



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:41 PM UTC

PDB ID : 1MSW / pdb\_00001msw  
Title : Structural basis for the transition from initiation to elongation transcription  
in T7 RNA polymerase  
Authors : Yin, Y.W.; Steitz, T.A.  
Deposited on : 2002-09-19  
Resolution : 2.10 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                                             |
| Xtriage (Phenix)               | : | <b>NOT EXECUTED</b>                                              |
| EDS                            | : | <b>NOT EXECUTED</b>                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

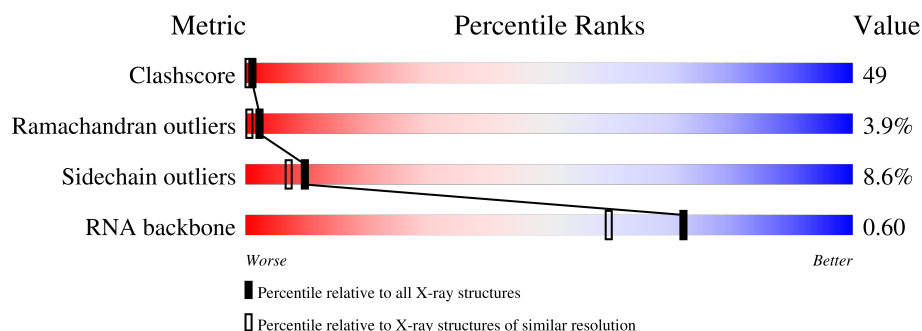
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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                      | 7164 (2.10-2.10)                                      |
| Ramachandran outliers | 187476                      | 7099 (2.10-2.10)                                      |
| Sidechain outliers    | 187428                      | 7100 (2.10-2.10)                                      |
| RNA backbone          | 3983                        | 1006 (2.42-1.78)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | T     | 20     | 5% 60% 20% 15%   |
| 2   | N     | 17     | 18% 82%          |
| 3   | R     | 10     | 20% 80%          |
| 4   | D     | 883    | 42% 46% 9% .     |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7956 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 DNA chain called Template DNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 1   | T     | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 405   | 193 | 71 | 122 | 19 |         |         |       |

- Molecule 2 is a DNA chain called Non-Template DNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 2   | N     | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 344   | 165 | 60 | 103 | 16 |         |         |       |

- Molecule 3 is a RNA chain called RNA message.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 3   | R     | 10       | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 215   | 97 | 44 | 65 | 9 |         |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 4   | D     | 863      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6802  | 4333 | 1182 | 1251 | 36 |         |         |       |

- Molecule 5 is water.

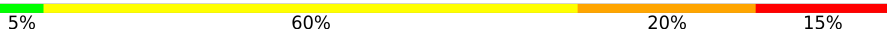
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 5   | T     | 13       | Total | O   | 0       | 0       |
|     |       |          | 13    | 13  |         |         |
| 5   | N     | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 5   | R     | 9        | Total | O   | 0       | 0       |
|     |       |          | 9     | 9   |         |         |
| 5   | D     | 166      | Total | O   | 0       | 0       |
|     |       |          | 166   | 166 |         |         |

### 3 Residue-property plots

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

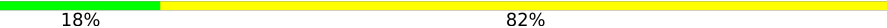
Note EDS was not executed.

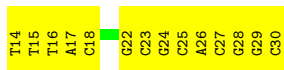
#### • Molecule 1: Template DNA

Chain T: 

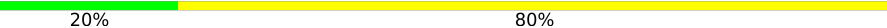


#### • Molecule 2: Non-Template DNA

Chain N: 



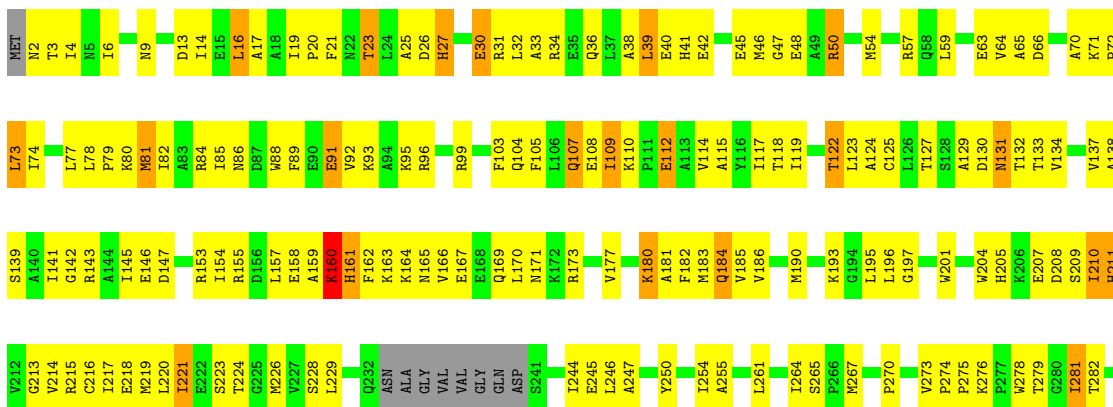
#### • Molecule 3: RNA message

Chain R: 



#### • Molecule 4: DNA-directed RNA polymerase

Chain D: 





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | C 2 2 21                                        | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 142.91Å 145.46Å 145.60Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 20.00 – 2.10                                    | Depositor |
| % Data completeness<br>(in resolution range)             | 85.0 (20.00-2.10)                               | Depositor |
| $R_{merge}$                                              | (Not available)                                 | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | CNS                                             | Depositor |
| R, $R_{free}$                                            | 0.241 , 0.275                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 7956                                            | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 75.0                                            | wwPDB-VP  |

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | T     | 0.35         | 0/452       | 1.02        | 6/696 (0.9%)    |
| 2   | N     | 0.27         | 0/384       | 0.57        | 0/591           |
| 3   | R     | 0.37         | 0/241       | 0.68        | 0/375           |
| 4   | D     | 0.54         | 0/6955      | 1.03        | 35/9407 (0.4%)  |
| All | All   | 0.52         | 0/8032      | 1.00        | 41/11069 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | T     | 0                   | 7                   |

There are no bond length outliers.

All (41) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 4   | D     | 160 | LYS  | N-CA-C      | -10.54 | 100.54      | 113.50   |
| 4   | D     | 860 | LYS  | N-CA-C      | -9.49  | 100.58      | 113.30   |
| 4   | D     | 500 | THR  | N-CA-C      | 7.78   | 122.48      | 113.38   |
| 4   | D     | 405 | ALA  | N-CA-C      | -7.38  | 103.24      | 112.90   |
| 1   | T     | 119 | DT   | N1-C1'-C2'  | -7.28  | 102.57      | 113.50   |
| 1   | T     | 119 | DT   | C4'-C3'-O3' | 6.96   | 120.44      | 110.00   |
| 1   | T     | 119 | DT   | C5'-C4'-C3' | -6.66  | 104.92      | 114.90   |
| 4   | D     | 783 | VAL  | CB-CA-C     | -6.55  | 103.30      | 112.14   |
| 4   | D     | 211 | HIS  | N-CA-C      | -6.41  | 104.38      | 111.82   |
| 4   | D     | 858 | LEU  | N-CA-C      | -6.40  | 105.05      | 112.92   |
| 1   | T     | 117 | DG   | C4'-C3'-O3' | 6.39   | 119.59      | 110.00   |
| 4   | D     | 555 | GLY  | N-CA-C      | -6.39  | 106.74      | 114.66   |
| 4   | D     | 131 | ASN  | N-CA-C      | -6.28  | 104.66      | 113.20   |
| 4   | D     | 184 | GLN  | N-CA-C      | -6.25  | 104.52      | 111.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | D     | 429 | VAL  | N-CA-C      | 6.14  | 117.69      | 111.00   |
| 4   | D     | 161 | HIS  | N-CA-C      | -6.13 | 104.37      | 112.34   |
| 4   | D     | 190 | MET  | N-CA-C      | -6.09 | 105.83      | 113.20   |
| 4   | D     | 347 | CYS  | CA-C-N      | 6.07  | 125.69      | 119.56   |
| 4   | D     | 347 | CYS  | C-N-CA      | 6.07  | 125.69      | 119.56   |
| 4   | D     | 833 | VAL  | N-CA-C      | 6.01  | 116.19      | 110.42   |
| 4   | D     | 821 | ALA  | N-CA-C      | 5.98  | 118.59      | 111.71   |
| 4   | D     | 825 | PHE  | N-CA-C      | -5.89 | 104.86      | 111.28   |
| 4   | D     | 527 | SER  | N-CA-C      | -5.63 | 106.25      | 113.01   |
| 4   | D     | 210 | ILE  | N-CA-C      | -5.46 | 108.53      | 113.71   |
| 4   | D     | 193 | LYS  | N-CA-C      | -5.42 | 107.21      | 113.88   |
| 4   | D     | 304 | ALA  | N-CA-C      | -5.41 | 105.46      | 111.36   |
| 4   | D     | 779 | ALA  | CA-C-N      | -5.37 | 113.09      | 119.05   |
| 4   | D     | 779 | ALA  | C-N-CA      | -5.37 | 113.09      | 119.05   |
| 4   | D     | 340 | VAL  | N-CA-C      | 5.36  | 116.44      | 111.45   |
| 4   | D     | 758 | GLN  | CA-C-N      | 5.35  | 125.52      | 119.90   |
| 4   | D     | 758 | GLN  | C-N-CA      | 5.35  | 125.52      | 119.90   |
| 4   | D     | 668 | THR  | N-CA-C      | -5.34 | 105.83      | 112.93   |
| 4   | D     | 832 | MET  | N-CA-C      | -5.33 | 104.71      | 111.11   |
| 4   | D     | 463 | HIS  | N-CA-C      | -5.32 | 105.38      | 111.07   |
| 4   | D     | 38  | ALA  | N-CA-C      | -5.26 | 105.63      | 111.36   |
| 4   | D     | 452 | ILE  | N-CA-C      | 5.23  | 115.85      | 110.36   |
| 1   | T     | 117 | DG   | N9-C1'-C2'  | -5.20 | 105.71      | 113.50   |
| 4   | D     | 279 | THR  | N-CA-C      | -5.15 | 106.92      | 114.39   |
| 4   | D     | 560 | ASN  | N-CA-C      | 5.11  | 118.78      | 112.24   |
| 1   | T     | 115 | DC   | C5'-C4'-C3' | -5.07 | 107.30      | 114.90   |
| 4   | D     | 23  | THR  | N-CA-C      | -5.04 | 105.87      | 111.36   |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | T     | 114 | DG   | Sidechain |
| 1   | T     | 115 | DC   | Sidechain |
| 1   | T     | 116 | DC   | Sidechain |
| 1   | T     | 117 | DG   | Sidechain |
| 1   | T     | 118 | DC   | Sidechain |
| 1   | T     | 119 | DT   | Sidechain |
| 1   | T     | 121 | DA   | Sidechain |



## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | T     | 405   | 0        | 227      | 49      | 0            |
| 2   | N     | 344   | 0        | 194      | 17      | 0            |
| 3   | R     | 215   | 0        | 112      | 15      | 0            |
| 4   | D     | 6802  | 0        | 6770     | 670     | 0            |
| 5   | D     | 166   | 0        | 0        | 253     | 0            |
| 5   | N     | 2     | 0        | 0        | 0       | 0            |
| 5   | R     | 9     | 0        | 0        | 8       | 0            |
| 5   | T     | 13    | 0        | 0        | 27      | 0            |
| All | All   | 7956  | 0        | 7303     | 740     | 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 49.

All (740) 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) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:360:LEU:HB2  | 5:D:968:HOH:O    | 1.29                     | 1.29              |
| 4:D:104:GLN:HB3  | 5:D:979:HOH:O    | 1.23                     | 1.27              |
| 4:D:276:LYS:HE2  | 5:D:1032:HOH:O   | 1.22                     | 1.26              |
| 4:D:217:ILE:O    | 4:D:221:ILE:HD13 | 1.24                     | 1.24              |
| 4:D:428:ALA:HA   | 5:D:944:HOH:O    | 1.39                     | 1.22              |
| 3:R:5:G:H3'      | 5:R:99:HOH:O     | 1.43                     | 1.18              |
| 4:D:383:ALA:HB3  | 5:D:986:HOH:O    | 1.42                     | 1.18              |
| 4:D:648:GLN:HA   | 5:D:1028:HOH:O   | 1.44                     | 1.17              |
| 4:D:647:ARG:HG2  | 5:D:958:HOH:O    | 1.42                     | 1.17              |
| 4:D:647:ARG:HD3  | 5:D:913:HOH:O    | 1.44                     | 1.15              |
| 1:T:111:DT:H3'   | 5:T:132:HOH:O    | 1.50                     | 1.12              |
| 4:D:360:LEU:HD23 | 5:D:917:HOH:O    | 1.49                     | 1.11              |
| 4:D:386:ARG:HG3  | 5:D:933:HOH:O    | 1.52                     | 1.08              |
| 4:D:285:GLY:HA2  | 5:D:928:HOH:O    | 1.54                     | 1.07              |
| 4:D:312:TYR:HB3  | 5:D:976:HOH:O    | 1.51                     | 1.06              |
| 4:D:735:VAL:HG12 | 5:D:1012:HOH:O   | 1.53                     | 1.05              |
| 1:T:119:DT:H71   | 5:T:141:HOH:O    | 1.55                     | 1.05              |
| 1:T:111:DT:C3'   | 5:T:132:HOH:O    | 2.02                     | 1.04              |
| 4:D:794:THR:HB   | 5:D:892:HOH:O    | 1.55                     | 1.04              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:330:ILE:HD13 | 5:D:895:HOH:O    | 1.54                     | 1.04              |
| 4:D:817:ILE:HD11 | 5:D:947:HOH:O    | 1.55                     | 1.03              |
| 4:D:141:ILE:O    | 4:D:145:ILE:HD13 | 1.57                     | 1.03              |
| 4:D:344:TRP:CB   | 5:D:1015:HOH:O   | 2.06                     | 1.02              |
| 4:D:96:ARG:HG3   | 5:D:891:HOH:O    | 1.60                     | 1.01              |
| 4:D:451:PRO:HD3  | 5:D:1001:HOH:O   | 1.59                     | 1.01              |
| 4:D:4:ILE:HG21   | 5:D:942:HOH:O    | 1.60                     | 1.00              |
| 4:D:445:THR:HA   | 5:D:974:HOH:O    | 1.60                     | 1.00              |
| 4:D:733:PHE:CZ   | 5:D:1002:HOH:O   | 2.15                     | 1.00              |
| 4:D:344:TRP:HB2  | 5:D:1015:HOH:O   | 1.63                     | 0.97              |
| 4:D:344:TRP:O    | 4:D:355:ILE:HD11 | 1.62                     | 0.97              |
| 4:D:177:VAL:O    | 4:D:180:LYS:HG3  | 1.64                     | 0.97              |
| 4:D:289:ASN:C    | 5:D:960:HOH:O    | 2.07                     | 0.97              |
| 4:D:296:LEU:HD21 | 4:D:320:ILE:HD13 | 1.45                     | 0.97              |
| 4:D:154:ILE:HD11 | 4:D:183:MET:HE3  | 1.47                     | 0.96              |
| 4:D:664:GLY:HA2  | 5:D:1031:HOH:O   | 1.66                     | 0.95              |
| 4:D:65:ALA:HA    | 5:D:1017:HOH:O   | 1.65                     | 0.94              |
| 4:D:118:THR:O    | 4:D:122:THR:HG23 | 1.67                     | 0.94              |
| 4:D:664:GLY:CA   | 5:D:1031:HOH:O   | 2.14                     | 0.94              |
| 4:D:270:PRO:HD3  | 5:D:935:HOH:O    | 1.69                     | 0.93              |
| 4:D:796:VAL:HB   | 5:D:1016:HOH:O   | 1.67                     | 0.93              |
| 4:D:419:ASN:C    | 5:D:957:HOH:O    | 2.10                     | 0.93              |
| 4:D:795:VAL:N    | 5:D:892:HOH:O    | 2.00                     | 0.93              |
| 4:D:816:THR:CG2  | 5:D:989:HOH:O    | 2.18                     | 0.92              |
| 4:D:132:THR:CG2  | 5:D:983:HOH:O    | 2.17                     | 0.92              |
| 4:D:464:GLY:HA3  | 5:D:1036:HOH:O   | 1.69                     | 0.91              |
| 4:D:74:ILE:HG13  | 5:D:1017:HOH:O   | 1.70                     | 0.90              |
| 4:D:355:ILE:HD13 | 4:D:355:ILE:H    | 1.35                     | 0.90              |
| 3:R:10:G:N3      | 5:R:46:HOH:O     | 2.05                     | 0.90              |
| 3:R:9:A:H1'      | 4:D:756:ARG:NH2  | 1.87                     | 0.90              |
| 4:D:433:ASN:HD22 | 4:D:435:GLN:H    | 1.15                     | 0.90              |
| 4:D:746:ARG:HE   | 4:D:754:GLN:HE22 | 1.14                     | 0.89              |
| 4:D:816:THR:HG22 | 5:D:989:HOH:O    | 1.72                     | 0.89              |
| 4:D:302:LYS:O    | 4:D:304:ALA:N    | 2.04                     | 0.89              |
| 4:D:378:LYS:HD2  | 4:D:379:ARG:N    | 1.88                     | 0.88              |
| 4:D:830:GLU:HB2  | 5:D:910:HOH:O    | 1.71                     | 0.88              |
| 4:D:270:PRO:CG   | 5:D:935:HOH:O    | 2.21                     | 0.88              |
| 4:D:137:VAL:HG21 | 4:D:244:ILE:HD11 | 1.54                     | 0.88              |
| 4:D:491:ALA:HB1  | 4:D:499:ASN:ND2  | 1.90                     | 0.87              |
| 3:R:10:G:C2      | 5:R:46:HOH:O     | 2.26                     | 0.87              |
| 4:D:217:ILE:N    | 5:D:1005:HOH:O   | 2.08                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:546:PHE:HB3  | 5:D:909:HOH:O    | 1.74                     | 0.86              |
| 4:D:118:THR:CA   | 5:D:955:HOH:O    | 2.23                     | 0.86              |
| 4:D:468:ALA:HB2  | 5:D:987:HOH:O    | 1.74                     | 0.86              |
| 4:D:118:THR:HA   | 5:D:955:HOH:O    | 1.74                     | 0.85              |
| 4:D:129:ALA:HB3  | 5:D:1045:HOH:O   | 1.75                     | 0.85              |
| 4:D:292:ARG:HE   | 4:D:292:ARG:HA   | 1.40                     | 0.85              |
| 4:D:720:ARG:CZ   | 5:D:1029:HOH:O   | 2.22                     | 0.85              |
| 3:R:9:A:H1'      | 4:D:756:ARG:HH21 | 1.42                     | 0.85              |
| 4:D:359:GLU:HA   | 5:D:917:HOH:O    | 1.75                     | 0.85              |
| 4:D:118:THR:N    | 5:D:955:HOH:O    | 2.10                     | 0.84              |
| 4:D:441:LYS:N    | 5:D:967:HOH:O    | 2.11                     | 0.84              |
| 3:R:3:C:H5'      | 5:R:91:HOH:O     | 1.76                     | 0.83              |
| 4:D:876:LEU:HD12 | 5:D:1018:HOH:O   | 1.78                     | 0.83              |
| 4:D:360:LEU:N    | 5:D:917:HOH:O    | 2.02                     | 0.83              |
| 4:D:3:THR:HA     | 5:D:985:HOH:O    | 1.78                     | 0.83              |
| 4:D:361:PRO:HD2  | 5:D:968:HOH:O    | 1.78                     | 0.83              |
| 1:T:126:DT:H2''  | 1:T:125:DG:H5'   | 1.58                     | 0.82              |
| 4:D:441:LYS:HG3  | 5:D:967:HOH:O    | 1.80                     | 0.82              |
| 4:D:780:PRO:CD   | 5:D:1010:HOH:O   | 2.26                     | 0.82              |
| 4:D:59:LEU:HD12  | 4:D:64:VAL:HG22  | 1.60                     | 0.82              |
| 4:D:875:ILE:HG13 | 5:D:1014:HOH:O   | 1.80                     | 0.82              |
| 4:D:270:PRO:CD   | 5:D:935:HOH:O    | 2.26                     | 0.81              |
| 4:D:428:ALA:CB   | 5:D:944:HOH:O    | 2.24                     | 0.81              |
| 4:D:359:GLU:CA   | 5:D:917:HOH:O    | 2.27                     | 0.81              |
| 4:D:281:ILE:HG12 | 4:D:282:THR:HG23 | 1.62                     | 0.81              |
| 4:D:632:ARG:HB3  | 5:D:916:HOH:O    | 1.80                     | 0.81              |
| 4:D:873:ARG:HD3  | 5:D:1018:HOH:O   | 1.79                     | 0.81              |
| 4:D:361:PRO:CD   | 5:D:968:HOH:O    | 2.29                     | 0.81              |
| 4:D:741:LYS:HZ2  | 4:D:742:PRO:HD3  | 1.45                     | 0.81              |
| 4:D:270:PRO:HG3  | 5:D:935:HOH:O    | 1.81                     | 0.81              |
| 1:T:121:DA:H1'   | 5:T:135:HOH:O    | 1.81                     | 0.80              |
| 4:D:733:PHE:HZ   | 5:D:1002:HOH:O   | 1.53                     | 0.80              |
| 4:D:780:PRO:HG3  | 5:D:1010:HOH:O   | 1.81                     | 0.80              |
| 4:D:473:VAL:HG22 | 4:D:474:PRO:HD2  | 1.63                     | 0.80              |
| 4:D:276:LYS:HG2  | 5:D:1032:HOH:O   | 1.80                     | 0.80              |
| 4:D:856:SER:HB3  | 5:D:884:HOH:O    | 1.82                     | 0.80              |
| 4:D:157:LEU:HG   | 4:D:158:GLU:HG2  | 1.63                     | 0.80              |
| 4:D:115:ALA:O    | 4:D:119:ILE:HG13 | 1.82                     | 0.80              |
| 4:D:117:ILE:C    | 5:D:955:HOH:O    | 2.25                     | 0.79              |
| 4:D:780:PRO:CG   | 5:D:1010:HOH:O   | 2.31                     | 0.79              |
| 4:D:741:LYS:HZ2  | 4:D:741:LYS:HA   | 1.47                     | 0.79              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:D:790:HIS:CD2 | 5:D:995:HOH:O    | 2.36                     | 0.79              |
| 4:D:505:GLN:OE1 | 5:D:1046:HOH:O   | 2.00                     | 0.78              |
| 1:T:128:DC:H1'  | 1:T:127:DG:N7    | 1.97                     | 0.78              |
| 4:D:561:LEU:O   | 5:D:1014:HOH:O   | 2.01                     | 0.78              |
| 4:D:361:PRO:N   | 5:D:968:HOH:O    | 2.17                     | 0.78              |
| 4:D:119:ILE:O   | 4:D:123:LEU:HB2  | 1.85                     | 0.77              |
| 4:D:756:ARG:HG3 | 4:D:756:ARG:HH11 | 1.48                     | 0.77              |
| 3:R:5:G:C8      | 5:R:99:HOH:O     | 2.37                     | 0.77              |
| 4:D:214:VAL:O   | 4:D:218:GLU:HG3  | 1.85                     | 0.77              |
| 4:D:716:GLY:O   | 5:D:1013:HOH:O   | 2.02                     | 0.77              |
| 4:D:666:MET:HE1 | 5:D:1031:HOH:O   | 1.85                     | 0.77              |
| 1:T:121:DA:C1'  | 5:T:135:HOH:O    | 2.33                     | 0.76              |
| 4:D:454:LYS:HE3 | 5:D:948:HOH:O    | 1.85                     | 0.76              |
| 4:D:433:ASN:ND2 | 4:D:435:GLN:H    | 1.84                     | 0.76              |
| 1:T:127:DG:H1'  | 1:T:126:DT:H5'   | 1.66                     | 0.76              |
| 4:D:817:ILE:CD1 | 5:D:947:HOH:O    | 2.23                     | 0.76              |
| 4:D:255:ALA:HA  | 5:D:942:HOH:O    | 1.84                     | 0.76              |
| 4:D:514:PHE:CE2 | 5:D:1036:HOH:O   | 2.39                     | 0.76              |
| 4:D:137:VAL:O   | 4:D:141:ILE:HD12 | 1.85                     | 0.76              |
| 4:D:289:ASN:CA  | 5:D:960:HOH:O    | 2.33                     | 0.75              |
| 4:D:791:LEU:O   | 5:D:892:HOH:O    | 2.04                     | 0.75              |
| 1:T:125:DG:H1'  | 1:T:124:DC:H5'   | 1.67                     | 0.75              |
| 4:D:741:LYS:NZ  | 4:D:742:PRO:HD3  | 2.01                     | 0.75              |
| 4:D:820:ASP:OD2 | 5:D:989:HOH:O    | 2.05                     | 0.75              |
| 4:D:428:ALA:CA  | 5:D:944:HOH:O    | 2.08                     | 0.74              |
| 5:T:139:HOH:O   | 4:D:780:PRO:HB2  | 1.87                     | 0.74              |
| 4:D:468:ALA:CB  | 5:D:987:HOH:O    | 2.33                     | 0.74              |
| 4:D:594:VAL:O   | 4:D:607:GLU:HB2  | 1.87                     | 0.74              |
| 4:D:688:THR:O   | 5:D:1007:HOH:O   | 2.04                     | 0.74              |
| 4:D:873:ARG:CA  | 5:D:1018:HOH:O   | 2.35                     | 0.74              |
| 4:D:103:PHE:HB3 | 5:D:946:HOH:O    | 1.87                     | 0.74              |
| 4:D:291:ARG:O   | 4:D:293:PRO:HD3  | 1.88                     | 0.74              |
| 4:D:748:ASN:OD1 | 4:D:754:GLN:HB3  | 1.86                     | 0.74              |
| 4:D:453:GLY:HA3 | 5:D:980:HOH:O    | 1.86                     | 0.74              |
| 4:D:213:GLY:O   | 4:D:217:ILE:HG12 | 1.88                     | 0.73              |
| 4:D:729:THR:HA  | 5:D:1041:HOH:O   | 1.88                     | 0.73              |
| 4:D:441:LYS:CG  | 5:D:967:HOH:O    | 2.35                     | 0.73              |
| 1:T:128:DC:O2   | 5:T:134:HOH:O    | 2.05                     | 0.73              |
| 4:D:454:LYS:O   | 5:D:951:HOH:O    | 2.06                     | 0.73              |
| 4:D:691:ALA:HB1 | 5:D:909:HOH:O    | 1.87                     | 0.73              |
| 4:D:129:ALA:O   | 5:D:983:HOH:O    | 2.04                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:552:ASP:HB2  | 4:D:691:ALA:HB2  | 1.68                     | 0.73              |
| 4:D:587:ILE:O    | 4:D:588:ASN:HB2  | 1.88                     | 0.73              |
| 4:D:787:ASP:HB3  | 5:D:1026:HOH:O   | 1.87                     | 0.73              |
| 4:D:54:MET:HG3   | 4:D:57:ARG:NH2   | 2.04                     | 0.73              |
| 4:D:352:ILE:HG22 | 4:D:352:ILE:O    | 1.89                     | 0.73              |
| 4:D:355:ILE:H    | 4:D:355:ILE:CD1  | 1.97                     | 0.73              |
| 4:D:360:LEU:HD23 | 4:D:360:LEU:H    | 1.53                     | 0.72              |
| 4:D:88:TRP:O     | 4:D:92:VAL:HG12  | 1.89                     | 0.72              |
| 4:D:289:ASN:N    | 5:D:960:HOH:O    | 2.21                     | 0.72              |
| 4:D:452:ILE:O    | 5:D:980:HOH:O    | 2.07                     | 0.72              |
| 4:D:819:ALA:HB3  | 5:D:947:HOH:O    | 1.88                     | 0.72              |
| 4:D:804:ILE:HD11 | 5:D:1004:HOH:O   | 1.88                     | 0.72              |
| 4:D:141:ILE:O    | 4:D:145:ILE:CD1  | 2.36                     | 0.72              |
| 4:D:247:ALA:HB3  | 4:D:250:TYR:HD2  | 1.55                     | 0.72              |
| 4:D:795:VAL:HG23 | 5:D:892:HOH:O    | 1.90                     | 0.71              |
| 4:D:804:ILE:HD12 | 4:D:820:ASP:CG   | 2.15                     | 0.71              |
| 4:D:682:TRP:O    | 4:D:686:SER:HB2  | 1.91                     | 0.71              |
| 3:R:5:G:O5'      | 5:R:99:HOH:O     | 2.09                     | 0.71              |
| 4:D:594:VAL:HA   | 4:D:608:LYS:O    | 1.90                     | 0.71              |
| 4:D:875:ILE:N    | 5:D:1014:HOH:O   | 2.23                     | 0.71              |
| 4:D:107:GLN:OE1  | 5:D:1011:HOH:O   | 2.09                     | 0.70              |
| 4:D:117:ILE:HG22 | 5:D:955:HOH:O    | 1.91                     | 0.70              |
| 4:D:585:ASP:O    | 4:D:614:LYS:HG2  | 1.91                     | 0.70              |
| 4:D:217:ILE:O    | 4:D:221:ILE:CD1  | 2.20                     | 0.70              |
| 4:D:546:PHE:C    | 5:D:909:HOH:O    | 2.33                     | 0.70              |
| 4:D:85:ILE:HA    | 4:D:219:MET:HE1  | 1.73                     | 0.70              |
| 4:D:70:ALA:O     | 4:D:74:ILE:HG12  | 1.90                     | 0.70              |
| 4:D:577:LYS:HB2  | 4:D:577:LYS:NZ   | 2.06                     | 0.70              |
| 4:D:741:LYS:HD3  | 4:D:742:PRO:HD2  | 1.73                     | 0.70              |
| 4:D:73:LEU:HD23  | 4:D:74:ILE:N     | 2.06                     | 0.69              |
| 4:D:278:TRP:H    | 4:D:321:ASN:HD21 | 1.38                     | 0.69              |
| 4:D:454:LYS:CD   | 5:D:948:HOH:O    | 2.40                     | 0.69              |
| 4:D:423:ARG:HH12 | 4:D:784:HIS:HD2  | 1.39                     | 0.69              |
| 1:T:111:DT:C2'   | 5:T:132:HOH:O    | 2.36                     | 0.69              |
| 4:D:4:ILE:N      | 5:D:985:HOH:O    | 2.05                     | 0.69              |
| 4:D:488:ASN:ND2  | 5:D:993:HOH:O    | 2.24                     | 0.69              |
| 4:D:538:GLY:O    | 5:D:984:HOH:O    | 2.09                     | 0.69              |
| 2:N:14:DT:H2''   | 2:N:15:DT:OP1    | 1.93                     | 0.69              |
| 4:D:488:ASN:CG   | 5:D:993:HOH:O    | 2.36                     | 0.69              |
| 4:D:859:ASP:O    | 5:D:988:HOH:O    | 2.11                     | 0.69              |
| 4:D:420:MET:CB   | 5:D:957:HOH:O    | 2.41                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:873:ARG:HA   | 5:D:1018:HOH:O   | 1.92                     | 0.69              |
| 4:D:473:VAL:CG2  | 4:D:474:PRO:HD2  | 2.23                     | 0.69              |
| 4:D:146:GLU:OE2  | 5:D:971:HOH:O    | 2.10                     | 0.69              |
| 4:D:709:GLU:CA   | 5:D:940:HOH:O    | 2.41                     | 0.68              |
| 4:D:730:PRO:HD3  | 5:D:1041:HOH:O   | 1.93                     | 0.68              |
| 3:R:1:A:H5"      | 5:R:75:HOH:O     | 1.93                     | 0.68              |
| 4:D:324:GLN:HB3  | 4:D:418:TYR:HD1  | 1.58                     | 0.68              |
| 4:D:765:LYS:HD3  | 4:D:766:ASP:N    | 2.09                     | 0.68              |
| 4:D:587:ILE:HA   | 4:D:614:LYS:HE3  | 1.76                     | 0.68              |
| 4:D:324:GLN:NE2  | 5:D:928:HOH:O    | 2.27                     | 0.67              |
| 4:D:546:PHE:O    | 5:D:909:HOH:O    | 2.11                     | 0.67              |
| 4:D:709:GLU:HA   | 5:D:940:HOH:O    | 1.93                     | 0.67              |
| 4:D:109:ILE:HD13 | 4:D:114:VAL:CG2  | 2.25                     | 0.67              |
| 4:D:755:PHE:HB2  | 5:D:1024:HOH:O   | 1.95                     | 0.67              |
| 4:D:803:GLY:O    | 5:D:966:HOH:O    | 2.13                     | 0.67              |
| 4:D:74:ILE:CG1   | 5:D:1017:HOH:O   | 2.36                     | 0.67              |
| 4:D:281:ILE:HD13 | 4:D:281:ILE:H    | 1.59                     | 0.67              |
| 1:T:130:DG:HO5'  | 1:T:130:DG:H8    | 1.41                     | 0.67              |
| 4:D:81:MET:O     | 4:D:85:ILE:HG12  | 1.95                     | 0.66              |
| 4:D:354:ALA:HB3  | 4:D:391:ARG:HD2  | 1.77                     | 0.66              |
| 4:D:458:TYR:O    | 4:D:462:ILE:HD12 | 1.95                     | 0.66              |
| 4:D:655:ILE:HD12 | 4:D:655:ILE:H    | 1.60                     | 0.66              |
| 1:T:127:DG:C5    | 5:T:134:HOH:O    | 2.47                     | 0.66              |
| 4:D:78:LEU:HD13  | 4:D:119:ILE:HD12 | 1.77                     | 0.66              |
| 4:D:209:SER:OG   | 5:D:971:HOH:O    | 2.12                     | 0.66              |
| 4:D:137:VAL:HG12 | 4:D:141:ILE:HD11 | 1.78                     | 0.66              |
| 4:D:857:GLN:OE1  | 4:D:857:GLN:HA   | 1.95                     | 0.66              |
| 4:D:95:LYS:O     | 5:D:902:HOH:O    | 2.12                     | 0.66              |
| 4:D:134:VAL:HG12 | 4:D:244:ILE:HG23 | 1.77                     | 0.66              |
| 4:D:756:ARG:HG3  | 4:D:756:ARG:NH1  | 2.07                     | 0.66              |
| 4:D:797:TRP:N    | 5:D:1016:HOH:O   | 2.27                     | 0.66              |
| 4:D:505:GLN:HB3  | 5:D:952:HOH:O    | 1.94                     | 0.66              |
| 4:D:807:PHE:O    | 5:D:941:HOH:O    | 2.13                     | 0.66              |
| 4:D:4:ILE:CG2    | 5:D:942:HOH:O    | 2.30                     | 0.66              |
| 4:D:196:LEU:H    | 4:D:196:LEU:HD22 | 1.61                     | 0.66              |
| 4:D:637:LEU:HG   | 4:D:696:MET:HE1  | 1.78                     | 0.66              |
| 4:D:344:TRP:CE3  | 5:D:1015:HOH:O   | 2.50                     | 0.65              |
| 4:D:537:ASP:OD2  | 5:D:984:HOH:O    | 2.13                     | 0.65              |
| 4:D:217:ILE:HD13 | 5:D:1005:HOH:O   | 1.95                     | 0.65              |
| 4:D:352:ILE:O    | 4:D:353:PRO:O    | 2.15                     | 0.65              |
| 4:D:54:MET:HG3   | 4:D:57:ARG:HH21  | 1.61                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:308:TYR:O    | 4:D:311:VAL:HG12 | 1.97                     | 0.65              |
| 4:D:779:ALA:O    | 4:D:783:VAL:HG23 | 1.96                     | 0.65              |
| 5:T:139:HOH:O    | 4:D:780:PRO:HG2  | 1.97                     | 0.65              |
| 4:D:829:ARG:NH2  | 4:D:882:PHE:HA   | 2.11                     | 0.65              |
| 4:D:861:MET:HE3  | 4:D:862:PRO:HD2  | 1.77                     | 0.65              |
| 1:T:119:DT:O4'   | 5:T:139:HOH:O    | 2.13                     | 0.65              |
| 4:D:25:ALA:HA    | 5:D:937:HOH:O    | 1.96                     | 0.65              |
| 4:D:500:THR:OG1  | 5:D:1009:HOH:O   | 2.15                     | 0.65              |
| 4:D:593:GLU:HG2  | 4:D:594:VAL:H    | 1.62                     | 0.65              |
| 4:D:228:SER:HB3  | 4:D:245:GLU:OE1  | 1.96                     | 0.64              |
| 4:D:360:LEU:HD23 | 4:D:360:LEU:N    | 2.13                     | 0.64              |
| 4:D:650:VAL:HG12 | 4:D:655:ILE:CD1  | 2.27                     | 0.64              |
| 4:D:669:GLN:HG3  | 4:D:672:GLN:HB2  | 1.79                     | 0.64              |
| 4:D:250:TYR:O    | 4:D:254:ILE:HD12 | 1.97                     | 0.64              |
| 4:D:355:ILE:HD13 | 4:D:355:ILE:N    | 2.09                     | 0.64              |
| 5:T:139:HOH:O    | 4:D:780:PRO:CG   | 2.46                     | 0.63              |
| 4:D:787:ASP:CB   | 5:D:1026:HOH:O   | 2.43                     | 0.63              |
| 1:T:126:DT:C4    | 5:T:134:HOH:O    | 2.51                     | 0.63              |
| 4:D:99:ARG:O     | 5:D:982:HOH:O    | 2.15                     | 0.63              |
| 4:D:169:GLN:CD   | 4:D:169:GLN:H    | 2.07                     | 0.63              |
| 4:D:13:ASP:CG    | 4:D:14:ILE:HD12  | 2.24                     | 0.63              |
| 4:D:71:LYS:HA    | 5:D:1034:HOH:O   | 1.98                     | 0.63              |
| 4:D:595:VAL:HB   | 4:D:607:GLU:HA   | 1.81                     | 0.63              |
| 4:D:664:GLY:HA3  | 5:D:1031:HOH:O   | 1.88                     | 0.63              |
| 4:D:746:ARG:HE   | 4:D:754:GLN:NE2  | 1.92                     | 0.63              |
| 4:D:720:ARG:NH2  | 5:D:1029:HOH:O   | 2.31                     | 0.63              |
| 4:D:353:PRO:HG3  | 4:D:394:ARG:HB2  | 1.80                     | 0.63              |
| 4:D:532:LEU:O    | 4:D:818:PRO:HD3  | 1.99                     | 0.63              |
| 4:D:141:ILE:C    | 4:D:145:ILE:HD13 | 2.25                     | 0.62              |
| 4:D:423:ARG:HH12 | 4:D:784:HIS:CD2  | 2.16                     | 0.62              |
| 4:D:579:ASN:HA   | 4:D:582:LEU:HB2  | 1.81                     | 0.62              |
| 4:D:74:ILE:CD1   | 5:D:1017:HOH:O   | 2.47                     | 0.62              |
| 4:D:577:LYS:HB2  | 4:D:577:LYS:HZ3  | 1.64                     | 0.62              |
| 1:T:119:DT:P     | 5:T:141:HOH:O    | 2.57                     | 0.62              |
| 4:D:153:ARG:C    | 4:D:155:ARG:H    | 2.06                     | 0.62              |
| 4:D:806:SER:O    | 4:D:816:THR:HG23 | 1.99                     | 0.62              |
| 1:T:119:DT:OP2   | 5:T:141:HOH:O    | 2.16                     | 0.62              |
| 4:D:130:ASP:C    | 4:D:132:THR:H    | 2.07                     | 0.62              |
| 4:D:207:GLU:HG2  | 4:D:211:HIS:HE1  | 1.65                     | 0.62              |
| 4:D:445:THR:CB   | 5:D:974:HOH:O    | 2.47                     | 0.62              |
| 1:T:123:DG:H2''  | 1:T:122:DC:H5'   | 1.82                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:562:LEU:HD21 | 4:D:870:LEU:CD1  | 2.30                     | 0.62              |
| 4:D:14:ILE:HG23  | 4:D:288:ALA:HB1  | 1.81                     | 0.61              |
| 4:D:180:LYS:HD2  | 4:D:181:ALA:N    | 2.15                     | 0.61              |
| 4:D:589:GLY:C    | 4:D:614:LYS:HG3  | 2.25                     | 0.61              |
| 4:D:490:MET:HE3  | 5:D:926:HOH:O    | 1.99                     | 0.61              |
| 4:D:689:VAL:C    | 5:D:972:HOH:O    | 2.42                     | 0.61              |
| 1:T:126:DT:C5    | 5:T:134:HOH:O    | 2.52                     | 0.61              |
| 4:D:420:MET:HE3  | 4:D:424:GLY:O    | 1.99                     | 0.61              |
| 4:D:208:ASP:C    | 4:D:210:ILE:H    | 2.09                     | 0.61              |
| 4:D:340:VAL:CG2  | 4:D:341:ILE:N    | 2.64                     | 0.61              |
| 4:D:725:VAL:HG23 | 4:D:774:GLN:NE2  | 2.15                     | 0.61              |
| 4:D:25:ALA:O     | 4:D:26:ASP:HB2   | 2.00                     | 0.61              |
| 4:D:50:ARG:NH2   | 4:D:267:MET:HG2  | 2.15                     | 0.61              |
| 4:D:117:ILE:HG21 | 4:D:145:ILE:HD12 | 1.80                     | 0.61              |
| 1:T:120:DT:H1'   | 1:T:119:DT:H71   | 1.81                     | 0.61              |
| 4:D:104:GLN:N    | 5:D:946:HOH:O    | 2.17                     | 0.61              |
| 4:D:330:ILE:N    | 4:D:330:ILE:HD12 | 2.16                     | 0.61              |
| 4:D:360:LEU:C    | 5:D:968:HOH:O    | 2.44                     | 0.60              |
| 4:D:710:VAL:HG13 | 4:D:720:ARG:H    | 1.64                     | 0.60              |
| 4:D:330:ILE:HD13 | 4:D:408:PHE:O    | 1.99                     | 0.60              |
| 4:D:790:HIS:HD2  | 5:D:995:HOH:O    | 1.80                     | 0.60              |
| 2:N:25:DC:H1'    | 2:N:26:DA:H5''   | 1.83                     | 0.60              |
| 3:R:4:G:O3'      | 4:D:394:ARG:NH1  | 2.33                     | 0.60              |
| 4:D:264:ILE:HB   | 4:D:292:ARG:HD2  | 1.83                     | 0.60              |
| 4:D:420:MET:N    | 5:D:957:HOH:O    | 2.28                     | 0.60              |
| 4:D:797:TRP:CE2  | 5:D:910:HOH:O    | 2.51                     | 0.60              |
| 4:D:873:ARG:O    | 5:D:1018:HOH:O   | 2.17                     | 0.60              |
| 4:D:746:ARG:NE   | 4:D:754:GLN:HE22 | 1.94                     | 0.60              |
| 4:D:19:ILE:HB    | 4:D:20:PRO:HD3   | 1.82                     | 0.60              |
| 4:D:292:ARG:HA   | 4:D:292:ARG:NE   | 2.14                     | 0.60              |
| 4:D:445:THR:CA   | 5:D:974:HOH:O    | 2.33                     | 0.60              |
| 1:T:119:DT:C4'   | 5:T:139:HOH:O    | 2.49                     | 0.60              |
| 4:D:816:THR:HG21 | 5:D:989:HOH:O    | 1.94                     | 0.60              |
| 4:D:141:ILE:CD1  | 4:D:217:ILE:HD11 | 2.32                     | 0.60              |
| 1:T:117:DG:H2''  | 1:T:116:DC:H5'   | 1.82                     | 0.59              |
| 4:D:82:ILE:HG12  | 4:D:112:GLU:HA   | 1.83                     | 0.59              |
| 4:D:157:LEU:HD23 | 4:D:196:LEU:HD12 | 1.83                     | 0.59              |
| 4:D:320:ILE:HD11 | 4:D:420:MET:SD   | 2.41                     | 0.59              |
| 4:D:360:LEU:HB3  | 4:D:384:VAL:HG21 | 1.83                     | 0.59              |
| 4:D:539:SER:O    | 4:D:540:CYS:HB2  | 2.03                     | 0.59              |
| 4:D:655:ILE:O    | 4:D:656:GLN:C    | 2.44                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:796:VAL:CB   | 5:D:1016:HOH:O   | 2.36                     | 0.59              |
| 4:D:16:LEU:HG    | 4:D:20:PRO:HB2   | 1.85                     | 0.59              |
| 4:D:141:ILE:HD13 | 4:D:217:ILE:HD11 | 1.84                     | 0.59              |
| 4:D:439:MET:HB2  | 5:D:934:HOH:O    | 2.03                     | 0.59              |
| 4:D:857:GLN:HE22 | 4:D:859:ASP:HB2  | 1.67                     | 0.59              |
| 1:T:119:DT:H6    | 5:T:141:HOH:O    | 1.85                     | 0.58              |
| 4:D:404:GLN:N    | 5:D:973:HOH:O    | 2.35                     | 0.58              |
| 4:D:655:ILE:O    | 4:D:658:ALA:N    | 2.34                     | 0.58              |
| 1:T:119:DT:C7    | 5:T:141:HOH:O    | 2.32                     | 0.58              |
| 3:R:9:A:H2       | 5:D:991:HOH:O    | 1.86                     | 0.58              |
| 4:D:157:LEU:O    | 4:D:159:ALA:N    | 2.35                     | 0.58              |
| 4:D:826:LYS:HE2  | 4:D:830:GLU:OE2  | 2.04                     | 0.58              |
| 2:N:17:DA:H3'    | 2:N:18:DC:H5''   | 1.85                     | 0.58              |
| 4:D:337:VAL:HG11 | 4:D:512:LEU:HD21 | 1.86                     | 0.58              |
| 4:D:562:LEU:HD21 | 4:D:870:LEU:HD12 | 1.84                     | 0.58              |
| 4:D:80:LYS:O     | 5:D:1048:HOH:O   | 2.16                     | 0.58              |
| 4:D:727:TRP:CD1  | 5:D:1037:HOH:O   | 2.56                     | 0.58              |
| 3:R:10:G:H8      | 4:D:301:SER:OG   | 1.87                     | 0.58              |
| 4:D:25:ALA:CA    | 5:D:937:HOH:O    | 2.52                     | 0.58              |
| 4:D:153:ARG:O    | 4:D:157:LEU:HB3  | 2.04                     | 0.58              |
| 4:D:812:ASP:OD2  | 5:D:984:HOH:O    | 2.17                     | 0.58              |
| 4:D:340:VAL:HG23 | 4:D:341:ILE:N    | 2.19                     | 0.58              |
| 4:D:344:TRP:HB3  | 5:D:1015:HOH:O   | 1.88                     | 0.57              |
| 4:D:318:LYS:O    | 4:D:322:ILE:HG12 | 2.03                     | 0.57              |
| 4:D:137:VAL:HG12 | 4:D:141:ILE:CD1  | 2.34                     | 0.57              |
| 4:D:420:MET:HB3  | 5:D:957:HOH:O    | 2.04                     | 0.57              |
| 4:D:454:LYS:CE   | 5:D:948:HOH:O    | 2.45                     | 0.57              |
| 4:D:557:ARG:O    | 4:D:568:GLN:HG3  | 2.04                     | 0.57              |
| 4:D:611:LEU:HD22 | 4:D:615:ALA:HB1  | 1.85                     | 0.57              |
| 4:D:633:SER:HA   | 4:D:649:GLN:HE22 | 1.69                     | 0.57              |
| 4:D:729:THR:HG22 | 5:D:1041:HOH:O   | 2.03                     | 0.57              |
| 4:D:217:ILE:C    | 4:D:221:ILE:HD13 | 2.22                     | 0.57              |
| 4:D:420:MET:CE   | 4:D:424:GLY:HA2  | 2.34                     | 0.57              |
| 4:D:335:LEU:HD22 | 4:D:339:ASN:ND2  | 2.19                     | 0.57              |
| 4:D:404:GLN:CA   | 5:D:973:HOH:O    | 2.53                     | 0.57              |
| 4:D:727:TRP:NE1  | 5:D:1037:HOH:O   | 2.38                     | 0.57              |
| 4:D:85:ILE:HA    | 4:D:219:MET:CE   | 2.34                     | 0.57              |
| 4:D:110:LYS:HB3  | 4:D:112:GLU:OE2  | 2.05                     | 0.57              |
| 4:D:797:TRP:CZ3  | 4:D:801:LYS:HE3  | 2.40                     | 0.57              |
| 4:D:14:ILE:HG13  | 4:D:290:GLY:HA2  | 1.87                     | 0.57              |
| 4:D:851:ASP:O    | 4:D:853:LEU:N    | 2.38                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:407:LYS:HB2  | 5:D:973:HOH:O    | 2.04                     | 0.56              |
| 1:T:120:DT:H1'   | 5:T:141:HOH:O    | 2.04                     | 0.56              |
| 2:N:22:DG:H2''   | 2:N:23:DC:C6     | 2.40                     | 0.56              |
| 4:D:25:ALA:HB2   | 5:D:937:HOH:O    | 2.03                     | 0.56              |
| 4:D:30:GLU:N     | 5:D:937:HOH:O    | 2.38                     | 0.56              |
| 4:D:147:ASP:HB3  | 4:D:751:PHE:HE2  | 1.70                     | 0.56              |
| 4:D:440:THR:HG22 | 5:D:967:HOH:O    | 2.04                     | 0.56              |
| 4:D:710:VAL:N    | 5:D:940:HOH:O    | 2.38                     | 0.56              |
| 4:D:281:ILE:H    | 4:D:281:ILE:CD1  | 2.19                     | 0.56              |
| 4:D:344:TRP:HE3  | 5:D:1015:HOH:O   | 1.87                     | 0.56              |
| 4:D:380:ALA:C    | 5:D:986:HOH:O    | 2.47                     | 0.56              |
| 1:T:111:DT:H3'   | 1:T:111:DT:OP2   | 2.05                     | 0.56              |
| 5:T:139:HOH:O    | 4:D:780:PRO:CB   | 2.50                     | 0.56              |
| 4:D:46:MET:HB3   | 4:D:267:MET:HE3  | 1.88                     | 0.56              |
| 4:D:517:GLU:HG3  | 4:D:532:LEU:HB2  | 1.86                     | 0.56              |
| 4:D:709:GLU:C    | 5:D:940:HOH:O    | 2.49                     | 0.56              |
| 4:D:325:ASN:HB3  | 5:D:919:HOH:O    | 2.06                     | 0.56              |
| 4:D:360:LEU:CB   | 5:D:968:HOH:O    | 2.12                     | 0.56              |
| 4:D:780:PRO:CB   | 5:D:975:HOH:O    | 2.54                     | 0.56              |
| 4:D:797:TRP:NE1  | 5:D:910:HOH:O    | 2.38                     | 0.56              |
| 4:D:684:SER:O    | 4:D:687:VAL:HG22 | 2.06                     | 0.56              |
| 4:D:454:LYS:HD3  | 5:D:948:HOH:O    | 2.05                     | 0.56              |
| 4:D:25:ALA:CB    | 5:D:937:HOH:O    | 2.54                     | 0.55              |
| 4:D:221:ILE:CD1  | 4:D:221:ILE:N    | 2.69                     | 0.55              |
| 4:D:255:ALA:CA   | 5:D:942:HOH:O    | 2.49                     | 0.55              |
| 1:T:114:DG:H4'   | 4:D:396:ILE:HG21 | 1.88                     | 0.55              |
| 4:D:134:VAL:HG11 | 4:D:229:LEU:CD2  | 2.36                     | 0.55              |
| 4:D:300:HIS:O    | 4:D:301:SER:HB2  | 2.06                     | 0.55              |
| 4:D:710:VAL:CG1  | 4:D:720:ARG:HB3  | 2.37                     | 0.55              |
| 4:D:726:HIS:HB2  | 4:D:736:TRP:CD1  | 2.41                     | 0.55              |
| 4:D:804:ILE:CD1  | 5:D:1004:HOH:O   | 2.50                     | 0.55              |
| 4:D:264:ILE:O    | 4:D:264:ILE:HD12 | 2.05                     | 0.55              |
| 4:D:471:ASP:OD1  | 4:D:472:LYS:HE2  | 2.06                     | 0.55              |
| 1:T:127:DG:H1'   | 1:T:126:DT:C5'   | 2.36                     | 0.55              |
| 4:D:593:GLU:HG2  | 4:D:594:VAL:N    | 2.22                     | 0.55              |
| 4:D:619:GLN:OE1  | 4:D:667:PHE:HA   | 2.06                     | 0.55              |
| 3:R:10:G:N2      | 5:R:46:HOH:O     | 2.31                     | 0.55              |
| 4:D:16:LEU:CG    | 4:D:20:PRO:HB2   | 2.37                     | 0.55              |
| 4:D:689:VAL:O    | 4:D:689:VAL:HG23 | 2.06                     | 0.55              |
| 4:D:779:ALA:O    | 4:D:783:VAL:CG2  | 2.55                     | 0.55              |
| 4:D:830:GLU:CB   | 5:D:910:HOH:O    | 2.43                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:81:MET:HE3   | 4:D:115:ALA:HA   | 1.89                     | 0.55              |
| 4:D:428:ALA:HB1  | 5:D:944:HOH:O    | 1.97                     | 0.55              |
| 4:D:829:ARG:NH1  | 4:D:878:SER:O    | 2.40                     | 0.55              |
| 4:D:420:MET:CG   | 5:D:957:HOH:O    | 2.54                     | 0.55              |
| 4:D:543:ILE:HD12 | 4:D:543:ILE:H    | 1.71                     | 0.54              |
| 4:D:379:ARG:C    | 4:D:381:ALA:H    | 2.15                     | 0.54              |
| 4:D:160:LYS:HD3  | 4:D:163:LYS:HD2  | 1.88                     | 0.54              |
| 4:D:853:LEU:O    | 4:D:854:HIS:HB2  | 2.08                     | 0.54              |
| 4:D:545:HIS:O    | 4:D:549:MET:HG2  | 2.07                     | 0.54              |
| 4:D:651:LEU:HG   | 4:D:656:GLN:HE21 | 1.73                     | 0.54              |
| 4:D:157:LEU:CD2  | 4:D:196:LEU:HD12 | 2.37                     | 0.54              |
| 4:D:590:THR:HG22 | 4:D:591:ASP:N    | 2.22                     | 0.54              |
| 4:D:553:GLU:HB3  | 5:D:893:HOH:O    | 2.06                     | 0.54              |
| 4:D:13:ASP:OD2   | 4:D:14:ILE:HD12  | 2.07                     | 0.54              |
| 4:D:254:ILE:C    | 5:D:942:HOH:O    | 2.49                     | 0.54              |
| 4:D:291:ARG:C    | 4:D:293:PRO:HD3  | 2.32                     | 0.54              |
| 4:D:347:CYS:HA   | 5:D:1015:HOH:O   | 2.06                     | 0.54              |
| 4:D:400:PHE:O    | 4:D:404:GLN:HB2  | 2.07                     | 0.54              |
| 4:D:570:ILE:O    | 4:D:574:VAL:HG23 | 2.08                     | 0.54              |
| 4:D:160:LYS:HZ3  | 4:D:160:LYS:HB2  | 1.73                     | 0.53              |
| 4:D:810:ILE:N    | 4:D:810:ILE:HD12 | 2.23                     | 0.53              |
| 4:D:195:LEU:C    | 4:D:197:GLY:H    | 2.16                     | 0.53              |
| 4:D:292:ARG:HE   | 4:D:292:ARG:CA   | 2.18                     | 0.53              |
| 4:D:410:ASN:N    | 5:D:903:HOH:O    | 2.21                     | 0.53              |
| 4:D:806:SER:HB2  | 5:D:1008:HOH:O   | 2.07                     | 0.53              |
| 4:D:92:VAL:HG11  | 4:D:103:PHE:CD1  | 2.43                     | 0.53              |
| 4:D:160:LYS:CD   | 4:D:163:LYS:HD2  | 2.39                     | 0.53              |
| 4:D:335:LEU:CD2  | 4:D:339:ASN:ND2  | 2.72                     | 0.53              |
| 4:D:791:LEU:HA   | 4:D:814:PHE:HE2  | 1.73                     | 0.53              |
| 1:T:126:DT:C2'   | 1:T:125:DG:H5'   | 2.33                     | 0.53              |
| 4:D:2:ASN:O      | 4:D:127:THR:HA   | 2.09                     | 0.53              |
| 4:D:196:LEU:HD22 | 4:D:196:LEU:N    | 2.23                     | 0.53              |
| 4:D:790:HIS:HD2  | 5:D:904:HOH:O    | 1.92                     | 0.53              |
| 4:D:6:ILE:N      | 4:D:6:ILE:HD12   | 2.24                     | 0.52              |
| 4:D:810:ILE:CD1  | 5:D:932:HOH:O    | 2.57                     | 0.52              |
| 4:D:153:ARG:NH2  | 4:D:201:TRP:HB2  | 2.24                     | 0.52              |
| 4:D:162:PHE:C    | 4:D:164:LYS:H    | 2.17                     | 0.52              |
| 4:D:379:ARG:C    | 4:D:381:ALA:N    | 2.65                     | 0.52              |
| 1:T:120:DT:H2''  | 5:T:141:HOH:O    | 2.09                     | 0.52              |
| 5:T:131:HOH:O    | 4:D:421:ASP:HB2  | 2.08                     | 0.52              |
| 4:D:6:ILE:HD12   | 4:D:6:ILE:H      | 1.75                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:122:DC:H2''  | 1:T:121:DA:O5'   | 2.10                     | 0.52              |
| 4:D:650:VAL:HG12 | 4:D:655:ILE:HD11 | 1.91                     | 0.52              |
| 4:D:765:LYS:HA   | 4:D:765:LYS:HZ3  | 1.75                     | 0.52              |
| 4:D:780:PRO:CA   | 5:D:975:HOH:O    | 2.58                     | 0.52              |
| 4:D:25:ALA:C     | 4:D:27:HIS:H     | 2.17                     | 0.52              |
| 4:D:335:LEU:HD21 | 4:D:406:ASN:OD1  | 2.10                     | 0.52              |
| 4:D:421:ASP:O    | 5:D:1002:HOH:O   | 2.18                     | 0.52              |
| 4:D:147:ASP:HB3  | 4:D:751:PHE:CE2  | 2.45                     | 0.52              |
| 4:D:226:MET:HA   | 4:D:250:TYR:CD2  | 2.44                     | 0.52              |
| 4:D:727:TRP:CZ3  | 5:D:1012:HOH:O   | 2.54                     | 0.52              |
| 4:D:765:LYS:HZ2  | 4:D:765:LYS:C    | 2.16                     | 0.52              |
| 4:D:533:PRO:CD   | 5:D:974:HOH:O    | 2.57                     | 0.52              |
| 4:D:610:LYS:HA   | 4:D:672:GLN:OE1  | 2.09                     | 0.52              |
| 3:R:10:G:C8      | 4:D:301:SER:OG   | 2.63                     | 0.51              |
| 4:D:181:ALA:O    | 4:D:185:VAL:HG23 | 2.10                     | 0.51              |
| 4:D:41:HIS:O     | 4:D:45:GLU:HG3   | 2.10                     | 0.51              |
| 1:T:111:DT:H3'   | 1:T:111:DT:P     | 2.49                     | 0.51              |
| 4:D:65:ALA:CA    | 5:D:1017:HOH:O   | 2.39                     | 0.51              |
| 4:D:169:GLN:CD   | 4:D:169:GLN:N    | 2.69                     | 0.51              |
| 4:D:2:ASN:OD1    | 4:D:245:GLU:HB2  | 2.11                     | 0.51              |
| 4:D:461:LYS:HA   | 5:D:1036:HOH:O   | 2.11                     | 0.51              |
| 1:T:120:DT:C2'   | 5:T:141:HOH:O    | 2.59                     | 0.51              |
| 4:D:182:PHE:O    | 4:D:186:VAL:HG23 | 2.11                     | 0.51              |
| 4:D:420:MET:HE3  | 4:D:424:GLY:HA2  | 1.93                     | 0.51              |
| 4:D:595:VAL:CG2  | 4:D:608:LYS:H    | 2.23                     | 0.51              |
| 4:D:118:THR:HG22 | 4:D:220:LEU:HD12 | 1.93                     | 0.51              |
| 4:D:433:ASN:HB2  | 4:D:434:PRO:CD   | 2.41                     | 0.51              |
| 4:D:652:GLU:O    | 4:D:657:PRO:HD3  | 2.11                     | 0.51              |
| 4:D:50:ARG:HG2   | 4:D:267:MET:HE2  | 1.93                     | 0.51              |
| 4:D:32:LEU:HG    | 5:D:1047:HOH:O   | 2.11                     | 0.50              |
| 4:D:255:ALA:N    | 5:D:942:HOH:O    | 2.44                     | 0.50              |
| 4:D:706:LEU:HA   | 5:D:1029:HOH:O   | 2.11                     | 0.50              |
| 4:D:709:GLU:CG   | 5:D:940:HOH:O    | 2.60                     | 0.50              |
| 4:D:30:GLU:HG3   | 4:D:34:ARG:HH21  | 1.76                     | 0.50              |
| 4:D:215:ARG:O    | 4:D:219:MET:HG3  | 2.11                     | 0.50              |
| 4:D:339:ASN:OD1  | 4:D:402:LEU:HD11 | 2.11                     | 0.50              |
| 4:D:804:ILE:HD12 | 4:D:820:ASP:HB3  | 1.93                     | 0.50              |
| 4:D:33:ALA:HB3   | 5:D:937:HOH:O    | 2.12                     | 0.50              |
| 4:D:210:ILE:O    | 4:D:214:VAL:HG23 | 2.11                     | 0.50              |
| 4:D:550:LEU:HB2  | 4:D:691:ALA:HB1  | 1.92                     | 0.50              |
| 4:D:30:GLU:HA    | 5:D:937:HOH:O    | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:85:ILE:HG22  | 4:D:89:PHE:CE2   | 2.46                     | 0.50              |
| 4:D:143:ARG:HG2  | 4:D:143:ARG:HH11 | 1.76                     | 0.50              |
| 4:D:160:LYS:C    | 4:D:162:PHE:N    | 2.68                     | 0.50              |
| 4:D:341:ILE:HD11 | 4:D:348:PRO:CG   | 2.40                     | 0.50              |
| 4:D:804:ILE:HD12 | 4:D:820:ASP:CB   | 2.42                     | 0.50              |
| 4:D:421:ASP:OD1  | 4:D:421:ASP:C    | 2.54                     | 0.50              |
| 4:D:778:ILE:HG23 | 4:D:779:ALA:N    | 2.26                     | 0.50              |
| 1:T:119:DT:C6    | 5:T:141:HOH:O    | 2.55                     | 0.50              |
| 4:D:551:ARG:HB2  | 4:D:868:GLY:H    | 1.76                     | 0.50              |
| 4:D:655:ILE:HG23 | 4:D:659:ILE:HD13 | 1.93                     | 0.50              |
| 4:D:217:ILE:CA   | 5:D:1005:HOH:O   | 2.57                     | 0.50              |
| 4:D:276:LYS:CE   | 5:D:1032:HOH:O   | 2.07                     | 0.50              |
| 4:D:631:LYS:HD3  | 4:D:635:MET:SD   | 2.51                     | 0.50              |
| 4:D:707:ALA:O    | 4:D:722:ARG:HG2  | 2.10                     | 0.50              |
| 4:D:711:LYS:NZ   | 5:D:1013:HOH:O   | 2.45                     | 0.50              |
| 4:D:324:GLN:CD   | 5:D:928:HOH:O    | 2.53                     | 0.50              |
| 4:D:417:PRO:HG2  | 4:D:429:VAL:HB   | 1.94                     | 0.50              |
| 4:D:621:LEU:C    | 4:D:623:TYR:H    | 2.19                     | 0.50              |
| 4:D:651:LEU:HG   | 4:D:656:GLN:NE2  | 2.26                     | 0.50              |
| 4:D:861:MET:HE3  | 4:D:862:PRO:CD   | 2.41                     | 0.50              |
| 4:D:312:TYR:HD2  | 5:D:976:HOH:O    | 1.94                     | 0.49              |
| 4:D:727:TRP:CE3  | 5:D:1012:HOH:O   | 2.64                     | 0.49              |
| 4:D:404:GLN:HA   | 5:D:973:HOH:O    | 2.12                     | 0.49              |
| 4:D:117:ILE:HG12 | 4:D:752:LEU:HD12 | 1.95                     | 0.49              |
| 4:D:157:LEU:HD12 | 4:D:158:GLU:H    | 1.78                     | 0.49              |
| 4:D:420:MET:HE2  | 4:D:733:PHE:CE1  | 2.47                     | 0.49              |
| 4:D:875:ILE:CG1  | 5:D:1014:HOH:O   | 2.50                     | 0.49              |
| 4:D:537:ASP:CG   | 5:D:984:HOH:O    | 2.55                     | 0.49              |
| 4:D:159:ALA:HA   | 4:D:195:LEU:HD21 | 1.94                     | 0.49              |
| 4:D:495:SER:HA   | 5:D:929:HOH:O    | 2.13                     | 0.49              |
| 4:D:710:VAL:HG13 | 4:D:720:ARG:N    | 2.28                     | 0.49              |
| 1:T:127:DG:H2"   | 1:T:126:DT:OP2   | 2.13                     | 0.49              |
| 4:D:417:PRO:O    | 5:D:944:HOH:O    | 2.20                     | 0.49              |
| 4:D:593:GLU:CG   | 4:D:594:VAL:H    | 2.25                     | 0.49              |
| 4:D:653:ASP:O    | 4:D:657:PRO:HG3  | 2.12                     | 0.49              |
| 4:D:47:GLY:HA3   | 4:D:265:SER:O    | 2.12                     | 0.49              |
| 4:D:352:ILE:O    | 4:D:352:ILE:CG2  | 2.61                     | 0.49              |
| 4:D:854:HIS:O    | 4:D:855:GLU:O    | 2.31                     | 0.49              |
| 4:D:654:THR:O    | 4:D:657:PRO:HG2  | 2.13                     | 0.48              |
| 4:D:473:VAL:HG11 | 4:D:477:GLU:OE2  | 2.13                     | 0.48              |
| 4:D:153:ARG:C    | 4:D:155:ARG:N    | 2.71                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:207:GLU:HG2  | 4:D:211:HIS:CE1  | 2.45                     | 0.48              |
| 4:D:543:ILE:HD12 | 4:D:543:ILE:N    | 2.27                     | 0.48              |
| 4:D:620:TRP:O    | 4:D:623:TYR:HB3  | 2.13                     | 0.48              |
| 4:D:744:GLN:NE2  | 4:D:758:GLN:NE2  | 2.61                     | 0.48              |
| 4:D:833:VAL:O    | 4:D:837:GLU:HB2  | 2.12                     | 0.48              |
| 4:D:873:ARG:CB   | 5:D:1018:HOH:O   | 2.57                     | 0.48              |
| 4:D:88:TRP:O     | 4:D:91:GLU:HG2   | 2.14                     | 0.48              |
| 4:D:349:VAL:HG13 | 4:D:508:PRO:HG3  | 1.96                     | 0.48              |
| 4:D:360:LEU:N    | 4:D:360:LEU:CD2  | 2.76                     | 0.48              |
| 4:D:584:ALA:O    | 4:D:588:ASN:HB3  | 2.14                     | 0.48              |
| 4:D:330:ILE:CD1  | 5:D:895:HOH:O    | 2.33                     | 0.48              |
| 4:D:661:SER:C    | 4:D:663:LYS:H    | 2.21                     | 0.48              |
| 4:D:729:THR:CB   | 5:D:1041:HOH:O   | 2.61                     | 0.48              |
| 4:D:533:PRO:HA   | 4:D:816:THR:O    | 2.13                     | 0.48              |
| 4:D:707:ALA:O    | 4:D:722:ARG:NH1  | 2.43                     | 0.48              |
| 2:N:28:DG:H2''   | 2:N:29:DG:H8     | 1.79                     | 0.48              |
| 4:D:13:ASP:OD1   | 4:D:14:ILE:HD12  | 2.12                     | 0.48              |
| 4:D:157:LEU:O    | 4:D:158:GLU:C    | 2.55                     | 0.48              |
| 2:N:22:DG:H2''   | 2:N:23:DC:C5     | 2.48                     | 0.48              |
| 4:D:468:ALA:HA   | 5:D:952:HOH:O    | 2.13                     | 0.48              |
| 4:D:828:VAL:HG11 | 4:D:882:PHE:O    | 2.13                     | 0.48              |
| 1:T:117:DG:H2''  | 1:T:116:DC:C5'   | 2.43                     | 0.48              |
| 4:D:276:LYS:CD   | 5:D:1032:HOH:O   | 2.55                     | 0.48              |
| 4:D:286:TYR:CZ   | 4:D:417:PRO:HG3  | 2.48                     | 0.48              |
| 4:D:320:ILE:O    | 4:D:324:GLN:HG2  | 2.14                     | 0.48              |
| 4:D:130:ASP:C    | 4:D:132:THR:N    | 2.71                     | 0.47              |
| 4:D:278:TRP:CH2  | 4:D:294:LEU:HB3  | 2.50                     | 0.47              |
| 4:D:595:VAL:CB   | 4:D:607:GLU:HA   | 2.43                     | 0.47              |
| 4:D:650:VAL:O    | 4:D:655:ILE:HD12 | 2.14                     | 0.47              |
| 4:D:735:VAL:C    | 5:D:1012:HOH:O   | 2.57                     | 0.47              |
| 1:T:128:DC:H42   | 2:N:27:DC:H42    | 1.61                     | 0.47              |
| 4:D:375:THR:O    | 4:D:376:ALA:HB3  | 2.14                     | 0.47              |
| 4:D:537:ASP:N    | 4:D:882:PHE:HD1  | 2.13                     | 0.47              |
| 4:D:669:GLN:HG2  | 4:D:672:GLN:NE2  | 2.30                     | 0.47              |
| 3:R:6:C:H5'      | 4:D:171:ASN:O    | 2.15                     | 0.47              |
| 4:D:32:LEU:O     | 4:D:33:ALA:C     | 2.58                     | 0.47              |
| 4:D:93:LYS:HE3   | 4:D:103:PHE:HZ   | 1.79                     | 0.47              |
| 4:D:109:ILE:HD12 | 4:D:109:ILE:H    | 1.80                     | 0.47              |
| 4:D:17:ALA:C     | 4:D:20:PRO:HD2   | 2.40                     | 0.47              |
| 4:D:20:PRO:O     | 4:D:23:THR:HB    | 2.14                     | 0.47              |
| 4:D:330:ILE:N    | 4:D:330:ILE:CD1  | 2.78                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:735:VAL:CG2  | 5:D:1037:HOH:O   | 2.63                     | 0.47              |
| 4:D:254:ILE:HG22 | 5:D:942:HOH:O    | 2.15                     | 0.46              |
| 4:D:676:TYR:O    | 4:D:679:LYS:HB3  | 2.16                     | 0.46              |
| 4:D:828:VAL:CG1  | 4:D:882:PHE:O    | 2.63                     | 0.46              |
| 4:D:577:LYS:HD3  | 4:D:687:VAL:CG2  | 2.45                     | 0.46              |
| 4:D:700:LYS:NZ   | 4:D:700:LYS:HB3  | 2.30                     | 0.46              |
| 4:D:4:ILE:HD13   | 4:D:254:ILE:HG21 | 1.98                     | 0.46              |
| 4:D:85:ILE:HD13  | 4:D:219:MET:SD   | 2.55                     | 0.46              |
| 4:D:208:ASP:C    | 4:D:210:ILE:N    | 2.74                     | 0.46              |
| 4:D:226:MET:O    | 4:D:246:LEU:HD12 | 2.16                     | 0.46              |
| 4:D:473:VAL:HG22 | 4:D:474:PRO:CD   | 2.40                     | 0.46              |
| 4:D:696:MET:O    | 4:D:700:LYS:HG3  | 2.16                     | 0.46              |
| 4:D:296:LEU:CD2  | 4:D:320:ILE:HD13 | 2.32                     | 0.46              |
| 4:D:802:TYR:OH   | 4:D:826:LYS:HD3  | 2.15                     | 0.46              |
| 4:D:93:LYS:NZ    | 5:D:1011:HOH:O   | 2.26                     | 0.46              |
| 2:N:27:DC:H2''   | 2:N:28:DG:H5''   | 1.98                     | 0.46              |
| 4:D:131:ASN:C    | 4:D:133:THR:H    | 2.24                     | 0.46              |
| 4:D:817:ILE:CG1  | 5:D:947:HOH:O    | 2.60                     | 0.46              |
| 4:D:42:GLU:CD    | 5:D:1035:HOH:O   | 2.59                     | 0.46              |
| 4:D:70:ALA:HB1   | 5:D:1017:HOH:O   | 2.15                     | 0.46              |
| 4:D:481:PHE:HE2  | 5:D:987:HOH:O    | 1.98                     | 0.46              |
| 4:D:765:LYS:HD3  | 4:D:766:ASP:H    | 1.78                     | 0.46              |
| 1:T:126:DT:H1'   | 1:T:125:DG:H5''  | 1.98                     | 0.45              |
| 4:D:379:ARG:O    | 5:D:986:HOH:O    | 2.21                     | 0.45              |
| 4:D:669:GLN:HG2  | 4:D:672:GLN:HE21 | 1.81                     | 0.45              |
| 4:D:855:GLU:HB3  | 4:D:856:SER:H    | 1.44                     | 0.45              |
| 4:D:157:LEU:HG   | 4:D:196:LEU:HD12 | 1.98                     | 0.45              |
| 4:D:763:THR:CG2  | 5:D:962:HOH:O    | 0.76                     | 0.45              |
| 1:T:112:DG:O4'   | 1:T:112:DG:N3    | 2.50                     | 0.45              |
| 4:D:360:LEU:O    | 4:D:362:MET:SD   | 2.75                     | 0.45              |
| 1:T:113:DT:H2'   | 4:D:57:ARG:NH1   | 2.31                     | 0.45              |
| 4:D:154:ILE:HD11 | 4:D:183:MET:CE   | 2.33                     | 0.45              |
| 4:D:505:GLN:CA   | 5:D:952:HOH:O    | 2.64                     | 0.45              |
| 4:D:105:PHE:O    | 4:D:108:GLU:HG2  | 2.17                     | 0.45              |
| 4:D:659:ILE:HD11 | 4:D:667:PHE:HD2  | 1.81                     | 0.45              |
| 4:D:74:ILE:HD11  | 5:D:1017:HOH:O   | 2.11                     | 0.45              |
| 4:D:330:ILE:HD11 | 4:D:408:PHE:CB   | 2.47                     | 0.45              |
| 4:D:398:LEU:O    | 4:D:402:LEU:HB2  | 2.17                     | 0.45              |
| 4:D:461:LYS:HE2  | 4:D:479:ILE:HD12 | 1.97                     | 0.45              |
| 4:D:655:ILE:CG2  | 4:D:659:ILE:HD13 | 2.47                     | 0.45              |
| 4:D:875:ILE:CA   | 5:D:1014:HOH:O   | 2.64                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:126:DT:H1'   | 1:T:125:DG:C5'   | 2.46                     | 0.45              |
| 4:D:162:PHE:O    | 4:D:167:GLU:N    | 2.49                     | 0.45              |
| 4:D:270:PRO:CB   | 5:D:935:HOH:O    | 2.62                     | 0.45              |
| 4:D:655:ILE:HD12 | 4:D:655:ILE:N    | 2.30                     | 0.45              |
| 4:D:816:THR:HG22 | 4:D:817:ILE:H    | 1.82                     | 0.45              |
| 1:T:115:DC:H2'   | 1:T:115:DC:O5'   | 2.17                     | 0.45              |
| 4:D:229:LEU:HD23 | 4:D:244:ILE:HG23 | 1.98                     | 0.45              |
| 4:D:321:ASN:O    | 4:D:325:ASN:HB2  | 2.17                     | 0.45              |
| 4:D:796:VAL:C    | 5:D:1016:HOH:O   | 2.60                     | 0.45              |
| 4:D:727:TRP:CZ2  | 4:D:782:PHE:HA   | 2.52                     | 0.45              |
| 1:T:123:DG:H2''  | 1:T:122:DC:C5'   | 2.47                     | 0.44              |
| 4:D:533:PRO:HD2  | 5:D:974:HOH:O    | 2.16                     | 0.44              |
| 4:D:633:SER:CA   | 4:D:649:GLN:HE22 | 2.30                     | 0.44              |
| 4:D:706:LEU:O    | 4:D:723:CYS:N    | 2.43                     | 0.44              |
| 4:D:276:LYS:CG   | 5:D:1032:HOH:O   | 2.50                     | 0.44              |
| 4:D:416:PHE:HE1  | 5:D:935:HOH:O    | 2.01                     | 0.44              |
| 2:N:17:DA:C3'    | 2:N:18:DC:H5''   | 2.46                     | 0.44              |
| 4:D:73:LEU:O     | 4:D:77:LEU:HG    | 2.17                     | 0.44              |
| 4:D:651:LEU:HA   | 4:D:655:ILE:HD13 | 1.99                     | 0.44              |
| 4:D:154:ILE:HG22 | 4:D:196:LEU:HD21 | 2.00                     | 0.44              |
| 4:D:395:ARG:O    | 4:D:399:GLU:HG3  | 2.17                     | 0.44              |
| 4:D:780:PRO:C    | 5:D:975:HOH:O    | 2.61                     | 0.44              |
| 4:D:30:GLU:O     | 4:D:31:ARG:C     | 2.60                     | 0.44              |
| 4:D:301:SER:O    | 4:D:302:LYS:C    | 2.61                     | 0.44              |
| 4:D:566:THR:HG23 | 4:D:568:GLN:HE22 | 1.83                     | 0.44              |
| 4:D:655:ILE:HG22 | 4:D:656:GLN:N    | 2.33                     | 0.44              |
| 4:D:145:ILE:HD12 | 4:D:145:ILE:N    | 2.32                     | 0.44              |
| 4:D:278:TRP:HH2  | 4:D:294:LEU:HB3  | 1.81                     | 0.44              |
| 4:D:873:ARG:HG3  | 4:D:873:ARG:HH11 | 1.83                     | 0.44              |
| 1:T:123:DG:H1'   | 1:T:122:DC:H5''  | 1.99                     | 0.44              |
| 1:T:118:DC:H2''  | 1:T:117:DG:OP2   | 2.18                     | 0.44              |
| 4:D:9:ASN:OD1    | 4:D:48:GLU:OE2   | 2.35                     | 0.44              |
| 4:D:655:ILE:HG23 | 4:D:659:ILE:CD1  | 2.48                     | 0.44              |
| 4:D:281:ILE:HD13 | 4:D:281:ILE:N    | 2.30                     | 0.44              |
| 2:N:24:DG:H2''   | 2:N:25:DC:C6     | 2.53                     | 0.44              |
| 4:D:33:ALA:CB    | 5:D:937:HOH:O    | 2.64                     | 0.44              |
| 4:D:208:ASP:O    | 4:D:210:ILE:N    | 2.51                     | 0.44              |
| 4:D:221:ILE:CD1  | 4:D:221:ILE:H    | 2.30                     | 0.44              |
| 4:D:78:LEU:HB3   | 4:D:79:PRO:HD3   | 2.00                     | 0.43              |
| 4:D:109:ILE:H    | 4:D:109:ILE:CD1  | 2.30                     | 0.43              |
| 4:D:275:PRO:HD3  | 4:D:415:TRP:HB3  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:452:ILE:HG23 | 4:D:453:GLY:N    | 2.32                     | 0.43              |
| 4:D:117:ILE:CG2  | 4:D:145:ILE:HD12 | 2.46                     | 0.43              |
| 4:D:353:PRO:HG3  | 4:D:394:ARG:CB   | 2.47                     | 0.43              |
| 4:D:846:TYR:HA   | 4:D:849:PHE:CE1  | 2.53                     | 0.43              |
| 4:D:690:VAL:N    | 5:D:972:HOH:O    | 2.48                     | 0.43              |
| 4:D:157:LEU:CG   | 4:D:196:LEU:HD12 | 2.48                     | 0.43              |
| 4:D:356:GLU:HG2  | 4:D:357:ARG:N    | 2.33                     | 0.43              |
| 4:D:124:ALA:O    | 4:D:125:CYS:C    | 2.61                     | 0.43              |
| 4:D:216:CYS:C    | 5:D:1005:HOH:O   | 2.57                     | 0.43              |
| 4:D:273:VAL:O    | 4:D:274:PRO:C    | 2.59                     | 0.43              |
| 4:D:652:GLU:OE2  | 5:D:1028:HOH:O   | 2.21                     | 0.43              |
| 4:D:744:GLN:HE21 | 4:D:758:GLN:NE2  | 2.17                     | 0.43              |
| 4:D:39:LEU:HD12  | 4:D:39:LEU:HA    | 1.73                     | 0.43              |
| 4:D:439:MET:HE2  | 4:D:439:MET:HB3  | 1.94                     | 0.43              |
| 4:D:109:ILE:HD13 | 4:D:114:VAL:HG22 | 2.00                     | 0.43              |
| 4:D:180:LYS:O    | 4:D:184:GLN:HG3  | 2.18                     | 0.43              |
| 4:D:873:ARG:C    | 5:D:1018:HOH:O   | 2.55                     | 0.43              |
| 4:D:17:ALA:O     | 4:D:21:PHE:HB2   | 2.18                     | 0.43              |
| 4:D:137:VAL:C    | 4:D:141:ILE:HD12 | 2.44                     | 0.43              |
| 4:D:386:ARG:CG   | 5:D:933:HOH:O    | 2.34                     | 0.43              |
| 4:D:388:ASP:OD1  | 4:D:388:ASP:C    | 2.62                     | 0.43              |
| 4:D:647:ARG:C    | 5:D:958:HOH:O    | 2.62                     | 0.43              |
| 1:T:119:DT:H4'   | 5:T:139:HOH:O    | 2.15                     | 0.42              |
| 2:N:27:DC:C2'    | 2:N:28:DG:H5''   | 2.49                     | 0.42              |
| 4:D:468:ALA:C    | 5:D:952:HOH:O    | 2.61                     | 0.42              |
| 4:D:632:ARG:HE   | 4:D:632:ARG:HA   | 1.84                     | 0.42              |
| 4:D:204:TRP:O    | 4:D:205:HIS:CB   | 2.66                     | 0.42              |
| 4:D:439:MET:O    | 4:D:443:LEU:HD22 | 2.18                     | 0.42              |
| 4:D:579:ASN:O    | 4:D:583:GLN:HG2  | 2.18                     | 0.42              |
| 4:D:582:LEU:HB3  | 4:D:621:LEU:HD21 | 2.01                     | 0.42              |
| 4:D:612:GLY:O    | 4:D:615:ALA:N    | 2.52                     | 0.42              |
| 4:D:160:LYS:NZ   | 4:D:160:LYS:HA   | 2.34                     | 0.42              |
| 4:D:463:HIS:CB   | 4:D:534:LEU:HD22 | 2.48                     | 0.42              |
| 4:D:593:GLU:CG   | 4:D:594:VAL:N    | 2.82                     | 0.42              |
| 4:D:138:ALA:O    | 4:D:213:GLY:HA3  | 2.19                     | 0.42              |
| 4:D:302:LYS:HG2  | 4:D:303:LYS:N    | 2.35                     | 0.42              |
| 4:D:464:GLY:CA   | 5:D:1036:HOH:O   | 2.44                     | 0.42              |
| 4:D:70:ALA:C     | 4:D:74:ILE:HG12  | 2.43                     | 0.42              |
| 4:D:78:LEU:HA    | 4:D:119:ILE:HD11 | 2.02                     | 0.42              |
| 4:D:166:VAL:HG12 | 4:D:166:VAL:O    | 2.20                     | 0.42              |
| 4:D:398:LEU:C    | 4:D:398:LEU:HD23 | 2.45                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:575:ALA:O    | 4:D:578:VAL:HB   | 2.19                     | 0.42              |
| 4:D:616:LEU:C    | 4:D:618:GLY:N    | 2.77                     | 0.42              |
| 4:D:64:VAL:HG21  | 4:D:127:THR:OG1  | 2.20                     | 0.42              |
| 4:D:84:ARG:HB2   | 4:D:223:SER:HB3  | 2.00                     | 0.42              |
| 1:T:128:DC:H42   | 2:N:27:DC:N4     | 2.17                     | 0.42              |
| 2:N:16:DT:H2''   | 2:N:17:DA:O5'    | 2.20                     | 0.42              |
| 2:N:26:DA:H2''   | 2:N:27:DC:O5'    | 2.19                     | 0.42              |
| 4:D:224:THR:C    | 4:D:226:MET:H    | 2.27                     | 0.42              |
| 4:D:729:THR:OG1  | 4:D:733:PHE:HB3  | 2.20                     | 0.42              |
| 4:D:729:THR:HB   | 4:D:789:SER:HB2  | 2.02                     | 0.42              |
| 4:D:758:GLN:HA   | 4:D:759:PRO:HD3  | 1.85                     | 0.42              |
| 2:N:29:DG:H2''   | 2:N:30:DC:H5     | 1.85                     | 0.42              |
| 4:D:65:ALA:HB2   | 4:D:123:LEU:HD23 | 2.01                     | 0.42              |
| 4:D:446:LEU:HD13 | 4:D:806:SER:HB3  | 2.02                     | 0.42              |
| 4:D:611:LEU:HD22 | 4:D:615:ALA:CB   | 2.48                     | 0.42              |
| 4:D:698:TRP:HZ3  | 4:D:845:PHE:HD2  | 1.68                     | 0.42              |
| 4:D:828:VAL:HG21 | 4:D:883:ALA:HA   | 2.01                     | 0.42              |
| 4:D:63:GLU:O     | 4:D:66:ASP:HB2   | 2.19                     | 0.41              |
| 4:D:330:ILE:HD11 | 4:D:408:PHE:HB2  | 2.02                     | 0.41              |
| 4:D:41:HIS:CE1   | 4:D:45:GLU:OE2   | 2.72                     | 0.41              |
| 4:D:86:ASN:HD22  | 4:D:86:ASN:HA    | 1.69                     | 0.41              |
| 4:D:141:ILE:HG23 | 4:D:145:ILE:HD11 | 2.02                     | 0.41              |
| 4:D:157:LEU:HG   | 4:D:158:GLU:N    | 2.36                     | 0.41              |
| 4:D:221:ILE:HD13 | 4:D:221:ILE:H    | 1.85                     | 0.41              |
| 4:D:686:SER:C    | 5:D:972:HOH:O    | 2.64                     | 0.41              |
| 4:D:749:LEU:HD23 | 4:D:749:LEU:HA   | 1.89                     | 0.41              |
| 4:D:790:HIS:CD2  | 5:D:904:HOH:O    | 2.70                     | 0.41              |
| 4:D:869:ASN:N    | 5:D:893:HOH:O    | 2.15                     | 0.41              |
| 4:D:16:LEU:HD21  | 4:D:20:PRO:HB2   | 2.02                     | 0.41              |
| 4:D:560:ASN:HA   | 5:D:938:HOH:O    | 2.19                     | 0.41              |
| 4:D:690:VAL:HG22 | 5:D:972:HOH:O    | 2.20                     | 0.41              |
| 4:D:710:VAL:HG12 | 4:D:720:ARG:HB3  | 2.02                     | 0.41              |
| 4:D:561:LEU:HA   | 4:D:561:LEU:HD12 | 1.88                     | 0.41              |
| 4:D:655:ILE:C    | 4:D:657:PRO:HD2  | 2.46                     | 0.41              |
| 2:N:27:DC:H2''   | 2:N:28:DG:OP1    | 2.21                     | 0.41              |
| 4:D:162:PHE:C    | 4:D:164:LYS:N    | 2.79                     | 0.41              |
| 4:D:744:GLN:HB3  | 4:D:757:LEU:O    | 2.21                     | 0.41              |
| 1:T:127:DG:N7    | 5:T:134:HOH:O    | 2.50                     | 0.41              |
| 4:D:71:LYS:N     | 4:D:72:PRO:HD2   | 2.36                     | 0.41              |
| 4:D:333:LYS:HB3  | 4:D:516:PHE:CE1  | 2.56                     | 0.41              |
| 4:D:608:LYS:HG3  | 4:D:609:VAL:N    | 2.36                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:378:LYS:HD2  | 4:D:379:ARG:H    | 1.77                     | 0.41              |
| 4:D:550:LEU:HD11 | 4:D:695:ALA:HB2  | 2.02                     | 0.41              |
| 4:D:828:VAL:CG2  | 4:D:883:ALA:HA   | 2.50                     | 0.41              |
| 2:N:17:DA:H2'    | 4:D:173:ARG:NH2  | 2.35                     | 0.41              |
| 4:D:88:TRP:CZ2   | 4:D:215:ARG:HD3  | 2.55                     | 0.41              |
| 4:D:139:SER:O    | 4:D:143:ARG:HG2  | 2.20                     | 0.41              |
| 4:D:142:GLY:HA3  | 5:D:924:HOH:O    | 2.21                     | 0.41              |
| 4:D:161:HIS:CE1  | 4:D:165:ASN:HB2  | 2.55                     | 0.41              |
| 4:D:285:GLY:CA   | 5:D:928:HOH:O    | 2.35                     | 0.41              |
| 4:D:551:ARG:HA   | 4:D:551:ARG:HD3  | 1.84                     | 0.41              |
| 4:D:595:VAL:HG23 | 4:D:608:LYS:H    | 1.84                     | 0.41              |
| 4:D:622:ALA:O    | 4:D:666:MET:HG2  | 2.21                     | 0.41              |
| 4:D:360:LEU:CD2  | 5:D:917:HOH:O    | 2.31                     | 0.41              |
| 4:D:404:GLN:HA   | 4:D:404:GLN:NE2  | 2.36                     | 0.41              |
| 4:D:577:LYS:HD3  | 4:D:687:VAL:HG21 | 2.03                     | 0.41              |
| 4:D:605:ILE:O    | 4:D:606:SER:HB3  | 2.21                     | 0.41              |
| 4:D:857:GLN:NE2  | 4:D:859:ASP:HB2  | 2.34                     | 0.41              |
| 4:D:36:GLN:HE21  | 4:D:40:GLU:CG    | 2.34                     | 0.40              |
| 1:T:125:DG:H2''  | 1:T:124:DC:OP2   | 2.20                     | 0.40              |
| 4:D:330:ILE:CD1  | 4:D:330:ILE:H    | 2.34                     | 0.40              |
| 4:D:770:ASP:CG   | 4:D:773:LYS:HB2  | 2.46                     | 0.40              |
| 4:D:590:THR:CG2  | 4:D:591:ASP:N    | 2.83                     | 0.40              |
| 4:D:74:ILE:HB    | 5:D:1034:HOH:O   | 2.21                     | 0.40              |
| 4:D:647:ARG:CD   | 5:D:913:HOH:O    | 2.29                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles       |
|-----|-------|---------------|-----------|---------|----------|-------------------|
| 4   | D     | 560/883 (63%) | 489 (87%) | 49 (9%) | 22 (4%)  | <b>2</b> <b>0</b> |

All (22) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 16  | LEU  |
| 4   | D     | 353 | PRO  |
| 4   | D     | 588 | ASN  |
| 4   | D     | 592 | ASN  |
| 4   | D     | 655 | ILE  |
| 4   | D     | 852 | GLN  |
| 4   | D     | 854 | HIS  |
| 4   | D     | 855 | GLU  |
| 4   | D     | 358 | GLU  |
| 4   | D     | 404 | GLN  |
| 4   | D     | 595 | VAL  |
| 4   | D     | 602 | THR  |
| 4   | D     | 606 | SER  |
| 4   | D     | 767 | SER  |
| 4   | D     | 851 | ASP  |
| 4   | D     | 853 | LEU  |
| 4   | D     | 30  | GLU  |
| 4   | D     | 859 | ASP  |
| 4   | D     | 882 | PHE  |
| 4   | D     | 656 | GLN  |
| 4   | D     | 766 | ASP  |
| 4   | D     | 603 | GLY  |

### 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 |
|-----|-------|---------------|-----------|----------|-------------|
| 4   | D     | 711/729 (98%) | 650 (91%) | 61 (9%)  | 10 7        |

All (61) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 27  | HIS  |
| 4   | D     | 39  | LEU  |
| 4   | D     | 50  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 73  | LEU  |
| 4   | D     | 81  | MET  |
| 4   | D     | 91  | GLU  |
| 4   | D     | 107 | GLN  |
| 4   | D     | 109 | ILE  |
| 4   | D     | 112 | GLU  |
| 4   | D     | 122 | THR  |
| 4   | D     | 160 | LYS  |
| 4   | D     | 170 | LEU  |
| 4   | D     | 180 | LYS  |
| 4   | D     | 221 | ILE  |
| 4   | D     | 261 | LEU  |
| 4   | D     | 281 | ILE  |
| 4   | D     | 294 | LEU  |
| 4   | D     | 296 | LEU  |
| 4   | D     | 330 | ILE  |
| 4   | D     | 335 | LEU  |
| 4   | D     | 337 | VAL  |
| 4   | D     | 340 | VAL  |
| 4   | D     | 346 | HIS  |
| 4   | D     | 353 | PRO  |
| 4   | D     | 355 | ILE  |
| 4   | D     | 358 | GLU  |
| 4   | D     | 360 | LEU  |
| 4   | D     | 362 | MET  |
| 4   | D     | 378 | LYS  |
| 4   | D     | 391 | ARG  |
| 4   | D     | 392 | LYS  |
| 4   | D     | 402 | LEU  |
| 4   | D     | 407 | LYS  |
| 4   | D     | 440 | THR  |
| 4   | D     | 443 | LEU  |
| 4   | D     | 462 | ILE  |
| 4   | D     | 507 | SER  |
| 4   | D     | 514 | PHE  |
| 4   | D     | 561 | LEU  |
| 4   | D     | 577 | LYS  |
| 4   | D     | 587 | ILE  |
| 4   | D     | 616 | LEU  |
| 4   | D     | 631 | LYS  |
| 4   | D     | 648 | GLN  |
| 4   | D     | 652 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 666 | MET  |
| 4   | D     | 672 | GLN  |
| 4   | D     | 686 | SER  |
| 4   | D     | 741 | LYS  |
| 4   | D     | 743 | ILE  |
| 4   | D     | 754 | GLN  |
| 4   | D     | 757 | LEU  |
| 4   | D     | 765 | LYS  |
| 4   | D     | 783 | VAL  |
| 4   | D     | 787 | ASP  |
| 4   | D     | 805 | GLU  |
| 4   | D     | 816 | THR  |
| 4   | D     | 834 | ASP  |
| 4   | D     | 837 | GLU  |
| 4   | D     | 847 | ASP  |
| 4   | D     | 857 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 9   | ASN  |
| 4   | D     | 27  | HIS  |
| 4   | D     | 41  | HIS  |
| 4   | D     | 86  | ASN  |
| 4   | D     | 131 | ASN  |
| 4   | D     | 161 | HIS  |
| 4   | D     | 176 | HIS  |
| 4   | D     | 184 | GLN  |
| 4   | D     | 321 | ASN  |
| 4   | D     | 404 | GLN  |
| 4   | D     | 410 | ASN  |
| 4   | D     | 433 | ASN  |
| 4   | D     | 529 | ASN  |
| 4   | D     | 544 | GLN  |
| 4   | D     | 579 | ASN  |
| 4   | D     | 649 | GLN  |
| 4   | D     | 656 | GLN  |
| 4   | D     | 672 | GLN  |
| 4   | D     | 697 | ASN  |
| 4   | D     | 726 | HIS  |
| 4   | D     | 744 | GLN  |
| 4   | D     | 754 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 758 | GLN  |
| 4   | D     | 772 | HIS  |
| 4   | D     | 781 | ASN  |
| 4   | D     | 784 | HIS  |
| 4   | D     | 848 | GLN  |
| 4   | D     | 871 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed   | Backbone Outliers | Pucker Outliers |
|-----|-------|------------|-------------------|-----------------|
| 3   | R     | 9/10 (90%) | 1 (11%)           | 0               |

All (1) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | R     | 8   | C    |

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.