



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:37 PM UTC

PDB ID : 5WTK / pdb\_00005wtk  
Title : Crystal structure of RNP complex  
Authors : Liu, L.; Wang, Y.  
Deposited on : 2016-12-13  
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

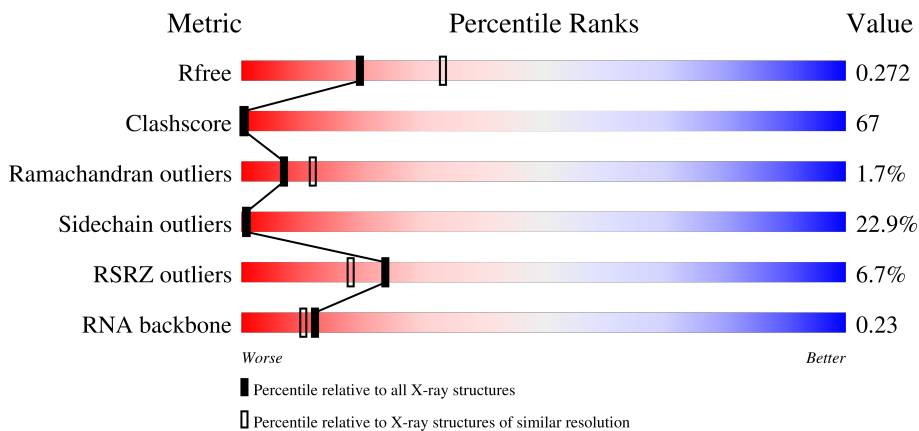
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|--------------------------|--|
| $R_{free}$            | 180053                   | 1110 (2.66-2.66)                                   |
| Clashscore            | 190562                   | 1141 (2.66-2.66)                                   |
| Ramachandran outliers | 187476                   | 1126 (2.66-2.66)                                   |
| Sidechain outliers    | 187428                   | 1126 (2.66-2.66)                                   |
| RSRZ outliers         | 180081                   | 1110 (2.66-2.66)                                   |
| RNA backbone          | 3983                     | 1090 (2.90-2.42)                                   |

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     | 1397   |                  |
| 2   | B     | 58     |                  |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10671 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 CRISPR-associated endoribonuclease C2c2.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
|     |       |          | Total | C    | N    | O    | S  |         |         |       |
| 1   | A     | 1215     | 9757  | 6260 | 1633 | 1846 | 18 | 0       | 0       | 0     |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1390    | LEU      | -      | expression tag | UNP P0DOC6 |
| A     | 1391    | GLU      | -      | expression tag | UNP P0DOC6 |
| A     | 1392    | HIS      | -      | expression tag | UNP P0DOC6 |
| A     | 1393    | HIS      | -      | expression tag | UNP P0DOC6 |
| A     | 1394    | HIS      | -      | expression tag | UNP P0DOC6 |
| A     | 1395    | HIS      | -      | expression tag | UNP P0DOC6 |
| A     | 1396    | HIS      | -      | expression tag | UNP P0DOC6 |
| A     | 1397    | HIS      | -      | expression tag | UNP P0DOC6 |

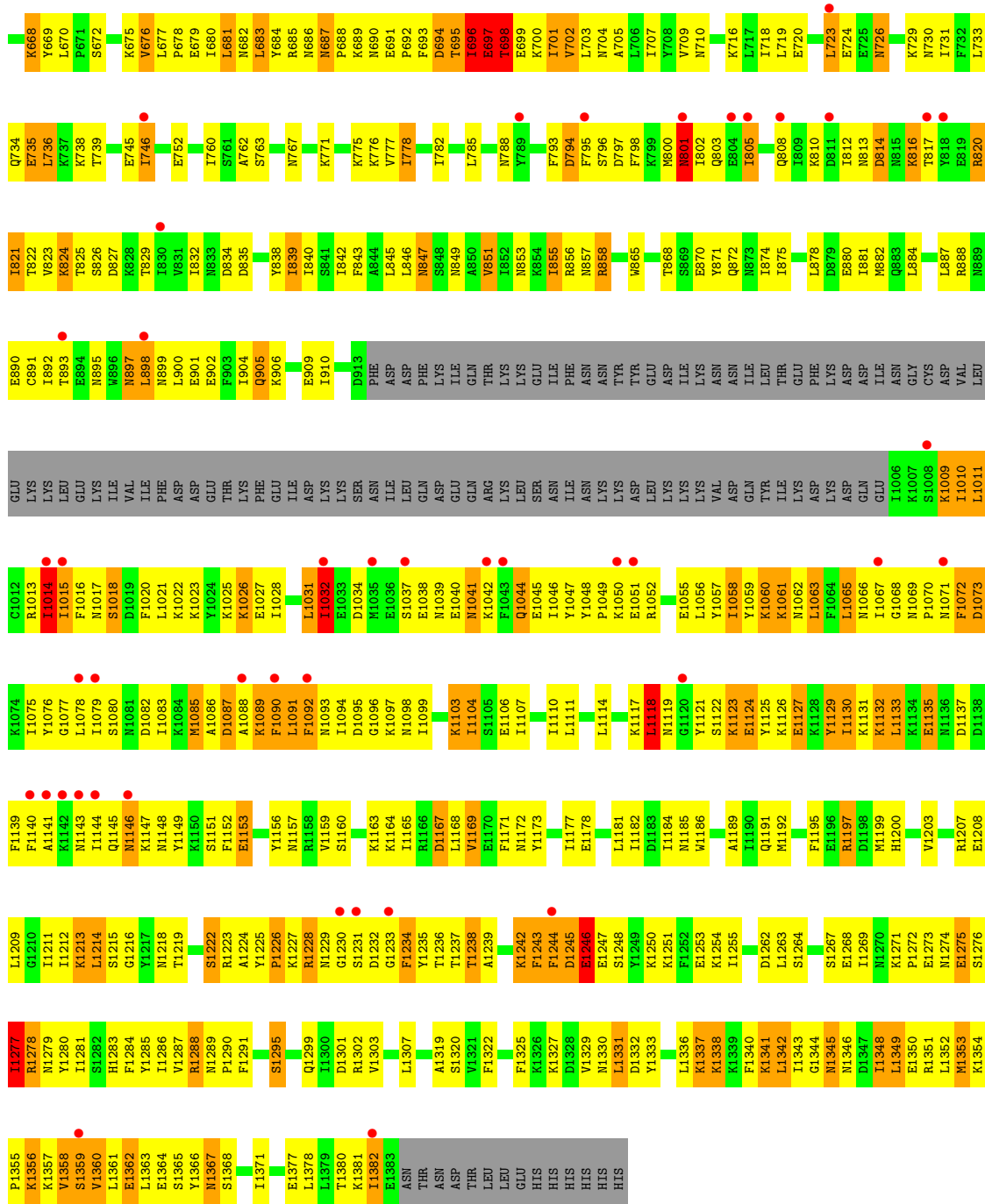
- Molecule 2 is a RNA chain called RNA (58-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | P  |         |         |       |
| 2   | B     | 40       | 849   | 383 | 161 | 266 | 39 | 0       | 0       | 0     |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 60       | Total | O  | 0       | 0       |
|     |       |          | 60    | 60 |         |         |
| 3   | B     | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 86.59Å 137.05Å 153.88Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)  | 40.41 – 2.65<br>40.41 – 2.65                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.5 (40.41-2.65)<br>98.4 (40.41-2.65)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.44 (at 2.65Å)   | Xtrriage         |
| Refinement program  | PHENIX (1.10.1_2155: ???)                                   | Depositor        |
| R, $R_{free}$   | 0.259 , 0.272<br>0.259 , 0.272                              | Depositor<br>DCC |
| $R_{free}$ test set   | 2621 reflections (4.86%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 56.2  | Xtrriage         |
| Anisotropy  | 0.112   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 30.4   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 10671   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 69.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.84         | 2/9906 (0.0%)  | 1.09        | 61/13336 (0.5%) |
| 2   | B     | 0.77         | 2/949 (0.2%)   | 0.93        | 2/1471 (0.1%)   |
| All | All   | 0.84         | 4/10855 (0.0%) | 1.08        | 63/14807 (0.4%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | B     | 16   | A    | O3'-P | -6.51 | 1.51        | 1.61     |
| 1   | A     | 1289 | ASN  | C-N   | 5.57  | 1.40        | 1.33     |
| 1   | A     | 1358 | VAL  | N-CA  | -5.19 | 1.40        | 1.46     |
| 2   | B     | 15   | A    | O3'-P | -5.04 | 1.53        | 1.61     |

All (63) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 215  | VAL  | N-CA-C  | 9.32  | 120.14      | 110.72   |
| 1   | A     | 462  | ILE  | N-CA-C  | -8.69 | 103.25      | 113.42   |
| 1   | A     | 1103 | LYS  | N-CA-C  | 8.29  | 124.58      | 113.97   |
| 1   | A     | 1209 | LEU  | N-CA-C  | -8.08 | 99.10       | 110.50   |
| 1   | A     | 367  | ILE  | N-CA-C  | 8.07  | 118.86      | 110.62   |
| 1   | A     | 1358 | VAL  | CB-CA-C | -7.92 | 100.23      | 111.40   |
| 1   | A     | 1118 | LEU  | N-CA-C  | 7.68  | 119.73      | 111.36   |
| 1   | A     | 524  | SER  | N-CA-C  | -7.50 | 104.65      | 113.88   |
| 1   | A     | 1288 | ARG  | N-CA-C  | 7.42  | 119.45      | 111.36   |
| 1   | A     | 397  | ASP  | N-CA-C  | 7.34  | 117.66      | 108.19   |
| 1   | A     | 539  | ASN  | N-CA-C  | 7.13  | 119.05      | 111.28   |
| 1   | A     | 1090 | PHE  | N-CA-C  | 7.08  | 122.58      | 113.88   |
| 1   | A     | 698  | THR  | N-CA-C  | 6.94  | 125.58      | 110.80   |
| 1   | A     | 91   | ILE  | N-CA-C  | 6.78  | 116.90      | 110.53   |
| 1   | A     | 377  | GLU  | N-CA-C  | -6.63 | 104.08      | 111.71   |
| 1   | A     | 1014 | ILE  | CB-CA-C | -6.56 | 103.28      | 112.14   |
| 1   | A     | 1345 | ASN  | CB-CA-C | -6.52 | 109.07      | 116.63   |
| 1   | A     | 1032 | ILE  | N-CA-C  | 6.49  | 117.28      | 110.72   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1289 | ASN  | CA-C-N      | -6.49 | 113.30      | 119.85   |
| 1   | A     | 1289 | ASN  | C-N-CA      | -6.49 | 113.30      | 119.85   |
| 2   | B     | 13   | C    | C4'-C3'-O3' | -6.47 | 103.30      | 113.00   |
| 1   | A     | 897  | ASN  | N-CA-C      | -6.38 | 99.63       | 109.14   |
| 1   | A     | 1360 | VAL  | CA-C-N      | 6.37  | 133.17      | 121.70   |
| 1   | A     | 1360 | VAL  | C-N-CA      | 6.37  | 133.17      | 121.70   |
| 1   | A     | 252  | ASN  | N-CA-C      | 6.31  | 117.82      | 111.07   |
| 1   | A     | 611  | GLN  | N-CA-C      | -6.29 | 104.42      | 111.28   |
| 1   | A     | 639  | ASN  | N-CA-C      | -6.20 | 99.76       | 109.25   |
| 1   | A     | 586  | ILE  | N-CA-C      | 6.17  | 116.91      | 110.62   |
| 1   | A     | 1129 | TYR  | N-CA-C      | -6.12 | 104.61      | 111.28   |
| 1   | A     | 1104 | ILE  | N-CA-C      | -6.01 | 104.49      | 110.62   |
| 1   | A     | 1364 | GLU  | CB-CA-C     | -6.01 | 100.28      | 109.89   |
| 1   | A     | 93   | ILE  | N-CA-C      | 5.97  | 116.23      | 107.75   |
| 1   | A     | 1277 | ILE  | N-CA-C      | -5.97 | 104.53      | 110.62   |
| 1   | A     | 1244 | PHE  | N-CA-C      | 5.85  | 117.33      | 111.07   |
| 1   | A     | 610  | LEU  | N-CA-C      | -5.84 | 101.19      | 109.96   |
| 1   | A     | 702  | VAL  | N-CA-C      | -5.75 | 106.21      | 111.67   |
| 1   | A     | 67   | ILE  | N-CA-C      | 5.74  | 115.93      | 110.42   |
| 1   | A     | 805  | ILE  | N-CA-C      | -5.65 | 104.85      | 110.62   |
| 1   | A     | 413  | ASP  | N-CA-C      | -5.59 | 103.16      | 110.53   |
| 1   | A     | 1135 | GLU  | N-CA-C      | 5.44  | 117.21      | 111.28   |
| 1   | A     | 1358 | VAL  | O-C-N       | 5.44  | 128.33      | 122.67   |
| 1   | A     | 810  | LYS  | N-CA-C      | -5.38 | 105.41      | 111.28   |
| 1   | A     | 564  | SER  | N-CA-C      | -5.37 | 105.08      | 111.69   |
| 2   | B     | 34   | A    | C3'-C2'-O2' | 5.36  | 118.75      | 110.70   |
| 1   | A     | 654  | ILE  | N-CA-C      | 5.32  | 116.09      | 110.72   |
| 1   | A     | 16   | LYS  | N-CA-C      | 5.29  | 117.13      | 111.36   |
| 1   | A     | 1238 | THR  | N-CA-C      | 5.27  | 117.11      | 111.36   |
| 1   | A     | 594  | THR  | N-CA-C      | 5.26  | 116.82      | 111.14   |
| 1   | A     | 598  | ASN  | N-CA-C      | 5.26  | 117.92      | 111.82   |
| 1   | A     | 851  | VAL  | N-CA-C      | 5.22  | 115.99      | 110.72   |
| 1   | A     | 1046 | ILE  | N-CA-C      | -5.21 | 107.08      | 111.56   |
| 1   | A     | 1246 | GLU  | N-CA-C      | -5.20 | 104.88      | 111.11   |
| 1   | A     | 895  | ASN  | N-CA-C      | 5.16  | 119.55      | 112.68   |
| 1   | A     | 239  | LEU  | N-CA-C      | -5.16 | 105.66      | 111.28   |
| 1   | A     | 640  | LEU  | N-CA-C      | 5.15  | 116.57      | 109.15   |
| 1   | A     | 1182 | ILE  | N-CA-C      | 5.14  | 115.86      | 110.62   |
| 1   | A     | 642  | VAL  | N-CA-C      | -5.11 | 105.41      | 110.62   |
| 1   | A     | 410  | VAL  | N-CA-C      | 5.10  | 115.32      | 110.53   |
| 1   | A     | 395  | ASN  | N-CA-C      | 5.09  | 116.91      | 111.36   |
| 1   | A     | 847  | ASN  | N-CA-C      | 5.07  | 116.69      | 109.14   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 428 | TYR  | N-CA-C | 5.06  | 116.61      | 111.14   |
| 1   | A     | 337 | LEU  | N-CA-C | 5.02  | 117.49      | 109.81   |
| 1   | A     | 814 | ASP  | N-CA-C | -5.01 | 101.42      | 109.39   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 9757  | 0        | 9502     | 1330    | 0            |
| 2   | B     | 849   | 0        | 438      | 78      | 0            |
| 3   | A     | 60    | 0        | 0        | 66      | 0            |
| 3   | B     | 5     | 0        | 0        | 5       | 0            |
| All | All   | 10671 | 0        | 9940     | 1383    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 67.

All (1383) 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:25:VAL:HG11  | 1:A:40:ILE:CD1    | 1.36                     | 1.52              |
| 1:A:898:LEU:HD13 | 1:A:1059:TYR:CD2  | 1.56                     | 1.37              |
| 1:A:604:ILE:HA   | 1:A:605:SER:CB    | 1.55                     | 1.34              |
| 1:A:633:GLU:CB   | 1:A:825:THR:HG21  | 1.58                     | 1.31              |
| 1:A:906:LYS:NZ   | 1:A:1022:LYS:HA   | 1.49                     | 1.28              |
| 1:A:83:LYS:HG2   | 1:A:85:LYS:CE     | 1.65                     | 1.26              |
| 1:A:899:ASN:CB   | 1:A:905:GLN:HG3   | 1.64                     | 1.25              |
| 1:A:246:ARG:HB2  | 3:A:1411:HOH:O    | 1.34                     | 1.23              |
| 1:A:407:HIS:CE1  | 3:A:1401:HOH:O    | 1.90                     | 1.21              |
| 1:A:94:GLU:CB    | 1:A:198:MET:HE1   | 1.72                     | 1.20              |
| 1:A:1011:LEU:O   | 1:A:1014:ILE:HG13 | 1.40                     | 1.20              |
| 1:A:76:HIS:CE1   | 1:A:79:ASN:HB3    | 1.78                     | 1.18              |
| 1:A:214:LYS:HA   | 3:A:1406:HOH:O    | 1.42                     | 1.17              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1271:LYS:HG2  | 3:A:1405:HOH:O    | 1.44                     | 1.16              |
| 1:A:1078:LEU:HD22 | 1:A:1377:GLU:HG2  | 1.21                     | 1.15              |
| 1:A:287:VAL:HG21  | 1:A:1125:TYR:OH   | 1.47                     | 1.15              |
| 1:A:84:LEU:HD11   | 1:A:194:LYS:HA    | 1.29                     | 1.14              |
| 1:A:1340:PHE:CE2  | 1:A:1342:LEU:HD11 | 1.83                     | 1.14              |
| 1:A:59:ILE:CG2    | 1:A:314:VAL:HG21  | 1.77                     | 1.13              |
| 1:A:906:LYS:CE    | 1:A:1022:LYS:HA   | 1.78                     | 1.13              |
| 1:A:80:ILE:HD11   | 1:A:200:LEU:HG    | 1.22                     | 1.13              |
| 1:A:1227:LYS:H    | 1:A:1238:THR:HG21 | 0.97                     | 1.13              |
| 1:A:83:LYS:HG2    | 1:A:85:LYS:HE2    | 1.14                     | 1.13              |
| 1:A:591:LYS:HE3   | 1:A:591:LYS:HA    | 1.14                     | 1.13              |
| 1:A:59:ILE:HG23   | 1:A:314:VAL:CG2   | 1.78                     | 1.12              |
| 1:A:76:HIS:CD2    | 1:A:79:ASN:HD22   | 1.67                     | 1.12              |
| 1:A:400:ILE:HD13  | 1:A:442:ILE:HD11  | 1.23                     | 1.12              |
| 1:A:548:GLY:N     | 1:A:594:THR:HG22  | 1.63                     | 1.11              |
| 1:A:1028:ILE:HA   | 1:A:1031:LEU:HD12 | 1.16                     | 1.11              |
| 1:A:1133:LEU:HD23 | 1:A:1139:PHE:CE2  | 1.86                     | 1.11              |
| 1:A:548:GLY:H     | 1:A:594:THR:CG2   | 1.64                     | 1.10              |
| 1:A:1271:LYS:CG   | 3:A:1405:HOH:O    | 1.98                     | 1.10              |
| 1:A:1340:PHE:HE2  | 1:A:1342:LEU:HD11 | 0.98                     | 1.10              |
| 1:A:25:VAL:CG1    | 1:A:40:ILE:HD11   | 1.81                     | 1.09              |
| 1:A:1342:LEU:HA   | 1:A:1349:LEU:HD23 | 1.21                     | 1.09              |
| 1:A:611:GLN:N     | 1:A:612:GLY:CA    | 2.16                     | 1.09              |
| 1:A:641:ASP:N     | 3:A:1403:HOH:O    | 1.85                     | 1.09              |
| 1:A:87:LYS:CB     | 1:A:90:ILE:HG12   | 1.84                     | 1.07              |
| 1:A:1350:GLU:HA   | 1:A:1352:LEU:H    | 1.04                     | 1.07              |
| 1:A:1083:ILE:HD13 | 1:A:1171:PHE:CE1  | 1.88                     | 1.07              |
| 1:A:1192:MET:HE2  | 1:A:1278:ARG:HA   | 1.08                     | 1.07              |
| 1:A:25:VAL:CG1    | 1:A:40:ILE:CD1    | 2.32                     | 1.07              |
| 1:A:407:HIS:NE2   | 3:A:1401:HOH:O    | 1.81                     | 1.06              |
| 1:A:80:ILE:CD1    | 1:A:200:LEU:HG    | 1.84                     | 1.06              |
| 1:A:724:GLU:OE1   | 1:A:724:GLU:N     | 1.88                     | 1.05              |
| 1:A:611:GLN:N     | 1:A:612:GLY:HA3   | 1.67                     | 1.05              |
| 1:A:525:THR:HG22  | 1:A:847:ASN:ND2   | 1.69                     | 1.05              |
| 1:A:548:GLY:H     | 1:A:594:THR:HG22  | 0.91                     | 1.05              |
| 1:A:638:LEU:HD13  | 1:A:638:LEU:H     | 1.22                     | 1.05              |
| 1:A:821:ILE:HD13  | 1:A:821:ILE:H     | 1.20                     | 1.04              |
| 1:A:1348:ILE:HB   | 1:A:1351:ARG:HH21 | 1.18                     | 1.04              |
| 1:A:1327:LYS:O    | 1:A:1356:LYS:HE3  | 1.56                     | 1.04              |
| 1:A:640:LEU:CD1   | 1:A:808:GLN:OE1   | 2.05                     | 1.04              |
| 1:A:1066:ASN:OD1  | 1:A:1067:ILE:N    | 1.89                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1086:ALA:HB1  | 1:A:1165:ILE:CG2  | 1.88                     | 1.04              |
| 1:A:1348:ILE:H    | 1:A:1348:ILE:HD12 | 1.20                     | 1.04              |
| 1:A:610:LEU:C     | 1:A:612:GLY:HA3   | 1.82                     | 1.04              |
| 2:B:14:G:P        | 3:B:102:HOH:O     | 2.14                     | 1.04              |
| 1:A:84:LEU:HD11   | 1:A:194:LYS:CA    | 1.88                     | 1.03              |
| 1:A:640:LEU:HD11  | 1:A:808:GLN:OE1   | 1.58                     | 1.03              |
| 1:A:1083:ILE:HD13 | 1:A:1171:PHE:HE1  | 1.17                     | 1.03              |
| 1:A:1230:GLY:HA2  | 1:A:1234:PHE:HB3  | 1.40                     | 1.03              |
| 1:A:1360:VAL:HG23 | 2:B:35:U:O2       | 1.58                     | 1.03              |
| 1:A:604:ILE:CA    | 1:A:605:SER:CB    | 2.37                     | 1.02              |
| 1:A:191:GLU:HG2   | 1:A:194:LYS:HE2   | 1.39                     | 1.02              |
| 1:A:438:ARG:NH2   | 3:A:1404:HOH:O    | 1.90                     | 1.02              |
| 1:A:1271:LYS:N    | 3:A:1405:HOH:O    | 1.91                     | 1.02              |
| 1:A:1359:SER:OG   | 1:A:1363:LEU:HG   | 1.59                     | 1.02              |
| 1:A:25:VAL:HG11   | 1:A:40:ILE:HD11   | 1.06                     | 1.02              |
| 1:A:1234:PHE:CD1  | 1:A:1235:TYR:N    | 2.26                     | 1.02              |
| 2:B:31:C:H2'      | 2:B:32:A:C4'      | 1.90                     | 1.02              |
| 1:A:243:MET:HA    | 3:A:1411:HOH:O    | 1.57                     | 1.02              |
| 1:A:1227:LYS:N    | 1:A:1238:THR:HG21 | 1.74                     | 1.01              |
| 1:A:1086:ALA:HB1  | 1:A:1165:ILE:HG23 | 1.02                     | 1.01              |
| 1:A:398:THR:C     | 3:A:1409:HOH:O    | 2.02                     | 1.01              |
| 1:A:1089:LYS:HA   | 1:A:1092:PHE:CB   | 1.91                     | 1.01              |
| 1:A:1060:LYS:NZ   | 1:A:1060:LYS:HA   | 1.76                     | 1.00              |
| 1:A:1086:ALA:CB   | 1:A:1165:ILE:HG23 | 1.90                     | 1.00              |
| 1:A:362:ILE:HG13  | 1:A:367:ILE:CD1   | 1.90                     | 1.00              |
| 1:A:1350:GLU:HA   | 1:A:1352:LEU:N    | 1.77                     | 0.99              |
| 1:A:399:GLU:N     | 3:A:1409:HOH:O    | 1.93                     | 0.99              |
| 1:A:898:LEU:CD1   | 1:A:1059:TYR:HD2  | 1.74                     | 0.99              |
| 1:A:326:ARG:NH1   | 1:A:327:ASN:OD1   | 1.95                     | 0.99              |
| 1:A:562:LEU:O     | 1:A:563:ASN:HB3   | 1.61                     | 0.98              |
| 1:A:801:ASN:ND2   | 1:A:802:ILE:HA    | 1.77                     | 0.98              |
| 1:A:25:VAL:HG11   | 1:A:40:ILE:HD12   | 1.44                     | 0.98              |
| 1:A:633:GLU:CB    | 1:A:825:THR:CG2   | 2.41                     | 0.98              |
| 2:B:18:G:O6       | 3:B:101:HOH:O     | 1.82                     | 0.97              |
| 1:A:1340:PHE:CE2  | 1:A:1342:LEU:CD1  | 2.46                     | 0.97              |
| 1:A:1133:LEU:CD2  | 1:A:1139:PHE:CE2  | 2.47                     | 0.97              |
| 1:A:1068:GLY:N    | 1:A:1069:ASN:HB2  | 1.80                     | 0.97              |
| 1:A:1028:ILE:HA   | 1:A:1031:LEU:CD1  | 1.93                     | 0.97              |
| 1:A:94:GLU:CB     | 1:A:198:MET:CE    | 2.42                     | 0.96              |
| 1:A:581:ILE:HD13  | 1:A:582:THR:N     | 1.80                     | 0.96              |
| 1:A:1133:LEU:HD23 | 1:A:1139:PHE:CD2  | 1.99                     | 0.96              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:344:LYS:HE2   | 1:A:500:VAL:O     | 1.64                     | 0.96              |
| 2:B:34:A:O2'      | 2:B:35:U:OP1      | 1.84                     | 0.95              |
| 1:A:76:HIS:CG     | 1:A:79:ASN:HD22   | 1.83                     | 0.95              |
| 1:A:636:LYS:HE3   | 1:A:887:LEU:HD23  | 1.48                     | 0.95              |
| 1:A:1359:SER:C    | 1:A:1361:LEU:HB2  | 1.91                     | 0.95              |
| 1:A:1359:SER:N    | 3:A:1408:HOH:O    | 1.92                     | 0.95              |
| 1:A:561:ILE:CD1   | 1:A:563:ASN:H     | 1.79                     | 0.95              |
| 1:A:1279:ASN:HD22 | 1:A:1283:HIS:HE1  | 1.02                     | 0.95              |
| 1:A:697:GLU:N     | 1:A:697:GLU:OE1   | 1.99                     | 0.95              |
| 1:A:390:GLU:HB2   | 1:A:403:ILE:HD11  | 1.47                     | 0.94              |
| 1:A:251:SER:OG    | 1:A:252:ASN:OD1   | 1.85                     | 0.94              |
| 1:A:80:ILE:HD11   | 1:A:200:LEU:CG    | 1.97                     | 0.94              |
| 1:A:1359:SER:CA   | 3:A:1408:HOH:O    | 2.16                     | 0.94              |
| 1:A:906:LYS:HZ1   | 1:A:1022:LYS:HA   | 1.31                     | 0.94              |
| 1:A:694:ASP:CB    | 1:A:800:MET:CB    | 2.45                     | 0.94              |
| 1:A:203:ILE:O     | 1:A:207:ILE:HD12  | 1.66                     | 0.93              |
| 1:A:641:ASP:CA    | 3:A:1403:HOH:O    | 2.13                     | 0.93              |
| 1:A:695:THR:O     | 1:A:696:ILE:HG23  | 1.67                     | 0.93              |
| 1:A:246:ARG:CB    | 3:A:1411:HOH:O    | 2.01                     | 0.93              |
| 1:A:243:MET:SD    | 1:A:246:ARG:NH1   | 2.42                     | 0.93              |
| 1:A:561:ILE:HD13  | 1:A:563:ASN:N     | 1.83                     | 0.92              |
| 1:A:525:THR:HG22  | 1:A:847:ASN:HD22  | 1.29                     | 0.92              |
| 1:A:898:LEU:HD13  | 1:A:1059:TYR:HD2  | 0.79                     | 0.92              |
| 1:A:449:VAL:CG1   | 1:A:456:LYS:H     | 1.82                     | 0.92              |
| 1:A:906:LYS:HE2   | 1:A:1022:LYS:HA   | 1.49                     | 0.92              |
| 1:A:1228:ARG:HG2  | 1:A:1228:ARG:HH11 | 1.35                     | 0.92              |
| 1:A:1348:ILE:HB   | 1:A:1351:ARG:NH2  | 1.83                     | 0.92              |
| 1:A:808:GLN:O     | 1:A:812:ILE:HG13  | 1.70                     | 0.92              |
| 1:A:1279:ASN:HD22 | 1:A:1283:HIS:CE1  | 1.86                     | 0.92              |
| 1:A:906:LYS:HE2   | 1:A:1022:LYS:CA   | 1.99                     | 0.92              |
| 1:A:1365:SER:OG   | 1:A:1368:SER:HB3  | 1.71                     | 0.91              |
| 1:A:686:ASN:HA    | 3:A:1423:HOH:O    | 1.68                     | 0.91              |
| 1:A:1028:ILE:CA   | 1:A:1031:LEU:HD12 | 2.00                     | 0.91              |
| 1:A:1342:LEU:HA   | 1:A:1349:LEU:CD2  | 2.00                     | 0.91              |
| 1:A:25:VAL:HG11   | 1:A:40:ILE:CG1    | 1.99                     | 0.91              |
| 1:A:73:ARG:HH21   | 1:A:73:ARG:HG3    | 1.35                     | 0.91              |
| 1:A:380:ILE:HD12  | 1:A:380:ILE:H     | 1.33                     | 0.91              |
| 1:A:76:HIS:NE2    | 1:A:79:ASN:HB3    | 1.84                     | 0.91              |
| 1:A:454:MET:HE2   | 1:A:455:GLU:N     | 1.86                     | 0.90              |
| 1:A:400:ILE:CD1   | 1:A:442:ILE:HD11  | 2.01                     | 0.90              |
| 1:A:272:SER:HB2   | 3:A:1421:HOH:O    | 1.72                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1278:ARG:HG2  | 1:A:1278:ARG:HH21 | 1.36                     | 0.90              |
| 1:A:681:LEU:HD21  | 1:A:707:ILE:HD11  | 1.52                     | 0.90              |
| 1:A:1254:LYS:NZ   | 3:A:1402:HOH:O    | 1.83                     | 0.90              |
| 1:A:690:ASN:OD1   | 1:A:795:PHE:HB2   | 1.72                     | 0.90              |
| 1:A:243:MET:CE    | 1:A:246:ARG:HH11  | 1.84                     | 0.90              |
| 1:A:362:ILE:HA    | 1:A:367:ILE:HD12  | 1.52                     | 0.89              |
| 1:A:1192:MET:CE   | 1:A:1278:ARG:HA   | 2.00                     | 0.89              |
| 2:B:34:A:H5''     | 2:B:34:A:H8       | 1.37                     | 0.89              |
| 1:A:362:ILE:CG1   | 1:A:367:ILE:CD1   | 2.51                     | 0.89              |
| 1:A:1268:GLU:O    | 1:A:1276:SER:HA   | 1.73                     | 0.89              |
| 1:A:20:LYS:O      | 1:A:20:LYS:NZ     | 2.06                     | 0.89              |
| 1:A:1192:MET:HE2  | 1:A:1278:ARG:CA   | 2.00                     | 0.88              |
| 2:B:14:G:OP2      | 3:B:102:HOH:O     | 1.91                     | 0.88              |
| 1:A:191:GLU:HG2   | 1:A:194:LYS:CE    | 2.02                     | 0.88              |
| 1:A:681:LEU:CD2   | 1:A:707:ILE:HD11  | 2.03                     | 0.88              |
| 1:A:1226:PRO:HA   | 1:A:1238:THR:CG2  | 2.03                     | 0.88              |
| 1:A:1234:PHE:HD1  | 1:A:1235:TYR:H    | 1.13                     | 0.88              |
| 1:A:677:LEU:HD11  | 1:A:707:ILE:HD12  | 1.53                     | 0.88              |
| 1:A:696:ILE:CG2   | 1:A:699:GLU:HB3   | 2.04                     | 0.88              |
| 1:A:1360:VAL:CG2  | 2:B:35:U:H1'      | 2.04                     | 0.87              |
| 1:A:199:SER:O     | 1:A:203:ILE:HG13  | 1.75                     | 0.87              |
| 1:A:213:GLU:O     | 3:A:1406:HOH:O    | 1.91                     | 0.87              |
| 1:A:816:LYS:HD3   | 1:A:816:LYS:H     | 1.38                     | 0.87              |
| 1:A:897:ASN:CB    | 1:A:1016:PHE:CZ   | 2.57                     | 0.87              |
| 1:A:528:GLU:HG3   | 1:A:847:ASN:HB3   | 1.57                     | 0.87              |
| 1:A:898:LEU:CD1   | 1:A:1059:TYR:CD2  | 2.52                     | 0.87              |
| 1:A:1275:GLU:N    | 3:A:1413:HOH:O    | 2.08                     | 0.87              |
| 1:A:407:HIS:CE1   | 1:A:411:ASN:HD22  | 1.92                     | 0.87              |
| 1:A:767:ASN:O     | 3:A:1407:HOH:O    | 1.92                     | 0.86              |
| 1:A:720:GLU:O     | 1:A:731:ILE:HD11  | 1.75                     | 0.86              |
| 1:A:87:LYS:CB     | 1:A:90:ILE:CG1    | 2.54                     | 0.86              |
| 1:A:696:ILE:HG21  | 1:A:699:GLU:HB3   | 1.57                     | 0.86              |
| 1:A:83:LYS:HG2    | 1:A:85:LYS:HE3    | 1.56                     | 0.86              |
| 1:A:900:LEU:O     | 1:A:1056:LEU:HA   | 1.76                     | 0.86              |
| 1:A:1047:TYR:C    | 1:A:1058:ILE:HG13 | 2.00                     | 0.86              |
| 1:A:1197:ARG:HH11 | 1:A:1197:ARG:HB3  | 1.41                     | 0.86              |
| 1:A:83:LYS:CG     | 1:A:85:LYS:HE2    | 2.05                     | 0.85              |
| 1:A:397:ASP:OD1   | 1:A:398:THR:N     | 2.09                     | 0.85              |
| 3:A:1409:HOH:O    | 2:B:16:A:C2       | 2.29                     | 0.85              |
| 1:A:248:LYS:C     | 1:A:256:LEU:HD12  | 2.01                     | 0.85              |
| 1:A:705:ALA:O     | 1:A:709:VAL:HG23  | 1.77                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1349:LEU:O    | 1:A:1351:ARG:HB3  | 1.77                     | 0.85              |
| 1:A:1078:LEU:HD22 | 1:A:1377:GLU:CG   | 2.07                     | 0.85              |
| 1:A:1227:LYS:O    | 1:A:1234:PHE:HD2  | 1.60                     | 0.85              |
| 1:A:314:VAL:N     | 3:A:1415:HOH:O    | 2.09                     | 0.84              |
| 1:A:384:ILE:HG12  | 1:A:463:LEU:HD12  | 1.59                     | 0.84              |
| 1:A:1047:TYR:C    | 1:A:1058:ILE:CG1  | 2.50                     | 0.84              |
| 1:A:528:GLU:O     | 3:A:1410:HOH:O    | 1.94                     | 0.84              |
| 1:A:561:ILE:CD1   | 1:A:563:ASN:N     | 2.39                     | 0.84              |
| 1:A:760:ILE:O     | 1:A:763:SER:HB3   | 1.77                     | 0.84              |
| 1:A:357:PHE:CD2   | 1:A:423:GLU:HG2   | 2.13                     | 0.84              |
| 2:B:31:C:H2'      | 2:B:32:A:C5'      | 2.08                     | 0.84              |
| 1:A:1047:TYR:O    | 1:A:1058:ILE:HG12 | 1.78                     | 0.83              |
| 1:A:1227:LYS:O    | 1:A:1234:PHE:CD2  | 2.31                     | 0.83              |
| 1:A:1085:MET:SD   | 1:A:1085:MET:N    | 2.52                     | 0.83              |
| 1:A:1359:SER:C    | 3:A:1408:HOH:O    | 2.20                     | 0.83              |
| 1:A:1060:LYS:HA   | 1:A:1060:LYS:CE   | 2.08                     | 0.83              |
| 1:A:245:ILE:O     | 1:A:249:ILE:HG22  | 1.78                     | 0.83              |
| 1:A:537:ASN:ND2   | 1:A:540:ASN:H     | 1.76                     | 0.83              |
| 1:A:591:LYS:HE3   | 1:A:591:LYS:CA    | 2.03                     | 0.83              |
| 1:A:192:ILE:HG22  | 1:A:245:ILE:HD11  | 1.61                     | 0.82              |
| 1:A:379:LYS:O     | 3:A:1401:HOH:O    | 1.95                     | 0.82              |
| 1:A:362:ILE:HG13  | 1:A:367:ILE:HD11  | 1.62                     | 0.82              |
| 2:B:15:A:O2'      | 2:B:16:A:OP2      | 1.96                     | 0.82              |
| 1:A:1050:LYS:N    | 1:A:1051:GLU:HA   | 1.94                     | 0.82              |
| 1:A:902:GLU:HG2   | 1:A:1057:TYR:CD1  | 2.14                     | 0.82              |
| 1:A:358:PHE:HB3   | 1:A:480:THR:HG21  | 1.62                     | 0.81              |
| 1:A:532:ILE:HD11  | 1:A:533:PHE:CE2   | 2.15                     | 0.81              |
| 1:A:591:LYS:HA    | 1:A:591:LYS:CE    | 2.04                     | 0.81              |
| 1:A:84:LEU:HD23   | 1:A:84:LEU:H      | 1.43                     | 0.81              |
| 1:A:1041:ASN:HD22 | 1:A:1042:LYS:H    | 1.26                     | 0.81              |
| 1:A:243:MET:HE1   | 1:A:246:ARG:NH1   | 1.96                     | 0.81              |
| 1:A:588:LYS:O     | 1:A:592:ILE:HD12  | 1.81                     | 0.81              |
| 1:A:630:SER:HB2   | 1:A:884:LEU:HD22  | 1.62                     | 0.81              |
| 1:A:76:HIS:CD2    | 1:A:79:ASN:ND2    | 2.47                     | 0.81              |
| 1:A:399:GLU:CA    | 3:A:1409:HOH:O    | 2.26                     | 0.81              |
| 1:A:525:THR:CG2   | 1:A:847:ASN:ND2   | 2.44                     | 0.81              |
| 1:A:1244:PHE:HB3  | 1:A:1245:ASP:OD1  | 1.80                     | 0.81              |
| 1:A:1088:ALA:O    | 1:A:1092:PHE:CB   | 2.28                     | 0.81              |
| 1:A:449:VAL:HG12  | 1:A:455:GLU:HA    | 1.61                     | 0.80              |
| 1:A:315:LYS:HG3   | 1:A:316:LYS:HE2   | 1.64                     | 0.80              |
| 1:A:454:MET:HE2   | 1:A:454:MET:C     | 2.06                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1059:TYR:HE1  | 1:A:1061:LYS:CB   | 1.94                     | 0.80              |
| 1:A:696:ILE:HA    | 1:A:697:GLU:C     | 2.04                     | 0.80              |
| 1:A:1226:PRO:HA   | 1:A:1238:THR:HG22 | 1.63                     | 0.80              |
| 1:A:270:LYS:HA    | 1:A:270:LYS:CE    | 2.09                     | 0.80              |
| 1:A:1360:VAL:N    | 1:A:1362:GLU:H    | 1.79                     | 0.80              |
| 1:A:906:LYS:HE2   | 1:A:1022:LYS:N    | 1.96                     | 0.80              |
| 1:A:906:LYS:NZ    | 1:A:1022:LYS:CA   | 2.40                     | 0.80              |
| 1:A:404:PHE:CG    | 1:A:439:ILE:CD1   | 2.65                     | 0.79              |
| 1:A:1340:PHE:CD2  | 1:A:1342:LEU:CD1  | 2.65                     | 0.79              |
| 1:A:1075:ILE:HG23 | 1:A:1177:ILE:HG21 | 1.64                     | 0.79              |
| 1:A:1103:LYS:HA   | 1:A:1106:GLU:HB2  | 1.62                     | 0.79              |
| 1:A:532:ILE:HD11  | 1:A:533:PHE:CD2   | 2.17                     | 0.79              |
| 1:A:1127:GLU:O    | 1:A:1130:ILE:HG22 | 1.80                     | 0.79              |
| 1:A:1147:LYS:N    | 3:A:1416:HOH:O    | 2.14                     | 0.79              |
| 1:A:270:LYS:HA    | 1:A:270:LYS:HE3   | 1.62                     | 0.79              |
| 1:A:315:LYS:HG3   | 1:A:316:LYS:CE    | 2.11                     | 0.79              |
| 1:A:358:PHE:CB    | 1:A:480:THR:HG21  | 2.12                     | 0.79              |
| 1:A:212:THR:N     | 1:A:213:GLU:HA    | 1.97                     | 0.78              |
| 1:A:614:GLN:CB    | 1:A:835:ASP:OD1   | 2.31                     | 0.78              |
| 1:A:532:ILE:O     | 1:A:557:LEU:CD1   | 2.30                     | 0.78              |
| 1:A:906:LYS:CE    | 1:A:1022:LYS:CA   | 2.58                     | 0.78              |
| 1:A:616:ASP:O     | 1:A:620:VAL:HG22  | 1.83                     | 0.78              |
| 1:A:891:CYS:SG    | 1:A:892:ILE:N     | 2.55                     | 0.78              |
| 1:A:1133:LEU:CD2  | 1:A:1139:PHE:CD2  | 2.67                     | 0.78              |
| 2:B:31:C:H2'      | 2:B:32:A:H4'      | 1.64                     | 0.78              |
| 1:A:557:LEU:HD12  | 1:A:558:ASP:N     | 1.98                     | 0.78              |
| 1:A:1118:LEU:HD13 | 1:A:1126:LYS:HG2  | 1.65                     | 0.78              |
| 1:A:102:THR:O     | 3:A:1412:HOH:O    | 2.02                     | 0.78              |
| 1:A:1278:ARG:HG2  | 1:A:1278:ARG:NH2  | 1.98                     | 0.77              |
| 1:A:505:PHE:HD2   | 2:B:22:C:O2'      | 1.66                     | 0.77              |
| 2:B:50:U:H6       | 2:B:50:U:H5'      | 1.48                     | 0.77              |
| 1:A:287:VAL:HG21  | 1:A:1125:TYR:HH   | 1.48                     | 0.77              |
| 1:A:316:LYS:CD    | 1:A:316:LYS:H     | 1.96                     | 0.77              |
| 1:A:314:VAL:CA    | 3:A:1415:HOH:O    | 2.33                     | 0.77              |
| 1:A:362:ILE:CA    | 1:A:367:ILE:HD12  | 2.15                     | 0.77              |
| 1:A:404:PHE:CD1   | 1:A:439:ILE:HD11  | 2.19                     | 0.77              |
| 1:A:898:LEU:HD13  | 1:A:1059:TYR:CE2  | 2.20                     | 0.77              |
| 1:A:263:LEU:O     | 1:A:264:ASN:ND2   | 2.18                     | 0.76              |
| 1:A:391:LEU:HD12  | 1:A:459:ILE:HD11  | 1.65                     | 0.76              |
| 1:A:74:LYS:HD3    | 1:A:74:LYS:N      | 1.99                     | 0.76              |
| 1:A:1059:TYR:CE1  | 1:A:1061:LYS:CB   | 2.68                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:413:ASP:HA    | 1:A:414:SER:HB3   | 1.67                     | 0.76              |
| 1:A:399:GLU:HA    | 3:A:1409:HOH:O    | 1.83                     | 0.76              |
| 1:A:816:LYS:H     | 1:A:816:LYS:CD    | 1.97                     | 0.76              |
| 1:A:1044:GLN:HA   | 1:A:1048:TYR:CE1  | 2.21                     | 0.76              |
| 1:A:32:ASP:C      | 3:A:1417:HOH:O    | 2.28                     | 0.76              |
| 1:A:68:LEU:HD23   | 1:A:208:ILE:CG2   | 2.15                     | 0.76              |
| 1:A:1359:SER:O    | 1:A:1361:LEU:HB2  | 1.84                     | 0.76              |
| 1:A:490:LEU:HD21  | 1:A:500:VAL:HG11  | 1.68                     | 0.76              |
| 1:A:570:ARG:HA    | 1:A:575:ILE:HG22  | 1.67                     | 0.76              |
| 1:A:1360:VAL:H    | 1:A:1362:GLU:H    | 1.33                     | 0.76              |
| 1:A:1340:PHE:CD2  | 1:A:1342:LEU:HD12 | 2.21                     | 0.75              |
| 1:A:291:VAL:O     | 1:A:294:ILE:HG22  | 1.85                     | 0.75              |
| 1:A:1360:VAL:HB   | 2:B:35:U:O4'      | 1.86                     | 0.75              |
| 1:A:1011:LEU:O    | 1:A:1014:ILE:CG1  | 2.31                     | 0.75              |
| 1:A:248:LYS:HB3   | 1:A:256:LEU:CD1   | 2.16                     | 0.75              |
| 1:A:1049:PRO:HA   | 1:A:1050:LYS:CB   | 2.17                     | 0.75              |
| 1:A:1146:ASN:N    | 3:A:1418:HOH:O    | 2.20                     | 0.75              |
| 1:A:1227:LYS:H    | 1:A:1238:THR:CG2  | 1.90                     | 0.75              |
| 1:A:235:ILE:HD13  | 1:A:291:VAL:HG22  | 1.67                     | 0.75              |
| 1:A:1093:ASN:HB2  | 1:A:1096:GLY:H    | 1.52                     | 0.74              |
| 1:A:1382:ILE:O    | 1:A:1382:ILE:HG13 | 1.87                     | 0.74              |
| 1:A:695:THR:HG23  | 1:A:696:ILE:N     | 2.01                     | 0.74              |
| 1:A:893:THR:O     | 1:A:897:ASN:O     | 2.05                     | 0.74              |
| 1:A:1060:LYS:HA   | 1:A:1060:LYS:HZ2  | 1.50                     | 0.74              |
| 1:A:853:ASN:ND2   | 2:B:30:A:N7       | 2.34                     | 0.74              |
| 1:A:638:LEU:HD13  | 1:A:638:LEU:N     | 1.99                     | 0.74              |
| 1:A:390:GLU:CB    | 1:A:403:ILE:HD11  | 2.18                     | 0.74              |
| 1:A:561:ILE:HD13  | 1:A:563:ASN:H     | 1.43                     | 0.74              |
| 1:A:640:LEU:O     | 1:A:643:VAL:HG23  | 1.88                     | 0.74              |
| 1:A:1118:LEU:HD12 | 1:A:1126:LYS:CD   | 2.17                     | 0.74              |
| 1:A:1041:ASN:O    | 1:A:1044:GLN:HB3  | 1.87                     | 0.74              |
| 1:A:561:ILE:HD11  | 1:A:563:ASN:H     | 1.50                     | 0.74              |
| 1:A:1168:LEU:H    | 1:A:1168:LEU:HD12 | 1.52                     | 0.74              |
| 1:A:84:LEU:CD1    | 1:A:194:LYS:CA    | 2.65                     | 0.74              |
| 1:A:801:ASN:CG    | 1:A:802:ILE:HA    | 2.13                     | 0.74              |
| 1:A:374:ILE:HD13  | 1:A:428:TYR:CE1   | 2.22                     | 0.73              |
| 1:A:1028:ILE:O    | 1:A:1032:ILE:HG13 | 1.87                     | 0.73              |
| 1:A:84:LEU:CD1    | 1:A:194:LYS:N     | 2.51                     | 0.73              |
| 1:A:1068:GLY:H    | 1:A:1069:ASN:HB2  | 1.52                     | 0.73              |
| 2:B:35:U:N3       | 3:B:103:HOH:O     | 2.10                     | 0.73              |
| 1:A:1348:ILE:O    | 1:A:1351:ARG:HB2  | 1.87                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:78:GLY:O      | 1:A:85:LYS:HG2    | 1.89                     | 0.73              |
| 1:A:404:PHE:CG    | 1:A:439:ILE:HD11  | 2.23                     | 0.73              |
| 1:A:32:ASP:HA     | 3:A:1417:HOH:O    | 1.88                     | 0.73              |
| 1:A:248:LYS:HB3   | 1:A:256:LEU:HD11  | 1.69                     | 0.73              |
| 1:A:359:VAL:HG12  | 1:A:1255:ILE:HD12 | 1.69                     | 0.73              |
| 1:A:617:TYR:HA    | 1:A:620:VAL:CG2   | 2.19                     | 0.73              |
| 1:A:1207:ARG:HD3  | 1:A:1214:LEU:HD22 | 1.71                     | 0.73              |
| 1:A:1360:VAL:HG21 | 2:B:35:U:H1'      | 1.70                     | 0.73              |
| 1:A:357:PHE:HD2   | 1:A:423:GLU:HG2   | 1.53                     | 0.73              |
| 1:A:83:LYS:O      | 1:A:83:LYS:HD3    | 1.88                     | 0.72              |
| 1:A:1360:VAL:HB   | 2:B:35:U:C1'      | 2.19                     | 0.72              |
| 1:A:84:LEU:H      | 1:A:84:LEU:CD2    | 2.01                     | 0.72              |
| 1:A:683:LEU:C     | 1:A:683:LEU:HD12  | 2.14                     | 0.72              |
| 1:A:617:TYR:HA    | 1:A:620:VAL:HG22  | 1.71                     | 0.72              |
| 1:A:449:VAL:HG11  | 1:A:456:LYS:H     | 1.51                     | 0.72              |
| 1:A:557:LEU:HD12  | 1:A:558:ASP:H     | 1.54                     | 0.72              |
| 1:A:249:ILE:HG13  | 1:A:257:GLY:HA2   | 1.72                     | 0.72              |
| 1:A:290:THR:HG22  | 1:A:292:GLU:H     | 1.54                     | 0.72              |
| 1:A:68:LEU:HD23   | 1:A:208:ILE:HG21  | 1.70                     | 0.72              |
| 1:A:436:LYS:HA    | 1:A:439:ILE:HD12  | 1.71                     | 0.72              |
| 1:A:639:ASN:H     | 1:A:639:ASN:HD22  | 1.37                     | 0.72              |
| 1:A:332:LYS:O     | 1:A:337:LEU:CD2   | 2.37                     | 0.72              |
| 1:A:1130:ILE:CD1  | 1:A:1361:LEU:H    | 2.02                     | 0.72              |
| 1:A:562:LEU:O     | 1:A:563:ASN:CB    | 2.38                     | 0.72              |
| 1:A:640:LEU:HD13  | 1:A:808:GLN:HB3   | 1.71                     | 0.72              |
| 1:A:213:GLU:OE1   | 1:A:213:GLU:N     | 2.23                     | 0.71              |
| 1:A:357:PHE:CD2   | 1:A:423:GLU:CB    | 2.73                     | 0.71              |
| 1:A:853:ASN:ND2   | 2:B:30:A:C8       | 2.58                     | 0.71              |
| 1:A:1359:SER:OG   | 1:A:1363:LEU:CG   | 2.35                     | 0.71              |
| 1:A:362:ILE:N     | 1:A:367:ILE:HD11  | 2.05                     | 0.71              |
| 1:A:626:ASN:OD1   | 1:A:845:LEU:HD21  | 1.88                     | 0.71              |
| 1:A:1076:TYR:CE1  | 1:A:1080:SER:HA   | 2.25                     | 0.71              |
| 1:A:345:ILE:HG13  | 1:A:346:GLU:N     | 2.05                     | 0.71              |
| 1:A:309:LYS:HD2   | 1:A:310:ARG:O     | 1.90                     | 0.71              |
| 1:A:599:ARG:NH2   | 1:A:608:ARG:HB2   | 2.05                     | 0.71              |
| 1:A:871:TYR:OH    | 3:A:1414:HOH:O    | 2.06                     | 0.71              |
| 1:A:1341:LYS:HZ2  | 1:A:1344:GLY:HA3  | 1.54                     | 0.71              |
| 1:A:243:MET:CE    | 1:A:246:ARG:NH1   | 2.54                     | 0.71              |
| 1:A:567:LYS:HB3   | 1:A:567:LYS:HZ3   | 1.55                     | 0.71              |
| 1:A:1044:GLN:O    | 1:A:1045:GLU:CB   | 2.38                     | 0.71              |
| 1:A:390:GLU:HB2   | 1:A:403:ILE:CD1   | 2.19                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:361:ASN:HB3   | 1:A:367:ILE:CG1   | 2.20                     | 0.71              |
| 1:A:442:ILE:HD12  | 1:A:443:LEU:N     | 2.06                     | 0.71              |
| 1:A:567:LYS:HB3   | 1:A:567:LYS:NZ    | 2.04                     | 0.71              |
| 1:A:696:ILE:HG22  | 1:A:697:GLU:O     | 1.90                     | 0.71              |
| 1:A:1047:TYR:C    | 1:A:1058:ILE:HG12 | 2.16                     | 0.71              |
| 1:A:249:ILE:C     | 1:A:249:ILE:HD13  | 2.16                     | 0.71              |
| 2:B:22:C:H5'      | 2:B:23:U:H2'      | 1.72                     | 0.71              |
| 1:A:442:ILE:HD12  | 1:A:442:ILE:C     | 2.15                     | 0.71              |
| 1:A:272:SER:CB    | 3:A:1421:HOH:O    | 2.34                     | 0.71              |
| 1:A:899:ASN:CB    | 1:A:905:GLN:CG    | 2.58                     | 0.71              |
| 1:A:449:VAL:HG12  | 1:A:456:LYS:H     | 1.54                     | 0.70              |
| 1:A:454:MET:HB3   | 1:A:455:GLU:HA    | 1.72                     | 0.70              |
| 1:A:505:PHE:CD2   | 2:B:22:C:O2'      | 2.44                     | 0.70              |
| 1:A:561:ILE:HD13  | 1:A:561:ILE:C     | 2.15                     | 0.70              |
| 1:A:1063:LEU:HD23 | 1:A:1171:PHE:CE2  | 2.26                     | 0.70              |
| 2:B:34:A:HO2'     | 2:B:35:U:P        | 2.14                     | 0.70              |
| 1:A:636:LYS:HE3   | 1:A:887:LEU:CD2   | 2.20                     | 0.70              |
| 1:A:641:ASP:HB2   | 1:A:821:ILE:CG1   | 2.21                     | 0.70              |
| 1:A:1118:LEU:HD12 | 1:A:1126:LYS:HD2  | 1.72                     | 0.70              |
| 1:A:182:GLU:OE1   | 1:A:184:GLU:HB2   | 1.91                     | 0.70              |
| 1:A:214:LYS:CA    | 3:A:1406:HOH:O    | 2.13                     | 0.70              |
| 1:A:636:LYS:CE    | 1:A:887:LEU:HD23  | 2.21                     | 0.70              |
| 1:A:1235:TYR:CE1  | 1:A:1236:THR:HG23 | 2.27                     | 0.70              |
| 1:A:374:ILE:HD13  | 1:A:428:TYR:CZ    | 2.26                     | 0.70              |
| 1:A:1110:ILE:HG12 | 1:A:1144:ILE:CB   | 2.22                     | 0.70              |
| 1:A:1236:THR:HB   | 1:A:1242:LYS:CG   | 2.21                     | 0.70              |
| 1:A:532:ILE:C     | 1:A:532:ILE:HD12  | 2.17                     | 0.70              |
| 1:A:263:LEU:C     | 1:A:264:ASN:HD22  | 1.99                     | 0.69              |
| 1:A:1236:THR:HB   | 1:A:1242:LYS:HG3  | 1.74                     | 0.69              |
| 1:A:1245:ASP:OD1  | 1:A:1245:ASP:N    | 2.24                     | 0.69              |
| 1:A:823:VAL:O     | 1:A:825:THR:HG23  | 1.92                     | 0.69              |
| 1:A:210:ASN:C     | 1:A:211:GLU:HG2   | 2.17                     | 0.69              |
| 1:A:1228:ARG:HG2  | 1:A:1228:ARG:NH1  | 2.07                     | 0.69              |
| 1:A:82:PHE:HB2    | 1:A:84:LEU:HD22   | 1.74                     | 0.69              |
| 1:A:400:ILE:HD12  | 1:A:443:LEU:HD13  | 1.74                     | 0.69              |
| 2:B:15:A:C8       | 2:B:15:A:H5''     | 2.28                     | 0.69              |
| 1:A:357:PHE:CD2   | 1:A:423:GLU:CG    | 2.75                     | 0.69              |
| 1:A:547:PHE:HA    | 1:A:594:THR:HG22  | 1.75                     | 0.69              |
| 1:A:200:LEU:HD12  | 1:A:200:LEU:O     | 1.91                     | 0.69              |
| 1:A:417:PHE:HD1   | 1:A:418:SER:HB3   | 1.58                     | 0.69              |
| 2:B:34:A:H5''     | 2:B:34:A:C8       | 2.24                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:435:LEU:CD2   | 1:A:468:LEU:CD1   | 2.71                     | 0.69              |
| 1:A:1342:LEU:HD12 | 1:A:1349:LEU:HD21 | 1.75                     | 0.69              |
| 1:A:286:ASN:H     | 1:A:286:ASN:HD22  | 1.41                     | 0.68              |
| 1:A:357:PHE:CE1   | 1:A:361:ASN:ND2   | 2.62                     | 0.68              |
| 1:A:1075:ILE:HD11 | 1:A:1290:PRO:HG2  | 1.74                     | 0.68              |
| 2:B:13:C:O3'      | 3:B:102:HOH:O     | 2.08                     | 0.68              |
| 1:A:20:LYS:HA     | 1:A:20:LYS:HZ3    | 1.56                     | 0.68              |
| 1:A:80:ILE:HG21   | 1:A:201:TYR:HB2   | 1.74                     | 0.68              |
| 1:A:1118:LEU:CD1  | 1:A:1126:LYS:CD   | 2.72                     | 0.68              |
| 1:A:626:ASN:O     | 1:A:629:ILE:HG13  | 1.94                     | 0.68              |
| 1:A:581:ILE:HD13  | 1:A:581:ILE:C     | 2.18                     | 0.68              |
| 1:A:1268:GLU:O    | 1:A:1276:SER:CA   | 2.41                     | 0.68              |
| 1:A:82:PHE:CB     | 1:A:84:LEU:HD22   | 2.24                     | 0.68              |
| 1:A:1044:GLN:HB2  | 1:A:1048:TYR:HE1  | 1.59                     | 0.68              |
| 1:A:210:ASN:HB3   | 3:A:1431:HOH:O    | 1.94                     | 0.68              |
| 1:A:404:PHE:CD2   | 1:A:439:ILE:CD1   | 2.77                     | 0.68              |
| 1:A:659:ILE:HD12  | 1:A:659:ILE:C     | 2.19                     | 0.68              |
| 1:A:821:ILE:HD13  | 1:A:821:ILE:N     | 2.03                     | 0.68              |
| 1:A:1066:ASN:CG   | 1:A:1067:ILE:H    | 1.94                     | 0.68              |
| 1:A:51:ASN:HB3    | 1:A:331:ILE:HD13  | 1.75                     | 0.68              |
| 1:A:73:ARG:HG3    | 1:A:73:ARG:NH2    | 1.99                     | 0.68              |
| 1:A:641:ASP:HB2   | 1:A:821:ILE:HD11  | 1.76                     | 0.68              |
| 1:A:662:GLU:HB3   | 3:A:1422:HOH:O    | 1.94                     | 0.68              |
| 1:A:1340:PHE:HD2  | 1:A:1342:LEU:HD12 | 1.59                     | 0.68              |
| 1:A:186:LYS:O     | 1:A:189:ILE:HG13  | 1.93                     | 0.67              |
| 1:A:413:ASP:HA    | 1:A:414:SER:CB    | 2.23                     | 0.67              |
| 1:A:1041:ASN:HD22 | 1:A:1042:LYS:N    | 1.92                     | 0.67              |
| 1:A:1047:TYR:HE1  | 1:A:1060:LYS:HG3  | 1.60                     | 0.67              |
| 1:A:289:LEU:HD23  | 1:A:290:THR:N     | 2.09                     | 0.67              |
| 1:A:1216:GLY:HA3  | 1:A:1242:LYS:HE3  | 1.74                     | 0.67              |
| 1:A:1235:TYR:CD1  | 1:A:1236:THR:HG23 | 2.29                     | 0.67              |
| 1:A:659:ILE:HD12  | 1:A:659:ILE:O     | 1.93                     | 0.67              |
| 1:A:646:ASP:HB3   | 1:A:647:LYS:CB    | 2.25                     | 0.67              |
| 1:A:1226:PRO:CB   | 1:A:1238:THR:HB   | 2.24                     | 0.67              |
| 1:A:1230:GLY:HA2  | 1:A:1234:PHE:CB   | 2.23                     | 0.67              |
| 1:A:249:ILE:N     | 1:A:256:LEU:HD12  | 2.10                     | 0.67              |
| 1:A:337:LEU:HD23  | 1:A:337:LEU:H     | 1.59                     | 0.67              |
| 1:A:735:GLU:O     | 1:A:739:THR:HG23  | 1.95                     | 0.67              |
| 1:A:1365:SER:OG   | 1:A:1368:SER:CB   | 2.41                     | 0.67              |
| 1:A:683:LEU:HD12  | 1:A:684:TYR:N     | 2.10                     | 0.67              |
| 1:A:687:ASN:CG    | 1:A:688:PRO:HD2   | 2.20                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:22:C:H4'      | 2:B:23:U:OP2      | 1.95                     | 0.67              |
| 1:A:314:VAL:HG12  | 1:A:315:LYS:N     | 2.10                     | 0.67              |
| 1:A:897:ASN:CB    | 1:A:898:LEU:HA    | 2.25                     | 0.67              |
| 1:A:906:LYS:O     | 1:A:910:ILE:HG13  | 1.96                     | 0.67              |
| 1:A:80:ILE:HD11   | 1:A:200:LEU:HB3   | 1.76                     | 0.66              |
| 1:A:316:LYS:HE2   | 1:A:316:LYS:H     | 1.59                     | 0.66              |
| 1:A:899:ASN:O     | 1:A:900:LEU:HB2   | 1.93                     | 0.66              |
| 1:A:906:LYS:HZ3   | 1:A:1022:LYS:HA   | 1.57                     | 0.66              |
| 1:A:94:GLU:CB     | 1:A:198:MET:SD    | 2.83                     | 0.66              |
| 1:A:316:LYS:CE    | 1:A:316:LYS:H     | 2.06                     | 0.66              |
| 1:A:44:ASN:C      | 1:A:44:ASN:HD22   | 2.04                     | 0.66              |
| 1:A:80:ILE:HD11   | 1:A:200:LEU:CB    | 2.25                     | 0.66              |
| 1:A:608:ARG:HA    | 1:A:609:ASP:CB    | 2.25                     | 0.66              |
| 1:A:1049:PRO:C    | 1:A:1051:GLU:HA   | 2.20                     | 0.66              |
| 1:A:610:LEU:CA    | 1:A:612:GLY:HA3   | 2.25                     | 0.66              |
| 1:A:1087:ASP:OD1  | 1:A:1087:ASP:N    | 2.22                     | 0.66              |
| 1:A:1149:TYR:CE1  | 1:A:1153:GLU:HG3  | 2.31                     | 0.66              |
| 1:A:1348:ILE:HD12 | 1:A:1348:ILE:N    | 2.03                     | 0.66              |
| 1:A:314:VAL:HB    | 3:A:1415:HOH:O    | 1.96                     | 0.66              |
| 1:A:536:GLU:OE2   | 1:A:556:VAL:HG21  | 1.95                     | 0.66              |
| 1:A:1228:ARG:HA   | 1:A:1234:PHE:CD2  | 2.30                     | 0.66              |
| 1:A:404:PHE:CG    | 1:A:439:ILE:HD13  | 2.30                     | 0.66              |
| 1:A:1117:LYS:HE2  | 1:A:1129:TYR:OH   | 1.96                     | 0.66              |
| 1:A:243:MET:HE1   | 1:A:246:ARG:HH11  | 1.56                     | 0.66              |
| 1:A:261:PHE:CB    | 1:A:283:LEU:CD1   | 2.74                     | 0.66              |
| 1:A:662:GLU:OE1   | 1:A:662:GLU:HA    | 1.95                     | 0.66              |
| 1:A:1272:PRO:HG2  | 1:A:1275:GLU:OE1  | 1.96                     | 0.66              |
| 1:A:395:ASN:HB3   | 1:A:399:GLU:OE2   | 1.96                     | 0.65              |
| 1:A:315:LYS:CG    | 1:A:316:LYS:HE2   | 2.26                     | 0.65              |
| 1:A:362:ILE:CG1   | 1:A:367:ILE:HD12  | 2.24                     | 0.65              |
| 1:A:900:LEU:HD23  | 1:A:1057:TYR:O    | 1.95                     | 0.65              |
| 1:A:359:VAL:CG1   | 1:A:1255:ILE:HD12 | 2.25                     | 0.65              |
| 1:A:592:ILE:HG22  | 1:A:839:ILE:HG21  | 1.78                     | 0.65              |
| 1:A:1040:GLU:HB3  | 1:A:1042:LYS:HG2  | 1.78                     | 0.65              |
| 1:A:1090:PHE:H    | 1:A:1091:LEU:CB   | 2.09                     | 0.65              |
| 1:A:1301:ASP:OD2  | 1:A:1343:ILE:CB   | 2.44                     | 0.65              |
| 1:A:1360:VAL:HG23 | 2:B:35:U:C2       | 2.31                     | 0.65              |
| 1:A:332:LYS:O     | 1:A:337:LEU:HD23  | 1.96                     | 0.65              |
| 1:A:449:VAL:HG12  | 1:A:454:MET:HB3   | 1.79                     | 0.65              |
| 1:A:1269:ILE:O    | 1:A:1276:SER:HB3  | 1.96                     | 0.65              |
| 1:A:268:ASP:CB    | 2:B:51:C:C2       | 2.80                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:35:U:H2'      | 2:B:36:C:C6       | 2.32                     | 0.65              |
| 1:A:617:TYR:CA    | 1:A:620:VAL:HG22  | 2.26                     | 0.65              |
| 1:A:361:ASN:HB3   | 1:A:367:ILE:HG13  | 1.77                     | 0.65              |
| 1:A:578:LYS:O     | 1:A:579:ASN:HB2   | 1.95                     | 0.65              |
| 1:A:1044:GLN:O    | 1:A:1045:GLU:HB2  | 1.96                     | 0.65              |
| 1:A:362:ILE:N     | 1:A:367:ILE:CD1   | 2.60                     | 0.64              |
| 1:A:448:LYS:O     | 1:A:454:MET:HB2   | 1.97                     | 0.64              |
| 1:A:261:PHE:HA    | 1:A:283:LEU:HD21  | 1.79                     | 0.64              |
| 1:A:391:LEU:CD1   | 1:A:459:ILE:HD11  | 2.27                     | 0.64              |
| 1:A:435:LEU:HD21  | 1:A:468:LEU:CD1   | 2.27                     | 0.64              |
| 1:A:464:ASN:HD22  | 1:A:467:ILE:HD12  | 1.61                     | 0.64              |
| 1:A:767:ASN:C     | 3:A:1407:HOH:O    | 2.39                     | 0.64              |
| 1:A:464:ASN:HB3   | 1:A:467:ILE:HB    | 1.78                     | 0.64              |
| 1:A:76:HIS:H      | 1:A:79:ASN:ND2    | 1.96                     | 0.64              |
| 1:A:32:ASP:O      | 3:A:1417:HOH:O    | 2.14                     | 0.64              |
| 1:A:1130:ILE:HD12 | 1:A:1361:LEU:H    | 1.62                     | 0.64              |
| 1:A:20:LYS:NZ     | 1:A:20:LYS:HA     | 2.13                     | 0.64              |
| 1:A:314:VAL:O     | 3:A:1415:HOH:O    | 2.15                     | 0.64              |
| 1:A:698:THR:O     | 1:A:702:VAL:N     | 2.31                     | 0.64              |
| 1:A:5:PHE:HA      | 1:A:27:VAL:O      | 1.98                     | 0.64              |
| 1:A:524:SER:O     | 1:A:527:MET:HG3   | 1.98                     | 0.64              |
| 1:A:1359:SER:O    | 1:A:1360:VAL:HG12 | 1.97                     | 0.64              |
| 1:A:338:ASP:OD1   | 1:A:341:GLU:HG2   | 1.97                     | 0.63              |
| 1:A:537:ASN:HD21  | 1:A:540:ASN:H     | 1.45                     | 0.63              |
| 1:A:76:HIS:CE1    | 1:A:79:ASN:CB     | 2.68                     | 0.63              |
| 1:A:387:LEU:HD23  | 1:A:403:ILE:CG2   | 2.29                     | 0.63              |
| 1:A:1349:LEU:C    | 1:A:1351:ARG:HB3  | 2.24                     | 0.63              |
| 1:A:695:THR:O     | 1:A:696:ILE:CG2   | 2.45                     | 0.63              |
| 1:A:726:ASN:ND2   | 1:A:726:ASN:H     | 1.97                     | 0.63              |
| 1:A:78:GLY:CA     | 1:A:197:ASN:OD1   | 2.47                     | 0.63              |
| 1:A:314:VAL:C     | 3:A:1415:HOH:O    | 2.41                     | 0.63              |
| 1:A:1067:ILE:HG12 | 1:A:1072:PHE:CD2  | 2.34                     | 0.63              |
| 1:A:400:ILE:HD13  | 1:A:442:ILE:CD1   | 2.16                     | 0.63              |
| 1:A:449:VAL:CG1   | 1:A:456:LYS:N     | 2.58                     | 0.63              |
| 1:A:683:LEU:HD11  | 1:A:793:PHE:CG    | 2.33                     | 0.63              |
| 1:A:1246:GLU:HB3  | 1:A:1250:LYS:HE2  | 1.80                     | 0.63              |
| 1:A:1360:VAL:N    | 3:A:1408:HOH:O    | 2.28                     | 0.63              |
| 1:A:192:ILE:HG21  | 1:A:245:ILE:CG1   | 2.29                     | 0.63              |
| 1:A:824:LYS:C     | 1:A:825:THR:HG23  | 2.23                     | 0.63              |
| 2:B:30:A:C2'      | 2:B:31:C:O5'      | 2.47                     | 0.63              |
| 1:A:248:LYS:CB    | 1:A:256:LEU:HD11  | 2.27                     | 0.63              |

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| Atom-1            | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------------|--------------------------|-------------------|
| 1:A:1090:PHE:HB2  | 1:A:1091:LEU:CB         | 2.29                     | 0.63              |
| 1:A:1332:ASP:HB2  | 1:A:1354:LYS:HE2        | 1.81                     | 0.63              |
| 1:A:316:LYS:H     | 1:A:316:LYS:HD3         | 1.62                     | 0.62              |
| 1:A:1034:ASP:HB3  | 1:A:1039:ASN:HA         | 1.80                     | 0.62              |
| 1:A:1059:TYR:CE1  | 1:A:1061:LYS:HB3        | 2.34                     | 0.62              |
| 1:A:1279:ASN:ND2  | 1:A:1283:HIS:HE1        | 1.85                     | 0.62              |
| 1:A:1234:PHE:CE1  | 1:A:1235:TYR:HB3        | 2.35                     | 0.62              |
| 1:A:371:ILE:HG21  | 1:A:472:ILE:HG22        | 1.80                     | 0.62              |
| 1:A:547:PHE:O     | 1:A:597:ARG:NH2         | 2.33                     | 0.62              |
| 1:A:1063:LEU:O    | 1:A:1063:LEU:HD12       | 1.98                     | 0.62              |
| 1:A:1359:SER:OG   | 1:A:1361:LEU:HB3        | 1.98                     | 0.62              |
| 1:A:1359:SER:O    | 1:A:1361:LEU:HD13       | 1.98                     | 0.62              |
| 1:A:81:LEU:C      | 1:A:81:LEU:HD23         | 2.24                     | 0.62              |
| 1:A:351:LYS:O     | 1:A:355:VAL:HG23        | 1.99                     | 0.62              |
| 1:A:463:LEU:O     | 1:A:468:LEU:HG          | 1.99                     | 0.62              |
| 1:A:1083:ILE:HD13 | 1:A:1171:PHE:CD1        | 2.34                     | 0.62              |
| 1:A:1279:ASN:O    | 1:A:1283:HIS:ND1        | 2.33                     | 0.62              |
| 1:A:339:LYS:HG3   | 2:B:6:C:H4 <sup>+</sup> | 1.81                     | 0.62              |
| 1:A:1197:ARG:HH11 | 1:A:1197:ARG:CB         | 2.12                     | 0.62              |
| 1:A:82:PHE:HD1    | 1:A:263:LEU:O           | 1.83                     | 0.62              |
| 1:A:821:ILE:H     | 1:A:821:ILE:CD1         | 1.96                     | 0.62              |
| 1:A:1269:ILE:O    | 1:A:1276:SER:CB         | 2.47                     | 0.62              |
| 1:A:1273:GLU:O    | 1:A:1274:ASN:HB2        | 2.00                     | 0.62              |
| 1:A:76:HIS:NE2    | 2:B:48:A:OP1            | 2.30                     | 0.62              |
| 1:A:435:LEU:CD2   | 1:A:468:LEU:HD11        | 2.30                     | 0.62              |
| 1:A:1133:LEU:HD21 | 1:A:1139:PHE:CE2        | 2.33                     | 0.62              |
| 1:A:246:ARG:HA    | 1:A:249:ILE:CG2         | 2.29                     | 0.62              |
| 1:A:316:LYS:HE2   | 1:A:316:LYS:N           | 2.14                     | 0.62              |
| 1:A:738:LYS:HA    | 1:A:746:ILE:HG12        | 1.81                     | 0.62              |
| 1:A:1075:ILE:CD1  | 1:A:1181:LEU:HD11       | 2.30                     | 0.62              |
| 1:A:248:LYS:CB    | 1:A:256:LEU:CD1         | 2.78                     | 0.61              |
| 1:A:261:PHE:CB    | 1:A:283:LEU:HD11        | 2.30                     | 0.61              |
| 1:A:286:ASN:OD1   | 1:A:1139:PHE:CD1        | 2.53                     | 0.61              |
| 1:A:1230:GLY:CA   | 1:A:1234:PHE:HB3        | 2.22                     | 0.61              |
| 1:A:1341:LYS:NZ   | 1:A:1344:GLY:HA3        | 2.16                     | 0.61              |
| 1:A:59:ILE:HG23   | 1:A:314:VAL:HG21        | 0.83                     | 0.61              |
| 1:A:418:SER:OG    | 1:A:420:LYS:HD2         | 2.00                     | 0.61              |
| 1:A:525:THR:CG2   | 1:A:847:ASN:HD21        | 2.12                     | 0.61              |
| 1:A:1067:ILE:HG12 | 1:A:1072:PHE:CE2        | 2.34                     | 0.61              |
| 1:A:183:LEU:HD22  | 1:A:253:LEU:CD1         | 2.30                     | 0.61              |
| 1:A:197:ASN:HD22  | 1:A:198:MET:N           | 1.98                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1075:ILE:HD11 | 1:A:1181:LEU:HD11 | 1.81                     | 0.61              |
| 1:A:1127:GLU:HA   | 1:A:1127:GLU:OE2  | 1.99                     | 0.61              |
| 1:A:287:VAL:HG21  | 1:A:1125:TYR:CZ   | 2.35                     | 0.61              |
| 1:A:374:ILE:CD1   | 1:A:428:TYR:CE1   | 2.84                     | 0.61              |
| 1:A:726:ASN:H     | 1:A:726:ASN:HD22  | 1.48                     | 0.61              |
| 1:A:1346:ASN:O    | 1:A:1349:LEU:HB2  | 2.01                     | 0.61              |
| 2:B:15:A:H5''     | 2:B:15:A:H8       | 1.66                     | 0.61              |
| 1:A:1067:ILE:HG22 | 1:A:1067:ILE:O    | 2.00                     | 0.61              |
| 1:A:1059:TYR:HE1  | 1:A:1061:LYS:HB3  | 1.64                     | 0.61              |
| 1:A:1083:ILE:CD1  | 1:A:1171:PHE:CE1  | 2.77                     | 0.61              |
| 1:A:446:GLU:HA    | 1:A:449:VAL:HG22  | 1.83                     | 0.61              |
| 1:A:1200:HIS:CE1  | 1:A:1224:ALA:HB2  | 2.36                     | 0.61              |
| 1:A:357:PHE:HE1   | 1:A:361:ASN:ND2   | 1.98                     | 0.61              |
| 2:B:9:A:C4        | 2:B:13:C:N4       | 2.68                     | 0.61              |
| 1:A:417:PHE:CD1   | 1:A:418:SER:HB3   | 2.35                     | 0.61              |
| 1:A:246:ARG:CG    | 3:A:1411:HOH:O    | 2.43                     | 0.60              |
| 1:A:286:ASN:O     | 1:A:1132:LYS:HG3  | 2.01                     | 0.60              |
| 1:A:802:ILE:HG23  | 1:A:805:ILE:HB    | 1.81                     | 0.60              |
| 1:A:1040:GLU:OE2  | 1:A:1040:GLU:HA   | 2.01                     | 0.60              |
| 1:A:1130:ILE:HD11 | 1:A:1361:LEU:HD12 | 1.82                     | 0.60              |
| 1:A:490:LEU:HD21  | 1:A:500:VAL:CG1   | 2.30                     | 0.60              |
| 1:A:1269:ILE:C    | 1:A:1276:SER:HB3  | 2.26                     | 0.60              |
| 1:A:83:LYS:HB2    | 1:A:265:VAL:HG22  | 1.82                     | 0.60              |
| 1:A:801:ASN:HA    | 1:A:803:GLN:N     | 2.16                     | 0.60              |
| 1:A:1076:TYR:CE1  | 1:A:1080:SER:CA   | 2.83                     | 0.60              |
| 1:A:262:TYR:C     | 1:A:264:ASN:H     | 2.08                     | 0.60              |
| 1:A:638:LEU:HD22  | 1:A:639:ASN:HD22  | 1.65                     | 0.60              |
| 1:A:1107:ILE:HD13 | 1:A:1156:TYR:HA   | 1.83                     | 0.60              |
| 1:A:56:ARG:HH21   | 1:A:56:ARG:CG     | 2.14                     | 0.60              |
| 1:A:501:ASN:OD1   | 1:A:503:ASP:HB2   | 2.02                     | 0.60              |
| 1:A:731:ILE:HG22  | 1:A:734:GLN:HG3   | 1.82                     | 0.60              |
| 1:A:1047:TYR:CA   | 1:A:1058:ILE:HG13 | 2.31                     | 0.60              |
| 1:A:1047:TYR:CE1  | 1:A:1060:LYS:HG3  | 2.35                     | 0.60              |
| 1:A:1268:GLU:O    | 1:A:1276:SER:CB   | 2.50                     | 0.60              |
| 1:A:84:LEU:HD23   | 1:A:84:LEU:N      | 2.13                     | 0.60              |
| 1:A:252:ASN:OD1   | 1:A:252:ASN:N     | 2.35                     | 0.60              |
| 1:A:449:VAL:CG1   | 1:A:454:MET:HB3   | 2.30                     | 0.60              |
| 1:A:576:ASP:HB3   | 1:A:580:ASN:O     | 2.02                     | 0.60              |
| 1:A:1118:LEU:HD13 | 1:A:1126:LYS:CG   | 2.31                     | 0.60              |
| 1:A:1213:LYS:C    | 1:A:1214:LEU:HD12 | 2.27                     | 0.60              |
| 1:A:183:LEU:CD1   | 1:A:255:ILE:HG21  | 2.31                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:638:LEU:HD22  | 1:A:639:ASN:N     | 2.16                     | 0.60              |
| 1:A:695:THR:OG1   | 1:A:696:ILE:N     | 2.35                     | 0.60              |
| 2:B:35:U:C4       | 2:B:36:C:N4       | 2.69                     | 0.60              |
| 1:A:76:HIS:CE1    | 1:A:79:ASN:N      | 2.70                     | 0.60              |
| 1:A:638:LEU:HD22  | 1:A:639:ASN:ND2   | 2.17                     | 0.60              |
| 1:A:1076:TYR:CE1  | 1:A:1080:SER:CB   | 2.85                     | 0.60              |
| 1:A:78:GLY:HA2    | 1:A:197:ASN:OD1   | 2.02                     | 0.59              |
| 1:A:1262:ASP:CG   | 1:A:1267:SER:HB2  | 2.27                     | 0.59              |
| 1:A:235:ILE:CD1   | 1:A:291:VAL:HG22  | 2.29                     | 0.59              |
| 1:A:802:ILE:O     | 1:A:805:ILE:N     | 2.34                     | 0.59              |
| 1:A:1185:ASN:ND2  | 1:A:1185:ASN:O    | 2.35                     | 0.59              |
| 1:A:698:THR:O     | 1:A:702:VAL:HG23  | 2.02                     | 0.59              |
| 1:A:1245:ASP:O    | 1:A:1246:GLU:C    | 2.37                     | 0.59              |
| 1:A:1278:ARG:HH21 | 1:A:1278:ARG:CG   | 2.11                     | 0.59              |
| 1:A:314:VAL:CB    | 3:A:1415:HOH:O    | 2.50                     | 0.59              |
| 1:A:84:LEU:HD13   | 1:A:193:PHE:HB3   | 1.85                     | 0.59              |
| 1:A:558:ASP:OD1   | 1:A:559:LYS:N     | 2.35                     | 0.59              |
| 1:A:1076:TYR:HE1  | 1:A:1080:SER:HA   | 1.66                     | 0.59              |
| 1:A:1164:LYS:O    | 1:A:1168:LEU:HD12 | 2.02                     | 0.59              |
| 1:A:1207:ARG:CD   | 1:A:1214:LEU:HD22 | 2.31                     | 0.59              |
| 1:A:387:LEU:HD23  | 1:A:403:ILE:HG21  | 1.85                     | 0.59              |
| 1:A:487:LEU:HD22  | 1:A:497:MET:HE2   | 1.84                     | 0.59              |
| 1:A:738:LYS:HA    | 1:A:746:ILE:CG1   | 2.33                     | 0.59              |
| 1:A:853:ASN:CB    | 1:A:882:MET:HE1   | 2.33                     | 0.59              |
| 1:A:1118:LEU:CD1  | 1:A:1126:LYS:CG   | 2.81                     | 0.59              |
| 1:A:1065:LEU:O    | 1:A:1066:ASN:CG   | 2.45                     | 0.59              |
| 1:A:76:HIS:CG     | 1:A:79:ASN:ND2    | 2.63                     | 0.59              |
| 1:A:700:LYS:O     | 1:A:704:ASN:ND2   | 2.36                     | 0.59              |
| 1:A:1218:ASN:ND2  | 1:A:1236:THR:O    | 2.36                     | 0.59              |
| 1:A:1226:PRO:HA   | 1:A:1238:THR:HG21 | 1.84                     | 0.59              |
| 1:A:1359:SER:CB   | 1:A:1363:LEU:HD12 | 2.33                     | 0.59              |
| 1:A:1044:GLN:O    | 1:A:1044:GLN:HG3  | 2.01                     | 0.59              |
| 1:A:371:ILE:HG21  | 1:A:472:ILE:CG2   | 2.33                     | 0.59              |
| 1:A:686:ASN:CG    | 3:A:1423:HOH:O    | 2.46                     | 0.59              |
| 1:A:693:PHE:O     | 1:A:694:ASP:O     | 2.21                     | 0.59              |
| 1:A:20:LYS:HZ2    | 1:A:20:LYS:C      | 2.06                     | 0.58              |
| 1:A:608:ARG:HH11  | 1:A:608:ARG:CG    | 2.16                     | 0.58              |
| 1:A:677:LEU:CD1   | 1:A:707:ILE:HD12  | 2.30                     | 0.58              |
| 1:A:1059:TYR:CE1  | 1:A:1061:LYS:HA   | 2.38                     | 0.58              |
| 1:A:1360:VAL:HG13 | 1:A:1360:VAL:O    | 2.02                     | 0.58              |
| 1:A:1164:LYS:CG   | 1:A:1366:TYR:O    | 2.52                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1267:SER:O    | 1:A:1268:GLU:HB2  | 2.03                     | 0.58              |
| 1:A:191:GLU:O     | 1:A:194:LYS:HG3   | 2.03                     | 0.58              |
| 1:A:375:LEU:O     | 1:A:378:PHE:HB2   | 2.03                     | 0.58              |
| 1:A:647:LYS:O     | 1:A:650:ILE:HD12  | 2.03                     | 0.58              |
| 1:A:691:GLU:CB    | 1:A:692:PRO:HD2   | 2.33                     | 0.58              |
| 1:A:84:LEU:HD11   | 1:A:194:LYS:N     | 2.16                     | 0.58              |
| 1:A:565:LYS:O     | 1:A:569:ILE:HG12  | 2.03                     | 0.58              |
| 1:A:814:ASP:HB3   | 1:A:817:THR:OG1   | 2.02                     | 0.58              |
| 1:A:1104:ILE:HG12 | 1:A:1159:VAL:HG13 | 1.84                     | 0.58              |
| 1:A:200:LEU:HD12  | 1:A:200:LEU:C     | 2.28                     | 0.58              |
| 1:A:359:VAL:HG13  | 1:A:1255:ILE:HG23 | 1.85                     | 0.58              |
| 1:A:384:ILE:HG12  | 1:A:463:LEU:CD1   | 2.34                     | 0.58              |
| 1:A:449:VAL:HG11  | 1:A:456:LYS:N     | 2.17                     | 0.58              |
| 1:A:801:ASN:HA    | 1:A:803:GLN:H     | 1.67                     | 0.58              |
| 1:A:640:LEU:HD13  | 1:A:808:GLN:CB    | 2.33                     | 0.58              |
| 1:A:1059:TYR:HE1  | 1:A:1061:LYS:HB2  | 1.65                     | 0.58              |
| 1:A:1141:ALA:HA   | 1:A:1147:LYS:CB   | 2.34                     | 0.58              |
| 1:A:1367:ASN:O    | 1:A:1367:ASN:ND2  | 2.35                     | 0.58              |
| 1:A:355:VAL:O     | 1:A:359:VAL:HG23  | 2.04                     | 0.58              |
| 1:A:547:PHE:CA    | 1:A:594:THR:HG22  | 2.33                     | 0.58              |
| 1:A:1271:LYS:CB   | 1:A:1275:GLU:HB3  | 2.34                     | 0.58              |
| 1:A:348:GLU:O     | 1:A:349:ASN:HB2   | 2.03                     | 0.58              |
| 1:A:239:LEU:O     | 1:A:243:MET:HG2   | 2.04                     | 0.58              |
| 1:A:362:ILE:CA    | 1:A:367:ILE:CD1   | 2.82                     | 0.58              |
| 1:A:853:ASN:HB2   | 1:A:882:MET:HE1   | 1.86                     | 0.58              |
| 1:A:390:GLU:OE2   | 1:A:403:ILE:HD11  | 2.04                     | 0.57              |
| 1:A:654:ILE:O     | 1:A:716:LYS:HE2   | 2.04                     | 0.57              |
| 1:A:676:VAL:HG12  | 1:A:778:ILE:HD13  | 1.85                     | 0.57              |
| 1:A:1034:ASP:HB3  | 1:A:1038:GLU:O    | 2.03                     | 0.57              |
| 1:A:186:LYS:HA    | 1:A:189:ILE:HG13  | 1.85                     | 0.57              |
| 1:A:310:ARG:HD2   | 1:A:312:GLU:HB3   | 1.86                     | 0.57              |
| 1:A:446:GLU:HA    | 1:A:446:GLU:OE2   | 2.03                     | 0.57              |
| 1:A:547:PHE:HA    | 1:A:594:THR:CG2   | 2.34                     | 0.57              |
| 1:A:246:ARG:O     | 1:A:249:ILE:HG23  | 2.04                     | 0.57              |
| 1:A:1226:PRO:HB3  | 1:A:1238:THR:HB   | 1.87                     | 0.57              |
| 1:A:246:ARG:HD2   | 1:A:285:ILE:HG22  | 1.86                     | 0.57              |
| 1:A:665:ASN:O     | 1:A:668:LYS:HD2   | 2.04                     | 0.57              |
| 1:A:210:ASN:O     | 1:A:211:GLU:HG2   | 2.03                     | 0.57              |
| 1:A:235:ILE:O     | 1:A:238:ILE:HB    | 2.04                     | 0.57              |
| 1:A:853:ASN:ND2   | 2:B:29:G:O2'      | 2.38                     | 0.57              |
| 1:A:1354:LYS:HB3  | 1:A:1355:PRO:HD2  | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:246:ARG:O     | 1:A:250:LYS:N     | 2.36                     | 0.57              |
| 1:A:362:ILE:HG12  | 1:A:367:ILE:CD1   | 2.35                     | 0.57              |
| 1:A:537:ASN:C     | 1:A:537:ASN:HD22  | 2.12                     | 0.57              |
| 1:A:572:LEU:O     | 1:A:573:ASP:HB3   | 2.04                     | 0.57              |
| 1:A:1069:ASN:O    | 1:A:1070:PRO:C    | 2.47                     | 0.57              |
| 1:A:1107:ILE:CD1  | 1:A:1156:TYR:HA   | 2.35                     | 0.57              |
| 1:A:1246:GLU:O    | 1:A:1247:GLU:C    | 2.45                     | 0.57              |
| 1:A:416:LYS:O     | 1:A:418:SER:HA    | 2.05                     | 0.57              |
| 1:A:390:GLU:O     | 1:A:393:LYS:N     | 2.38                     | 0.57              |
| 1:A:83:LYS:HA     | 1:A:85:LYS:HE2    | 1.87                     | 0.56              |
| 1:A:561:ILE:HD11  | 1:A:566:ILE:HG13  | 1.87                     | 0.56              |
| 1:A:332:LYS:HA    | 1:A:336:LEU:HB2   | 1.86                     | 0.56              |
| 1:A:641:ASP:HB2   | 1:A:821:ILE:CD1   | 2.33                     | 0.56              |
| 1:A:697:GLU:HA    | 1:A:701:ILE:HD13  | 1.86                     | 0.56              |
| 1:A:1049:PRO:O    | 1:A:1052:ARG:HA   | 2.05                     | 0.56              |
| 1:A:1342:LEU:HD13 | 1:A:1342:LEU:H    | 1.69                     | 0.56              |
| 1:A:183:LEU:HD11  | 1:A:255:ILE:HD13  | 1.86                     | 0.56              |
| 1:A:681:LEU:HD23  | 1:A:707:ILE:HD11  | 1.83                     | 0.56              |
| 1:A:824:LYS:O     | 1:A:825:THR:OG1   | 2.19                     | 0.56              |
| 1:A:1165:ILE:O    | 1:A:1169:VAL:HG13 | 2.05                     | 0.56              |
| 1:A:1247:GLU:HA   | 1:A:1250:LYS:HE3  | 1.86                     | 0.56              |
| 2:B:30:A:H2'      | 2:B:31:C:O5'      | 2.04                     | 0.56              |
| 2:B:31:C:O5'      | 2:B:31:C:H6       | 1.88                     | 0.56              |
| 1:A:547:PHE:C     | 1:A:594:THR:HG22  | 2.29                     | 0.56              |
| 1:A:1041:ASN:ND2  | 1:A:1041:ASN:H    | 2.02                     | 0.56              |
| 1:A:1327:LYS:O    | 1:A:1356:LYS:CE   | 2.43                     | 0.56              |
| 1:A:1360:VAL:CG2  | 2:B:35:U:O2       | 2.43                     | 0.56              |
| 1:A:530:ASN:HD21  | 1:A:543:ASN:HA    | 1.71                     | 0.56              |
| 1:A:532:ILE:O     | 1:A:557:LEU:HD13  | 2.04                     | 0.56              |
| 1:A:449:VAL:HG12  | 1:A:456:LYS:N     | 2.20                     | 0.56              |
| 1:A:1061:LYS:HG3  | 1:A:1062:ASN:N    | 2.21                     | 0.56              |
| 1:A:636:LYS:NZ    | 1:A:887:LEU:HG    | 2.21                     | 0.56              |
| 1:A:698:THR:OG1   | 1:A:699:GLU:N     | 2.38                     | 0.56              |
| 1:A:59:ILE:HD11   | 1:A:330:TYR:CD2   | 2.41                     | 0.56              |
| 1:A:76:HIS:N      | 1:A:79:ASN:ND2    | 2.53                     | 0.56              |
| 1:A:390:GLU:CB    | 1:A:403:ILE:CD1   | 2.81                     | 0.56              |
| 1:A:1360:VAL:CB   | 2:B:35:U:H1'      | 2.36                     | 0.56              |
| 1:A:358:PHE:HB2   | 1:A:480:THR:HG21  | 1.86                     | 0.56              |
| 1:A:435:LEU:HD21  | 1:A:468:LEU:HD13  | 1.88                     | 0.56              |
| 1:A:589:PHE:CE1   | 1:A:842:ILE:HG21  | 2.40                     | 0.56              |
| 1:A:610:LEU:C     | 1:A:612:GLY:CA    | 2.64                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1068:GLY:CA   | 1:A:1069:ASN:HB2  | 2.36                     | 0.56              |
| 1:A:1336:LEU:HG   | 1:A:1352:LEU:HD22 | 1.88                     | 0.56              |
| 1:A:317:VAL:HG11  | 1:A:323:GLU:HB2   | 1.87                     | 0.55              |
| 1:A:517:GLU:HG3   | 1:A:858:ARG:HD2   | 1.88                     | 0.55              |
| 1:A:731:ILE:HG22  | 1:A:734:GLN:CG    | 2.35                     | 0.55              |
| 1:A:87:LYS:HA     | 1:A:97:ASP:O      | 2.05                     | 0.55              |
| 1:A:377:GLU:HG2   | 1:A:412:PHE:CE2   | 2.41                     | 0.55              |
| 1:A:561:ILE:HD13  | 1:A:562:LEU:N     | 2.21                     | 0.55              |
| 1:A:616:ASP:O     | 1:A:620:VAL:N     | 2.36                     | 0.55              |
| 1:A:1218:ASN:ND2  | 1:A:1242:LYS:HD3  | 2.21                     | 0.55              |
| 1:A:1342:LEU:CA   | 1:A:1349:LEU:HD23 | 2.15                     | 0.55              |
| 1:A:1359:SER:OG   | 1:A:1361:LEU:CB   | 2.54                     | 0.55              |
| 1:A:514:LEU:HD23  | 1:A:858:ARG:CG    | 2.36                     | 0.55              |
| 1:A:248:LYS:HB3   | 1:A:256:LEU:HD12  | 1.88                     | 0.55              |
| 1:A:805:ILE:O     | 1:A:808:GLN:HG2   | 2.07                     | 0.55              |
| 1:A:1083:ILE:CD1  | 1:A:1171:PHE:CD1  | 2.90                     | 0.55              |
| 1:A:357:PHE:HE1   | 1:A:361:ASN:HD22  | 1.52                     | 0.55              |
| 1:A:639:ASN:HD22  | 1:A:639:ASN:N     | 2.05                     | 0.55              |
| 1:A:682:ASN:O     | 1:A:686:ASN:HB2   | 2.06                     | 0.55              |
| 1:A:514:LEU:HD23  | 1:A:858:ARG:HG3   | 1.89                     | 0.55              |
| 1:A:1059:TYR:CE1  | 1:A:1061:LYS:CA   | 2.89                     | 0.55              |
| 1:A:1146:ASN:HD21 | 1:A:1152:PHE:N    | 2.05                     | 0.55              |
| 1:A:357:PHE:CE2   | 1:A:423:GLU:HB2   | 2.41                     | 0.55              |
| 1:A:696:ILE:HA    | 1:A:697:GLU:O     | 2.06                     | 0.55              |
| 1:A:1090:PHE:H    | 1:A:1092:PHE:H    | 1.54                     | 0.55              |
| 1:A:1285:TYR:HA   | 1:A:1288:ARG:HG2  | 1.89                     | 0.55              |
| 1:A:344:LYS:CE    | 1:A:500:VAL:O     | 2.49                     | 0.55              |
| 1:A:1044:GLN:HB2  | 1:A:1048:TYR:CE1  | 2.41                     | 0.55              |
| 1:A:1130:ILE:HD11 | 1:A:1361:LEU:CD1  | 2.36                     | 0.55              |
| 1:A:1223:ARG:HD3  | 1:A:1225:TYR:CZ   | 2.42                     | 0.55              |
| 1:A:382:GLU:O     | 1:A:386:LYS:N     | 2.32                     | 0.55              |
| 1:A:670:LEU:HD12  | 1:A:718:ILE:HD13  | 1.88                     | 0.55              |
| 1:A:263:LEU:C     | 1:A:264:ASN:ND2   | 2.63                     | 0.54              |
| 1:A:687:ASN:ND2   | 1:A:689:LYS:H     | 2.05                     | 0.54              |
| 1:A:731:ILE:CG2   | 1:A:734:GLN:CG    | 2.85                     | 0.54              |
| 2:B:14:G:C6       | 2:B:16:A:C6       | 2.94                     | 0.54              |
| 1:A:663:ASN:O     | 1:A:665:ASN:N     | 2.35                     | 0.54              |
| 1:A:1072:PHE:CD1  | 1:A:1072:PHE:C    | 2.85                     | 0.54              |
| 1:A:286:ASN:H     | 1:A:286:ASN:ND2   | 2.05                     | 0.54              |
| 1:A:561:ILE:CD1   | 1:A:566:ILE:HG13  | 2.37                     | 0.54              |
| 1:A:608:ARG:CA    | 1:A:609:ASP:CB    | 2.84                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1009:LYS:CB   | 1:A:1010:ILE:CB   | 2.85                     | 0.54              |
| 1:A:1277:ILE:HG13 | 1:A:1302:ARG:HB3  | 1.88                     | 0.54              |
| 1:A:319:ASN:OD1   | 1:A:322:LEU:HD12  | 2.07                     | 0.54              |
| 1:A:357:PHE:CD1   | 1:A:357:PHE:C     | 2.85                     | 0.54              |
| 1:A:358:PHE:HB2   | 1:A:480:THR:CG2   | 2.37                     | 0.54              |
| 1:A:454:MET:H     | 1:A:455:GLU:CB    | 2.21                     | 0.54              |
| 1:A:1164:LYS:O    | 1:A:1168:LEU:CD1  | 2.55                     | 0.54              |
| 1:A:646:ASP:CB    | 1:A:647:LYS:CB    | 2.85                     | 0.54              |
| 1:A:26:LYS:HG3    | 1:A:41:ASN:O      | 2.08                     | 0.54              |
| 1:A:608:ARG:HD2   | 1:A:608:ARG:O     | 2.07                     | 0.54              |
| 1:A:1164:LYS:HG2  | 1:A:1366:TYR:O    | 2.07                     | 0.54              |
| 1:A:1280:TYR:CD2  | 1:A:1299:GLN:NE2  | 2.71                     | 0.54              |
| 1:A:1333:TYR:O    | 1:A:1337:LYS:HG2  | 2.08                     | 0.54              |
| 1:A:1077:GLY:O    | 1:A:1078:LEU:HB3  | 2.06                     | 0.54              |
| 1:A:1078:LEU:HG   | 1:A:1078:LEU:O    | 2.08                     | 0.54              |
| 1:A:25:VAL:HG11   | 1:A:40:ILE:HG13   | 1.85                     | 0.54              |
| 1:A:249:ILE:N     | 1:A:256:LEU:CD1   | 2.70                     | 0.54              |
| 1:A:413:ASP:CA    | 1:A:414:SER:CB    | 2.85                     | 0.54              |
| 1:A:1329:VAL:HG23 | 1:A:1331:LEU:HD13 | 1.90                     | 0.54              |
| 1:A:235:ILE:HD11  | 1:A:294:ILE:CG2   | 2.38                     | 0.54              |
| 1:A:1063:LEU:HD12 | 1:A:1063:LEU:C    | 2.33                     | 0.54              |
| 2:B:29:G:H4'      | 2:B:30:A:OP1      | 2.08                     | 0.54              |
| 1:A:213:GLU:HG3   | 1:A:216:PHE:HD2   | 1.73                     | 0.54              |
| 1:A:289:LEU:HD23  | 1:A:289:LEU:C     | 2.33                     | 0.54              |
| 1:A:1366:TYR:CE1  | 1:A:1367:ASN:CG   | 2.86                     | 0.53              |
| 1:A:25:VAL:HG13   | 1:A:42:GLU:HG2    | 1.90                     | 0.53              |
| 1:A:261:PHE:CB    | 1:A:283:LEU:CD2   | 2.87                     | 0.53              |
| 1:A:763:SER:OG    | 2:B:21:A:H5''     | 2.07                     | 0.53              |
| 1:A:183:LEU:HD22  | 1:A:253:LEU:HD13  | 1.90                     | 0.53              |
| 1:A:640:LEU:HD13  | 1:A:808:GLN:OE1   | 2.07                     | 0.53              |
| 1:A:185:THR:O     | 1:A:188:SER:HB3   | 2.07                     | 0.53              |
| 1:A:584:ASN:ND2   | 1:A:588:LYS:CB    | 2.72                     | 0.53              |
| 1:A:78:GLY:N      | 1:A:197:ASN:OD1   | 2.41                     | 0.53              |
| 1:A:270:LYS:HD3   | 1:A:271:LYS:H     | 1.74                     | 0.53              |
| 1:A:358:PHE:CB    | 1:A:480:THR:CG2   | 2.85                     | 0.53              |
| 1:A:608:ARG:NH1   | 1:A:608:ARG:HG3   | 2.23                     | 0.53              |
| 1:A:1360:VAL:HB   | 2:B:35:U:H1'      | 1.91                     | 0.53              |
| 1:A:1366:TYR:C    | 1:A:1366:TYR:CD1  | 2.85                     | 0.53              |
| 1:A:1367:ASN:O    | 1:A:1371:ILE:HG22 | 2.08                     | 0.53              |
| 1:A:205:GLU:O     | 1:A:209:GLU:HB2   | 2.08                     | 0.53              |
| 1:A:442:ILE:O     | 1:A:446:GLU:HG2   | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1090:PHE:CA   | 1:A:1091:LEU:CB   | 2.86                     | 0.53              |
| 2:B:15:A:HO2'     | 2:B:16:A:P        | 2.26                     | 0.53              |
| 1:A:25:VAL:CG1    | 1:A:40:ILE:HG13   | 2.38                     | 0.53              |
| 1:A:536:GLU:OE2   | 1:A:556:VAL:CG2   | 2.56                     | 0.53              |
| 1:A:1017:ASN:HB3  | 1:A:1020:PHE:CD2  | 2.43                     | 0.53              |
| 1:A:84:LEU:HD13   | 1:A:193:PHE:CB    | 2.38                     | 0.53              |
| 1:A:364:ASN:O     | 1:A:365:ASN:HB2   | 2.08                     | 0.53              |
| 1:A:703:LEU:O     | 1:A:707:ILE:HG12  | 2.09                     | 0.53              |
| 1:A:84:LEU:HD12   | 1:A:194:LYS:HB3   | 1.90                     | 0.53              |
| 1:A:235:ILE:HG23  | 1:A:236:ASP:N     | 2.24                     | 0.53              |
| 1:A:400:ILE:HG22  | 1:A:439:ILE:HG23  | 1.89                     | 0.53              |
| 1:A:1236:THR:HG22 | 1:A:1243:PHE:O    | 2.09                     | 0.53              |
| 1:A:1271:LYS:HB3  | 1:A:1275:GLU:HB3  | 1.90                     | 0.53              |
| 1:A:77:ALA:HB2    | 1:A:201:TYR:CD2   | 2.45                     | 0.52              |
| 1:A:520:THR:HG23  | 1:A:1189:ALA:HB1  | 1.89                     | 0.52              |
| 1:A:599:ARG:HA    | 1:A:604:ILE:HB    | 1.90                     | 0.52              |
| 1:A:1243:PHE:CD1  | 1:A:1243:PHE:N    | 2.75                     | 0.52              |
| 1:A:362:ILE:HG13  | 1:A:367:ILE:HD13  | 1.87                     | 0.52              |
| 1:A:853:ASN:HB2   | 1:A:882:MET:CE    | 2.39                     | 0.52              |
| 1:A:1234:PHE:CD1  | 1:A:1234:PHE:C    | 2.85                     | 0.52              |
| 2:B:50:U:H6       | 2:B:50:U:C5'      | 2.20                     | 0.52              |
| 1:A:289:LEU:HD23  | 1:A:290:THR:O     | 2.08                     | 0.52              |
| 1:A:1009:LYS:N    | 1:A:1010:ILE:CB   | 2.72                     | 0.52              |
| 1:A:78:GLY:O      | 1:A:85:LYS:HD3    | 2.09                     | 0.52              |
| 1:A:290:THR:HG22  | 1:A:291:VAL:N     | 2.25                     | 0.52              |
| 1:A:767:ASN:OD1   | 1:A:767:ASN:N     | 2.38                     | 0.52              |
| 1:A:1028:ILE:HG22 | 1:A:1032:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:1359:SER:HB3  | 1:A:1363:LEU:HD12 | 1.92                     | 0.52              |
| 1:A:354:ILE:O     | 1:A:357:PHE:HB3   | 2.08                     | 0.52              |
| 1:A:372:GLU:HG3   | 1:A:469:SER:OG    | 2.10                     | 0.52              |
| 1:A:404:PHE:CD2   | 1:A:439:ILE:HD13  | 2.43                     | 0.52              |
| 1:A:454:MET:N     | 1:A:455:GLU:CA    | 2.73                     | 0.52              |
| 1:A:454:MET:N     | 1:A:455:GLU:CB    | 2.73                     | 0.52              |
| 1:A:1060:LYS:CE   | 1:A:1060:LYS:CA   | 2.85                     | 0.52              |
| 1:A:1329:VAL:HG21 | 1:A:1353:MET:HE2  | 1.90                     | 0.52              |
| 2:B:49:C:H2'      | 2:B:50:U:H5'      | 1.91                     | 0.52              |
| 1:A:611:GLN:H     | 1:A:612:GLY:CA    | 2.17                     | 0.52              |
| 1:A:1009:LYS:CB   | 1:A:1010:ILE:CA   | 2.88                     | 0.52              |
| 1:A:1146:ASN:HB3  | 3:A:1418:HOH:O    | 2.09                     | 0.52              |
| 1:A:251:SER:OG    | 1:A:252:ASN:N     | 2.41                     | 0.52              |
| 1:A:359:VAL:CG1   | 1:A:1255:ILE:HG23 | 2.40                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1040:GLU:OE1  | 1:A:1042:LYS:HD3  | 2.10                     | 0.52              |
| 1:A:1277:ILE:HG13 | 1:A:1302:ARG:CB   | 2.40                     | 0.52              |
| 1:A:261:PHE:CA    | 1:A:283:LEU:HD21  | 2.39                     | 0.52              |
| 1:A:337:LEU:CD2   | 1:A:337:LEU:N     | 2.73                     | 0.52              |
| 1:A:726:ASN:HD22  | 1:A:726:ASN:N     | 2.08                     | 0.52              |
| 1:A:881:ILE:O     | 1:A:881:ILE:HG22  | 2.09                     | 0.52              |
| 1:A:1090:PHE:N    | 1:A:1091:LEU:CB   | 2.72                     | 0.52              |
| 1:A:1140:PHE:CD1  | 1:A:1140:PHE:C    | 2.87                     | 0.52              |
| 1:A:1226:PRO:CA   | 1:A:1238:THR:CG2  | 2.84                     | 0.52              |
| 1:A:71:PHE:HA     | 1:A:307:ILE:HD13  | 1.92                     | 0.52              |
| 1:A:397:ASP:CG    | 1:A:398:THR:H     | 2.04                     | 0.52              |
| 1:A:1367:ASN:C    | 1:A:1367:ASN:HD22 | 2.17                     | 0.52              |
| 1:A:25:VAL:CG1    | 1:A:40:ILE:CG1    | 2.80                     | 0.51              |
| 1:A:261:PHE:CB    | 1:A:283:LEU:HD21  | 2.41                     | 0.51              |
| 1:A:292:GLU:N     | 1:A:292:GLU:OE2   | 2.44                     | 0.51              |
| 1:A:638:LEU:CD2   | 1:A:639:ASN:ND2   | 2.73                     | 0.51              |
| 1:A:1200:HIS:ND1  | 1:A:1224:ALA:HB2  | 2.25                     | 0.51              |
| 1:A:608:ARG:CG    | 1:A:608:ARG:NH1   | 2.73                     | 0.51              |
| 1:A:669:TYR:CE2   | 1:A:752:GLU:HB2   | 2.45                     | 0.51              |
| 1:A:1059:TYR:N    | 3:A:1427:HOH:O    | 2.42                     | 0.51              |
| 1:A:1118:LEU:CD1  | 1:A:1126:LYS:HG2  | 2.36                     | 0.51              |
| 1:A:80:ILE:CD1    | 1:A:200:LEU:CG    | 2.70                     | 0.51              |
| 1:A:235:ILE:HD11  | 1:A:294:ILE:HG23  | 1.91                     | 0.51              |
| 1:A:679:GLU:HB3   | 1:A:782:ILE:HD11  | 1.92                     | 0.51              |
| 1:A:906:LYS:HZ3   | 1:A:1022:LYS:CB   | 2.23                     | 0.51              |
| 1:A:1278:ARG:HH22 | 1:A:1279:ASN:ND2  | 2.08                     | 0.51              |
| 1:A:1090:PHE:H    | 1:A:1092:PHE:N    | 2.08                     | 0.51              |
| 1:A:1214:LEU:N    | 1:A:1214:LEU:CD1  | 2.73                     | 0.51              |
| 1:A:402:GLY:O     | 1:A:403:ILE:C     | 2.51                     | 0.51              |
| 1:A:192:ILE:CG2   | 1:A:245:ILE:CG1   | 2.89                     | 0.51              |
| 1:A:272:SER:HB3   | 1:A:304:PHE:CE2   | 2.46                     | 0.51              |
| 1:A:662:GLU:O     | 1:A:663:ASN:HB2   | 2.10                     | 0.51              |
| 1:A:1130:ILE:HD11 | 1:A:1361:LEU:HG   | 1.91                     | 0.51              |
| 1:A:84:LEU:HD21   | 1:A:197:ASN:CG    | 2.36                     | 0.51              |
| 1:A:314:VAL:HG12  | 1:A:315:LYS:H     | 1.74                     | 0.51              |
| 1:A:585:PHE:C     | 1:A:585:PHE:CD1   | 2.89                     | 0.51              |
| 1:A:677:LEU:HD13  | 1:A:707:ILE:HG23  | 1.93                     | 0.51              |
| 1:A:1041:ASN:O    | 1:A:1042:LYS:C    | 2.53                     | 0.51              |
| 1:A:1146:ASN:ND2  | 1:A:1151:SER:OG   | 2.33                     | 0.51              |
| 1:A:378:PHE:HA    | 1:A:412:PHE:HE1   | 1.75                     | 0.51              |
| 1:A:417:PHE:HA    | 1:A:418:SER:CB    | 2.40                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:449:VAL:HG12  | 1:A:455:GLU:CA    | 2.39                     | 0.51              |
| 1:A:192:ILE:HG22  | 1:A:245:ILE:CD1   | 2.39                     | 0.51              |
| 1:A:641:ASP:HA    | 3:A:1403:HOH:O    | 1.93                     | 0.51              |
| 1:A:802:ILE:O     | 1:A:802:ILE:HG22  | 2.10                     | 0.51              |
| 1:A:1234:PHE:HE1  | 1:A:1235:TYR:HD2  | 1.57                     | 0.51              |
| 1:A:1342:LEU:CD1  | 1:A:1342:LEU:N    | 2.73                     | 0.51              |
| 1:A:1026:LYS:HG3  | 1:A:1027:GLU:N    | 2.26                     | 0.50              |
| 1:A:1063:LEU:HD12 | 1:A:1067:ILE:HD11 | 1.93                     | 0.50              |
| 1:A:1228:ARG:HA   | 1:A:1234:PHE:CE2  | 2.47                     | 0.50              |
| 1:A:213:GLU:CG    | 1:A:216:PHE:HD2   | 2.24                     | 0.50              |
| 1:A:683:LEU:HD11  | 1:A:793:PHE:CD2   | 2.46                     | 0.50              |
| 1:A:695:THR:C     | 1:A:696:ILE:CG1   | 2.82                     | 0.50              |
| 1:A:1228:ARG:NH1  | 1:A:1228:ARG:CG   | 2.73                     | 0.50              |
| 1:A:767:ASN:HA    | 3:A:1407:HOH:O    | 2.11                     | 0.50              |
| 2:B:14:G:C2       | 2:B:16:A:C4       | 2.99                     | 0.50              |
| 1:A:361:ASN:HB3   | 1:A:367:ILE:HG12  | 1.92                     | 0.50              |
| 1:A:584:ASN:HD21  | 1:A:588:LYS:CB    | 2.25                     | 0.50              |
| 1:A:701:ILE:O     | 1:A:701:ILE:CG2   | 2.60                     | 0.50              |
| 1:A:192:ILE:CG2   | 1:A:245:ILE:HD11  | 2.37                     | 0.50              |
| 1:A:315:LYS:CG    | 1:A:316:LYS:CE    | 2.86                     | 0.50              |
| 1:A:501:ASN:OD1   | 1:A:503:ASP:N     | 2.43                     | 0.50              |
| 1:A:871:TYR:O     | 1:A:874:ILE:HG22  | 2.12                     | 0.50              |
| 1:A:1366:TYR:CD1  | 1:A:1367:ASN:N    | 2.79                     | 0.50              |
| 1:A:197:ASN:ND2   | 1:A:198:MET:N     | 2.60                     | 0.50              |
| 1:A:315:LYS:HG3   | 1:A:316:LYS:NZ    | 2.27                     | 0.50              |
| 1:A:1234:PHE:HA   | 1:A:1237:THR:OG1  | 2.12                     | 0.50              |
| 1:A:664:ASN:O     | 1:A:665:ASN:ND2   | 2.44                     | 0.50              |
| 1:A:906:LYS:HE2   | 1:A:1021:LEU:C    | 2.37                     | 0.50              |
| 1:A:1130:ILE:HD11 | 1:A:1361:LEU:CG   | 2.41                     | 0.50              |
| 1:A:1322:PHE:O    | 1:A:1331:LEU:HD21 | 2.11                     | 0.50              |
| 1:A:70:GLU:OE2    | 1:A:70:GLU:HA     | 2.12                     | 0.50              |
| 1:A:262:TYR:O     | 1:A:264:ASN:N     | 2.37                     | 0.50              |
| 1:A:696:ILE:CG2   | 1:A:699:GLU:CB    | 2.86                     | 0.50              |
| 1:A:893:THR:O     | 1:A:897:ASN:C     | 2.55                     | 0.50              |
| 1:A:901:GLU:O     | 1:A:904:ILE:HB    | 2.12                     | 0.50              |
| 1:A:1167:ASP:HA   | 1:A:1172:ASN:OD1  | 2.11                     | 0.50              |
| 1:A:1290:PRO:O    | 1:A:1291:PHE:HB2  | 2.12                     | 0.50              |
| 1:A:1380:THR:O    | 1:A:1381:LYS:C    | 2.55                     | 0.50              |
| 1:A:183:LEU:HD11  | 1:A:255:ILE:CD1   | 2.41                     | 0.49              |
| 1:A:636:LYS:HE3   | 1:A:887:LEU:CG    | 2.42                     | 0.49              |
| 1:A:693:PHE:C     | 1:A:694:ASP:O     | 2.51                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:695:THR:HG23  | 1:A:696:ILE:H    | 1.75                     | 0.49              |
| 1:A:76:HIS:C      | 1:A:76:HIS:ND1   | 2.70                     | 0.49              |
| 1:A:675:LYS:O     | 1:A:678:PRO:HD2  | 2.12                     | 0.49              |
| 1:A:686:ASN:CA    | 3:A:1423:HOH:O   | 2.41                     | 0.49              |
| 1:A:56:ARG:CG     | 1:A:56:ARG:NH2   | 2.73                     | 0.49              |
| 1:A:270:LYS:HE3   | 1:A:270:LYS:CA   | 2.30                     | 0.49              |
| 1:A:377:GLU:HB3   | 1:A:412:PHE:HZ   | 1.78                     | 0.49              |
| 1:A:407:HIS:CE1   | 1:A:411:ASN:ND2  | 2.73                     | 0.49              |
| 1:A:1356:LYS:HG3  | 1:A:1357:LYS:N   | 2.27                     | 0.49              |
| 1:A:87:LYS:CA     | 1:A:97:ASP:O     | 2.61                     | 0.49              |
| 1:A:237:VAL:O     | 1:A:240:THR:HB   | 2.13                     | 0.49              |
| 1:A:249:ILE:HG13  | 1:A:257:GLY:CA   | 2.41                     | 0.49              |
| 1:A:357:PHE:CD2   | 1:A:423:GLU:HB3  | 2.46                     | 0.49              |
| 1:A:631:ASP:OD2   | 1:A:891:CYS:SG   | 2.70                     | 0.49              |
| 1:A:1124:GLU:OE2  | 1:A:1124:GLU:HA  | 2.12                     | 0.49              |
| 1:A:1253:GLU:OE1  | 1:A:1264:SER:HB3 | 2.12                     | 0.49              |
| 2:B:15:A:H4'      | 2:B:15:A:OP2     | 2.13                     | 0.49              |
| 1:A:561:ILE:HD11  | 1:A:563:ASN:N    | 2.19                     | 0.49              |
| 1:A:597:ARG:NH1   | 1:A:1222:SER:OG  | 2.46                     | 0.49              |
| 1:A:1090:PHE:N    | 1:A:1092:PHE:N   | 2.60                     | 0.49              |
| 1:A:1146:ASN:HD21 | 1:A:1152:PHE:CA  | 2.25                     | 0.49              |
| 2:B:31:C:H2'      | 2:B:32:A:O4'     | 2.12                     | 0.49              |
| 1:A:56:ARG:HH21   | 1:A:56:ARG:HG3   | 1.76                     | 0.49              |
| 1:A:81:LEU:C      | 1:A:81:LEU:CD2   | 2.86                     | 0.49              |
| 1:A:1069:ASN:O    | 1:A:1071:ASN:N   | 2.46                     | 0.49              |
| 1:A:1079:ILE:HD13 | 1:A:1173:TYR:HB2 | 1.95                     | 0.49              |
| 1:A:192:ILE:HG21  | 1:A:245:ILE:HG13 | 1.95                     | 0.49              |
| 1:A:1122:SER:O    | 1:A:1126:LYS:HG3 | 2.13                     | 0.49              |
| 1:A:192:ILE:HG21  | 1:A:245:ILE:HG12 | 1.94                     | 0.49              |
| 1:A:207:ILE:O     | 1:A:210:ASN:HB2  | 2.13                     | 0.49              |
| 1:A:400:ILE:HD12  | 1:A:443:LEU:CD1  | 2.41                     | 0.49              |
| 1:A:1049:PRO:HB3  | 1:A:1050:LYS:C   | 2.37                     | 0.49              |
| 1:A:4:LEU:HD12    | 1:A:54:PHE:HZ    | 1.78                     | 0.49              |
| 1:A:1168:LEU:HD12 | 1:A:1168:LEU:N   | 2.26                     | 0.49              |
| 1:A:352:ASP:OD1   | 1:A:352:ASP:N    | 2.46                     | 0.48              |
| 1:A:611:GLN:N     | 1:A:612:GLY:HA2  | 2.17                     | 0.48              |
| 1:A:638:LEU:CD2   | 1:A:638:LEU:C    | 2.85                     | 0.48              |
| 1:A:684:TYR:OH    | 1:A:693:PHE:CZ   | 2.63                     | 0.48              |
| 1:A:1009:LYS:CA   | 1:A:1010:ILE:CB  | 2.91                     | 0.48              |
| 1:A:631:ASP:OD2   | 1:A:891:CYS:HB3  | 2.12                     | 0.48              |
| 1:A:1049:PRO:CA   | 1:A:1050:LYS:CB  | 2.90                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1227:LYS:CB   | 1:A:1229:ASN:ND2  | 2.75                     | 0.48              |
| 1:A:390:GLU:O     | 1:A:393:LYS:CB    | 2.62                     | 0.48              |
| 1:A:534:SER:O     | 1:A:556:VAL:O     | 2.32                     | 0.48              |
| 1:A:288:ASP:OD1   | 1:A:289:LEU:N     | 2.47                     | 0.48              |
| 2:B:31:C:H6       | 2:B:31:C:P        | 2.36                     | 0.48              |
| 1:A:183:LEU:HD22  | 1:A:253:LEU:HD11  | 1.95                     | 0.48              |
| 1:A:405:LYS:NZ    | 2:B:16:A:N7       | 2.43                     | 0.48              |
| 1:A:641:ASP:CB    | 1:A:821:ILE:HG12  | 2.44                     | 0.48              |
| 1:A:731:ILE:CG2   | 1:A:734:GLN:HG2   | 2.43                     | 0.48              |
| 1:A:1026:LYS:HB2  | 1:A:1026:LYS:HE2  | 1.63                     | 0.48              |
| 1:A:1079:ILE:HG22 | 1:A:1083:ILE:HD11 | 1.94                     | 0.48              |
| 1:A:1094:ILE:O    | 1:A:1098:ASN:HB2  | 2.12                     | 0.48              |
| 2:B:46:A:H2'      | 2:B:47:A:O4'      | 2.13                     | 0.48              |
| 1:A:58:TYR:O      | 1:A:62:LYS:HG3    | 2.13                     | 0.48              |
| 1:A:84:LEU:O      | 1:A:84:LEU:HG     | 2.13                     | 0.48              |
| 1:A:270:LYS:HD3   | 1:A:271:LYS:N     | 2.29                     | 0.48              |
| 1:A:316:LYS:CE    | 1:A:316:LYS:N     | 2.73                     | 0.48              |
| 1:A:532:ILE:O     | 1:A:532:ILE:HD12  | 2.13                     | 0.48              |
| 1:A:608:ARG:HH11  | 1:A:608:ARG:CB    | 2.26                     | 0.48              |
| 1:A:808:GLN:O     | 1:A:812:ILE:CG1   | 2.51                     | 0.48              |
| 1:A:1346:ASN:CG   | 1:A:1349:LEU:HD22 | 2.38                     | 0.48              |
| 1:A:19:PHE:CD1    | 1:A:19:PHE:N      | 2.82                     | 0.48              |
| 1:A:25:VAL:HG13   | 1:A:42:GLU:CG     | 2.44                     | 0.48              |
| 1:A:362:ILE:HG12  | 1:A:367:ILE:HD12  | 1.93                     | 0.48              |
| 1:A:377:GLU:OE2   | 1:A:417:PHE:HZ    | 1.97                     | 0.48              |
| 1:A:495:ILE:HD11  | 1:A:508:LEU:CD1   | 2.44                     | 0.48              |
| 1:A:1095:ASP:O    | 1:A:1099:ILE:HG13 | 2.13                     | 0.48              |
| 1:A:1163:LYS:HD3  | 1:A:1366:TYR:CD2  | 2.49                     | 0.48              |
| 1:A:84:LEU:CD1    | 1:A:194:LYS:HB3   | 2.43                     | 0.48              |
| 1:A:337:LEU:HD23  | 1:A:337:LEU:N     | 2.24                     | 0.48              |
| 1:A:346:GLU:HB2   | 1:A:347:ARG:CB    | 2.43                     | 0.48              |
| 1:A:641:ASP:HB2   | 1:A:821:ILE:HG12  | 1.96                     | 0.48              |
| 1:A:1041:ASN:ND2  | 1:A:1041:ASN:N    | 2.60                     | 0.48              |
| 2:B:14:G:C2       | 2:B:16:A:C2       | 3.02                     | 0.48              |
| 1:A:182:GLU:CD    | 1:A:184:GLU:HB2   | 2.38                     | 0.48              |
| 1:A:517:GLU:HG3   | 1:A:858:ARG:CD    | 2.44                     | 0.48              |
| 1:A:668:LYS:HG2   | 1:A:669:TYR:N     | 2.29                     | 0.48              |
| 1:A:893:THR:CB    | 1:A:1059:TYR:OH   | 2.62                     | 0.48              |
| 1:A:1069:ASN:ND2  | 1:A:1178:GLU:OE2  | 2.47                     | 0.48              |
| 1:A:1090:PHE:CB   | 1:A:1091:LEU:CB   | 2.92                     | 0.48              |
| 1:A:1130:ILE:CD1  | 1:A:1361:LEU:N    | 2.74                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1346:ASN:HB3  | 1:A:1349:LEU:HB2 | 1.94                     | 0.48              |
| 2:B:31:C:H2'      | 2:B:32:A:O5'     | 2.13                     | 0.48              |
| 1:A:362:ILE:CG1   | 1:A:367:ILE:HD13 | 2.41                     | 0.47              |
| 1:A:639:ASN:N     | 1:A:639:ASN:ND2  | 2.60                     | 0.47              |
| 1:A:1049:PRO:HD3  | 1:A:1058:ILE:CD1 | 2.44                     | 0.47              |
| 1:A:249:ILE:CG1   | 1:A:257:GLY:CA   | 2.92                     | 0.47              |
| 1:A:1069:ASN:C    | 1:A:1071:ASN:N   | 2.69                     | 0.47              |
| 1:A:95:ASN:C      | 1:A:95:ASN:ND2   | 2.73                     | 0.47              |
| 1:A:213:GLU:CB    | 3:A:1431:HOH:O   | 2.61                     | 0.47              |
| 1:A:583:ASN:OD1   | 1:A:583:ASN:N    | 2.48                     | 0.47              |
| 1:A:622:ASN:HD21  | 1:A:842:ILE:HG13 | 1.79                     | 0.47              |
| 1:A:668:LYS:HD3   | 1:A:669:TYR:CZ   | 2.49                     | 0.47              |
| 1:A:683:LEU:C     | 1:A:683:LEU:CD1  | 2.85                     | 0.47              |
| 1:A:664:ASN:OD1   | 1:A:719:LEU:HD23 | 2.15                     | 0.47              |
| 1:A:90:ILE:HD11   | 1:A:97:ASP:H     | 1.79                     | 0.47              |
| 1:A:610:LEU:CB    | 1:A:612:GLY:HA3  | 2.44                     | 0.47              |
| 1:A:181:ASP:HA    | 1:A:182:GLU:HA   | 1.63                     | 0.47              |
| 1:A:454:MET:H     | 1:A:455:GLU:CA   | 2.28                     | 0.47              |
| 1:A:630:SER:HB2   | 1:A:884:LEU:CD2  | 2.41                     | 0.47              |
| 1:A:687:ASN:ND2   | 1:A:687:ASN:C    | 2.73                     | 0.47              |
| 1:A:785:LEU:HD23  | 1:A:785:LEU:HA   | 1.77                     | 0.47              |
| 1:A:855:ILE:HG13  | 1:A:856:ARG:N    | 2.27                     | 0.47              |
| 1:A:1069:ASN:O    | 1:A:1072:PHE:N   | 2.36                     | 0.47              |
| 1:A:1090:PHE:N    | 1:A:1091:LEU:C   | 2.73                     | 0.47              |
| 1:A:1227:LYS:CB   | 1:A:1229:ASN:CG  | 2.88                     | 0.47              |
| 1:A:53:LYS:O      | 1:A:57:LYS:HG2   | 2.14                     | 0.47              |
| 1:A:95:ASN:C      | 1:A:95:ASN:HD22  | 2.23                     | 0.47              |
| 1:A:193:PHE:HE2   | 1:A:263:LEU:HD23 | 1.79                     | 0.47              |
| 1:A:454:MET:CB    | 1:A:455:GLU:HA   | 2.39                     | 0.47              |
| 1:A:546:PHE:O     | 1:A:590:THR:HG23 | 2.15                     | 0.47              |
| 1:A:794:ASP:O     | 1:A:795:PHE:HD1  | 1.98                     | 0.47              |
| 1:A:893:THR:CB    | 1:A:1059:TYR:CZ  | 2.98                     | 0.47              |
| 1:A:1044:GLN:CB   | 1:A:1048:TYR:CE1 | 2.97                     | 0.47              |
| 1:A:1047:TYR:O    | 1:A:1058:ILE:CG1 | 2.52                     | 0.47              |
| 1:A:1358:VAL:O    | 1:A:1363:LEU:N   | 2.48                     | 0.47              |
| 1:A:1367:ASN:HD22 | 1:A:1367:ASN:H   | 1.63                     | 0.47              |
| 1:A:80:ILE:HD12   | 1:A:200:LEU:HG   | 1.89                     | 0.47              |
| 1:A:90:ILE:O      | 1:A:90:ILE:HG13  | 2.14                     | 0.47              |
| 1:A:249:ILE:CG1   | 1:A:257:GLY:HA2  | 2.44                     | 0.47              |
| 1:A:402:GLY:O     | 1:A:405:LYS:N    | 2.48                     | 0.47              |
| 1:A:687:ASN:ND2   | 1:A:689:LYS:N    | 2.62                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1075:ILE:HG23 | 1:A:1177:ILE:CG2  | 2.41                     | 0.47              |
| 1:A:1211:ILE:HG22 | 1:A:1211:ILE:O    | 2.15                     | 0.47              |
| 1:A:1233:GLY:O    | 1:A:1237:THR:HG23 | 2.15                     | 0.47              |
| 1:A:1341:LYS:O    | 1:A:1341:LYS:HG3  | 2.14                     | 0.47              |
| 1:A:19:PHE:HD1    | 1:A:19:PHE:H      | 1.62                     | 0.47              |
| 1:A:191:GLU:CG    | 1:A:194:LYS:HE2   | 2.28                     | 0.47              |
| 1:A:1011:LEU:C    | 1:A:1013:ARG:H    | 2.23                     | 0.47              |
| 1:A:1295:SER:N    | 1:A:1382:ILE:HD12 | 2.30                     | 0.47              |
| 1:A:4:LEU:O       | 2:B:19:G:OP1      | 2.33                     | 0.47              |
| 1:A:695:THR:CG2   | 1:A:696:ILE:H     | 2.27                     | 0.47              |
| 2:B:14:G:C5       | 2:B:16:A:C6       | 3.03                     | 0.47              |
| 1:A:287:VAL:HG11  | 1:A:1129:TYR:HD2  | 1.79                     | 0.46              |
| 1:A:184:GLU:HA    | 1:A:184:GLU:OE1   | 2.15                     | 0.46              |
| 1:A:197:ASN:ND2   | 1:A:197:ASN:C     | 2.73                     | 0.46              |
| 1:A:448:LYS:C     | 1:A:454:MET:HB2   | 2.39                     | 0.46              |
| 1:A:640:LEU:C     | 1:A:642:VAL:N     | 2.72                     | 0.46              |
| 1:A:1228:ARG:HA   | 1:A:1234:PHE:HD2  | 1.77                     | 0.46              |
| 1:A:1325:PHE:CD2  | 1:A:1353:MET:HE1  | 2.50                     | 0.46              |
| 1:A:407:HIS:ND1   | 1:A:407:HIS:C     | 2.73                     | 0.46              |
| 1:A:664:ASN:OD1   | 1:A:719:LEU:CD2   | 2.64                     | 0.46              |
| 1:A:26:LYS:CG     | 1:A:41:ASN:O      | 2.62                     | 0.46              |
| 1:A:82:PHE:HB3    | 1:A:84:LEU:HD22   | 1.94                     | 0.46              |
| 1:A:213:GLU:HB3   | 3:A:1431:HOH:O    | 2.14                     | 0.46              |
| 1:A:222:GLU:CD    | 1:A:222:GLU:H     | 2.23                     | 0.46              |
| 1:A:314:VAL:CG1   | 1:A:315:LYS:N     | 2.76                     | 0.46              |
| 1:A:592:ILE:HG22  | 1:A:839:ILE:CG2   | 2.44                     | 0.46              |
| 1:A:808:GLN:O     | 1:A:812:ILE:N     | 2.46                     | 0.46              |
| 1:A:1011:LEU:C    | 1:A:1013:ARG:N    | 2.70                     | 0.46              |
| 1:A:1145:GLN:C    | 3:A:1416:HOH:O    | 2.58                     | 0.46              |
| 1:A:1157:ASN:HA   | 1:A:1160:SER:HB3  | 1.98                     | 0.46              |
| 1:A:1345:ASN:O    | 1:A:1346:ASN:C    | 2.58                     | 0.46              |
| 1:A:638:LEU:HD22  | 1:A:639:ASN:H     | 1.78                     | 0.46              |
| 1:A:677:LEU:HB3   | 1:A:678:PRO:HD3   | 1.98                     | 0.46              |
| 1:A:874:ILE:O     | 1:A:878:LEU:HG    | 2.16                     | 0.46              |
| 1:A:1060:LYS:HA   | 1:A:1060:LYS:HZ3  | 1.75                     | 0.46              |
| 1:A:355:VAL:HG21  | 1:A:483:HIS:CD2   | 2.51                     | 0.46              |
| 1:A:377:GLU:HB3   | 1:A:412:PHE:CZ    | 2.50                     | 0.46              |
| 1:A:505:PHE:HB3   | 2:B:22:C:H1'      | 1.96                     | 0.46              |
| 1:A:532:ILE:CD1   | 1:A:533:PHE:CD2   | 2.95                     | 0.46              |
| 1:A:1184:ILE:HD11 | 1:A:1325:PHE:CZ   | 2.51                     | 0.46              |
| 1:A:1340:PHE:HD2  | 1:A:1349:LEU:HD21 | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1346:ASN:HB3  | 1:A:1349:LEU:HD22 | 1.96                     | 0.46              |
| 1:A:1348:ILE:H    | 1:A:1348:ILE:CD1  | 1.94                     | 0.46              |
| 1:A:369:GLU:HA    | 1:A:372:GLU:HB2   | 1.98                     | 0.46              |
| 1:A:510:ALA:HB2   | 1:A:865:TRP:CE2   | 2.51                     | 0.46              |
| 1:A:581:ILE:C     | 1:A:581:ILE:CD1   | 2.87                     | 0.46              |
| 1:A:638:LEU:H     | 1:A:638:LEU:CD1   | 2.03                     | 0.46              |
| 1:A:888:ARG:O     | 1:A:891:CYS:SG    | 2.73                     | 0.46              |
| 1:A:96:ASN:HA     | 1:A:97:ASP:HA     | 1.73                     | 0.46              |
| 1:A:378:PHE:O     | 3:A:1401:HOH:O    | 2.21                     | 0.46              |
| 1:A:576:ASP:N     | 1:A:580:ASN:O     | 2.47                     | 0.46              |
| 1:A:632:GLU:O     | 1:A:635:SER:HB3   | 2.16                     | 0.46              |
| 1:A:665:ASN:ND2   | 1:A:665:ASN:C     | 2.73                     | 0.46              |
| 1:A:1063:LEU:CD2  | 1:A:1171:PHE:CE2  | 2.98                     | 0.46              |
| 1:A:1073:ASP:OD1  | 1:A:1073:ASP:N    | 2.47                     | 0.46              |
| 1:A:1195:PHE:CZ   | 1:A:1269:ILE:HD11 | 2.51                     | 0.46              |
| 1:A:1235:TYR:CD1  | 1:A:1236:THR:CG2  | 2.99                     | 0.46              |
| 1:A:317:VAL:HG21  | 1:A:323:GLU:N     | 2.31                     | 0.46              |
| 1:A:361:ASN:C     | 1:A:367:ILE:HG13  | 2.41                     | 0.46              |
| 1:A:1015:ILE:HD12 | 1:A:1015:ILE:HA   | 1.71                     | 0.46              |
| 1:A:83:LYS:CG     | 1:A:85:LYS:HE3    | 2.38                     | 0.45              |
| 3:A:1409:HOH:O    | 2:B:16:A:N3       | 2.42                     | 0.45              |
| 1:A:906:LYS:HZ3   | 1:A:1022:LYS:CA   | 2.21                     | 0.45              |
| 1:A:1197:ARG:HH11 | 1:A:1197:ARG:CG   | 2.28                     | 0.45              |
| 1:A:1340:PHE:CD2  | 1:A:1349:LEU:HD21 | 2.51                     | 0.45              |
| 1:A:1039:ASN:C    | 1:A:1040:GLU:HG2  | 2.41                     | 0.45              |
| 1:A:442:ILE:CD1   | 1:A:443:LEU:N     | 2.79                     | 0.45              |
| 1:A:357:PHE:C     | 1:A:357:PHE:HD1   | 2.25                     | 0.45              |
| 1:A:574:PHE:O     | 1:A:582:THR:CB    | 2.65                     | 0.45              |
| 1:A:631:ASP:OD2   | 1:A:891:CYS:CB    | 2.65                     | 0.45              |
| 1:A:897:ASN:CB    | 1:A:1016:PHE:HZ   | 2.24                     | 0.45              |
| 1:A:1299:GLN:OE1  | 1:A:1302:ARG:HD3  | 2.17                     | 0.45              |
| 1:A:1319:ALA:O    | 1:A:1320:SER:C    | 2.59                     | 0.45              |
| 1:A:397:ASP:HA    | 1:A:443:LEU:HD11  | 1.98                     | 0.45              |
| 1:A:1213:LYS:C    | 1:A:1214:LEU:CD1  | 2.89                     | 0.45              |
| 2:B:14:G:N1       | 2:B:16:A:C2       | 2.84                     | 0.45              |
| 1:A:345:ILE:CG1   | 1:A:346:GLU:N     | 2.78                     | 0.45              |
| 1:A:1050:LYS:N    | 1:A:1051:GLU:CA   | 2.72                     | 0.45              |
| 1:A:1059:TYR:CE1  | 1:A:1061:LYS:HB2  | 2.46                     | 0.45              |
| 1:A:1106:GLU:O    | 1:A:1110:ILE:HG13 | 2.15                     | 0.45              |
| 1:A:1349:LEU:O    | 1:A:1349:LEU:HD12 | 2.15                     | 0.45              |
| 1:A:286:ASN:ND2   | 1:A:286:ASN:N     | 2.65                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:368:LYS:HB2   | 1:A:368:LYS:HE3   | 1.65                     | 0.45              |
| 1:A:617:TYR:C     | 1:A:620:VAL:HG22  | 2.42                     | 0.45              |
| 1:A:662:GLU:O     | 1:A:663:ASN:CB    | 2.65                     | 0.45              |
| 1:A:897:ASN:CB    | 1:A:898:LEU:CA    | 2.94                     | 0.45              |
| 1:A:1264:SER:O    | 1:A:1267:SER:HB3  | 2.17                     | 0.45              |
| 1:A:1325:PHE:O    | 1:A:1329:VAL:HG22 | 2.16                     | 0.45              |
| 1:A:54:PHE:CD1    | 1:A:54:PHE:C      | 2.94                     | 0.45              |
| 1:A:201:TYR:CE2   | 1:A:205:GLU:OE2   | 2.70                     | 0.45              |
| 1:A:235:ILE:CG2   | 1:A:236:ASP:N     | 2.80                     | 0.45              |
| 1:A:284:ASN:OD1   | 1:A:287:VAL:N     | 2.44                     | 0.45              |
| 1:A:442:ILE:C     | 1:A:442:ILE:CD1   | 2.85                     | 0.45              |
| 1:A:454:MET:H     | 1:A:455:GLU:HA    | 1.82                     | 0.45              |
| 1:A:575:ILE:HG12  | 1:A:579:ASN:HA    | 1.99                     | 0.45              |
| 1:A:1039:ASN:O    | 1:A:1040:GLU:HG2  | 2.17                     | 0.45              |
| 1:A:82:PHE:CD1    | 1:A:263:LEU:O     | 2.68                     | 0.45              |
| 1:A:262:TYR:O     | 1:A:262:TYR:CD1   | 2.70                     | 0.45              |
| 1:A:445:ASN:O     | 1:A:449:VAL:N     | 2.49                     | 0.45              |
| 1:A:636:LYS:O     | 1:A:636:LYS:HG2   | 2.17                     | 0.45              |
| 1:A:1076:TYR:O    | 1:A:1076:TYR:CD1  | 2.70                     | 0.45              |
| 1:A:1291:PHE:HE1  | 1:A:1378:LEU:O    | 2.00                     | 0.45              |
| 1:A:249:ILE:HA    | 1:A:256:LEU:HB3   | 1.99                     | 0.44              |
| 1:A:491:ARG:O     | 1:A:494:ASP:N     | 2.49                     | 0.44              |
| 1:A:638:LEU:HD22  | 1:A:638:LEU:C     | 2.42                     | 0.44              |
| 1:A:1185:ASN:OD1  | 1:A:1284:PHE:HA   | 2.17                     | 0.44              |
| 1:A:194:LYS:HG3   | 1:A:195:ASN:N     | 2.32                     | 0.44              |
| 1:A:259:VAL:HG23  | 1:A:260:LYS:N     | 2.33                     | 0.44              |
| 1:A:851:VAL:HG13  | 1:A:1186:TRP:CZ3  | 2.53                     | 0.44              |
| 2:B:31:C:C2'      | 2:B:32:A:C5'      | 2.88                     | 0.44              |
| 1:A:96:ASN:CB     | 1:A:97:ASP:HA     | 2.45                     | 0.44              |
| 1:A:380:ILE:HD12  | 1:A:380:ILE:N     | 2.16                     | 0.44              |
| 1:A:613:THR:O     | 1:A:835:ASP:OD2   | 2.36                     | 0.44              |
| 1:A:636:LYS:CE    | 1:A:887:LEU:CD2   | 2.90                     | 0.44              |
| 1:A:644:PHE:O     | 1:A:646:ASP:N     | 2.46                     | 0.44              |
| 1:A:1118:LEU:O    | 1:A:1121:TYR:CD1  | 2.70                     | 0.44              |
| 1:A:1278:ARG:HH22 | 1:A:1279:ASN:HD21 | 1.65                     | 0.44              |
| 2:B:31:C:C6       | 2:B:31:C:OP2      | 2.70                     | 0.44              |
| 1:A:454:MET:C     | 1:A:454:MET:CE    | 2.86                     | 0.44              |
| 1:A:898:LEU:CD1   | 1:A:1059:TYR:CE2  | 2.94                     | 0.44              |
| 1:A:1140:PHE:CD1  | 1:A:1140:PHE:O    | 2.70                     | 0.44              |
| 1:A:1226:PRO:CA   | 1:A:1238:THR:HG21 | 2.46                     | 0.44              |
| 1:A:1271:LYS:HB2  | 1:A:1275:GLU:HB3  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1281:ILE:HD13 | 1:A:1303:VAL:HG11 | 1.99                     | 0.44              |
| 1:A:1342:LEU:CD1  | 1:A:1342:LEU:H    | 2.31                     | 0.44              |
| 1:A:1367:ASN:ND2  | 1:A:1367:ASN:C    | 2.76                     | 0.44              |
| 1:A:31:TYR:CE2    | 1:A:33:GLY:O      | 2.70                     | 0.44              |
| 1:A:1048:TYR:CD1  | 1:A:1048:TYR:O    | 2.71                     | 0.44              |
| 1:A:1236:THR:CB   | 1:A:1242:LYS:HG3  | 2.45                     | 0.44              |
| 1:A:1271:LYS:HG3  | 3:A:1405:HOH:O    | 1.92                     | 0.44              |
| 1:A:1354:LYS:HE3  | 1:A:1354:LYS:HB2  | 1.58                     | 0.44              |
| 1:A:200:LEU:C     | 1:A:200:LEU:CD1   | 2.91                     | 0.44              |
| 1:A:527:MET:HE1   | 1:A:1287:VAL:HG23 | 2.00                     | 0.44              |
| 1:A:573:ASP:O     | 1:A:582:THR:CB    | 2.65                     | 0.44              |
| 1:A:623:ILE:O     | 1:A:627:LEU:HG    | 2.18                     | 0.44              |
| 1:A:625:GLN:HG2   | 1:A:845:LEU:CD1   | 2.47                     | 0.44              |
| 1:A:729:LYS:HE3   | 1:A:788:ASN:OD1   | 2.18                     | 0.44              |
| 1:A:839:ILE:HG13  | 1:A:840:ILE:N     | 2.32                     | 0.44              |
| 1:A:193:PHE:O     | 1:A:196:ILE:HB    | 2.17                     | 0.44              |
| 1:A:193:PHE:HZ    | 1:A:260:LYS:HA    | 1.82                     | 0.44              |
| 1:A:547:PHE:CZ    | 1:A:843:PHE:CZ    | 3.05                     | 0.44              |
| 1:A:785:LEU:HD13  | 1:A:793:PHE:HZ    | 1.81                     | 0.44              |
| 1:A:1044:GLN:CA   | 1:A:1048:TYR:CE1  | 2.97                     | 0.44              |
| 1:A:1111:LEU:HD22 | 1:A:1359:SER:CB   | 2.48                     | 0.44              |
| 2:B:32:A:O5'      | 2:B:32:A:C8       | 2.70                     | 0.44              |
| 1:A:210:ASN:ND2   | 1:A:228:LYS:NZ    | 2.66                     | 0.44              |
| 1:A:290:THR:CG2   | 1:A:291:VAL:N     | 2.80                     | 0.44              |
| 2:B:31:C:O5'      | 2:B:31:C:C6       | 2.70                     | 0.44              |
| 2:B:51:C:H3'      | 2:B:51:C:H6       | 1.83                     | 0.44              |
| 1:A:268:ASP:CB    | 2:B:51:C:O2       | 2.65                     | 0.44              |
| 1:A:567:LYS:NZ    | 1:A:567:LYS:CB    | 2.73                     | 0.44              |
| 1:A:1118:LEU:CD1  | 1:A:1126:LYS:HD3  | 2.48                     | 0.44              |
| 1:A:1338:LYS:HE2  | 1:A:1338:LYS:HB2  | 1.60                     | 0.44              |
| 1:A:640:LEU:C     | 1:A:642:VAL:H     | 2.26                     | 0.43              |
| 1:A:644:PHE:O     | 1:A:647:LYS:C     | 2.61                     | 0.43              |
| 1:A:1017:ASN:OD1  | 1:A:1018:SER:N    | 2.51                     | 0.43              |
| 1:A:1118:LEU:HD13 | 1:A:1126:LYS:CD   | 2.47                     | 0.43              |
| 1:A:1357:LYS:HB3  | 1:A:1362:GLU:HA   | 2.00                     | 0.43              |
| 2:B:35:U:C3'      | 2:B:35:U:C6       | 3.01                     | 0.43              |
| 1:A:59:ILE:HD11   | 1:A:330:TYR:HD2   | 1.82                     | 0.43              |
| 1:A:261:PHE:CB    | 1:A:283:LEU:HD13  | 2.46                     | 0.43              |
| 1:A:357:PHE:CE2   | 1:A:423:GLU:CB    | 3.00                     | 0.43              |
| 1:A:371:ILE:CG2   | 1:A:472:ILE:HG21  | 2.48                     | 0.43              |
| 1:A:641:ASP:CB    | 1:A:821:ILE:HD11  | 2.47                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1063:LEU:HB2  | 1:A:1171:PHE:CD2  | 2.53                     | 0.43              |
| 1:A:1143:ASN:HA   | 1:A:1144:ILE:HA   | 1.59                     | 0.43              |
| 1:A:213:GLU:N     | 1:A:213:GLU:CD    | 2.73                     | 0.43              |
| 1:A:265:VAL:HA    | 1:A:266:GLY:HA3   | 1.79                     | 0.43              |
| 1:A:423:GLU:CD    | 1:A:423:GLU:H     | 2.25                     | 0.43              |
| 1:A:1076:TYR:CE1  | 1:A:1080:SER:HB3  | 2.54                     | 0.43              |
| 1:A:435:LEU:CD2   | 1:A:468:LEU:HD13  | 2.46                     | 0.43              |
| 1:A:532:ILE:HD11  | 1:A:533:PHE:CZ    | 2.51                     | 0.43              |
| 1:A:832:ILE:HG21  | 1:A:838:TYR:HB2   | 2.01                     | 0.43              |
| 1:A:1146:ASN:HD21 | 1:A:1152:PHE:HA   | 1.82                     | 0.43              |
| 1:A:442:ILE:HD12  | 1:A:443:LEU:CA    | 2.48                     | 0.43              |
| 1:A:641:ASP:CB    | 3:A:1403:HOH:O    | 2.60                     | 0.43              |
| 1:A:696:ILE:CA    | 1:A:697:GLU:C     | 2.84                     | 0.43              |
| 1:A:776:LYS:O     | 1:A:777:VAL:C     | 2.60                     | 0.43              |
| 1:A:802:ILE:CG2   | 1:A:805:ILE:HB    | 2.47                     | 0.43              |
| 1:A:1126:LYS:O    | 1:A:1130:ILE:HB   | 2.18                     | 0.43              |
| 1:A:69:LYS:O      | 1:A:73:ARG:HB2    | 2.18                     | 0.43              |
| 1:A:294:ILE:O     | 1:A:298:VAL:HG23  | 2.18                     | 0.43              |
| 1:A:400:ILE:CG2   | 1:A:439:ILE:HG23  | 2.49                     | 0.43              |
| 1:A:576:ASP:CG    | 1:A:577:ASN:N     | 2.76                     | 0.43              |
| 2:B:35:U:C6       | 2:B:35:U:H3'      | 2.53                     | 0.43              |
| 1:A:213:GLU:CD    | 1:A:213:GLU:H     | 2.27                     | 0.43              |
| 1:A:436:LYS:NZ    | 2:B:15:A:O2'      | 2.35                     | 0.43              |
| 1:A:1093:ASN:O    | 1:A:1096:GLY:N    | 2.52                     | 0.43              |
| 1:A:1250:LYS:HE3  | 1:A:1250:LYS:HB2  | 1.80                     | 0.43              |
| 1:A:255:ILE:O     | 1:A:259:VAL:HG22  | 2.18                     | 0.43              |
| 1:A:278:LEU:O     | 1:A:282:ILE:HG13  | 2.18                     | 0.43              |
| 1:A:397:ASP:O     | 1:A:400:ILE:HG13  | 2.19                     | 0.43              |
| 1:A:429:LYS:O     | 1:A:433:ARG:HG3   | 2.19                     | 0.43              |
| 1:A:80:ILE:HG13   | 1:A:81:LEU:N      | 2.34                     | 0.43              |
| 1:A:272:SER:O     | 1:A:273:LYS:C     | 2.61                     | 0.43              |
| 1:A:495:ILE:HD11  | 1:A:508:LEU:HD12  | 2.01                     | 0.43              |
| 1:A:522:PHE:CD2   | 1:A:843:PHE:HE2   | 2.36                     | 0.43              |
| 1:A:1048:TYR:CD1  | 1:A:1048:TYR:C    | 2.97                     | 0.43              |
| 1:A:1137:ASP:OD1  | 1:A:1148:ASN:CB   | 2.67                     | 0.43              |
| 1:A:1243:PHE:N    | 1:A:1243:PHE:HD1  | 2.17                     | 0.43              |
| 1:A:1251:LYS:O    | 1:A:1255:ILE:HG12 | 2.17                     | 0.43              |
| 1:A:1359:SER:C    | 1:A:1360:VAL:HG12 | 2.43                     | 0.43              |
| 1:A:222:GLU:HG2   | 1:A:223:GLU:N     | 2.33                     | 0.43              |
| 1:A:301:GLU:OE2   | 1:A:301:GLU:HA    | 2.19                     | 0.43              |
| 1:A:820:ARG:O     | 1:A:822:THR:HG23  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:880:GLU:O     | 1:A:884:LEU:HG    | 2.18                     | 0.43              |
| 1:A:1276:SER:N    | 3:A:1413:HOH:O    | 2.02                     | 0.43              |
| 1:A:1359:SER:CB   | 1:A:1361:LEU:HB2  | 2.49                     | 0.43              |
| 1:A:680:ILE:HD13  | 1:A:710:ASN:HB3   | 2.01                     | 0.42              |
| 1:A:189:ILE:HG22  | 1:A:192:ILE:HD12  | 2.01                     | 0.42              |
| 1:A:219:ARG:NH2   | 1:A:220:TYR:OH    | 2.48                     | 0.42              |
| 1:A:625:GLN:HG2   | 1:A:845:LEU:HD13  | 2.02                     | 0.42              |
| 1:A:723:LEU:HD12  | 1:A:723:LEU:HA    | 1.89                     | 0.42              |
| 1:A:20:LYS:NZ     | 1:A:20:LYS:CA     | 2.81                     | 0.42              |
| 1:A:46:LYS:HE2    | 1:A:46:LYS:HA     | 2.00                     | 0.42              |
| 1:A:279:VAL:O     | 1:A:282:ILE:N     | 2.52                     | 0.42              |
| 1:A:317:VAL:HG21  | 1:A:322:LEU:C     | 2.44                     | 0.42              |
| 1:A:695:THR:O     | 1:A:696:ILE:CB    | 2.64                     | 0.42              |
| 1:A:1199:MET:O    | 1:A:1203:VAL:HG23 | 2.18                     | 0.42              |
| 1:A:25:VAL:HG21   | 1:A:40:ILE:HD11   | 2.00                     | 0.42              |
| 1:A:191:GLU:HG2   | 1:A:194:LYS:HE3   | 1.94                     | 0.42              |
| 1:A:640:LEU:O     | 1:A:643:VAL:CG2   | 2.64                     | 0.42              |
| 1:A:691:GLU:CB    | 1:A:692:PRO:CD    | 2.97                     | 0.42              |
| 1:A:812:ILE:O     | 1:A:813:ASN:CB    | 2.67                     | 0.42              |
| 1:A:1123:LYS:HA   | 1:A:1123:LYS:HD3  | 1.80                     | 0.42              |
| 1:A:1133:LEU:HD23 | 1:A:1139:PHE:HE2  | 1.70                     | 0.42              |
| 1:A:1208:GLU:OE1  | 1:A:1208:GLU:HA   | 2.19                     | 0.42              |
| 1:A:25:VAL:CG2    | 1:A:40:ILE:HD11   | 2.49                     | 0.42              |
| 1:A:78:GLY:O      | 1:A:85:LYS:CG     | 2.62                     | 0.42              |
| 1:A:84:LEU:HD11   | 1:A:194:LYS:CB    | 2.48                     | 0.42              |
| 1:A:87:LYS:CB     | 1:A:90:ILE:HG13   | 2.46                     | 0.42              |
| 1:A:183:LEU:HD23  | 1:A:183:LEU:HA    | 1.87                     | 0.42              |
| 1:A:250:LYS:CB    | 1:A:285:ILE:HG21  | 2.49                     | 0.42              |
| 1:A:315:LYS:CA    | 1:A:316:LYS:HE2   | 2.49                     | 0.42              |
| 1:A:659:ILE:C     | 1:A:659:ILE:CD1   | 2.87                     | 0.42              |
| 1:A:1063:LEU:C    | 1:A:1063:LEU:CD1  | 2.92                     | 0.42              |
| 2:B:49:C:H2'      | 2:B:50:U:C5'      | 2.49                     | 0.42              |
| 1:A:249:ILE:C     | 1:A:249:ILE:CD1   | 2.85                     | 0.42              |
| 1:A:374:ILE:CD1   | 1:A:428:TYR:CZ    | 3.00                     | 0.42              |
| 1:A:537:ASN:ND2   | 1:A:537:ASN:C     | 2.77                     | 0.42              |
| 1:A:1049:PRO:HD3  | 1:A:1058:ILE:HD11 | 2.01                     | 0.42              |
| 1:A:211:GLU:HG3   | 1:A:212:THR:H     | 1.85                     | 0.42              |
| 1:A:337:LEU:CD2   | 1:A:337:LEU:H     | 2.25                     | 0.42              |
| 1:A:1090:PHE:N    | 1:A:1091:LEU:CA   | 2.83                     | 0.42              |
| 1:A:236:ASP:N     | 1:A:236:ASP:OD1   | 2.53                     | 0.42              |
| 1:A:467:ILE:O     | 1:A:470:GLU:HG3   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1048:TYR:O    | 1:A:1048:TYR:HD1  | 2.02                     | 0.42              |
| 1:A:4:LEU:HA      | 1:A:10:TRP:HE1    | 1.84                     | 0.42              |
| 1:A:186:LYS:HA    | 1:A:189:ILE:CG1   | 2.48                     | 0.42              |
| 1:A:726:ASN:ND2   | 1:A:726:ASN:N     | 2.60                     | 0.42              |
| 1:A:829:THR:O     | 1:A:829:THR:OG1   | 2.27                     | 0.42              |
| 1:A:846:LEU:HD23  | 1:A:846:LEU:HA    | 1.80                     | 0.42              |
| 1:A:1076:TYR:CD1  | 1:A:1076:TYR:C    | 2.96                     | 0.42              |
| 1:A:1340:PHE:HD2  | 1:A:1342:LEU:CD1  | 2.22                     | 0.42              |
| 1:A:1346:ASN:CB   | 1:A:1349:LEU:HD22 | 2.50                     | 0.42              |
| 1:A:204:ILE:O     | 1:A:208:ILE:HG13  | 2.19                     | 0.42              |
| 1:A:289:LEU:C     | 1:A:289:LEU:CD2   | 2.93                     | 0.42              |
| 1:A:641:ASP:HB3   | 3:A:1403:HOH:O    | 2.18                     | 0.42              |
| 1:A:1013:ARG:O    | 1:A:1016:PHE:HB2  | 2.19                     | 0.42              |
| 1:A:1111:LEU:HD22 | 1:A:1359:SER:HA   | 2.02                     | 0.42              |
| 1:A:1358:VAL:O    | 1:A:1358:VAL:HG23 | 2.18                     | 0.42              |
| 1:A:189:ILE:O     | 1:A:190:TYR:C     | 2.63                     | 0.41              |
| 1:A:514:LEU:HD23  | 1:A:858:ARG:HG2   | 2.02                     | 0.41              |
| 1:A:1235:TYR:CE1  | 1:A:1236:THR:CG2  | 2.98                     | 0.41              |
| 1:A:40:ILE:HG13   | 1:A:41:ASN:N      | 2.35                     | 0.41              |
| 1:A:376:ALA:O     | 1:A:377:GLU:C     | 2.61                     | 0.41              |
| 1:A:383:LEU:HA    | 1:A:386:LYS:HB2   | 2.02                     | 0.41              |
| 1:A:539:ASN:OD1   | 1:A:539:ASN:N     | 2.51                     | 0.41              |
| 1:A:736:LEU:C     | 1:A:736:LEU:CD2   | 2.92                     | 0.41              |
| 1:A:823:VAL:HG12  | 1:A:824:LYS:H     | 1.85                     | 0.41              |
| 1:A:1048:TYR:C    | 1:A:1058:ILE:HD11 | 2.45                     | 0.41              |
| 1:A:771:LYS:HE3   | 2:B:28:C:OP1      | 2.20                     | 0.41              |
| 1:A:1070:PRO:HB2  | 1:A:1288:ARG:O    | 2.20                     | 0.41              |
| 1:A:1277:ILE:HG12 | 1:A:1302:ARG:CZ   | 2.50                     | 0.41              |
| 1:A:638:LEU:N     | 1:A:638:LEU:CD1   | 2.73                     | 0.41              |
| 1:A:76:HIS:ND1    | 1:A:77:ALA:O      | 2.54                     | 0.41              |
| 1:A:190:TYR:C     | 1:A:190:TYR:CD1   | 2.98                     | 0.41              |
| 1:A:210:ASN:C     | 1:A:211:GLU:CG    | 2.88                     | 0.41              |
| 1:A:253:LEU:HB2   | 1:A:256:LEU:HB2   | 2.02                     | 0.41              |
| 1:A:303:GLU:O     | 1:A:304:PHE:C     | 2.62                     | 0.41              |
| 1:A:427:LEU:HA    | 1:A:427:LEU:HD23  | 1.79                     | 0.41              |
| 1:A:464:ASN:O     | 1:A:467:ILE:N     | 2.53                     | 0.41              |
| 1:A:1342:LEU:HD12 | 1:A:1349:LEU:CD2  | 2.47                     | 0.41              |
| 1:A:84:LEU:CD1    | 1:A:194:LYS:CB    | 2.99                     | 0.41              |
| 1:A:191:GLU:HA    | 1:A:194:LYS:HG2   | 2.02                     | 0.41              |
| 1:A:1129:TYR:CD1  | 1:A:1129:TYR:C    | 2.99                     | 0.41              |
| 1:A:1336:LEU:HG   | 1:A:1352:LEU:CD2  | 2.50                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:15:A:C8       | 2:B:15:A:C5'      | 3.03                     | 0.41              |
| 1:A:194:LYS:HG3   | 1:A:195:ASN:H     | 1.85                     | 0.41              |
| 1:A:371:ILE:CG2   | 1:A:472:ILE:CG2   | 2.97                     | 0.41              |
| 1:A:527:MET:CE    | 1:A:1287:VAL:CG2  | 2.99                     | 0.41              |
| 1:A:636:LYS:CD    | 1:A:887:LEU:HD23  | 2.49                     | 0.41              |
| 1:A:801:ASN:ND2   | 1:A:805:ILE:CG1   | 2.84                     | 0.41              |
| 1:A:1093:ASN:HB2  | 1:A:1096:GLY:N    | 2.29                     | 0.41              |
| 1:A:1286:ILE:O    | 1:A:1290:PRO:HG3  | 2.21                     | 0.41              |
| 2:B:14:G:N1       | 2:B:16:A:N1       | 2.68                     | 0.41              |
| 1:A:241:ASN:O     | 1:A:245:ILE:HG13  | 2.20                     | 0.41              |
| 1:A:407:HIS:HE1   | 1:A:411:ASN:HD22  | 1.58                     | 0.41              |
| 1:A:413:ASP:CB    | 1:A:414:SER:C     | 2.94                     | 0.41              |
| 1:A:529:LEU:HD23  | 1:A:529:LEU:HA    | 1.95                     | 0.41              |
| 1:A:1069:ASN:HA   | 1:A:1070:PRO:HD2  | 1.83                     | 0.41              |
| 1:A:1118:LEU:HD22 | 1:A:1118:LEU:HA   | 1.96                     | 0.41              |
| 2:B:14:G:C4       | 2:B:16:A:C5       | 3.09                     | 0.41              |
| 1:A:49:ILE:CG2    | 1:A:54:PHE:HB2    | 2.50                     | 0.41              |
| 1:A:256:LEU:O     | 1:A:259:VAL:HG22  | 2.20                     | 0.41              |
| 1:A:262:TYR:C     | 1:A:264:ASN:N     | 2.73                     | 0.41              |
| 1:A:436:LYS:HZ1   | 2:B:15:A:HO2'     | 1.59                     | 0.41              |
| 1:A:532:ILE:HD11  | 1:A:533:PHE:CG    | 2.55                     | 0.41              |
| 1:A:801:ASN:ND2   | 1:A:805:ILE:HG13  | 2.36                     | 0.41              |
| 1:A:1066:ASN:O    | 1:A:1067:ILE:C    | 2.61                     | 0.41              |
| 1:A:1076:TYR:O    | 1:A:1076:TYR:HD1  | 2.04                     | 0.41              |
| 1:A:1089:LYS:HA   | 1:A:1092:PHE:CA   | 2.48                     | 0.41              |
| 1:A:1191:GLN:HG2  | 1:A:1307:LEU:HD21 | 2.03                     | 0.41              |
| 1:A:1226:PRO:HD3  | 1:A:1239:ALA:HB2  | 2.03                     | 0.41              |
| 1:A:1234:PHE:HD1  | 1:A:1235:TYR:N    | 1.83                     | 0.41              |
| 1:A:1360:VAL:O    | 1:A:1360:VAL:HG22 | 2.21                     | 0.41              |
| 1:A:100:LEU:O     | 1:A:102:THR:HG23  | 2.21                     | 0.41              |
| 1:A:327:ASN:OD1   | 1:A:327:ASN:N     | 2.53                     | 0.41              |
| 1:A:399:GLU:H     | 1:A:399:GLU:HG3   | 1.54                     | 0.41              |
| 1:A:1147:LYS:CB   | 3:A:1416:HOH:O    | 2.69                     | 0.41              |
| 1:A:409:LYS:NZ    | 3:A:1430:HOH:O    | 2.45                     | 0.40              |
| 1:A:416:LYS:CB    | 3:A:1424:HOH:O    | 2.68                     | 0.40              |
| 1:A:441:LYS:HA    | 1:A:441:LYS:HD2   | 1.84                     | 0.40              |
| 1:A:1049:PRO:CB   | 1:A:1050:LYS:C    | 2.94                     | 0.40              |
| 1:A:1063:LEU:CD1  | 1:A:1067:ILE:HD11 | 2.51                     | 0.40              |
| 2:B:16:A:H4'      | 2:B:17:G:OP2      | 2.21                     | 0.40              |
| 1:A:557:LEU:CD1   | 1:A:558:ASP:H     | 2.27                     | 0.40              |
| 1:A:865:TRP:CD1   | 1:A:865:TRP:C     | 3.00                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1262:ASP:CG   | 1:A:1267:SER:CB  | 2.93                     | 0.40              |
| 1:A:1353:MET:HE2  | 1:A:1353:MET:HB3 | 1.88                     | 0.40              |
| 2:B:15:A:OP2      | 2:B:15:A:C4'     | 2.70                     | 0.40              |
| 1:A:528:GLU:HA    | 1:A:528:GLU:OE1  | 2.20                     | 0.40              |
| 1:A:596:GLU:HA    | 1:A:599:ARG:HG3  | 2.03                     | 0.40              |
| 1:A:868:THR:OG1   | 1:A:870:GLU:HG3  | 2.21                     | 0.40              |
| 1:A:210:ASN:O     | 1:A:211:GLU:CB   | 2.69                     | 0.40              |
| 1:A:574:PHE:N     | 1:A:574:PHE:CD1  | 2.88                     | 0.40              |
| 1:A:588:LYS:O     | 1:A:592:ILE:CD1  | 2.61                     | 0.40              |
| 1:A:627:LEU:N     | 1:A:627:LEU:HD23 | 2.37                     | 0.40              |
| 1:A:902:GLU:HG2   | 1:A:1057:TYR:CG  | 2.54                     | 0.40              |
| 1:A:1079:ILE:HG22 | 1:A:1083:ILE:CD1 | 2.51                     | 0.40              |
| 1:A:93:ILE:CB     | 1:A:96:ASN:O     | 2.70                     | 0.40              |
| 1:A:183:LEU:HD11  | 1:A:255:ILE:HG21 | 2.03                     | 0.40              |
| 1:A:314:VAL:CG1   | 1:A:315:LYS:H    | 2.34                     | 0.40              |
| 1:A:400:ILE:CD1   | 1:A:442:ILE:CD1  | 2.88                     | 0.40              |
| 1:A:577:ASN:O     | 1:A:578:LYS:CB   | 2.68                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles        |
|-----|-------|-----------------|------------|---------|----------|--------------------|
| 1   | A     | 1207/1397 (86%) | 1100 (91%) | 86 (7%) | 21 (2%)  | <b>7</b> <b>12</b> |

All (21) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 211 | GLU  |
| 1   | A     | 268 | ASP  |
| 1   | A     | 269 | LYS  |
| 1   | A     | 694 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 695  | THR  |
| 1   | A     | 696  | ILE  |
| 1   | A     | 697  | GLU  |
| 1   | A     | 698  | THR  |
| 1   | A     | 1009 | LYS  |
| 1   | A     | 1010 | ILE  |
| 1   | A     | 1011 | LEU  |
| 1   | A     | 464  | ASN  |
| 1   | A     | 605  | SER  |
| 1   | A     | 609  | ASP  |
| 1   | A     | 614  | GLN  |
| 1   | A     | 1359 | SER  |
| 1   | A     | 762  | ALA  |
| 1   | A     | 1091 | LEU  |
| 1   | A     | 1092 | PHE  |
| 1   | A     | 801  | ASN  |
| 1   | A     | 1226 | PRO  |

### 5.3.2 Protein sidechains [i](#)

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     | 1024/1332 (77%) | 790 (77%) | 234 (23%) | <b>1</b> <b>1</b> |

All (234) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | LEU  |
| 1   | A     | 20  | LYS  |
| 1   | A     | 22  | LYS  |
| 1   | A     | 24  | LYS  |
| 1   | A     | 40  | ILE  |
| 1   | A     | 44  | ASN  |
| 1   | A     | 46  | LYS  |
| 1   | A     | 56  | ARG  |
| 1   | A     | 63  | LYS  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 65         | ASP         |
| 1          | A            | 68         | LEU         |
| 1          | A            | 70         | GLU         |
| 1          | A            | 73         | ARG         |
| 1          | A            | 79         | ASN         |
| 1          | A            | 80         | ILE         |
| 1          | A            | 84         | LEU         |
| 1          | A            | 85         | LYS         |
| 1          | A            | 95         | ASN         |
| 1          | A            | 182        | GLU         |
| 1          | A            | 184        | GLU         |
| 1          | A            | 187        | LYS         |
| 1          | A            | 194        | LYS         |
| 1          | A            | 197        | ASN         |
| 1          | A            | 200        | LEU         |
| 1          | A            | 202        | LYS         |
| 1          | A            | 207        | ILE         |
| 1          | A            | 209        | GLU         |
| 1          | A            | 213        | GLU         |
| 1          | A            | 226        | ARG         |
| 1          | A            | 229        | LEU         |
| 1          | A            | 230        | LEU         |
| 1          | A            | 231        | LYS         |
| 1          | A            | 233        | ASP         |
| 1          | A            | 237        | VAL         |
| 1          | A            | 239        | LEU         |
| 1          | A            | 248        | LYS         |
| 1          | A            | 249        | ILE         |
| 1          | A            | 252        | ASN         |
| 1          | A            | 256        | LEU         |
| 1          | A            | 263        | LEU         |
| 1          | A            | 265        | VAL         |
| 1          | A            | 270        | LYS         |
| 1          | A            | 285        | ILE         |
| 1          | A            | 286        | ASN         |
| 1          | A            | 292        | GLU         |
| 1          | A            | 294        | ILE         |
| 1          | A            | 302        | LEU         |
| 1          | A            | 309        | LYS         |
| 1          | A            | 310        | ARG         |
| 1          | A            | 316        | LYS         |
| 1          | A            | 337        | LEU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 346        | GLU         |
| 1          | A            | 351        | LYS         |
| 1          | A            | 363        | LYS         |
| 1          | A            | 366        | SER         |
| 1          | A            | 370        | LYS         |
| 1          | A            | 372        | GLU         |
| 1          | A            | 377        | GLU         |
| 1          | A            | 380        | ILE         |
| 1          | A            | 386        | LYS         |
| 1          | A            | 388        | GLU         |
| 1          | A            | 393        | LYS         |
| 1          | A            | 395        | ASN         |
| 1          | A            | 399        | GLU         |
| 1          | A            | 409        | LYS         |
| 1          | A            | 414        | SER         |
| 1          | A            | 418        | SER         |
| 1          | A            | 419        | LYS         |
| 1          | A            | 420        | LYS         |
| 1          | A            | 441        | LYS         |
| 1          | A            | 442        | ILE         |
| 1          | A            | 450        | ARG         |
| 1          | A            | 451        | LEU         |
| 1          | A            | 454        | MET         |
| 1          | A            | 458        | GLU         |
| 1          | A            | 468        | LEU         |
| 1          | A            | 469        | SER         |
| 1          | A            | 471        | LYS         |
| 1          | A            | 480        | THR         |
| 1          | A            | 485        | MET         |
| 1          | A            | 495        | ILE         |
| 1          | A            | 498        | THR         |
| 1          | A            | 500        | VAL         |
| 1          | A            | 514        | LEU         |
| 1          | A            | 520        | THR         |
| 1          | A            | 526        | ASN         |
| 1          | A            | 527        | MET         |
| 1          | A            | 532        | ILE         |
| 1          | A            | 535        | ARG         |
| 1          | A            | 537        | ASN         |
| 1          | A            | 539        | ASN         |
| 1          | A            | 557        | LEU         |
| 1          | A            | 561        | ILE         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 567        | LYS         |
| 1          | A            | 575        | ILE         |
| 1          | A            | 581        | ILE         |
| 1          | A            | 583        | ASN         |
| 1          | A            | 591        | LYS         |
| 1          | A            | 595        | ASN         |
| 1          | A            | 597        | ARG         |
| 1          | A            | 608        | ARG         |
| 1          | A            | 613        | THR         |
| 1          | A            | 622        | ASN         |
| 1          | A            | 624        | ILE         |
| 1          | A            | 625        | GLN         |
| 1          | A            | 629        | ILE         |
| 1          | A            | 630        | SER         |
| 1          | A            | 638        | LEU         |
| 1          | A            | 639        | ASN         |
| 1          | A            | 646        | ASP         |
| 1          | A            | 649        | ASN         |
| 1          | A            | 650        | ILE         |
| 1          | A            | 651        | ILE         |
| 1          | A            | 658        | LYS         |
| 1          | A            | 660        | SER         |
| 1          | A            | 662        | GLU         |
| 1          | A            | 665        | ASN         |
| 1          | A            | 668        | LYS         |
| 1          | A            | 672        | SER         |
| 1          | A            | 676        | VAL         |
| 1          | A            | 681        | LEU         |
| 1          | A            | 683        | LEU         |
| 1          | A            | 685        | ARG         |
| 1          | A            | 687        | ASN         |
| 1          | A            | 696        | ILE         |
| 1          | A            | 697        | GLU         |
| 1          | A            | 698        | THR         |
| 1          | A            | 701        | ILE         |
| 1          | A            | 723        | LEU         |
| 1          | A            | 726        | ASN         |
| 1          | A            | 730        | ASN         |
| 1          | A            | 733        | LEU         |
| 1          | A            | 735        | GLU         |
| 1          | A            | 736        | LEU         |
| 1          | A            | 745        | GLU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 746        | ILE         |
| 1          | A            | 775        | LYS         |
| 1          | A            | 778        | ILE         |
| 1          | A            | 794        | ASP         |
| 1          | A            | 796        | SER         |
| 1          | A            | 797        | ASP         |
| 1          | A            | 798        | PHE         |
| 1          | A            | 801        | ASN         |
| 1          | A            | 816        | LYS         |
| 1          | A            | 820        | ARG         |
| 1          | A            | 821        | ILE         |
| 1          | A            | 824        | LYS         |
| 1          | A            | 826        | SER         |
| 1          | A            | 827        | ASP         |
| 1          | A            | 834        | ASP         |
| 1          | A            | 839        | ILE         |
| 1          | A            | 849        | ASN         |
| 1          | A            | 855        | ILE         |
| 1          | A            | 857        | ASN         |
| 1          | A            | 858        | ARG         |
| 1          | A            | 872        | GLN         |
| 1          | A            | 875        | ILE         |
| 1          | A            | 890        | GLU         |
| 1          | A            | 898        | LEU         |
| 1          | A            | 905        | GLN         |
| 1          | A            | 909        | GLU         |
| 1          | A            | 1014       | ILE         |
| 1          | A            | 1015       | ILE         |
| 1          | A            | 1018       | SER         |
| 1          | A            | 1023       | LYS         |
| 1          | A            | 1025       | LYS         |
| 1          | A            | 1026       | LYS         |
| 1          | A            | 1031       | LEU         |
| 1          | A            | 1032       | ILE         |
| 1          | A            | 1037       | SER         |
| 1          | A            | 1041       | ASN         |
| 1          | A            | 1044       | GLN         |
| 1          | A            | 1055       | GLU         |
| 1          | A            | 1058       | ILE         |
| 1          | A            | 1060       | LYS         |
| 1          | A            | 1061       | LYS         |
| 1          | A            | 1063       | LEU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 1065       | LEU         |
| 1          | A            | 1072       | PHE         |
| 1          | A            | 1073       | ASP         |
| 1          | A            | 1082       | ASP         |
| 1          | A            | 1085       | MET         |
| 1          | A            | 1087       | ASP         |
| 1          | A            | 1089       | LYS         |
| 1          | A            | 1097       | LYS         |
| 1          | A            | 1114       | LEU         |
| 1          | A            | 1118       | LEU         |
| 1          | A            | 1119       | ASN         |
| 1          | A            | 1123       | LYS         |
| 1          | A            | 1124       | GLU         |
| 1          | A            | 1127       | GLU         |
| 1          | A            | 1130       | ILE         |
| 1          | A            | 1131       | LYS         |
| 1          | A            | 1132       | LYS         |
| 1          | A            | 1133       | LEU         |
| 1          | A            | 1135       | GLU         |
| 1          | A            | 1146       | ASN         |
| 1          | A            | 1153       | GLU         |
| 1          | A            | 1167       | ASP         |
| 1          | A            | 1169       | VAL         |
| 1          | A            | 1197       | ARG         |
| 1          | A            | 1212       | ILE         |
| 1          | A            | 1213       | LYS         |
| 1          | A            | 1214       | LEU         |
| 1          | A            | 1215       | SER         |
| 1          | A            | 1219       | THR         |
| 1          | A            | 1222       | SER         |
| 1          | A            | 1228       | ARG         |
| 1          | A            | 1231       | SER         |
| 1          | A            | 1232       | ASP         |
| 1          | A            | 1234       | PHE         |
| 1          | A            | 1242       | LYS         |
| 1          | A            | 1243       | PHE         |
| 1          | A            | 1245       | ASP         |
| 1          | A            | 1246       | GLU         |
| 1          | A            | 1248       | SER         |
| 1          | A            | 1263       | LEU         |
| 1          | A            | 1275       | GLU         |
| 1          | A            | 1277       | ILE         |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1278 | ARG  |
| 1   | A     | 1295 | SER  |
| 1   | A     | 1330 | ASN  |
| 1   | A     | 1331 | LEU  |
| 1   | A     | 1337 | LYS  |
| 1   | A     | 1338 | LYS  |
| 1   | A     | 1341 | LYS  |
| 1   | A     | 1342 | LEU  |
| 1   | A     | 1348 | ILE  |
| 1   | A     | 1349 | LEU  |
| 1   | A     | 1353 | MET  |
| 1   | A     | 1356 | LYS  |
| 1   | A     | 1362 | GLU  |
| 1   | A     | 1367 | ASN  |
| 1   | A     | 1382 | ILE  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 30  | ASN  |
| 1   | A     | 34  | ASN  |
| 1   | A     | 39  | ASN  |
| 1   | A     | 44  | ASN  |
| 1   | A     | 79  | ASN  |
| 1   | A     | 95  | ASN  |
| 1   | A     | 210 | ASN  |
| 1   | A     | 224 | HIS  |
| 1   | A     | 264 | ASN  |
| 1   | A     | 286 | ASN  |
| 1   | A     | 306 | ASN  |
| 1   | A     | 365 | ASN  |
| 1   | A     | 407 | HIS  |
| 1   | A     | 464 | ASN  |
| 1   | A     | 483 | HIS  |
| 1   | A     | 537 | ASN  |
| 1   | A     | 543 | ASN  |
| 1   | A     | 598 | ASN  |
| 1   | A     | 622 | ASN  |
| 1   | A     | 625 | GLN  |
| 1   | A     | 639 | ASN  |
| 1   | A     | 649 | ASN  |
| 1   | A     | 665 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 682  | ASN  |
| 1   | A     | 687  | ASN  |
| 1   | A     | 726  | ASN  |
| 1   | A     | 730  | ASN  |
| 1   | A     | 734  | GLN  |
| 1   | A     | 801  | ASN  |
| 1   | A     | 803  | GLN  |
| 1   | A     | 847  | ASN  |
| 1   | A     | 853  | ASN  |
| 1   | A     | 857  | ASN  |
| 1   | A     | 1041 | ASN  |
| 1   | A     | 1069 | ASN  |
| 1   | A     | 1146 | ASN  |
| 1   | A     | 1172 | ASN  |
| 1   | A     | 1218 | ASN  |
| 1   | A     | 1279 | ASN  |
| 1   | A     | 1283 | HIS  |
| 1   | A     | 1367 | ASN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 2   | B     | 38/58 (65%) | 18 (47%)          | 6 (15%)         |

All (18) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 3   | A    |
| 2   | B     | 8   | A    |
| 2   | B     | 9   | A    |
| 2   | B     | 14  | G    |
| 2   | B     | 15  | A    |
| 2   | B     | 16  | A    |
| 2   | B     | 21  | A    |
| 2   | B     | 22  | C    |
| 2   | B     | 23  | U    |
| 2   | B     | 29  | G    |
| 2   | B     | 30  | A    |
| 2   | B     | 31  | C    |
| 2   | B     | 32  | A    |
| 2   | B     | 35  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 36  | C    |
| 2   | B     | 49  | C    |
| 2   | B     | 50  | U    |
| 2   | B     | 51  | C    |

All (6) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 15  | A    |
| 2   | B     | 21  | A    |
| 2   | B     | 22  | C    |
| 2   | B     | 29  | G    |
| 2   | B     | 34  | A    |
| 2   | B     | 35  | U    |

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

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

#### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 1215/1397 (86%) | 0.40   | 83 (6%) 23 17 | 28, 69, 112, 156      | 0     |
| 2   | B     | 40/58 (68%)     | -0.18  | 1 (2%) 58 52  | 32, 55, 111, 123      | 0     |
| All | All   | 1255/1455 (86%) | 0.38   | 84 (6%) 24 18 | 28, 68, 112, 156      | 0     |

All (84) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 804  | GLU  | 8.7  |
| 1   | A     | 1359 | SER  | 5.7  |
| 1   | A     | 177  | ILE  | 5.2  |
| 1   | A     | 1037 | SER  | 4.8  |
| 1   | A     | 615  | ASP  | 4.5  |
| 1   | A     | 1120 | GLY  | 4.4  |
| 1   | A     | 414  | SER  | 4.3  |
| 1   | A     | 1088 | ALA  | 4.1  |
| 1   | A     | 181  | ASP  | 4.1  |
| 1   | A     | 92   | ARG  | 4.1  |
| 1   | A     | 811  | ASP  | 3.7  |
| 1   | A     | 637  | ALA  | 3.7  |
| 1   | A     | 212  | THR  | 3.6  |
| 1   | A     | 631  | ASP  | 3.4  |
| 1   | A     | 1015 | ILE  | 3.4  |
| 1   | A     | 1382 | ILE  | 3.2  |
| 2   | B     | 32   | A    | 3.1  |
| 1   | A     | 1043 | PHE  | 3.1  |
| 1   | A     | 579  | ASN  | 3.1  |
| 1   | A     | 102  | THR  | 3.1  |
| 1   | A     | 533  | PHE  | 3.1  |
| 1   | A     | 74   | LYS  | 3.0  |
| 1   | A     | 99   | PHE  | 3.0  |
| 1   | A     | 86   | GLY  | 3.0  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | A            | 1092       | PHE         | 3.0         |
| 1          | A            | 263        | LEU         | 2.9         |
| 1          | A            | 265        | VAL         | 2.9         |
| 1          | A            | 259        | VAL         | 2.9         |
| 1          | A            | 1051       | GLU         | 2.8         |
| 1          | A            | 1090       | PHE         | 2.8         |
| 1          | A            | 746        | ILE         | 2.7         |
| 1          | A            | 562        | LEU         | 2.7         |
| 1          | A            | 817        | THR         | 2.7         |
| 1          | A            | 413        | ASP         | 2.7         |
| 1          | A            | 1078       | LEU         | 2.6         |
| 1          | A            | 91         | ILE         | 2.6         |
| 1          | A            | 255        | ILE         | 2.6         |
| 1          | A            | 638        | LEU         | 2.5         |
| 1          | A            | 555        | TYR         | 2.5         |
| 1          | A            | 1141       | ALA         | 2.5         |
| 1          | A            | 1071       | ASN         | 2.5         |
| 1          | A            | 898        | LEU         | 2.5         |
| 1          | A            | 640        | LEU         | 2.4         |
| 1          | A            | 893        | THR         | 2.4         |
| 1          | A            | 1067       | ILE         | 2.4         |
| 1          | A            | 549        | GLY         | 2.4         |
| 1          | A            | 1014       | ILE         | 2.4         |
| 1          | A            | 1146       | ASN         | 2.4         |
| 1          | A            | 1142       | LYS         | 2.4         |
| 1          | A            | 801        | ASN         | 2.3         |
| 1          | A            | 1050       | LYS         | 2.3         |
| 1          | A            | 1244       | PHE         | 2.3         |
| 1          | A            | 1008       | SER         | 2.3         |
| 1          | A            | 1231       | SER         | 2.3         |
| 1          | A            | 1144       | ILE         | 2.3         |
| 1          | A            | 622        | ASN         | 2.3         |
| 1          | A            | 789        | TYR         | 2.2         |
| 1          | A            | 818        | TYR         | 2.2         |
| 1          | A            | 609        | ASP         | 2.2         |
| 1          | A            | 93         | ILE         | 2.2         |
| 1          | A            | 581        | ILE         | 2.2         |
| 1          | A            | 1143       | ASN         | 2.2         |
| 1          | A            | 808        | GLN         | 2.2         |
| 1          | A            | 282        | ILE         | 2.2         |
| 1          | A            | 795        | PHE         | 2.2         |
| 1          | A            | 805        | ILE         | 2.2         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 612  | GLY  | 2.2  |
| 1   | A     | 644  | PHE  | 2.2  |
| 1   | A     | 195  | ASN  | 2.1  |
| 1   | A     | 572  | LEU  | 2.1  |
| 1   | A     | 1032 | ILE  | 2.1  |
| 1   | A     | 1079 | ILE  | 2.1  |
| 1   | A     | 1042 | LYS  | 2.1  |
| 1   | A     | 613  | THR  | 2.1  |
| 1   | A     | 723  | LEU  | 2.1  |
| 1   | A     | 1233 | GLY  | 2.1  |
| 1   | A     | 830  | ILE  | 2.1  |
| 1   | A     | 100  | LEU  | 2.0  |
| 1   | A     | 13   | VAL  | 2.0  |
| 1   | A     | 1140 | PHE  | 2.0  |
| 1   | A     | 18   | ASP  | 2.0  |
| 1   | A     | 1035 | MET  | 2.0  |
| 1   | A     | 307  | ILE  | 2.0  |
| 1   | A     | 1230 | GLY  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.