



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:05 PM UTC

PDB ID : 3HTX / pdb\_00003htx  
Title : Crystal structure of small RNA methyltransferase HEN1  
Authors : Huang, Y.; Ji, L.-J.; Huang, Q.-C.; Vassylyev, D.G.; Chen, X.-M.; Ma, J.-B.  
Deposited on : 2009-06-12  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

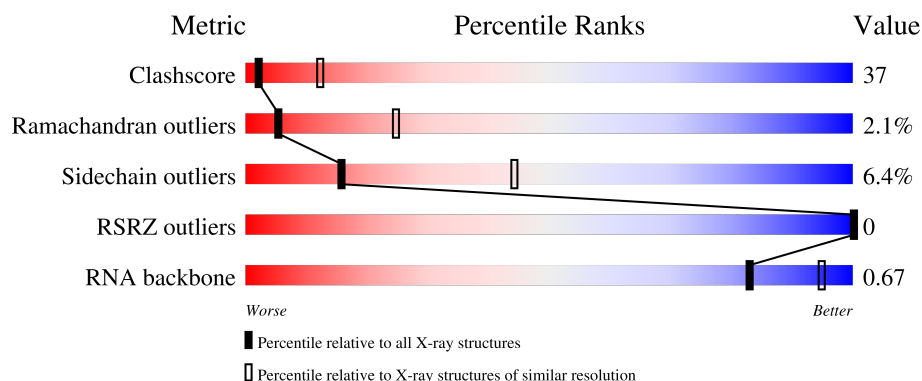
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |
| RNA backbone          | 3983                        | 1022 (3.32-2.88)                                      |

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     | 950    | <div> <div>35%</div> <div>40%</div> <div>6%</div> <div>18%</div> </div> |
| 1   | D     | 950    | <div> <div>34%</div> <div>43%</div> <div>6%</div> <div>16%</div> </div> |
| 2   | B     | 22     | <div> <div>9%</div> <div>77%</div> <div>14%</div> </div>                |
| 2   | E     | 22     | <div> <div>32%</div> <div>59%</div> <div>9%</div> </div>                |
| 3   | C     | 22     | <div> <div>27%</div> <div>64%</div> <div>9%</div> </div>                |

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| Mol | Chain | Length | Quality of chain                                                                                                                                                                                                                                                                        |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 3   | F     | 22     |  A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (55%), yellow (27%), orange (14%), and red (5%). The percentages are labeled below each segment. |

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14269 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 HEN1.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 779      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6093  | 3847 | 1046 | 1170 | 30 |         |         |       |
| 1   | D     | 795      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6217  | 3928 | 1065 | 1194 | 30 |         |         |       |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | -7      | MET      | -      | expression tag      | UNP Q945R3 |
| A     | -6      | GLY      | -      | expression tag      | UNP Q945R3 |
| A     | -5      | HIS      | -      | expression tag      | UNP Q945R3 |
| A     | -4      | HIS      | -      | expression tag      | UNP Q945R3 |
| A     | -3      | HIS      | -      | expression tag      | UNP Q945R3 |
| A     | -2      | HIS      | -      | expression tag      | UNP Q945R3 |
| A     | -1      | HIS      | -      | expression tag      | UNP Q945R3 |
| A     | 0       | HIS      | -      | expression tag      | UNP Q945R3 |
| A     | 604     | PRO      | LEU    | engineered mutation | UNP Q945R3 |
| A     | 640     | LYS      | ARG    | engineered mutation | UNP Q945R3 |
| D     | -7      | MET      | -      | expression tag      | UNP Q945R3 |
| D     | -6      | GLY      | -      | expression tag      | UNP Q945R3 |
| D     | -5      | HIS      | -      | expression tag      | UNP Q945R3 |
| D     | -4      | HIS      | -      | expression tag      | UNP Q945R3 |
| D     | -3      | HIS      | -      | expression tag      | UNP Q945R3 |
| D     | -2      | HIS      | -      | expression tag      | UNP Q945R3 |
| D     | -1      | HIS      | -      | expression tag      | UNP Q945R3 |
| D     | 0       | HIS      | -      | expression tag      | UNP Q945R3 |
| D     | 604     | PRO      | LEU    | engineered mutation | UNP Q945R3 |
| D     | 640     | LYS      | ARG    | engineered mutation | UNP Q945R3 |

- Molecule 2 is a RNA chain called 5'-R(\*GP\*AP\*UP\*UP\*UP\*CP\*UP\*CP\*UP\*CP\*UP\*GP\*CP\*AP\*AP\*GP\*CP\*GP\*AP\*AP\*AP\*G)-3'.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 2   | B     | 22       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 464   | 209 | 82 | 152 | 21 |         |         |       |
| 2   | E     | 22       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 464   | 209 | 82 | 152 | 21 |         |         |       |

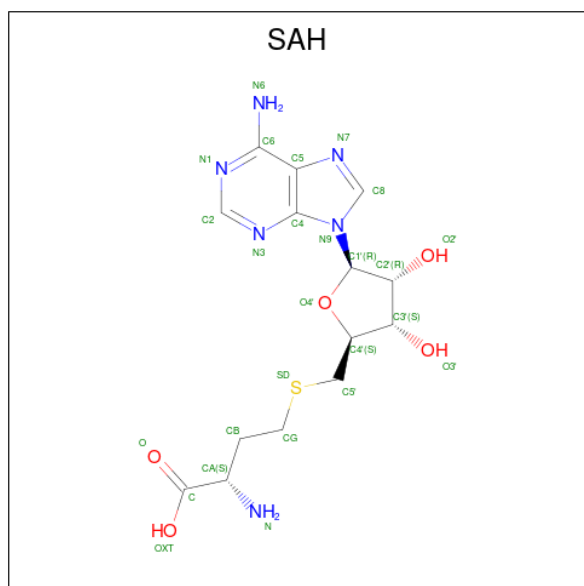
- Molecule 3 is a RNA chain called 5'-R(P\*UP\*UP\*CP\*GP\*CP\*UP\*UP\*GP\*CP\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*AP\*UP\*CP\*AP\*C)-3'.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 3   | C     | 22       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 470   | 210 | 85 | 153 | 22 |         |         |       |
| 3   | F     | 22       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 470   | 210 | 85 | 153 | 22 |         |         |       |

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

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

- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 5   | A     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 26    | 14 | 6 | 5 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 5   | D     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 26    | 14 | 6 | 5 | 1 |         |         |

- Molecule 6 is water.

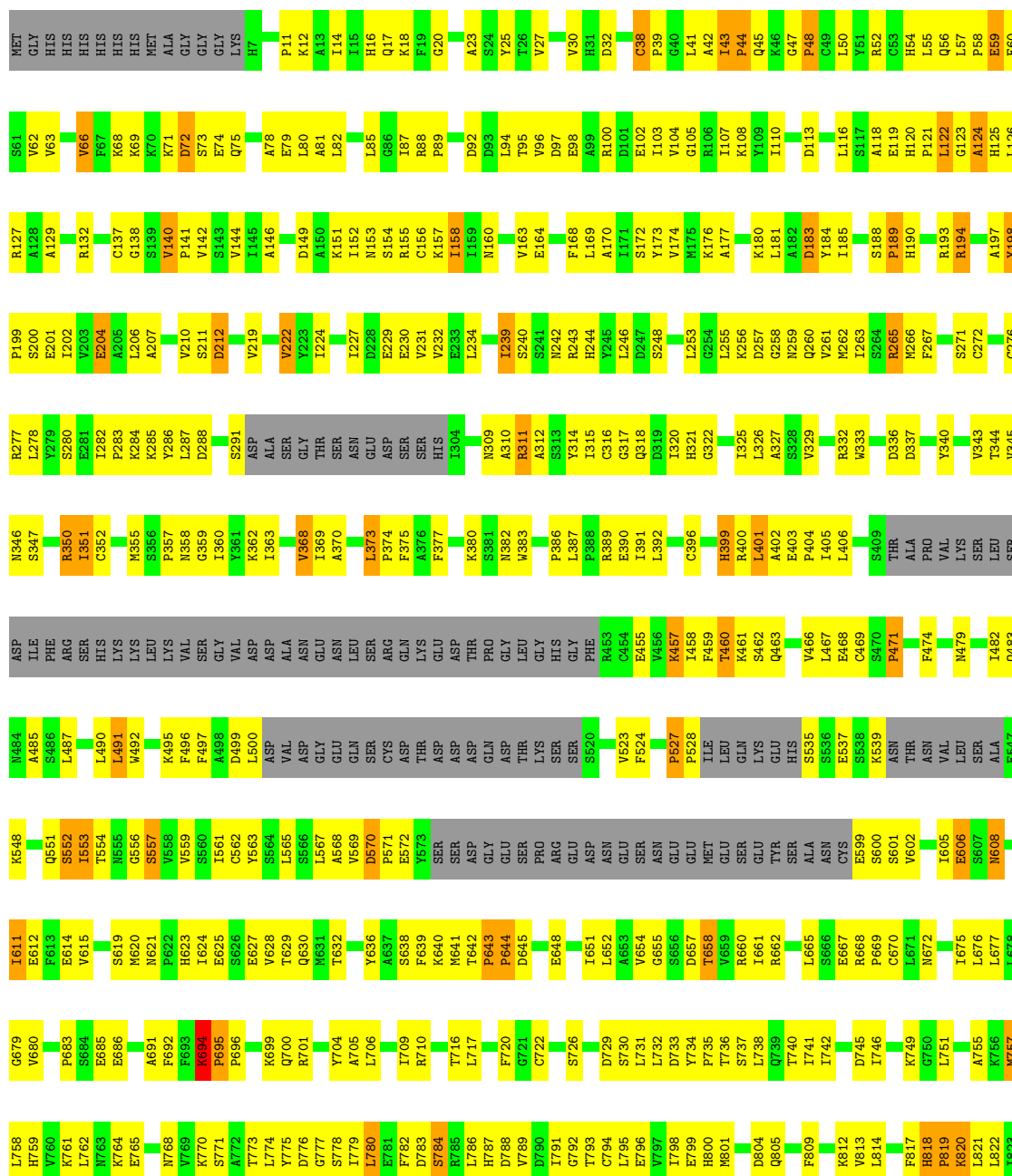
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 6   | B     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 6   | C     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 6   | D     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 6   | E     | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 6   | F     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |





• Molecule 1: HEN1

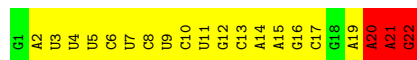
Chain D: 34% 43% 6% 16%





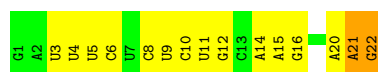
• Molecule 2: 5'-R(\*GP\*AP\*UP\*UP\*UP\*CP\*UP\*CP\*UP\*CP\*UP\*GP\*CP\*AP\*AP\*GP\*CP\*GP\*AP\*AP\*AP\*G)-3'

Chain B: 9% 77% 14%



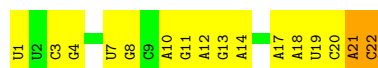
• Molecule 2: 5'-R(\*GP\*AP\*UP\*UP\*UP\*CP\*UP\*CP\*UP\*CP\*UP\*GP\*CP\*AP\*AP\*GP\*CP\*GP\*AP\*AP\*AP\*G)-3'

Chain E: 32% 59% 9%



• Molecule 3: 5'-R(P\*UP\*UP\*CP\*GP\*CP\*UP\*UP\*GP\*CP\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*AP\*AP\*UP\*CP\*AP\*C)-3'

Chain C: 27% 64% 9%



• Molecule 3: 5'-R(P\*UP\*UP\*CP\*GP\*CP\*UP\*UP\*GP\*CP\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*AP\*AP\*UP\*CP\*AP\*C)-3'

Chain F: 55% 27% 14% 5%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 97.00Å 124.35Å 101.38Å<br>90.00° 93.47° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 20.00 – 3.10<br>20.00 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 92.8 (20.00-3.10)<br>77.9 (20.00-3.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.59 (at 3.09Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.260 , 0.288<br>0.244 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 72.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.237                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.21 , 32.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$ | Xtriage          |
| Estimated twinning fraction                                             | 0.054 for l,-k,h                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 14269                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 106.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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     | 0.64         | 1/6214 (0.0%)  | 1.17        | 58/8395 (0.7%)   |
| 1   | D     | 0.64         | 2/6343 (0.0%)  | 1.20        | 54/8573 (0.6%)   |
| 2   | B     | 0.38         | 0/518          | 0.94        | 6/805 (0.7%)     |
| 2   | E     | 0.36         | 0/518          | 0.76        | 1/805 (0.1%)     |
| 3   | C     | 0.42         | 0/525          | 0.61        | 0/814            |
| 3   | F     | 0.44         | 0/525          | 0.81        | 1/814 (0.1%)     |
| All | All   | 0.61         | 3/14643 (0.0%) | 1.13        | 120/20206 (0.6%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 927 | ILE  | CA-CB | -5.61 | 1.48        | 1.54     |
| 1   | D     | 553 | ILE  | N-CA  | -5.31 | 1.39        | 1.46     |
| 1   | A     | 852 | LEU  | N-CA  | -5.25 | 1.40        | 1.46     |

All (120) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1   | D     | 818 | HIS  | CA-C-N      | 15.28  | 136.50      | 119.99   |
| 1   | D     | 818 | HIS  | C-N-CA      | 15.28  | 136.50      | 119.99   |
| 1   | D     | 695 | PRO  | N-CA-C      | -12.58 | 95.36       | 110.70   |
| 2   | B     | 20  | A    | C2'-C3'-O3' | 11.75  | 131.33      | 113.70   |
| 1   | A     | 764 | LYS  | N-CA-C      | -10.76 | 96.33       | 110.43   |
| 1   | D     | 694 | LYS  | CA-C-N      | -10.29 | 109.78      | 120.38   |
| 1   | D     | 694 | LYS  | C-N-CA      | -10.29 | 109.78      | 120.38   |
| 1   | A     | 852 | LEU  | N-CA-C      | -9.97  | 99.25       | 108.22   |
| 1   | A     | 695 | PRO  | N-CA-C      | -9.83  | 98.71       | 110.70   |
| 1   | A     | 789 | VAL  | CB-CA-C     | -9.56  | 97.08       | 111.33   |
| 3   | F     | 19  | U    | C2'-C3'-O3' | 9.37   | 127.75      | 113.70   |
| 1   | A     | 818 | HIS  | CA-C-N      | -8.93  | 110.83      | 119.76   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 818 | HIS  | C-N-CA      | -8.93 | 110.83      | 119.76   |
| 1   | D     | 768 | ASN  | N-CA-C      | -8.84 | 103.34      | 114.56   |
| 1   | D     | 499 | ASP  | N-CA-C      | -8.77 | 95.64       | 109.50   |
| 1   | D     | 523 | VAL  | N-CA-C      | 8.64  | 120.21      | 108.11   |
| 1   | A     | 643 | PRO  | N-CA-C      | -8.45 | 100.39      | 110.70   |
| 1   | A     | 336 | ASP  | N-CA-C      | -8.40 | 103.04      | 113.38   |
| 1   | D     | 527 | PRO  | N-CA-C      | 8.18  | 120.68      | 110.70   |
| 1   | A     | 656 | SER  | N-CA-C      | 8.08  | 119.71      | 111.07   |
| 1   | D     | 66  | VAL  | N-CA-C      | 8.05  | 121.22      | 109.63   |
| 1   | D     | 399 | HIS  | N-CA-C      | -8.01 | 98.61       | 110.46   |
| 1   | A     | 694 | LYS  | CA-C-N      | -7.97 | 112.17      | 120.38   |
| 1   | A     | 694 | LYS  | C-N-CA      | -7.97 | 112.17      | 120.38   |
| 2   | B     | 21  | A    | C2'-C3'-O3' | 7.73  | 121.09      | 109.50   |
| 1   | A     | 554 | THR  | N-CA-C      | 7.71  | 122.92      | 109.96   |
| 1   | D     | 122 | LEU  | N-CA-C      | 7.67  | 119.64      | 111.28   |
| 1   | D     | 20  | GLY  | N-CA-C      | -7.62 | 95.12       | 113.18   |
| 1   | D     | 288 | ASP  | N-CA-C      | 7.61  | 119.21      | 111.07   |
| 1   | A     | 95  | THR  | N-CA-C      | -7.50 | 98.35       | 110.20   |
| 1   | D     | 317 | GLY  | N-CA-C      | -7.49 | 104.52      | 114.25   |
| 1   | A     | 261 | VAL  | N-CA-C      | 7.31  | 119.00      | 109.58   |
| 1   | D     | 780 | LEU  | N-CA-C      | -7.27 | 104.67      | 113.97   |
| 1   | A     | 276 | CYS  | N-CA-C      | 7.25  | 121.47      | 109.95   |
| 1   | D     | 819 | PRO  | N-CA-C      | -7.23 | 98.95       | 111.32   |
| 1   | D     | 814 | LEU  | N-CA-C      | 7.20  | 118.77      | 111.07   |
| 1   | A     | 858 | HIS  | N-CA-C      | -7.09 | 104.99      | 112.93   |
| 1   | D     | 38  | CYS  | CA-C-N      | 7.01  | 127.18      | 120.31   |
| 1   | D     | 38  | CYS  | C-N-CA      | 7.01  | 127.18      | 120.31   |
| 1   | A     | 385 | GLY  | CA-C-N      | 6.99  | 127.41      | 119.93   |
| 1   | A     | 385 | GLY  | C-N-CA      | 6.99  | 127.41      | 119.93   |
| 1   | A     | 94  | LEU  | N-CA-C      | 6.97  | 121.68      | 109.96   |
| 1   | D     | 552 | SER  | N-CA-C      | -6.96 | 99.59       | 109.96   |
| 1   | D     | 327 | ALA  | N-CA-C      | 6.85  | 118.60      | 108.60   |
| 1   | D     | 692 | PHE  | N-CA-C      | 6.81  | 119.28      | 111.11   |
| 1   | A     | 347 | SER  | N-CA-C      | -6.79 | 103.96      | 111.36   |
| 1   | A     | 163 | VAL  | CB-CA-C     | -6.73 | 103.05      | 112.14   |
| 1   | A     | 712 | SER  | N-CA-C      | -6.62 | 97.94       | 108.73   |
| 1   | A     | 633 | VAL  | N-CA-C      | 6.61  | 117.86      | 108.93   |
| 2   | E     | 22  | G    | C4'-C3'-O3' | -6.57 | 103.14      | 113.00   |
| 1   | D     | 222 | VAL  | N-CA-C      | 6.44  | 117.12      | 108.11   |
| 1   | A     | 498 | ALA  | N-CA-C      | 6.42  | 119.03      | 109.59   |
| 1   | A     | 675 | ILE  | N-CA-C      | 6.35  | 117.06      | 108.17   |
| 2   | B     | 21  | A    | C5'-C4'-C3' | -6.31 | 105.74      | 115.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 22  | G    | C2'-C3'-O3' | 6.27  | 123.10      | 113.70   |
| 1   | A     | 682 | GLY  | CA-C-N      | 6.25  | 126.22      | 120.03   |
| 1   | A     | 682 | GLY  | C-N-CA      | 6.25  | 126.22      | 120.03   |
| 2   | B     | 21  | A    | C4'-C3'-O3' | 6.24  | 118.77      | 109.40   |
| 1   | A     | 75  | GLN  | N-CA-C      | -6.20 | 104.44      | 111.14   |
| 1   | D     | 884 | VAL  | N-CA-C      | 6.12  | 117.02      | 107.28   |
| 1   | D     | 903 | ILE  | N-CA-C      | 6.09  | 117.06      | 108.17   |
| 1   | D     | 212 | ASP  | N-CA-C      | 6.08  | 118.81      | 111.40   |
| 1   | D     | 373 | LEU  | CA-C-N      | 6.07  | 125.98      | 119.85   |
| 1   | D     | 373 | LEU  | C-N-CA      | 6.07  | 125.98      | 119.85   |
| 1   | D     | 321 | HIS  | N-CA-C      | 6.06  | 119.42      | 109.85   |
| 1   | D     | 557 | SER  | N-CA-C      | 6.05  | 119.03      | 110.50   |
| 1   | A     | 864 | TRP  | N-CA-C      | 6.04  | 119.50      | 110.14   |
| 1   | D     | 860 | HIS  | N-CA-C      | -5.99 | 100.04      | 109.50   |
| 1   | D     | 124 | ALA  | N-CA-C      | -5.95 | 104.79      | 111.28   |
| 1   | A     | 562 | CYS  | N-CA-C      | -5.95 | 97.43       | 108.02   |
| 1   | A     | 635 | GLU  | N-CA-C      | 5.91  | 118.84      | 110.50   |
| 1   | A     | 151 | LYS  | N-CA-C      | -5.85 | 104.81      | 111.07   |
| 1   | A     | 769 | VAL  | N-CA-C      | 5.82  | 117.58      | 109.55   |
| 2   | B     | 22  | G    | C4'-C3'-O3' | -5.81 | 104.28      | 113.00   |
| 1   | D     | 658 | THR  | N-CA-C      | 5.80  | 119.17      | 111.75   |
| 1   | D     | 310 | ALA  | N-CA-C      | 5.79  | 118.08      | 111.02   |
| 1   | D     | 820 | LYS  | N-CA-C      | -5.72 | 105.56      | 112.54   |
| 1   | A     | 259 | ASN  | N-CA-C      | -5.71 | 106.15      | 113.01   |
| 1   | A     | 183 | ASP  | N-CA-C      | 5.69  | 118.25      | 111.71   |
| 1   | A     | 198 | TYR  | N-CA-C      | -5.62 | 102.70      | 109.83   |
| 1   | D     | 360 | ILE  | CB-CA-C     | -5.61 | 104.78      | 111.97   |
| 1   | D     | 930 | TRP  | N-CA-C      | 5.59  | 117.33      | 107.61   |
| 1   | D     | 800 | HIS  | N-CA-C      | -5.56 | 106.70      | 112.93   |
| 1   | A     | 224 | ILE  | CB-CA-C     | -5.56 | 104.39      | 110.78   |
| 1   | A     | 654 | VAL  | N-CA-C      | 5.56  | 117.06      | 111.00   |
| 1   | A     | 642 | THR  | N-CA-C      | -5.55 | 105.06      | 112.55   |
| 1   | D     | 474 | PHE  | N-CA-C      | 5.53  | 117.72      | 109.59   |
| 1   | A     | 865 | THR  | N-CA-C      | -5.52 | 103.40      | 110.53   |
| 1   | A     | 884 | VAL  | N-CA-C      | 5.52  | 115.89      | 108.17   |
| 1   | A     | 654 | VAL  | CB-CA-C     | -5.50 | 104.87      | 112.24   |
| 1   | A     | 96  | VAL  | N-CA-C      | 5.49  | 116.13      | 110.36   |
| 1   | D     | 52  | ARG  | N-CA-C      | -5.44 | 100.81      | 109.23   |
| 1   | A     | 628 | VAL  | N-CA-C      | 5.41  | 116.18      | 110.72   |
| 1   | A     | 233 | GLU  | N-CA-C      | 5.39  | 117.87      | 109.52   |
| 1   | A     | 780 | LEU  | N-CA-C      | -5.39 | 106.74      | 113.15   |
| 1   | A     | 614 | GLU  | N-CA-C      | -5.35 | 102.36      | 110.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 540 | ASN  | N-CA-C  | 5.35  | 116.14      | 107.32   |
| 1   | D     | 368 | VAL  | N-CA-C  | 5.33  | 116.70      | 110.62   |
| 1   | D     | 198 | TYR  | CA-C-N  | -5.31 | 114.48      | 119.90   |
| 1   | D     | 198 | TYR  | C-N-CA  | -5.31 | 114.48      | 119.90   |
| 1   | D     | 460 | THR  | CA-C-N  | -5.31 | 115.71      | 122.77   |
| 1   | D     | 460 | THR  | C-N-CA  | -5.31 | 115.71      | 122.77   |
| 1   | D     | 788 | ASP  | N-CA-C  | 5.30  | 118.75      | 111.54   |
| 1   | A     | 258 | GLY  | N-CA-C  | -5.26 | 100.71      | 113.18   |
| 1   | D     | 198 | TYR  | N-CA-C  | -5.23 | 103.19      | 109.83   |
| 1   | D     | 645 | ASP  | N-CA-C  | 5.19  | 118.39      | 111.75   |
| 1   | A     | 796 | GLU  | N-CA-C  | 5.17  | 118.86      | 112.24   |
| 1   | D     | 818 | HIS  | N-CA-C  | 5.16  | 119.88      | 108.27   |
| 1   | A     | 166 | ASP  | CA-C-N  | 5.15  | 124.81      | 119.56   |
| 1   | A     | 166 | ASP  | C-N-CA  | 5.15  | 124.81      | 119.56   |
| 1   | A     | 806 | ALA  | N-CA-C  | -5.10 | 105.64      | 111.14   |
| 1   | A     | 655 | GLY  | N-CA-C  | 5.09  | 125.25      | 113.18   |
| 1   | D     | 784 | SER  | N-CA-C  | 5.07  | 118.24      | 111.75   |
| 1   | A     | 815 | SER  | N-CA-C  | 5.06  | 117.91      | 111.69   |
| 1   | D     | 351 | ILE  | CB-CA-C | -5.05 | 105.47      | 112.24   |
| 1   | A     | 360 | ILE  | CB-CA-C | -5.02 | 105.47      | 112.04   |
| 1   | A     | 789 | VAL  | N-CA-CB | 5.02  | 116.48      | 110.31   |
| 1   | A     | 488 | LYS  | N-CA-C  | -5.00 | 105.72      | 111.07   |
| 1   | D     | 140 | VAL  | CA-C-N  | 5.00  | 125.23      | 119.83   |
| 1   | D     | 140 | VAL  | C-N-CA  | 5.00  | 125.23      | 119.83   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 6093  | 0        | 6031     | 447     | 0            |
| 1   | D     | 6217  | 0        | 6139     | 512     | 0            |
| 2   | B     | 464   | 0        | 236      | 36      | 0            |
| 2   | E     | 464   | 0        | 236      | 20      | 0            |
| 3   | C     | 470   | 0        | 238      | 20      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | F     | 470   | 0        | 238      | 17      | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 26    | 0        | 19       | 2       | 0            |
| 5   | D     | 26    | 0        | 19       | 1       | 0            |
| 6   | A     | 14    | 0        | 0        | 5       | 0            |
| 6   | B     | 2     | 0        | 0        | 2       | 0            |
| 6   | C     | 2     | 0        | 0        | 0       | 0            |
| 6   | D     | 16    | 0        | 0        | 2       | 0            |
| 6   | E     | 1     | 0        | 0        | 0       | 0            |
| 6   | F     | 2     | 0        | 0        | 1       | 0            |
| All | All   | 14269 | 0        | 13156    | 1019    | 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 37.

All (1019) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:802:GLU:HB2  | 1:A:805:GLN:HG3  | 1.21                     | 1.20              |
| 3:F:21:A:H2'     | 6:F:226:HOH:O    | 1.45                     | 1.12              |
| 1:D:776:ASP:HB2  | 1:D:927:ILE:HD11 | 1.34                     | 1.07              |
| 1:A:45:GLN:HE21  | 1:A:752:ALA:HB1  | 1.18                     | 1.07              |
| 1:A:401:LEU:HD22 | 1:A:461:LYS:HB2  | 1.39                     | 1.03              |
| 1:A:142:VAL:HG11 | 1:A:171:ILE:HG23 | 1.43                     | 1.01              |
| 1:A:15:ILE:HG21  | 1:A:82:LEU:HD11  | 1.43                     | 1.00              |
| 1:D:570:ASP:H    | 1:D:571:PRO:HD2  | 1.27                     | 0.98              |
| 1:D:457:LYS:HE2  | 1:D:457:LYS:HA   | 1.46                     | 0.97              |
| 1:A:183:ASP:HA   | 6:A:947:HOH:O    | 1.66                     | 0.95              |
| 1:D:43:ILE:N     | 1:D:44:PRO:HD3   | 1.82                     | 0.94              |
| 1:D:836:GLN:HE22 | 1:D:854:LYS:HB2  | 1.29                     | 0.94              |
| 1:A:45:GLN:NE2   | 1:A:752:ALA:HB1  | 1.82                     | 0.93              |
| 1:D:401:LEU:HD22 | 1:D:461:LYS:HD3  | 1.51                     | 0.93              |
| 1:A:82:LEU:HD23  | 1:A:85:LEU:HD12  | 1.50                     | 0.92              |
| 1:D:262:MET:HB2  | 1:D:282:ILE:HG12 | 1.52                     | 0.92              |
| 1:A:405:ILE:HB   | 1:A:458:ILE:HG12 | 1.53                     | 0.91              |
| 1:A:798:ILE:HA   | 1:A:801:MET:HE3  | 1.55                     | 0.89              |
| 1:D:116:LEU:HG   | 1:D:206:LEU:HD11 | 1.53                     | 0.89              |
| 1:D:757:MET:HG3  | 1:D:758:LEU:N    | 1.85                     | 0.89              |
| 1:D:265:ARG:H    | 1:D:318:GLN:NE2  | 1.71                     | 0.88              |
| 1:A:244:HIS:HD2  | 1:A:246:LEU:H    | 1.18                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:244:HIS:CD2  | 1:D:246:LEU:HB2  | 2.09                     | 0.88              |
| 1:A:400:ARG:O    | 1:A:401:LEU:HD23 | 1.74                     | 0.87              |
| 1:D:570:ASP:H    | 1:D:571:PRO:CD   | 1.88                     | 0.87              |
| 1:D:716:THR:HG22 | 1:D:740:THR:HB   | 1.56                     | 0.87              |
| 1:A:810:GLY:HA3  | 1:A:876:LEU:HD21 | 1.57                     | 0.86              |
| 1:A:457:LYS:HZ3  | 1:A:486:SER:HA   | 1.41                     | 0.86              |
| 1:A:401:LEU:HD22 | 1:A:461:LYS:CB   | 2.04                     | 0.86              |
| 1:D:88:ARG:HG2   | 1:D:89:PRO:HD2   | 1.57                     | 0.86              |
| 1:D:262:MET:HB2  | 1:D:282:ILE:CG1  | 2.06                     | 0.86              |
| 1:D:817:PHE:O    | 1:D:819:PRO:HD2  | 1.77                     | 0.85              |
| 1:D:817:PHE:C    | 1:D:819:PRO:HD2  | 2.02                     | 0.84              |
| 1:D:43:ILE:N     | 1:D:44:PRO:CD    | 2.39                     | 0.84              |
| 1:D:262:MET:HE3  | 1:D:263:ILE:H    | 1.41                     | 0.83              |
| 1:A:831:PHE:O    | 1:A:834:ILE:HG22 | 1.76                     | 0.83              |
| 1:A:365:ARG:HG3  | 1:A:365:ARG:HH11 | 1.44                     | 0.83              |
| 1:D:265:ARG:H    | 1:D:318:GLN:HE22 | 1.21                     | 0.83              |
| 1:D:729:ASP:HB2  | 1:D:757:MET:SD   | 2.19                     | 0.83              |
| 1:D:710:ARG:NH2  | 1:D:734:TYR:HB2  | 1.92                     | 0.83              |
| 1:D:776:ASP:HB2  | 1:D:927:ILE:CD1  | 2.07                     | 0.83              |
| 1:A:255:LEU:HD11 | 1:A:281:GLU:HB2  | 1.62                     | 0.82              |
| 1:A:88:ARG:HG3   | 1:A:89:PRO:HD3   | 1.59                     | 0.82              |
| 1:A:742:ILE:HD13 | 1:A:786:LEU:HD22 | 1.62                     | 0.82              |
| 1:A:757:MET:HE3  | 1:A:761:LYS:HG3  | 1.61                     | 0.82              |
| 1:D:387:LEU:HB3  | 1:D:483:GLN:HE22 | 1.45                     | 0.82              |
| 1:D:23:ALA:CB    | 1:D:57:LEU:HD23  | 2.09                     | 0.81              |
| 1:A:405:ILE:HD12 | 1:A:458:ILE:HD11 | 1.61                     | 0.81              |
| 1:A:127:ARG:HG3  | 1:A:206:LEU:HD21 | 1.63                     | 0.81              |
| 1:D:124:ALA:HA   | 1:D:127:ARG:NH1  | 1.96                     | 0.81              |
| 1:D:621:ASN:HD22 | 1:D:624:ILE:HG13 | 1.45                     | 0.81              |
| 1:D:548:LYS:O    | 1:D:552:SER:HB2  | 1.80                     | 0.81              |
| 1:D:892:SER:HB2  | 1:D:895:VAL:HG23 | 1.62                     | 0.80              |
| 1:A:126:LEU:HD23 | 1:A:140:VAL:HG21 | 1.63                     | 0.80              |
| 1:D:43:ILE:HD11  | 1:D:927:ILE:HD13 | 1.64                     | 0.80              |
| 1:A:262:MET:HE3  | 1:A:263:ILE:H    | 1.46                     | 0.80              |
| 1:A:569:VAL:HG23 | 1:A:601:SER:HB2  | 1.61                     | 0.80              |
| 1:A:865:THR:H    | 1:A:868:GLN:NE2  | 1.80                     | 0.80              |
| 1:A:624:ILE:HG23 | 1:A:675:ILE:HD11 | 1.65                     | 0.79              |
| 1:D:57:LEU:HB3   | 1:D:58:PRO:HD2   | 1.62                     | 0.79              |
| 1:D:105:GLY:O    | 1:D:108:LYS:HG2  | 1.82                     | 0.79              |
| 1:D:570:ASP:N    | 1:D:571:PRO:HD2  | 1.96                     | 0.79              |
| 1:A:895:VAL:HG12 | 1:A:897:PRO:HD2  | 1.64                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:387:LEU:HB3  | 1:D:483:GLN:NE2  | 1.98                     | 0.79              |
| 1:A:537:GLU:HB3  | 1:A:641:MET:CE   | 2.12                     | 0.79              |
| 1:D:559:VAL:HG12 | 1:D:561:ILE:HG23 | 1.63                     | 0.79              |
| 1:D:799:GLU:HG3  | 1:D:860:HIS:CD2  | 2.18                     | 0.79              |
| 1:D:740:THR:HG23 | 1:D:771:SER:HB3  | 1.66                     | 0.78              |
| 1:D:829:TYR:HD1  | 1:D:832:ASN:HD21 | 1.29                     | 0.78              |
| 1:D:266:MET:HB3  | 1:D:277:ARG:HE   | 1.47                     | 0.78              |
| 1:A:457:LYS:NZ   | 1:A:486:SER:HA   | 1.98                     | 0.78              |
| 1:D:405:ILE:HB   | 1:D:458:ILE:HG13 | 1.66                     | 0.78              |
| 2:E:8:C:H2'      | 2:E:9:U:C6       | 2.20                     | 0.77              |
| 1:A:108:LYS:HD2  | 1:A:181:LEU:HD21 | 1.66                     | 0.77              |
| 1:A:151:LYS:O    | 1:A:155:ARG:HG2  | 1.85                     | 0.77              |
| 1:D:557:SER:O    | 1:D:615:VAL:HG23 | 1.84                     | 0.77              |
| 1:D:461:LYS:HG3  | 1:D:466:VAL:HG21 | 1.65                     | 0.77              |
| 1:A:123:GLY:O    | 1:A:127:ARG:HB2  | 1.86                     | 0.76              |
| 1:D:552:SER:HA   | 1:D:629:THR:O    | 1.86                     | 0.76              |
| 1:A:852:LEU:HB2  | 1:A:855:PHE:CE1  | 2.20                     | 0.76              |
| 1:A:865:THR:H    | 1:A:868:GLN:HE21 | 1.30                     | 0.76              |
| 1:A:537:GLU:HB3  | 1:A:641:MET:HE1  | 1.67                     | 0.76              |
| 3:F:19:U:O2'     | 3:F:20:C:H5'     | 1.86                     | 0.76              |
| 1:D:164:GLU:HB3  | 1:D:400:ARG:HH12 | 1.48                     | 0.75              |
| 1:A:318:GLN:HG3  | 1:A:400:ARG:HH22 | 1.50                     | 0.75              |
| 1:D:895:VAL:HG12 | 1:D:897:PRO:HD2  | 1.67                     | 0.75              |
| 1:A:827:PRO:HA   | 1:A:901:SER:HA   | 1.68                     | 0.75              |
| 3:F:18:A:H2'     | 3:F:19:U:C6      | 2.21                     | 0.75              |
| 1:A:553:ILE:HD12 | 1:A:629:THR:HA   | 1.68                     | 0.75              |
| 1:D:568:ALA:HB1  | 1:D:601:SER:O    | 1.85                     | 0.75              |
| 1:D:830:GLU:HG3  | 1:D:865:THR:HG23 | 1.69                     | 0.75              |
| 1:D:181:LEU:HG   | 1:D:184:TYR:HB2  | 1.68                     | 0.74              |
| 1:A:704:TYR:HA   | 1:A:707:LYS:HE3  | 1.69                     | 0.74              |
| 1:D:41:LEU:HD21  | 1:D:755:ALA:HB1  | 1.69                     | 0.74              |
| 1:D:606:GLU:HB3  | 1:D:654:VAL:HG11 | 1.70                     | 0.74              |
| 1:A:650:LEU:O    | 1:A:654:VAL:HG23 | 1.86                     | 0.74              |
| 1:D:552:SER:HA   | 1:D:629:THR:HG22 | 1.68                     | 0.74              |
| 1:D:12:LYS:HG3   | 1:D:79:GLU:HB2   | 1.69                     | 0.74              |
| 1:A:368:VAL:HB   | 1:A:650:LEU:HD11 | 1.68                     | 0.74              |
| 1:D:16:HIS:NE2   | 1:D:82:LEU:HG    | 2.03                     | 0.74              |
| 3:F:19:U:H2'     | 3:F:20:C:H6      | 1.53                     | 0.73              |
| 1:A:47:GLY:HA2   | 2:B:15:A:H4'     | 1.69                     | 0.73              |
| 1:D:283:PRO:HG2  | 1:D:286:TYR:HD1  | 1.54                     | 0.73              |
| 1:D:627:GLU:HB2  | 6:D:955:HOH:O    | 1.86                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:731:LEU:HD21 | 1:D:738:LEU:HD13 | 1.71                     | 0.73              |
| 1:A:392:LEU:HD22 | 1:A:457:LYS:HZ2  | 1.54                     | 0.73              |
| 1:A:864:TRP:HA   | 1:A:868:GLN:NE2  | 2.03                     | 0.73              |
| 1:D:866:ARG:NH1  | 1:D:898:GLY:HA3  | 2.03                     | 0.73              |
| 1:A:10:THR:HG21  | 1:A:90:GLN:HG2   | 1.69                     | 0.72              |
| 1:D:836:GLN:NE2  | 1:D:854:LYS:HB2  | 2.04                     | 0.72              |
| 1:A:94:LEU:HD23  | 1:A:99:ALA:HB2   | 1.72                     | 0.72              |
| 1:A:569:VAL:O    | 1:A:571:PRO:HD3  | 1.88                     | 0.72              |
| 1:D:710:ARG:CZ   | 1:D:734:TYR:HB2  | 2.19                     | 0.72              |
| 1:D:88:ARG:CG    | 1:D:89:PRO:HD2   | 2.20                     | 0.72              |
| 1:A:364:SER:HB3  | 1:A:386:PRO:HG2  | 1.70                     | 0.72              |
| 1:D:784:SER:HB3  | 1:D:920:SER:HA   | 1.73                     | 0.71              |
| 1:D:628:VAL:CG2  | 1:D:675:ILE:HD12 | 2.21                     | 0.71              |
| 1:D:731:LEU:HD11 | 1:D:738:LEU:HD12 | 1.72                     | 0.71              |
| 1:D:164:GLU:HB3  | 1:D:400:ARG:NH1  | 2.05                     | 0.71              |
| 1:A:253:LEU:HD21 | 1:A:325:ILE:HG12 | 1.72                     | 0.71              |
| 1:A:262:MET:CE   | 1:A:263:ILE:H    | 2.04                     | 0.71              |
| 1:D:244:HIS:HD2  | 1:D:246:LEU:HB2  | 1.54                     | 0.71              |
| 1:D:402:ALA:HB3  | 1:D:460:THR:O    | 1.91                     | 0.71              |
| 1:A:364:SER:CB   | 1:A:386:PRO:HG2  | 2.21                     | 0.71              |
| 1:D:283:PRO:HG2  | 1:D:286:TYR:CD1  | 2.26                     | 0.71              |
| 1:D:553:ILE:H    | 1:D:629:THR:HG23 | 1.56                     | 0.71              |
| 1:D:278:LEU:HD21 | 1:D:312:ALA:HB1  | 1.73                     | 0.70              |
| 1:A:888:GLY:C    | 1:A:899:PHE:CD2  | 2.70                     | 0.70              |
| 1:D:742:ILE:HG21 | 1:D:786:LEU:HD21 | 1.73                     | 0.70              |
| 1:D:628:VAL:HG22 | 1:D:675:ILE:HD12 | 1.72                     | 0.70              |
| 1:D:160:ASN:O    | 1:D:163:VAL:HG23 | 1.92                     | 0.70              |
| 1:D:232:VAL:HG23 | 1:D:311:ARG:NH2  | 2.07                     | 0.70              |
| 1:A:332:ARG:HG2  | 1:A:333:TRP:H    | 1.57                     | 0.70              |
| 1:A:392:LEU:HD11 | 1:A:459:PHE:HE1  | 1.57                     | 0.70              |
| 1:D:567:LEU:HB2  | 1:D:605:ILE:HD11 | 1.72                     | 0.70              |
| 1:D:827:PRO:HB3  | 1:D:856:ARG:HD2  | 1.72                     | 0.69              |
| 1:A:367:ALA:HB1  | 1:A:370:ALA:HB3  | 1.74                     | 0.69              |
| 1:A:255:LEU:HB3  | 1:A:260:GLN:OE1  | 1.92                     | 0.69              |
| 1:A:667:GLU:O    | 1:A:669:PRO:HD3  | 1.93                     | 0.69              |
| 1:A:887:SER:O    | 1:A:903:ILE:HB   | 1.93                     | 0.69              |
| 1:A:369:ILE:HG21 | 1:A:565:LEU:HD11 | 1.74                     | 0.69              |
| 1:D:81:ALA:O     | 1:D:85:LEU:HG    | 1.93                     | 0.69              |
| 1:A:809:PHE:O    | 1:A:813:VAL:HG23 | 1.93                     | 0.69              |
| 1:A:108:LYS:HB2  | 1:A:181:LEU:HD21 | 1.74                     | 0.69              |
| 3:C:7:U:H2'      | 3:C:8:G:C8       | 2.28                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:110:ILE:HG22 | 1:A:126:LEU:HD11 | 1.74                     | 0.68              |
| 3:F:21:A:H1'     | 3:F:22:C:H5      | 1.57                     | 0.68              |
| 1:D:731:LEU:HD21 | 1:D:738:LEU:CD1  | 2.23                     | 0.68              |
| 1:D:639:PHE:CD1  | 1:D:641:MET:HE3  | 2.29                     | 0.68              |
| 1:D:219:VAL:HG21 | 1:D:239:ILE:HD11 | 1.74                     | 0.68              |
| 1:A:244:HIS:CD2  | 1:A:246:LEU:H    | 2.06                     | 0.68              |
| 1:D:257:ASP:H    | 1:D:260:GLN:HE21 | 1.42                     | 0.68              |
| 1:D:809:PHE:O    | 1:D:813:VAL:HG23 | 1.93                     | 0.68              |
| 1:A:721:GLY:HA3  | 1:A:797:VAL:HG21 | 1.75                     | 0.68              |
| 1:D:559:VAL:CG1  | 1:D:561:ILE:HG23 | 2.23                     | 0.68              |
| 1:D:406:LEU:HD13 | 1:D:457:LYS:HE3  | 1.74                     | 0.68              |
| 1:A:362:LYS:HB3  | 1:A:368:VAL:HA   | 1.76                     | 0.67              |
| 1:A:18:LYS:HE2   | 3:C:19:U:H4'     | 1.75                     | 0.67              |
| 1:A:117:SER:HB3  | 1:A:206:LEU:HD13 | 1.77                     | 0.67              |
| 1:D:43:ILE:O     | 1:D:43:ILE:HG22  | 1.91                     | 0.67              |
| 1:D:152:ILE:O    | 1:D:156:CYS:HB2  | 1.94                     | 0.67              |
| 1:D:265:ARG:HH12 | 1:D:400:ARG:HE   | 1.42                     | 0.67              |
| 1:D:828:ASN:HA   | 1:D:902:GLN:NE2  | 2.10                     | 0.67              |
| 1:D:30:VAL:HG12  | 1:D:32:ASP:H     | 1.58                     | 0.67              |
| 1:D:124:ALA:HA   | 1:D:127:ARG:HH12 | 1.57                     | 0.67              |
| 1:D:194:ARG:HH12 | 1:D:198:TYR:HA   | 1.60                     | 0.67              |
| 1:D:344:THR:H    | 1:D:347:SER:HB2  | 1.60                     | 0.67              |
| 1:A:108:LYS:HB2  | 1:A:181:LEU:CD2  | 2.24                     | 0.67              |
| 1:D:43:ILE:HD11  | 1:D:927:ILE:CD1  | 2.23                     | 0.67              |
| 1:A:742:ILE:HD13 | 1:A:786:LEU:CD2  | 2.24                     | 0.67              |
| 1:D:459:PHE:HB2  | 1:D:466:VAL:HB   | 1.76                     | 0.67              |
| 1:D:691:ALA:HB2  | 2:E:20:A:H5''    | 1.75                     | 0.67              |
| 1:D:347:SER:O    | 1:D:351:ILE:HG12 | 1.94                     | 0.66              |
| 1:A:94:LEU:HB2   | 1:A:158:ILE:HD13 | 1.78                     | 0.66              |
| 1:D:283:PRO:C    | 1:D:285:LYS:H    | 2.02                     | 0.66              |
| 3:C:7:U:H2'      | 3:C:8:G:H8       | 1.59                     | 0.66              |
| 3:C:21:A:H5'     | 3:C:22:C:OP1     | 1.96                     | 0.66              |
| 1:A:753:ARG:O    | 1:A:756:LYS:HG2  | 1.94                     | 0.66              |
| 1:D:23:ALA:HB1   | 1:D:56:GLN:O     | 1.95                     | 0.66              |
| 1:D:458:ILE:HG22 | 1:D:468:GLU:HA   | 1.76                     | 0.66              |
| 1:A:658:THR:O    | 1:A:662:ARG:CG   | 2.43                     | 0.66              |
| 1:A:149:ASP:OD1  | 1:A:151:LYS:HB2  | 1.95                     | 0.65              |
| 1:D:567:LEU:CB   | 1:D:605:ILE:HD11 | 2.26                     | 0.65              |
| 1:A:561:ILE:HD11 | 1:A:613:PHE:HE1  | 1.62                     | 0.65              |
| 1:A:829:TYR:HD1  | 1:A:863:GLU:HB3  | 1.61                     | 0.65              |
| 1:A:888:GLY:O    | 1:A:899:PHE:CE2  | 2.50                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:113:ASP:HB3  | 1:A:202:ILE:HD13 | 1.78                     | 0.65              |
| 1:D:257:ASP:H    | 1:D:260:GLN:NE2  | 1.94                     | 0.65              |
| 1:D:467:LEU:HD13 | 1:D:492:TRP:CZ3  | 2.31                     | 0.65              |
| 1:A:168:PHE:HE2  | 1:A:282:ILE:HA   | 1.62                     | 0.65              |
| 1:A:639:PHE:HE1  | 1:A:641:MET:HE3  | 1.61                     | 0.65              |
| 1:A:921:MET:C    | 1:A:923:PRO:HD3  | 2.22                     | 0.65              |
| 1:A:639:PHE:CE1  | 1:A:641:MET:HE3  | 2.32                     | 0.65              |
| 1:A:779:ILE:HD11 | 1:A:801:MET:HE1  | 1.78                     | 0.65              |
| 1:A:57:LEU:HG    | 1:A:58:PRO:HD2   | 1.79                     | 0.64              |
| 1:D:210:VAL:HG12 | 1:D:211:SER:N    | 2.12                     | 0.64              |
| 1:D:655:GLY:HA3  | 1:D:661:ILE:HD11 | 1.78                     | 0.64              |
| 1:D:798:ILE:HA   | 1:D:801:MET:HE3  | 1.79                     | 0.64              |
| 1:D:362:LYS:HD3  | 1:D:368:VAL:O    | 1.97                     | 0.64              |
| 1:A:85:LEU:HD22  | 1:A:88:ARG:NH2   | 2.12                     | 0.64              |
| 1:D:798:ILE:HD11 | 1:D:826:THR:OG1  | 1.98                     | 0.64              |
| 3:F:21:A:H1'     | 3:F:22:C:C5      | 2.33                     | 0.64              |
| 1:A:239:ILE:N    | 1:A:239:ILE:HD12 | 2.13                     | 0.64              |
| 1:D:168:PHE:CD2  | 1:D:282:ILE:HG23 | 2.32                     | 0.64              |
| 1:D:265:ARG:HH12 | 1:D:400:ARG:NE   | 1.94                     | 0.64              |
| 1:D:701:ARG:NH1  | 1:D:796:GLU:HG2  | 2.13                     | 0.64              |
| 1:A:88:ARG:CG    | 1:A:89:PRO:HD3   | 2.28                     | 0.63              |
| 1:A:392:LEU:HD13 | 1:A:457:LYS:HZ1  | 1.63                     | 0.63              |
| 1:D:60:PHE:HE1   | 1:D:62:VAL:HG22  | 1.64                     | 0.63              |
| 1:A:365:ARG:HH11 | 1:A:365:ARG:CG   | 2.12                     | 0.63              |
| 1:A:624:ILE:HG23 | 1:A:675:ILE:CD1  | 2.28                     | 0.63              |
| 1:A:12:LYS:HA    | 1:A:15:ILE:HD12  | 1.79                     | 0.63              |
| 1:A:658:THR:O    | 1:A:662:ARG:HG2  | 1.98                     | 0.63              |
| 1:A:883:SER:HB3  | 1:A:907:ARG:HB2  | 1.78                     | 0.63              |
| 1:D:14:ILE:HD11  | 2:E:5:U:H1'      | 1.81                     | 0.63              |
| 1:D:50:LEU:HD22  | 1:D:68:LYS:HA    | 1.79                     | 0.63              |
| 1:D:401:LEU:HA   | 1:D:461:LYS:HG2  | 1.78                     | 0.63              |
| 1:D:627:GLU:N    | 6:D:955:HOH:O    | 2.31                     | 0.63              |
| 1:D:929:GLU:HG3  | 1:D:930:TRP:N    | 2.13                     | 0.63              |
| 1:A:796:GLU:HA   | 1:A:825:SER:O    | 1.99                     | 0.63              |
| 1:D:240:SER:HB2  | 1:D:242:ASN:OD1  | 1.98                     | 0.63              |
| 1:A:795:LEU:O    | 1:A:796:GLU:HG3  | 1.99                     | 0.63              |
| 1:D:243:ARG:HH11 | 1:D:248:SER:HB3  | 1.63                     | 0.63              |
| 1:A:565:LEU:HD21 | 1:A:673:TYR:CE2  | 2.33                     | 0.63              |
| 1:A:813:VAL:HA   | 1:A:817:PHE:HD1  | 1.64                     | 0.63              |
| 1:A:852:LEU:HB2  | 1:A:855:PHE:HE1  | 1.62                     | 0.63              |
| 1:D:278:LEU:HD23 | 1:D:320:ILE:HG13 | 1.81                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:69:LYS:HE3   | 3:C:8:G:OP1      | 1.98                     | 0.62              |
| 1:A:895:VAL:C    | 1:A:897:PRO:HD2  | 2.24                     | 0.62              |
| 1:D:455:GLU:HG2  | 1:D:482:ILE:HA   | 1.81                     | 0.62              |
| 1:D:661:ILE:O    | 1:D:665:LEU:HG   | 1.99                     | 0.62              |
| 1:A:329:VAL:HG12 | 1:A:340:TYR:HB3  | 1.82                     | 0.62              |
| 1:D:102:GLU:HG3  | 1:D:155:ARG:HD2  | 1.81                     | 0.62              |
| 1:D:710:ARG:HH22 | 1:D:734:TYR:HB2  | 1.65                     | 0.62              |
| 1:A:717:LEU:HD12 | 1:A:718:VAL:N    | 2.14                     | 0.62              |
| 2:B:2:A:H2'      | 2:B:3:U:O4'      | 1.99                     | 0.62              |
| 1:D:373:LEU:HD12 | 1:D:374:PRO:HD2  | 1.81                     | 0.62              |
| 1:D:751:LEU:HD13 | 1:D:927:ILE:HD13 | 1.81                     | 0.62              |
| 1:A:238:TYR:HE1  | 1:A:252:ARG:HH22 | 1.46                     | 0.62              |
| 1:A:255:LEU:HD22 | 1:A:260:GLN:NE2  | 2.15                     | 0.62              |
| 1:D:23:ALA:HB2   | 1:D:57:LEU:HD23  | 1.81                     | 0.62              |
| 1:D:256:LYS:H    | 1:D:260:GLN:HE22 | 1.46                     | 0.62              |
| 1:D:169:LEU:HB3  | 1:D:173:TYR:CE1  | 2.34                     | 0.62              |
| 1:D:729:ASP:HB2  | 1:D:757:MET:CE   | 2.30                     | 0.62              |
| 1:A:182:ALA:O    | 6:A:947:HOH:O    | 2.16                     | 0.62              |
| 1:D:467:LEU:HD22 | 1:D:492:TRP:CE3  | 2.34                     | 0.62              |
| 1:A:368:VAL:CG2  | 1:A:654:VAL:HG22 | 2.30                     | 0.62              |
| 1:D:45:GLN:HE22  | 1:D:749:LYS:HA   | 1.65                     | 0.62              |
| 1:A:694:LYS:HB3  | 1:A:695:PRO:CD   | 2.29                     | 0.61              |
| 1:D:43:ILE:H     | 1:D:44:PRO:HD3   | 1.63                     | 0.61              |
| 1:D:41:LEU:HD21  | 1:D:755:ALA:CB   | 2.29                     | 0.61              |
| 1:D:387:LEU:O    | 1:D:391:ILE:HG13 | 2.00                     | 0.61              |
| 1:D:716:THR:HA   | 1:D:740:THR:O    | 2.00                     | 0.61              |
| 1:A:60:PHE:HB2   | 6:A:948:HOH:O    | 2.01                     | 0.61              |
| 1:A:710:ARG:HG2  | 1:A:711:GLU:N    | 2.11                     | 0.61              |
| 3:C:19:U:O2'     | 3:C:20:C:H5'     | 2.01                     | 0.61              |
| 1:D:95:THR:HG22  | 1:D:97:ASP:H     | 1.64                     | 0.61              |
| 1:A:41:LEU:HG    | 1:A:43:ILE:H     | 1.66                     | 0.61              |
| 1:D:636:TYR:HD1  | 1:D:676:LEU:HD13 | 1.65                     | 0.61              |
| 1:A:17:GLN:NE2   | 2:B:4:U:O2'      | 2.28                     | 0.61              |
| 1:D:309:ASN:HB2  | 1:D:322:GLY:O    | 2.00                     | 0.61              |
| 1:D:782:PHE:HE2  | 1:D:921:MET:HE3  | 1.65                     | 0.61              |
| 1:A:400:ARG:C    | 1:A:401:LEU:HD23 | 2.26                     | 0.61              |
| 1:D:170:ALA:HA   | 1:D:173:TYR:HD1  | 1.66                     | 0.61              |
| 1:A:856:ARG:HD3  | 2:B:21:A:O2'     | 2.01                     | 0.60              |
| 2:B:22:G:H1'     | 3:C:1:U:O2       | 2.01                     | 0.60              |
| 1:D:219:VAL:CG2  | 1:D:239:ILE:HD11 | 2.30                     | 0.60              |
| 1:D:694:LYS:HB2  | 1:D:695:PRO:HD2  | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:133:ASP:O    | 1:A:136:ARG:HB2  | 2.01                     | 0.60              |
| 1:D:358:ASN:ND2  | 1:D:373:LEU:H    | 1.99                     | 0.60              |
| 1:A:828:ASN:HA   | 1:A:902:GLN:NE2  | 2.16                     | 0.60              |
| 1:D:120:HIS:ND1  | 1:D:121:PRO:HD2  | 2.16                     | 0.60              |
| 1:D:732:LEU:HD23 | 1:D:761:LYS:HB3  | 1.84                     | 0.60              |
| 1:A:308:ARG:HD3  | 1:A:321:HIS:CE1  | 2.36                     | 0.60              |
| 1:D:642:THR:O    | 1:D:644:PRO:HD3  | 2.02                     | 0.60              |
| 1:A:870:ASN:HA   | 1:A:886:PHE:CE2  | 2.36                     | 0.60              |
| 1:D:183:ASP:OD2  | 1:D:183:ASP:N    | 2.32                     | 0.60              |
| 1:A:103:ILE:O    | 1:A:107:ILE:HG13 | 2.00                     | 0.60              |
| 1:D:11:PRO:HD2   | 1:D:14:ILE:HD12  | 1.83                     | 0.60              |
| 1:D:113:ASP:HB3  | 1:D:202:ILE:HD13 | 1.83                     | 0.60              |
| 1:D:141:PRO:HB2  | 1:D:144:VAL:HG23 | 1.84                     | 0.60              |
| 1:D:537:GLU:HA   | 1:D:641:MET:CE   | 2.31                     | 0.60              |
| 3:F:19:U:H2'     | 3:F:20:C:C6      | 2.36                     | 0.60              |
| 1:D:368:VAL:HB   | 1:D:654:VAL:CG2  | 2.32                     | 0.60              |
| 1:D:780:LEU:O    | 1:D:812:LYS:HD2  | 2.01                     | 0.60              |
| 1:A:255:LEU:HD22 | 1:A:260:GLN:HE22 | 1.66                     | 0.59              |
| 1:D:401:LEU:CD1  | 1:D:461:LYS:HE2  | 2.33                     | 0.59              |
| 1:D:406:LEU:HD21 | 1:D:482:ILE:HD13 | 1.82                     | 0.59              |
| 1:D:731:LEU:HD11 | 1:D:738:LEU:CD1  | 2.32                     | 0.59              |
| 1:A:633:VAL:HG22 | 1:A:677:LEU:HD12 | 1.84                     | 0.59              |
| 2:B:8:C:H2'      | 2:B:9:U:C6       | 2.38                     | 0.59              |
| 1:A:266:MET:SD   | 1:A:275:GLU:HB3  | 2.43                     | 0.59              |
| 1:D:559:VAL:HG23 | 1:D:615:VAL:CG2  | 2.33                     | 0.59              |
| 1:D:716:THR:HG22 | 1:D:740:THR:CB   | 2.32                     | 0.59              |
| 1:D:243:ARG:NH1  | 1:D:248:SER:HB3  | 2.18                     | 0.59              |
| 1:A:697:LEU:HD23 | 2:B:22:G:OP2     | 2.03                     | 0.59              |
| 1:D:404:PRO:HB3  | 1:D:459:PHE:CE2  | 2.38                     | 0.59              |
| 1:D:764:LYS:HG3  | 1:D:765:GLU:HG3  | 1.83                     | 0.59              |
| 1:D:386:PRO:HG2  | 1:D:391:ILE:HD11 | 1.85                     | 0.59              |
| 3:C:18:A:H2'     | 3:C:19:U:C6      | 2.38                     | 0.58              |
| 3:C:21:A:H5'     | 3:C:22:C:P       | 2.42                     | 0.58              |
| 1:A:810:GLY:CA   | 1:A:876:LEU:HD21 | 2.32                     | 0.58              |
| 1:D:265:ARG:NH1  | 1:D:400:ARG:HH21 | 2.01                     | 0.58              |
| 1:D:362:LYS:HB3  | 1:D:368:VAL:HA   | 1.85                     | 0.58              |
| 3:F:2:U:H2'      | 3:F:3:C:C6       | 2.38                     | 0.58              |
| 1:A:392:LEU:HD22 | 1:A:457:LYS:NZ   | 2.18                     | 0.58              |
| 1:A:818:HIS:O    | 1:A:908:ARG:NH1  | 2.36                     | 0.58              |
| 1:A:473:LYS:HE3  | 1:A:484:ASN:ND2  | 2.18                     | 0.58              |
| 1:A:560:SER:O    | 1:A:678:LEU:HB2  | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:642:THR:HB   | 1:A:643:PRO:CD   | 2.33                     | 0.58              |
| 1:D:559:VAL:O    | 1:D:612:GLU:HA   | 2.04                     | 0.58              |
| 1:D:866:ARG:HD2  | 1:D:897:PRO:O    | 2.04                     | 0.58              |
| 1:A:12:LYS:HE3   | 1:A:79:GLU:CD    | 2.29                     | 0.58              |
| 1:A:499:ASP:O    | 1:A:500:LEU:HB2  | 2.02                     | 0.58              |
| 1:D:60:PHE:CE1   | 1:D:62:VAL:HG22  | 2.38                     | 0.58              |
| 1:D:95:THR:HB    | 1:D:98:GLU:HG3   | 1.86                     | 0.58              |
| 1:D:777:GLY:HA3  | 1:D:924:TYR:CD1  | 2.39                     | 0.58              |
| 1:D:829:TYR:HA   | 1:D:832:ASN:ND2  | 2.18                     | 0.58              |
| 1:A:567:LEU:HB2  | 1:A:605:ILE:HD11 | 1.85                     | 0.58              |
| 1:A:642:THR:O    | 1:A:644:PRO:HD3  | 2.04                     | 0.57              |
| 1:D:16:HIS:CD2   | 1:D:78:ALA:HB1   | 2.38                     | 0.57              |
| 1:D:870:ASN:HA   | 1:D:886:PHE:CE2  | 2.39                     | 0.57              |
| 1:A:835:LEU:HD13 | 2:B:21:A:H1'     | 1.87                     | 0.57              |
| 1:D:210:VAL:HG12 | 1:D:211:SER:H    | 1.69                     | 0.57              |
| 1:A:46:LYS:HE3   | 2:B:14:A:O3'     | 2.04                     | 0.57              |
| 1:A:537:GLU:HB3  | 1:A:641:MET:HE2  | 1.87                     | 0.57              |
| 1:D:539:LYS:HG3  | 1:D:638:SER:O    | 2.04                     | 0.57              |
| 1:A:207:ALA:HA   | 1:A:210:VAL:HG23 | 1.84                     | 0.57              |
| 1:A:332:ARG:HB2  | 1:A:339:ASP:OD2  | 2.04                     | 0.57              |
| 2:B:15:A:H2'     | 2:B:16:G:H8      | 1.69                     | 0.57              |
| 1:D:315:ILE:HD11 | 1:D:352:CYS:SG   | 2.45                     | 0.57              |
| 1:A:460:THR:HG23 | 6:A:944:HOH:O    | 2.04                     | 0.57              |
| 1:D:813:VAL:O    | 1:D:817:PHE:O    | 2.21                     | 0.57              |
| 1:D:829:TYR:HA   | 1:D:832:ASN:HD21 | 1.69                     | 0.57              |
| 1:D:266:MET:HA   | 1:D:276:CYS:O    | 2.05                     | 0.57              |
| 1:A:368:VAL:HG23 | 1:A:369:ILE:N    | 2.20                     | 0.57              |
| 1:D:98:GLU:O     | 1:D:102:GLU:HG2  | 2.03                     | 0.57              |
| 1:D:113:ASP:HB3  | 1:D:202:ILE:CD1  | 2.35                     | 0.57              |
| 1:D:255:LEU:HD13 | 1:D:260:GLN:HB2  | 1.85                     | 0.57              |
| 1:A:374:PRO:HG3  | 1:A:619:SER:HB3  | 1.87                     | 0.57              |
| 1:D:368:VAL:HB   | 1:D:654:VAL:HG21 | 1.86                     | 0.57              |
| 1:D:374:PRO:HG3  | 1:D:619:SER:HA   | 1.86                     | 0.57              |
| 1:A:94:LEU:CB    | 1:A:158:ILE:HD13 | 2.34                     | 0.57              |
| 1:A:142:VAL:CG1  | 1:A:171:ILE:HG23 | 2.26                     | 0.57              |
| 1:D:94:LEU:HD12  | 1:D:158:ILE:HD13 | 1.87                     | 0.57              |
| 3:F:21:A:C2      | 3:F:21:A:OP2     | 2.58                     | 0.57              |
| 1:A:658:THR:O    | 1:A:662:ARG:HG3  | 2.04                     | 0.57              |
| 1:A:81:ALA:O     | 1:A:85:LEU:HG    | 2.05                     | 0.56              |
| 1:A:694:LYS:CB   | 1:A:695:PRO:CD   | 2.83                     | 0.56              |
| 1:A:762:LEU:HD13 | 1:A:930:TRP:CE3  | 2.40                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:798:ILE:O    | 1:A:801:MET:HG2  | 2.06                     | 0.56              |
| 2:B:20:A:O2'     | 2:B:21:A:H5''    | 2.05                     | 0.56              |
| 1:D:720:PHE:HB3  | 1:D:779:ILE:HG21 | 1.86                     | 0.56              |
| 1:A:46:LYS:HZ1   | 2:B:14:A:H5''    | 1.70                     | 0.56              |
| 1:A:360:ILE:HD11 | 1:A:398:GLN:NE2  | 2.20                     | 0.56              |
| 1:D:142:VAL:HG23 | 1:D:259:ASN:OD1  | 2.05                     | 0.56              |
| 1:D:390:GLU:OE1  | 1:D:390:GLU:HA   | 2.06                     | 0.56              |
| 1:D:694:LYS:HB2  | 1:D:695:PRO:CD   | 2.36                     | 0.56              |
| 3:F:18:A:H2'     | 3:F:19:U:H6      | 1.70                     | 0.56              |
| 1:A:43:ILE:CD1   | 1:A:927:ILE:HD13 | 2.35                     | 0.56              |
| 1:D:467:LEU:HG   | 1:D:468:GLU:N    | 2.20                     | 0.56              |
| 1:A:603:GLU:HG3  | 1:A:604:PRO:HD2  | 1.88                     | 0.56              |
| 2:B:4:U:H2'      | 2:B:5:U:C6       | 2.40                     | 0.56              |
| 1:A:46:LYS:NZ    | 2:B:14:A:H5''    | 2.20                     | 0.56              |
| 1:A:405:ILE:CD1  | 1:A:458:ILE:HD11 | 2.35                     | 0.56              |
| 1:A:828:ASN:CG   | 1:A:866:ARG:HG3  | 2.30                     | 0.56              |
| 1:D:624:ILE:HG22 | 1:D:624:ILE:O    | 2.05                     | 0.56              |
| 2:B:15:A:H2'     | 2:B:16:G:C8      | 2.40                     | 0.56              |
| 1:D:567:LEU:HB2  | 1:D:605:ILE:CD1  | 2.35                     | 0.56              |
| 1:A:365:ARG:CG   | 1:A:365:ARG:NH1  | 2.67                     | 0.56              |
| 1:D:11:PRO:HD2   | 1:D:14:ILE:CD1   | 2.35                     | 0.56              |
| 1:D:563:TYR:CE2  | 1:D:608:ASN:HB2  | 2.41                     | 0.56              |
| 1:D:570:ASP:N    | 1:D:571:PRO:CD   | 2.51                     | 0.56              |
| 1:D:570:ASP:HB3  | 1:D:640:LYS:NZ   | 2.21                     | 0.56              |
| 1:D:865:THR:HG22 | 1:D:866:ARG:N    | 2.21                     | 0.56              |
| 1:A:493:PHE:HA   | 1:A:496:PHE:CD1  | 2.41                     | 0.56              |
| 1:D:122:LEU:O    | 1:D:125:HIS:HB2  | 2.06                     | 0.56              |
| 1:D:551:GLN:O    | 1:D:629:THR:O    | 2.24                     | 0.56              |
| 1:A:568:ALA:HA   | 1:A:601:SER:O    | 2.06                     | 0.56              |
| 1:A:814:LEU:HD12 | 1:A:876:LEU:HG   | 1.86                     | 0.56              |
| 1:A:719:ASP:HB3  | 1:A:722:CYS:HB3  | 1.89                     | 0.55              |
| 1:D:369:ILE:HG21 | 1:D:565:LEU:CD2  | 2.36                     | 0.55              |
| 1:D:568:ALA:HB2  | 1:D:602:VAL:HA   | 1.88                     | 0.55              |
| 1:A:57:LEU:O     | 1:A:58:PRO:C     | 2.49                     | 0.55              |
| 1:A:169:LEU:O    | 1:A:173:TYR:CD1  | 2.59                     | 0.55              |
| 1:A:725:GLY:O    | 1:A:729:ASP:N    | 2.38                     | 0.55              |
| 1:D:222:VAL:HB   | 1:D:326:LEU:HB3  | 1.87                     | 0.55              |
| 1:D:401:LEU:HD13 | 1:D:461:LYS:HE2  | 1.88                     | 0.55              |
| 1:A:369:ILE:CG2  | 1:A:565:LEU:HD11 | 2.35                     | 0.55              |
| 1:A:387:LEU:O    | 1:A:391:ILE:HG22 | 2.06                     | 0.55              |
| 1:A:405:ILE:HB   | 1:A:458:ILE:CG1  | 2.32                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:253:LEU:HD13 | 1:D:325:ILE:HG12 | 1.87                     | 0.55              |
| 1:D:455:GLU:O    | 1:D:471:PRO:HD2  | 2.06                     | 0.55              |
| 1:A:283:PRO:O    | 1:A:285:LYS:N    | 2.39                     | 0.55              |
| 1:A:392:LEU:O    | 1:A:395:PHE:HB3  | 2.07                     | 0.55              |
| 1:A:852:LEU:HB2  | 1:A:855:PHE:CD1  | 2.42                     | 0.55              |
| 1:D:606:GLU:CB   | 1:D:654:VAL:HG11 | 2.35                     | 0.55              |
| 1:A:146:ALA:HB2  | 1:A:174:VAL:HG21 | 1.88                     | 0.55              |
| 1:A:160:ASN:HD21 | 1:A:169:LEU:HD13 | 1.71                     | 0.55              |
| 1:A:908:ARG:HE   | 1:A:911:SER:HB3  | 1.71                     | 0.55              |
| 1:A:7:HIS:C      | 1:A:9:PRO:HD2    | 2.32                     | 0.55              |
| 1:D:345:VAL:CG1  | 1:D:658:THR:HG21 | 2.37                     | 0.55              |
| 1:D:553:ILE:H    | 1:D:629:THR:CG2  | 2.20                     | 0.55              |
| 1:D:821:LEU:HD12 | 1:D:906:PHE:O    | 2.06                     | 0.55              |
| 1:A:27:VAL:HG11  | 1:A:70:LYS:HE2   | 1.89                     | 0.55              |
| 1:A:132:ARG:NH2  | 1:A:257:ASP:OD1  | 2.39                     | 0.55              |
| 1:A:360:ILE:HD11 | 1:A:398:GLN:HE22 | 1.72                     | 0.55              |
| 1:A:864:TRP:HA   | 1:A:868:GLN:HE22 | 1.72                     | 0.55              |
| 1:A:865:THR:N    | 1:A:868:GLN:HE21 | 2.04                     | 0.55              |
| 1:A:365:ARG:HG3  | 1:A:365:ARG:NH1  | 2.18                     | 0.55              |
| 1:D:103:ILE:HG23 | 1:D:152:ILE:HD12 | 1.87                     | 0.55              |
| 1:D:496:PHE:N    | 1:D:496:PHE:CD2  | 2.74                     | 0.55              |
| 1:D:570:ASP:O    | 1:D:572:GLU:HG3  | 2.07                     | 0.55              |
| 1:D:829:TYR:OH   | 1:D:853:PRO:HG2  | 2.07                     | 0.55              |
| 2:B:13:C:O2'     | 2:B:14:A:H5'     | 2.07                     | 0.55              |
| 1:D:643:PRO:O    | 1:D:644:PRO:C    | 2.48                     | 0.55              |
| 1:D:12:LYS:HD2   | 1:D:82:LEU:HD12  | 1.90                     | 0.54              |
| 1:D:168:PHE:HD2  | 1:D:282:ILE:HG23 | 1.71                     | 0.54              |
| 1:D:392:LEU:HD13 | 1:D:490:LEU:HG   | 1.89                     | 0.54              |
| 1:D:568:ALA:CB   | 1:D:601:SER:O    | 2.53                     | 0.54              |
| 1:A:358:ASN:HA   | 1:A:373:LEU:HB2  | 1.90                     | 0.54              |
| 1:A:558:VAL:CG1  | 1:A:681:LYS:HD3  | 2.37                     | 0.54              |
| 1:A:851:GLN:O    | 1:A:852:LEU:HG   | 2.08                     | 0.54              |
| 1:D:569:VAL:HG22 | 1:D:668:ARG:O    | 2.08                     | 0.54              |
| 1:D:710:ARG:NH1  | 1:D:734:TYR:HB2  | 2.22                     | 0.54              |
| 1:A:365:ARG:HD2  | 1:A:385:GLY:HA3  | 1.89                     | 0.54              |
| 1:A:855:PHE:HZ   | 1:A:862:PHE:HA   | 1.73                     | 0.54              |
| 1:D:88:ARG:CB    | 1:D:89:PRO:HD2   | 2.37                     | 0.54              |
| 1:A:374:PRO:HG3  | 1:A:619:SER:CB   | 2.38                     | 0.54              |
| 1:A:757:MET:HE3  | 1:A:761:LYS:CG   | 2.36                     | 0.54              |
| 1:D:11:PRO:HB2   | 1:D:75:GLN:HE22  | 1.72                     | 0.54              |
| 1:D:17:GLN:O     | 1:D:17:GLN:HG3   | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:736:THR:HG22 | 1:D:737:SER:N    | 2.23                     | 0.54              |
| 1:D:829:TYR:HB2  | 1:D:863:GLU:O    | 2.07                     | 0.54              |
| 1:A:171:ILE:HD13 | 1:A:282:ILE:HD13 | 1.89                     | 0.54              |
| 1:A:255:LEU:HD13 | 1:A:260:GLN:HB3  | 1.90                     | 0.54              |
| 1:A:62:VAL:HG11  | 1:A:80:LEU:HB2   | 1.90                     | 0.54              |
| 1:A:168:PHE:CE2  | 1:A:282:ILE:HA   | 2.42                     | 0.54              |
| 1:A:188:SER:C    | 1:A:190:HIS:H    | 2.15                     | 0.54              |
| 1:A:700:GLN:HB2  | 1:A:889:VAL:HG11 | 1.90                     | 0.54              |
| 1:D:42:ALA:C     | 1:D:44:PRO:HD3   | 2.33                     | 0.54              |
| 1:D:121:PRO:HD3  | 1:D:333:TRP:CD2  | 2.43                     | 0.54              |
| 1:D:571:PRO:HD3  | 1:D:670:CYS:HB2  | 1.88                     | 0.54              |
| 1:A:252:ARG:HG3  | 1:A:252:ARG:HH11 | 1.73                     | 0.54              |
| 1:A:871:GLN:O    | 1:A:875:LYS:HG3  | 2.08                     | 0.54              |
| 1:D:257:ASP:N    | 1:D:260:GLN:HE21 | 2.03                     | 0.54              |
| 1:D:627:GLU:O    | 1:D:630:GLN:HG2  | 2.07                     | 0.54              |
| 1:D:895:VAL:HG12 | 1:D:896:GLU:N    | 2.22                     | 0.54              |
| 1:A:12:LYS:HB3   | 1:A:78:ALA:CB    | 2.39                     | 0.53              |
| 2:B:10:C:H2'     | 2:B:11:U:C6      | 2.43                     | 0.53              |
| 1:A:392:LEU:HD21 | 1:A:404:PRO:HG3  | 1.90                     | 0.53              |
| 1:D:704:TYR:HH   | 1:D:887:SER:HG   | 1.55                     | 0.53              |
| 1:D:18:LYS:HD3   | 3:F:19:U:O2'     | 2.08                     | 0.53              |
| 1:D:265:ARG:N    | 1:D:318:GLN:HE22 | 1.98                     | 0.53              |
| 1:A:23:ALA:HB2   | 1:A:57:LEU:CD1   | 2.38                     | 0.53              |
| 1:D:392:LEU:HD21 | 1:D:459:PHE:HZ   | 1.74                     | 0.53              |
| 1:D:685:GLU:HG3  | 1:D:686:GLU:H    | 1.73                     | 0.53              |
| 1:D:857:ASN:OD1  | 3:F:2:U:H4'      | 2.08                     | 0.53              |
| 1:D:188:SER:O    | 1:D:190:HIS:N    | 2.41                     | 0.53              |
| 1:D:257:ASP:OD1  | 1:D:258:GLY:N    | 2.42                     | 0.53              |
| 1:A:278:LEU:HD23 | 1:A:320:ILE:HD12 | 1.90                     | 0.53              |
| 1:A:677:LEU:HD13 | 1:A:678:LEU:N    | 2.23                     | 0.53              |
| 1:D:194:ARG:HH12 | 1:D:198:TYR:CA   | 2.20                     | 0.53              |
| 1:D:551:GLN:O    | 1:D:553:ILE:HG13 | 2.08                     | 0.53              |
| 1:D:896:GLU:HB2  | 1:D:897:PRO:HD3  | 1.91                     | 0.53              |
| 1:D:39:PRO:HD2   | 1:D:759:HIS:CD2  | 2.44                     | 0.53              |
| 1:D:119:GLU:HA   | 1:D:119:GLU:OE1  | 2.08                     | 0.53              |
| 1:D:201:GLU:HA   | 1:D:204:GLU:OE1  | 2.09                     | 0.53              |
| 1:D:146:ALA:HB2  | 1:D:174:VAL:HG21 | 1.91                     | 0.53              |
| 1:D:537:GLU:HA   | 1:D:641:MET:HE1  | 1.89                     | 0.53              |
| 1:D:828:ASN:HA   | 1:D:902:GLN:HE21 | 1.74                     | 0.53              |
| 1:A:246:LEU:HD22 | 1:A:261:VAL:HG11 | 1.90                     | 0.53              |
| 1:A:829:TYR:OH   | 1:A:853:PRO:O    | 2.26                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:19:U:H2'     | 3:F:20:C:O4'     | 2.09                     | 0.53              |
| 1:A:160:ASN:ND2  | 1:A:169:LEU:HD13 | 2.24                     | 0.53              |
| 1:A:392:LEU:HA   | 1:A:490:LEU:HD21 | 1.91                     | 0.53              |
| 1:A:407:SER:HB2  | 1:A:456:VAL:HB   | 1.90                     | 0.53              |
| 1:D:50:LEU:CD2   | 1:D:68:LYS:HG3   | 2.39                     | 0.53              |
| 1:D:188:SER:O    | 1:D:189:PRO:C    | 2.52                     | 0.53              |
| 1:D:818:HIS:N    | 1:D:819:PRO:HD2  | 2.11                     | 0.53              |
| 1:A:8:THR:O      | 1:A:10:THR:N     | 2.42                     | 0.52              |
| 1:A:813:VAL:HG11 | 1:A:822:LEU:HD11 | 1.92                     | 0.52              |
| 1:A:365:ARG:NH2  | 1:A:612:GLU:O    | 2.42                     | 0.52              |
| 1:A:368:VAL:HG21 | 1:A:654:VAL:HG22 | 1.90                     | 0.52              |
| 1:A:642:THR:HB   | 1:A:643:PRO:HD2  | 1.90                     | 0.52              |
| 1:D:357:PRO:HB3  | 1:D:490:LEU:HD22 | 1.90                     | 0.52              |
| 1:D:655:GLY:HA3  | 1:D:661:ILE:CD1  | 2.38                     | 0.52              |
| 1:A:221:ALA:O    | 1:A:234:LEU:HD12 | 2.09                     | 0.52              |
| 1:A:278:LEU:HD21 | 1:A:312:ALA:HB1  | 1.90                     | 0.52              |
| 1:A:793:THR:CG2  | 1:A:795:LEU:HG   | 2.39                     | 0.52              |
| 1:D:123:GLY:HA2  | 1:D:126:LEU:HB2  | 1.91                     | 0.52              |
| 1:D:375:PHE:HA   | 1:D:491:LEU:HD11 | 1.92                     | 0.52              |
| 1:A:267:PHE:CE1  | 1:A:315:ILE:HG22 | 2.45                     | 0.52              |
| 1:D:14:ILE:CD1   | 2:E:5:U:H1'      | 2.39                     | 0.52              |
| 1:D:265:ARG:NH1  | 1:D:400:ARG:HE   | 2.07                     | 0.52              |
| 1:D:359:GLY:O    | 1:D:363:ILE:HG13 | 2.09                     | 0.52              |
| 1:D:829:TYR:HD1  | 1:D:832:ASN:ND2  | 2.04                     | 0.52              |
| 1:D:621:ASN:HD21 | 1:D:623:HIS:HB2  | 1.73                     | 0.52              |
| 1:D:679:GLY:O    | 1:D:680:VAL:HG23 | 2.10                     | 0.52              |
| 1:A:155:ARG:O    | 1:A:159:ILE:HG13 | 2.10                     | 0.52              |
| 1:A:318:GLN:HG3  | 1:A:400:ARG:NH2  | 2.24                     | 0.52              |
| 1:A:391:ILE:HG23 | 1:A:490:LEU:HD11 | 1.90                     | 0.52              |
| 1:A:680:VAL:C    | 1:A:681:LYS:HD2  | 2.35                     | 0.52              |
| 1:D:132:ARG:O    | 1:D:137:CYS:HB2  | 2.10                     | 0.52              |
| 1:D:789:VAL:O    | 1:D:819:PRO:HA   | 2.10                     | 0.52              |
| 2:E:14:A:H2'     | 2:E:15:A:C8      | 2.44                     | 0.52              |
| 1:A:693:PHE:O    | 1:A:694:LYS:C    | 2.51                     | 0.52              |
| 1:D:358:ASN:HD21 | 1:D:373:LEU:H    | 1.58                     | 0.52              |
| 1:D:570:ASP:O    | 1:D:572:GLU:N    | 2.39                     | 0.52              |
| 1:D:778:SER:HA   | 5:D:951:SAH:N1   | 2.24                     | 0.52              |
| 2:B:4:U:H5'      | 6:B:23:HOH:O     | 2.10                     | 0.52              |
| 1:D:176:LYS:O    | 1:D:180:LYS:HG3  | 2.10                     | 0.51              |
| 1:D:729:ASP:HB2  | 1:D:757:MET:HE1  | 1.92                     | 0.51              |
| 1:A:353:CYS:O    | 1:A:359:GLY:HA3  | 2.09                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:621:ASN:HD22 | 1:A:622:PRO:N    | 2.08                     | 0.51              |
| 1:D:121:PRO:HD3  | 1:D:333:TRP:CE2  | 2.45                     | 0.51              |
| 1:A:23:ALA:HA    | 1:A:56:GLN:O     | 2.09                     | 0.51              |
| 1:A:895:VAL:HG12 | 1:A:897:PRO:CD   | 2.37                     | 0.51              |
| 1:D:18:LYS:HD3   | 3:F:20:C:H5'     | 1.92                     | 0.51              |
| 1:D:459:PHE:CB   | 1:D:466:VAL:HB   | 2.41                     | 0.51              |
| 1:A:35:GLN:NE2   | 1:A:47:GLY:HA3   | 2.25                     | 0.51              |
| 1:D:921:MET:O    | 1:D:923:PRO:HD3  | 2.11                     | 0.51              |
| 1:A:160:ASN:ND2  | 1:A:173:TYR:OH   | 2.42                     | 0.51              |
| 1:A:378:THR:CG2  | 1:A:382:ASN:HD22 | 2.24                     | 0.51              |
| 1:A:389:ARG:O    | 1:A:392:LEU:HB3  | 2.10                     | 0.51              |
| 1:A:704:TYR:CD2  | 1:A:903:ILE:HD13 | 2.46                     | 0.51              |
| 1:A:886:PHE:N    | 1:A:886:PHE:CD1  | 2.78                     | 0.51              |
| 1:D:779:ILE:HD11 | 1:D:801:MET:HE1  | 1.93                     | 0.51              |
| 1:D:867:GLU:HG3  | 1:D:868:GLN:N    | 2.25                     | 0.51              |
| 1:D:921:MET:O    | 1:D:921:MET:HG2  | 2.10                     | 0.51              |
| 1:A:43:ILE:HG22  | 1:A:44:PRO:N     | 2.25                     | 0.51              |
| 1:D:639:PHE:HD1  | 1:D:641:MET:HE3  | 1.74                     | 0.51              |
| 1:D:932:LYS:C    | 1:D:932:LYS:HD3  | 2.35                     | 0.51              |
| 1:D:373:LEU:HD12 | 1:D:374:PRO:CD   | 2.41                     | 0.51              |
| 1:D:406:LEU:HD11 | 1:D:482:ILE:HG23 | 1.91                     | 0.51              |
| 1:D:224:ILE:HG22 | 1:D:309:ASN:HD21 | 1.76                     | 0.51              |
| 1:D:701:ARG:NH1  | 1:D:796:GLU:CG   | 2.73                     | 0.51              |
| 1:D:479:ASN:O    | 1:D:483:GLN:HG2  | 2.11                     | 0.51              |
| 1:D:48:PRO:HD2   | 1:D:48:PRO:O     | 2.12                     | 0.50              |
| 1:D:401:LEU:HD13 | 1:D:461:LYS:CG   | 2.41                     | 0.50              |
| 1:D:496:PHE:HB3  | 1:D:524:PHE:CD1  | 2.46                     | 0.50              |
| 1:A:558:VAL:HG12 | 1:A:681:LYS:HB2  | 1.92                     | 0.50              |
| 1:D:780:LEU:CD1  | 1:D:805:GLN:HB3  | 2.41                     | 0.50              |
| 1:A:258:GLY:HA2  | 1:A:261:VAL:HG23 | 1.94                     | 0.50              |
| 1:D:605:ILE:HD13 | 1:D:651:ILE:HG23 | 1.94                     | 0.50              |
| 1:D:778:SER:C    | 1:D:780:LEU:H    | 2.20                     | 0.50              |
| 1:D:818:HIS:N    | 1:D:819:PRO:CD   | 2.69                     | 0.50              |
| 1:A:697:LEU:HD23 | 2:B:22:G:P       | 2.50                     | 0.50              |
| 1:D:819:PRO:HB2  | 1:D:821:LEU:O    | 2.12                     | 0.50              |
| 1:A:12:LYS:O     | 1:A:15:ILE:HB    | 2.11                     | 0.50              |
| 1:A:22:LYS:O     | 1:A:22:LYS:HG3   | 2.10                     | 0.50              |
| 1:A:865:THR:N    | 1:A:868:GLN:NE2  | 2.55                     | 0.50              |
| 1:A:920:SER:O    | 1:A:921:MET:HG3  | 2.11                     | 0.50              |
| 1:D:47:GLY:HA2   | 2:E:14:A:O2'     | 2.11                     | 0.50              |
| 1:D:706:LEU:HD11 | 1:D:730:SER:HB2  | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:741:ILE:C    | 1:D:742:ILE:HG13 | 2.35                     | 0.50              |
| 3:F:8:G:H2'      | 3:F:9:C:C6       | 2.46                     | 0.50              |
| 1:A:283:PRO:C    | 1:A:285:LYS:H    | 2.20                     | 0.50              |
| 1:A:369:ILE:HG21 | 1:A:565:LEU:CD1  | 2.41                     | 0.50              |
| 1:A:769:VAL:HG12 | 1:A:770:LYS:N    | 2.27                     | 0.50              |
| 1:A:567:LEU:HB2  | 1:A:605:ILE:CD1  | 2.42                     | 0.50              |
| 1:A:706:LEU:HA   | 1:A:709:ILE:HD12 | 1.94                     | 0.50              |
| 1:D:25:TYR:CD2   | 1:D:55:LEU:HD13  | 2.47                     | 0.50              |
| 1:D:396:CYS:O    | 1:D:401:LEU:HB2  | 2.11                     | 0.50              |
| 1:D:553:ILE:HG22 | 1:D:557:SER:HB2  | 1.94                     | 0.50              |
| 1:D:103:ILE:O    | 1:D:107:ILE:HG13 | 2.12                     | 0.50              |
| 1:D:640:LYS:HD2  | 1:D:670:CYS:SG   | 2.51                     | 0.50              |
| 1:D:621:ASN:ND2  | 1:D:624:ILE:HG13 | 2.23                     | 0.49              |
| 1:D:773:THR:C    | 1:D:774:LEU:HD23 | 2.36                     | 0.49              |
| 1:A:7:HIS:NE2    | 3:C:17:A:H4'     | 2.27                     | 0.49              |
| 1:A:379:THR:C    | 1:A:381:SER:H    | 2.20                     | 0.49              |
| 1:D:770:LYS:O    | 1:D:931:LYS:HA   | 2.12                     | 0.49              |
| 1:A:694:LYS:HB3  | 1:A:695:PRO:HD3  | 1.93                     | 0.49              |
| 1:D:246:LEU:HD22 | 1:D:261:VAL:HB   | 1.92                     | 0.49              |
| 1:D:403:GLU:HG3  | 1:D:404:PRO:HD2  | 1.93                     | 0.49              |
| 1:A:487:LEU:O    | 1:A:491:LEU:HG   | 2.12                     | 0.49              |
| 1:A:18:LYS:CE    | 3:C:19:U:H4'     | 2.42                     | 0.49              |
| 1:D:567:LEU:O    | 1:D:568:ALA:HB2  | 2.12                     | 0.49              |
| 1:A:87:ILE:O     | 1:A:91:ASN:HB2   | 2.13                     | 0.49              |
| 1:A:396:CYS:SG   | 1:A:459:PHE:CZ   | 3.02                     | 0.49              |
| 1:D:16:HIS:HD2   | 1:D:78:ALA:HB1   | 1.78                     | 0.49              |
| 1:D:262:MET:HA   | 1:D:282:ILE:HD11 | 1.94                     | 0.49              |
| 1:A:315:ILE:HD11 | 1:A:348:PHE:HE1  | 1.77                     | 0.49              |
| 1:A:329:VAL:HG12 | 1:A:340:TYR:CB   | 2.43                     | 0.49              |
| 1:A:798:ILE:HG13 | 1:A:799:GLU:N    | 2.28                     | 0.49              |
| 1:A:43:ILE:CG2   | 1:A:44:PRO:CD    | 2.91                     | 0.49              |
| 1:A:265:ARG:HG2  | 1:A:266:MET:N    | 2.28                     | 0.49              |
| 1:A:565:LEU:HD21 | 1:A:673:TYR:CZ   | 2.48                     | 0.49              |
| 1:A:642:THR:CB   | 1:A:643:PRO:CD   | 2.91                     | 0.49              |
| 1:A:803:GLU:HG2  | 1:A:862:PHE:CD2  | 2.48                     | 0.49              |
| 1:D:704:TYR:CE2  | 1:D:903:ILE:HD11 | 2.47                     | 0.49              |
| 1:A:142:VAL:CG2  | 1:A:175:MET:HE3  | 2.43                     | 0.49              |
| 1:A:358:ASN:ND2  | 1:A:373:LEU:H    | 2.11                     | 0.49              |
| 1:A:621:ASN:C    | 1:A:621:ASN:ND2  | 2.70                     | 0.49              |
| 1:D:43:ILE:HD11  | 1:D:927:ILE:CG1  | 2.43                     | 0.49              |
| 1:A:106:ARG:HD3  | 1:A:151:LYS:HD2  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:265:ARG:HG2  | 1:A:266:MET:H    | 1.76                     | 0.48              |
| 1:D:242:ASN:OD1  | 1:D:243:ARG:N    | 2.46                     | 0.48              |
| 1:A:401:LEU:CD2  | 1:A:461:LYS:HB2  | 2.26                     | 0.48              |
| 1:D:287:LEU:O    | 1:D:291:SER:HB3  | 2.13                     | 0.48              |
| 1:D:462:SER:O    | 1:D:463:GLN:HB2  | 2.13                     | 0.48              |
| 1:D:467:LEU:HD22 | 1:D:492:TRP:HE3  | 1.76                     | 0.48              |
| 1:D:757:MET:HG3  | 1:D:758:LEU:H    | 1.73                     | 0.48              |
| 1:D:887:SER:O    | 1:D:903:ILE:HG12 | 2.13                     | 0.48              |
| 1:A:357:PRO:HB3  | 1:A:490:LEU:HD22 | 1.95                     | 0.48              |
| 1:A:700:GLN:HB2  | 1:A:889:VAL:CG1  | 2.44                     | 0.48              |
| 1:D:780:LEU:HD21 | 1:D:801:MET:SD   | 2.53                     | 0.48              |
| 1:A:110:ILE:HG23 | 1:A:115:PHE:CE2  | 2.48                     | 0.48              |
| 1:A:120:HIS:O    | 1:A:121:PRO:C    | 2.56                     | 0.48              |
| 1:A:392:LEU:CD2  | 1:A:404:PRO:HG3  | 2.44                     | 0.48              |
| 1:D:138:GLY:O    | 1:D:193:ARG:HG3  | 2.12                     | 0.48              |
| 1:D:189:PRO:O    | 1:D:259:ASN:ND2  | 2.46                     | 0.48              |
| 1:D:820:LYS:HG2  | 1:D:908:ARG:NH2  | 2.29                     | 0.48              |
| 1:D:278:LEU:HD22 | 1:D:316:CYS:SG   | 2.54                     | 0.48              |
| 1:D:357:PRO:CB   | 1:D:490:LEU:HD22 | 2.44                     | 0.48              |
| 1:D:657:ASP:CG   | 1:D:660:ARG:HE   | 2.22                     | 0.48              |
| 1:D:832:ASN:HB3  | 1:D:856:ARG:HE   | 1.79                     | 0.48              |
| 2:E:15:A:H2'     | 2:E:16:G:C8      | 2.49                     | 0.48              |
| 1:A:779:ILE:HD12 | 1:A:809:PHE:CE1  | 2.48                     | 0.48              |
| 1:A:905:ILE:N    | 1:A:905:ILE:HD12 | 2.29                     | 0.48              |
| 1:A:907:ARG:HG3  | 6:A:952:HOH:O    | 2.13                     | 0.48              |
| 1:D:87:ILE:O     | 1:D:87:ILE:HG22  | 2.13                     | 0.48              |
| 1:D:567:LEU:HD12 | 1:D:670:CYS:O    | 2.13                     | 0.48              |
| 1:A:170:ALA:O    | 1:A:174:VAL:HG23 | 2.13                     | 0.48              |
| 1:A:920:SER:C    | 1:A:921:MET:HG3  | 2.39                     | 0.48              |
| 2:B:19:A:O2'     | 2:B:20:A:H5'     | 2.14                     | 0.48              |
| 1:A:23:ALA:HB2   | 1:A:57:LEU:HD12  | 1.95                     | 0.48              |
| 1:A:43:ILE:HD11  | 1:A:927:ILE:HD13 | 1.96                     | 0.48              |
| 1:D:50:LEU:HB3   | 1:D:66:VAL:CG1   | 2.43                     | 0.48              |
| 1:D:107:ILE:HG22 | 1:D:185:ILE:HD13 | 1.96                     | 0.48              |
| 1:D:181:LEU:HD11 | 1:D:184:TYR:CD1  | 2.49                     | 0.48              |
| 1:D:537:GLU:CB   | 1:D:641:MET:HE1  | 2.44                     | 0.48              |
| 2:E:11:U:H2'     | 2:E:12:G:H8      | 1.78                     | 0.48              |
| 1:A:822:LEU:HD23 | 1:A:823:ILE:N    | 2.29                     | 0.48              |
| 1:D:315:ILE:HG23 | 1:D:351:ILE:HG21 | 1.95                     | 0.48              |
| 1:D:852:LEU:N    | 1:D:853:PRO:CD   | 2.77                     | 0.48              |
| 1:A:11:PRO:O     | 1:A:12:LYS:C     | 2.57                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:35:GLN:HE22  | 1:A:47:GLY:HA3   | 1.79                     | 0.47              |
| 1:A:380:LYS:O    | 1:A:380:LYS:HG2  | 2.14                     | 0.47              |
| 1:A:462:SER:O    | 1:A:463:GLN:HB2  | 2.13                     | 0.47              |
| 1:A:467:LEU:HD22 | 1:A:492:TRP:HE3  | 1.79                     | 0.47              |
| 1:D:43:ILE:HG13  | 1:D:927:ILE:HG23 | 1.96                     | 0.47              |
| 1:D:345:VAL:HG12 | 1:D:658:THR:HG21 | 1.96                     | 0.47              |
| 1:D:825:SER:HA   | 1:D:903:ILE:HG22 | 1.96                     | 0.47              |
| 2:E:9:U:C2       | 3:F:13:G:N2      | 2.82                     | 0.47              |
| 3:F:19:U:O2'     | 3:F:20:C:C5'     | 2.61                     | 0.47              |
| 1:A:461:LYS:HE2  | 1:A:466:VAL:HG21 | 1.97                     | 0.47              |
| 1:D:71:LYS:HD2   | 2:E:6:C:OP2      | 2.14                     | 0.47              |
| 1:A:59:GLU:HB3   | 1:A:60:PHE:HD1   | 1.79                     | 0.47              |
| 1:A:467:LEU:HD13 | 1:A:492:TRP:CE3  | 2.50                     | 0.47              |
| 1:A:834:ILE:HG23 | 1:A:835:LEU:N    | 2.29                     | 0.47              |
| 1:D:283:PRO:C    | 1:D:285:LYS:N    | 2.68                     | 0.47              |
| 1:D:552:SER:CA   | 1:D:629:THR:O    | 2.61                     | 0.47              |
| 3:C:10:A:O2'     | 3:C:11:G:H5'     | 2.14                     | 0.47              |
| 1:D:632:THR:C    | 1:D:677:LEU:HD23 | 2.39                     | 0.47              |
| 1:D:642:THR:HB   | 1:D:643:PRO:HD3  | 1.97                     | 0.47              |
| 1:A:365:ARG:NH2  | 1:A:384:ARG:HB3  | 2.29                     | 0.47              |
| 1:A:538:SER:O    | 1:A:639:PHE:HB2  | 2.14                     | 0.47              |
| 1:A:709:ILE:O    | 1:A:712:SER:O    | 2.33                     | 0.47              |
| 1:D:272:CYS:HB2  | 1:D:351:ILE:HD11 | 1.97                     | 0.47              |
| 1:A:160:ASN:O    | 1:A:163:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:188:SER:C    | 1:A:190:HIS:N    | 2.70                     | 0.47              |
| 1:A:382:ASN:HD21 | 1:A:684:SER:HB2  | 1.79                     | 0.47              |
| 1:A:383:TRP:HH2  | 1:A:487:LEU:HD21 | 1.79                     | 0.47              |
| 1:A:795:LEU:C    | 1:A:796:GLU:HG3  | 2.40                     | 0.47              |
| 1:A:796:GLU:O    | 1:A:796:GLU:CD   | 2.58                     | 0.47              |
| 1:D:392:LEU:HD11 | 1:D:459:PHE:CZ   | 2.50                     | 0.47              |
| 1:D:599:GLU:C    | 1:D:601:SER:H    | 2.22                     | 0.47              |
| 1:D:639:PHE:CE1  | 1:D:641:MET:HE3  | 2.50                     | 0.47              |
| 1:D:856:ARG:HB3  | 2:E:21:A:O2'     | 2.13                     | 0.47              |
| 1:D:870:ASN:C    | 1:D:870:ASN:OD1  | 2.56                     | 0.47              |
| 1:A:22:LYS:HE2   | 1:A:22:LYS:HA    | 1.97                     | 0.47              |
| 1:A:739:GLN:HE22 | 1:A:770:LYS:NZ   | 2.12                     | 0.47              |
| 1:A:821:LEU:HD11 | 1:A:905:ILE:CG2  | 2.45                     | 0.47              |
| 1:D:210:VAL:CG1  | 1:D:211:SER:N    | 2.77                     | 0.47              |
| 1:D:382:ASN:O    | 1:D:614:GLU:HG3  | 2.14                     | 0.47              |
| 1:D:795:LEU:HA   | 1:D:825:SER:HB3  | 1.95                     | 0.47              |
| 1:A:190:HIS:HA   | 1:A:257:ASP:OD2  | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:383:TRP:CH2  | 1:A:487:LEU:HD21 | 2.50                     | 0.47              |
| 1:A:745:ASP:HB3  | 1:A:751:LEU:HD21 | 1.96                     | 0.47              |
| 2:E:10:C:O2'     | 2:E:11:U:H5'     | 2.15                     | 0.47              |
| 1:A:43:ILE:HD12  | 1:A:927:ILE:HD13 | 1.97                     | 0.47              |
| 1:D:210:VAL:CG1  | 1:D:211:SER:H    | 2.28                     | 0.47              |
| 1:D:377:PHE:C    | 1:D:377:PHE:CD2  | 2.93                     | 0.47              |
| 1:D:691:ALA:CB   | 2:E:20:A:H5''    | 2.45                     | 0.47              |
| 1:D:764:LYS:HG3  | 1:D:765:GLU:N    | 2.30                     | 0.47              |
| 1:A:160:ASN:ND2  | 1:A:162:SER:OG   | 2.47                     | 0.46              |
| 1:A:392:LEU:HD11 | 1:A:459:PHE:CE1  | 2.45                     | 0.46              |
| 2:B:8:C:H2'      | 2:B:9:U:H6       | 1.80                     | 0.46              |
| 1:D:266:MET:HE2  | 1:D:277:ARG:NH2  | 2.29                     | 0.46              |
| 1:D:401:LEU:HD22 | 1:D:461:LYS:CD   | 2.33                     | 0.46              |
| 1:A:22:LYS:HG2   | 1:A:58:PRO:HG3   | 1.97                     | 0.46              |
| 1:A:199:PRO:HD2  | 1:A:202:ILE:HD12 | 1.96                     | 0.46              |
| 1:A:365:ARG:O    | 1:A:366:GLN:HB2  | 2.15                     | 0.46              |
| 1:A:59:GLU:HB3   | 1:A:60:PHE:CD1   | 2.51                     | 0.46              |
| 1:A:223:TYR:HB2  | 1:A:235:ASP:HB2  | 1.97                     | 0.46              |
| 1:A:557:SER:HB2  | 1:A:681:LYS:O    | 2.15                     | 0.46              |
| 1:D:181:LEU:CG   | 1:D:184:TYR:HB2  | 2.42                     | 0.46              |
| 1:D:190:HIS:O    | 1:D:259:ASN:HB2  | 2.15                     | 0.46              |
| 1:D:599:GLU:HG2  | 1:D:600:SER:N    | 2.31                     | 0.46              |
| 1:A:46:LYS:CE    | 2:B:14:A:H4'     | 2.45                     | 0.46              |
| 1:A:110:ILE:CG2  | 1:A:126:LEU:HD11 | 2.44                     | 0.46              |
| 1:A:372:GLN:O    | 1:A:374:PRO:HD3  | 2.15                     | 0.46              |
| 1:A:486:SER:O    | 1:A:490:LEU:HG   | 2.16                     | 0.46              |
| 1:A:797:VAL:O    | 1:A:800:HIS:HB2  | 2.16                     | 0.46              |
| 1:D:54:HIS:ND1   | 1:D:63:VAL:HG22  | 2.30                     | 0.46              |
| 1:D:642:THR:N    | 1:D:643:PRO:CD   | 2.78                     | 0.46              |
| 1:D:199:PRO:HG2  | 1:D:202:ILE:HD12 | 1.98                     | 0.46              |
| 1:A:106:ARG:O    | 1:A:110:ILE:HG13 | 2.16                     | 0.46              |
| 1:A:305:VAL:HG12 | 1:A:306:LYS:N    | 2.31                     | 0.46              |
| 1:A:931:LYS:HG3  | 1:A:931:LYS:O    | 2.16                     | 0.46              |
| 1:D:537:GLU:HA   | 1:D:641:MET:HE2  | 1.96                     | 0.46              |
| 1:D:817:PHE:C    | 1:D:819:PRO:CD   | 2.81                     | 0.46              |
| 1:A:689:GLU:OE2  | 3:C:3:C:H1'      | 2.16                     | 0.46              |
| 1:A:870:ASN:HA   | 1:A:886:PHE:HE2  | 1.78                     | 0.46              |
| 1:D:43:ILE:O     | 1:D:44:PRO:C     | 2.58                     | 0.46              |
| 1:D:55:LEU:HD23  | 1:D:81:ALA:HB2   | 1.97                     | 0.46              |
| 1:D:396:CYS:O    | 1:D:399:HIS:O    | 2.33                     | 0.46              |
| 1:D:705:ALA:O    | 1:D:709:ILE:HG13 | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:221:ALA:HB1  | 1:A:326:LEU:O    | 2.16                     | 0.46              |
| 1:A:636:TYR:HA   | 1:A:675:ILE:O    | 2.16                     | 0.46              |
| 1:D:12:LYS:HD2   | 1:D:79:GLU:HA    | 1.97                     | 0.46              |
| 1:A:315:ILE:HD11 | 1:A:348:PHE:CE1  | 2.51                     | 0.45              |
| 1:A:796:GLU:OE2  | 5:A:951:SAH:HB2  | 2.16                     | 0.45              |
| 1:D:232:VAL:HG23 | 1:D:311:ARG:HH21 | 1.79                     | 0.45              |
| 1:A:621:ASN:HD22 | 1:A:621:ASN:C    | 2.25                     | 0.45              |
| 2:B:14:A:O2'     | 2:B:15:A:H5'     | 2.17                     | 0.45              |
| 1:D:282:ILE:HG23 | 1:D:283:PRO:HD2  | 1.98                     | 0.45              |
| 1:A:17:GLN:NE2   | 2:B:4:U:H4'      | 2.31                     | 0.45              |
| 1:A:237:LEU:CD2  | 1:A:249:ILE:HG12 | 2.46                     | 0.45              |
| 1:A:368:VAL:CG2  | 1:A:654:VAL:CG2  | 2.94                     | 0.45              |
| 1:A:565:LEU:HD21 | 1:A:673:TYR:CD2  | 2.52                     | 0.45              |
| 1:D:107:ILE:HG22 | 1:D:185:ILE:CD1  | 2.46                     | 0.45              |
| 1:D:265:ARG:HH12 | 1:D:400:ARG:CZ   | 2.29                     | 0.45              |
| 1:D:524:PHE:CD1  | 1:D:524:PHE:O    | 2.70                     | 0.45              |
| 1:D:783:ASP:H    | 1:D:817:PHE:HZ   | 1.65                     | 0.45              |
| 1:A:271:SER:HB3  | 1:A:351:ILE:HA   | 1.98                     | 0.45              |
| 1:A:714:ALA:O    | 1:A:737:SER:O    | 2.34                     | 0.45              |
| 1:D:100:ARG:O    | 1:D:104:VAL:HG23 | 2.16                     | 0.45              |
| 1:D:104:VAL:HG22 | 1:D:177:ALA:HB1  | 1.99                     | 0.45              |
| 1:D:88:ARG:HG2   | 1:D:89:PRO:CD    | 2.38                     | 0.45              |
| 1:D:700:GLN:HB3  | 1:D:889:VAL:HG11 | 1.97                     | 0.45              |
| 1:D:826:THR:HG23 | 1:D:827:PRO:HD2  | 1.98                     | 0.45              |
| 1:A:231:VAL:HG12 | 1:A:232:VAL:N    | 2.32                     | 0.45              |
| 1:D:628:VAL:HG23 | 1:D:675:ILE:HD12 | 1.98                     | 0.45              |
| 1:A:12:LYS:HB3   | 1:A:78:ALA:HB1   | 1.99                     | 0.45              |
| 1:A:169:LEU:O    | 1:A:173:TYR:HD1  | 1.97                     | 0.45              |
| 1:A:255:LEU:CD1  | 1:A:281:GLU:HB2  | 2.40                     | 0.45              |
| 1:A:333:TRP:C    | 1:A:335:SER:H    | 2.25                     | 0.45              |
| 1:A:821:LEU:HD11 | 1:A:905:ILE:HG23 | 1.99                     | 0.45              |
| 1:A:822:LEU:HB3  | 1:A:906:PHE:HB2  | 1.99                     | 0.45              |
| 3:C:13:G:H2'     | 3:C:14:A:C8      | 2.52                     | 0.45              |
| 1:D:116:LEU:HG   | 1:D:206:LEU:CD1  | 2.36                     | 0.45              |
| 1:D:553:ILE:HG22 | 1:D:554:THR:N    | 2.32                     | 0.45              |
| 1:D:717:LEU:HD12 | 1:D:791:ILE:O    | 2.16                     | 0.45              |
| 1:D:792:GLY:O    | 1:D:822:LEU:HD12 | 2.16                     | 0.45              |
| 1:A:142:VAL:HG22 | 1:A:175:MET:HE3  | 1.97                     | 0.45              |
| 1:A:719:ASP:OD2  | 1:A:727:LEU:HD23 | 2.17                     | 0.45              |
| 1:A:727:LEU:CD2  | 1:A:793:THR:HG21 | 2.46                     | 0.45              |
| 1:D:11:PRO:HG3   | 2:E:5:U:O2'      | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:696:PRO:O    | 1:D:699:LYS:HB2  | 2.17                     | 0.45              |
| 1:D:775:TYR:HB3  | 1:D:924:TYR:HB3  | 1.97                     | 0.45              |
| 1:A:108:LYS:CD   | 1:A:181:LEU:HD21 | 2.43                     | 0.45              |
| 1:A:235:ASP:OD1  | 1:A:252:ARG:HD2  | 2.18                     | 0.45              |
| 1:D:118:ALA:C    | 1:D:120:HIS:H    | 2.24                     | 0.45              |
| 1:A:896:GLU:N    | 1:A:897:PRO:HD2  | 2.31                     | 0.44              |
| 1:D:169:LEU:O    | 1:D:173:TYR:CD1  | 2.70                     | 0.44              |
| 1:D:267:PHE:CE1  | 1:D:315:ILE:HG22 | 2.52                     | 0.44              |
| 1:D:401:LEU:HD11 | 1:D:461:LYS:HE2  | 1.99                     | 0.44              |
| 2:E:20:A:O2'     | 2:E:21:A:H5''    | 2.17                     | 0.44              |
| 1:D:358:ASN:ND2  | 1:D:373:LEU:N    | 2.65                     | 0.44              |
| 1:D:733:ASP:OD1  | 1:D:761:LYS:HE2  | 2.17                     | 0.44              |
| 1:A:347:SER:O    | 1:A:351:ILE:HG13 | 2.18                     | 0.44              |
| 1:D:59:GLU:HB3   | 1:D:60:PHE:HD2   | 1.82                     | 0.44              |
| 1:D:278:LEU:CD2  | 1:D:320:ILE:HG13 | 2.46                     | 0.44              |
| 1:A:211:SER:O    | 1:A:212:ASP:C    | 2.60                     | 0.44              |
| 1:A:219:VAL:HG23 | 1:A:239:ILE:HD13 | 1.99                     | 0.44              |
| 1:D:127:ARG:NH1  | 1:D:336:ASP:OD1  | 2.50                     | 0.44              |
| 1:D:396:CYS:HA   | 1:D:401:LEU:HG   | 1.99                     | 0.44              |
| 1:D:570:ASP:HB3  | 1:D:640:LYS:HZ3  | 1.81                     | 0.44              |
| 1:D:620:MET:HE3  | 1:D:625:GLU:CG   | 2.47                     | 0.44              |
| 1:D:745:ASP:O    | 1:D:776:ASP:HA   | 2.18                     | 0.44              |
| 1:A:113:ASP:HB3  | 1:A:202:ILE:CD1  | 2.46                     | 0.44              |
| 1:A:759:HIS:O    | 1:A:763:ASN:ND2  | 2.51                     | 0.44              |
| 1:A:837:ARG:O    | 1:A:838:SER:HB3  | 2.17                     | 0.44              |
| 2:B:7:U:O2       | 2:B:7:U:H2'      | 2.18                     | 0.44              |
| 1:D:487:LEU:HD23 | 1:D:491:LEU:HD12 | 2.00                     | 0.44              |
| 1:D:556:GLY:HA3  | 1:D:683:PRO:HB3  | 1.99                     | 0.44              |
| 1:D:648:GLU:OE1  | 1:D:665:LEU:HD13 | 2.18                     | 0.44              |
| 1:A:48:PRO:HD3   | 2:B:15:A:O2'     | 2.18                     | 0.44              |
| 1:A:222:VAL:CG1  | 1:A:223:TYR:N    | 2.81                     | 0.44              |
| 2:B:11:U:O2'     | 2:B:12:G:H5'     | 2.17                     | 0.44              |
| 1:A:94:LEU:HB3   | 1:A:158:ILE:HG21 | 2.00                     | 0.44              |
| 3:C:19:U:H2'     | 3:C:20:C:H6      | 1.83                     | 0.44              |
| 1:D:172:SER:O    | 1:D:176:LYS:HG3  | 2.18                     | 0.44              |
| 1:D:559:VAL:HG23 | 1:D:615:VAL:HG22 | 1.99                     | 0.44              |
| 1:A:8:THR:N      | 1:A:9:PRO:CD     | 2.81                     | 0.43              |
| 1:A:696:PRO:HD2  | 1:A:699:LYS:HD2  | 2.00                     | 0.43              |
| 1:A:763:ASN:C    | 1:A:764:LYS:O    | 2.58                     | 0.43              |
| 1:A:921:MET:HE3  | 1:A:921:MET:HB2  | 1.78                     | 0.43              |
| 3:C:11:G:H2'     | 3:C:12:A:H8      | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:110:ILE:HD13 | 1:D:122:LEU:HD13 | 2.00                     | 0.43              |
| 1:A:50:LEU:HD23  | 1:A:50:LEU:N     | 2.32                     | 0.43              |
| 1:A:340:TYR:CD1  | 1:A:340:TYR:C    | 2.96                     | 0.43              |
| 1:A:467:LEU:HD22 | 1:A:492:TRP:CE3  | 2.53                     | 0.43              |
| 1:D:121:PRO:O    | 1:D:124:ALA:HB3  | 2.18                     | 0.43              |
| 1:D:153:ASN:O    | 1:D:157:LYS:HG3  | 2.18                     | 0.43              |
| 1:A:121:PRO:HB2  | 1:A:148:VAL:CG1  | 2.48                     | 0.43              |
| 1:A:217:ARG:HD3  | 1:A:340:TYR:CE2  | 2.53                     | 0.43              |
| 1:A:318:GLN:CG   | 1:A:400:ARG:HH22 | 2.24                     | 0.43              |
| 1:A:356:SER:O    | 1:A:360:ILE:HG13 | 2.18                     | 0.43              |
| 1:A:407:SER:HB2  | 1:A:456:VAL:O    | 2.18                     | 0.43              |
| 1:A:620:MET:HE2  | 1:A:624:ILE:HG22 | 2.00                     | 0.43              |
| 2:B:16:G:O2'     | 2:B:17:C:H5'     | 2.19                     | 0.43              |
| 1:D:164:GLU:CB   | 1:D:400:ARG:HH12 | 2.24                     | 0.43              |
| 1:D:389:ARG:HD2  | 1:D:389:ARG:O    | 2.18                     | 0.43              |
| 1:D:461:LYS:HG3  | 1:D:466:VAL:CG2  | 2.41                     | 0.43              |
| 1:D:496:PHE:N    | 1:D:496:PHE:HD2  | 2.14                     | 0.43              |
| 1:D:652:LEU:HD23 | 1:D:661:ILE:HG21 | 1.99                     | 0.43              |
| 1:D:695:PRO:HG2  | 1:D:700:GLN:NE2  | 2.33                     | 0.43              |
| 2:E:4:U:H2'      | 2:E:5:U:C6       | 2.53                     | 0.43              |
| 1:A:71:LYS:HE2   | 2:B:6:C:P        | 2.58                     | 0.43              |
| 1:A:896:GLU:O    | 1:A:897:PRO:C    | 2.60                     | 0.43              |
| 3:C:10:A:H2'     | 3:C:11:G:C8      | 2.53                     | 0.43              |
| 1:D:126:LEU:O    | 1:D:129:ALA:HB3  | 2.18                     | 0.43              |
| 1:D:257:ASP:N    | 1:D:260:GLN:NE2  | 2.65                     | 0.43              |
| 1:D:391:ILE:HB   | 1:D:490:LEU:HD11 | 2.00                     | 0.43              |
| 1:D:406:LEU:HD13 | 1:D:457:LYS:CE   | 2.44                     | 0.43              |
| 1:D:824:VAL:HG12 | 1:D:825:SER:N    | 2.33                     | 0.43              |
| 1:D:227:ILE:HB   | 1:D:230:GLU:OE2  | 2.18                     | 0.43              |
| 1:D:234:LEU:HB2  | 1:D:345:VAL:HG23 | 1.99                     | 0.43              |
| 1:D:667:GLU:O    | 1:D:669:PRO:HD3  | 2.19                     | 0.43              |
| 1:D:832:ASN:O    | 1:D:836:GLN:HG3  | 2.18                     | 0.43              |
| 1:A:57:LEU:CG    | 1:A:58:PRO:HD2   | 2.48                     | 0.43              |
| 1:A:680:VAL:HG12 | 1:A:681:LYS:N    | 2.34                     | 0.43              |
| 1:A:785:ARG:NH2  | 1:A:922:GLN:HB3  | 2.34                     | 0.43              |
| 1:A:694:LYS:CB   | 1:A:695:PRO:HD2  | 2.48                     | 0.43              |
| 1:D:158:ILE:H    | 1:D:158:ILE:HG13 | 1.66                     | 0.43              |
| 1:D:265:ARG:HH12 | 1:D:400:ARG:NH2  | 2.17                     | 0.43              |
| 1:D:732:LEU:HD21 | 1:D:762:LEU:HD23 | 2.00                     | 0.43              |
| 1:D:895:VAL:HG12 | 1:D:896:GLU:H    | 1.83                     | 0.43              |
| 1:D:12:LYS:CD    | 1:D:82:LEU:HD12  | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:69:LYS:HB2   | 1:D:72:ASP:HB2   | 2.00                     | 0.43              |
| 1:D:314:TYR:CE2  | 1:D:355:MET:HG3  | 2.54                     | 0.43              |
| 1:D:329:VAL:HG12 | 1:D:340:TYR:HB3  | 2.00                     | 0.43              |
| 1:A:120:HIS:HD2  | 1:A:122:LEU:HB2  | 1.84                     | 0.43              |
| 1:A:160:ASN:HB2  | 1:A:173:TYR:OH   | 2.19                     | 0.43              |
| 1:A:624:ILE:O    | 1:A:628:VAL:HG23 | 2.18                     | 0.43              |
| 1:D:92:ASP:O     | 1:D:94:LEU:HG    | 2.19                     | 0.43              |
| 1:D:492:TRP:CD1  | 1:D:495:LYS:HD3  | 2.53                     | 0.43              |
| 1:D:742:ILE:HD13 | 1:D:786:LEU:CD2  | 2.48                     | 0.43              |
| 1:A:126:LEU:HD23 | 1:A:140:VAL:CG2  | 2.42                     | 0.43              |
| 1:A:742:ILE:HG21 | 1:A:786:LEU:CD2  | 2.49                     | 0.43              |
| 1:A:834:ILE:CG2  | 1:A:835:LEU:N    | 2.82                     | 0.43              |
| 1:D:42:ALA:C     | 1:D:44:PRO:CD    | 2.91                     | 0.43              |
| 1:D:326:LEU:HG   | 1:D:343:VAL:HG11 | 2.01                     | 0.43              |
| 1:D:762:LEU:HD13 | 1:D:930:TRP:CE3  | 2.54                     | 0.43              |
| 1:A:120:HIS:O    | 1:A:122:LEU:N    | 2.52                     | 0.42              |
| 1:A:741:ILE:HG13 | 1:A:772:ALA:HA   | 2.00                     | 0.42              |
| 1:A:796:GLU:HB3  | 1:A:825:SER:OG   | 2.19                     | 0.42              |
| 1:D:11:PRO:HB2   | 1:D:75:GLN:NE2   | 2.34                     | 0.42              |
| 1:D:329:VAL:HG12 | 1:D:340:TYR:CB   | 2.49                     | 0.42              |
| 1:A:10:THR:CG2   | 1:A:90:GLN:HG2   | 2.45                     | 0.42              |
| 1:A:225:PRO:HG3  | 1:A:230:GLU:HG2  | 2.01                     | 0.42              |
| 1:A:695:PRO:HA   | 1:A:696:PRO:HD3  | 1.88                     | 0.42              |
| 1:D:255:LEU:HD13 | 1:D:260:GLN:CB   | 2.48                     | 0.42              |
| 1:D:624:ILE:O    | 1:D:624:ILE:CG2  | 2.66                     | 0.42              |
| 1:A:127:ARG:CG   | 1:A:206:LEU:HD21 | 2.42                     | 0.42              |
| 1:A:250:ALA:HB2  | 1:A:261:VAL:CG2  | 2.49                     | 0.42              |
| 1:A:864:TRP:CA   | 1:A:868:GLN:NE2  | 2.78                     | 0.42              |
| 1:A:924:TYR:N    | 1:A:924:TYR:CD2  | 2.86                     | 0.42              |
| 5:A:951:SAH:HG2  | 2:B:22:G:N2      | 2.34                     | 0.42              |
| 2:B:20:A:O2'     | 2:B:21:A:C5'     | 2.68                     | 0.42              |
| 2:B:4:U:O2'      | 2:B:5:U:H5'      | 2.19                     | 0.42              |
| 1:D:12:LYS:HE3   | 1:D:79:GLU:OE2   | 2.19                     | 0.42              |
| 1:D:94:LEU:HD12  | 1:D:158:ILE:CD1  | 2.49                     | 0.42              |
| 1:D:818:HIS:HA   | 1:D:819:PRO:HD2  | 1.34                     | 0.42              |
| 1:A:8:THR:O      | 1:A:8:THR:HG22   | 2.19                     | 0.42              |
| 1:A:621:ASN:HD22 | 1:A:622:PRO:CD   | 2.33                     | 0.42              |
| 3:C:11:G:H2'     | 3:C:12:A:C8      | 2.54                     | 0.42              |
| 1:D:12:LYS:HE3   | 1:D:79:GLU:CD    | 2.44                     | 0.42              |
| 1:D:262:MET:CA   | 1:D:282:ILE:HD11 | 2.49                     | 0.42              |
| 1:D:608:ASN:ND2  | 1:D:611:ILE:HD11 | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:742:ILE:HD13 | 1:D:786:LEU:HD23 | 2.01                     | 0.42              |
| 1:D:895:VAL:CG1  | 1:D:897:PRO:HD2  | 2.43                     | 0.42              |
| 1:A:822:LEU:HD23 | 1:A:822:LEU:C    | 2.44                     | 0.42              |
| 1:D:198:TYR:O    | 1:D:199:PRO:C    | 2.61                     | 0.42              |
| 1:D:227:ILE:HG22 | 1:D:229:GLU:H    | 1.84                     | 0.42              |
| 1:D:271:SER:O    | 1:D:350:ARG:NH1  | 2.52                     | 0.42              |
| 1:D:694:LYS:CB   | 1:D:695:PRO:CD   | 2.97                     | 0.42              |
| 2:E:3:U:H2'      | 2:E:4:U:O4'      | 2.20                     | 0.42              |
| 1:A:119:GLU:O    | 1:A:120:HIS:C    | 2.63                     | 0.42              |
| 1:A:218:GLU:OE1  | 1:A:236:THR:HG21 | 2.20                     | 0.42              |
| 2:B:6:C:H2'      | 2:B:7:U:O4'      | 2.19                     | 0.42              |
| 1:A:39:PRO:HD2   | 1:A:759:HIS:NE2  | 2.34                     | 0.42              |
| 1:A:827:PRO:C    | 1:A:902:GLN:HE21 | 2.27                     | 0.42              |
| 1:A:857:ASN:HB3  | 1:A:859:ASP:H    | 1.84                     | 0.42              |
| 1:D:14:ILE:O     | 1:D:17:GLN:HB3   | 2.20                     | 0.42              |
| 1:D:126:LEU:HD23 | 1:D:140:VAL:HG21 | 2.02                     | 0.42              |
| 1:D:151:LYS:O    | 1:D:155:ARG:HG2  | 2.19                     | 0.42              |
| 1:D:833:THR:O    | 1:D:837:ARG:HG3  | 2.19                     | 0.42              |
| 1:D:834:ILE:HD12 | 1:D:897:PRO:HB3  | 2.01                     | 0.42              |
| 1:D:283:PRO:O    | 1:D:285:LYS:N    | 2.52                     | 0.42              |
| 1:D:387:LEU:CB   | 1:D:483:GLN:HE22 | 2.24                     | 0.42              |
| 1:D:537:GLU:CA   | 1:D:641:MET:HE1  | 2.49                     | 0.42              |
| 1:D:746:ILE:C    | 1:D:746:ILE:HD12 | 2.45                     | 0.42              |
| 1:D:908:ARG:HG2  | 1:D:909:GLU:H    | 1.84                     | 0.42              |
| 1:A:391:ILE:O    | 1:A:391:ILE:HG12 | 2.20                     | 0.42              |
| 1:A:693:PHE:CD1  | 1:A:693:PHE:N    | 2.88                     | 0.42              |
| 1:A:822:LEU:CD2  | 1:A:824:VAL:HG23 | 2.50                     | 0.42              |
| 3:C:13:G:H2'     | 3:C:14:A:H8      | 1.85                     | 0.42              |
| 1:D:535:SER:N    | 1:D:643:PRO:HB2  | 2.35                     | 0.42              |
| 1:D:559:VAL:HG13 | 1:D:677:LEU:HD11 | 2.01                     | 0.42              |
| 1:D:836:GLN:HG2  | 2:E:21:A:N1      | 2.34                     | 0.42              |
| 1:D:919:SER:OG   | 1:D:921:MET:HE1  | 2.19                     | 0.42              |
| 1:A:39:PRO:HD2   | 1:A:759:HIS:CD2  | 2.55                     | 0.41              |
| 1:A:71:LYS:NZ    | 2:B:7:U:OP2      | 2.50                     | 0.41              |
| 1:A:368:VAL:HG22 | 1:A:654:VAL:HG22 | 1.99                     | 0.41              |
| 1:A:559:VAL:HG23 | 1:A:615:VAL:CG2  | 2.50                     | 0.41              |
| 1:A:745:ASP:OD1  | 1:A:746:ILE:N    | 2.53                     | 0.41              |
| 1:D:62:VAL:HG11  | 1:D:80:LEU:HB3   | 2.02                     | 0.41              |
| 1:D:96:VAL:O     | 1:D:100:ARG:HD2  | 2.19                     | 0.41              |
| 1:D:383:TRP:HZ2  | 1:D:386:PRO:O    | 2.03                     | 0.41              |
| 1:D:387:LEU:HD13 | 1:D:483:GLN:NE2  | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:12:LYS:CB    | 1:A:78:ALA:HB3   | 2.51                     | 0.41              |
| 1:A:30:VAL:HG12  | 1:A:31:HIS:N     | 2.34                     | 0.41              |
| 1:A:209:HIS:O    | 1:A:209:HIS:CG   | 2.71                     | 0.41              |
| 1:A:255:LEU:HB3  | 1:A:260:GLN:CD   | 2.44                     | 0.41              |
| 1:D:524:PHE:O    | 1:D:524:PHE:CG   | 2.74                     | 0.41              |
| 1:D:658:THR:O    | 1:D:662:ARG:HG3  | 2.20                     | 0.41              |
| 1:D:18:LYS:O     | 1:D:18:LYS:HG3   | 2.19                     | 0.41              |
| 1:D:47:GLY:HA3   | 1:D:48:PRO:HD3   | 1.91                     | 0.41              |
| 1:D:548:LYS:C    | 1:D:552:SER:HB2  | 2.43                     | 0.41              |
| 1:A:168:PHE:HD2  | 1:A:282:ILE:HG23 | 1.84                     | 0.41              |
| 1:A:246:LEU:HD22 | 1:A:261:VAL:CG1  | 2.50                     | 0.41              |
| 1:A:368:VAL:CG2  | 1:A:369:ILE:N    | 2.82                     | 0.41              |
| 1:A:864:TRP:CA   | 1:A:868:GLN:HE21 | 2.32                     | 0.41              |
| 2:B:13:C:H2'     | 2:B:14:A:H8      | 1.85                     | 0.41              |
| 1:D:380:LYS:HD2  | 1:D:479:ASN:ND2  | 2.35                     | 0.41              |
| 1:D:783:ASP:OD1  | 1:D:922:GLN:HA   | 2.19                     | 0.41              |
| 1:D:857:ASN:HB3  | 1:D:860:HIS:CE1  | 2.56                     | 0.41              |
| 1:A:32:ASP:HB2   | 1:A:50:LEU:CD1   | 2.50                     | 0.41              |
| 1:A:52:ARG:HB2   | 1:A:64:SER:O     | 2.21                     | 0.41              |
| 1:A:356:SER:HA   | 1:A:497:PHE:CE1  | 2.55                     | 0.41              |
| 1:D:38:CYS:HB3   | 1:D:41:LEU:CD1   | 2.50                     | 0.41              |
| 1:D:231:VAL:HG12 | 1:D:232:VAL:O    | 2.21                     | 0.41              |
| 1:D:243:ARG:O    | 1:D:244:HIS:C    | 2.63                     | 0.41              |
| 1:D:272:CYS:HB2  | 1:D:351:ILE:CD1  | 2.51                     | 0.41              |
| 1:D:482:ILE:O    | 1:D:485:ALA:HB3  | 2.20                     | 0.41              |
| 1:D:773:THR:O    | 1:D:774:LEU:HD23 | 2.20                     | 0.41              |
| 1:A:631:MET:HA   | 1:A:635:GLU:OE1  | 2.20                     | 0.41              |
| 1:D:527:PRO:N    | 1:D:528:PRO:CD   | 2.84                     | 0.41              |
| 1:D:679:GLY:C    | 1:D:680:VAL:HG23 | 2.45                     | 0.41              |
| 1:D:793:THR:HG22 | 1:D:795:LEU:HG   | 2.02                     | 0.41              |
| 3:C:3:C:H2'      | 3:C:4:G:C8       | 2.55                     | 0.41              |
| 1:D:358:ASN:HA   | 1:D:373:LEU:HB2  | 2.02                     | 0.41              |
| 1:D:370:ALA:O    | 1:D:620:MET:HB2  | 2.20                     | 0.41              |
| 1:D:561:ILE:HG22 | 1:D:677:LEU:HD12 | 2.02                     | 0.41              |
| 2:E:11:U:O2'     | 2:E:12:G:H5'     | 2.21                     | 0.41              |
| 1:A:244:HIS:HD2  | 1:A:246:LEU:N    | 2.01                     | 0.41              |
| 1:A:667:GLU:O    | 1:A:669:PRO:CD   | 2.64                     | 0.41              |
| 1:D:95:THR:C     | 1:D:97:ASP:N     | 2.78                     | 0.41              |
| 1:D:154:SER:O    | 1:D:158:ILE:HG13 | 2.20                     | 0.41              |
| 1:D:168:PHE:HE2  | 1:D:282:ILE:HG12 | 1.86                     | 0.41              |
| 1:D:262:MET:N    | 1:D:280:SER:O    | 2.46                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:186:VAL:CG2  | 1:A:195:LYS:HG3  | 2.50                     | 0.41              |
| 1:A:237:LEU:HD22 | 1:A:249:ILE:HG12 | 2.03                     | 0.41              |
| 1:A:263:ILE:HG12 | 1:A:279:TYR:CE2  | 2.56                     | 0.41              |
| 1:A:392:LEU:HD21 | 1:A:404:PRO:CG   | 2.51                     | 0.41              |
| 1:A:470:SER:HA   | 1:A:471:PRO:HD3  | 1.83                     | 0.41              |
| 1:A:753:ARG:HA   | 1:A:756:LYS:HE2  | 2.03                     | 0.41              |
| 1:D:18:LYS:O     | 1:D:18:LYS:CG    | 2.69                     | 0.41              |
| 1:D:199:PRO:HB2  | 1:D:201:GLU:OE1  | 2.20                     | 0.41              |
| 1:D:782:PHE:HD1  | 1:D:817:PHE:CE1  | 2.39                     | 0.41              |
| 1:D:857:ASN:HB3  | 1:D:860:HIS:ND1  | 2.36                     | 0.41              |
| 1:A:401:LEU:HD22 | 1:A:461:LYS:HB3  | 1.98                     | 0.41              |
| 1:A:696:PRO:O    | 1:A:697:LEU:C    | 2.63                     | 0.41              |
| 1:A:728:LEU:HD22 | 1:A:741:ILE:HD12 | 2.03                     | 0.41              |
| 1:A:783:ASP:OD1  | 1:A:922:GLN:HA   | 2.21                     | 0.41              |
| 1:A:821:LEU:HD12 | 1:A:906:PHE:O    | 2.21                     | 0.41              |
| 1:A:827:PRO:HB2  | 1:A:856:ARG:CZ   | 2.50                     | 0.41              |
| 1:A:887:SER:O    | 1:A:903:ILE:N    | 2.54                     | 0.41              |
| 1:D:212:ASP:HB3  | 1:D:337:ASP:OD1  | 2.21                     | 0.41              |
| 1:D:401:LEU:CD2  | 1:D:461:LYS:HD3  | 2.37                     | 0.41              |
| 1:D:780:LEU:HD11 | 1:D:805:GLN:HB3  | 2.03                     | 0.41              |
| 2:E:11:U:H2'     | 2:E:12:G:C8      | 2.55                     | 0.41              |
| 1:A:160:ASN:CB   | 1:A:173:TYR:OH   | 2.69                     | 0.40              |
| 1:A:624:ILE:HD11 | 1:A:673:TYR:CE2  | 2.55                     | 0.40              |
| 1:A:719:ASP:O    | 1:A:721:GLY:N    | 2.54                     | 0.40              |
| 1:D:43:ILE:O     | 1:D:43:ILE:CG2   | 2.62                     | 0.40              |
| 1:A:12:LYS:HE2   | 1:A:90:GLN:HE22  | 1.85                     | 0.40              |
| 1:A:82:LEU:CD2   | 1:A:85:LEU:HD12  | 2.37                     | 0.40              |
| 1:A:120:HIS:CD2  | 1:A:122:LEU:H    | 2.38                     | 0.40              |
| 1:A:252:ARG:HH11 | 1:A:252:ARG:CG   | 2.33                     | 0.40              |
| 1:A:361:TYR:HB2  | 1:A:391:ILE:CD1  | 2.52                     | 0.40              |
| 1:A:457:LYS:NZ   | 1:A:489:ALA:HB3  | 2.36                     | 0.40              |
| 1:A:493:PHE:HA   | 1:A:496:PHE:HD1  | 1.84                     | 0.40              |
| 2:B:20:A:C2'     | 2:B:21:A:H5''    | 2.51                     | 0.40              |
| 1:D:73:SER:OG    | 1:D:74:GLU:N     | 2.53                     | 0.40              |
| 1:D:483:GLN:HA   | 1:D:483:GLN:OE1  | 2.21                     | 0.40              |
| 1:D:570:ASP:OD2  | 1:D:672:ASN:OD1  | 2.38                     | 0.40              |
| 1:D:695:PRO:HG2  | 1:D:700:GLN:CG   | 2.50                     | 0.40              |
| 1:A:493:PHE:HA   | 1:A:496:PHE:CE1  | 2.55                     | 0.40              |
| 1:A:605:ILE:HD13 | 1:A:651:ILE:HG23 | 2.03                     | 0.40              |
| 1:D:38:CYS:HA    | 1:D:39:PRO:HD3   | 1.86                     | 0.40              |
| 1:D:62:VAL:HG21  | 1:D:81:ALA:HA    | 2.02                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:373:LEU:HA   | 1:D:374:PRO:HD3  | 1.80                     | 0.40              |
| 1:D:824:VAL:O    | 1:D:903:ILE:HB   | 2.21                     | 0.40              |
| 1:A:17:GLN:HG2   | 6:B:23:HOH:O     | 2.22                     | 0.40              |
| 1:A:100:ARG:O    | 1:A:104:VAL:HG23 | 2.22                     | 0.40              |
| 1:D:149:ASP:OD2  | 1:D:152:ILE:HG12 | 2.21                     | 0.40              |
| 1:D:392:LEU:HD11 | 1:D:459:PHE:HZ   | 1.87                     | 0.40              |
| 1:D:648:GLU:OE1  | 1:D:665:LEU:HD22 | 2.22                     | 0.40              |
| 1:D:736:THR:CG2  | 1:D:738:LEU:HG   | 2.52                     | 0.40              |
| 1:A:12:LYS:HB3   | 1:A:78:ALA:HB3   | 2.04                     | 0.40              |
| 1:A:217:ARG:HD3  | 1:A:340:TYR:HE2  | 1.85                     | 0.40              |
| 1:A:457:LYS:HZ3  | 1:A:489:ALA:HB3  | 1.87                     | 0.40              |
| 1:A:813:VAL:HA   | 1:A:817:PHE:CD1  | 2.50                     | 0.40              |
| 1:D:777:GLY:HA3  | 1:D:924:TYR:CE1  | 2.57                     | 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     | 761/950 (80%)   | 671 (88%)  | 72 (10%) | 18 (2%)  | 4           | 22 |
| 1   | D     | 777/950 (82%)   | 692 (89%)  | 70 (9%)  | 15 (2%)  | 6           | 27 |
| All | All   | 1538/1900 (81%) | 1363 (89%) | 142 (9%) | 33 (2%)  | 5           | 25 |

All (33) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 44  | PRO  |
| 1   | A     | 59  | GLU  |
| 1   | A     | 284 | LYS  |
| 1   | D     | 48  | PRO  |
| 1   | D     | 854 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 682 | GLY  |
| 1   | A     | 687 | ARG  |
| 1   | A     | 720 | PHE  |
| 1   | A     | 924 | TYR  |
| 1   | D     | 644 | PRO  |
| 1   | A     | 58  | PRO  |
| 1   | A     | 694 | LYS  |
| 1   | A     | 722 | CYS  |
| 1   | A     | 723 | GLY  |
| 1   | D     | 44  | PRO  |
| 1   | D     | 284 | LYS  |
| 1   | A     | 310 | ALA  |
| 1   | A     | 380 | LYS  |
| 1   | D     | 197 | ALA  |
| 1   | D     | 207 | ALA  |
| 1   | D     | 895 | VAL  |
| 1   | A     | 121 | PRO  |
| 1   | A     | 334 | LYS  |
| 1   | A     | 669 | PRO  |
| 1   | D     | 189 | PRO  |
| 1   | A     | 8   | THR  |
| 1   | D     | 570 | ASP  |
| 1   | D     | 643 | PRO  |
| 1   | D     | 694 | LYS  |
| 1   | A     | 735 | PRO  |
| 1   | D     | 43  | ILE  |
| 1   | D     | 471 | PRO  |
| 1   | D     | 735 | PRO  |

### 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     | 676/828 (82%)   | 624 (92%)  | 52 (8%)  | 12          | 38 |
| 1   | D     | 689/828 (83%)   | 653 (95%)  | 36 (5%)  | 21          | 51 |
| All | All   | 1365/1656 (82%) | 1277 (94%) | 88 (6%)  | 16          | 44 |

All (88) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 22  | LYS  |
| 1   | A     | 49  | CYS  |
| 1   | A     | 58  | PRO  |
| 1   | A     | 63  | VAL  |
| 1   | A     | 64  | SER  |
| 1   | A     | 91  | ASN  |
| 1   | A     | 121 | PRO  |
| 1   | A     | 143 | SER  |
| 1   | A     | 167 | PRO  |
| 1   | A     | 173 | TYR  |
| 1   | A     | 175 | MET  |
| 1   | A     | 183 | ASP  |
| 1   | A     | 193 | ARG  |
| 1   | A     | 209 | HIS  |
| 1   | A     | 218 | GLU  |
| 1   | A     | 230 | GLU  |
| 1   | A     | 251 | GLU  |
| 1   | A     | 311 | ARG  |
| 1   | A     | 339 | ASP  |
| 1   | A     | 365 | ARG  |
| 1   | A     | 392 | LEU  |
| 1   | A     | 396 | CYS  |
| 1   | A     | 458 | ILE  |
| 1   | A     | 462 | SER  |
| 1   | A     | 473 | LYS  |
| 1   | A     | 497 | PHE  |
| 1   | A     | 537 | GLU  |
| 1   | A     | 538 | SER  |
| 1   | A     | 541 | THR  |
| 1   | A     | 560 | SER  |
| 1   | A     | 621 | ASN  |
| 1   | A     | 660 | ARG  |
| 1   | A     | 667 | GLU  |
| 1   | A     | 677 | LEU  |
| 1   | A     | 701 | ARG  |
| 1   | A     | 703 | GLU  |
| 1   | A     | 710 | ARG  |
| 1   | A     | 715 | SER  |
| 1   | A     | 717 | LEU  |
| 1   | A     | 738 | LEU  |
| 1   | A     | 757 | MET  |
| 1   | A     | 784 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 796 | GLU  |
| 1   | A     | 799 | GLU  |
| 1   | A     | 804 | ASP  |
| 1   | A     | 825 | SER  |
| 1   | A     | 826 | THR  |
| 1   | A     | 855 | PHE  |
| 1   | A     | 857 | ASN  |
| 1   | A     | 865 | THR  |
| 1   | A     | 886 | PHE  |
| 1   | A     | 927 | ILE  |
| 1   | D     | 27  | VAL  |
| 1   | D     | 59  | GLU  |
| 1   | D     | 72  | ASP  |
| 1   | D     | 158 | ILE  |
| 1   | D     | 183 | ASP  |
| 1   | D     | 194 | ARG  |
| 1   | D     | 200 | SER  |
| 1   | D     | 204 | GLU  |
| 1   | D     | 239 | ILE  |
| 1   | D     | 265 | ARG  |
| 1   | D     | 311 | ARG  |
| 1   | D     | 332 | ARG  |
| 1   | D     | 346 | ASN  |
| 1   | D     | 350 | ARG  |
| 1   | D     | 401 | LEU  |
| 1   | D     | 457 | LYS  |
| 1   | D     | 469 | CYS  |
| 1   | D     | 491 | LEU  |
| 1   | D     | 497 | PHE  |
| 1   | D     | 500 | LEU  |
| 1   | D     | 562 | CYS  |
| 1   | D     | 606 | GLU  |
| 1   | D     | 608 | ASN  |
| 1   | D     | 611 | ILE  |
| 1   | D     | 722 | CYS  |
| 1   | D     | 726 | SER  |
| 1   | D     | 757 | MET  |
| 1   | D     | 787 | HIS  |
| 1   | D     | 794 | CYS  |
| 1   | D     | 804 | ASP  |
| 1   | D     | 863 | GLU  |
| 1   | D     | 867 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 870 | ASN  |
| 1   | D     | 878 | LYS  |
| 1   | D     | 929 | GLU  |
| 1   | D     | 933 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 17  | GLN  |
| 1   | A     | 35  | GLN  |
| 1   | A     | 45  | GLN  |
| 1   | A     | 90  | GLN  |
| 1   | A     | 91  | ASN  |
| 1   | A     | 120 | HIS  |
| 1   | A     | 244 | HIS  |
| 1   | A     | 321 | HIS  |
| 1   | A     | 358 | ASN  |
| 1   | A     | 372 | GLN  |
| 1   | A     | 382 | ASN  |
| 1   | A     | 398 | GLN  |
| 1   | A     | 484 | ASN  |
| 1   | A     | 621 | ASN  |
| 1   | A     | 739 | GLN  |
| 1   | A     | 836 | GLN  |
| 1   | A     | 868 | GLN  |
| 1   | A     | 870 | ASN  |
| 1   | A     | 922 | GLN  |
| 1   | D     | 45  | GLN  |
| 1   | D     | 244 | HIS  |
| 1   | D     | 260 | GLN  |
| 1   | D     | 318 | GLN  |
| 1   | D     | 358 | ASN  |
| 1   | D     | 479 | ASN  |
| 1   | D     | 484 | ASN  |
| 1   | D     | 608 | ASN  |
| 1   | D     | 621 | ASN  |
| 1   | D     | 672 | ASN  |
| 1   | D     | 700 | GLN  |
| 1   | D     | 832 | ASN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 2   | B     | 21/22 (95%) | 3 (14%)           | 2 (9%)          |
| 2   | E     | 21/22 (95%) | 2 (9%)            | 0               |
| 3   | C     | 21/22 (95%) | 2 (9%)            | 0               |
| 3   | F     | 21/22 (95%) | 4 (19%)           | 1 (4%)          |
| All | All   | 84/88 (95%) | 11 (13%)          | 3 (3%)          |

All (11) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 20  | A    |
| 2   | B     | 21  | A    |
| 2   | B     | 22  | G    |
| 3   | C     | 21  | A    |
| 3   | C     | 22  | C    |
| 2   | E     | 21  | A    |
| 2   | E     | 22  | G    |
| 3   | F     | 19  | U    |
| 3   | F     | 20  | C    |
| 3   | F     | 21  | A    |
| 3   | F     | 22  | C    |

All (3) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 20  | A    |
| 2   | B     | 21  | A    |
| 3   | F     | 19  | U    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | SAH  | A     | 951 | -    | 27,28,28     | 0.95 | 1 (3%)      | 36,40,40    | 0.72 | 1 (2%)      |
| 5   | SAH  | D     | 951 | -    | 27,28,28     | 0.86 | 0           | 36,40,40    | 0.64 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | SAH  | A     | 951 | -    | -       | 5/15/31/31 | 0/3/3/3 |
| 5   | SAH  | D     | 951 | -    | -       | 3/15/31/31 | 0/3/3/3 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 5   | A     | 951 | SAH  | O-C   | 2.45 | 1.29        | 1.22     |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | A     | 951 | SAH  | O4'-C1'-C2' | -2.52 | 101.23      | 106.62   |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 5   | A     | 951 | SAH  | N-CA-CB-CG   |
| 5   | A     | 951 | SAH  | C-CA-CB-CG   |
| 5   | D     | 951 | SAH  | N-CA-CB-CG   |
| 5   | D     | 951 | SAH  | C-CA-CB-CG   |
| 5   | D     | 951 | SAH  | OXT-C-CA-N   |
| 5   | A     | 951 | SAH  | O-C-CA-N     |
| 5   | A     | 951 | SAH  | CB-CG-SD-C5' |

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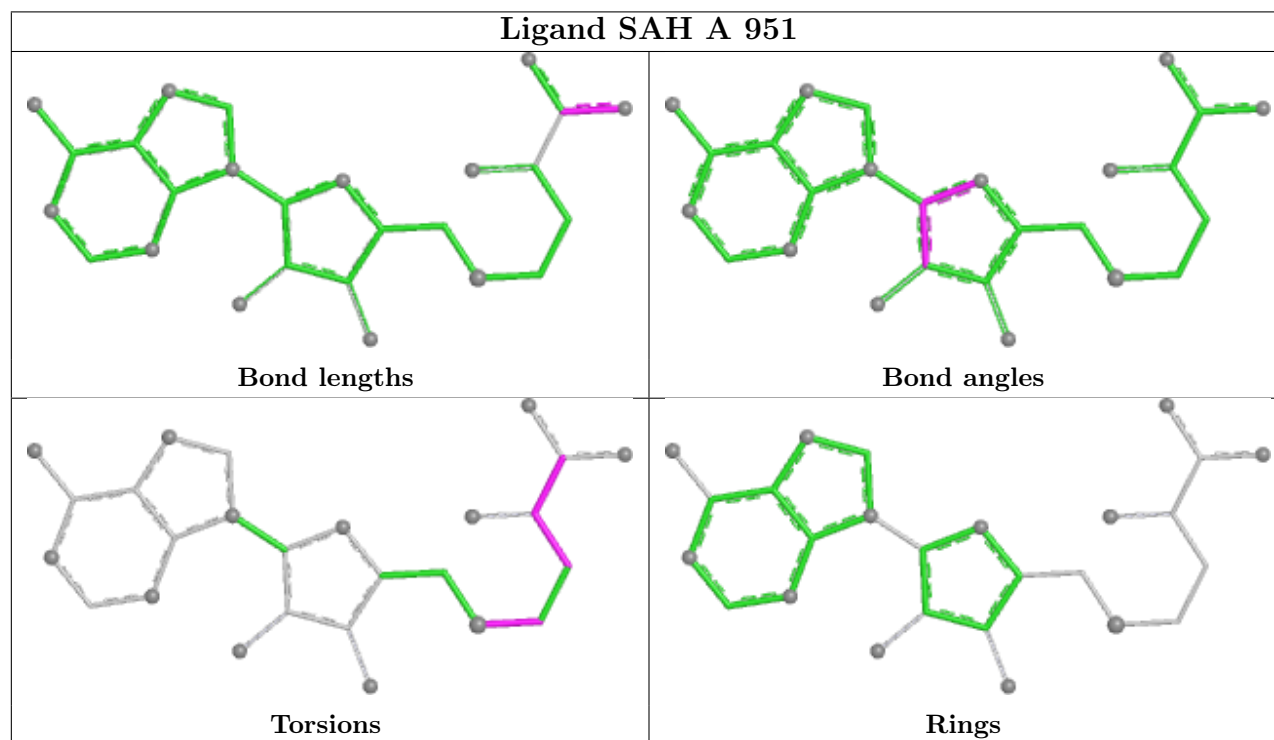
| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 5   | A     | 951 | SAH  | OXT-C-CA-N |

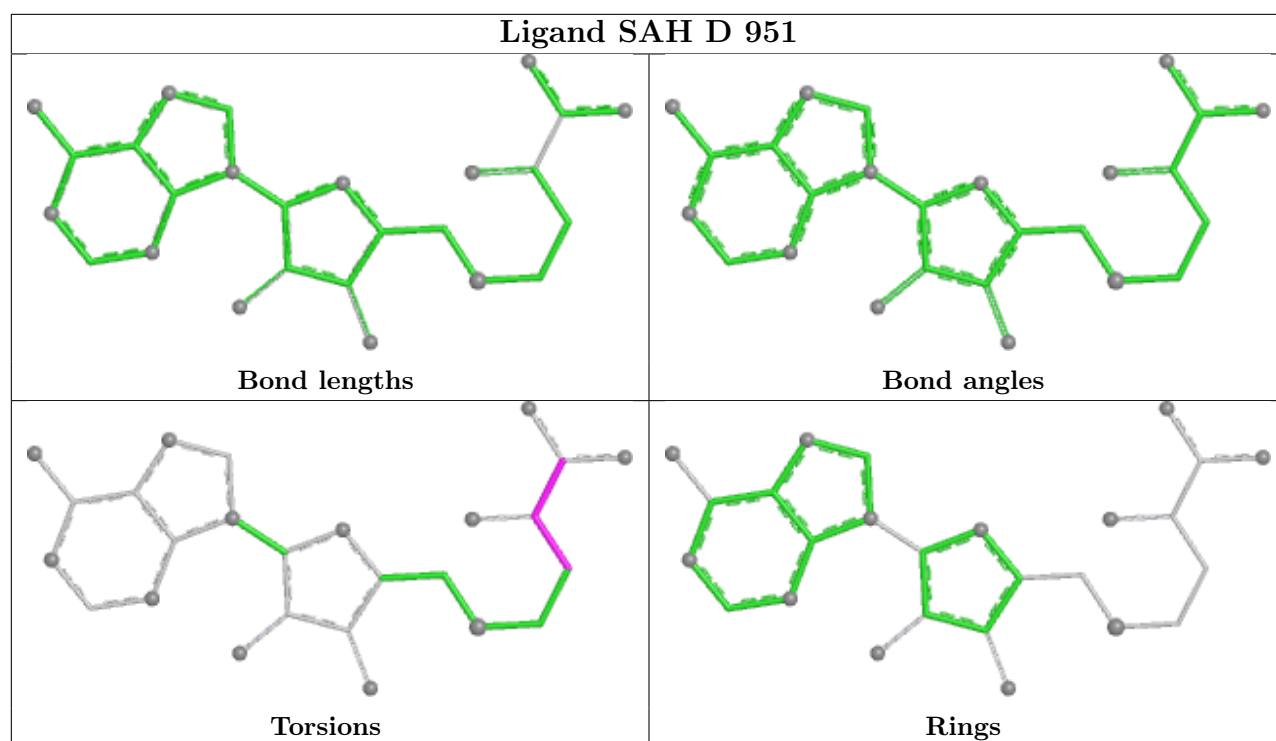
There are no ring outliers.

2 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | A     | 951 | SAH  | 2       | 0            |
| 5   | D     | 951 | SAH  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 779/950 (82%)   | -1.55  | 0 100 100 | 60, 96, 160, 193      | 0     |
| 1   | D     | 795/950 (83%)   | -1.57  | 0 100 100 | 55, 98, 154, 188      | 0     |
| 2   | B     | 22/22 (100%)    | -2.06  | 0 100 100 | 91, 120, 146, 151     | 0     |
| 2   | E     | 22/22 (100%)    | -2.14  | 0 100 100 | 99, 114, 123, 130     | 0     |
| 3   | C     | 22/22 (100%)    | -2.02  | 0 100 100 | 89, 137, 168, 199     | 0     |
| 3   | F     | 22/22 (100%)    | -2.08  | 0 100 100 | 91, 125, 144, 186     | 0     |
| All | All   | 1662/1988 (83%) | -1.58  | 0 100 100 | 55, 98, 159, 199      | 0     |

There are no RSRZ outliers to report.

### 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.

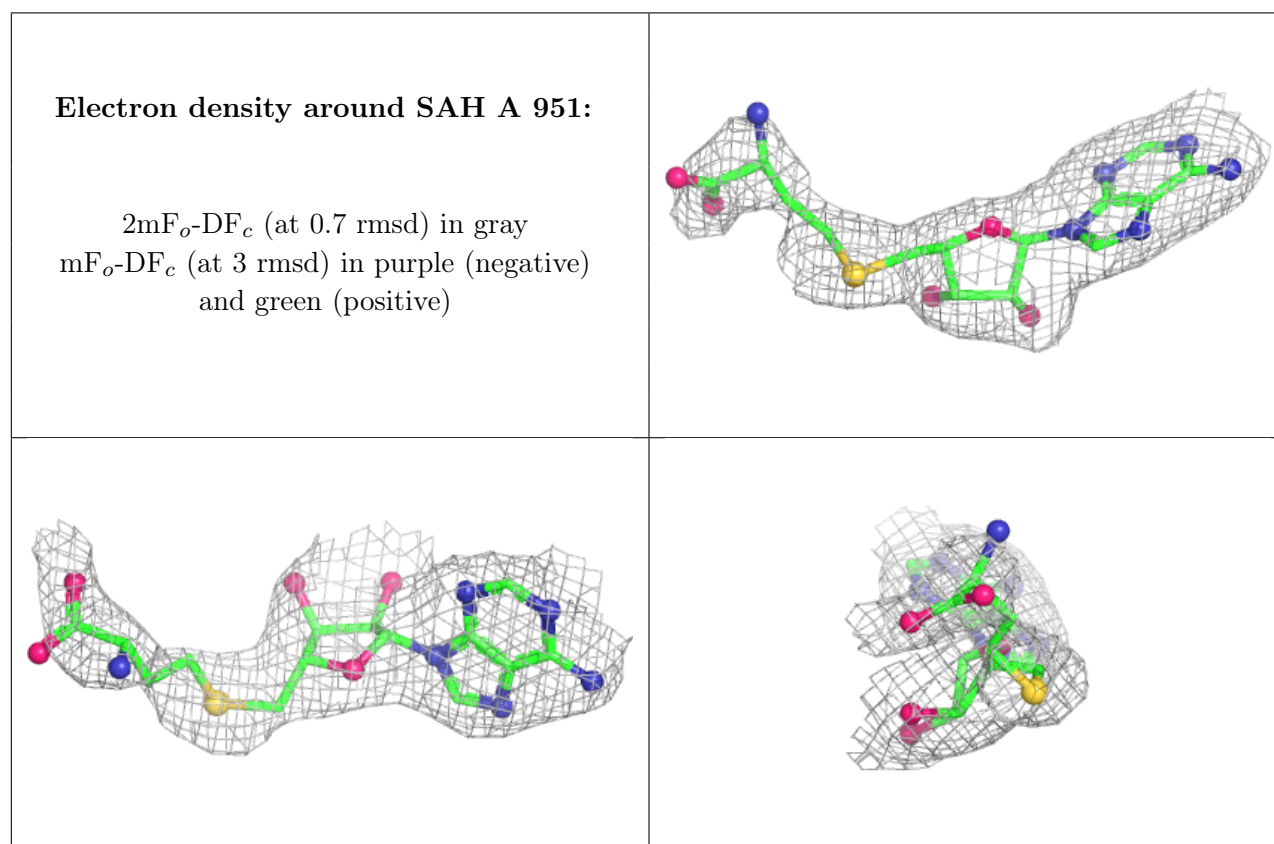
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 5   | SAH  | A     | 951 | 26/26 | 0.99 | 0.03 | 62,68,85,86                | 0     |

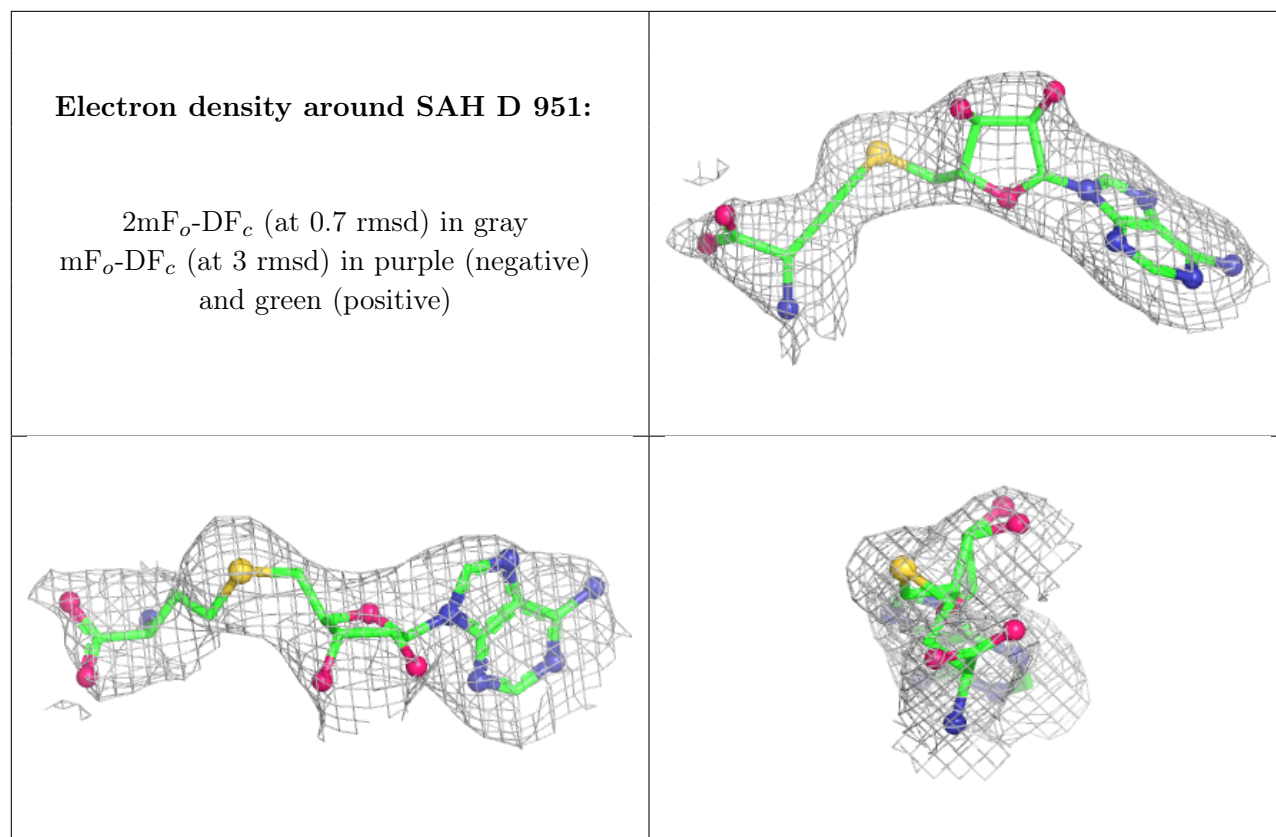
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 5   | SAH  | D     | 951 | 26/26 | 0.99 | 0.03 | 70,74,86,87                 | 0     |
| 4   | MG   | A     | 950 | 1/1   | 1.00 | 0.01 | 60,60,60,60                 | 0     |
| 4   | MG   | D     | 950 | 1/1   | 1.00 | 0.02 | 36,36,36,36                 | 0     |

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.