



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:35 PM EDT

PDB ID : 3PU1 / pdb\_00003pu1  
Title : Crystal Structure of a vesicular stomatitis virus nucleocapsid-polyG complex  
Authors : Luo, M.; Green, T.J.; Rowse, M.  
Deposited on : 2010-12-03  
Resolution : 3.14 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                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

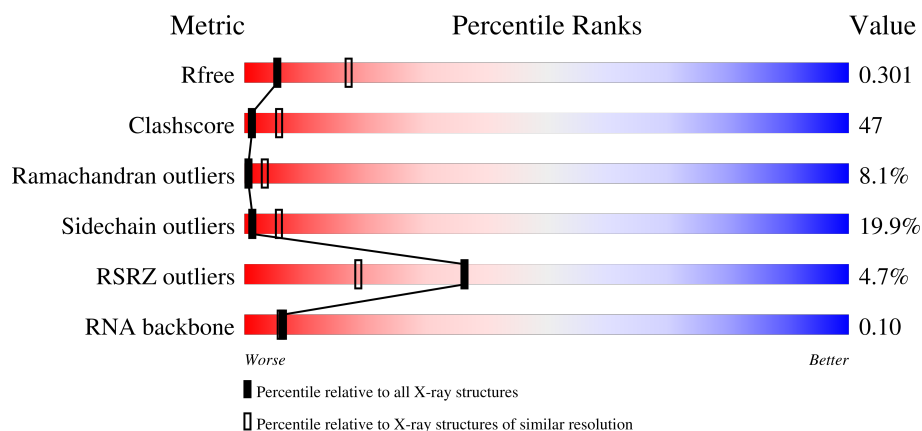
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.14 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2351 (3.18-3.10)                                      |
| Clashscore            | 190562                      | 2452 (3.18-3.10)                                      |
| Ramachandran outliers | 187476                      | 2324 (3.18-3.10)                                      |
| Sidechain outliers    | 187428                      | 2324 (3.18-3.10)                                      |
| RSRZ outliers         | 180081                      | 2351 (3.18-3.10)                                      |
| RNA backbone          | 3983                        | 1040 (3.38-2.90)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                              |
|-----|-------|--------|---------------------------------------------------------------------------------------------------------------|
| 1   | A     | 421    | <div> <div>3%</div> <div> <div></div> <div>40%</div> <div>43%</div> <div>14%</div> <div>.</div> </div> </div> |
| 1   | B     | 421    | <div> <div>5%</div> <div> <div></div> <div>40%</div> <div>41%</div> <div>14%</div> <div>.</div> </div> </div> |
| 1   | C     | 421    | <div> <div>5%</div> <div> <div></div> <div>39%</div> <div>43%</div> <div>13%</div> <div>.</div> </div> </div> |
| 1   | D     | 421    | <div> <div>4%</div> <div> <div></div> <div>39%</div> <div>42%</div> <div>14%</div> <div>.</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 1   | E     | 421    | <div><div>5%</div><div><div></div><div>42%</div><div>42%</div><div>14%</div></div><div></div></div> |
| 2   | R     | 45     | <div><div>7%</div><div><div></div><div>42%</div><div>56%</div></div><div></div></div>               |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17572 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.

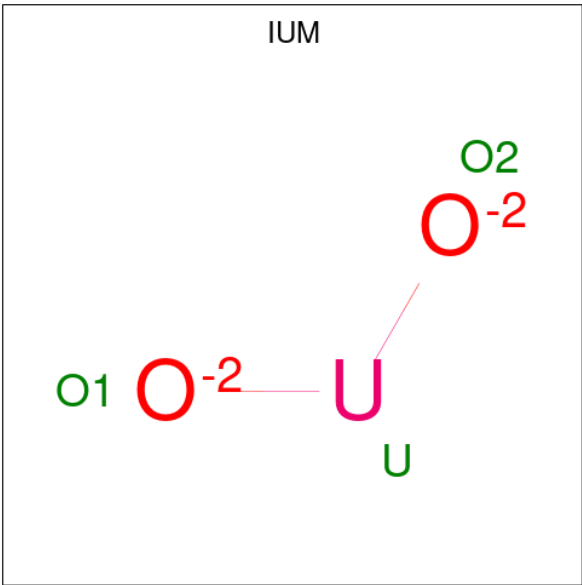
- Molecule 1 is a protein called Nucleoprotein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 421      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3327  | 2118 | 558 | 633 | 18 |         |         |       |
| 1   | B     | 415      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3290  | 2097 | 552 | 623 | 18 |         |         |       |
| 1   | C     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3275  | 2089 | 550 | 618 | 18 |         |         |       |
| 1   | D     | 416      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3298  | 2103 | 553 | 624 | 18 |         |         |       |
| 1   | E     | 421      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3327  | 2118 | 558 | 633 | 18 |         |         |       |

- Molecule 2 is a RNA chain called RNA (45-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2   | R     | 45       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1035  | 450 | 225 | 315 | 45 |         |         |       |

- Molecule 3 is URANYL (VI) ION (CCD ID: IUM) (formula: O<sub>2</sub>U).



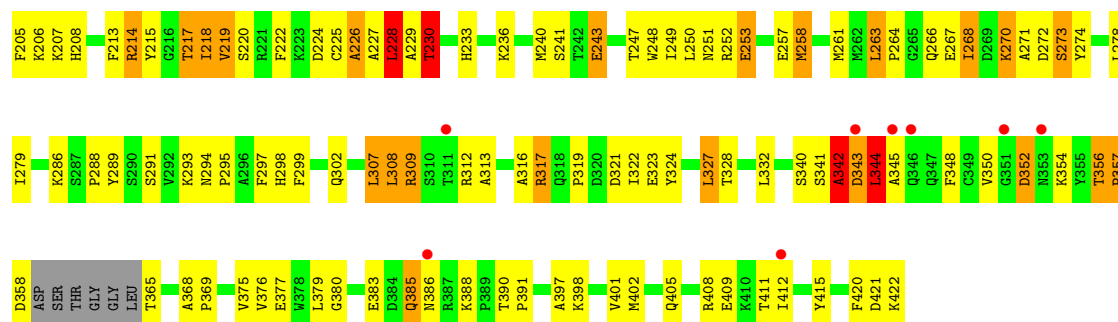
| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 3   | A     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | A     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | B     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | B     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | B     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | C     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | C     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | C     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | D     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | D     | 1        | Total U<br>1 1 | 0       | 0       |
| 3   | E     | 1        | Total U<br>1 1 | 0       | 0       |

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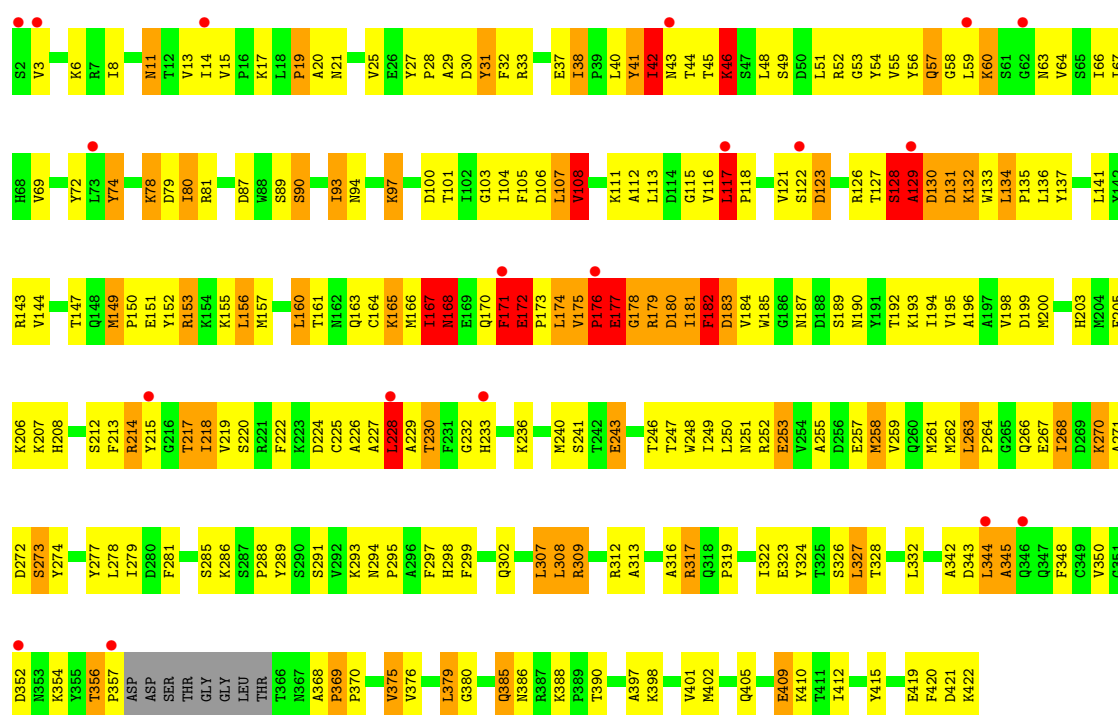
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| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 3   | E     | 1        | Total<br>1 | U<br>1 | 0       | 0       |
| 3   | R     | 1        | Total<br>1 | U<br>1 | 0       | 0       |
| 3   | R     | 1        | Total<br>1 | U<br>1 | 0       | 0       |
| 3   | R     | 1        | Total<br>1 | U<br>1 | 0       | 0       |
| 3   | R     | 1        | Total<br>1 | U<br>1 | 0       | 0       |
| 3   | R     | 1        | Total<br>1 | U<br>1 | 0       | 0       |

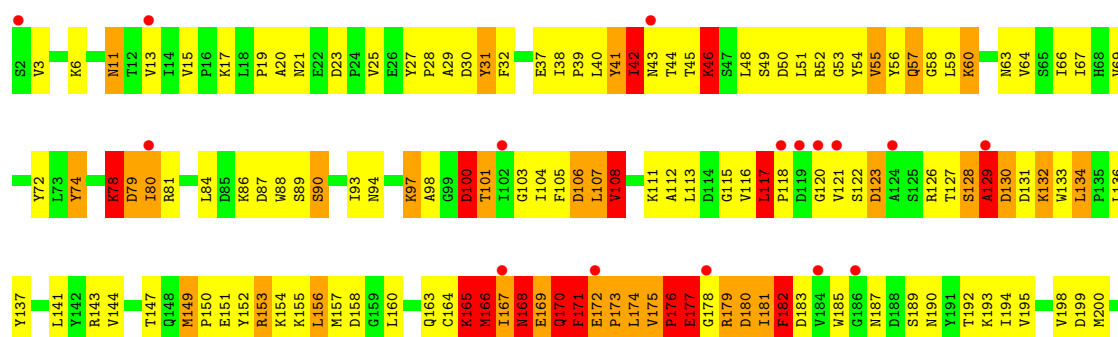


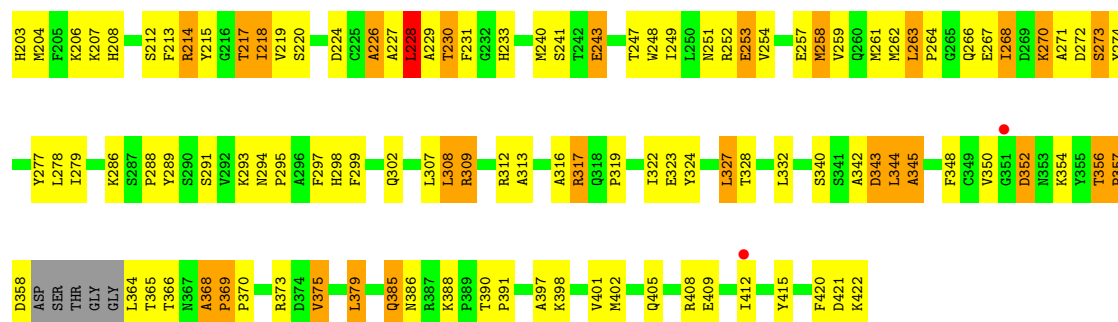


### • Molecule 1: Nucleoprotein

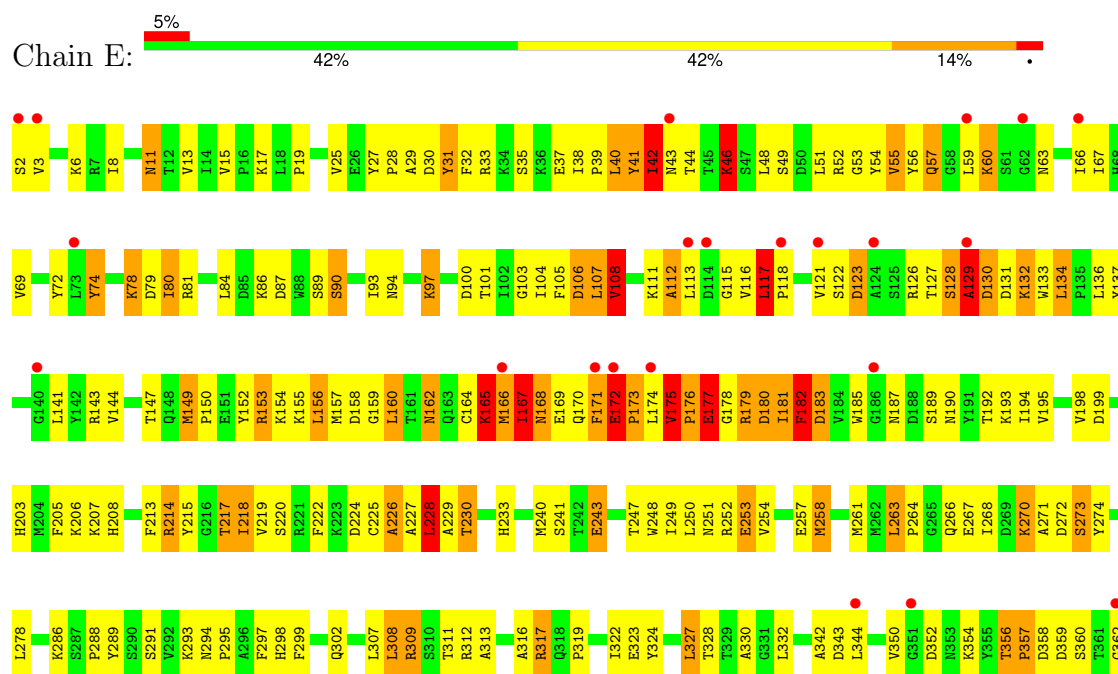


### • Molecule 1: Nucleoprotein

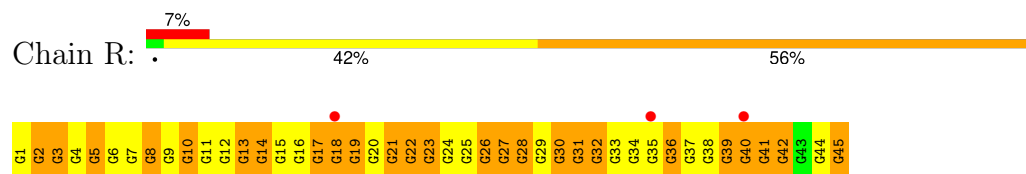




### • Molecule 1: Nucleoprotein



### • Molecule 2: RNA (45-MER)



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 163.22Å 233.19Å 75.57Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 45.10 – 3.14<br>45.10 – 3.14                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 79.0 (45.10-3.14)<br>79.0 (45.10-3.14)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.92 (at 3.12Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.6.1 _357                                           | Depositor        |
| R, $R_{free}$                                                           | 0.259 , 0.305<br>0.254 , 0.301                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2000 reflections (4.75%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 76.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.674                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 44.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.89                                                        | EDS              |
| Total number of atoms                                                   | 17572                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 97.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.65         | 0/3403      | 1.09        | 20/4607 (0.4%)  |
| 1   | B     | 0.65         | 0/3365      | 0.98        | 11/4554 (0.2%)  |
| 1   | C     | 0.68         | 0/3350      | 1.10        | 19/4533 (0.4%)  |
| 1   | D     | 0.62         | 0/3373      | 1.01        | 15/4565 (0.3%)  |
| 1   | E     | 0.61         | 0/3403      | 1.06        | 19/4607 (0.4%)  |
| 2   | R     | 0.47         | 0/1169      | 0.55        | 0/1841          |
| All | All   | 0.63         | 0/18063     | 1.02        | 84/24707 (0.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 5                   |
| 1   | B     | 0                   | 8                   |
| 1   | C     | 0                   | 4                   |
| 1   | D     | 0                   | 6                   |
| 1   | E     | 0                   | 7                   |
| All | All   | 0                   | 30                  |

There are no bond length outliers.

All (84) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | C     | 171 | PHE  | CB-CA-C | -16.64 | 89.33       | 109.80   |
| 1   | C     | 171 | PHE  | N-CA-C  | 15.68  | 133.85      | 110.64   |
| 1   | A     | 177 | GLU  | N-CA-CB | -14.48 | 86.01       | 110.49   |
| 1   | E     | 177 | GLU  | N-CA-CB | -14.40 | 86.15       | 110.49   |
| 1   | E     | 167 | ILE  | N-CA-C  | 14.24  | 124.63      | 110.82   |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | C     | 176 | PRO  | CB-CA-C | -11.70 | 93.56       | 111.22   |
| 1   | A     | 176 | PRO  | CB-CA-C | -10.54 | 94.17       | 111.56   |
| 1   | C     | 172 | GLU  | N-CA-C  | 10.21  | 132.38      | 109.81   |
| 1   | E     | 176 | PRO  | CB-CA-C | -9.95  | 95.14       | 111.56   |
| 1   | D     | 130 | ASP  | N-CA-CB | -9.95  | 93.68       | 110.49   |
| 1   | C     | 130 | ASP  | N-CA-CB | -9.94  | 93.69       | 110.49   |
| 1   | B     | 130 | ASP  | N-CA-CB | -9.88  | 93.80       | 110.49   |
| 1   | A     | 177 | GLU  | N-CA-C  | 9.72   | 131.50      | 110.80   |
| 1   | E     | 130 | ASP  | N-CA-CB | -9.56  | 94.34       | 110.49   |
| 1   | E     | 177 | GLU  | N-CA-C  | 9.55   | 131.15      | 110.80   |
| 1   | D     | 368 | ALA  | CA-C-N  | 9.46   | 126.56      | 119.66   |
| 1   | D     | 368 | ALA  | C-N-CA  | 9.46   | 126.56      | 119.66   |
| 1   | A     | 130 | ASP  | N-CA-CB | -9.32  | 94.73       | 110.49   |
| 1   | A     | 368 | ALA  | CA-C-N  | 9.12   | 126.32      | 119.66   |
| 1   | A     | 368 | ALA  | C-N-CA  | 9.12   | 126.32      | 119.66   |
| 1   | B     | 368 | ALA  | CA-C-N  | 8.99   | 126.22      | 119.66   |
| 1   | B     | 368 | ALA  | C-N-CA  | 8.99   | 126.22      | 119.66   |
| 1   | D     | 176 | PRO  | CB-CA-C | -8.80  | 97.04       | 111.56   |
| 1   | C     | 172 | GLU  | N-CA-CB | -8.74  | 94.81       | 110.37   |
| 1   | E     | 112 | ALA  | N-CA-C  | 8.53   | 118.30      | 108.49   |
| 1   | C     | 177 | GLU  | N-CA-CB | -8.47  | 96.17       | 110.49   |
| 1   | A     | 112 | ALA  | N-CA-C  | 8.46   | 118.22      | 108.49   |
| 1   | E     | 175 | VAL  | CA-C-N  | 8.35   | 130.28      | 119.84   |
| 1   | E     | 175 | VAL  | C-N-CA  | 8.35   | 130.28      | 119.84   |
| 1   | E     | 368 | ALA  | CA-C-N  | 8.29   | 125.71      | 119.66   |
| 1   | E     | 368 | ALA  | C-N-CA  | 8.29   | 125.71      | 119.66   |
| 1   | A     | 175 | VAL  | CA-C-N  | 8.13   | 130.00      | 119.84   |
| 1   | A     | 175 | VAL  | C-N-CA  | 8.13   | 130.00      | 119.84   |
| 1   | E     | 230 | THR  | N-CA-C  | -8.10  | 102.43      | 111.82   |
| 1   | A     | 169 | GLU  | N-CA-C  | 7.71   | 120.45      | 108.96   |
| 1   | B     | 230 | THR  | N-CA-C  | -7.61  | 103.00      | 111.82   |
| 1   | C     | 230 | THR  | N-CA-C  | -7.33  | 103.32      | 111.82   |
| 1   | C     | 368 | ALA  | CA-C-N  | 7.33   | 125.01      | 119.66   |
| 1   | C     | 368 | ALA  | C-N-CA  | 7.33   | 125.01      | 119.66   |
| 1   | A     | 230 | THR  | N-CA-C  | -7.32  | 103.33      | 111.82   |
| 1   | E     | 369 | PRO  | CA-C-N  | 7.27   | 128.93      | 119.84   |
| 1   | E     | 369 | PRO  | C-N-CA  | 7.27   | 128.93      | 119.84   |
| 1   | A     | 369 | PRO  | CA-C-N  | 7.27   | 128.93      | 119.84   |
| 1   | A     | 369 | PRO  | C-N-CA  | 7.27   | 128.93      | 119.84   |
| 1   | A     | 345 | ALA  | N-CA-CB | -7.27  | 98.33       | 110.32   |
| 1   | D     | 369 | PRO  | CA-C-N  | 7.19   | 128.82      | 119.84   |
| 1   | D     | 369 | PRO  | C-N-CA  | 7.19   | 128.82      | 119.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 168 | ASN  | N-CA-C  | 7.03  | 119.17      | 109.54   |
| 1   | D     | 230 | THR  | N-CA-C  | -6.91 | 103.81      | 111.82   |
| 1   | E     | 167 | ILE  | N-CA-CB | -6.84 | 100.66      | 110.52   |
| 1   | C     | 369 | PRO  | CA-C-N  | 6.79  | 128.32      | 119.84   |
| 1   | C     | 369 | PRO  | C-N-CA  | 6.79  | 128.32      | 119.84   |
| 1   | A     | 369 | PRO  | O-C-N   | 6.71  | 124.40      | 121.31   |
| 1   | D     | 177 | GLU  | N-CA-CB | -6.70 | 99.17       | 110.49   |
| 1   | B     | 108 | VAL  | N-CA-C  | 6.47  | 122.79      | 109.34   |
| 1   | B     | 369 | PRO  | CA-C-N  | 6.45  | 127.90      | 119.84   |
| 1   | B     | 369 | PRO  | C-N-CA  | 6.45  | 127.90      | 119.84   |
| 1   | E     | 108 | VAL  | N-CA-C  | 6.21  | 122.25      | 109.34   |
| 1   | C     | 168 | ASN  | N-CA-C  | 6.16  | 123.92      | 110.80   |
| 1   | A     | 108 | VAL  | N-CA-C  | 6.08  | 121.98      | 109.34   |
| 1   | C     | 108 | VAL  | N-CA-C  | 5.84  | 121.48      | 109.34   |
| 1   | D     | 108 | VAL  | N-CA-C  | 5.80  | 121.39      | 109.34   |
| 1   | B     | 218 | ILE  | N-CA-C  | 5.72  | 115.91      | 110.53   |
| 1   | D     | 98  | ALA  | N-CA-C  | 5.72  | 118.36      | 110.35   |
| 1   | E     | 183 | ASP  | N-CA-C  | -5.70 | 106.46      | 113.41   |
| 1   | C     | 369 | PRO  | O-C-N   | 5.54  | 123.86      | 121.31   |
| 1   | E     | 176 | PRO  | N-CA-C  | -5.48 | 101.18      | 112.47   |
| 1   | A     | 361 | THR  | N-CA-C  | 5.48  | 113.27      | 108.78   |
| 1   | D     | 388 | LYS  | CA-C-N  | 5.42  | 125.42      | 119.90   |
| 1   | D     | 388 | LYS  | C-N-CA  | 5.42  | 125.42      | 119.90   |
| 1   | D     | 171 | PHE  | N-CA-CB | 5.41  | 119.51      | 110.59   |
| 1   | A     | 176 | PRO  | N-CA-C  | -5.39 | 101.36      | 112.47   |
| 1   | B     | 388 | LYS  | CA-C-N  | 5.37  | 125.68      | 119.93   |
| 1   | B     | 388 | LYS  | C-N-CA  | 5.37  | 125.68      | 119.93   |
| 1   | C     | 38  | ILE  | CA-C-N  | 5.36  | 126.83      | 120.23   |
| 1   | C     | 38  | ILE  | C-N-CA  | 5.36  | 126.83      | 120.23   |
| 1   | E     | 401 | VAL  | N-CA-C  | 5.32  | 115.83      | 111.62   |
| 1   | D     | 170 | GLN  | N-CA-C  | 5.32  | 122.13      | 110.80   |
| 1   | A     | 361 | THR  | CB-CA-C | -5.29 | 109.46      | 117.07   |
| 1   | C     | 167 | ILE  | N-CA-C  | 5.16  | 120.06      | 109.34   |
| 1   | B     | 369 | PRO  | O-C-N   | 5.15  | 123.68      | 121.31   |
| 1   | A     | 109 | SER  | N-CA-C  | 5.12  | 117.09      | 109.25   |
| 1   | E     | 311 | THR  | N-CA-C  | -5.07 | 106.78      | 113.12   |
| 1   | C     | 183 | ASP  | N-CA-C  | -5.07 | 107.27      | 113.50   |

There are no chirality outliers.

All (30) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 107 | LEU  | Peptide   |
| 1   | A     | 129 | ALA  | Peptide   |
| 1   | A     | 169 | GLU  | Peptide   |
| 1   | A     | 317 | ARG  | Sidechain |
| 1   | A     | 41  | TYR  | Peptide   |
| 1   | B     | 107 | LEU  | Peptide   |
| 1   | B     | 129 | ALA  | Peptide   |
| 1   | B     | 176 | PRO  | Peptide   |
| 1   | B     | 342 | ALA  | Peptide   |
| 1   | B     | 343 | ASP  | Peptide   |
| 1   | B     | 344 | LEU  | Peptide   |
| 1   | B     | 41  | TYR  | Peptide   |
| 1   | B     | 78  | LYS  | Peptide   |
| 1   | C     | 107 | LEU  | Peptide   |
| 1   | C     | 129 | ALA  | Peptide   |
| 1   | C     | 176 | PRO  | Peptide   |
| 1   | C     | 41  | TYR  | Peptide   |
| 1   | D     | 107 | LEU  | Peptide   |
| 1   | D     | 129 | ALA  | Peptide   |
| 1   | D     | 170 | GLN  | Peptide   |
| 1   | D     | 176 | PRO  | Peptide   |
| 1   | D     | 41  | TYR  | Peptide   |
| 1   | D     | 78  | LYS  | Peptide   |
| 1   | E     | 107 | LEU  | Peptide   |
| 1   | E     | 129 | ALA  | Peptide   |
| 1   | E     | 165 | LYS  | Peptide   |
| 1   | E     | 169 | GLU  | Peptide   |
| 1   | E     | 172 | GLU  | Peptide   |
| 1   | E     | 363 | GLY  | Peptide   |
| 1   | E     | 41  | TYR  | Peptide   |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3327  | 0        | 3287     | 343     | 0            |
| 1   | B     | 3290  | 0        | 3253     | 355     | 0            |
| 1   | C     | 3275  | 0        | 3242     | 344     | 0            |
| 1   | D     | 3298  | 0        | 3264     | 337     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | E     | 3327  | 0        | 3287     | 297     | 0            |
| 2   | R     | 1035  | 0        | 496      | 127     | 0            |
| 3   | A     | 5     | 0        | 0        | 0       | 0            |
| 3   | B     | 3     | 0        | 0        | 0       | 0            |
| 3   | C     | 3     | 0        | 0        | 0       | 0            |
| 3   | D     | 2     | 0        | 0        | 0       | 0            |
| 3   | E     | 2     | 0        | 0        | 0       | 0            |
| 3   | R     | 5     | 0        | 0        | 0       | 0            |
| All | All   | 17572 | 0        | 16829    | 1628    | 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 47.

All (1628) 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:C:171:PHE:CG   | 1:C:171:PHE:O    | 1.78                     | 1.31              |
| 1:C:171:PHE:O    | 1:C:171:PHE:CD2  | 1.91                     | 1.23              |
| 1:A:326:SER:HB3  | 1:B:343:ASP:CB   | 1.72                     | 1.19              |
| 1:D:166:MET:O    | 1:D:167:ILE:HG13 | 1.42                     | 1.17              |
| 1:D:317:ARG:H    | 1:D:317:ARG:CZ   | 1.56                     | 1.17              |
| 1:C:177:GLU:HA   | 1:C:181:ILE:HD11 | 1.20                     | 1.16              |
| 1:D:212:SER:HA   | 2:R:9:G:C2       | 1.80                     | 1.15              |
| 1:D:170:GLN:CG   | 1:D:171:PHE:HB3  | 1.75                     | 1.15              |
| 1:A:326:SER:HB3  | 1:B:343:ASP:HB2  | 1.24                     | 1.14              |
| 1:D:170:GLN:HG3  | 1:D:171:PHE:HB3  | 1.23                     | 1.13              |
| 1:B:317:ARG:CZ   | 1:B:317:ARG:H    | 1.61                     | 1.12              |
| 1:B:164:CYS:HA   | 1:B:168:ASN:HA   | 1.18                     | 1.10              |
| 1:B:177:GLU:HA   | 1:B:181:ILE:HD11 | 1.28                     | 1.09              |
| 1:E:59:LEU:HB3   | 1:E:172:GLU:HG2  | 1.33                     | 1.09              |
| 1:A:317:ARG:CZ   | 1:A:317:ARG:H    | 1.65                     | 1.08              |
| 1:D:177:GLU:HA   | 1:D:181:ILE:HD11 | 1.10                     | 1.07              |
| 1:E:149:MET:HG3  | 2:R:42:G:O4'     | 1.55                     | 1.06              |
| 1:E:317:ARG:CZ   | 1:E:317:ARG:H    | 1.67                     | 1.05              |
| 1:C:143:ARG:HH22 | 2:R:17:G:H3'     | 1.18                     | 1.04              |
| 1:C:317:ARG:CZ   | 1:C:317:ARG:H    | 1.71                     | 1.04              |
| 1:E:43:ASN:HA    | 1:E:112:ALA:H    | 1.24                     | 1.03              |
| 1:D:170:GLN:HG3  | 1:D:171:PHE:CB   | 1.89                     | 1.03              |
| 1:D:43:ASN:HA    | 1:D:112:ALA:H    | 1.24                     | 1.02              |
| 1:A:317:ARG:HH21 | 2:R:32:G:P       | 1.82                     | 1.02              |
| 1:C:43:ASN:HA    | 1:C:112:ALA:H    | 1.21                     | 1.02              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:187:ASN:CG   | 1:C:165:LYS:HE3  | 1.85                     | 1.02              |
| 1:C:181:ILE:H    | 1:C:181:ILE:HD12 | 1.25                     | 0.99              |
| 1:A:166:MET:O    | 1:A:167:ILE:HG13 | 1.59                     | 0.98              |
| 1:A:326:SER:CB   | 1:B:343:ASP:HB2  | 1.94                     | 0.98              |
| 1:A:57:GLN:HE21  | 1:A:60:LYS:HZ2   | 0.98                     | 0.98              |
| 1:A:43:ASN:HA    | 1:A:112:ALA:H    | 1.25                     | 0.97              |
| 1:B:43:ASN:HA    | 1:B:112:ALA:H    | 1.28                     | 0.97              |
| 1:E:177:GLU:HA   | 1:E:181:ILE:HD11 | 1.44                     | 0.96              |
| 1:E:57:GLN:HE21  | 1:E:60:LYS:HZ2   | 0.96                     | 0.96              |
| 1:A:177:GLU:HA   | 1:A:181:ILE:HD11 | 1.45                     | 0.96              |
| 1:B:42:ILE:HG13  | 1:B:74:TYR:HD2   | 1.30                     | 0.95              |
| 1:D:165:LYS:O    | 1:D:166:MET:HB2  | 1.60                     | 0.95              |
| 1:A:141:LEU:HD22 | 1:A:182:PHE:HE1  | 1.31                     | 0.95              |
| 1:C:42:ILE:HG13  | 1:C:74:TYR:HD2   | 1.27                     | 0.95              |
| 1:A:42:ILE:HG13  | 1:A:74:TYR:HD2   | 1.29                     | 0.94              |
| 1:D:170:GLN:HG3  | 1:D:171:PHE:N    | 1.83                     | 0.94              |
| 1:C:57:GLN:HE21  | 1:C:60:LYS:HZ2   | 0.94                     | 0.94              |
| 1:B:181:ILE:HD12 | 1:B:181:ILE:H    | 1.33                     | 0.94              |
| 1:C:324:TYR:O    | 1:C:328:THR:HG23 | 1.68                     | 0.94              |
| 1:E:37:GLU:HB2   | 1:E:108:VAL:HG11 | 1.46                     | 0.94              |
| 1:C:141:LEU:HD22 | 1:C:182:PHE:HE1  | 1.32                     | 0.93              |
| 1:E:133:TRP:CD1  | 1:E:167:ILE:HG12 | 2.04                     | 0.93              |
| 1:C:37:GLU:HB2   | 1:C:108:VAL:HG11 | 1.52                     | 0.92              |
| 1:D:149:MET:HG3  | 2:R:6:G:O4'      | 1.70                     | 0.92              |
| 1:A:181:ILE:HD12 | 1:A:181:ILE:H    | 1.34                     | 0.92              |
| 1:B:380:GLY:HA2  | 1:C:354:LYS:NZ   | 1.85                     | 0.92              |
| 1:D:42:ILE:HG13  | 1:D:74:TYR:HD2   | 1.33                     | 0.92              |
| 1:B:97:LYS:O     | 1:B:100:ASP:HB2  | 1.70                     | 0.91              |
| 1:D:143:ARG:HH22 | 2:R:8:G:H3'      | 1.33                     | 0.91              |
| 1:A:163:GLN:O    | 1:A:167:ILE:HB   | 1.70                     | 0.91              |
| 1:E:42:ILE:HG13  | 1:E:74:TYR:HD2   | 1.33                     | 0.90              |
| 1:B:176:PRO:O    | 1:B:181:ILE:HG12 | 1.72                     | 0.90              |
| 1:D:177:GLU:CA   | 1:D:181:ILE:HD11 | 2.00                     | 0.90              |
| 1:A:37:GLU:HB2   | 1:A:108:VAL:HG11 | 1.51                     | 0.90              |
| 1:C:226:ALA:HB2  | 2:R:13:G:H5''    | 1.51                     | 0.90              |
| 1:B:57:GLN:HE21  | 1:B:60:LYS:HZ2   | 0.95                     | 0.89              |
| 1:D:141:LEU:HD22 | 1:D:182:PHE:HE1  | 1.35                     | 0.89              |
| 1:D:37:GLU:HB2   | 1:D:108:VAL:HG11 | 1.54                     | 0.89              |
| 1:D:117:LEU:HB2  | 1:D:118:PRO:HD2  | 1.54                     | 0.89              |
| 1:D:324:TYR:O    | 1:D:328:THR:HG23 | 1.72                     | 0.89              |
| 1:B:37:GLU:HB2   | 1:B:108:VAL:HG11 | 1.52                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:143:ARG:HH22 | 2:R:17:G:C3'     | 1.85                     | 0.89              |
| 1:E:141:LEU:HD22 | 1:E:182:PHE:HE1  | 1.36                     | 0.89              |
| 1:D:177:GLU:HA   | 1:D:181:ILE:CD1  | 2.01                     | 0.88              |
| 1:C:143:ARG:NH2  | 2:R:17:G:H3'     | 1.87                     | 0.88              |
| 1:B:141:LEU:HD22 | 1:B:182:PHE:HE1  | 1.37                     | 0.88              |
| 1:C:132:LYS:HB3  | 1:C:167:ILE:HD12 | 1.56                     | 0.88              |
| 1:D:181:ILE:HD12 | 1:D:181:ILE:H    | 1.36                     | 0.88              |
| 1:B:286:LYS:HD2  | 2:R:20:G:OP1     | 1.73                     | 0.88              |
| 1:E:143:ARG:HH22 | 2:R:44:G:H3'     | 1.39                     | 0.88              |
| 1:C:117:LEU:HB2  | 1:C:118:PRO:HD2  | 1.56                     | 0.88              |
| 1:C:149:MET:HG3  | 2:R:15:G:O4'     | 1.74                     | 0.87              |
| 1:B:383:GLU:HG3  | 1:C:354:LYS:HE2  | 1.55                     | 0.87              |
| 1:A:324:TYR:O    | 1:A:328:THR:HG23 | 1.75                     | 0.87              |
| 1:D:97:LYS:O     | 1:D:100:ASP:HB2  | 1.74                     | 0.87              |
| 1:A:165:LYS:O    | 1:A:167:ILE:HD12 | 1.74                     | 0.87              |
| 1:B:57:GLN:HE21  | 1:B:60:LYS:NZ    | 1.71                     | 0.87              |
| 1:B:117:LEU:HB2  | 1:B:118:PRO:HD2  | 1.56                     | 0.87              |
| 1:C:214:ARG:HA   | 1:C:217:THR:HG22 | 1.54                     | 0.87              |
| 1:E:214:ARG:HA   | 1:E:217:THR:HG22 | 1.56                     | 0.86              |
| 1:E:117:LEU:HB2  | 1:E:118:PRO:HD2  | 1.57                     | 0.86              |
| 1:A:97:LYS:O     | 1:A:100:ASP:HB2  | 1.76                     | 0.85              |
| 1:B:133:TRP:CZ3  | 1:B:169:GLU:HG3  | 2.11                     | 0.85              |
| 1:E:97:LYS:O     | 1:E:100:ASP:HB2  | 1.76                     | 0.85              |
| 1:B:126:ARG:HH11 | 1:B:127:THR:H    | 1.24                     | 0.85              |
| 1:A:126:ARG:HH11 | 1:A:127:THR:H    | 1.24                     | 0.85              |
| 1:E:133:TRP:NE1  | 1:E:167:ILE:HG12 | 1.92                     | 0.85              |
| 1:E:171:PHE:O    | 1:E:171:PHE:CD2  | 2.30                     | 0.85              |
| 1:E:181:ILE:H    | 1:E:181:ILE:HD12 | 1.40                     | 0.85              |
| 1:D:126:ARG:HH11 | 1:D:127:THR:H    | 1.22                     | 0.84              |
| 1:C:97:LYS:O     | 1:C:100:ASP:HB2  | 1.77                     | 0.84              |
| 1:C:57:GLN:HE21  | 1:C:60:LYS:NZ    | 1.76                     | 0.84              |
| 1:A:326:SER:HB3  | 1:B:343:ASP:HB3  | 1.60                     | 0.84              |
| 1:C:263:LEU:HD12 | 1:C:264:PRO:HD2  | 1.58                     | 0.84              |
| 1:C:42:ILE:HG13  | 1:C:74:TYR:CD2   | 2.13                     | 0.83              |
| 1:C:166:MET:C    | 1:C:167:ILE:HD13 | 2.01                     | 0.83              |
| 1:D:214:ARG:HA   | 1:D:217:THR:HG22 | 1.57                     | 0.83              |
| 1:D:317:ARG:CZ   | 1:D:317:ARG:N    | 2.40                     | 0.83              |
| 1:A:165:LYS:HZ3  | 1:A:165:LYS:HB2  | 1.43                     | 0.83              |
| 1:B:42:ILE:HG13  | 1:B:74:TYR:CD2   | 2.14                     | 0.83              |
| 1:A:117:LEU:HB2  | 1:A:118:PRO:HD2  | 1.59                     | 0.83              |
| 1:A:42:ILE:HG13  | 1:A:74:TYR:CD2   | 2.13                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:172:GLU:CB   | 1:E:173:PRO:HD3  | 2.07                     | 0.83              |
| 1:D:170:GLN:HG3  | 1:D:171:PHE:CA   | 2.09                     | 0.82              |
| 1:C:126:ARG:HH11 | 1:C:127:THR:H    | 1.27                     | 0.82              |
| 1:B:324:TYR:O    | 1:B:328:THR:HG23 | 1.80                     | 0.81              |
| 1:D:72:TYR:CE1   | 1:D:134:LEU:HD12 | 2.15                     | 0.81              |
| 1:B:214:ARG:HA   | 1:B:217:THR:HG22 | 1.60                     | 0.81              |
| 1:E:57:GLN:HE21  | 1:E:60:LYS:NZ    | 1.77                     | 0.81              |
| 1:C:177:GLU:CA   | 1:C:181:ILE:HD11 | 2.07                     | 0.81              |
| 1:E:126:ARG:HH11 | 1:E:127:THR:H    | 1.25                     | 0.81              |
| 1:B:169:GLU:HA   | 1:B:169:GLU:OE1  | 1.78                     | 0.81              |
| 1:A:57:GLN:HE21  | 1:A:60:LYS:NZ    | 1.79                     | 0.81              |
| 1:A:326:SER:CB   | 1:B:343:ASP:CB   | 2.56                     | 0.81              |
| 1:D:175:VAL:HG23 | 1:D:176:PRO:O    | 1.79                     | 0.81              |
| 1:A:317:ARG:NH1  | 1:A:317:ARG:N    | 2.29                     | 0.81              |
| 1:B:176:PRO:O    | 1:B:181:ILE:CG1  | 2.29                     | 0.80              |
| 1:E:324:TYR:O    | 1:E:328:THR:HG23 | 1.82                     | 0.80              |
| 1:A:214:ARG:HA   | 1:A:217:THR:HG22 | 1.62                     | 0.80              |
| 1:B:72:TYR:CE1   | 1:B:134:LEU:HD12 | 2.17                     | 0.80              |
| 1:C:177:GLU:HA   | 1:C:181:ILE:CD1  | 2.08                     | 0.80              |
| 1:A:143:ARG:HH12 | 2:R:36:G:C5'     | 1.95                     | 0.79              |
| 1:B:164:CYS:CA   | 1:B:168:ASN:HA   | 2.08                     | 0.79              |
| 1:B:165:LYS:HB2  | 1:B:165:LYS:HZ3  | 1.47                     | 0.79              |
| 1:C:175:VAL:HG23 | 1:C:176:PRO:O    | 1.82                     | 0.79              |
| 1:D:42:ILE:HG13  | 1:D:74:TYR:CD2   | 2.18                     | 0.78              |
| 1:C:72:TYR:CE1   | 1:C:134:LEU:HD12 | 2.17                     | 0.78              |
| 1:A:317:ARG:H    | 1:A:317:ARG:NH1  | 1.80                     | 0.78              |
| 1:C:356:THR:HG23 | 1:C:357:PRO:HD3  | 1.64                     | 0.78              |
| 1:E:72:TYR:CE1   | 1:E:134:LEU:HD12 | 2.19                     | 0.78              |
| 1:B:133:TRP:CE3  | 1:B:169:GLU:HG3  | 2.18                     | 0.78              |
| 1:A:354:LYS:HE3  | 1:A:356:THR:HA   | 1.64                     | 0.78              |
| 1:B:122:SER:O    | 1:B:123:ASP:HB3  | 1.83                     | 0.78              |
| 1:C:312:ARG:HG3  | 2:R:14:G:C5      | 2.18                     | 0.78              |
| 1:E:214:ARG:HA   | 1:E:217:THR:CG2  | 2.14                     | 0.78              |
| 1:A:356:THR:HG23 | 1:A:357:PRO:HD3  | 1.65                     | 0.78              |
| 1:E:354:LYS:HE3  | 1:E:356:THR:HA   | 1.64                     | 0.78              |
| 1:B:57:GLN:NE2   | 1:B:60:LYS:HZ2   | 1.79                     | 0.77              |
| 1:A:365:THR:O    | 1:A:366:THR:HB   | 1.83                     | 0.77              |
| 1:B:152:TYR:HE1  | 1:B:153:ARG:CZ   | 1.97                     | 0.77              |
| 1:B:149:MET:HG3  | 2:R:24:G:O4'     | 1.84                     | 0.77              |
| 1:A:72:TYR:CE1   | 1:A:134:LEU:HD12 | 2.20                     | 0.77              |
| 1:D:179:ARG:HA   | 1:D:183:ASP:OD1  | 1.85                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:365:THR:HG23 | 1:D:366:THR:H    | 1.49                     | 0.77              |
| 1:E:263:LEU:HD12 | 1:E:264:PRO:HD2  | 1.64                     | 0.77              |
| 1:E:179:ARG:HA   | 1:E:183:ASP:OD1  | 1.85                     | 0.77              |
| 1:B:354:LYS:HE3  | 1:B:356:THR:HA   | 1.65                     | 0.77              |
| 1:C:214:ARG:HA   | 1:C:217:THR:CG2  | 2.15                     | 0.77              |
| 1:D:152:TYR:HE1  | 1:D:153:ARG:CZ   | 1.97                     | 0.77              |
| 1:D:166:MET:O    | 1:D:167:ILE:CG1  | 2.30                     | 0.77              |
| 1:A:152:TYR:HE1  | 1:A:153:ARG:CZ   | 1.98                     | 0.76              |
| 1:E:59:LEU:HB3   | 1:E:172:GLU:CG   | 2.12                     | 0.76              |
| 1:A:317:ARG:CZ   | 1:A:317:ARG:N    | 2.47                     | 0.76              |
| 1:B:224:ASP:CG   | 2:R:21:G:H4'     | 2.10                     | 0.76              |
| 1:E:122:SER:O    | 1:E:123:ASP:HB3  | 1.84                     | 0.76              |
| 1:B:214:ARG:HA   | 1:B:217:THR:CG2  | 2.15                     | 0.76              |
| 1:E:167:ILE:HG22 | 1:E:168:ASN:H    | 1.50                     | 0.76              |
| 1:E:172:GLU:HB2  | 1:E:173:PRO:HD3  | 1.68                     | 0.76              |
| 1:C:354:LYS:HE3  | 1:C:356:THR:HA   | 1.66                     | 0.76              |
| 1:B:312:ARG:HG3  | 2:R:23:G:C4      | 2.21                     | 0.75              |
| 1:B:18:LEU:HD12  | 1:C:232:GLY:CA   | 2.16                     | 0.75              |
| 1:D:356:THR:HG23 | 1:D:357:PRO:HD3  | 1.68                     | 0.75              |
| 1:B:250:LEU:HD13 | 1:C:344:LEU:HD12 | 1.66                     | 0.75              |
| 1:D:224:ASP:CG   | 2:R:3:G:H4'      | 2.11                     | 0.75              |
| 1:E:42:ILE:HG13  | 1:E:74:TYR:CD2   | 2.19                     | 0.75              |
| 1:D:175:VAL:CG2  | 1:D:176:PRO:O    | 2.35                     | 0.75              |
| 1:B:356:THR:HG23 | 1:B:357:PRO:HD3  | 1.67                     | 0.75              |
| 1:A:214:ARG:HA   | 1:A:217:THR:CG2  | 2.16                     | 0.75              |
| 1:D:214:ARG:HA   | 1:D:217:THR:CG2  | 2.17                     | 0.75              |
| 1:A:359:ASP:C    | 1:A:361:THR:H    | 1.94                     | 0.74              |
| 1:C:165:LYS:HZ3  | 1:C:165:LYS:HB2  | 1.52                     | 0.74              |
| 1:D:354:LYS:HE3  | 1:D:356:THR:HA   | 1.67                     | 0.74              |
| 2:R:19:G:H2'     | 2:R:20:G:H5'     | 1.67                     | 0.74              |
| 1:B:380:GLY:HA2  | 1:C:354:LYS:HZ3  | 1.50                     | 0.74              |
| 1:A:122:SER:O    | 1:A:123:ASP:HB3  | 1.87                     | 0.74              |
| 1:B:383:GLU:HG3  | 1:C:354:LYS:CE   | 2.15                     | 0.74              |
| 1:D:122:SER:O    | 1:D:123:ASP:HB3  | 1.85                     | 0.74              |
| 1:A:105:PHE:C    | 1:A:107:LEU:H    | 1.94                     | 0.74              |
| 1:C:122:SER:O    | 1:C:123:ASP:HB3  | 1.85                     | 0.74              |
| 1:C:179:ARG:HA   | 1:C:183:ASP:OD1  | 1.88                     | 0.74              |
| 1:E:152:TYR:HE1  | 1:E:153:ARG:CZ   | 2.01                     | 0.74              |
| 1:C:152:TYR:HE1  | 1:C:153:ARG:CZ   | 2.00                     | 0.74              |
| 1:C:250:LEU:HD13 | 1:D:344:LEU:HD12 | 1.68                     | 0.74              |
| 1:C:376:VAL:HG13 | 1:D:354:LYS:HB2  | 1.68                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:263:LEU:HD12 | 1:D:264:PRO:HD2  | 1.68                     | 0.74              |
| 1:E:167:ILE:HG22 | 1:E:168:ASN:N    | 2.03                     | 0.74              |
| 1:D:343:ASP:OD2  | 1:D:373:ARG:NH2  | 2.21                     | 0.74              |
| 1:E:288:PRO:HG2  | 1:E:289:TYR:CE2  | 2.24                     | 0.73              |
| 1:D:74:TYR:CE1   | 1:D:78:LYS:HD2   | 2.24                     | 0.73              |
| 1:C:56:TYR:HD1   | 1:C:126:ARG:HB2  | 1.54                     | 0.73              |
| 1:A:263:LEU:HD12 | 1:A:264:PRO:HD2  | 1.70                     | 0.73              |
| 1:B:141:LEU:HD12 | 1:B:185:TRP:CZ3  | 2.24                     | 0.73              |
| 1:D:56:TYR:HD1   | 1:D:126:ARG:HB2  | 1.53                     | 0.73              |
| 1:D:170:GLN:CD   | 1:D:171:PHE:HB3  | 2.14                     | 0.72              |
| 1:B:165:LYS:O    | 1:B:167:ILE:HD12 | 1.87                     | 0.72              |
| 1:A:317:ARG:NH2  | 2:R:32:G:OP2     | 2.22                     | 0.72              |
| 1:A:56:TYR:HD1   | 1:A:126:ARG:HB2  | 1.55                     | 0.72              |
| 1:A:224:ASP:CG   | 2:R:30:G:H4'     | 2.14                     | 0.72              |
| 1:D:57:GLN:HE21  | 1:D:60:LYS:HZ2   | 1.36                     | 0.72              |
| 1:E:56:TYR:HD1   | 1:E:126:ARG:HB2  | 1.54                     | 0.72              |
| 1:B:133:TRP:CH2  | 1:B:169:GLU:HG3  | 2.24                     | 0.72              |
| 1:D:57:GLN:HE21  | 1:D:60:LYS:NZ    | 1.87                     | 0.72              |
| 1:B:179:ARG:HA   | 1:B:183:ASP:OD1  | 1.89                     | 0.72              |
| 1:C:263:LEU:HD12 | 1:C:264:PRO:CD   | 2.19                     | 0.72              |
| 1:A:179:ARG:HA   | 1:A:183:ASP:OD1  | 1.89                     | 0.72              |
| 1:C:141:LEU:HD13 | 1:C:182:PHE:HD1  | 1.54                     | 0.71              |
| 1:E:317:ARG:CZ   | 1:E:317:ARG:N    | 2.50                     | 0.71              |
| 1:E:177:GLU:CA   | 1:E:181:ILE:HD11 | 2.20                     | 0.71              |
| 1:B:166:MET:O    | 1:B:167:ILE:HG13 | 1.89                     | 0.71              |
| 1:E:167:ILE:CG2  | 1:E:168:ASN:N    | 2.52                     | 0.71              |
| 2:R:30:G:H2'     | 2:R:31:G:O4'     | 1.90                     | 0.71              |
| 2:R:36:G:C2      | 2:R:37:G:H1'     | 2.25                     | 0.71              |
| 1:E:117:LEU:CB   | 1:E:118:PRO:HD2  | 2.19                     | 0.71              |
| 1:A:143:ARG:HH12 | 2:R:36:G:H5'     | 1.54                     | 0.71              |
| 1:D:117:LEU:CB   | 1:D:118:PRO:HD2  | 2.21                     | 0.71              |
| 1:D:143:ARG:HE   | 1:D:155:LYS:HZ1  | 1.36                     | 0.71              |
| 1:E:312:ARG:HG3  | 2:R:41:G:C2      | 2.26                     | 0.71              |
| 1:A:344:LEU:N    | 1:A:344:LEU:CD2  | 2.52                     | 0.71              |
| 1:B:263:LEU:HD12 | 1:B:264:PRO:HD2  | 1.72                     | 0.71              |
| 1:B:317:ARG:CZ   | 1:B:317:ARG:N    | 2.46                     | 0.71              |
| 1:A:344:LEU:HD11 | 1:E:330:ALA:HA   | 1.73                     | 0.71              |
| 1:D:288:PRO:HG2  | 1:D:289:TYR:CE2  | 2.25                     | 0.71              |
| 1:E:398:LYS:O    | 1:E:402:MET:HG2  | 1.91                     | 0.71              |
| 1:D:261:MET:HE1  | 1:D:297:PHE:CD2  | 2.26                     | 0.71              |
| 1:B:18:LEU:HD12  | 1:C:232:GLY:HA2  | 1.72                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:364:LEU:HD12 | 1:E:386:ASN:HD21 | 1.56                     | 0.70              |
| 1:B:56:TYR:HD1   | 1:B:126:ARG:HB2  | 1.55                     | 0.70              |
| 1:A:165:LYS:HB2  | 1:A:165:LYS:NZ   | 2.05                     | 0.70              |
| 1:E:356:THR:HG23 | 1:E:357:PRO:HD3  | 1.71                     | 0.70              |
| 1:B:408:ARG:NH1  | 2:R:24:G:C8      | 2.59                     | 0.70              |
| 1:E:105:PHE:C    | 1:E:107:LEU:H    | 2.00                     | 0.70              |
| 1:A:166:MET:C    | 1:A:167:ILE:HG13 | 2.16                     | 0.70              |
| 1:A:299:PHE:CE1  | 1:A:328:THR:HG22 | 2.26                     | 0.70              |
| 1:B:105:PHE:C    | 1:B:107:LEU:H    | 2.00                     | 0.70              |
| 1:B:169:GLU:O    | 1:B:170:GLN:HB2  | 1.92                     | 0.70              |
| 1:D:316:ALA:HA   | 1:D:317:ARG:NH2  | 2.06                     | 0.70              |
| 1:C:250:LEU:HD13 | 1:D:344:LEU:CD1  | 2.20                     | 0.70              |
| 1:C:298:HIS:NE2  | 1:C:317:ARG:NH1  | 2.39                     | 0.70              |
| 1:D:308:LEU:O    | 1:D:309:ARG:HB2  | 1.90                     | 0.70              |
| 1:A:316:ALA:HB1  | 1:A:317:ARG:HH12 | 1.57                     | 0.70              |
| 1:C:117:LEU:CB   | 1:C:118:PRO:HD2  | 2.22                     | 0.70              |
| 1:E:261:MET:HE1  | 1:E:297:PHE:CD2  | 2.27                     | 0.70              |
| 1:B:308:LEU:O    | 1:B:309:ARG:HB2  | 1.91                     | 0.70              |
| 1:B:79:ASP:HB2   | 1:B:81:ARG:HB2   | 1.72                     | 0.69              |
| 1:B:288:PRO:HG2  | 1:B:289:TYR:CE2  | 2.27                     | 0.69              |
| 1:D:29:ALA:C     | 1:D:31:TYR:H     | 1.99                     | 0.69              |
| 1:B:133:TRP:CD2  | 1:B:169:GLU:CG   | 2.74                     | 0.69              |
| 1:C:181:ILE:HD12 | 1:C:181:ILE:N    | 2.04                     | 0.69              |
| 1:C:105:PHE:C    | 1:C:107:LEU:H    | 1.98                     | 0.69              |
| 1:D:164:CYS:CB   | 1:D:168:ASN:HB3  | 2.22                     | 0.69              |
| 1:A:141:LEU:HD13 | 1:A:182:PHE:HD1  | 1.57                     | 0.69              |
| 1:A:199:ASP:HB2  | 1:A:217:THR:HG23 | 1.74                     | 0.69              |
| 1:C:233:HIS:HB2  | 1:C:312:ARG:NH1  | 2.07                     | 0.69              |
| 1:B:141:LEU:HD13 | 1:B:182:PHE:HD1  | 1.56                     | 0.69              |
| 1:B:167:ILE:O    | 1:B:168:ASN:O    | 2.10                     | 0.69              |
| 1:A:117:LEU:CB   | 1:A:118:PRO:HD2  | 2.22                     | 0.69              |
| 1:A:175:VAL:HG23 | 1:A:176:PRO:O    | 1.93                     | 0.69              |
| 1:B:2:SER:HA     | 1:D:350:VAL:HG11 | 1.75                     | 0.69              |
| 1:D:170:GLN:CG   | 1:D:171:PHE:N    | 2.55                     | 0.69              |
| 1:E:59:LEU:CB    | 1:E:172:GLU:HG2  | 2.18                     | 0.69              |
| 1:E:79:ASP:HB2   | 1:E:81:ARG:HB2   | 1.74                     | 0.69              |
| 1:D:299:PHE:CE1  | 1:D:328:THR:HG22 | 2.27                     | 0.69              |
| 1:A:29:ALA:C     | 1:A:31:TYR:H     | 2.01                     | 0.69              |
| 1:A:74:TYR:CE1   | 1:A:78:LYS:HD2   | 2.27                     | 0.69              |
| 1:B:133:TRP:CD2  | 1:B:169:GLU:HG2  | 2.28                     | 0.69              |
| 1:E:29:ALA:C     | 1:E:31:TYR:H     | 2.01                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:288:PRO:HG2  | 1:A:289:TYR:CE2  | 2.28                     | 0.68              |
| 1:C:179:ARG:HH22 | 2:R:11:G:N2      | 1.91                     | 0.68              |
| 1:C:288:PRO:HG2  | 1:C:289:TYR:CE2  | 2.27                     | 0.68              |
| 1:C:79:ASP:HB2   | 1:C:81:ARG:HB2   | 1.75                     | 0.68              |
| 1:D:79:ASP:HB2   | 1:D:81:ARG:HB2   | 1.75                     | 0.68              |
| 1:A:141:LEU:HD22 | 1:A:182:PHE:CE1  | 2.23                     | 0.68              |
| 1:B:141:LEU:HB3  | 1:B:182:PHE:CE1  | 2.27                     | 0.68              |
| 1:C:385:GLN:HG2  | 1:C:390:THR:HG22 | 1.75                     | 0.68              |
| 1:E:167:ILE:O    | 1:E:168:ASN:HB2  | 1.93                     | 0.68              |
| 1:A:117:LEU:HD23 | 1:A:117:LEU:N    | 2.09                     | 0.68              |
| 1:B:143:ARG:HH22 | 2:R:26:G:H3'     | 1.57                     | 0.68              |
| 1:A:376:VAL:HG13 | 1:B:354:LYS:HB2  | 1.76                     | 0.68              |
| 1:C:308:LEU:O    | 1:C:309:ARG:HB2  | 1.93                     | 0.68              |
| 1:D:105:PHE:C    | 1:D:107:LEU:H    | 2.01                     | 0.68              |
| 1:D:141:LEU:HD13 | 1:D:182:PHE:HD1  | 1.58                     | 0.68              |
| 1:E:364:LEU:O    | 1:E:365:THR:C    | 2.36                     | 0.68              |
| 1:C:117:LEU:N    | 1:C:117:LEU:HD23 | 2.08                     | 0.68              |
| 1:D:212:SER:HA   | 2:R:9:G:N1       | 2.09                     | 0.68              |
| 1:C:165:LYS:HB2  | 1:C:165:LYS:NZ   | 2.08                     | 0.68              |
| 1:D:51:LEU:O     | 1:D:55:VAL:HG22  | 1.94                     | 0.68              |
| 1:D:317:ARG:H    | 1:D:317:ARG:NH1  | 1.92                     | 0.68              |
| 1:E:141:LEU:HD12 | 1:E:185:TRP:CZ3  | 2.29                     | 0.68              |
| 1:E:263:LEU:HD12 | 1:E:264:PRO:CD   | 2.24                     | 0.68              |
| 1:B:117:LEU:CB   | 1:B:118:PRO:HD2  | 2.23                     | 0.67              |
| 1:B:350:VAL:HG11 | 1:E:2:SER:HA     | 1.76                     | 0.67              |
| 1:B:181:ILE:H    | 1:B:181:ILE:CD1  | 2.02                     | 0.67              |
| 1:D:398:LYS:O    | 1:D:402:MET:HG2  | 1.93                     | 0.67              |
| 1:A:181:ILE:H    | 1:A:181:ILE:CD1  | 2.03                     | 0.67              |
| 1:E:317:ARG:HG3  | 2:R:40:G:C4      | 2.29                     | 0.67              |
| 1:D:143:ARG:NH2  | 2:R:8:G:H3'      | 2.07                     | 0.67              |
| 1:A:261:MET:HE1  | 1:A:297:PHE:CD2  | 2.30                     | 0.67              |
| 1:C:141:LEU:HD22 | 1:C:182:PHE:CE1  | 2.24                     | 0.67              |
| 1:D:56:TYR:CD1   | 1:D:126:ARG:HB2  | 2.30                     | 0.67              |
| 1:A:79:ASP:HB2   | 1:A:81:ARG:HB2   | 1.76                     | 0.67              |
| 1:C:299:PHE:CE1  | 1:C:328:THR:HG22 | 2.29                     | 0.67              |
| 1:B:165:LYS:HB2  | 1:B:165:LYS:NZ   | 2.07                     | 0.67              |
| 1:E:141:LEU:HD13 | 1:E:182:PHE:HD1  | 1.59                     | 0.67              |
| 1:B:132:LYS:HB3  | 1:B:167:ILE:HG12 | 1.77                     | 0.67              |
| 1:E:117:LEU:N    | 1:E:117:LEU:HD23 | 2.10                     | 0.67              |
| 1:A:344:LEU:N    | 1:A:344:LEU:HD23 | 2.09                     | 0.66              |
| 1:A:380:GLY:HA2  | 1:B:354:LYS:NZ   | 2.10                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:141:LEU:HD13 | 1:C:182:PHE:CD1  | 2.30                     | 0.66              |
| 1:E:175:VAL:HG23 | 1:E:176:PRO:O    | 1.95                     | 0.66              |
| 1:B:51:LEU:O     | 1:B:55:VAL:HG22  | 1.96                     | 0.66              |
| 1:D:212:SER:HA   | 2:R:9:G:N2       | 2.10                     | 0.66              |
| 1:C:66:ILE:HD12  | 1:C:69:VAL:HG21  | 1.78                     | 0.66              |
| 1:A:250:LEU:HD13 | 1:B:344:LEU:HD12 | 1.77                     | 0.66              |
| 1:B:29:ALA:C     | 1:B:31:TYR:H     | 2.02                     | 0.66              |
| 1:C:326:SER:CB   | 1:D:343:ASP:OD1  | 2.44                     | 0.66              |
| 1:D:166:MET:C    | 1:D:167:ILE:HG13 | 2.20                     | 0.66              |
| 1:E:358:ASP:CG   | 1:E:359:ASP:H    | 2.04                     | 0.66              |
| 1:C:56:TYR:CD1   | 1:C:126:ARG:HB2  | 2.30                     | 0.66              |
| 1:C:57:GLN:NE2   | 1:C:60:LYS:HZ2   | 1.80                     | 0.66              |
| 1:D:44:THR:HG21  | 1:D:116:VAL:CG1  | 2.25                     | 0.66              |
| 1:D:263:LEU:HD12 | 1:D:264:PRO:CD   | 2.25                     | 0.66              |
| 1:B:133:TRP:CE3  | 1:B:169:GLU:CG   | 2.78                     | 0.66              |
| 1:B:317:ARG:H    | 1:B:317:ARG:NH1  | 1.94                     | 0.66              |
| 1:D:141:LEU:HD12 | 1:D:185:TRP:CZ3  | 2.31                     | 0.66              |
| 2:R:16:G:H2'     | 2:R:17:G:H5'     | 1.76                     | 0.66              |
| 1:A:253:GLU:N    | 1:A:253:GLU:CD   | 2.54                     | 0.65              |
| 1:A:385:GLN:HG2  | 1:A:390:THR:HG22 | 1.76                     | 0.65              |
| 1:E:74:TYR:CE1   | 1:E:78:LYS:HD2   | 2.31                     | 0.65              |
| 1:A:141:LEU:HD12 | 1:A:185:TRP:CZ3  | 2.31                     | 0.65              |
| 1:A:358:ASP:CG   | 1:A:359:ASP:H    | 2.01                     | 0.65              |
| 1:A:398:LYS:O    | 1:A:402:MET:HG2  | 1.95                     | 0.65              |
| 1:B:298:HIS:NE2  | 1:B:317:ARG:NH1  | 2.44                     | 0.65              |
| 1:E:308:LEU:O    | 1:E:309:ARG:HB2  | 1.95                     | 0.65              |
| 1:B:385:GLN:HG2  | 1:B:390:THR:HG22 | 1.77                     | 0.65              |
| 1:E:299:PHE:CE1  | 1:E:328:THR:HG22 | 2.32                     | 0.65              |
| 1:C:74:TYR:CE1   | 1:C:78:LYS:HD2   | 2.32                     | 0.65              |
| 1:C:344:LEU:O    | 1:C:345:ALA:HB2  | 1.95                     | 0.65              |
| 1:D:129:ALA:HB1  | 1:D:167:ILE:HD13 | 1.79                     | 0.65              |
| 1:D:141:LEU:HB3  | 1:D:182:PHE:CE1  | 2.30                     | 0.65              |
| 1:E:298:HIS:NE2  | 1:E:317:ARG:NH1  | 2.43                     | 0.65              |
| 1:C:261:MET:HE1  | 1:C:297:PHE:CD2  | 2.32                     | 0.65              |
| 1:A:56:TYR:CD1   | 1:A:126:ARG:HB2  | 2.31                     | 0.65              |
| 1:B:383:GLU:HG3  | 1:C:354:LYS:NZ   | 2.12                     | 0.65              |
| 2:R:34:G:H2'     | 2:R:35:G:O4'     | 1.96                     | 0.65              |
| 1:A:385:GLN:HG2  | 1:A:390:THR:CG2  | 2.27                     | 0.65              |
| 1:B:56:TYR:CD1   | 1:B:126:ARG:HB2  | 2.32                     | 0.65              |
| 1:D:317:ARG:NH2  | 2:R:5:G:P        | 2.70                     | 0.65              |
| 1:A:44:THR:HG21  | 1:A:116:VAL:CG1  | 2.27                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:141:LEU:HD12 | 1:C:185:TRP:CZ3  | 2.32                     | 0.65              |
| 1:D:152:TYR:CE1  | 1:D:153:ARG:CZ   | 2.80                     | 0.65              |
| 1:D:317:ARG:HH21 | 2:R:5:G:P        | 2.19                     | 0.65              |
| 1:E:28:PRO:O     | 1:E:31:TYR:HB3   | 1.97                     | 0.65              |
| 1:C:247:THR:HA   | 1:D:348:PHE:HB2  | 1.79                     | 0.64              |
| 1:A:398:LYS:HG2  | 1:A:402:MET:HE3  | 1.79                     | 0.64              |
| 1:B:74:TYR:CE1   | 1:B:78:LYS:HD2   | 2.33                     | 0.64              |
| 1:D:192:THR:HA   | 1:D:195:VAL:HG12 | 1.79                     | 0.64              |
| 1:E:56:TYR:CD1   | 1:E:126:ARG:HB2  | 2.31                     | 0.64              |
| 1:B:66:ILE:HD12  | 1:B:69:VAL:HG21  | 1.79                     | 0.64              |
| 1:D:79:ASP:O     | 1:D:81:ARG:N     | 2.29                     | 0.64              |
| 1:A:133:TRP:CG   | 1:A:167:ILE:HG21 | 2.33                     | 0.64              |
| 1:A:177:GLU:CA   | 1:A:181:ILE:HD11 | 2.22                     | 0.64              |
| 1:D:181:ILE:CD1  | 1:D:181:ILE:H    | 2.03                     | 0.64              |
| 1:E:141:LEU:HB3  | 1:E:182:PHE:CE1  | 2.32                     | 0.64              |
| 1:A:233:HIS:HB2  | 1:A:312:ARG:NH1  | 2.12                     | 0.64              |
| 1:B:233:HIS:HB2  | 1:B:312:ARG:NH1  | 2.13                     | 0.64              |
| 1:C:29:ALA:C     | 1:C:31:TYR:H     | 2.04                     | 0.64              |
| 1:C:170:GLN:HG2  | 1:C:171:PHE:N    | 2.13                     | 0.64              |
| 1:D:29:ALA:O     | 1:D:31:TYR:N     | 2.31                     | 0.64              |
| 1:D:253:GLU:N    | 1:D:253:GLU:CD   | 2.53                     | 0.64              |
| 1:D:317:ARG:NH2  | 2:R:5:G:OP2      | 2.31                     | 0.64              |
| 1:E:141:LEU:HD22 | 1:E:182:PHE:CE1  | 2.28                     | 0.64              |
| 1:E:385:GLN:HG2  | 1:E:390:THR:HG22 | 1.79                     | 0.64              |
| 1:A:263:LEU:HD12 | 1:A:264:PRO:CD   | 2.27                     | 0.64              |
| 1:A:66:ILE:HD12  | 1:A:69:VAL:HG21  | 1.80                     | 0.64              |
| 1:B:321:ASP:OD1  | 1:C:233:HIS:ND1  | 2.31                     | 0.64              |
| 1:D:179:ARG:HG2  | 1:D:183:ASP:HB3  | 1.78                     | 0.64              |
| 2:R:36:G:H2'     | 2:R:37:G:O4'     | 1.98                     | 0.64              |
| 1:A:179:ARG:HG2  | 1:A:183:ASP:HB3  | 1.80                     | 0.64              |
| 1:B:133:TRP:HB3  | 1:B:167:ILE:HD13 | 1.80                     | 0.64              |
| 1:E:179:ARG:HG2  | 1:E:183:ASP:HB3  | 1.80                     | 0.64              |
| 1:C:55:VAL:HG23  | 1:C:56:TYR:H     | 1.63                     | 0.63              |
| 1:A:308:LEU:O    | 1:A:309:ARG:HB2  | 1.97                     | 0.63              |
| 1:D:28:PRO:O     | 1:D:31:TYR:HB3   | 1.98                     | 0.63              |
| 1:B:55:VAL:HG23  | 1:B:56:TYR:H     | 1.63                     | 0.63              |
| 1:A:141:LEU:HB3  | 1:A:182:PHE:CE1  | 2.33                     | 0.63              |
| 1:A:152:TYR:CE1  | 1:A:153:ARG:CZ   | 2.81                     | 0.63              |
| 1:B:316:ALA:HA   | 1:B:317:ARG:NH2  | 2.14                     | 0.63              |
| 1:B:152:TYR:CE1  | 1:B:153:ARG:CZ   | 2.80                     | 0.63              |
| 1:D:141:LEU:HD22 | 1:D:182:PHE:CE1  | 2.26                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:302:GLN:HE21 | 1:A:313:ALA:HB2  | 1.64                     | 0.63              |
| 1:D:365:THR:HG23 | 1:D:366:THR:N    | 2.14                     | 0.63              |
| 1:E:44:THR:HG21  | 1:E:116:VAL:CG1  | 2.27                     | 0.63              |
| 1:E:171:PHE:CZ   | 1:E:173:PRO:O    | 2.51                     | 0.63              |
| 1:A:344:LEU:HD23 | 1:A:344:LEU:H    | 1.64                     | 0.63              |
| 1:B:44:THR:HG21  | 1:B:116:VAL:CG1  | 2.28                     | 0.63              |
| 1:B:141:LEU:HD22 | 1:B:182:PHE:CE1  | 2.27                     | 0.63              |
| 1:B:143:ARG:HE   | 1:B:155:LYS:HZ1  | 1.47                     | 0.63              |
| 1:C:28:PRO:O     | 1:C:31:TYR:HB3   | 1.99                     | 0.63              |
| 1:E:328:THR:HG21 | 1:E:415:TYR:OH   | 1.98                     | 0.63              |
| 1:A:141:LEU:HD13 | 1:A:182:PHE:CD1  | 2.34                     | 0.63              |
| 1:A:227:ALA:C    | 1:A:229:ALA:H    | 2.07                     | 0.63              |
| 1:A:299:PHE:HE1  | 1:A:328:THR:HG22 | 1.62                     | 0.63              |
| 1:B:192:THR:HA   | 1:B:195:VAL:HG12 | 1.81                     | 0.63              |
| 2:R:16:G:C2'     | 2:R:17:G:H5'     | 2.28                     | 0.63              |
| 1:B:179:ARG:HG2  | 1:B:183:ASP:HB3  | 1.81                     | 0.63              |
| 1:B:299:PHE:CE1  | 1:B:328:THR:HG22 | 2.34                     | 0.63              |
| 1:C:199:ASP:HB2  | 1:C:217:THR:HG23 | 1.81                     | 0.63              |
| 2:R:37:G:C8      | 2:R:38:G:C8      | 2.88                     | 0.62              |
| 1:D:199:ASP:HB2  | 1:D:217:THR:HG23 | 1.79                     | 0.62              |
| 1:D:385:GLN:O    | 1:D:386:ASN:HB2  | 1.99                     | 0.62              |
| 1:D:57:GLN:HA    | 1:D:60:LYS:HD3   | 1.81                     | 0.62              |
| 1:E:171:PHE:CD2  | 1:E:171:PHE:C    | 2.77                     | 0.62              |
| 1:C:263:LEU:CD1  | 1:C:264:PRO:HD2  | 2.27                     | 0.62              |
| 1:D:117:LEU:CB   | 1:D:118:PRO:CD   | 2.78                     | 0.62              |
| 1:E:342:ALA:HB1  | 1:E:344:LEU:HD23 | 1.80                     | 0.62              |
| 1:A:175:VAL:CG2  | 1:A:176:PRO:O    | 2.48                     | 0.62              |
| 1:B:117:LEU:CB   | 1:B:118:PRO:CD   | 2.77                     | 0.62              |
| 1:B:250:LEU:HD13 | 1:C:344:LEU:CD1  | 2.30                     | 0.62              |
| 1:B:253:GLU:N    | 1:B:253:GLU:CD   | 2.56                     | 0.62              |
| 1:C:117:LEU:CB   | 1:C:118:PRO:CD   | 2.77                     | 0.62              |
| 1:D:298:HIS:NE2  | 1:D:317:ARG:NH1  | 2.47                     | 0.62              |
| 1:A:240:MET:HE1  | 1:A:248:TRP:CD1  | 2.34                     | 0.62              |
| 1:C:184:VAL:HG13 | 1:D:165:LYS:HG3  | 1.81                     | 0.62              |
| 1:D:117:LEU:HD23 | 1:D:117:LEU:N    | 2.14                     | 0.62              |
| 1:B:263:LEU:HD12 | 1:B:264:PRO:CD   | 2.29                     | 0.62              |
| 1:D:137:TYR:O    | 1:D:141:LEU:HG   | 2.00                     | 0.62              |
| 1:D:385:GLN:HG2  | 1:D:390:THR:HG22 | 1.80                     | 0.62              |
| 1:D:385:GLN:HG2  | 1:D:390:THR:CG2  | 2.30                     | 0.62              |
| 1:E:253:GLU:CD   | 1:E:253:GLU:N    | 2.58                     | 0.62              |
| 1:A:137:TYR:O    | 1:A:141:LEU:HG   | 2.00                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:141:LEU:HB3  | 1:C:182:PHE:CE1  | 2.35                     | 0.62              |
| 1:D:141:LEU:HD13 | 1:D:182:PHE:CD1  | 2.34                     | 0.62              |
| 1:E:137:TYR:O    | 1:E:141:LEU:HG   | 1.99                     | 0.62              |
| 1:B:317:ARG:O    | 1:B:319:PRO:HD3  | 2.00                     | 0.62              |
| 1:C:44:THR:HG21  | 1:C:116:VAL:CG1  | 2.30                     | 0.62              |
| 1:D:66:ILE:HD12  | 1:D:69:VAL:HG21  | 1.82                     | 0.62              |
| 1:D:227:ALA:C    | 1:D:229:ALA:H    | 2.07                     | 0.62              |
| 1:E:87:ASP:OD2   | 1:E:97:LYS:HG2   | 2.00                     | 0.62              |
| 1:E:164:CYS:O    | 1:E:165:LYS:C    | 2.40                     | 0.62              |
| 1:E:117:LEU:CB   | 1:E:118:PRO:CD   | 2.77                     | 0.62              |
| 1:B:18:LEU:CD1   | 1:C:232:GLY:HA2  | 2.29                     | 0.61              |
| 1:B:57:GLN:HA    | 1:B:60:LYS:HD3   | 1.82                     | 0.61              |
| 1:C:179:ARG:HG2  | 1:C:183:ASP:HB3  | 1.81                     | 0.61              |
| 1:E:316:ALA:HA   | 1:E:317:ARG:NH2  | 2.15                     | 0.61              |
| 1:A:79:ASP:O     | 1:A:81:ARG:N     | 2.33                     | 0.61              |
| 1:E:52:ARG:HD3   | 1:E:126:ARG:HG3  | 1.82                     | 0.61              |
| 1:E:302:GLN:HE21 | 1:E:313:ALA:HB2  | 1.65                     | 0.61              |
| 1:A:385:GLN:O    | 1:A:386:ASN:HB2  | 1.98                     | 0.61              |
| 1:B:117:LEU:N    | 1:B:117:LEU:HD23 | 2.15                     | 0.61              |
| 1:B:141:LEU:HD13 | 1:B:182:PHE:CD1  | 2.34                     | 0.61              |
| 1:D:299:PHE:HE1  | 1:D:328:THR:HG22 | 1.65                     | 0.61              |
| 1:D:343:ASP:OD2  | 1:D:373:ARG:CZ   | 2.48                     | 0.61              |
| 1:E:66:ILE:HD12  | 1:E:69:VAL:HG21  | 1.81                     | 0.61              |
| 1:E:141:LEU:HD13 | 1:E:182:PHE:CD1  | 2.35                     | 0.61              |
| 1:E:199:ASP:HB2  | 1:E:217:THR:HG23 | 1.82                     | 0.61              |
| 1:B:28:PRO:O     | 1:B:31:TYR:HB3   | 2.00                     | 0.61              |
| 1:C:246:THR:HG22 | 1:D:348:PHE:CG   | 2.35                     | 0.61              |
| 1:D:412:ILE:C    | 1:D:412:ILE:HD12 | 2.25                     | 0.61              |
| 1:C:192:THR:HA   | 1:C:195:VAL:HG12 | 1.82                     | 0.61              |
| 1:E:175:VAL:CG2  | 1:E:176:PRO:O    | 2.48                     | 0.61              |
| 1:A:192:THR:HA   | 1:A:195:VAL:HG12 | 1.82                     | 0.61              |
| 1:A:199:ASP:CB   | 1:A:217:THR:HG23 | 2.30                     | 0.61              |
| 1:B:261:MET:HE1  | 1:B:297:PHE:CD2  | 2.35                     | 0.61              |
| 1:E:316:ALA:HB1  | 1:E:317:ARG:HH12 | 1.64                     | 0.61              |
| 1:E:342:ALA:CB   | 1:E:344:LEU:HD23 | 2.30                     | 0.61              |
| 1:E:364:LEU:HB2  | 1:E:368:ALA:HB2  | 1.83                     | 0.61              |
| 1:C:66:ILE:HD12  | 1:C:69:VAL:CG2   | 2.31                     | 0.61              |
| 1:C:87:ASP:OD2   | 1:C:97:LYS:HG2   | 2.01                     | 0.61              |
| 1:C:107:LEU:HD23 | 1:C:274:TYR:CE2  | 2.36                     | 0.61              |
| 1:C:227:ALA:C    | 1:C:229:ALA:H    | 2.09                     | 0.61              |
| 1:A:51:LEU:O     | 1:A:55:VAL:HG22  | 2.01                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:55:VAL:HG23  | 1:A:56:TYR:H     | 1.66                     | 0.61              |
| 1:A:57:GLN:NE2   | 1:A:60:LYS:HZ2   | 1.83                     | 0.61              |
| 1:D:59:LEU:HD13  | 1:D:172:GLU:HG2  | 1.83                     | 0.61              |
| 1:E:385:GLN:O    | 1:E:386:ASN:HB2  | 2.00                     | 0.61              |
| 1:C:51:LEU:O     | 1:C:55:VAL:HG22  | 2.01                     | 0.60              |
| 1:C:317:ARG:CZ   | 1:C:317:ARG:N    | 2.55                     | 0.60              |
| 1:C:385:GLN:HG2  | 1:C:390:THR:CG2  | 2.31                     | 0.60              |
| 2:R:20:G:H2'     | 2:R:21:G:O4'     | 2.01                     | 0.60              |
| 1:A:365:THR:O    | 1:A:366:THR:CB   | 2.49                     | 0.60              |
| 1:B:149:MET:HG3  | 2:R:24:G:C1'     | 2.32                     | 0.60              |
| 1:B:166:MET:C    | 1:B:167:ILE:HG13 | 2.26                     | 0.60              |
| 1:D:126:ARG:HD3  | 1:D:127:THR:N    | 2.17                     | 0.60              |
| 1:D:136:LEU:HD23 | 1:D:136:LEU:O    | 2.00                     | 0.60              |
| 1:D:408:ARG:NH1  | 2:R:6:G:C8       | 2.69                     | 0.60              |
| 1:E:354:LYS:CE   | 1:E:356:THR:HA   | 2.31                     | 0.60              |
| 1:B:133:TRP:CD2  | 1:B:169:GLU:HG3  | 2.37                     | 0.60              |
| 1:B:137:TYR:CE2  | 1:B:141:LEU:HD21 | 2.36                     | 0.60              |
| 1:B:137:TYR:O    | 1:B:141:LEU:HG   | 2.01                     | 0.60              |
| 1:B:398:LYS:O    | 1:B:402:MET:HG2  | 2.00                     | 0.60              |
| 1:C:133:TRP:HB3  | 1:C:167:ILE:HG13 | 1.83                     | 0.60              |
| 1:C:385:GLN:O    | 1:C:386:ASN:HB2  | 2.00                     | 0.60              |
| 1:D:87:ASP:OD2   | 1:D:97:LYS:HG2   | 2.01                     | 0.60              |
| 1:D:328:THR:HG21 | 1:D:415:TYR:OH   | 2.00                     | 0.60              |
| 1:C:397:ALA:O    | 1:C:401:VAL:HG22 | 2.01                     | 0.60              |
| 1:E:79:ASP:O     | 1:E:81:ARG:N     | 2.34                     | 0.60              |
| 1:E:385:GLN:HG2  | 1:E:390:THR:CG2  | 2.30                     | 0.60              |
| 2:R:32:G:H5''    | 2:R:33:G:OP1     | 2.01                     | 0.60              |
| 1:E:317:ARG:HG3  | 2:R:40:G:C5      | 2.36                     | 0.60              |
| 1:A:344:LEU:HD12 | 1:E:250:LEU:HD13 | 1.83                     | 0.60              |
| 1:B:240:MET:HE1  | 1:B:248:TRP:CD1  | 2.37                     | 0.60              |
| 1:B:385:GLN:O    | 1:B:386:ASN:HB2  | 2.02                     | 0.60              |
| 1:D:317:ARG:N    | 1:D:317:ARG:NH1  | 2.49                     | 0.60              |
| 1:E:263:LEU:CD1  | 1:E:264:PRO:HD2  | 2.32                     | 0.60              |
| 1:A:117:LEU:CB   | 1:A:118:PRO:CD   | 2.79                     | 0.60              |
| 1:C:152:TYR:CE1  | 1:C:153:ARG:CZ   | 2.83                     | 0.60              |
| 1:D:117:LEU:HB2  | 1:D:118:PRO:CD   | 2.31                     | 0.60              |
| 1:E:57:GLN:HA    | 1:E:60:LYS:HD3   | 1.84                     | 0.60              |
| 1:E:152:TYR:CE1  | 1:E:153:ARG:CZ   | 2.85                     | 0.60              |
| 1:A:52:ARG:HD3   | 1:A:126:ARG:HG3  | 1.83                     | 0.60              |
| 1:B:316:ALA:HB1  | 1:B:317:ARG:HH12 | 1.66                     | 0.60              |
| 1:B:328:THR:HG21 | 1:B:415:TYR:OH   | 2.00                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:6:G:C8       | 2:R:6:G:O5'      | 2.55                     | 0.60              |
| 1:D:59:LEU:HB3   | 1:D:172:GLU:HG3  | 1.84                     | 0.60              |
| 1:E:51:LEU:O     | 1:E:55:VAL:HG22  | 2.01                     | 0.60              |
| 1:A:28:PRO:O     | 1:A:31:TYR:HB3   | 2.02                     | 0.59              |
| 1:C:117:LEU:HB2  | 1:C:118:PRO:CD   | 2.31                     | 0.59              |
| 1:C:143:ARG:HE   | 1:C:155:LYS:HZ1  | 1.49                     | 0.59              |
| 1:C:212:SER:HB2  | 2:R:18:G:C6      | 2.36                     | 0.59              |
| 1:C:246:THR:HG22 | 1:D:348:PHE:CD1  | 2.36                     | 0.59              |
| 1:C:350:VAL:HG12 | 1:C:350:VAL:O    | 2.02                     | 0.59              |
| 1:D:350:VAL:HG12 | 1:D:350:VAL:O    | 2.01                     | 0.59              |
| 1:E:167:ILE:O    | 1:E:168:ASN:CB   | 2.50                     | 0.59              |
| 1:E:227:ALA:C    | 1:E:229:ALA:H    | 2.09                     | 0.59              |
| 1:B:227:ALA:C    | 1:B:229:ALA:H    | 2.09                     | 0.59              |
| 1:C:57:GLN:HA    | 1:C:60:LYS:HD3   | 1.84                     | 0.59              |
| 1:C:164:CYS:HA   | 1:C:168:ASN:HA   | 1.83                     | 0.59              |
| 1:A:87:ASP:OD2   | 1:A:97:LYS:HG2   | 2.02                     | 0.59              |
| 1:A:228:LEU:O    | 1:A:228:LEU:HD22 | 2.02                     | 0.59              |
| 1:B:385:GLN:HG2  | 1:B:390:THR:CG2  | 2.31                     | 0.59              |
| 1:C:143:ARG:HH22 | 2:R:17:G:C2'     | 2.15                     | 0.59              |
| 1:D:263:LEU:CD1  | 1:D:264:PRO:HD2  | 2.32                     | 0.59              |
| 1:E:365:THR:OG1  | 1:E:366:THR:N    | 2.33                     | 0.59              |
| 2:R:17:G:O2'     | 2:R:18:G:P       | 2.59                     | 0.59              |
| 1:A:107:LEU:HD23 | 1:A:274:TYR:CE2  | 2.37                     | 0.59              |
| 1:A:133:TRP:HB3  | 1:A:167:ILE:HD13 | 1.84                     | 0.59              |
| 1:B:181:ILE:HD12 | 1:B:181:ILE:N    | 2.13                     | 0.59              |
| 1:B:187:ASN:ND2  | 1:C:165:LYS:HD3  | 2.18                     | 0.59              |
| 1:B:302:GLN:HE21 | 1:B:313:ALA:HB2  | 1.67                     | 0.59              |
| 1:D:55:VAL:HG23  | 1:D:56:TYR:H     | 1.67                     | 0.59              |
| 1:D:240:MET:HE1  | 1:D:248:TRP:CD1  | 2.37                     | 0.59              |
| 1:B:80:ILE:HA    | 1:B:103:GLY:HA3  | 1.85                     | 0.59              |
| 1:C:354:LYS:CE   | 1:C:356:THR:HA   | 2.33                     | 0.59              |
| 1:E:350:VAL:HG12 | 1:E:350:VAL:O    | 2.02                     | 0.59              |
| 1:B:59:LEU:HB3   | 1:B:172:GLU:HG2  | 1.85                     | 0.59              |
| 1:B:126:ARG:HD3  | 1:B:127:THR:N    | 2.18                     | 0.59              |
| 1:A:66:ILE:HD13  | 1:A:185:TRP:CD1  | 2.38                     | 0.59              |
| 1:B:153:ARG:HH12 | 1:B:176:PRO:HA   | 1.66                     | 0.59              |
| 1:B:169:GLU:O    | 1:B:170:GLN:CB   | 2.51                     | 0.59              |
| 1:B:267:GLU:HB3  | 1:B:270:LYS:HB2  | 1.83                     | 0.59              |
| 1:C:261:MET:HE2  | 1:C:294:ASN:CG   | 2.28                     | 0.59              |
| 1:A:57:GLN:HA    | 1:A:60:LYS:HD3   | 1.85                     | 0.58              |
| 1:A:218:ILE:C    | 1:A:220:SER:H    | 2.11                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:170:GLN:OE1  | 1:D:171:PHE:HB3  | 2.03                     | 0.58              |
| 1:E:412:ILE:C    | 1:E:412:ILE:HD12 | 2.28                     | 0.58              |
| 1:B:354:LYS:CE   | 1:B:356:THR:HA   | 2.33                     | 0.58              |
| 1:C:52:ARG:HD3   | 1:C:126:ARG:HG3  | 1.84                     | 0.58              |
| 1:D:317:ARG:CZ   | 2:R:5:G:OP2      | 2.51                     | 0.58              |
| 1:C:253:GLU:CD   | 1:C:253:GLU:N    | 2.59                     | 0.58              |
| 1:C:317:ARG:O    | 1:C:319:PRO:HD3  | 2.03                     | 0.58              |
| 1:D:354:LYS:CE   | 1:D:356:THR:HA   | 2.33                     | 0.58              |
| 1:A:344:LEU:HD11 | 1:E:330:ALA:CA   | 2.34                     | 0.58              |
| 1:B:17:LYS:O     | 1:C:262:MET:HE1  | 2.02                     | 0.58              |
| 1:D:66:ILE:HD13  | 1:D:185:TRP:CD1  | 2.39                     | 0.58              |
| 1:C:14:ILE:HD12  | 1:D:259:VAL:HG22 | 1.86                     | 0.58              |
| 1:D:286:LYS:HD2  | 2:R:2:G:OP1      | 2.04                     | 0.58              |
| 1:C:153:ARG:HH12 | 1:C:176:PRO:HA   | 1.69                     | 0.58              |
| 1:D:107:LEU:HD23 | 1:D:274:TYR:CE2  | 2.38                     | 0.58              |
| 1:D:364:LEU:HD23 | 1:D:366:THR:N    | 2.19                     | 0.58              |
| 1:D:153:ARG:HH12 | 1:D:176:PRO:HA   | 1.68                     | 0.58              |
| 1:B:117:LEU:HB2  | 1:B:118:PRO:CD   | 2.31                     | 0.58              |
| 1:C:171:PHE:O    | 1:C:171:PHE:CD1  | 2.53                     | 0.58              |
| 1:D:126:ARG:HA   | 1:D:126:ARG:NH1  | 2.19                     | 0.58              |
| 1:E:66:ILE:HD13  | 1:E:185:TRP:CD1  | 2.38                     | 0.58              |
| 1:E:192:THR:HA   | 1:E:195:VAL:HG12 | 1.86                     | 0.58              |
| 1:B:177:GLU:HA   | 1:B:181:ILE:CD1  | 2.19                     | 0.58              |
| 1:B:341:SER:O    | 1:B:342:ALA:O    | 2.22                     | 0.58              |
| 1:D:151:GLU:HB2  | 2:R:6:G:O2'      | 2.04                     | 0.58              |
| 1:B:194:ILE:O    | 1:B:198:VAL:HG23 | 2.04                     | 0.57              |
| 1:B:227:ALA:O    | 1:B:229:ALA:N    | 2.37                     | 0.57              |
| 1:C:194:ILE:O    | 1:C:198:VAL:HG23 | 2.03                     | 0.57              |
| 1:E:107:LEU:HD23 | 1:E:274:TYR:CE2  | 2.38                     | 0.57              |
| 1:A:380:GLY:HA2  | 1:B:354:LYS:HZ3  | 1.69                     | 0.57              |
| 1:B:218:ILE:C    | 1:B:220:SER:H    | 2.11                     | 0.57              |
| 1:D:302:GLN:HE21 | 1:D:313:ALA:HB2  | 1.69                     | 0.57              |
| 1:D:316:ALA:HB1  | 1:D:317:ARG:HH12 | 1.68                     | 0.57              |
| 1:A:29:ALA:O     | 1:A:31:TYR:N     | 2.36                     | 0.57              |
| 1:A:181:ILE:HD12 | 1:A:181:ILE:N    | 2.13                     | 0.57              |
| 1:B:199:ASP:HB2  | 1:B:217:THR:HG23 | 1.87                     | 0.57              |
| 1:C:137:TYR:O    | 1:C:141:LEU:HG   | 2.04                     | 0.57              |
| 1:D:164:CYS:O    | 1:D:166:MET:N    | 2.31                     | 0.57              |
| 1:D:344:LEU:O    | 1:D:345:ALA:HB2  | 2.03                     | 0.57              |
| 1:A:317:ARG:O    | 1:A:319:PRO:HD3  | 2.03                     | 0.57              |
| 1:C:175:VAL:CG2  | 1:C:176:PRO:O    | 2.50                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:57:GLN:HG3   | 1:D:60:LYS:HZ2   | 1.69                     | 0.57              |
| 1:D:172:GLU:CB   | 1:D:173:PRO:HD3  | 2.34                     | 0.57              |
| 1:E:29:ALA:O     | 1:E:31:TYR:N     | 2.35                     | 0.57              |
| 1:B:107:LEU:HD23 | 1:B:274:TYR:CE2  | 2.39                     | 0.57              |
| 1:C:59:LEU:HB3   | 1:C:172:GLU:HG2  | 1.86                     | 0.57              |
| 1:C:240:MET:HE1  | 1:C:248:TRP:CD1  | 2.40                     | 0.57              |
| 1:D:54:TYR:CD1   | 1:D:122:SER:HB3  | 2.39                     | 0.57              |
| 1:A:397:ALA:O    | 1:A:401:VAL:HG22 | 2.05                     | 0.57              |
| 1:C:302:GLN:HE21 | 1:C:313:ALA:HB2  | 1.67                     | 0.57              |
| 1:C:317:ARG:H    | 1:C:317:ARG:NH1  | 2.03                     | 0.57              |
| 1:D:149:MET:HG3  | 2:R:6:G:C1'      | 2.34                     | 0.57              |
| 1:A:143:ARG:NH2  | 2:R:35:G:C8      | 2.73                     | 0.57              |
| 1:B:126:ARG:HD3  | 1:B:127:THR:H    | 1.69                     | 0.57              |
| 1:C:288:PRO:HG2  | 1:C:289:TYR:CD2  | 2.40                     | 0.57              |
| 1:C:421:ASP:O    | 1:C:422:LYS:HB3  | 2.04                     | 0.57              |
| 1:D:215:TYR:C    | 1:D:215:TYR:CD2  | 2.83                     | 0.57              |
| 1:E:181:ILE:H    | 1:E:181:ILE:CD1  | 2.05                     | 0.57              |
| 1:A:59:LEU:HB3   | 1:A:172:GLU:HG2  | 1.87                     | 0.57              |
| 1:B:52:ARG:HD3   | 1:B:126:ARG:HG3  | 1.86                     | 0.57              |
| 1:B:153:ARG:O    | 1:B:157:MET:HG3  | 2.05                     | 0.57              |
| 1:C:328:THR:HG21 | 1:C:415:TYR:OH   | 2.05                     | 0.57              |
| 1:C:19:PRO:HA    | 1:D:268:ILE:O    | 2.04                     | 0.57              |
| 1:C:199:ASP:CB   | 1:C:217:THR:HG23 | 2.34                     | 0.57              |
| 1:C:299:PHE:HE1  | 1:C:328:THR:HG22 | 1.67                     | 0.57              |
| 1:E:179:ARG:HA   | 1:E:183:ASP:CB   | 2.35                     | 0.57              |
| 1:C:376:VAL:HG13 | 1:D:354:LYS:CB   | 2.35                     | 0.57              |
| 1:D:267:GLU:HB3  | 1:D:270:LYS:HB2  | 1.87                     | 0.57              |
| 1:C:137:TYR:CE2  | 1:C:141:LEU:HD21 | 2.39                     | 0.56              |
| 1:C:326:SER:HB3  | 1:D:343:ASP:OD1  | 2.05                     | 0.56              |
| 1:D:137:TYR:CE2  | 1:D:141:LEU:HD21 | 2.39                     | 0.56              |
| 1:E:66:ILE:HD12  | 1:E:69:VAL:CG2   | 2.34                     | 0.56              |
| 1:E:228:LEU:HD22 | 1:E:228:LEU:O    | 2.05                     | 0.56              |
| 2:R:15:G:O5'     | 2:R:15:G:H8      | 1.88                     | 0.56              |
| 1:A:182:PHE:N    | 1:A:182:PHE:HD2  | 2.03                     | 0.56              |
| 1:D:199:ASP:CB   | 1:D:217:THR:HG23 | 2.35                     | 0.56              |
| 1:A:143:ARG:HH12 | 2:R:36:G:H5''    | 1.68                     | 0.56              |
| 1:A:143:ARG:HE   | 1:A:155:LYS:HZ1  | 1.53                     | 0.56              |
| 1:A:194:ILE:O    | 1:A:198:VAL:HG23 | 2.06                     | 0.56              |
| 1:A:267:GLU:HB3  | 1:A:270:LYS:HB2  | 1.86                     | 0.56              |
| 1:B:317:ARG:N    | 1:B:317:ARG:NH1  | 2.53                     | 0.56              |
| 1:D:52:ARG:HD3   | 1:D:126:ARG:HG3  | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:317:ARG:O    | 1:D:319:PRO:HD3  | 2.05                     | 0.56              |
| 1:E:80:ILE:HA    | 1:E:103:GLY:HA3  | 1.87                     | 0.56              |
| 1:B:2:SER:O      | 1:C:243:GLU:HG3  | 2.05                     | 0.56              |
| 1:D:164:CYS:HA   | 1:D:168:ASN:HB3  | 1.87                     | 0.56              |
| 1:E:214:ARG:CA   | 1:E:217:THR:HG22 | 2.31                     | 0.56              |
| 1:E:317:ARG:O    | 1:E:319:PRO:HD3  | 2.05                     | 0.56              |
| 1:A:149:MET:HG3  | 2:R:33:G:C8      | 2.40                     | 0.56              |
| 1:B:66:ILE:HD12  | 1:B:69:VAL:CG2   | 2.35                     | 0.56              |
| 1:D:179:ARG:HA   | 1:D:183:ASP:CB   | 2.35                     | 0.56              |
| 1:E:288:PRO:HG2  | 1:E:289:TYR:CD2  | 2.40                     | 0.56              |
| 1:C:179:ARG:HA   | 1:C:183:ASP:CB   | 2.36                     | 0.56              |
| 1:D:44:THR:HG21  | 1:D:116:VAL:HG13 | 1.86                     | 0.56              |
| 1:B:79:ASP:O     | 1:B:81:ARG:N     | 2.38                     | 0.56              |
| 1:B:261:MET:HE2  | 1:B:294:ASN:CG   | 2.30                     | 0.56              |
| 1:E:41:TYR:HB2   | 1:E:190:ASN:HD21 | 1.70                     | 0.56              |
| 1:C:226:ALA:HB2  | 2:R:13:G:C5'     | 2.30                     | 0.56              |
| 1:D:59:LEU:HB3   | 1:D:172:GLU:CG   | 2.36                     | 0.56              |
| 1:D:153:ARG:O    | 1:D:157:MET:HG3  | 2.06                     | 0.56              |
| 1:D:401:VAL:HG21 | 1:D:420:PHE:HB2  | 1.88                     | 0.56              |
| 1:C:79:ASP:O     | 1:C:81:ARG:N     | 2.37                     | 0.56              |
| 1:D:126:ARG:HD3  | 1:D:127:THR:H    | 1.70                     | 0.56              |
| 1:E:199:ASP:CB   | 1:E:217:THR:HG23 | 2.34                     | 0.56              |
| 1:C:66:ILE:HD13  | 1:C:185:TRP:CD1  | 2.42                     | 0.55              |
| 1:C:151:GLU:HB2  | 2:R:15:G:O2'     | 2.06                     | 0.55              |
| 1:D:74:TYR:CD1   | 1:D:78:LYS:HD2   | 2.41                     | 0.55              |
| 1:A:388:LYS:HE2  | 1:B:340:SER:HB2  | 1.87                     | 0.55              |
| 1:B:164:CYS:HA   | 1:B:168:ASN:CA   | 2.12                     | 0.55              |
| 1:B:179:ARG:HA   | 1:B:183:ASP:CB   | 2.36                     | 0.55              |
| 1:B:228:LEU:O    | 1:B:228:LEU:HD22 | 2.07                     | 0.55              |
| 1:D:129:ALA:O    | 1:D:133:TRP:NE1  | 2.39                     | 0.55              |
| 1:E:55:VAL:HG23  | 1:E:56:TYR:H     | 1.71                     | 0.55              |
| 1:A:137:TYR:CE2  | 1:A:141:LEU:HD21 | 2.42                     | 0.55              |
| 1:A:179:ARG:HA   | 1:A:183:ASP:CB   | 2.37                     | 0.55              |
| 1:A:261:MET:HE2  | 1:A:294:ASN:CG   | 2.31                     | 0.55              |
| 1:C:170:GLN:HG2  | 1:C:171:PHE:HB3  | 1.89                     | 0.55              |
| 1:C:228:LEU:HD22 | 1:C:228:LEU:O    | 2.06                     | 0.55              |
| 1:D:74:TYR:O     | 1:D:78:LYS:HD3   | 2.06                     | 0.55              |
| 1:A:43:ASN:OD1   | 1:A:112:ALA:HB3  | 2.06                     | 0.55              |
| 1:A:263:LEU:CD1  | 1:A:264:PRO:HD2  | 2.37                     | 0.55              |
| 1:B:31:TYR:CD1   | 1:B:31:TYR:C     | 2.85                     | 0.55              |
| 1:B:401:VAL:HG21 | 1:B:420:PHE:HB2  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:31:TYR:CD1   | 1:C:31:TYR:C     | 2.85                     | 0.55              |
| 1:D:122:SER:O    | 1:D:123:ASP:CB   | 2.54                     | 0.55              |
| 1:B:343:ASP:H    | 1:B:344:LEU:HD23 | 1.70                     | 0.55              |
| 1:C:74:TYR:CD1   | 1:C:74:TYR:C     | 2.85                     | 0.55              |
| 1:C:398:LYS:O    | 1:C:402:MET:HG2  | 2.05                     | 0.55              |
| 1:D:286:LYS:HE2  | 1:D:293:LYS:HD3  | 1.87                     | 0.55              |
| 1:D:295:PRO:HB2  | 1:D:322:ILE:CG2  | 2.37                     | 0.55              |
| 1:A:317:ARG:NH2  | 2:R:32:G:OP1     | 2.40                     | 0.55              |
| 1:B:44:THR:HG21  | 1:B:116:VAL:HG13 | 1.88                     | 0.55              |
| 1:B:87:ASP:OD2   | 1:B:97:LYS:HG2   | 2.06                     | 0.55              |
| 1:C:29:ALA:O     | 1:C:31:TYR:N     | 2.38                     | 0.55              |
| 1:D:72:TYR:HE1   | 1:D:134:LEU:HB3  | 1.70                     | 0.55              |
| 1:A:350:VAL:HG12 | 1:A:350:VAL:O    | 2.07                     | 0.55              |
| 1:B:2:SER:HA     | 1:D:350:VAL:CG1  | 2.37                     | 0.55              |
| 1:C:182:PHE:HD2  | 1:C:182:PHE:N    | 2.04                     | 0.55              |
| 1:D:164:CYS:SG   | 1:D:168:ASN:HB3  | 2.47                     | 0.55              |
| 1:E:31:TYR:CD1   | 1:E:31:TYR:C     | 2.84                     | 0.55              |
| 1:E:182:PHE:HD2  | 1:E:182:PHE:N    | 2.05                     | 0.55              |
| 1:A:354:LYS:CE   | 1:A:356:THR:HA   | 2.34                     | 0.55              |
| 1:C:182:PHE:N    | 1:C:182:PHE:CD2  | 2.75                     | 0.55              |
| 1:E:117:LEU:HB2  | 1:E:118:PRO:CD   | 2.34                     | 0.55              |
| 1:A:136:LEU:HD23 | 1:A:136:LEU:O    | 2.07                     | 0.55              |
| 1:C:72:TYR:HE1   | 1:C:134:LEU:HB3  | 1.71                     | 0.55              |
| 1:D:288:PRO:HG2  | 1:D:289:TYR:CD2  | 2.42                     | 0.55              |
| 1:E:149:MET:HG3  | 2:R:42:G:C1'     | 2.36                     | 0.55              |
| 1:B:136:LEU:HD23 | 1:B:136:LEU:O    | 2.05                     | 0.54              |
| 1:E:171:PHE:CE1  | 1:E:173:PRO:O    | 2.60                     | 0.54              |
| 1:E:267:GLU:HB3  | 1:E:270:LYS:HB2  | 1.89                     | 0.54              |
| 1:A:66:ILE:HD12  | 1:A:69:VAL:CG2   | 2.37                     | 0.54              |
| 1:A:117:LEU:HB2  | 1:A:118:PRO:CD   | 2.35                     | 0.54              |
| 1:C:74:TYR:C     | 1:C:74:TYR:HD1   | 2.15                     | 0.54              |
| 1:A:286:LYS:HE2  | 1:A:293:LYS:HD3  | 1.88                     | 0.54              |
| 1:B:182:PHE:HD2  | 1:B:182:PHE:N    | 2.05                     | 0.54              |
| 1:E:43:ASN:HA    | 1:E:112:ALA:N    | 2.08                     | 0.54              |
| 1:A:182:PHE:N    | 1:A:182:PHE:CD2  | 2.74                     | 0.54              |
| 1:B:126:ARG:NH1  | 1:B:127:THR:HG22 | 2.22                     | 0.54              |
| 1:D:72:TYR:CE1   | 1:D:134:LEU:HB3  | 2.42                     | 0.54              |
| 1:D:80:ILE:HA    | 1:D:103:GLY:HA3  | 1.89                     | 0.54              |
| 1:D:170:GLN:CG   | 1:D:171:PHE:CB   | 2.61                     | 0.54              |
| 1:A:317:ARG:NE   | 2:R:32:G:OP2     | 2.40                     | 0.54              |
| 1:B:41:TYR:HB2   | 1:B:190:ASN:HD21 | 1.72                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:214:ARG:CA   | 1:C:217:THR:HG22 | 2.31                     | 0.54              |
| 1:C:263:LEU:HD12 | 1:C:264:PRO:N    | 2.23                     | 0.54              |
| 1:C:316:ALA:HB1  | 1:C:317:ARG:HH12 | 1.72                     | 0.54              |
| 1:C:342:ALA:CB   | 1:C:344:LEU:HD23 | 2.38                     | 0.54              |
| 1:C:398:LYS:HG2  | 1:C:402:MET:HE3  | 1.90                     | 0.54              |
| 1:D:74:TYR:CD1   | 1:D:74:TYR:C     | 2.86                     | 0.54              |
| 1:D:253:GLU:CD   | 1:D:253:GLU:H    | 2.15                     | 0.54              |
| 1:E:299:PHE:HE1  | 1:E:328:THR:HG22 | 1.69                     | 0.54              |
| 1:E:126:ARG:HA   | 1:E:126:ARG:NH1  | 2.22                     | 0.54              |
| 1:B:179:ARG:O    | 1:C:161:THR:HG21 | 2.07                     | 0.54              |
| 1:C:388:LYS:HE2  | 1:D:340:SER:HB2  | 1.89                     | 0.54              |
| 1:C:401:VAL:HG21 | 1:C:420:PHE:HB2  | 1.90                     | 0.54              |
| 1:E:137:TYR:CE2  | 1:E:141:LEU:HD21 | 2.43                     | 0.54              |
| 1:A:31:TYR:CD1   | 1:A:31:TYR:C     | 2.86                     | 0.54              |
| 1:D:228:LEU:O    | 1:D:228:LEU:HD22 | 2.08                     | 0.54              |
| 1:B:54:TYR:CD1   | 1:B:122:SER:HB3  | 2.43                     | 0.54              |
| 1:B:182:PHE:N    | 1:B:182:PHE:CD2  | 2.76                     | 0.54              |
| 1:C:52:ARG:CD    | 1:C:126:ARG:HG3  | 2.38                     | 0.54              |
| 1:D:74:TYR:O     | 1:D:74:TYR:HD1   | 1.91                     | 0.54              |
| 1:E:44:THR:HG21  | 1:E:116:VAL:HG13 | 1.88                     | 0.54              |
| 1:B:288:PRO:HG2  | 1:B:289:TYR:CD2  | 2.44                     | 0.53              |
| 1:A:126:ARG:HD3  | 1:A:127:THR:N    | 2.24                     | 0.53              |
| 1:A:250:LEU:HD13 | 1:B:344:LEU:CD1  | 2.38                     | 0.53              |
| 1:B:74:TYR:O     | 1:B:78:LYS:HD3   | 2.09                     | 0.53              |
| 1:B:299:PHE:HE1  | 1:B:328:THR:HG22 | 1.73                     | 0.53              |
| 1:C:192:THR:HA   | 1:C:195:VAL:CG1  | 2.39                     | 0.53              |
| 1:E:52:ARG:CD    | 1:E:126:ARG:HG3  | 2.37                     | 0.53              |
| 1:D:263:LEU:HD12 | 1:D:264:PRO:N    | 2.23                     | 0.53              |
| 1:E:72:TYR:HE1   | 1:E:134:LEU:HB3  | 1.73                     | 0.53              |
| 1:E:397:ALA:O    | 1:E:401:VAL:HG22 | 2.08                     | 0.53              |
| 1:A:263:LEU:HD12 | 1:A:264:PRO:N    | 2.23                     | 0.53              |
| 1:A:401:VAL:HG21 | 1:A:420:PHE:HB2  | 1.90                     | 0.53              |
| 1:B:72:TYR:HE1   | 1:B:134:LEU:HB3  | 1.72                     | 0.53              |
| 1:B:263:LEU:CD1  | 1:B:264:PRO:HD2  | 2.38                     | 0.53              |
| 1:A:31:TYR:CD1   | 1:A:32:PHE:N     | 2.77                     | 0.53              |
| 1:B:31:TYR:CD1   | 1:B:32:PHE:N     | 2.77                     | 0.53              |
| 1:B:66:ILE:HD13  | 1:B:185:TRP:CD1  | 2.44                     | 0.53              |
| 1:B:263:LEU:HD12 | 1:B:264:PRO:N    | 2.23                     | 0.53              |
| 1:B:356:THR:O    | 1:B:358:ASP:N    | 2.38                     | 0.53              |
| 1:D:66:ILE:HD12  | 1:D:69:VAL:CG2   | 2.38                     | 0.53              |
| 1:D:136:LEU:HB2  | 1:D:213:PHE:CE2  | 2.43                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:27:TYR:CZ    | 1:A:263:LEU:HD23 | 2.43                     | 0.53              |
| 1:B:192:THR:HA   | 1:B:195:VAL:CG1  | 2.39                     | 0.53              |
| 1:E:74:TYR:CD1   | 1:E:74:TYR:C     | 2.86                     | 0.53              |
| 1:E:398:LYS:HG2  | 1:E:402:MET:HE3  | 1.90                     | 0.53              |
| 1:A:44:THR:HG21  | 1:A:116:VAL:HG13 | 1.89                     | 0.53              |
| 1:A:79:ASP:C     | 1:A:81:ARG:N     | 2.67                     | 0.53              |
| 1:B:72:TYR:CE1   | 1:B:134:LEU:HB3  | 2.43                     | 0.53              |
| 1:B:226:ALA:HB3  | 1:B:291:SER:HB3  | 1.91                     | 0.53              |
| 2:R:19:G:C2'     | 2:R:20:G:H5'     | 2.37                     | 0.53              |
| 1:A:226:ALA:O    | 1:A:227:ALA:C    | 2.51                     | 0.53              |
| 1:A:317:ARG:H    | 1:A:317:ARG:NE   | 2.06                     | 0.53              |
| 1:B:397:ALA:O    | 1:B:401:VAL:HG22 | 2.09                     | 0.53              |
| 1:C:166:MET:O    | 1:C:167:ILE:HD13 | 2.08                     | 0.53              |
| 1:D:227:ALA:O    | 1:D:229:ALA:N    | 2.40                     | 0.53              |
| 1:E:317:ARG:N    | 1:E:317:ARG:NH1  | 2.57                     | 0.53              |
| 1:E:317:ARG:H    | 1:E:317:ARG:NH1  | 2.03                     | 0.53              |
| 1:A:126:ARG:NH1  | 1:A:126:ARG:HA   | 2.23                     | 0.53              |
| 1:A:340:SER:HB2  | 1:E:388:LYS:HE2  | 1.91                     | 0.53              |
| 1:A:421:ASP:O    | 1:A:422:LYS:HB3  | 2.07                     | 0.53              |
| 1:B:129:ALA:O    | 1:B:133:TRP:NE1  | 2.42                     | 0.53              |
| 1:C:31:TYR:CD1   | 1:C:32:PHE:N     | 2.77                     | 0.53              |
| 1:C:179:ARG:HH22 | 2:R:11:G:H22     | 1.56                     | 0.53              |
| 1:C:227:ALA:O    | 1:C:229:ALA:N    | 2.41                     | 0.53              |
| 1:E:54:TYR:CD1   | 1:E:122:SER:HB3  | 2.44                     | 0.53              |
| 1:A:169:GLU:HA   | 1:A:170:GLN:OE1  | 2.08                     | 0.52              |
| 1:B:164:CYS:O    | 1:B:168:ASN:N    | 2.31                     | 0.52              |
| 1:C:72:TYR:CE1   | 1:C:134:LEU:HB3  | 2.44                     | 0.52              |
| 1:C:181:ILE:H    | 1:C:181:ILE:CD1  | 1.97                     | 0.52              |
| 1:D:43:ASN:HA    | 1:D:112:ALA:N    | 2.09                     | 0.52              |
| 2:R:17:G:O2'     | 2:R:18:G:O5'     | 2.24                     | 0.52              |
| 1:A:177:GLU:HA   | 1:A:181:ILE:CD1  | 2.31                     | 0.52              |
| 1:B:143:ARG:NH2  | 2:R:26:G:H2'     | 2.24                     | 0.52              |
| 1:B:215:TYR:C    | 1:B:215:TYR:CD2  | 2.88                     | 0.52              |
| 1:C:212:SER:CB   | 2:R:18:G:C6      | 2.92                     | 0.52              |
| 1:C:316:ALA:HA   | 1:C:317:ARG:NH2  | 2.25                     | 0.52              |
| 1:C:326:SER:OG   | 1:D:343:ASP:OD1  | 2.26                     | 0.52              |
| 1:A:80:ILE:HA    | 1:A:103:GLY:HA3  | 1.91                     | 0.52              |
| 1:A:133:TRP:HB3  | 1:A:167:ILE:CD1  | 2.39                     | 0.52              |
| 1:B:162:ASN:N    | 1:B:162:ASN:HD22 | 2.07                     | 0.52              |
| 1:B:199:ASP:CB   | 1:B:217:THR:HG23 | 2.39                     | 0.52              |
| 1:C:27:TYR:CZ    | 1:C:263:LEU:HD23 | 2.45                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:126:ARG:NH1  | 1:C:127:THR:HG22 | 2.24                     | 0.52              |
| 1:C:267:GLU:HB3  | 1:C:270:LYS:HB2  | 1.89                     | 0.52              |
| 1:D:31:TYR:C     | 1:D:31:TYR:CD1   | 2.87                     | 0.52              |
| 1:D:79:ASP:C     | 1:D:81:ARG:N     | 2.66                     | 0.52              |
| 1:E:218:ILE:C    | 1:E:220:SER:H    | 2.18                     | 0.52              |
| 1:B:52:ARG:CD    | 1:B:126:ARG:HG3  | 2.40                     | 0.52              |
| 1:B:421:ASP:O    | 1:B:422:LYS:HB3  | 2.09                     | 0.52              |
| 1:D:317:ARG:H    | 1:D:317:ARG:NE   | 2.03                     | 0.52              |
| 1:E:74:TYR:C     | 1:E:74:TYR:HD1   | 2.17                     | 0.52              |
| 1:A:273:SER:OG   | 1:A:274:TYR:N    | 2.40                     | 0.52              |
| 1:A:359:ASP:C    | 1:A:361:THR:N    | 2.61                     | 0.52              |
| 1:C:126:ARG:HD3  | 1:C:127:THR:N    | 2.24                     | 0.52              |
| 1:C:177:GLU:HG2  | 1:C:181:ILE:HD11 | 1.92                     | 0.52              |
| 1:E:74:TYR:CD1   | 1:E:78:LYS:HD2   | 2.45                     | 0.52              |
| 1:E:143:ARG:NH2  | 2:R:44:G:H5'     | 2.25                     | 0.52              |
| 1:C:72:TYR:HE1   | 1:C:134:LEU:HD12 | 1.73                     | 0.52              |
| 1:C:89:SER:O     | 1:C:90:SER:HB2   | 2.09                     | 0.52              |
| 1:C:155:LYS:HE3  | 2:R:17:G:OP2     | 2.09                     | 0.52              |
| 1:D:214:ARG:CA   | 1:D:217:THR:HG22 | 2.34                     | 0.52              |
| 1:E:129:ALA:HB1  | 1:E:167:ILE:HD11 | 1.91                     | 0.52              |
| 1:E:215:TYR:C    | 1:E:215:TYR:CD2  | 2.87                     | 0.52              |
| 1:E:240:MET:HE1  | 1:E:248:TRP:CD1  | 2.44                     | 0.52              |
| 1:C:129:ALA:HB1  | 1:C:133:TRP:HE1  | 1.75                     | 0.52              |
| 1:C:136:LEU:O    | 1:C:136:LEU:HD23 | 2.09                     | 0.52              |
| 1:D:189:SER:O    | 1:D:193:LYS:HG3  | 2.10                     | 0.52              |
| 1:E:129:ALA:O    | 1:E:133:TRP:NE1  | 2.43                     | 0.52              |
| 1:A:169:GLU:HA   | 1:A:170:GLN:CD   | 2.35                     | 0.52              |
| 1:A:356:THR:O    | 1:A:358:ASP:N    | 2.38                     | 0.52              |
| 1:B:143:ARG:HH22 | 2:R:26:G:C3'     | 2.23                     | 0.52              |
| 1:B:162:ASN:HD22 | 1:B:162:ASN:H    | 1.56                     | 0.52              |
| 1:B:224:ASP:OD1  | 2:R:21:G:H4'     | 2.10                     | 0.52              |
| 1:B:228:LEU:O    | 1:B:228:LEU:HD13 | 2.10                     | 0.52              |
| 1:C:43:ASN:OD1   | 1:C:112:ALA:HB3  | 2.10                     | 0.52              |
| 1:D:74:TYR:C     | 1:D:74:TYR:HD1   | 2.17                     | 0.52              |
| 1:E:31:TYR:CD1   | 1:E:32:PHE:N     | 2.77                     | 0.52              |
| 1:B:29:ALA:O     | 1:B:31:TYR:N     | 2.36                     | 0.52              |
| 1:B:57:GLN:C     | 1:B:59:LEU:N     | 2.68                     | 0.52              |
| 1:B:253:GLU:CD   | 1:B:253:GLU:H    | 2.17                     | 0.52              |
| 1:C:44:THR:HG21  | 1:C:116:VAL:HG13 | 1.90                     | 0.52              |
| 1:C:107:LEU:CD2  | 1:C:274:TYR:HE2  | 2.22                     | 0.52              |
| 1:E:177:GLU:HA   | 1:E:181:ILE:CD1  | 2.30                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:356:THR:O    | 1:E:358:ASP:N    | 2.40                     | 0.52              |
| 1:A:74:TYR:CD1   | 1:A:74:TYR:C     | 2.87                     | 0.52              |
| 1:A:328:THR:HG21 | 1:A:415:TYR:OH   | 2.10                     | 0.52              |
| 1:B:133:TRP:CZ2  | 1:B:169:GLU:HG3  | 2.45                     | 0.52              |
| 1:C:80:ILE:HA    | 1:C:103:GLY:HA3  | 1.93                     | 0.52              |
| 1:D:29:ALA:C     | 1:D:31:TYR:N     | 2.66                     | 0.52              |
| 1:E:136:LEU:O    | 1:E:136:LEU:HD23 | 2.10                     | 0.52              |
| 1:A:189:SER:O    | 1:A:193:LYS:HG3  | 2.11                     | 0.51              |
| 1:B:28:PRO:HD2   | 1:B:266:GLN:NE2  | 2.25                     | 0.51              |
| 1:B:45:THR:CB    | 1:B:111:LYS:HZ1  | 2.23                     | 0.51              |
| 1:B:74:TYR:CD1   | 1:B:78:LYS:HD2   | 2.45                     | 0.51              |
| 1:B:214:ARG:CA   | 1:B:217:THR:HG22 | 2.34                     | 0.51              |
| 1:C:153:ARG:O    | 1:C:157:MET:HG3  | 2.10                     | 0.51              |
| 1:B:350:VAL:HG12 | 1:B:350:VAL:O    | 2.11                     | 0.51              |
| 1:C:129:ALA:O    | 1:C:133:TRP:NE1  | 2.43                     | 0.51              |
| 1:E:126:ARG:NH1  | 1:E:127:THR:HG22 | 2.25                     | 0.51              |
| 2:R:38:G:H2'     | 2:R:39:G:O4'     | 2.10                     | 0.51              |
| 1:A:52:ARG:CD    | 1:A:126:ARG:HG3  | 2.40                     | 0.51              |
| 1:A:107:LEU:CD2  | 1:A:274:TYR:HE2  | 2.22                     | 0.51              |
| 1:A:227:ALA:O    | 1:A:229:ALA:N    | 2.43                     | 0.51              |
| 1:B:152:TYR:CD1  | 1:B:177:GLU:HG3  | 2.44                     | 0.51              |
| 1:C:41:TYR:HB2   | 1:C:190:ASN:HD21 | 1.75                     | 0.51              |
| 1:D:168:ASN:OD1  | 1:D:168:ASN:N    | 2.43                     | 0.51              |
| 1:E:107:LEU:CD2  | 1:E:274:TYR:HE2  | 2.24                     | 0.51              |
| 1:E:267:GLU:OE1  | 1:E:273:SER:HB2  | 2.10                     | 0.51              |
| 1:A:241:SER:OG   | 1:A:243:GLU:HG2  | 2.09                     | 0.51              |
| 1:A:376:VAL:HG13 | 1:B:354:LYS:CB   | 2.39                     | 0.51              |
| 1:B:74:TYR:CD1   | 1:B:74:TYR:C     | 2.88                     | 0.51              |
| 1:C:79:ASP:C     | 1:C:81:ARG:N     | 2.68                     | 0.51              |
| 2:R:1:G:C2'      | 2:R:2:G:H5'      | 2.40                     | 0.51              |
| 1:B:412:ILE:C    | 1:B:412:ILE:HD12 | 2.35                     | 0.51              |
| 1:D:89:SER:O     | 1:D:90:SER:HB2   | 2.11                     | 0.51              |
| 1:E:153:ARG:O    | 1:E:157:MET:HG3  | 2.10                     | 0.51              |
| 1:E:261:MET:HE2  | 1:E:294:ASN:CG   | 2.35                     | 0.51              |
| 1:A:126:ARG:NH1  | 1:A:127:THR:HG22 | 2.26                     | 0.51              |
| 1:A:358:ASP:OD2  | 1:A:359:ASP:N    | 2.33                     | 0.51              |
| 1:D:52:ARG:CD    | 1:D:126:ARG:HG3  | 2.40                     | 0.51              |
| 1:E:6:LYS:NZ     | 1:E:11:ASN:HD21  | 2.09                     | 0.51              |
| 1:E:263:LEU:HD12 | 1:E:264:PRO:N    | 2.26                     | 0.51              |
| 1:E:317:ARG:H    | 1:E:317:ARG:NE   | 2.06                     | 0.51              |
| 1:A:295:PRO:HB2  | 1:A:322:ILE:CG2  | 2.41                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:187:ASN:ND2  | 1:C:165:LYS:HE3  | 2.26                     | 0.51              |
| 1:C:74:TYR:O     | 1:C:78:LYS:HD3   | 2.11                     | 0.51              |
| 1:C:79:ASP:O     | 1:C:79:ASP:OD1   | 2.29                     | 0.51              |
| 1:C:130:ASP:C    | 1:C:132:LYS:N    | 2.66                     | 0.51              |
| 1:C:412:ILE:HD12 | 1:C:412:ILE:C    | 2.36                     | 0.51              |
| 1:E:79:ASP:C     | 1:E:81:ARG:N     | 2.68                     | 0.51              |
| 1:E:126:ARG:HD3  | 1:E:127:THR:N    | 2.25                     | 0.51              |
| 1:E:291:SER:OG   | 2:R:40:G:H5''    | 2.11                     | 0.51              |
| 1:A:43:ASN:HA    | 1:A:112:ALA:N    | 2.08                     | 0.51              |
| 1:B:81:ARG:HD2   | 1:B:208:HIS:CE1  | 2.46                     | 0.51              |
| 1:C:380:GLY:HA2  | 1:D:354:LYS:NZ   | 2.25                     | 0.51              |
| 1:D:72:TYR:HE1   | 1:D:134:LEU:HD12 | 1.73                     | 0.51              |
| 1:D:356:THR:O    | 1:D:358:ASP:N    | 2.38                     | 0.51              |
| 1:E:72:TYR:CE1   | 1:E:134:LEU:HB3  | 2.45                     | 0.51              |
| 2:R:10:G:C8      | 2:R:11:G:C8      | 2.99                     | 0.51              |
| 1:B:104:ILE:HD13 | 1:B:198:VAL:HG22 | 1.93                     | 0.51              |
| 1:B:415:TYR:HE2  | 1:C:309:ARG:HG2  | 1.76                     | 0.51              |
| 1:C:184:VAL:HG11 | 1:D:166:MET:HE2  | 1.92                     | 0.51              |
| 1:C:226:ALA:HB3  | 1:C:291:SER:HB3  | 1.93                     | 0.51              |
| 1:E:172:GLU:N    | 1:E:173:PRO:CD   | 2.74                     | 0.51              |
| 1:B:27:TYR:CZ    | 1:B:263:LEU:HD23 | 2.45                     | 0.51              |
| 1:C:203:HIS:O    | 1:C:206:LYS:HG3  | 2.11                     | 0.51              |
| 1:C:215:TYR:C    | 1:C:215:TYR:CD2  | 2.89                     | 0.51              |
| 1:D:421:ASP:O    | 1:D:422:LYS:HB3  | 2.11                     | 0.51              |
| 1:E:203:HIS:O    | 1:E:206:LYS:HG3  | 2.11                     | 0.51              |
| 1:A:74:TYR:C     | 1:A:74:TYR:HD1   | 2.19                     | 0.50              |
| 1:A:97:LYS:HB2   | 1:A:97:LYS:NZ    | 2.26                     | 0.50              |
| 1:A:354:LYS:HB2  | 1:E:376:VAL:HG13 | 1.91                     | 0.50              |
| 1:B:43:ASN:OD1   | 1:B:112:ALA:HB3  | 2.10                     | 0.50              |
| 1:D:182:PHE:N    | 1:D:182:PHE:HD2  | 2.08                     | 0.50              |
| 1:E:43:ASN:OD1   | 1:E:112:ALA:HB3  | 2.11                     | 0.50              |
| 1:A:72:TYR:HE1   | 1:A:134:LEU:HB3  | 1.76                     | 0.50              |
| 1:A:74:TYR:CD1   | 1:A:78:LYS:HD2   | 2.46                     | 0.50              |
| 1:D:213:PHE:C    | 1:D:215:TYR:H    | 2.19                     | 0.50              |
| 1:E:97:LYS:HB2   | 1:E:97:LYS:NZ    | 2.27                     | 0.50              |
| 1:E:182:PHE:N    | 1:E:182:PHE:CD2  | 2.76                     | 0.50              |
| 1:A:214:ARG:CA   | 1:A:217:THR:HG22 | 2.36                     | 0.50              |
| 1:C:38:ILE:HD11  | 1:C:107:LEU:O    | 2.11                     | 0.50              |
| 1:C:43:ASN:HA    | 1:C:112:ALA:N    | 2.07                     | 0.50              |
| 1:A:288:PRO:HG2  | 1:A:289:TYR:CD2  | 2.46                     | 0.50              |
| 1:D:107:LEU:CD2  | 1:D:274:TYR:HE2  | 2.24                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:181:ILE:HD12 | 1:D:181:ILE:N    | 2.16                     | 0.50              |
| 1:E:129:ALA:HB1  | 1:E:133:TRP:HE1  | 1.76                     | 0.50              |
| 1:A:412:ILE:HD12 | 1:A:412:ILE:C    | 2.37                     | 0.50              |
| 1:B:29:ALA:C     | 1:B:31:TYR:N     | 2.70                     | 0.50              |
| 1:B:74:TYR:C     | 1:B:74:TYR:HD1   | 2.20                     | 0.50              |
| 1:D:27:TYR:CZ    | 1:D:263:LEU:HD23 | 2.47                     | 0.50              |
| 1:D:81:ARG:HD2   | 1:D:208:HIS:CE1  | 2.47                     | 0.50              |
| 1:A:129:ALA:HB1  | 1:A:133:TRP:HE1  | 1.76                     | 0.50              |
| 1:B:2:SER:CA     | 1:D:350:VAL:HG11 | 2.42                     | 0.50              |
| 1:C:126:ARG:NH1  | 1:C:126:ARG:HA   | 2.26                     | 0.50              |
| 1:D:179:ARG:HA   | 1:D:183:ASP:CG   | 2.37                     | 0.50              |
| 2:R:19:G:H2'     | 2:R:20:G:C5'     | 2.38                     | 0.50              |
| 1:A:74:TYR:O     | 1:A:78:LYS:HD3   | 2.12                     | 0.50              |
| 1:A:218:ILE:C    | 1:A:220:SER:N    | 2.69                     | 0.50              |
| 1:B:218:ILE:C    | 1:B:220:SER:N    | 2.68                     | 0.50              |
| 1:D:203:HIS:O    | 1:D:206:LYS:HG3  | 2.12                     | 0.50              |
| 1:E:74:TYR:O     | 1:E:78:LYS:HD3   | 2.11                     | 0.50              |
| 2:R:6:G:C8       | 2:R:6:G:H3'      | 2.47                     | 0.50              |
| 1:A:41:TYR:HB2   | 1:A:190:ASN:HD21 | 1.77                     | 0.50              |
| 1:A:126:ARG:HD3  | 1:A:127:THR:H    | 1.76                     | 0.50              |
| 1:B:184:VAL:HG21 | 1:C:164:CYS:HB3  | 1.94                     | 0.50              |
| 1:D:126:ARG:NH1  | 1:D:127:THR:HG22 | 2.27                     | 0.50              |
| 1:D:182:PHE:N    | 1:D:182:PHE:CD2  | 2.79                     | 0.50              |
| 1:D:398:LYS:HG2  | 1:D:402:MET:HE3  | 1.94                     | 0.50              |
| 1:E:194:ILE:O    | 1:E:198:VAL:HG23 | 2.12                     | 0.50              |
| 1:E:286:LYS:HE2  | 1:E:293:LYS:HD3  | 1.93                     | 0.50              |
| 1:A:122:SER:O    | 1:A:123:ASP:CB   | 2.59                     | 0.50              |
| 1:A:152:TYR:CE1  | 1:A:177:GLU:HG3  | 2.47                     | 0.50              |
| 1:B:136:LEU:HB2  | 1:B:213:PHE:CE2  | 2.47                     | 0.50              |
| 1:C:286:LYS:HE2  | 1:C:293:LYS:HD3  | 1.94                     | 0.50              |
| 1:D:41:TYR:HB2   | 1:D:190:ASN:HD21 | 1.77                     | 0.50              |
| 1:D:43:ASN:OD1   | 1:D:112:ALA:HB3  | 2.11                     | 0.50              |
| 1:D:192:THR:HA   | 1:D:195:VAL:CG1  | 2.40                     | 0.50              |
| 1:B:187:ASN:CG   | 1:C:165:LYS:CE   | 2.74                     | 0.49              |
| 1:C:45:THR:CB    | 1:C:111:LYS:HZ2  | 2.24                     | 0.49              |
| 1:C:126:ARG:HD3  | 1:C:127:THR:H    | 1.76                     | 0.49              |
| 1:E:27:TYR:CZ    | 1:E:263:LEU:HD23 | 2.46                     | 0.49              |
| 1:A:48:LEU:HD12  | 1:A:48:LEU:O     | 2.12                     | 0.49              |
| 1:A:165:LYS:O    | 1:A:167:ILE:CD1  | 2.55                     | 0.49              |
| 1:B:79:ASP:O     | 1:B:79:ASP:OD1   | 2.29                     | 0.49              |
| 1:B:224:ASP:OD2  | 2:R:20:G:O2'     | 2.27                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:179:ARG:HA   | 1:E:183:ASP:CG   | 2.37                     | 0.49              |
| 1:E:421:ASP:O    | 1:E:422:LYS:HB3  | 2.10                     | 0.49              |
| 2:R:3:G:H2'      | 2:R:4:G:O4'      | 2.12                     | 0.49              |
| 1:A:136:LEU:HB2  | 1:A:213:PHE:CE2  | 2.48                     | 0.49              |
| 1:A:224:ASP:OD1  | 2:R:30:G:H4'     | 2.12                     | 0.49              |
| 1:B:74:TYR:O     | 1:B:74:TYR:HD1   | 1.96                     | 0.49              |
| 1:B:133:TRP:CE2  | 1:B:169:GLU:CG   | 2.95                     | 0.49              |
| 1:C:107:LEU:HD23 | 1:C:274:TYR:HE2  | 1.78                     | 0.49              |
| 1:E:107:LEU:HD23 | 1:E:274:TYR:HE2  | 1.77                     | 0.49              |
| 2:R:6:G:H3'      | 2:R:6:G:H8       | 1.76                     | 0.49              |
| 1:A:130:ASP:C    | 1:A:132:LYS:N    | 2.69                     | 0.49              |
| 1:A:153:ARG:O    | 1:A:157:MET:HG3  | 2.12                     | 0.49              |
| 1:B:126:ARG:NH1  | 1:B:126:ARG:HA   | 2.28                     | 0.49              |
| 1:D:56:TYR:CE1   | 1:D:126:ARG:NE   | 2.81                     | 0.49              |
| 1:D:57:GLN:C     | 1:D:59:LEU:N     | 2.69                     | 0.49              |
| 1:E:181:ILE:HD12 | 1:E:181:ILE:N    | 2.17                     | 0.49              |
| 1:A:364:LEU:CD1  | 1:E:386:ASN:HD21 | 2.26                     | 0.49              |
| 1:C:48:LEU:HD12  | 1:C:48:LEU:O     | 2.12                     | 0.49              |
| 1:D:79:ASP:HB2   | 1:D:81:ARG:NE    | 2.27                     | 0.49              |
| 1:E:401:VAL:HG21 | 1:E:420:PHE:HB2  | 1.92                     | 0.49              |
| 1:A:57:GLN:C     | 1:A:59:LEU:N     | 2.70                     | 0.49              |
| 1:A:192:THR:HA   | 1:A:195:VAL:CG1  | 2.42                     | 0.49              |
| 1:A:253:GLU:CD   | 1:A:253:GLU:H    | 2.19                     | 0.49              |
| 1:B:162:ASN:N    | 1:B:162:ASN:ND2  | 2.60                     | 0.49              |
| 1:B:295:PRO:HB2  | 1:B:322:ILE:CG2  | 2.42                     | 0.49              |
| 1:C:170:GLN:NE2  | 1:C:171:PHE:HD2  | 2.11                     | 0.49              |
| 1:E:81:ARG:HD2   | 1:E:208:HIS:CE1  | 2.47                     | 0.49              |
| 1:E:226:ALA:O    | 1:E:227:ALA:C    | 2.55                     | 0.49              |
| 1:A:81:ARG:HD2   | 1:A:208:HIS:CE1  | 2.48                     | 0.49              |
| 1:A:249:ILE:CD1  | 1:A:258:MET:HG3  | 2.43                     | 0.49              |
| 1:B:97:LYS:HB2   | 1:B:97:LYS:NZ    | 2.28                     | 0.49              |
| 1:B:133:TRP:CE2  | 1:B:169:GLU:HG3  | 2.47                     | 0.49              |
| 1:C:136:LEU:HB2  | 1:C:213:PHE:CE2  | 2.48                     | 0.49              |
| 1:E:89:SER:O     | 1:E:90:SER:HB2   | 2.12                     | 0.49              |
| 1:E:152:TYR:CE1  | 1:E:177:GLU:HG3  | 2.47                     | 0.49              |
| 1:B:46:LYS:HA    | 1:B:46:LYS:HD3   | 1.52                     | 0.49              |
| 1:E:53:GLY:O     | 1:E:54:TYR:C     | 2.56                     | 0.49              |
| 2:R:8:G:H5''     | 2:R:9:G:OP2      | 2.13                     | 0.49              |
| 1:B:107:LEU:CD2  | 1:B:274:TYR:HE2  | 2.26                     | 0.49              |
| 1:C:74:TYR:CD1   | 1:C:78:LYS:HD2   | 2.47                     | 0.49              |
| 1:C:380:GLY:HA2  | 1:D:354:LYS:HZ3  | 1.77                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:104:ILE:HD13 | 1:D:198:VAL:HG22 | 1.95                     | 0.49              |
| 1:D:233:HIS:HB2  | 1:D:312:ARG:NH1  | 2.27                     | 0.49              |
| 1:E:15:VAL:O     | 1:E:17:LYS:HG2   | 2.12                     | 0.49              |
| 2:R:27:G:N3      | 2:R:27:G:O4'     | 2.45                     | 0.49              |
| 1:C:117:LEU:N    | 1:C:117:LEU:CD2  | 2.74                     | 0.49              |
| 1:D:45:THR:CB    | 1:D:111:LYS:HZ2  | 2.26                     | 0.49              |
| 1:D:136:LEU:HD23 | 1:D:136:LEU:C    | 2.37                     | 0.49              |
| 1:A:45:THR:CB    | 1:A:111:LYS:HZ2  | 2.26                     | 0.48              |
| 1:B:55:VAL:O     | 1:B:56:TYR:C     | 2.56                     | 0.48              |
| 1:B:79:ASP:C     | 1:B:81:ARG:N     | 2.69                     | 0.48              |
| 1:B:226:ALA:O    | 1:B:227:ALA:C    | 2.56                     | 0.48              |
| 1:B:317:ARG:H    | 1:B:317:ARG:NE   | 2.05                     | 0.48              |
| 1:C:74:TYR:HD1   | 1:C:74:TYR:O     | 1.96                     | 0.48              |
| 1:C:342:ALA:HB1  | 1:C:344:LEU:HD23 | 1.95                     | 0.48              |
| 1:D:105:PHE:C    | 1:D:107:LEU:N    | 2.71                     | 0.48              |
| 1:D:218:ILE:C    | 1:D:220:SER:H    | 2.21                     | 0.48              |
| 1:A:358:ASP:CG   | 1:A:359:ASP:N    | 2.69                     | 0.48              |
| 1:B:48:LEU:HD12  | 1:B:48:LEU:O     | 2.13                     | 0.48              |
| 1:E:105:PHE:C    | 1:E:107:LEU:N    | 2.69                     | 0.48              |
| 1:A:54:TYR:CD1   | 1:A:122:SER:HB3  | 2.48                     | 0.48              |
| 1:A:203:HIS:O    | 1:A:206:LYS:HG3  | 2.14                     | 0.48              |
| 1:A:286:LYS:HD2  | 2:R:29:G:OP1     | 2.14                     | 0.48              |
| 1:A:326:SER:OG   | 1:B:343:ASP:HB2  | 2.14                     | 0.48              |
| 1:B:122:SER:O    | 1:B:123:ASP:CB   | 2.55                     | 0.48              |
| 1:C:249:ILE:CD1  | 1:C:258:MET:HG3  | 2.43                     | 0.48              |
| 1:D:164:CYS:CA   | 1:D:168:ASN:HB3  | 2.42                     | 0.48              |
| 1:A:175:VAL:HG13 | 1:A:181:ILE:HG23 | 1.96                     | 0.48              |
| 1:B:165:LYS:O    | 1:B:166:MET:HB2  | 2.11                     | 0.48              |
| 1:B:376:VAL:HG13 | 1:C:354:LYS:HB2  | 1.96                     | 0.48              |
| 1:C:29:ALA:C     | 1:C:31:TYR:N     | 2.71                     | 0.48              |
| 1:C:54:TYR:CD1   | 1:C:122:SER:HB3  | 2.48                     | 0.48              |
| 1:C:218:ILE:C    | 1:C:220:SER:H    | 2.21                     | 0.48              |
| 1:D:136:LEU:HB2  | 1:D:213:PHE:CD2  | 2.47                     | 0.48              |
| 1:D:397:ALA:O    | 1:D:401:VAL:HG22 | 2.13                     | 0.48              |
| 1:E:74:TYR:HD1   | 1:E:74:TYR:O     | 1.97                     | 0.48              |
| 1:E:323:GLU:O    | 1:E:327:LEU:HB2  | 2.14                     | 0.48              |
| 1:B:56:TYR:CE1   | 1:B:126:ARG:NE   | 2.82                     | 0.48              |
| 1:B:312:ARG:HG3  | 2:R:23:G:C5      | 2.49                     | 0.48              |
| 1:D:213:PHE:O    | 1:D:215:TYR:N    | 2.46                     | 0.48              |
| 1:E:6:LYS:HZ3    | 1:E:11:ASN:HD21  | 1.62                     | 0.48              |
| 1:A:15:VAL:O     | 1:A:17:LYS:HG2   | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:72:TYR:CE1   | 1:A:134:LEU:HB3  | 2.48                     | 0.48              |
| 1:A:226:ALA:HB3  | 1:A:291:SER:HB3  | 1.96                     | 0.48              |
| 1:A:269:ASP:HB3  | 1:E:17:LYS:HB2   | 1.95                     | 0.48              |
| 1:B:129:ALA:HB1  | 1:B:133:TRP:HE1  | 1.78                     | 0.48              |
| 1:C:317:ARG:NH1  | 1:C:317:ARG:N    | 2.60                     | 0.48              |
| 1:C:344:LEU:O    | 1:C:345:ALA:CB   | 2.60                     | 0.48              |
| 1:D:227:ALA:C    | 1:D:229:ALA:N    | 2.71                     | 0.48              |
| 1:E:189:SER:O    | 1:E:193:LYS:HG3  | 2.14                     | 0.48              |
| 1:B:107:LEU:C    | 1:B:108:VAL:HG23 | 2.38                     | 0.48              |
| 1:A:117:LEU:N    | 1:A:117:LEU:CD2  | 2.77                     | 0.48              |
| 1:B:172:GLU:H    | 1:B:173:PRO:CD   | 2.26                     | 0.48              |
| 1:B:189:SER:O    | 1:B:193:LYS:HG3  | 2.14                     | 0.48              |
| 1:C:97:LYS:HB2   | 1:C:97:LYS:NZ    | 2.29                     | 0.48              |
| 1:C:179:ARG:HA   | 1:C:183:ASP:CG   | 2.38                     | 0.48              |
| 1:D:243:GLU:O    | 1:D:247:THR:HG23 | 2.14                     | 0.48              |
| 1:A:133:TRP:CB   | 1:A:167:ILE:HG21 | 2.43                     | 0.48              |
| 1:D:267:GLU:OE1  | 1:D:273:SER:HB2  | 2.14                     | 0.48              |
| 1:E:233:HIS:CD2  | 1:E:312:ARG:HD2  | 2.48                     | 0.48              |
| 1:E:253:GLU:CD   | 1:E:253:GLU:H    | 2.20                     | 0.48              |
| 1:E:358:ASP:CG   | 1:E:359:ASP:N    | 2.71                     | 0.48              |
| 1:A:25:VAL:HG11  | 1:A:288:PRO:HA   | 1.96                     | 0.48              |
| 1:A:247:THR:HA   | 1:B:348:PHE:HB2  | 1.95                     | 0.48              |
| 1:C:226:ALA:O    | 1:C:227:ALA:C    | 2.57                     | 0.48              |
| 1:E:162:ASN:HA   | 1:E:165:LYS:NZ   | 2.28                     | 0.48              |
| 1:A:383:GLU:HG3  | 1:B:354:LYS:HE2  | 1.96                     | 0.47              |
| 1:B:182:PHE:HB2  | 1:B:185:TRP:CE2  | 2.48                     | 0.47              |
| 1:C:175:VAL:HG13 | 1:C:181:ILE:HG23 | 1.96                     | 0.47              |
| 1:D:143:ARG:HH22 | 2:R:8:G:C3'      | 2.18                     | 0.47              |
| 1:E:192:THR:HA   | 1:E:195:VAL:CG1  | 2.44                     | 0.47              |
| 1:A:136:LEU:HD23 | 1:A:136:LEU:C    | 2.39                     | 0.47              |
| 1:D:107:LEU:C    | 1:D:108:VAL:HG23 | 2.39                     | 0.47              |
| 1:E:117:LEU:N    | 1:E:117:LEU:CD2  | 2.77                     | 0.47              |
| 1:B:136:LEU:HD23 | 1:B:136:LEU:C    | 2.39                     | 0.47              |
| 1:B:222:PHE:O    | 1:B:225:CYS:HB2  | 2.14                     | 0.47              |
| 1:D:177:GLU:HG2  | 1:D:181:ILE:HD11 | 1.96                     | 0.47              |
| 1:B:126:ARG:HH11 | 1:B:127:THR:HG22 | 1.78                     | 0.47              |
| 1:D:97:LYS:HB2   | 1:D:97:LYS:NZ    | 2.30                     | 0.47              |
| 1:D:152:TYR:CE1  | 1:D:153:ARG:NH1  | 2.82                     | 0.47              |
| 1:D:261:MET:HE2  | 1:D:294:ASN:CG   | 2.39                     | 0.47              |
| 1:A:79:ASP:HB2   | 1:A:81:ARG:NE    | 2.29                     | 0.47              |
| 1:B:213:PHE:C    | 1:B:215:TYR:H    | 2.23                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:213:PHE:C    | 1:E:215:TYR:H    | 2.23                     | 0.47              |
| 1:B:57:GLN:C     | 1:B:59:LEU:H     | 2.23                     | 0.47              |
| 1:B:153:ARG:HH21 | 1:B:156:LEU:CD1  | 2.28                     | 0.47              |
| 1:D:258:MET:HE1  | 1:D:262:MET:HE3  | 1.96                     | 0.47              |
| 1:A:317:ARG:CZ   | 2:R:32:G:OP2     | 2.63                     | 0.47              |
| 1:B:343:ASP:C    | 1:B:344:LEU:HD22 | 2.40                     | 0.47              |
| 1:C:143:ARG:HH22 | 2:R:17:G:H2'     | 1.77                     | 0.47              |
| 1:D:129:ALA:HB1  | 1:D:133:TRP:HE1  | 1.79                     | 0.47              |
| 1:D:286:LYS:HE3  | 2:R:3:G:OP2      | 2.14                     | 0.47              |
| 1:E:79:ASP:HB2   | 1:E:81:ARG:NE    | 2.30                     | 0.47              |
| 1:E:227:ALA:O    | 1:E:229:ALA:N    | 2.48                     | 0.47              |
| 1:B:25:VAL:HG11  | 1:B:288:PRO:HA   | 1.97                     | 0.47              |
| 1:C:38:ILE:HD12  | 1:C:38:ILE:O     | 2.14                     | 0.47              |
| 1:E:160:LEU:HD12 | 1:E:160:LEU:O    | 2.15                     | 0.47              |
| 1:A:179:ARG:HA   | 1:A:183:ASP:CG   | 2.39                     | 0.47              |
| 1:A:267:GLU:OE1  | 1:A:273:SER:HB2  | 2.15                     | 0.47              |
| 1:A:359:ASP:HB3  | 1:A:361:THR:OG1  | 2.15                     | 0.47              |
| 1:B:143:ARG:HH22 | 2:R:26:G:H2'     | 1.79                     | 0.47              |
| 1:C:81:ARG:HD2   | 1:C:208:HIS:CE1  | 2.49                     | 0.47              |
| 1:C:344:LEU:N    | 1:C:344:LEU:CD2  | 2.77                     | 0.47              |
| 1:E:295:PRO:HB2  | 1:E:322:ILE:CG2  | 2.45                     | 0.47              |
| 2:R:9:G:H2'      | 2:R:10:G:O4'     | 2.15                     | 0.47              |
| 1:A:55:VAL:O     | 1:A:56:TYR:C     | 2.58                     | 0.47              |
| 1:B:107:LEU:HD23 | 1:B:274:TYR:HE2  | 1.79                     | 0.47              |
| 1:C:126:ARG:HH11 | 1:C:127:THR:HG22 | 1.80                     | 0.47              |
| 2:R:28:G:C8      | 2:R:29:G:N7      | 2.83                     | 0.47              |
| 1:A:31:TYR:C     | 1:A:33:ARG:H     | 2.23                     | 0.46              |
| 1:A:249:ILE:HD11 | 1:A:258:MET:HG3  | 1.98                     | 0.46              |
| 1:B:141:LEU:HD12 | 1:B:185:TRP:CH2  | 2.49                     | 0.46              |
| 1:B:179:ARG:HA   | 1:B:183:ASP:CG   | 2.39                     | 0.46              |
| 1:C:136:LEU:HD23 | 1:C:136:LEU:C    | 2.40                     | 0.46              |
| 1:C:152:TYR:HE1  | 1:C:153:ARG:NH1  | 2.13                     | 0.46              |
| 1:C:170:GLN:HG2  | 1:C:171:PHE:H    | 1.80                     | 0.46              |
| 1:D:31:TYR:CD1   | 1:D:32:PHE:N     | 2.83                     | 0.46              |
| 1:D:107:LEU:HD23 | 1:D:274:TYR:HE2  | 1.80                     | 0.46              |
| 1:E:249:ILE:CD1  | 1:E:258:MET:HG3  | 2.45                     | 0.46              |
| 1:E:302:GLN:HG2  | 1:E:316:ALA:CB   | 2.45                     | 0.46              |
| 1:A:215:TYR:HD1  | 2:R:36:G:C8      | 2.33                     | 0.46              |
| 1:B:18:LEU:HD12  | 1:C:232:GLY:HA3  | 1.94                     | 0.46              |
| 1:B:130:ASP:C    | 1:B:132:LYS:N    | 2.69                     | 0.46              |
| 1:E:25:VAL:HG11  | 1:E:288:PRO:HA   | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:126:ARG:HD3  | 1:E:127:THR:H    | 1.79                     | 0.46              |
| 1:E:136:LEU:HD23 | 1:E:136:LEU:C    | 2.41                     | 0.46              |
| 1:E:136:LEU:HB2  | 1:E:213:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:89:SER:O     | 1:A:90:SER:HB2   | 2.15                     | 0.46              |
| 1:A:179:ARG:HA   | 1:A:183:ASP:HB2  | 1.97                     | 0.46              |
| 1:B:175:VAL:CG2  | 1:B:176:PRO:O    | 2.63                     | 0.46              |
| 1:E:57:GLN:C     | 1:E:59:LEU:N     | 2.73                     | 0.46              |
| 1:E:226:ALA:HB3  | 1:E:291:SER:HB3  | 1.95                     | 0.46              |
| 1:E:233:HIS:HB2  | 1:E:312:ARG:NH1  | 2.30                     | 0.46              |
| 1:A:28:PRO:HD2   | 1:A:266:GLN:NE2  | 2.31                     | 0.46              |
| 1:B:152:TYR:CE1  | 1:B:177:GLU:HG3  | 2.49                     | 0.46              |
| 1:B:160:LEU:HD12 | 1:B:160:LEU:O    | 2.15                     | 0.46              |
| 1:C:189:SER:O    | 1:C:193:LYS:HG3  | 2.16                     | 0.46              |
| 1:C:218:ILE:HG23 | 1:C:219:VAL:N    | 2.30                     | 0.46              |
| 1:C:249:ILE:HD11 | 1:C:258:MET:HG3  | 1.98                     | 0.46              |
| 1:D:200:MET:HB2  | 1:D:277:TYR:CE2  | 2.50                     | 0.46              |
| 1:E:111:LYS:HE2  | 1:E:111:LYS:HB3  | 1.68                     | 0.46              |
| 1:E:317:ARG:CG   | 2:R:40:G:C5      | 2.99                     | 0.46              |
| 2:R:5:G:C2       | 2:R:7:G:H1'      | 2.51                     | 0.46              |
| 1:B:179:ARG:HA   | 1:B:183:ASP:HB2  | 1.97                     | 0.46              |
| 1:B:203:HIS:O    | 1:B:206:LYS:HG3  | 2.16                     | 0.46              |
| 1:B:227:ALA:C    | 1:B:229:ALA:N    | 2.74                     | 0.46              |
| 1:C:25:VAL:HG11  | 1:C:288:PRO:HA   | 1.98                     | 0.46              |
| 1:D:218:ILE:HG23 | 1:D:219:VAL:N    | 2.30                     | 0.46              |
| 1:E:81:ARG:HB3   | 1:E:208:HIS:HE2  | 1.80                     | 0.46              |
| 1:B:43:ASN:HA    | 1:B:112:ALA:N    | 2.12                     | 0.46              |
| 1:B:89:SER:O     | 1:B:90:SER:HB2   | 2.15                     | 0.46              |
| 1:B:249:ILE:CD1  | 1:B:258:MET:HG3  | 2.45                     | 0.46              |
| 1:B:286:LYS:HE2  | 1:B:293:LYS:HD3  | 1.96                     | 0.46              |
| 1:C:227:ALA:C    | 1:C:229:ALA:N    | 2.74                     | 0.46              |
| 1:C:228:LEU:O    | 1:C:228:LEU:HD13 | 2.16                     | 0.46              |
| 1:E:104:ILE:HD13 | 1:E:198:VAL:HG22 | 1.98                     | 0.46              |
| 1:E:107:LEU:C    | 1:E:108:VAL:HG23 | 2.40                     | 0.46              |
| 1:A:169:GLU:HB3  | 1:A:170:GLN:NE2  | 2.31                     | 0.46              |
| 2:R:11:G:H2'     | 2:R:12:G:O4'     | 2.15                     | 0.46              |
| 1:A:53:GLY:O     | 1:A:54:TYR:C     | 2.59                     | 0.46              |
| 1:A:103:GLY:N    | 1:A:106:ASP:OD2  | 2.40                     | 0.46              |
| 1:A:170:GLN:CD   | 1:A:170:GLN:N    | 2.74                     | 0.46              |
| 1:B:136:LEU:HB2  | 1:B:213:PHE:CD2  | 2.50                     | 0.46              |
| 1:B:352:ASP:OD1  | 1:B:352:ASP:O    | 2.34                     | 0.46              |
| 1:C:15:VAL:O     | 1:C:17:LYS:HG2   | 2.16                     | 0.46              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:106:ASP:C   | 1:E:107:LEU:HD12 | 2.41                     | 0.46              |
| 1:A:46:LYS:HA   | 1:A:46:LYS:HD3   | 1.57                     | 0.46              |
| 1:A:72:TYR:HE1  | 1:A:134:LEU:HD12 | 1.75                     | 0.46              |
| 1:A:133:TRP:HB3 | 1:A:167:ILE:CG1  | 2.45                     | 0.46              |
| 1:A:133:TRP:HB3 | 1:A:167:ILE:HG12 | 1.98                     | 0.46              |
| 1:A:134:LEU:HA  | 1:A:134:LEU:HD22 | 1.80                     | 0.46              |
| 1:A:152:TYR:CD1 | 1:A:177:GLU:HG3  | 2.51                     | 0.46              |
| 1:A:228:LEU:O   | 1:A:228:LEU:HD13 | 2.15                     | 0.46              |
| 1:B:38:ILE:HD11 | 1:B:107:LEU:O    | 2.15                     | 0.46              |
| 1:B:141:LEU:HB3 | 1:B:182:PHE:CD1  | 2.51                     | 0.46              |
| 1:B:257:GLU:O   | 1:B:261:MET:HG3  | 2.16                     | 0.46              |
| 1:B:302:GLN:HG2 | 1:B:316:ALA:CB   | 2.46                     | 0.46              |
| 1:C:356:THR:CG2 | 1:C:357:PRO:HD3  | 2.41                     | 0.46              |
| 1:D:153:ARG:HE  | 1:D:156:LEU:HD13 | 1.80                     | 0.46              |
| 2:R:34:G:H4'    | 2:R:34:G:OP2     | 2.15                     | 0.46              |
| 1:B:408:ARG:HD3 | 2:R:24:G:N7      | 2.31                     | 0.46              |
| 1:C:46:LYS:HD3  | 1:C:46:LYS:HA    | 1.49                     | 0.46              |
| 1:C:160:LEU:O   | 1:C:160:LEU:HD12 | 2.16                     | 0.46              |
| 1:C:317:ARG:NH2 | 2:R:13:G:O2'     | 2.48                     | 0.46              |
| 1:D:46:LYS:HA   | 1:D:46:LYS:HD3   | 1.62                     | 0.46              |
| 1:D:56:TYR:CE1  | 1:D:126:ARG:NH2  | 2.84                     | 0.46              |
| 1:E:218:ILE:C   | 1:E:220:SER:N    | 2.73                     | 0.46              |
| 1:A:6:LYS:NZ    | 1:A:11:ASN:HD21  | 2.14                     | 0.45              |
| 1:A:133:TRP:CB  | 1:A:167:ILE:HD13 | 2.46                     | 0.45              |
| 1:B:323:GLU:O   | 1:B:327:LEU:HB2  | 2.15                     | 0.45              |
| 1:B:380:GLY:HA2 | 1:C:354:LYS:HZ2  | 1.75                     | 0.45              |
| 1:D:194:ILE:O   | 1:D:198:VAL:HG23 | 2.16                     | 0.45              |
| 1:D:249:ILE:CD1 | 1:D:258:MET:HG3  | 2.47                     | 0.45              |
| 1:E:243:GLU:O   | 1:E:247:THR:HG23 | 2.16                     | 0.45              |
| 1:A:20:ALA:O    | 1:A:21:ASN:HB2   | 2.17                     | 0.45              |
| 1:B:53:GLY:O    | 1:B:54:TYR:C     | 2.59                     | 0.45              |
| 1:B:79:ASP:HB2  | 1:B:81:ARG:NE    | 2.31                     | 0.45              |
| 1:D:79:ASP:O    | 1:D:79:ASP:OD1   | 2.33                     | 0.45              |
| 1:E:409:GLU:O   | 1:E:410:LYS:HB2  | 2.15                     | 0.45              |
| 1:B:343:ASP:H   | 1:B:344:LEU:CD2  | 2.29                     | 0.45              |
| 1:C:56:TYR:CE1  | 1:C:126:ARG:NE   | 2.84                     | 0.45              |
| 1:C:81:ARG:HB3  | 1:C:208:HIS:HE2  | 1.80                     | 0.45              |
| 1:C:130:ASP:C   | 1:C:132:LYS:H    | 2.24                     | 0.45              |
| 1:C:179:ARG:HA  | 1:C:183:ASP:HB2  | 1.97                     | 0.45              |
| 1:D:56:TYR:HE1  | 1:D:126:ARG:NH2  | 2.14                     | 0.45              |
| 1:D:365:THR:CG2 | 1:D:366:THR:H    | 2.26                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:129:ALA:O    | 1:A:133:TRP:NE1  | 2.50                     | 0.45              |
| 1:B:218:ILE:O    | 1:B:220:SER:N    | 2.49                     | 0.45              |
| 1:C:31:TYR:HD1   | 1:C:32:PHE:N     | 2.15                     | 0.45              |
| 1:D:152:TYR:HE1  | 1:D:153:ARG:NH1  | 2.12                     | 0.45              |
| 1:D:299:PHE:CZ   | 1:D:328:THR:HG22 | 2.51                     | 0.45              |
| 1:E:38:ILE:HD11  | 1:E:107:LEU:O    | 2.17                     | 0.45              |
| 1:E:228:LEU:O    | 1:E:228:LEU:HD13 | 2.17                     | 0.45              |
| 1:A:299:PHE:CZ   | 1:A:328:THR:HG22 | 2.52                     | 0.45              |
| 1:B:218:ILE:HG23 | 1:B:219:VAL:N    | 2.32                     | 0.45              |
| 1:C:152:TYR:CE1  | 1:C:153:ARG:NH1  | 2.84                     | 0.45              |
| 1:C:273:SER:OG   | 1:C:274:TYR:N    | 2.47                     | 0.45              |
| 1:D:182:PHE:HB2  | 1:D:185:TRP:CE2  | 2.52                     | 0.45              |
| 1:E:79:ASP:O     | 1:E:79:ASP:OD1   | 2.35                     | 0.45              |
| 1:E:172:GLU:CB   | 1:E:173:PRO:CD   | 2.83                     | 0.45              |
| 1:E:224:ASP:CG   | 2:R:39:G:H4'     | 2.42                     | 0.45              |
| 2:R:6:G:C8       | 2:R:6:G:C3'      | 2.99                     | 0.45              |
| 1:A:218:ILE:HG23 | 1:A:219:VAL:N    | 2.32                     | 0.45              |
| 1:A:222:PHE:O    | 1:A:225:CYS:HB2  | 2.17                     | 0.45              |
| 1:B:72:TYR:HE1   | 1:B:134:LEU:HD12 | 1.76                     | 0.45              |
| 1:C:38:ILE:CD1   | 1:C:107:LEU:O    | 2.65                     | 0.45              |
| 1:C:295:PRO:HB2  | 1:C:322:ILE:CG2  | 2.46                     | 0.45              |
| 1:D:127:THR:OG1  | 1:D:128:SER:N    | 2.50                     | 0.45              |
| 1:E:31:TYR:HD1   | 1:E:32:PHE:N     | 2.15                     | 0.45              |
| 1:E:46:LYS:HA    | 1:E:46:LYS:HD3   | 1.57                     | 0.45              |
| 1:E:152:TYR:CD1  | 1:E:177:GLU:HG3  | 2.52                     | 0.45              |
| 1:E:172:GLU:N    | 1:E:173:PRO:HD3  | 2.31                     | 0.45              |
| 1:E:177:GLU:HB3  | 1:E:178:GLY:H    | 1.54                     | 0.45              |
| 1:A:80:ILE:HA    | 1:A:103:GLY:CA   | 2.47                     | 0.45              |
| 1:C:57:GLN:C     | 1:C:59:LEU:N     | 2.70                     | 0.45              |
| 1:C:79:ASP:HB2   | 1:C:81:ARG:NE    | 2.32                     | 0.45              |
| 1:D:15:VAL:O     | 1:D:17:LYS:HG2   | 2.16                     | 0.45              |
| 1:D:48:LEU:HD12  | 1:D:48:LEU:O     | 2.16                     | 0.45              |
| 1:D:226:ALA:HB3  | 1:D:291:SER:HB3  | 1.98                     | 0.45              |
| 1:A:302:GLN:HG2  | 1:A:316:ALA:CB   | 2.47                     | 0.45              |
| 1:D:25:VAL:HG11  | 1:D:288:PRO:HA   | 1.99                     | 0.45              |
| 1:D:28:PRO:HD2   | 1:D:266:GLN:NE2  | 2.32                     | 0.45              |
| 1:D:107:LEU:HD23 | 1:D:274:TYR:OH   | 2.17                     | 0.45              |
| 1:A:160:LEU:HD12 | 1:A:160:LEU:O    | 2.17                     | 0.45              |
| 1:A:163:GLN:OE1  | 1:A:163:GLN:N    | 2.49                     | 0.45              |
| 1:A:246:THR:HG22 | 1:B:348:PHE:CD1  | 2.52                     | 0.45              |
| 1:B:176:PRO:O    | 1:B:181:ILE:HG13 | 2.11                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:55:VAL:HG23  | 1:C:56:TYR:N     | 2.30                     | 0.45              |
| 1:D:152:TYR:OH   | 1:D:153:ARG:NH1  | 2.50                     | 0.45              |
| 1:A:2:SER:O      | 1:B:243:GLU:HG3  | 2.17                     | 0.45              |
| 1:A:359:ASP:O    | 1:A:361:THR:N    | 2.45                     | 0.45              |
| 1:B:152:TYR:CE1  | 1:B:153:ARG:NH1  | 2.85                     | 0.45              |
| 1:C:298:HIS:CD2  | 1:C:317:ARG:NH1  | 2.85                     | 0.45              |
| 1:D:130:ASP:C    | 1:D:132:LYS:N    | 2.73                     | 0.45              |
| 1:D:153:ARG:HH21 | 1:D:156:LEU:CD1  | 2.29                     | 0.45              |
| 1:D:323:GLU:O    | 1:D:327:LEU:HB2  | 2.16                     | 0.45              |
| 1:E:6:LYS:HD2    | 1:E:11:ASN:OD1   | 2.17                     | 0.45              |
| 1:E:126:ARG:HH11 | 1:E:127:THR:HG22 | 1.82                     | 0.45              |
| 1:E:130:ASP:C    | 1:E:132:LYS:N    | 2.72                     | 0.45              |
| 1:E:213:PHE:O    | 1:E:215:TYR:N    | 2.50                     | 0.45              |
| 1:A:105:PHE:O    | 1:A:107:LEU:N    | 2.50                     | 0.44              |
| 1:A:246:THR:HG22 | 1:B:348:PHE:CG   | 2.52                     | 0.44              |
| 1:B:55:VAL:HG23  | 1:B:56:TYR:N     | 2.30                     | 0.44              |
| 1:B:133:TRP:HB3  | 1:B:167:ILE:CD1  | 2.47                     | 0.44              |
| 1:C:196:ALA:HB3  | 1:C:281:PHE:CE1  | 2.52                     | 0.44              |
| 1:C:299:PHE:CZ   | 1:C:328:THR:HG22 | 2.52                     | 0.44              |
| 1:D:179:ARG:HA   | 1:D:183:ASP:HB2  | 1.98                     | 0.44              |
| 1:E:390:THR:HB   | 1:E:391:PRO:CD   | 2.47                     | 0.44              |
| 1:A:170:GLN:HB2  | 1:A:171:PHE:H    | 1.66                     | 0.44              |
| 1:B:149:MET:HB3  | 2:R:24:G:N3      | 2.32                     | 0.44              |
| 1:B:175:VAL:HG22 | 1:B:176:PRO:O    | 2.16                     | 0.44              |
| 1:C:233:HIS:CD2  | 1:C:312:ARG:HD2  | 2.52                     | 0.44              |
| 1:D:163:GLN:N    | 1:D:163:GLN:OE1  | 2.48                     | 0.44              |
| 1:E:273:SER:OG   | 1:E:274:TYR:N    | 2.50                     | 0.44              |
| 1:E:385:GLN:CG   | 1:E:390:THR:HG22 | 2.47                     | 0.44              |
| 2:R:18:G:H2'     | 2:R:19:G:C8      | 2.53                     | 0.44              |
| 1:A:31:TYR:C     | 1:A:33:ARG:N     | 2.76                     | 0.44              |
| 1:B:40:LEU:HD11  | 1:B:194:ILE:HG12 | 2.00                     | 0.44              |
| 1:B:166:MET:C    | 1:B:167:ILE:CG1  | 2.89                     | 0.44              |
| 1:B:267:GLU:OE1  | 1:B:273:SER:HB2  | 2.17                     | 0.44              |
| 1:C:122:SER:O    | 1:C:123:ASP:CB   | 2.59                     | 0.44              |
| 1:C:163:GLN:O    | 1:C:167:ILE:HG12 | 2.18                     | 0.44              |
| 1:D:141:LEU:HB3  | 1:D:182:PHE:CD1  | 2.52                     | 0.44              |
| 1:D:231:PHE:HB2  | 1:D:297:PHE:CZ   | 2.53                     | 0.44              |
| 1:D:299:PHE:HZ   | 1:D:415:TYR:CE1  | 2.36                     | 0.44              |
| 1:E:31:TYR:C     | 1:E:33:ARG:H     | 2.25                     | 0.44              |
| 1:E:84:LEU:HB3   | 1:E:86:LYS:O     | 2.16                     | 0.44              |
| 1:B:31:TYR:C     | 1:B:33:ARG:H     | 2.26                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:236:LYS:HD3  | 1:B:236:LYS:HA   | 1.84                     | 0.44              |
| 1:B:398:LYS:HG2  | 1:B:402:MET:HE3  | 1.98                     | 0.44              |
| 1:C:213:PHE:C    | 1:C:215:TYR:H    | 2.25                     | 0.44              |
| 1:D:342:ALA:CB   | 1:D:344:LEU:HD23 | 2.48                     | 0.44              |
| 1:A:57:GLN:C     | 1:A:59:LEU:H     | 2.25                     | 0.44              |
| 1:A:73:LEU:O     | 1:A:74:TYR:C     | 2.60                     | 0.44              |
| 1:A:105:PHE:C    | 1:A:107:LEU:N    | 2.64                     | 0.44              |
| 1:A:127:THR:OG1  | 1:A:128:SER:N    | 2.50                     | 0.44              |
| 1:A:215:TYR:C    | 1:A:215:TYR:CD2  | 2.94                     | 0.44              |
| 1:A:236:LYS:HD3  | 1:A:236:LYS:HA   | 1.84                     | 0.44              |
| 1:C:53:GLY:O     | 1:C:54:TYR:C     | 2.59                     | 0.44              |
| 1:C:104:ILE:HD13 | 1:C:198:VAL:HG22 | 2.00                     | 0.44              |
| 1:D:53:GLY:O     | 1:D:54:TYR:C     | 2.59                     | 0.44              |
| 1:A:79:ASP:O     | 1:A:79:ASP:OD1   | 2.36                     | 0.44              |
| 1:A:126:ARG:HH11 | 1:A:127:THR:HG22 | 1.82                     | 0.44              |
| 1:A:215:TYR:HD1  | 2:R:36:G:H8      | 1.66                     | 0.44              |
| 1:B:56:TYR:HE1   | 1:B:126:ARG:NH2  | 2.16                     | 0.44              |
| 1:B:299:PHE:CZ   | 1:B:328:THR:HG22 | 2.53                     | 0.44              |
| 1:C:241:SER:OG   | 1:C:243:GLU:HG2  | 2.16                     | 0.44              |
| 1:D:55:VAL:HG23  | 1:D:56:TYR:N     | 2.32                     | 0.44              |
| 1:D:175:VAL:HG13 | 1:D:181:ILE:HG23 | 1.99                     | 0.44              |
| 1:A:81:ARG:HB3   | 1:A:208:HIS:HE2  | 1.82                     | 0.44              |
| 1:A:164:CYS:HA   | 1:A:168:ASN:HA   | 1.98                     | 0.44              |
| 1:A:243:GLU:HG3  | 1:E:2:SER:O      | 2.18                     | 0.44              |
| 1:A:356:THR:CG2  | 1:A:357:PRO:HD3  | 2.42                     | 0.44              |
| 1:B:56:TYR:CE1   | 1:B:126:ARG:NH2  | 2.86                     | 0.44              |
| 1:B:81:ARG:HB3   | 1:B:208:HIS:HE2  | 1.82                     | 0.44              |
| 1:B:163:GLN:OE1  | 1:B:163:GLN:N    | 2.50                     | 0.44              |
| 1:C:56:TYR:CE1   | 1:C:126:ARG:NH2  | 2.85                     | 0.44              |
| 1:C:302:GLN:HG2  | 1:C:316:ALA:CB   | 2.47                     | 0.44              |
| 1:D:164:CYS:HB3  | 1:D:168:ASN:HB3  | 1.97                     | 0.44              |
| 1:D:302:GLN:HG2  | 1:D:316:ALA:CB   | 2.48                     | 0.44              |
| 1:E:57:GLN:NE2   | 1:E:60:LYS:HZ2   | 1.82                     | 0.44              |
| 1:E:247:THR:O    | 1:E:375:VAL:HG11 | 2.18                     | 0.44              |
| 1:A:243:GLU:HG2  | 1:A:243:GLU:H    | 1.47                     | 0.44              |
| 1:C:20:ALA:O     | 1:C:21:ASN:HB2   | 2.18                     | 0.44              |
| 1:C:233:HIS:HB2  | 1:C:312:ARG:HH11 | 1.82                     | 0.44              |
| 1:C:236:LYS:HD3  | 1:C:236:LYS:HA   | 1.83                     | 0.44              |
| 1:D:57:GLN:C     | 1:D:59:LEU:H     | 2.26                     | 0.44              |
| 1:D:352:ASP:OD1  | 1:D:352:ASP:O    | 2.36                     | 0.44              |
| 1:D:390:THR:HB   | 1:D:391:PRO:CD   | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:241:SER:OG   | 1:E:243:GLU:HG2  | 2.16                     | 0.44              |
| 1:E:243:GLU:H    | 1:E:243:GLU:HG2  | 1.50                     | 0.44              |
| 1:B:152:TYR:HE1  | 1:B:153:ARG:NH1  | 2.15                     | 0.44              |
| 1:C:134:LEU:N    | 1:C:135:PRO:CD   | 2.80                     | 0.44              |
| 1:D:106:ASP:C    | 1:D:107:LEU:HD12 | 2.43                     | 0.44              |
| 1:A:153:ARG:HH21 | 1:A:156:LEU:CD1  | 2.31                     | 0.43              |
| 1:B:171:PHE:CG   | 1:B:172:GLU:N    | 2.85                     | 0.43              |
| 1:C:103:GLY:N    | 1:C:106:ASP:OD2  | 2.39                     | 0.43              |
| 1:E:153:ARG:HE   | 1:E:156:LEU:HD13 | 1.83                     | 0.43              |
| 1:C:224:ASP:HB2  | 1:C:279:ILE:HG13 | 2.00                     | 0.43              |
| 1:E:55:VAL:HG23  | 1:E:56:TYR:N     | 2.34                     | 0.43              |
| 1:E:122:SER:O    | 1:E:123:ASP:CB   | 2.57                     | 0.43              |
| 1:E:141:LEU:HD12 | 1:E:185:TRP:CH2  | 2.53                     | 0.43              |
| 1:E:179:ARG:HA   | 1:E:183:ASP:HB2  | 2.00                     | 0.43              |
| 1:B:15:VAL:O     | 1:B:17:LYS:HG2   | 2.18                     | 0.43              |
| 1:B:317:ARG:NE   | 2:R:22:G:O2'     | 2.51                     | 0.43              |
| 1:C:29:ALA:H     | 1:C:266:GLN:HE22 | 1.65                     | 0.43              |
| 1:C:177:GLU:HG2  | 1:C:181:ILE:CD1  | 2.48                     | 0.43              |
| 1:C:218:ILE:C    | 1:C:220:SER:N    | 2.75                     | 0.43              |
| 1:D:54:TYR:CD1   | 1:D:122:SER:CB   | 3.01                     | 0.43              |
| 1:D:55:VAL:O     | 1:D:56:TYR:C     | 2.61                     | 0.43              |
| 1:D:168:ASN:C    | 1:D:169:GLU:O    | 2.60                     | 0.43              |
| 1:E:222:PHE:O    | 1:E:225:CYS:HB2  | 2.18                     | 0.43              |
| 1:A:55:VAL:HG23  | 1:A:56:TYR:N     | 2.31                     | 0.43              |
| 1:A:152:TYR:HE1  | 1:A:153:ARG:NH1  | 2.16                     | 0.43              |
| 1:A:227:ALA:HA   | 1:A:230:THR:HG23 | 2.00                     | 0.43              |
| 1:B:249:ILE:HD11 | 1:B:258:MET:HG3  | 2.01                     | 0.43              |
| 1:C:164:CYS:HA   | 1:C:168:ASN:CA   | 2.48                     | 0.43              |
| 1:D:316:ALA:HA   | 1:D:317:ARG:HH22 | 1.82                     | 0.43              |
| 1:E:152:TYR:HE1  | 1:E:153:ARG:NH1  | 2.16                     | 0.43              |
| 1:E:175:VAL:HG13 | 1:E:181:ILE:HG23 | 2.00                     | 0.43              |
| 1:A:172:GLU:H    | 1:A:173:PRO:CD   | 2.30                     | 0.43              |
| 1:B:187:ASN:ND2  | 1:C:165:LYS:CD   | 2.82                     | 0.43              |
| 1:C:55:VAL:O     | 1:C:56:TYR:C     | 2.62                     | 0.43              |
| 1:C:267:GLU:OE1  | 1:C:273:SER:HB2  | 2.18                     | 0.43              |
| 1:D:218:ILE:C    | 1:D:220:SER:N    | 2.76                     | 0.43              |
| 1:D:364:LEU:HD22 | 1:D:368:ALA:CB   | 2.48                     | 0.43              |
| 1:E:55:VAL:O     | 1:E:56:TYR:C     | 2.62                     | 0.43              |
| 1:A:66:ILE:HD13  | 1:A:185:TRP:CG   | 2.53                     | 0.43              |
| 1:A:136:LEU:HB2  | 1:A:213:PHE:CD2  | 2.54                     | 0.43              |
| 1:B:316:ALA:O    | 1:B:411:THR:HA   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:369:PRO:HA   | 1:C:370:PRO:HD3  | 1.86                     | 0.43              |
| 1:E:80:ILE:HA    | 1:E:103:GLY:CA   | 2.48                     | 0.43              |
| 1:A:149:MET:HG3  | 2:R:33:G:O4'     | 2.18                     | 0.43              |
| 1:A:152:TYR:C    | 1:A:154:LYS:N    | 2.77                     | 0.43              |
| 1:B:19:PRO:HD3   | 1:C:228:LEU:CD2  | 2.49                     | 0.43              |
| 1:C:107:LEU:C    | 1:C:108:VAL:HG23 | 2.44                     | 0.43              |
| 1:E:56:TYR:CE1   | 1:E:126:ARG:NE   | 2.87                     | 0.43              |
| 1:E:127:THR:OG1  | 1:E:128:SER:N    | 2.51                     | 0.43              |
| 2:R:27:G:N3      | 2:R:27:G:H5'     | 2.34                     | 0.43              |
| 1:A:31:TYR:HD1   | 1:A:32:PHE:N     | 2.16                     | 0.43              |
| 1:B:213:PHE:O    | 1:B:215:TYR:N    | 2.52                     | 0.43              |
| 1:C:111:LYS:HB3  | 1:C:111:LYS:HE2  | 1.71                     | 0.43              |
| 1:D:294:ASN:N    | 1:D:295:PRO:HD3  | 2.34                     | 0.43              |
| 1:E:298:HIS:CD2  | 1:E:317:ARG:NH1  | 2.86                     | 0.43              |
| 1:E:299:PHE:CZ   | 1:E:328:THR:HG22 | 2.54                     | 0.43              |
| 2:R:6:G:O5'      | 2:R:6:G:H8       | 2.02                     | 0.43              |
| 1:A:111:LYS:HB3  | 1:A:111:LYS:HE2  | 1.73                     | 0.43              |
| 1:A:213:PHE:C    | 1:A:215:TYR:H    | 2.27                     | 0.43              |
| 1:A:218:ILE:O    | 1:A:220:SER:N    | 2.51                     | 0.43              |
| 1:C:56:TYR:HE1   | 1:C:126:ARG:NH2  | 2.17                     | 0.43              |
| 1:C:200:MET:HE1  | 1:C:274:TYR:CD2  | 2.53                     | 0.43              |
| 1:C:253:GLU:CD   | 1:C:253:GLU:H    | 2.24                     | 0.43              |
| 1:D:111:LYS:HE2  | 1:D:111:LYS:HB3  | 1.67                     | 0.43              |
| 1:D:241:SER:OG   | 1:D:243:GLU:HG2  | 2.17                     | 0.43              |
| 1:A:56:TYR:CE1   | 1:A:126:ARG:NE   | 2.86                     | 0.43              |
| 1:A:133:TRP:CD1  | 1:A:167:ILE:HG23 | 2.54                     | 0.43              |
| 1:C:323:GLU:O    | 1:C:327:LEU:HB2  | 2.18                     | 0.43              |
| 1:C:342:ALA:HB3  | 1:C:344:LEU:HD23 | 2.01                     | 0.43              |
| 1:D:81:ARG:HB3   | 1:D:208:HIS:HE2  | 1.83                     | 0.43              |
| 1:D:88:TRP:CE2   | 1:D:204:MET:HE2  | 2.54                     | 0.43              |
| 2:R:17:G:HO2'    | 2:R:18:G:P       | 2.42                     | 0.43              |
| 1:A:323:GLU:O    | 1:A:327:LEU:HB2  | 2.19                     | 0.42              |
| 1:B:175:VAL:HG13 | 1:B:181:ILE:HG23 | 2.01                     | 0.42              |
| 1:C:57:GLN:C     | 1:C:59:LEU:H     | 2.26                     | 0.42              |
| 1:D:52:ARG:O     | 1:D:55:VAL:HG23  | 2.19                     | 0.42              |
| 1:E:152:TYR:C    | 1:E:154:LYS:N    | 2.77                     | 0.42              |
| 1:A:385:GLN:CG   | 1:A:390:THR:HG22 | 2.46                     | 0.42              |
| 1:B:31:TYR:HD1   | 1:B:32:PHE:N     | 2.16                     | 0.42              |
| 1:B:241:SER:OG   | 1:B:243:GLU:HG2  | 2.19                     | 0.42              |
| 1:B:307:LEU:HD12 | 1:B:307:LEU:HA   | 1.85                     | 0.42              |
| 1:C:58:GLY:C     | 1:C:64:VAL:HB    | 2.44                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:136:LEU:HB2  | 1:C:213:PHE:CD2  | 2.54                     | 0.42              |
| 1:D:103:GLY:O    | 1:D:104:ILE:C    | 2.62                     | 0.42              |
| 1:E:28:PRO:HD2   | 1:E:266:GLN:NE2  | 2.34                     | 0.42              |
| 2:R:18:G:H3'     | 2:R:19:G:C8      | 2.54                     | 0.42              |
| 2:R:27:G:H3'     | 2:R:28:G:C8      | 2.53                     | 0.42              |
| 1:A:171:PHE:O    | 1:A:172:GLU:OE2  | 2.36                     | 0.42              |
| 1:A:352:ASP:OD1  | 1:A:352:ASP:O    | 2.37                     | 0.42              |
| 1:B:117:LEU:N    | 1:B:117:LEU:CD2  | 2.81                     | 0.42              |
| 1:C:106:ASP:C    | 1:C:107:LEU:HD12 | 2.44                     | 0.42              |
| 1:C:285:SER:HB3  | 1:D:207:LYS:NZ   | 2.35                     | 0.42              |
| 1:D:6:LYS:NZ     | 1:D:11:ASN:HD21  | 2.17                     | 0.42              |
| 1:D:177:GLU:HG2  | 1:D:181:ILE:CD1  | 2.49                     | 0.42              |
| 1:D:195:VAL:HG23 | 1:D:217:THR:OG1  | 2.19                     | 0.42              |
| 1:D:254:VAL:HG13 | 1:D:297:PHE:HA   | 2.01                     | 0.42              |
| 1:A:58:GLY:C     | 1:A:64:VAL:HB    | 2.44                     | 0.42              |
| 1:A:134:LEU:N    | 1:A:135:PRO:CD   | 2.81                     | 0.42              |
| 1:A:227:ALA:C    | 1:A:229:ALA:N    | 2.73                     | 0.42              |
| 1:A:270:LYS:HE2  | 1:A:270:LYS:HB3  | 1.83                     | 0.42              |
| 1:A:345:ALA:O    | 1:A:346:GLN:C    | 2.61                     | 0.42              |
| 1:B:57:GLN:O     | 1:B:59:LEU:N     | 2.52                     | 0.42              |
| 1:C:31:TYR:C     | 1:C:33:ARG:H     | 2.27                     | 0.42              |
| 1:C:107:LEU:HD23 | 1:C:274:TYR:OH   | 2.19                     | 0.42              |
| 1:C:149:MET:HG3  | 2:R:15:G:C8      | 2.55                     | 0.42              |
| 1:C:285:SER:OG   | 1:D:207:LYS:HE2  | 2.19                     | 0.42              |
| 1:D:38:ILE:HA    | 1:D:39:PRO:HD2   | 1.87                     | 0.42              |
| 1:D:344:LEU:O    | 1:D:345:ALA:CB   | 2.68                     | 0.42              |
| 1:E:205:PHE:C    | 1:E:207:LYS:H    | 2.27                     | 0.42              |
| 1:B:247:THR:HA   | 1:C:348:PHE:HB2  | 2.01                     | 0.42              |
| 1:D:38:ILE:HD11  | 1:D:107:LEU:O    | 2.19                     | 0.42              |
| 1:D:213:PHE:C    | 1:D:215:TYR:N    | 2.77                     | 0.42              |
| 1:E:38:ILE:HD12  | 1:E:38:ILE:O     | 2.20                     | 0.42              |
| 1:E:316:ALA:HB1  | 1:E:317:ARG:NH1  | 2.33                     | 0.42              |
| 1:A:152:TYR:CE1  | 1:A:153:ARG:NH1  | 2.87                     | 0.42              |
| 1:A:153:ARG:HE   | 1:A:156:LEU:HD13 | 1.84                     | 0.42              |
| 1:B:17:LYS:HG3   | 1:C:268:ILE:HD11 | 2.02                     | 0.42              |
| 1:B:171:PHE:CD1  | 1:B:172:GLU:N    | 2.87                     | 0.42              |
| 1:B:356:THR:CG2  | 1:B:357:PRO:HD3  | 2.44                     | 0.42              |
| 2:R:30:G:H2'     | 2:R:31:G:C1'     | 2.49                     | 0.42              |
| 1:A:66:ILE:HA    | 1:A:69:VAL:HG22  | 2.02                     | 0.42              |
| 1:A:84:LEU:HB3   | 1:A:86:LYS:O     | 2.19                     | 0.42              |
| 1:B:20:ALA:O     | 1:B:21:ASN:HB2   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:106:ASP:C    | 1:B:107:LEU:HD12 | 2.45                     | 0.42              |
| 1:B:273:SER:OG   | 1:B:274:TYR:N    | 2.53                     | 0.42              |
| 1:C:57:GLN:O     | 1:C:59:LEU:N     | 2.53                     | 0.42              |
| 1:C:153:ARG:HE   | 1:C:156:LEU:HD13 | 1.83                     | 0.42              |
| 1:C:375:VAL:O    | 1:C:379:LEU:HB2  | 2.20                     | 0.42              |
| 1:D:257:GLU:O    | 1:D:261:MET:HG3  | 2.19                     | 0.42              |
| 1:E:317:ARG:HE   | 2:R:40:G:H3'     | 1.84                     | 0.42              |
| 1:A:74:TYR:HD1   | 1:A:74:TYR:O     | 2.02                     | 0.42              |
| 1:A:112:ALA:O    | 1:A:113:LEU:O    | 2.38                     | 0.42              |
| 1:A:355:TYR:HD2  | 1:A:355:TYR:HA   | 1.74                     | 0.42              |
| 1:B:6:LYS:NZ     | 1:B:11:ASN:HD21  | 2.17                     | 0.42              |
| 1:C:149:MET:O    | 1:C:151:GLU:N    | 2.53                     | 0.42              |
| 1:D:134:LEU:HD22 | 1:D:134:LEU:HA   | 1.78                     | 0.42              |
| 1:A:143:ARG:HD2  | 1:A:216:GLY:HA2  | 2.02                     | 0.42              |
| 1:A:151:GLU:CD   | 2:R:33:G:H4'     | 2.45                     | 0.42              |
| 1:B:224:ASP:HB2  | 1:B:279:ILE:HG13 | 2.02                     | 0.42              |
| 1:B:376:VAL:O    | 1:B:377:GLU:C    | 2.63                     | 0.42              |
| 1:C:80:ILE:HA    | 1:C:103:GLY:CA   | 2.50                     | 0.42              |
| 1:C:141:LEU:HD12 | 1:C:185:TRP:CH2  | 2.54                     | 0.42              |
| 1:D:385:GLN:O    | 1:D:386:ASN:CB   | 2.68                     | 0.42              |
| 1:E:134:LEU:HD22 | 1:E:134:LEU:HA   | 1.84                     | 0.42              |
| 1:A:56:TYR:CE1   | 1:A:126:ARG:NH2  | 2.88                     | 0.42              |
| 1:C:31:TYR:C     | 1:C:33:ARG:N     | 2.78                     | 0.42              |
| 1:E:31:TYR:C     | 1:E:33:ARG:N     | 2.77                     | 0.42              |
| 1:E:48:LEU:O     | 1:E:48:LEU:HD12  | 2.20                     | 0.42              |
| 1:E:153:ARG:HH21 | 1:E:156:LEU:CD1  | 2.33                     | 0.42              |
| 1:A:224:ASP:HB2  | 1:A:279:ILE:HG13 | 2.02                     | 0.41              |
| 1:B:66:ILE:HA    | 1:B:69:VAL:HG22  | 2.02                     | 0.41              |
| 1:C:177:GLU:HB3  | 1:C:178:GLY:H    | 1.72                     | 0.41              |
| 1:D:270:LYS:HB3  | 1:D:270:LYS:HE2  | 1.79                     | 0.41              |
| 1:E:56:TYR:CE1   | 1:E:126:ARG:NH2  | 2.88                     | 0.41              |
| 1:E:154:LYS:O    | 1:E:158:ASP:OD1  | 2.38                     | 0.41              |
| 1:E:257:GLU:O    | 1:E:261:MET:HG3  | 2.19                     | 0.41              |
| 1:E:369:PRO:HA   | 1:E:370:PRO:HD3  | 1.80                     | 0.41              |
| 1:E:402:MET:O    | 1:E:403:SER:OG   | 2.31                     | 0.41              |
| 1:A:88:TRP:CE2   | 1:A:204:MET:HE2  | 2.55                     | 0.41              |
| 1:B:80:ILE:HA    | 1:B:103:GLY:CA   | 2.50                     | 0.41              |
| 1:B:127:THR:OG1  | 1:B:128:SER:N    | 2.53                     | 0.41              |
| 1:C:127:THR:OG1  | 1:C:128:SER:N    | 2.54                     | 0.41              |
| 1:C:261:MET:HE2  | 1:C:294:ASN:OD1  | 2.20                     | 0.41              |
| 1:E:141:LEU:HB3  | 1:E:182:PHE:CD1  | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:358:ASP:OD2  | 1:E:359:ASP:N    | 2.50                     | 0.41              |
| 1:A:141:LEU:HB3  | 1:A:182:PHE:CD1  | 2.56                     | 0.41              |
| 1:A:167:ILE:O    | 1:A:168:ASN:HB2  | 2.20                     | 0.41              |
| 1:A:383:GLU:HG3  | 1:B:354:LYS:NZ   | 2.34                     | 0.41              |
| 1:B:93:ILE:HD12  | 1:B:93:ILE:H     | 1.84                     | 0.41              |
| 1:B:298:HIS:CD2  | 1:B:317:ARG:NH1  | 2.88                     | 0.41              |
| 1:C:182:PHE:HB2  | 1:C:185:TRP:CE2  | 2.55                     | 0.41              |
| 1:C:213:PHE:O    | 1:C:215:TYR:N    | 2.53                     | 0.41              |
| 1:E:376:VAL:O    | 1:E:377:GLU:C    | 2.63                     | 0.41              |
| 1:A:165:LYS:HG2  | 1:A:166:MET:HE2  | 2.02                     | 0.41              |
| 1:A:290:SER:HA   | 2:R:31:G:OP1     | 2.20                     | 0.41              |
| 1:B:58:GLY:C     | 1:B:64:VAL:HB    | 2.45                     | 0.41              |
| 1:B:175:VAL:HG22 | 1:B:181:ILE:HG23 | 2.02                     | 0.41              |
| 1:C:153:ARG:HH21 | 1:C:156:LEU:CD1  | 2.34                     | 0.41              |
| 1:C:184:VAL:HG13 | 1:D:165:LYS:CG   | 2.50                     | 0.41              |
| 1:E:40:LEU:HD11  | 1:E:194:ILE:HG12 | 2.02                     | 0.41              |
| 1:A:42:ILE:N     | 1:A:42:ILE:HD13  | 2.36                     | 0.41              |
| 1:B:205:PHE:C    | 1:B:207:LYS:H    | 2.28                     | 0.41              |
| 1:B:257:GLU:OE1  | 1:B:295:PRO:HD2  | 2.20                     | 0.41              |
| 1:C:105:PHE:C    | 1:C:107:LEU:N    | 2.68                     | 0.41              |
| 1:C:222:PHE:O    | 1:C:225:CYS:HB2  | 2.20                     | 0.41              |
| 1:D:57:GLN:OE1   | 1:D:123:ASP:CB   | 2.68                     | 0.41              |
| 1:E:66:ILE:HD13  | 1:E:185:TRP:CG   | 2.55                     | 0.41              |
| 1:E:205:PHE:C    | 1:E:207:LYS:N    | 2.78                     | 0.41              |
| 2:R:7:G:C2       | 2:R:8:G:C4       | 3.08                     | 0.41              |
| 1:B:187:ASN:OD1  | 1:C:165:LYS:HE3  | 2.14                     | 0.41              |
| 1:C:200:MET:HB2  | 1:C:277:TYR:CE2  | 2.56                     | 0.41              |
| 1:C:212:SER:HB2  | 2:R:18:G:C5      | 2.55                     | 0.41              |
| 1:C:285:SER:CB   | 1:D:207:LYS:NZ   | 2.84                     | 0.41              |
| 1:C:307:LEU:HD12 | 1:C:307:LEU:HA   | 1.92                     | 0.41              |
| 1:D:50:ASP:CG    | 1:D:120:GLY:O    | 2.64                     | 0.41              |
| 1:D:154:LYS:O    | 1:D:158:ASP:OD1  | 2.38                     | 0.41              |
| 1:E:149:MET:HG3  | 2:R:42:G:C8      | 2.55                     | 0.41              |
| 1:E:155:LYS:O    | 1:E:159:GLY:N    | 2.48                     | 0.41              |
| 1:A:205:PHE:C    | 1:A:207:LYS:H    | 2.29                     | 0.41              |
| 1:B:84:LEU:HB3   | 1:B:86:LYS:O     | 2.20                     | 0.41              |
| 1:B:385:GLN:CG   | 1:B:390:THR:HG22 | 2.48                     | 0.41              |
| 1:C:6:LYS:NZ     | 1:C:11:ASN:HD21  | 2.18                     | 0.41              |
| 1:C:255:ALA:O    | 1:C:259:VAL:HG23 | 2.21                     | 0.41              |
| 1:D:66:ILE:HD13  | 1:D:185:TRP:CG   | 2.56                     | 0.41              |
| 1:D:164:CYS:C    | 1:D:166:MET:N    | 2.77                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:215:TYR:HA   | 2:R:9:G:O4'      | 2.20                     | 0.41              |
| 1:D:298:HIS:CD2  | 1:D:317:ARG:NH1  | 2.88                     | 0.41              |
| 1:D:385:GLN:CG   | 1:D:390:THR:HG22 | 2.49                     | 0.41              |
| 1:E:132:LYS:HE2  | 1:E:166:MET:HE2  | 2.02                     | 0.41              |
| 1:E:182:PHE:HB2  | 1:E:185:TRP:CE2  | 2.56                     | 0.41              |
| 1:A:38:ILE:HD12  | 1:A:38:ILE:O     | 2.21                     | 0.41              |
| 1:C:257:GLU:O    | 1:C:261:MET:HG3  | 2.21                     | 0.41              |
| 1:C:294:ASN:N    | 1:C:295:PRO:HD3  | 2.36                     | 0.41              |
| 1:D:57:GLN:O     | 1:D:59:LEU:N     | 2.54                     | 0.41              |
| 1:D:101:THR:O    | 1:D:101:THR:HG22 | 2.21                     | 0.41              |
| 1:D:175:VAL:HG22 | 1:D:176:PRO:O    | 2.19                     | 0.41              |
| 1:D:228:LEU:O    | 1:D:228:LEU:HD13 | 2.20                     | 0.41              |
| 1:E:143:ARG:HH22 | 2:R:44:G:H5''    | 1.85                     | 0.41              |
| 1:E:215:TYR:CD1  | 2:R:45:G:H5''    | 2.56                     | 0.41              |
| 1:A:60:LYS:HB2   | 1:A:60:LYS:HE2   | 1.85                     | 0.41              |
| 1:A:316:ALA:HB1  | 1:A:317:ARG:NH1  | 2.31                     | 0.41              |
| 1:A:344:LEU:N    | 1:A:344:LEU:HD22 | 2.35                     | 0.41              |
| 1:A:344:LEU:HD11 | 1:E:330:ALA:CB   | 2.50                     | 0.41              |
| 1:B:38:ILE:HA    | 1:B:39:PRO:HD2   | 1.86                     | 0.41              |
| 1:C:28:PRO:HD2   | 1:C:266:GLN:NE2  | 2.35                     | 0.41              |
| 1:C:184:VAL:CG1  | 1:D:166:MET:HE2  | 2.51                     | 0.41              |
| 1:C:200:MET:SD   | 1:C:274:TYR:CD2  | 3.14                     | 0.41              |
| 1:C:409:GLU:O    | 1:C:410:LYS:HB2  | 2.21                     | 0.41              |
| 1:D:58:GLY:C     | 1:D:64:VAL:HB    | 2.46                     | 0.41              |
| 1:D:117:LEU:N    | 1:D:117:LEU:CD2  | 2.82                     | 0.41              |
| 1:D:141:LEU:HD12 | 1:D:185:TRP:CH2  | 2.55                     | 0.41              |
| 1:E:38:ILE:HA    | 1:E:39:PRO:HD2   | 1.83                     | 0.41              |
| 1:E:152:TYR:CE1  | 1:E:153:ARG:NH1  | 2.88                     | 0.41              |
| 1:A:56:TYR:HE1   | 1:A:126:ARG:NH2  | 2.19                     | 0.41              |
| 1:A:200:MET:SD   | 1:A:274:TYR:HD2  | 2.44                     | 0.41              |
| 1:A:257:GLU:HG2  | 1:A:294:ASN:HA   | 2.03                     | 0.41              |
| 1:B:205:PHE:C    | 1:B:207:LYS:N    | 2.79                     | 0.41              |
| 1:C:93:ILE:H     | 1:C:93:ILE:HD12  | 1.85                     | 0.41              |
| 1:C:165:LYS:HD2  | 2:R:18:G:O6      | 2.20                     | 0.41              |
| 1:C:205:PHE:C    | 1:C:207:LYS:H    | 2.29                     | 0.41              |
| 1:D:54:TYR:HD1   | 1:D:122:SER:HB3  | 1.85                     | 0.41              |
| 1:D:84:LEU:HB3   | 1:D:86:LYS:O     | 2.20                     | 0.41              |
| 1:E:270:LYS:HE2  | 1:E:270:LYS:HB3  | 1.85                     | 0.41              |
| 1:B:233:HIS:CD2  | 1:B:312:ARG:HD2  | 2.55                     | 0.40              |
| 1:C:312:ARG:HG3  | 2:R:14:G:C6      | 2.56                     | 0.40              |
| 1:D:342:ALA:HB3  | 1:D:344:LEU:HD23 | 2.01                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:365:THR:CG2  | 1:D:366:THR:N    | 2.82                     | 0.40              |
| 1:D:369:PRO:HA   | 1:D:370:PRO:HD3  | 1.83                     | 0.40              |
| 1:D:375:VAL:O    | 1:D:379:LEU:HB2  | 2.21                     | 0.40              |
| 1:E:143:ARG:NH2  | 2:R:44:G:H3'     | 2.21                     | 0.40              |
| 1:A:40:LEU:HD11  | 1:A:194:ILE:HG12 | 2.03                     | 0.40              |
| 1:A:106:ASP:C    | 1:A:107:LEU:HD12 | 2.46                     | 0.40              |
| 1:A:182:PHE:HB2  | 1:A:185:TRP:CE2  | 2.56                     | 0.40              |
| 1:B:152:TYR:C    | 1:B:154:LYS:N    | 2.80                     | 0.40              |
| 1:B:390:THR:HB   | 1:B:391:PRO:CD   | 2.51                     | 0.40              |
| 1:C:6:LYS:HD2    | 1:C:11:ASN:OD1   | 2.22                     | 0.40              |
| 1:C:133:TRP:CH2  | 1:C:134:LEU:HD23 | 2.57                     | 0.40              |
| 1:D:247:THR:O    | 1:D:375:VAL:HG11 | 2.21                     | 0.40              |
| 1:D:408:ARG:NH1  | 2:R:6:G:N7       | 2.69                     | 0.40              |
| 1:E:54:TYR:CD1   | 1:E:122:SER:CB   | 3.04                     | 0.40              |
| 1:E:218:ILE:HG23 | 1:E:219:VAL:N    | 2.37                     | 0.40              |
| 1:A:224:ASP:HA   | 2:R:30:G:O3'     | 2.22                     | 0.40              |
| 1:A:231:PHE:HB2  | 1:A:297:PHE:CZ   | 2.56                     | 0.40              |
| 1:A:390:THR:HB   | 1:A:391:PRO:CD   | 2.51                     | 0.40              |
| 1:C:317:ARG:H    | 1:C:317:ARG:NE   | 2.12                     | 0.40              |
| 1:C:419:GLU:O    | 1:C:419:GLU:HG3  | 2.22                     | 0.40              |
| 1:D:126:ARG:HH11 | 1:D:127:THR:HG22 | 1.83                     | 0.40              |
| 1:D:177:GLU:HB3  | 1:D:178:GLY:H    | 1.67                     | 0.40              |
| 1:D:356:THR:CG2  | 1:D:357:PRO:HD3  | 2.45                     | 0.40              |
| 1:E:136:LEU:HB2  | 1:E:213:PHE:CD2  | 2.56                     | 0.40              |
| 1:A:154:LYS:O    | 1:A:158:ASP:OD1  | 2.39                     | 0.40              |
| 1:A:171:PHE:CD1  | 1:A:172:GLU:N    | 2.90                     | 0.40              |
| 1:A:200:MET:SD   | 1:A:274:TYR:CD2  | 3.15                     | 0.40              |
| 1:A:243:GLU:O    | 1:A:247:THR:HG23 | 2.22                     | 0.40              |
| 1:A:375:VAL:O    | 1:A:379:LEU:HB2  | 2.22                     | 0.40              |
| 1:A:376:VAL:HG13 | 1:B:354:LYS:CA   | 2.51                     | 0.40              |
| 1:B:38:ILE:CD1   | 1:B:107:LEU:O    | 2.70                     | 0.40              |
| 1:B:227:ALA:HA   | 1:B:230:THR:HG23 | 2.02                     | 0.40              |
| 1:D:20:ALA:O     | 1:D:21:ASN:HB2   | 2.21                     | 0.40              |
| 1:D:129:ALA:O    | 1:D:133:TRP:CD1  | 2.74                     | 0.40              |
| 1:D:224:ASP:HB2  | 1:D:279:ILE:HG13 | 2.04                     | 0.40              |
| 1:D:249:ILE:HD11 | 1:D:258:MET:HG3  | 2.04                     | 0.40              |
| 1:A:19:PRO:HA    | 1:B:268:ILE:O    | 2.21                     | 0.40              |
| 1:A:104:ILE:HD13 | 1:A:198:VAL:HG22 | 2.04                     | 0.40              |
| 1:A:130:ASP:C    | 1:A:132:LYS:H    | 2.29                     | 0.40              |
| 1:A:177:GLU:HG2  | 1:A:181:ILE:HD11 | 2.02                     | 0.40              |
| 1:A:299:PHE:HZ   | 1:A:415:TYR:CE1  | 2.40                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:354:LYS:HZ3  | 1:E:380:GLY:HA2 | 1.85                     | 0.40              |
| 1:B:93:ILE:HD12  | 1:B:93:ILE:N    | 2.36                     | 0.40              |
| 1:B:316:ALA:HB1  | 1:B:317:ARG:NH1 | 2.36                     | 0.40              |
| 1:E:254:VAL:HG13 | 1:E:297:PHE:HA  | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|-----------|----------|-------------|---|
| 1   | A     | 419/421 (100%)  | 319 (76%)  | 66 (16%)  | 34 (8%)  | 1           | 3 |
| 1   | B     | 411/421 (98%)   | 321 (78%)  | 53 (13%)  | 37 (9%)  | 0           | 3 |
| 1   | C     | 409/421 (97%)   | 312 (76%)  | 67 (16%)  | 30 (7%)  | 1           | 4 |
| 1   | D     | 412/421 (98%)   | 317 (77%)  | 59 (14%)  | 36 (9%)  | 0           | 3 |
| 1   | E     | 419/421 (100%)  | 322 (77%)  | 66 (16%)  | 31 (7%)  | 1           | 4 |
| All | All   | 2070/2105 (98%) | 1591 (77%) | 311 (15%) | 168 (8%) | 1           | 3 |

All (168) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 63  | ASN  |
| 1   | A     | 113 | LEU  |
| 1   | A     | 117 | LEU  |
| 1   | A     | 167 | ILE  |
| 1   | A     | 173 | PRO  |
| 1   | A     | 174 | LEU  |
| 1   | A     | 182 | PHE  |
| 1   | A     | 358 | ASP  |
| 1   | A     | 365 | THR  |
| 1   | A     | 366 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 63  | ASN  |
| 1   | B     | 113 | LEU  |
| 1   | B     | 117 | LEU  |
| 1   | B     | 168 | ASN  |
| 1   | B     | 170 | GLN  |
| 1   | B     | 173 | PRO  |
| 1   | B     | 174 | LEU  |
| 1   | B     | 182 | PHE  |
| 1   | B     | 228 | LEU  |
| 1   | B     | 342 | ALA  |
| 1   | B     | 345 | ALA  |
| 1   | C     | 63  | ASN  |
| 1   | C     | 113 | LEU  |
| 1   | C     | 117 | LEU  |
| 1   | C     | 173 | PRO  |
| 1   | C     | 174 | LEU  |
| 1   | C     | 182 | PHE  |
| 1   | C     | 228 | LEU  |
| 1   | C     | 345 | ALA  |
| 1   | D     | 63  | ASN  |
| 1   | D     | 113 | LEU  |
| 1   | D     | 117 | LEU  |
| 1   | D     | 165 | LYS  |
| 1   | D     | 166 | MET  |
| 1   | D     | 169 | GLU  |
| 1   | D     | 173 | PRO  |
| 1   | D     | 174 | LEU  |
| 1   | D     | 182 | PHE  |
| 1   | D     | 228 | LEU  |
| 1   | D     | 345 | ALA  |
| 1   | E     | 63  | ASN  |
| 1   | E     | 113 | LEU  |
| 1   | E     | 117 | LEU  |
| 1   | E     | 182 | PHE  |
| 1   | E     | 362 | GLY  |
| 1   | E     | 365 | THR  |
| 1   | A     | 80  | ILE  |
| 1   | A     | 115 | GLY  |
| 1   | A     | 168 | ASN  |
| 1   | A     | 180 | ASP  |
| 1   | A     | 228 | LEU  |
| 1   | A     | 271 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 360 | SER  |
| 1   | B     | 80  | ILE  |
| 1   | B     | 115 | GLY  |
| 1   | B     | 167 | ILE  |
| 1   | B     | 176 | PRO  |
| 1   | B     | 180 | ASP  |
| 1   | B     | 271 | ALA  |
| 1   | C     | 80  | ILE  |
| 1   | C     | 108 | VAL  |
| 1   | C     | 115 | GLY  |
| 1   | C     | 167 | ILE  |
| 1   | C     | 180 | ASP  |
| 1   | C     | 214 | ARG  |
| 1   | C     | 271 | ALA  |
| 1   | D     | 80  | ILE  |
| 1   | D     | 115 | GLY  |
| 1   | D     | 180 | ASP  |
| 1   | D     | 214 | ARG  |
| 1   | D     | 271 | ALA  |
| 1   | E     | 80  | ILE  |
| 1   | E     | 115 | GLY  |
| 1   | E     | 168 | ASN  |
| 1   | E     | 180 | ASP  |
| 1   | E     | 228 | LEU  |
| 1   | E     | 271 | ALA  |
| 1   | E     | 363 | GLY  |
| 1   | A     | 90  | SER  |
| 1   | A     | 123 | ASP  |
| 1   | A     | 172 | GLU  |
| 1   | A     | 179 | ARG  |
| 1   | A     | 226 | ALA  |
| 1   | B     | 30  | ASP  |
| 1   | B     | 123 | ASP  |
| 1   | B     | 172 | GLU  |
| 1   | B     | 179 | ARG  |
| 1   | C     | 30  | ASP  |
| 1   | C     | 90  | SER  |
| 1   | C     | 123 | ASP  |
| 1   | C     | 128 | SER  |
| 1   | C     | 129 | ALA  |
| 1   | C     | 168 | ASN  |
| 1   | D     | 30  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 123 | ASP  |
| 1   | D     | 167 | ILE  |
| 1   | D     | 179 | ARG  |
| 1   | E     | 30  | ASP  |
| 1   | E     | 90  | SER  |
| 1   | E     | 123 | ASP  |
| 1   | E     | 129 | ALA  |
| 1   | E     | 214 | ARG  |
| 1   | E     | 226 | ALA  |
| 1   | A     | 30  | ASP  |
| 1   | A     | 128 | SER  |
| 1   | A     | 129 | ALA  |
| 1   | A     | 189 | SER  |
| 1   | A     | 309 | ARG  |
| 1   | A     | 342 | ALA  |
| 1   | A     | 357 | PRO  |
| 1   | B     | 90  | SER  |
| 1   | B     | 108 | VAL  |
| 1   | B     | 129 | ALA  |
| 1   | B     | 214 | ARG  |
| 1   | B     | 226 | ALA  |
| 1   | C     | 150 | PRO  |
| 1   | C     | 179 | ARG  |
| 1   | D     | 46  | LYS  |
| 1   | D     | 90  | SER  |
| 1   | D     | 108 | VAL  |
| 1   | D     | 129 | ALA  |
| 1   | D     | 226 | ALA  |
| 1   | D     | 309 | ARG  |
| 1   | D     | 357 | PRO  |
| 1   | E     | 108 | VAL  |
| 1   | E     | 128 | SER  |
| 1   | E     | 173 | PRO  |
| 1   | E     | 179 | ARG  |
| 1   | A     | 46  | LYS  |
| 1   | A     | 100 | ASP  |
| 1   | A     | 108 | VAL  |
| 1   | B     | 46  | LYS  |
| 1   | B     | 100 | ASP  |
| 1   | B     | 128 | SER  |
| 1   | B     | 309 | ARG  |
| 1   | B     | 357 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 131 | ASP  |
| 1   | C     | 309 | ARG  |
| 1   | D     | 79  | ASP  |
| 1   | D     | 128 | SER  |
| 1   | E     | 309 | ARG  |
| 1   | E     | 357 | PRO  |
| 1   | A     | 42  | ILE  |
| 1   | A     | 150 | PRO  |
| 1   | C     | 46  | LYS  |
| 1   | D     | 100 | ASP  |
| 1   | D     | 106 | ASP  |
| 1   | D     | 150 | PRO  |
| 1   | E     | 46  | LYS  |
| 1   | E     | 106 | ASP  |
| 1   | B     | 42  | ILE  |
| 1   | D     | 19  | PRO  |
| 1   | E     | 19  | PRO  |
| 1   | E     | 150 | PRO  |
| 1   | B     | 19  | PRO  |
| 1   | B     | 93  | ILE  |
| 1   | B     | 150 | PRO  |
| 1   | B     | 219 | VAL  |
| 1   | C     | 93  | ILE  |
| 1   | C     | 178 | GLY  |
| 1   | D     | 93  | ILE  |
| 1   | B     | 23  | ASP  |
| 1   | D     | 23  | ASP  |
| 1   | E     | 42  | ILE  |
| 1   | E     | 93  | ILE  |
| 1   | C     | 19  | PRO  |
| 1   | C     | 42  | ILE  |
| 1   | D     | 42  | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |   |
|-----|-------|-----------------|------------|-----------|-------------|---|
| 1   | A     | 362/362 (100%)  | 293 (81%)  | 69 (19%)  | 1           | 7 |
| 1   | B     | 358/362 (99%)   | 286 (80%)  | 72 (20%)  | 1           | 5 |
| 1   | C     | 356/362 (98%)   | 286 (80%)  | 70 (20%)  | 1           | 6 |
| 1   | D     | 359/362 (99%)   | 287 (80%)  | 72 (20%)  | 1           | 5 |
| 1   | E     | 362/362 (100%)  | 287 (79%)  | 75 (21%)  | 1           | 5 |
| All | All   | 1797/1810 (99%) | 1439 (80%) | 358 (20%) | 1           | 6 |

All (358) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | VAL  |
| 1   | A     | 11  | ASN  |
| 1   | A     | 13  | VAL  |
| 1   | A     | 31  | TYR  |
| 1   | A     | 40  | LEU  |
| 1   | A     | 42  | ILE  |
| 1   | A     | 46  | LYS  |
| 1   | A     | 55  | VAL  |
| 1   | A     | 57  | GLN  |
| 1   | A     | 60  | LYS  |
| 1   | A     | 67  | ILE  |
| 1   | A     | 74  | TYR  |
| 1   | A     | 78  | LYS  |
| 1   | A     | 94  | ASN  |
| 1   | A     | 97  | LYS  |
| 1   | A     | 101 | THR  |
| 1   | A     | 108 | VAL  |
| 1   | A     | 117 | LEU  |
| 1   | A     | 121 | VAL  |
| 1   | A     | 131 | ASP  |
| 1   | A     | 132 | LYS  |
| 1   | A     | 134 | LEU  |
| 1   | A     | 144 | VAL  |
| 1   | A     | 147 | THR  |
| 1   | A     | 149 | MET  |
| 1   | A     | 153 | ARG  |
| 1   | A     | 156 | LEU  |
| 1   | A     | 160 | LEU  |
| 1   | A     | 165 | LYS  |
| 1   | A     | 169 | GLU  |
| 1   | A     | 170 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 171 | PHE  |
| 1   | A     | 172 | GLU  |
| 1   | A     | 174 | LEU  |
| 1   | A     | 175 | VAL  |
| 1   | A     | 177 | GLU  |
| 1   | A     | 180 | ASP  |
| 1   | A     | 181 | ILE  |
| 1   | A     | 182 | PHE  |
| 1   | A     | 187 | ASN  |
| 1   | A     | 217 | THR  |
| 1   | A     | 218 | ILE  |
| 1   | A     | 228 | LEU  |
| 1   | A     | 230 | THR  |
| 1   | A     | 243 | GLU  |
| 1   | A     | 251 | ASN  |
| 1   | A     | 252 | ARG  |
| 1   | A     | 253 | GLU  |
| 1   | A     | 258 | MET  |
| 1   | A     | 263 | LEU  |
| 1   | A     | 268 | ILE  |
| 1   | A     | 270 | LYS  |
| 1   | A     | 272 | ASP  |
| 1   | A     | 273 | SER  |
| 1   | A     | 278 | LEU  |
| 1   | A     | 307 | LEU  |
| 1   | A     | 308 | LEU  |
| 1   | A     | 317 | ARG  |
| 1   | A     | 327 | LEU  |
| 1   | A     | 332 | LEU  |
| 1   | A     | 344 | LEU  |
| 1   | A     | 352 | ASP  |
| 1   | A     | 356 | THR  |
| 1   | A     | 361 | THR  |
| 1   | A     | 375 | VAL  |
| 1   | A     | 379 | LEU  |
| 1   | A     | 385 | GLN  |
| 1   | A     | 405 | GLN  |
| 1   | A     | 409 | GLU  |
| 1   | B     | 3   | VAL  |
| 1   | B     | 11  | ASN  |
| 1   | B     | 13  | VAL  |
| 1   | B     | 31  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 40  | LEU  |
| 1   | B     | 42  | ILE  |
| 1   | B     | 46  | LYS  |
| 1   | B     | 49  | SER  |
| 1   | B     | 55  | VAL  |
| 1   | B     | 57  | GLN  |
| 1   | B     | 60  | LYS  |
| 1   | B     | 67  | ILE  |
| 1   | B     | 74  | TYR  |
| 1   | B     | 78  | LYS  |
| 1   | B     | 94  | ASN  |
| 1   | B     | 97  | LYS  |
| 1   | B     | 101 | THR  |
| 1   | B     | 108 | VAL  |
| 1   | B     | 117 | LEU  |
| 1   | B     | 121 | VAL  |
| 1   | B     | 128 | SER  |
| 1   | B     | 131 | ASP  |
| 1   | B     | 132 | LYS  |
| 1   | B     | 134 | LEU  |
| 1   | B     | 144 | VAL  |
| 1   | B     | 147 | THR  |
| 1   | B     | 149 | MET  |
| 1   | B     | 153 | ARG  |
| 1   | B     | 156 | LEU  |
| 1   | B     | 160 | LEU  |
| 1   | B     | 162 | ASN  |
| 1   | B     | 165 | LYS  |
| 1   | B     | 167 | ILE  |
| 1   | B     | 169 | GLU  |
| 1   | B     | 170 | GLN  |
| 1   | B     | 171 | PHE  |
| 1   | B     | 172 | GLU  |
| 1   | B     | 174 | LEU  |
| 1   | B     | 175 | VAL  |
| 1   | B     | 177 | GLU  |
| 1   | B     | 180 | ASP  |
| 1   | B     | 181 | ILE  |
| 1   | B     | 182 | PHE  |
| 1   | B     | 187 | ASN  |
| 1   | B     | 217 | THR  |
| 1   | B     | 228 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 230 | THR  |
| 1   | B     | 243 | GLU  |
| 1   | B     | 251 | ASN  |
| 1   | B     | 252 | ARG  |
| 1   | B     | 253 | GLU  |
| 1   | B     | 258 | MET  |
| 1   | B     | 263 | LEU  |
| 1   | B     | 268 | ILE  |
| 1   | B     | 270 | LYS  |
| 1   | B     | 272 | ASP  |
| 1   | B     | 273 | SER  |
| 1   | B     | 278 | LEU  |
| 1   | B     | 307 | LEU  |
| 1   | B     | 308 | LEU  |
| 1   | B     | 317 | ARG  |
| 1   | B     | 327 | LEU  |
| 1   | B     | 332 | LEU  |
| 1   | B     | 344 | LEU  |
| 1   | B     | 352 | ASP  |
| 1   | B     | 356 | THR  |
| 1   | B     | 365 | THR  |
| 1   | B     | 375 | VAL  |
| 1   | B     | 379 | LEU  |
| 1   | B     | 385 | GLN  |
| 1   | B     | 405 | GLN  |
| 1   | B     | 409 | GLU  |
| 1   | C     | 3   | VAL  |
| 1   | C     | 8   | ILE  |
| 1   | C     | 11  | ASN  |
| 1   | C     | 13  | VAL  |
| 1   | C     | 31  | TYR  |
| 1   | C     | 40  | LEU  |
| 1   | C     | 42  | ILE  |
| 1   | C     | 46  | LYS  |
| 1   | C     | 49  | SER  |
| 1   | C     | 57  | GLN  |
| 1   | C     | 60  | LYS  |
| 1   | C     | 67  | ILE  |
| 1   | C     | 74  | TYR  |
| 1   | C     | 78  | LYS  |
| 1   | C     | 94  | ASN  |
| 1   | C     | 97  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 101 | THR  |
| 1   | C     | 108 | VAL  |
| 1   | C     | 117 | LEU  |
| 1   | C     | 121 | VAL  |
| 1   | C     | 128 | SER  |
| 1   | C     | 131 | ASP  |
| 1   | C     | 132 | LYS  |
| 1   | C     | 134 | LEU  |
| 1   | C     | 144 | VAL  |
| 1   | C     | 147 | THR  |
| 1   | C     | 149 | MET  |
| 1   | C     | 153 | ARG  |
| 1   | C     | 156 | LEU  |
| 1   | C     | 160 | LEU  |
| 1   | C     | 165 | LYS  |
| 1   | C     | 167 | ILE  |
| 1   | C     | 171 | PHE  |
| 1   | C     | 172 | GLU  |
| 1   | C     | 174 | LEU  |
| 1   | C     | 175 | VAL  |
| 1   | C     | 177 | GLU  |
| 1   | C     | 180 | ASP  |
| 1   | C     | 181 | ILE  |
| 1   | C     | 182 | PHE  |
| 1   | C     | 187 | ASN  |
| 1   | C     | 217 | THR  |
| 1   | C     | 218 | ILE  |
| 1   | C     | 228 | LEU  |
| 1   | C     | 230 | THR  |
| 1   | C     | 243 | GLU  |
| 1   | C     | 251 | ASN  |
| 1   | C     | 252 | ARG  |
| 1   | C     | 253 | GLU  |
| 1   | C     | 258 | MET  |
| 1   | C     | 263 | LEU  |
| 1   | C     | 268 | ILE  |
| 1   | C     | 270 | LYS  |
| 1   | C     | 272 | ASP  |
| 1   | C     | 273 | SER  |
| 1   | C     | 278 | LEU  |
| 1   | C     | 307 | LEU  |
| 1   | C     | 308 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 317 | ARG  |
| 1   | C     | 327 | LEU  |
| 1   | C     | 332 | LEU  |
| 1   | C     | 343 | ASP  |
| 1   | C     | 344 | LEU  |
| 1   | C     | 352 | ASP  |
| 1   | C     | 356 | THR  |
| 1   | C     | 375 | VAL  |
| 1   | C     | 379 | LEU  |
| 1   | C     | 385 | GLN  |
| 1   | C     | 405 | GLN  |
| 1   | C     | 409 | GLU  |
| 1   | D     | 3   | VAL  |
| 1   | D     | 11  | ASN  |
| 1   | D     | 13  | VAL  |
| 1   | D     | 31  | TYR  |
| 1   | D     | 40  | LEU  |
| 1   | D     | 42  | ILE  |
| 1   | D     | 46  | LYS  |
| 1   | D     | 49  | SER  |
| 1   | D     | 55  | VAL  |
| 1   | D     | 57  | GLN  |
| 1   | D     | 60  | LYS  |
| 1   | D     | 67  | ILE  |
| 1   | D     | 74  | TYR  |
| 1   | D     | 78  | LYS  |
| 1   | D     | 94  | ASN  |
| 1   | D     | 97  | LYS  |
| 1   | D     | 100 | ASP  |
| 1   | D     | 101 | THR  |
| 1   | D     | 108 | VAL  |
| 1   | D     | 117 | LEU  |
| 1   | D     | 121 | VAL  |
| 1   | D     | 131 | ASP  |
| 1   | D     | 132 | LYS  |
| 1   | D     | 134 | LEU  |
| 1   | D     | 144 | VAL  |
| 1   | D     | 147 | THR  |
| 1   | D     | 149 | MET  |
| 1   | D     | 153 | ARG  |
| 1   | D     | 156 | LEU  |
| 1   | D     | 160 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 165 | LYS  |
| 1   | D     | 166 | MET  |
| 1   | D     | 168 | ASN  |
| 1   | D     | 170 | GLN  |
| 1   | D     | 171 | PHE  |
| 1   | D     | 172 | GLU  |
| 1   | D     | 174 | LEU  |
| 1   | D     | 175 | VAL  |
| 1   | D     | 177 | GLU  |
| 1   | D     | 180 | ASP  |
| 1   | D     | 181 | ILE  |
| 1   | D     | 182 | PHE  |
| 1   | D     | 187 | ASN  |
| 1   | D     | 217 | THR  |
| 1   | D     | 218 | ILE  |
| 1   | D     | 228 | LEU  |
| 1   | D     | 230 | THR  |
| 1   | D     | 243 | GLU  |
| 1   | D     | 251 | ASN  |
| 1   | D     | 252 | ARG  |
| 1   | D     | 253 | GLU  |
| 1   | D     | 258 | MET  |
| 1   | D     | 263 | LEU  |
| 1   | D     | 268 | ILE  |
| 1   | D     | 270 | LYS  |
| 1   | D     | 272 | ASP  |
| 1   | D     | 273 | SER  |
| 1   | D     | 278 | LEU  |
| 1   | D     | 307 | LEU  |
| 1   | D     | 308 | LEU  |
| 1   | D     | 317 | ARG  |
| 1   | D     | 327 | LEU  |
| 1   | D     | 332 | LEU  |
| 1   | D     | 343 | ASP  |
| 1   | D     | 344 | LEU  |
| 1   | D     | 352 | ASP  |
| 1   | D     | 356 | THR  |
| 1   | D     | 375 | VAL  |
| 1   | D     | 379 | LEU  |
| 1   | D     | 385 | GLN  |
| 1   | D     | 405 | GLN  |
| 1   | D     | 409 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 3   | VAL  |
| 1   | E     | 8   | ILE  |
| 1   | E     | 11  | ASN  |
| 1   | E     | 13  | VAL  |
| 1   | E     | 31  | TYR  |
| 1   | E     | 35  | SER  |
| 1   | E     | 40  | LEU  |
| 1   | E     | 42  | ILE  |
| 1   | E     | 46  | LYS  |
| 1   | E     | 49  | SER  |
| 1   | E     | 55  | VAL  |
| 1   | E     | 57  | GLN  |
| 1   | E     | 60  | LYS  |
| 1   | E     | 67  | ILE  |
| 1   | E     | 74  | TYR  |
| 1   | E     | 78  | LYS  |
| 1   | E     | 94  | ASN  |
| 1   | E     | 97  | LYS  |
| 1   | E     | 101 | THR  |
| 1   | E     | 108 | VAL  |
| 1   | E     | 117 | LEU  |
| 1   | E     | 121 | VAL  |
| 1   | E     | 131 | ASP  |
| 1   | E     | 132 | LYS  |
| 1   | E     | 134 | LEU  |
| 1   | E     | 144 | VAL  |
| 1   | E     | 147 | THR  |
| 1   | E     | 149 | MET  |
| 1   | E     | 153 | ARG  |
| 1   | E     | 156 | LEU  |
| 1   | E     | 160 | LEU  |
| 1   | E     | 162 | ASN  |
| 1   | E     | 165 | LYS  |
| 1   | E     | 166 | MET  |
| 1   | E     | 167 | ILE  |
| 1   | E     | 170 | GLN  |
| 1   | E     | 171 | PHE  |
| 1   | E     | 172 | GLU  |
| 1   | E     | 174 | LEU  |
| 1   | E     | 175 | VAL  |
| 1   | E     | 177 | GLU  |
| 1   | E     | 180 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 181 | ILE  |
| 1   | E     | 182 | PHE  |
| 1   | E     | 187 | ASN  |
| 1   | E     | 217 | THR  |
| 1   | E     | 218 | ILE  |
| 1   | E     | 228 | LEU  |
| 1   | E     | 230 | THR  |
| 1   | E     | 243 | GLU  |
| 1   | E     | 251 | ASN  |
| 1   | E     | 252 | ARG  |
| 1   | E     | 253 | GLU  |
| 1   | E     | 258 | MET  |
| 1   | E     | 263 | LEU  |
| 1   | E     | 268 | ILE  |
| 1   | E     | 270 | LYS  |
| 1   | E     | 272 | ASP  |
| 1   | E     | 273 | SER  |
| 1   | E     | 278 | LEU  |
| 1   | E     | 307 | LEU  |
| 1   | E     | 308 | LEU  |
| 1   | E     | 317 | ARG  |
| 1   | E     | 327 | LEU  |
| 1   | E     | 332 | LEU  |
| 1   | E     | 343 | ASP  |
| 1   | E     | 352 | ASP  |
| 1   | E     | 356 | THR  |
| 1   | E     | 360 | SER  |
| 1   | E     | 365 | THR  |
| 1   | E     | 375 | VAL  |
| 1   | E     | 379 | LEU  |
| 1   | E     | 385 | GLN  |
| 1   | E     | 405 | GLN  |
| 1   | E     | 409 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | ASN  |
| 1   | A     | 57  | GLN  |
| 1   | A     | 68  | HIS  |
| 1   | A     | 70  | ASN  |
| 1   | A     | 162 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 170 | GLN  |
| 1   | A     | 190 | ASN  |
| 1   | A     | 266 | GLN  |
| 1   | A     | 302 | GLN  |
| 1   | A     | 347 | GLN  |
| 1   | A     | 353 | ASN  |
| 1   | A     | 395 | GLN  |
| 1   | B     | 11  | ASN  |
| 1   | B     | 57  | GLN  |
| 1   | B     | 68  | HIS  |
| 1   | B     | 70  | ASN  |
| 1   | B     | 162 | ASN  |
| 1   | B     | 190 | ASN  |
| 1   | B     | 266 | GLN  |
| 1   | B     | 302 | GLN  |
| 1   | B     | 347 | GLN  |
| 1   | B     | 353 | ASN  |
| 1   | B     | 395 | GLN  |
| 1   | C     | 11  | ASN  |
| 1   | C     | 57  | GLN  |
| 1   | C     | 68  | HIS  |
| 1   | C     | 170 | GLN  |
| 1   | C     | 190 | ASN  |
| 1   | C     | 266 | GLN  |
| 1   | C     | 302 | GLN  |
| 1   | C     | 347 | GLN  |
| 1   | C     | 353 | ASN  |
| 1   | C     | 395 | GLN  |
| 1   | D     | 11  | ASN  |
| 1   | D     | 57  | GLN  |
| 1   | D     | 68  | HIS  |
| 1   | D     | 70  | ASN  |
| 1   | D     | 162 | ASN  |
| 1   | D     | 190 | ASN  |
| 1   | D     | 266 | GLN  |
| 1   | D     | 347 | GLN  |
| 1   | D     | 395 | GLN  |
| 1   | E     | 11  | ASN  |
| 1   | E     | 57  | GLN  |
| 1   | E     | 68  | HIS  |
| 1   | E     | 70  | ASN  |
| 1   | E     | 190 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 203 | HIS  |
| 1   | E     | 266 | GLN  |
| 1   | E     | 302 | GLN  |
| 1   | E     | 347 | GLN  |
| 1   | E     | 385 | GLN  |
| 1   | E     | 386 | ASN  |
| 1   | E     | 395 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 2   | R     | 44/45 (97%) | 25 (56%)          | 3 (6%)          |

All (25) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R     | 2   | G    |
| 2   | R     | 3   | G    |
| 2   | R     | 5   | G    |
| 2   | R     | 8   | G    |
| 2   | R     | 10  | G    |
| 2   | R     | 13  | G    |
| 2   | R     | 14  | G    |
| 2   | R     | 18  | G    |
| 2   | R     | 19  | G    |
| 2   | R     | 21  | G    |
| 2   | R     | 22  | G    |
| 2   | R     | 23  | G    |
| 2   | R     | 25  | G    |
| 2   | R     | 26  | G    |
| 2   | R     | 27  | G    |
| 2   | R     | 28  | G    |
| 2   | R     | 30  | G    |
| 2   | R     | 31  | G    |
| 2   | R     | 32  | G    |
| 2   | R     | 36  | G    |
| 2   | R     | 39  | G    |
| 2   | R     | 40  | G    |
| 2   | R     | 41  | G    |
| 2   | R     | 42  | G    |
| 2   | R     | 45  | G    |

All (3) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R     | 17  | G    |
| 2   | R     | 18  | G    |
| 2   | R     | 26  | G    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 20 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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     | 421/421 (100%)  | 0.32   | 14 (3%)  | 49 | 28 | 56, 92, 130, 142      | 0     |
| 1   | B     | 415/421 (98%)   | 0.40   | 23 (5%)  | 30 | 16 | 57, 91, 130, 141      | 0     |
| 1   | C     | 413/421 (98%)   | 0.38   | 19 (4%)  | 37 | 19 | 56, 92, 129, 142      | 0     |
| 1   | D     | 416/421 (98%)   | 0.52   | 18 (4%)  | 40 | 21 | 56, 92, 130, 141      | 0     |
| 1   | E     | 421/421 (100%)  | 0.37   | 23 (5%)  | 30 | 16 | 57, 93, 131, 147      | 0     |
| 2   | R     | 45/45 (100%)    | 1.10   | 3 (6%)   | 24 | 12 | 118, 132, 143, 145    | 0     |
| All | All   | 2131/2150 (99%) | 0.41   | 100 (4%) | 36 | 19 | 56, 93, 131, 147      | 0     |

All (100) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 2   | SER  | 11.0 |
| 1   | A     | 2   | SER  | 8.3  |
| 1   | E     | 2   | SER  | 7.4  |
| 1   | D     | 43  | ASN  | 5.9  |
| 1   | C     | 2   | SER  | 4.4  |
| 1   | D     | 121 | VAL  | 4.4  |
| 1   | D     | 172 | GLU  | 4.3  |
| 1   | E     | 43  | ASN  | 3.9  |
| 1   | B     | 169 | GLU  | 3.8  |
| 1   | B     | 80  | ILE  | 3.8  |
| 1   | B     | 351 | GLY  | 3.8  |
| 1   | C     | 73  | LEU  | 3.8  |
| 1   | E     | 363 | GLY  | 3.6  |
| 1   | B     | 386 | ASN  | 3.5  |
| 1   | B     | 118 | PRO  | 3.5  |
| 1   | B     | 353 | ASN  | 3.5  |
| 1   | B     | 121 | VAL  | 3.4  |
| 1   | E     | 118 | PRO  | 3.4  |
| 1   | E     | 362 | GLY  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 215 | TYR  | 3.3  |
| 1   | C     | 59  | LEU  | 3.3  |
| 1   | D     | 13  | VAL  | 3.3  |
| 1   | B     | 129 | ALA  | 3.3  |
| 1   | B     | 346 | GLN  | 3.2  |
| 1   | A     | 129 | ALA  | 3.2  |
| 1   | B     | 120 | GLY  | 3.1  |
| 1   | C     | 129 | ALA  | 3.1  |
| 1   | D     | 2   | SER  | 3.1  |
| 1   | E     | 172 | GLU  | 3.0  |
| 1   | A     | 118 | PRO  | 2.9  |
| 1   | D     | 129 | ALA  | 2.9  |
| 1   | A     | 269 | ASP  | 2.9  |
| 1   | D     | 118 | PRO  | 2.9  |
| 1   | E     | 113 | LEU  | 2.9  |
| 1   | C     | 357 | PRO  | 2.8  |
| 1   | B     | 119 | ASP  | 2.7  |
| 1   | C     | 171 | PHE  | 2.7  |
| 1   | B     | 163 | GLN  | 2.7  |
| 1   | D     | 119 | ASP  | 2.7  |
| 1   | D     | 120 | GLY  | 2.7  |
| 1   | E     | 174 | LEU  | 2.7  |
| 1   | B     | 343 | ASP  | 2.7  |
| 1   | D     | 124 | ALA  | 2.6  |
| 1   | A     | 75  | GLY  | 2.6  |
| 1   | B     | 412 | ILE  | 2.6  |
| 1   | C     | 14  | ILE  | 2.6  |
| 1   | C     | 3   | VAL  | 2.6  |
| 1   | C     | 233 | HIS  | 2.6  |
| 1   | C     | 43  | ASN  | 2.6  |
| 1   | E     | 344 | LEU  | 2.6  |
| 1   | C     | 346 | GLN  | 2.5  |
| 1   | D     | 186 | GLY  | 2.5  |
| 1   | B     | 172 | GLU  | 2.5  |
| 1   | E     | 129 | ALA  | 2.5  |
| 1   | C     | 352 | ASP  | 2.5  |
| 1   | A     | 361 | THR  | 2.5  |
| 1   | A     | 357 | PRO  | 2.5  |
| 1   | E     | 3   | VAL  | 2.4  |
| 1   | C     | 228 | LEU  | 2.4  |
| 1   | B     | 185 | TRP  | 2.4  |
| 1   | D     | 178 | GLY  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 80  | ILE  | 2.4  |
| 1   | B     | 3   | VAL  | 2.4  |
| 1   | A     | 344 | LEU  | 2.3  |
| 1   | B     | 345 | ALA  | 2.3  |
| 1   | E     | 62  | GLY  | 2.3  |
| 1   | E     | 73  | LEU  | 2.3  |
| 1   | D     | 102 | ILE  | 2.3  |
| 1   | E     | 121 | VAL  | 2.3  |
| 1   | B     | 122 | SER  | 2.2  |
| 1   | D     | 412 | ILE  | 2.2  |
| 1   | E     | 66  | ILE  | 2.2  |
| 1   | E     | 124 | ALA  | 2.2  |
| 1   | E     | 140 | GLY  | 2.2  |
| 1   | A     | 356 | THR  | 2.2  |
| 1   | A     | 59  | LEU  | 2.2  |
| 1   | C     | 62  | GLY  | 2.2  |
| 1   | C     | 176 | PRO  | 2.2  |
| 1   | B     | 167 | ILE  | 2.2  |
| 1   | A     | 351 | GLY  | 2.2  |
| 1   | E     | 351 | GLY  | 2.2  |
| 2   | R     | 18  | G    | 2.2  |
| 1   | C     | 344 | LEU  | 2.1  |
| 1   | E     | 171 | PHE  | 2.1  |
| 1   | E     | 114 | ASP  | 2.1  |
| 1   | A     | 174 | LEU  | 2.1  |
| 1   | E     | 59  | LEU  | 2.1  |
| 2   | R     | 35  | G    | 2.1  |
| 2   | R     | 40  | G    | 2.1  |
| 1   | A     | 363 | GLY  | 2.1  |
| 1   | E     | 186 | GLY  | 2.1  |
| 1   | E     | 166 | MET  | 2.1  |
| 1   | D     | 184 | VAL  | 2.1  |
| 1   | A     | 184 | VAL  | 2.0  |
| 1   | B     | 43  | ASN  | 2.0  |
| 1   | C     | 117 | LEU  | 2.0  |
| 1   | C     | 122 | SER  | 2.0  |
| 1   | B     | 311 | THR  | 2.0  |
| 1   | D     | 351 | GLY  | 2.0  |
| 1   | D     | 167 | ILE  | 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](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | IUM  | R     | 540 | 1/3   | 0.73 | 0.07 | 238,238,238,238            | 1     |
| 3   | IUM  | R     | 536 | 1/3   | 0.78 | 0.09 | 212,212,212,212            | 1     |
| 3   | IUM  | R     | 537 | 1/3   | 0.79 | 0.09 | 161,161,161,161            | 1     |
| 3   | IUM  | R     | 538 | 1/3   | 0.84 | 0.09 | 234,234,234,234            | 1     |
| 3   | IUM  | B     | 525 | 1/3   | 0.84 | 0.07 | 157,157,157,157            | 1     |
| 3   | IUM  | R     | 539 | 1/3   | 0.87 | 0.06 | 156,156,156,156            | 1     |
| 3   | IUM  | B     | 527 | 1/3   | 0.90 | 0.05 | 168,168,168,168            | 1     |
| 3   | IUM  | E     | 535 | 1/3   | 0.92 | 0.07 | 160,160,160,160            | 1     |
| 3   | IUM  | D     | 531 | 1/3   | 0.93 | 0.07 | 144,144,144,144            | 1     |
| 3   | IUM  | A     | 521 | 1/3   | 0.95 | 0.04 | 171,171,171,171            | 1     |
| 3   | IUM  | A     | 523 | 1/3   | 0.97 | 0.04 | 177,177,177,177            | 1     |
| 3   | IUM  | E     | 533 | 1/3   | 0.97 | 0.04 | 152,152,152,152            | 1     |
| 3   | IUM  | A     | 524 | 1/3   | 0.98 | 0.04 | 159,159,159,159            | 1     |
| 3   | IUM  | C     | 528 | 1/3   | 0.99 | 0.02 | 130,130,130,130            | 1     |
| 3   | IUM  | C     | 529 | 1/3   | 0.99 | 0.03 | 108,108,108,108            | 1     |
| 3   | IUM  | C     | 530 | 1/3   | 0.99 | 0.03 | 151,151,151,151            | 1     |
| 3   | IUM  | A     | 522 | 1/3   | 0.99 | 0.04 | 113,113,113,113            | 1     |
| 3   | IUM  | D     | 532 | 1/3   | 0.99 | 0.03 | 119,119,119,119            | 0     |
| 3   | IUM  | A     | 534 | 1/3   | 0.99 | 0.04 | 128,128,128,128            | 0     |
| 3   | IUM  | B     | 526 | 1/3   | 1.00 | 0.05 | 103,103,103,103            | 1     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.