1:A:92:THR:H     | 1.66                     | 0.43              |
| 1:A:153:PHE:O    | 1:A:154:SER:C    | 2.61                     | 0.43              |
| 1:A:399:LEU:H    | 1:A:401:PRO:CG   | 2.31                     | 0.43              |
| 1:A:653:LEU:O    | 1:A:656:LEU:N    | 2.51                     | 0.43              |
| 1:A:833:VAL:O    | 1:A:835:PRO:CD   | 2.51                     | 0.43              |
| 3:C:62:SER:O     | 3:C:63:LEU:HD23  | 2.18                     | 0.43              |
| 1:A:75:GLN:NE2   | 1:A:95:ASN:HB2   | 2.31                     | 0.43              |
| 1:A:168:GLU:HG3  | 1:A:170:GLN:HE22 | 1.83                     | 0.43              |
| 1:A:181:GLY:O    | 1:A:182:LYS:C    | 2.58                     | 0.43              |
| 1:A:272:VAL:C    | 1:A:281:ASN:HD21 | 2.27                     | 0.43              |
| 1:A:353:ALA:O    | 1:A:356:LEU:HB2  | 2.18                     | 0.43              |
| 1:A:397:ALA:O    | 1:A:398:LEU:HD12 | 2.18                     | 0.43              |
| 1:A:399:LEU:HA   | 1:A:399:LEU:HD23 | 1.68                     | 0.43              |
| 1:A:667:PHE:N    | 1:A:667:PHE:CD2  | 2.87                     | 0.43              |
| 1:A:764:ALA:C    | 1:A:766:VAL:N    | 2.77                     | 0.43              |
| 1:A:240:SER:C    | 1:A:241:SER:O    | 2.62                     | 0.43              |
| 1:A:286:TYR:CE1  | 1:A:312:ILE:HB   | 2.54                     | 0.43              |
| 1:A:364:LYS:CB   | 1:A:373:GLU:CB   | 2.97                     | 0.43              |
| 1:A:719:ARG:HD2  | 1:A:719:ARG:HA   | 1.71                     | 0.43              |
| 1:A:773:MET:O    | 1:A:777:ARG:N    | 2.48                     | 0.43              |
| 2:B:90:ARG:HH11  | 2:B:142:VAL:HG13 | 1.83                     | 0.43              |
| 2:B:147:MET:HE3  | 2:B:151:SER:OG   | 2.19                     | 0.43              |
| 3:C:49:VAL:HA    | 3:C:52:VAL:HG23  | 2.00                     | 0.43              |
| 1:A:272:VAL:HG12 | 1:A:273:THR:HG23 | 2.01                     | 0.43              |
| 1:A:371:GLN:HE21 | 1:A:371:GLN:N    | 2.15                     | 0.43              |
| 1:A:374:SER:O    | 1:A:375:ASP:C    | 2.62                     | 0.43              |
| 1:A:532:ILE:O    | 1:A:533:LEU:C    | 2.61                     | 0.43              |
| 1:A:803:ASP:O    | 2:B:95:MET:HE1   | 2.18                     | 0.43              |
| 2:B:96:PHE:C     | 2:B:98:GLU:OE2   | 2.61                     | 0.43              |
| 1:A:43:PHE:CG    | 1:A:97:ALA:HB2   | 2.53                     | 0.42              |
| 1:A:417:ASN:CG   | 1:A:418:GLN:N    | 2.77                     | 0.42              |
| 2:B:146:ALA:O    | 2:B:151:SER:HB3  | 2.18                     | 0.42              |
| 1:A:214:SER:O    | 1:A:215:LEU:C    | 2.62                     | 0.42              |
| 1:A:288:ILE:HD12 | 1:A:352:THR:HG21 | 2.01                     | 0.42              |
| 1:A:560:ARG:H    | 1:A:560:ARG:HG2  | 1.55                     | 0.42              |
| 1:A:804:GLN:HB3  | 2:B:96:PHE:CZ    | 2.54                     | 0.42              |
| 1:A:807:GLY:CA   | 2:B:95:MET:CE    | 2.97                     | 0.42              |
| 3:C:5:GLN:O      | 3:C:9:ASP:OD1    | 2.37                     | 0.42              |
| 3:C:109:VAL:CA   | 3:C:113:LEU:HD13 | 2.47                     | 0.42              |
| 1:A:100:LEU:HD22 | 1:A:688:LEU:HD11 | 2.02                     | 0.42              |
| 1:A:271:ARG:NH1  | 1:A:280:ARG:O    | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:417:ASN:ND2  | 1:A:418:GLN:N    | 2.66                     | 0.42              |
| 1:A:495:LEU:O    | 1:A:498:GLU:CB   | 2.68                     | 0.42              |
| 1:A:812:GLN:HB2  | 2:B:120:PHE:CE1  | 2.54                     | 0.42              |
| 2:B:24:PHE:CE2   | 2:B:69:PHE:CA    | 3.03                     | 0.42              |
| 1:A:6:SER:OG     | 1:A:7:ASP:N      | 2.51                     | 0.42              |
| 1:A:189:VAL:HG12 | 1:A:193:LEU:HD11 | 2.02                     | 0.42              |
| 1:A:216:GLU:N    | 1:A:216:GLU:OE1  | 2.52                     | 0.42              |
| 1:A:287:GLN:HB2  | 1:A:328:PHE:HB2  | 2.00                     | 0.42              |
| 1:A:294:PRO:HB3  | 1:A:297:ASN:HD21 | 1.83                     | 0.42              |
| 1:A:764:ALA:O    | 1:A:766:VAL:HG22 | 2.20                     | 0.42              |
| 1:A:379:GLU:HA   | 1:A:382:LYS:CE   | 2.45                     | 0.42              |
| 1:A:485:GLN:OE1  | 1:A:485:GLN:HA   | 2.19                     | 0.42              |
| 2:B:97:ASP:OD1   | 2:B:101:THR:HG23 | 2.20                     | 0.42              |
| 2:B:99:GLN:C     | 2:B:100:GLU:HG3  | 2.45                     | 0.42              |
| 3:C:126:ILE:HG23 | 3:C:131:LEU:HB3  | 2.01                     | 0.42              |
| 1:A:171:SER:HB3  | 1:A:663:THR:OG1  | 2.20                     | 0.42              |
| 1:A:293:ILE:CD1  | 1:A:296:LEU:CD1  | 2.97                     | 0.42              |
| 1:A:567:LYS:HA   | 1:A:568:PRO:HD2  | 1.70                     | 0.42              |
| 1:A:762:PHE:CB   | 1:A:766:VAL:HG21 | 2.49                     | 0.42              |
| 2:B:24:PHE:CE1   | 2:B:35:VAL:HG22  | 2.55                     | 0.42              |
| 2:B:101:THR:OG1  | 2:B:103:LYS:O    | 2.37                     | 0.42              |
| 1:A:28:PHE:CD1   | 1:A:29:ASP:N     | 2.87                     | 0.42              |
| 1:A:223:ASN:O    | 1:A:225:VAL:N    | 2.52                     | 0.42              |
| 1:A:341:THR:OG1  | 1:A:344:GLU:HB2  | 2.18                     | 0.42              |
| 1:A:530:LEU:CD1  | 1:A:646:SER:OG   | 2.68                     | 0.42              |
| 1:A:530:LEU:CD2  | 1:A:650:ARG:HE   | 2.32                     | 0.42              |
| 1:A:534:GLU:C    | 1:A:537:CYS:SG   | 3.03                     | 0.42              |
| 1:A:614:LYS:O    | 1:A:616:PRO:HD3  | 2.20                     | 0.42              |
| 1:A:788:HIS:O    | 1:A:789:ILE:C    | 2.61                     | 0.42              |
| 2:B:125:MET:O    | 2:B:128:THR:N    | 2.51                     | 0.42              |
| 2:B:138:LYS:HD2  | 2:B:138:LYS:N    | 2.30                     | 0.42              |
| 1:A:33:ASN:O     | 1:A:34:CYS:HB3   | 2.20                     | 0.42              |
| 1:A:85:LEU:HB3   | 1:A:102:ASN:ND2  | 2.27                     | 0.42              |
| 1:A:271:ARG:NH2  | 1:A:279:GLU:CG   | 2.79                     | 0.42              |
| 1:A:404:LYS:HA   | 1:A:409:MET:CG   | 2.50                     | 0.42              |
| 1:A:447:ASP:CG   | 1:A:449:LYS:HZ2  | 2.28                     | 0.42              |
| 1:A:532:ILE:HG23 | 1:A:535:GLU:HG2  | 2.01                     | 0.42              |
| 2:B:147:MET:HE1  | 2:B:151:SER:OG   | 2.19                     | 0.42              |
| 3:C:122:VAL:C    | 3:C:125:ILE:HG22 | 2.45                     | 0.42              |
| 1:A:477:ILE:H    | 1:A:477:ILE:CD1  | 2.33                     | 0.42              |
| 2:B:54:LYS:HA    | 2:B:57:THR:OG1   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:46:ASN:O     | 3:C:47:GLU:C     | 2.62                     | 0.42              |
| 3:C:129:THR:O    | 3:C:130:ASP:C    | 2.63                     | 0.42              |
| 1:A:11:GLN:O     | 1:A:12:TYR:CD1   | 2.73                     | 0.42              |
| 1:A:24:GLN:O     | 1:A:81:LYS:HE3   | 2.20                     | 0.42              |
| 1:A:29:ASP:CG    | 1:A:30:GLY:N     | 2.78                     | 0.42              |
| 1:A:400:LYS:HA   | 1:A:414:GLN:N    | 2.35                     | 0.42              |
| 1:A:748:MET:O    | 1:A:750:PRO:HD3  | 2.20                     | 0.42              |
| 1:A:237:ASN:HD21 | 5:A:999:ANP:PA   | 2.43                     | 0.41              |
| 1:A:262:ILE:N    | 1:A:443:ASN:OD1  | 2.39                     | 0.41              |
| 1:A:390:ASN:ND2  | 1:A:393:ASP:N    | 2.58                     | 0.41              |
| 1:A:467:PHE:CD1  | 1:A:467:PHE:N    | 2.86                     | 0.41              |
| 1:A:532:ILE:C    | 1:A:535:GLU:H    | 2.28                     | 0.41              |
| 2:B:121:ASN:O    | 2:B:124:GLU:N    | 2.53                     | 0.41              |
| 1:A:327:GLU:O    | 1:A:330:LEU:HB2  | 2.20                     | 0.41              |
| 1:A:387:CYS:O    | 1:A:615:GLU:HB2  | 2.20                     | 0.41              |
| 1:A:418:GLN:O    | 1:A:422:SER:HB2  | 2.20                     | 0.41              |
| 1:A:535:GLU:O    | 1:A:537:CYS:N    | 2.46                     | 0.41              |
| 1:A:582:HIS:C    | 1:A:584:ALA:N    | 2.77                     | 0.41              |
| 1:A:783:SER:HB3  | 3:C:115:GLU:HG3  | 2.01                     | 0.41              |
| 1:A:795:ARG:C    | 1:A:797:ALA:H    | 2.27                     | 0.41              |
| 2:B:52:ASP:O     | 2:B:56:LEU:HG    | 2.20                     | 0.41              |
| 2:B:52:ASP:O     | 2:B:55:GLU:HB2   | 2.19                     | 0.41              |
| 2:B:72:PHE:C     | 2:B:74:SER:H     | 2.28                     | 0.41              |
| 1:A:85:LEU:CD2   | 1:A:91:MET:HG3   | 2.50                     | 0.41              |
| 1:A:120:CYS:O    | 1:A:669:ARG:N    | 2.51                     | 0.41              |
| 1:A:126:TYR:CD1  | 1:A:677:LYS:C    | 2.98                     | 0.41              |
| 1:A:134:ASP:O    | 1:A:135:SER:C    | 2.62                     | 0.41              |
| 1:A:248:ARG:NE   | 1:A:261:ASP:OD2  | 2.53                     | 0.41              |
| 1:A:397:ALA:O    | 1:A:401:PRO:HG2  | 2.05                     | 0.41              |
| 1:A:429:SER:OG   | 1:A:602:ILE:HD13 | 2.19                     | 0.41              |
| 1:A:684:ALA:HB3  | 1:A:685:GLU:OE2  | 2.20                     | 0.41              |
| 1:A:766:VAL:O    | 1:A:767:LEU:C    | 2.63                     | 0.41              |
| 1:A:794:ILE:O    | 1:A:794:ILE:CG2  | 2.65                     | 0.41              |
| 3:C:30:ALA:CB    | 3:C:55:THR:HB    | 2.46                     | 0.41              |
| 3:C:40:LEU:CB    | 3:C:72:TYR:OH    | 2.64                     | 0.41              |
| 3:C:91:LYS:C     | 3:C:93:PHE:H     | 2.29                     | 0.41              |
| 3:C:106:LEU:HD23 | 3:C:110:LEU:HD11 | 2.02                     | 0.41              |
| 3:C:130:ASP:O    | 3:C:130:ASP:CG   | 2.60                     | 0.41              |
| 1:A:95:ASN:O     | 1:A:95:ASN:OD1   | 2.38                     | 0.41              |
| 1:A:170:GLN:C    | 1:A:663:THR:HB   | 2.46                     | 0.41              |
| 1:A:234:THR:HA   | 1:A:279:GLU:OE1  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:251:PHE:HE1  | 1:A:456:ILE:HG12 | 1.86                     | 0.41              |
| 1:A:418:GLN:O    | 1:A:422:SER:CB   | 2.68                     | 0.41              |
| 1:A:429:SER:CB   | 1:A:602:ILE:HG23 | 2.51                     | 0.41              |
| 1:A:474:GLN:N    | 1:A:474:GLN:CD   | 2.78                     | 0.41              |
| 1:A:716:PHE:HE1  | 1:A:720:TYR:HD2  | 1.68                     | 0.41              |
| 1:A:763:LYS:O    | 1:A:766:VAL:HG21 | 2.18                     | 0.41              |
| 1:A:798:TYR:CE1  | 3:C:17:LEU:HD23  | 2.55                     | 0.41              |
| 1:A:805:ARG:HG2  | 3:C:20:PHE:CZ    | 2.55                     | 0.41              |
| 2:B:43:ILE:HD12  | 2:B:43:ILE:O     | 2.20                     | 0.41              |
| 2:B:147:MET:C    | 2:B:149:LYS:N    | 2.74                     | 0.41              |
| 3:C:58:MET:O     | 3:C:59:GLY:C     | 2.62                     | 0.41              |
| 3:C:122:VAL:O    | 3:C:126:ILE:CG1  | 2.65                     | 0.41              |
| 1:A:472:PHE:HB2  | 1:A:594:TRP:CZ3  | 2.55                     | 0.41              |
| 1:A:537:CYS:HA   | 1:A:595:LEU:HD21 | 2.01                     | 0.41              |
| 1:A:561:MET:HA   | 1:A:561:MET:HE2  | 2.03                     | 0.41              |
| 2:B:36:SER:O     | 2:B:39:ASP:N     | 2.53                     | 0.41              |
| 2:B:129:PHE:O    | 2:B:131:GLU:N    | 2.53                     | 0.41              |
| 3:C:106:LEU:O    | 3:C:110:LEU:CD1  | 2.69                     | 0.41              |
| 1:A:35:TRP:CE2   | 1:A:77:MET:HE2   | 2.56                     | 0.41              |
| 1:A:134:ASP:OD2  | 1:A:195:LYS:HG2  | 2.21                     | 0.41              |
| 1:A:185:ASN:C    | 1:A:187:LYS:N    | 2.78                     | 0.41              |
| 1:A:291:ASN:HD21 | 1:A:297:ASN:HD21 | 1.68                     | 0.41              |
| 1:A:308:LEU:HD23 | 1:A:308:LEU:HA   | 1.61                     | 0.41              |
| 1:A:488:PHE:O    | 1:A:492:MET:HG2  | 2.21                     | 0.41              |
| 1:A:604:GLU:CD   | 1:A:604:GLU:H    | 2.28                     | 0.41              |
| 3:C:70:PRO:HA    | 3:C:73:GLU:CG    | 2.51                     | 0.41              |
| 1:A:12:TYR:HD1   | 1:A:12:TYR:N     | 2.16                     | 0.41              |
| 1:A:186:THR:HG21 | 1:A:460:ASP:HB2  | 2.02                     | 0.41              |
| 1:A:447:ASP:OD1  | 1:A:447:ASP:C    | 2.63                     | 0.41              |
| 1:A:472:PHE:HB2  | 1:A:594:TRP:CE3  | 2.55                     | 0.41              |
| 1:A:721:SER:HA   | 1:A:742:ILE:HD13 | 2.03                     | 0.41              |
| 2:B:125:MET:O    | 2:B:128:THR:HB   | 2.21                     | 0.41              |
| 2:B:129:PHE:C    | 2:B:131:GLU:N    | 2.78                     | 0.41              |
| 3:C:87:MET:HE1   | 3:C:142:GLU:CG   | 2.51                     | 0.41              |
| 3:C:111:THR:HG22 | 3:C:122:VAL:HG21 | 2.02                     | 0.41              |
| 1:A:219:ILE:CG2  | 1:A:220:ILE:N    | 2.83                     | 0.41              |
| 1:A:290:SER:OG   | 1:A:325:VAL:HG12 | 2.21                     | 0.41              |
| 2:B:99:GLN:O     | 2:B:99:GLN:NE2   | 2.54                     | 0.41              |
| 2:B:119:ASN:O    | 2:B:120:PHE:C    | 2.63                     | 0.41              |
| 3:C:25:ASP:OD2   | 3:C:27:ALA:HB3   | 2.19                     | 0.41              |
| 1:A:55:GLU:C     | 1:A:56:ILE:HD13  | 2.46                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:126:TYR:CD1  | 1:A:677:LYS:CA   | 3.02                     | 0.41              |
| 1:A:129:LEU:HB2  | 1:A:131:ILE:CD1  | 2.51                     | 0.41              |
| 1:A:152:LEU:HD12 | 1:A:152:LEU:C    | 2.45                     | 0.41              |
| 1:A:286:TYR:HH   | 1:A:312:ILE:C    | 2.10                     | 0.41              |
| 1:A:334:ALA:O    | 1:A:338:LEU:HD23 | 2.20                     | 0.41              |
| 1:A:438:LEU:C    | 1:A:438:LEU:HD22 | 2.45                     | 0.41              |
| 1:A:537:CYS:CB   | 1:A:595:LEU:HD11 | 2.51                     | 0.41              |
| 1:A:577:HIS:CD2  | 1:A:591:ILE:H    | 2.39                     | 0.41              |
| 2:B:29:VAL:C     | 2:B:31:ARG:H     | 2.26                     | 0.41              |
| 2:B:76:PHE:C     | 2:B:78:ASP:N     | 2.79                     | 0.41              |
| 2:B:121:ASN:ND2  | 2:B:124:GLU:CG   | 2.78                     | 0.41              |
| 2:B:121:ASN:OD1  | 2:B:123:ASP:HB2  | 2.21                     | 0.41              |
| 3:C:5:GLN:C      | 3:C:7:GLU:N      | 2.78                     | 0.41              |
| 1:A:100:LEU:HB2  | 1:A:688:LEU:HD21 | 2.03                     | 0.41              |
| 1:A:128:ARG:HH12 | 1:A:188:LYS:HZ1  | 1.68                     | 0.41              |
| 1:A:250:HIS:ND1  | 1:A:455:TYR:HB3  | 2.35                     | 0.41              |
| 1:A:274:TYR:CD1  | 1:A:274:TYR:C    | 2.97                     | 0.41              |
| 1:A:325:VAL:CG2  | 1:A:326:GLU:N    | 2.82                     | 0.41              |
| 1:A:390:ASN:HB3  | 1:A:393:ASP:OD1  | 2.21                     | 0.41              |
| 1:A:447:ASP:O    | 1:A:448:THR:C    | 2.61                     | 0.41              |
| 1:A:534:GLU:OE2  | 1:A:646:SER:HB3  | 2.22                     | 0.41              |
| 1:A:788:HIS:CD2  | 3:C:149:MET:HA   | 2.56                     | 0.41              |
| 2:B:132:ALA:HA   | 2:B:133:PRO:HD3  | 1.70                     | 0.41              |
| 1:A:60:ILE:HG22  | 1:A:63:ASP:HB3   | 1.96                     | 0.40              |
| 1:A:173:LEU:HD21 | 1:A:660:LEU:CD2  | 2.50                     | 0.40              |
| 1:A:530:LEU:O    | 1:A:534:GLU:CG   | 2.53                     | 0.40              |
| 1:A:790:ARG:O    | 1:A:793:LEU:HB2  | 2.21                     | 0.40              |
| 2:B:24:PHE:HE2   | 2:B:69:PHE:CA    | 2.31                     | 0.40              |
| 2:B:99:GLN:O     | 2:B:99:GLN:HG3   | 2.21                     | 0.40              |
| 3:C:48:ASP:C     | 3:C:50:PHE:N     | 2.79                     | 0.40              |
| 1:A:135:SER:O    | 1:A:138:ALA:HB3  | 2.22                     | 0.40              |
| 1:A:645:ILE:O    | 1:A:645:ILE:HG22 | 2.20                     | 0.40              |
| 1:A:720:TYR:O    | 1:A:721:SER:C    | 2.64                     | 0.40              |
| 2:B:32:ASP:OD1   | 2:B:32:ASP:C     | 2.64                     | 0.40              |
| 2:B:101:THR:O    | 2:B:102:LYS:HB2  | 2.21                     | 0.40              |
| 1:A:66:THR:H     | 1:A:66:THR:HG23  | 1.63                     | 0.40              |
| 1:A:107:TYR:C    | 1:A:109:SER:N    | 2.78                     | 0.40              |
| 1:A:649:HIS:O    | 1:A:650:ARG:C    | 2.63                     | 0.40              |
| 1:A:737:THR:O    | 1:A:739:SER:N    | 2.54                     | 0.40              |
| 3:C:106:LEU:HA   | 3:C:109:VAL:CG2  | 2.51                     | 0.40              |
| 3:C:141:TYR:O    | 3:C:145:VAL:HG23 | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:174:ILE:CG2  | 1:A:668:VAL:HB   | 2.41                     | 0.40              |
| 1:A:288:ILE:HD11 | 1:A:352:THR:HG21 | 2.03                     | 0.40              |
| 1:A:598:ASN:O    | 1:A:598:ASN:CG   | 2.65                     | 0.40              |
| 1:A:741:LYS:O    | 1:A:745:GLY:N    | 2.36                     | 0.40              |
| 1:A:794:ILE:HD11 | 3:C:35:ASP:CB    | 2.52                     | 0.40              |
| 2:B:47:LEU:HD23  | 2:B:47:LEU:HA    | 1.75                     | 0.40              |
| 2:B:102:LYS:HA   | 2:B:141:TYR:OH   | 2.20                     | 0.40              |
| 2:B:106:ILE:O    | 2:B:106:ILE:CG1  | 2.69                     | 0.40              |
| 2:B:114:GLU:O    | 2:B:114:GLU:HG2  | 2.20                     | 0.40              |
| 3:C:33:LEU:O     | 3:C:34:GLY:C     | 2.64                     | 0.40              |
| 3:C:40:LEU:CD1   | 3:C:72:TYR:CE1   | 3.03                     | 0.40              |
| 3:C:109:VAL:O    | 3:C:113:LEU:CD1  | 2.69                     | 0.40              |
| 1:A:9:ASP:N      | 1:A:9:ASP:OD1    | 2.54                     | 0.40              |
| 1:A:221:GLN:C    | 1:A:223:ASN:N    | 2.79                     | 0.40              |
| 1:A:223:ASN:C    | 1:A:225:VAL:N    | 2.78                     | 0.40              |
| 1:A:319:VAL:HG23 | 1:A:322:ILE:HB   | 2.02                     | 0.40              |
| 1:A:322:ILE:HD13 | 1:A:322:ILE:HA   | 1.87                     | 0.40              |
| 1:A:468:ASP:OD1  | 1:A:468:ASP:N    | 2.54                     | 0.40              |
| 1:A:496:GLU:OE1  | 1:A:496:GLU:HA   | 2.21                     | 0.40              |
| 1:A:645:ILE:O    | 1:A:645:ILE:CG2  | 2.70                     | 0.40              |
| 3:C:99:GLY:C     | 3:C:141:TYR:CE2  | 2.96                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------------|--------------------------|-------------------|
| 1:A:452:ARG:O | 1:A:572:ASN:OD1[1_655] | 2.18                     | 0.02              |

## 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     | 757/835 (91%)   | 551 (73%) | 156 (21%) | 50 (7%)  | 1           | 5 |
| 2   | B     | 140/156 (90%)   | 93 (66%)  | 30 (21%)  | 17 (12%) | 0           | 1 |
| 3   | C     | 151/156 (97%)   | 100 (66%) | 35 (23%)  | 16 (11%) | 0           | 2 |
| All | All   | 1048/1147 (91%) | 744 (71%) | 221 (21%) | 83 (8%)  | 1           | 3 |

All (83) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 361 | MET  |
| 1   | A     | 413 | GLY  |
| 1   | A     | 504 | GLY  |
| 1   | A     | 526 | PRO  |
| 1   | A     | 604 | GLU  |
| 1   | A     | 645 | ILE  |
| 1   | A     | 718 | GLN  |
| 2   | B     | 41  | LYS  |
| 2   | B     | 94  | ALA  |
| 3   | C     | 54  | GLY  |
| 1   | A     | 8   | PRO  |
| 1   | A     | 81  | LYS  |
| 1   | A     | 164 | VAL  |
| 1   | A     | 193 | LEU  |
| 1   | A     | 272 | VAL  |
| 1   | A     | 307 | GLY  |
| 1   | A     | 316 | CYS  |
| 1   | A     | 335 | PHE  |
| 1   | A     | 373 | GLU  |
| 1   | A     | 375 | ASP  |
| 1   | A     | 416 | MET  |
| 1   | A     | 462 | ALA  |
| 1   | A     | 603 | ASN  |
| 1   | A     | 706 | GLY  |
| 1   | A     | 736 | LYS  |
| 2   | B     | 67  | LEU  |
| 2   | B     | 119 | ASN  |
| 3   | C     | 59  | GLY  |
| 3   | C     | 116 | ARG  |
| 3   | C     | 144 | PHE  |
| 3   | C     | 151 | GLY  |
| 3   | C     | 152 | PRO  |
| 1   | A     | 80  | PRO  |
| 1   | A     | 188 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 241 | SER  |
| 1   | A     | 429 | SER  |
| 1   | A     | 513 | GLY  |
| 1   | A     | 529 | ILE  |
| 1   | A     | 583 | TYR  |
| 1   | A     | 717 | LYS  |
| 1   | A     | 752 | GLU  |
| 1   | A     | 765 | GLY  |
| 1   | A     | 781 | ILE  |
| 2   | B     | 73  | LEU  |
| 2   | B     | 77  | SER  |
| 2   | B     | 80  | LEU  |
| 2   | B     | 112 | LEU  |
| 2   | B     | 113 | LEU  |
| 2   | B     | 120 | PHE  |
| 2   | B     | 130 | LYS  |
| 2   | B     | 146 | ALA  |
| 3   | C     | 33  | LEU  |
| 3   | C     | 56  | HIS  |
| 3   | C     | 71  | ALA  |
| 3   | C     | 129 | THR  |
| 1   | A     | 214 | SER  |
| 1   | A     | 277 | SER  |
| 1   | A     | 794 | ILE  |
| 1   | A     | 816 | ARG  |
| 1   | A     | 825 | GLN  |
| 2   | B     | 90  | ARG  |
| 3   | C     | 53  | GLY  |
| 3   | C     | 72  | TYR  |
| 3   | C     | 75  | LEU  |
| 1   | A     | 337 | ILE  |
| 1   | A     | 616 | PRO  |
| 2   | B     | 82  | GLY  |
| 1   | A     | 61  | VAL  |
| 1   | A     | 102 | ASN  |
| 1   | A     | 242 | ARG  |
| 1   | A     | 400 | LYS  |
| 1   | A     | 571 | PRO  |
| 1   | A     | 625 | PRO  |
| 2   | B     | 98  | GLU  |
| 3   | C     | 85  | ASP  |
| 3   | C     | 128 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 125 | ILE  |
| 2   | B     | 136 | GLY  |
| 1   | A     | 745 | GLY  |
| 2   | B     | 51  | PRO  |
| 1   | A     | 811 | ILE  |
| 1   | A     | 131 | ILE  |
| 1   | A     | 766 | VAL  |

### 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     | 614/728 (84%) | 487 (79%) | 127 (21%) | 1           | 7  |
| 2   | B     | 115/133 (86%) | 84 (73%)  | 31 (27%)  | 0           | 2  |
| 3   | C     | 119/132 (90%) | 99 (83%)  | 20 (17%)  | 2           | 11 |
| All | All   | 848/993 (85%) | 670 (79%) | 178 (21%) | 1           | 6  |

All (178) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | PHE  |
| 1   | A     | 7   | ASP  |
| 1   | A     | 12  | TYR  |
| 1   | A     | 48  | ILE  |
| 1   | A     | 51  | SER  |
| 1   | A     | 55  | GLU  |
| 1   | A     | 63  | ASP  |
| 1   | A     | 68  | THR  |
| 1   | A     | 72  | ASP  |
| 1   | A     | 94  | LEU  |
| 1   | A     | 96  | GLU  |
| 1   | A     | 111 | LEU  |
| 1   | A     | 112 | ILE  |
| 1   | A     | 115 | TYR  |
| 1   | A     | 118 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 120 | CYS  |
| 1   | A     | 121 | ILE  |
| 1   | A     | 131 | ILE  |
| 1   | A     | 133 | THR  |
| 1   | A     | 143 | LYS  |
| 1   | A     | 145 | LYS  |
| 1   | A     | 147 | GLU  |
| 1   | A     | 152 | LEU  |
| 1   | A     | 165 | THR  |
| 1   | A     | 166 | ASP  |
| 1   | A     | 174 | ILE  |
| 1   | A     | 190 | ILE  |
| 1   | A     | 196 | VAL  |
| 1   | A     | 214 | SER  |
| 1   | A     | 216 | GLU  |
| 1   | A     | 224 | PRO  |
| 1   | A     | 234 | THR  |
| 1   | A     | 257 | ILE  |
| 1   | A     | 266 | LEU  |
| 1   | A     | 284 | ILE  |
| 1   | A     | 288 | ILE  |
| 1   | A     | 300 | MET  |
| 1   | A     | 303 | THR  |
| 1   | A     | 305 | ASP  |
| 1   | A     | 314 | GLN  |
| 1   | A     | 321 | ASN  |
| 1   | A     | 324 | ASP  |
| 1   | A     | 335 | PHE  |
| 1   | A     | 343 | GLU  |
| 1   | A     | 347 | SER  |
| 1   | A     | 349 | PHE  |
| 1   | A     | 352 | THR  |
| 1   | A     | 361 | MET  |
| 1   | A     | 371 | GLN  |
| 1   | A     | 382 | LYS  |
| 1   | A     | 389 | ILE  |
| 1   | A     | 403 | VAL  |
| 1   | A     | 410 | VAL  |
| 1   | A     | 415 | ASN  |
| 1   | A     | 416 | MET  |
| 1   | A     | 417 | ASN  |
| 1   | A     | 418 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 426 | LEU  |
| 1   | A     | 436 | ASN  |
| 1   | A     | 438 | LEU  |
| 1   | A     | 452 | ARG  |
| 1   | A     | 455 | TYR  |
| 1   | A     | 459 | LEU  |
| 1   | A     | 467 | PHE  |
| 1   | A     | 470 | ASN  |
| 1   | A     | 472 | PHE  |
| 1   | A     | 475 | LEU  |
| 1   | A     | 476 | CYS  |
| 1   | A     | 482 | GLU  |
| 1   | A     | 501 | LYS  |
| 1   | A     | 507 | TRP  |
| 1   | A     | 512 | PHE  |
| 1   | A     | 515 | ASP  |
| 1   | A     | 517 | GLN  |
| 1   | A     | 526 | PRO  |
| 1   | A     | 529 | ILE  |
| 1   | A     | 543 | ASP  |
| 1   | A     | 544 | ASP  |
| 1   | A     | 546 | SER  |
| 1   | A     | 558 | LYS  |
| 1   | A     | 561 | MET  |
| 1   | A     | 587 | VAL  |
| 1   | A     | 591 | ILE  |
| 1   | A     | 595 | LEU  |
| 1   | A     | 599 | LYS  |
| 1   | A     | 602 | ILE  |
| 1   | A     | 604 | GLU  |
| 1   | A     | 610 | LEU  |
| 1   | A     | 615 | GLU  |
| 1   | A     | 617 | LEU  |
| 1   | A     | 627 | GLU  |
| 1   | A     | 644 | THR  |
| 1   | A     | 654 | ASN  |
| 1   | A     | 655 | LYS  |
| 1   | A     | 668 | VAL  |
| 1   | A     | 675 | GLU  |
| 1   | A     | 687 | VAL  |
| 1   | A     | 692 | GLN  |
| 1   | A     | 694 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 696 | VAL  |
| 1   | A     | 697 | LEU  |
| 1   | A     | 698 | GLU  |
| 1   | A     | 709 | SER  |
| 1   | A     | 711 | LEU  |
| 1   | A     | 722 | ILE  |
| 1   | A     | 726 | ASN  |
| 1   | A     | 737 | THR  |
| 1   | A     | 739 | SER  |
| 1   | A     | 746 | LEU  |
| 1   | A     | 755 | LEU  |
| 1   | A     | 757 | THR  |
| 1   | A     | 758 | THR  |
| 1   | A     | 760 | VAL  |
| 1   | A     | 766 | VAL  |
| 1   | A     | 769 | ASN  |
| 1   | A     | 774 | ARG  |
| 1   | A     | 777 | ARG  |
| 1   | A     | 783 | SER  |
| 1   | A     | 784 | MET  |
| 1   | A     | 789 | ILE  |
| 1   | A     | 792 | TYR  |
| 1   | A     | 794 | ILE  |
| 1   | A     | 805 | ARG  |
| 1   | A     | 806 | ILE  |
| 1   | A     | 808 | LEU  |
| 1   | A     | 814 | ASN  |
| 1   | A     | 823 | ASN  |
| 2   | B     | 14  | GLN  |
| 2   | B     | 30  | ASP  |
| 2   | B     | 35  | VAL  |
| 2   | B     | 36  | SER  |
| 2   | B     | 43  | ILE  |
| 2   | B     | 46  | GLN  |
| 2   | B     | 49  | ARG  |
| 2   | B     | 52  | ASP  |
| 2   | B     | 67  | LEU  |
| 2   | B     | 68  | ASN  |
| 2   | B     | 70  | THR  |
| 2   | B     | 71  | MET  |
| 2   | B     | 76  | PHE  |
| 2   | B     | 78  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 80  | LEU  |
| 2   | B     | 88  | THR  |
| 2   | B     | 96  | PHE  |
| 2   | B     | 98  | GLU  |
| 2   | B     | 100 | GLU  |
| 2   | B     | 102 | LYS  |
| 2   | B     | 106 | ILE  |
| 2   | B     | 107 | GLU  |
| 2   | B     | 109 | ILE  |
| 2   | B     | 119 | ASN  |
| 2   | B     | 130 | LYS  |
| 2   | B     | 134 | VAL  |
| 2   | B     | 139 | PHE  |
| 2   | B     | 145 | THR  |
| 2   | B     | 147 | MET  |
| 2   | B     | 149 | LYS  |
| 2   | B     | 154 | GLU  |
| 3   | C     | 5   | GLN  |
| 3   | C     | 15  | PHE  |
| 3   | C     | 22  | ASP  |
| 3   | C     | 24  | ARG  |
| 3   | C     | 33  | LEU  |
| 3   | C     | 36  | VAL  |
| 3   | C     | 55  | THR  |
| 3   | C     | 73  | GLU  |
| 3   | C     | 88  | GLU  |
| 3   | C     | 92  | THR  |
| 3   | C     | 98  | GLN  |
| 3   | C     | 100 | PHE  |
| 3   | C     | 102 | SER  |
| 3   | C     | 110 | LEU  |
| 3   | C     | 118 | SER  |
| 3   | C     | 135 | LEU  |
| 3   | C     | 140 | LYS  |
| 3   | C     | 141 | TYR  |
| 3   | C     | 148 | VAL  |
| 3   | C     | 153 | TYR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 75  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 218 | GLN  |
| 1   | A     | 223 | ASN  |
| 1   | A     | 275 | GLN  |
| 1   | A     | 276 | GLN  |
| 1   | A     | 297 | ASN  |
| 1   | A     | 313 | ASN  |
| 1   | A     | 314 | GLN  |
| 1   | A     | 321 | ASN  |
| 1   | A     | 346 | GLN  |
| 1   | A     | 357 | HIS  |
| 1   | A     | 371 | GLN  |
| 1   | A     | 390 | ASN  |
| 1   | A     | 417 | ASN  |
| 1   | A     | 418 | GLN  |
| 1   | A     | 421 | ASN  |
| 1   | A     | 478 | ASN  |
| 1   | A     | 486 | GLN  |
| 1   | A     | 517 | GLN  |
| 1   | A     | 554 | ASN  |
| 1   | A     | 559 | ASN  |
| 1   | A     | 577 | HIS  |
| 1   | A     | 582 | HIS  |
| 1   | A     | 586 | ASN  |
| 1   | A     | 598 | ASN  |
| 1   | A     | 603 | ASN  |
| 1   | A     | 605 | ASN  |
| 1   | A     | 654 | ASN  |
| 1   | A     | 664 | HIS  |
| 1   | A     | 694 | ASN  |
| 1   | A     | 769 | ASN  |
| 1   | A     | 802 | GLN  |
| 1   | A     | 823 | ASN  |
| 2   | B     | 68  | ASN  |
| 2   | B     | 91  | ASN  |
| 2   | B     | 99  | GLN  |
| 2   | B     | 119 | ASN  |
| 3   | C     | 43  | ASN  |
| 3   | C     | 46  | ASN  |
| 3   | C     | 98  | GLN  |
| 3   | C     | 132 | GLN  |
| 3   | C     | 138 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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 | $\# Z  > 2$ |
| 5   | ANP  | A     | 999 | 4    | 33,33,33     | 1.64 | 7 (21%)     | 45,52,52    | 1.53 | 6 (13%)     |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | ANP  | A     | 999 | 4    | -       | 6/18/38/38 | 0/3/3/3 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | A     | 999 | ANP  | PG-O1G | 3.93  | 1.52        | 1.46     |
| 5   | A     | 999 | ANP  | PG-N3B | 2.82  | 1.70        | 1.63     |
| 5   | A     | 999 | ANP  | C8-N9  | -2.66 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | A     | 999 | ANP  | PB-O3A  | 2.64  | 1.62        | 1.59     |
| 5   | A     | 999 | ANP  | O4'-C1' | -2.42 | 1.36        | 1.42     |
| 5   | A     | 999 | ANP  | PG-O2G  | -2.13 | 1.51        | 1.56     |
| 5   | A     | 999 | ANP  | C2'-C3' | -2.05 | 1.47        | 1.53     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 5   | A     | 999 | ANP  | O1G-PG-N3B | -4.45 | 105.22      | 111.77   |
| 5   | A     | 999 | ANP  | C2-N1-C6   | 4.08  | 125.43      | 118.73   |
| 5   | A     | 999 | ANP  | C5-C6-N6   | 2.96  | 130.62      | 123.29   |
| 5   | A     | 999 | ANP  | N3-C2-N1   | -2.92 | 124.17      | 128.58   |
| 5   | A     | 999 | ANP  | C5-C6-N1   | -2.54 | 111.06      | 117.51   |
| 5   | A     | 999 | ANP  | O4'-C1'-N9 | 2.32  | 112.55      | 108.09   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | A     | 999 | ANP  | PB-N3B-PG-O1G   |
| 5   | A     | 999 | ANP  | PG-N3B-PB-O1B   |
| 5   | A     | 999 | ANP  | C3'-C4'-C5'-O5' |
| 5   | A     | 999 | ANP  | O4'-C4'-C5'-O5' |
| 5   | A     | 999 | ANP  | PA-O3A-PB-O2B   |
| 5   | A     | 999 | ANP  | PA-O3A-PB-O1B   |

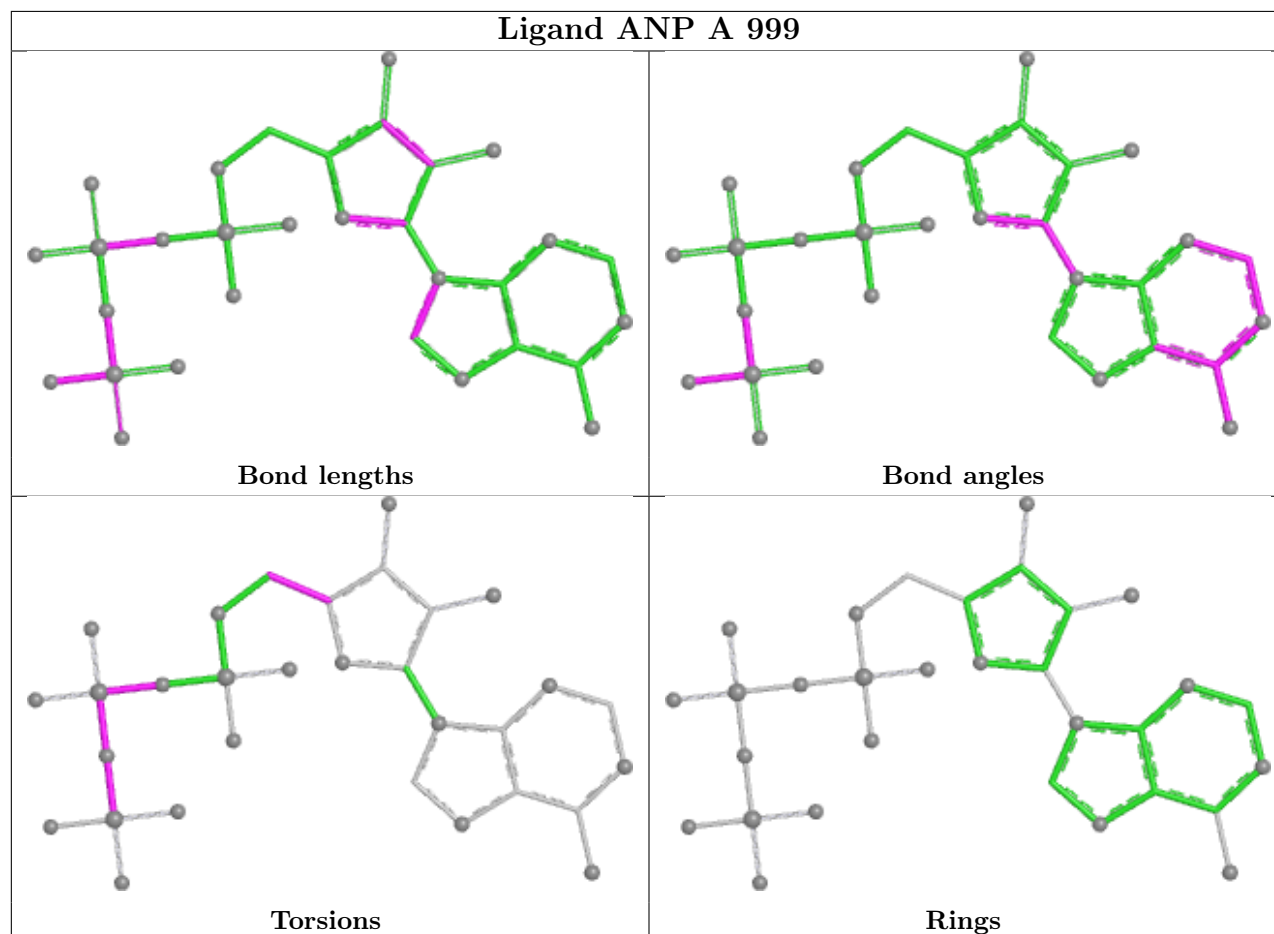
There are no ring outliers.

1 monomer is involved in 15 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | A     | 999 | ANP  | 15      | 0            |

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

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2 |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------|-------|-----------------------|-------|
| 1   | A     | 777/835 (93%)   | 0.07   | 12 (1%) | 72 49 | 25, 81, 106, 108      | 0     |
| 2   | B     | 142/156 (91%)   | -0.15  | 1 (0%)  | 84 66 | 41, 76, 103, 108      | 0     |
| 3   | C     | 153/156 (98%)   | -0.23  | 2 (1%)  | 75 53 | 28, 75, 99, 105       | 0     |
| All | All   | 1072/1147 (93%) | 0.00   | 15 (1%) | 73 51 | 25, 79, 106, 108      | 0     |

All (15) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 695 | GLY  | 4.3  |
| 2   | B     | 116 | MET  | 4.3  |
| 1   | A     | 253 | PRO  | 3.1  |
| 1   | A     | 738 | VAL  | 2.7  |
| 3   | C     | 21  | TRP  | 2.7  |
| 3   | C     | 90  | PHE  | 2.6  |
| 1   | A     | 394 | LEU  | 2.6  |
| 1   | A     | 28  | PHE  | 2.5  |
| 1   | A     | 350 | LYS  | 2.4  |
| 1   | A     | 728 | ILE  | 2.3  |
| 1   | A     | 110 | GLY  | 2.3  |
| 1   | A     | 830 | TYR  | 2.2  |
| 1   | A     | 122 | ALA  | 2.2  |
| 1   | A     | 109 | SER  | 2.1  |
| 1   | A     | 511 | ASP  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

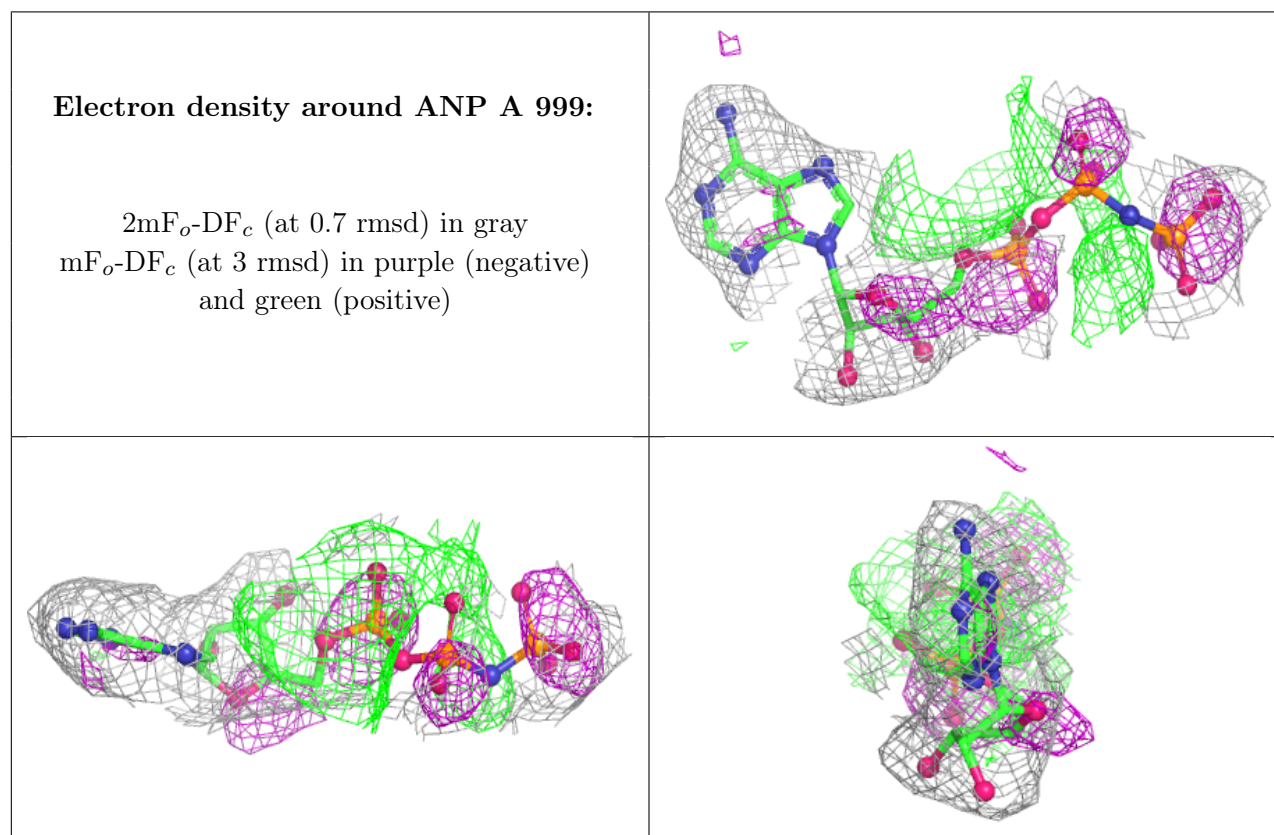
There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | MG   | A     | 903 | 1/1   | 0.79 | 0.17 | 58,58,58,58                 | 0     |
| 5   | ANP  | A     | 999 | 31/31 | 0.85 | 0.12 | 9,22,37,49                  | 0     |
| 6   | CA   | C     | 501 | 1/1   | 0.97 | 0.06 | 70,70,70,70                 | 0     |
| 4   | MG   | B     | 502 | 1/1   | 0.98 | 0.04 | 99,99,99,99                 | 0     |

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.