



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:08 am BST

PDB ID : 2JA8  
Title : CPD lesion containing RNA Polymerase II elongation complex D  
Authors : Brueckner, F.; Hennecke, U.; Carell, T.; Cramer, P.  
Deposited on : 2006-11-23  
Resolution : 3.80 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.

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

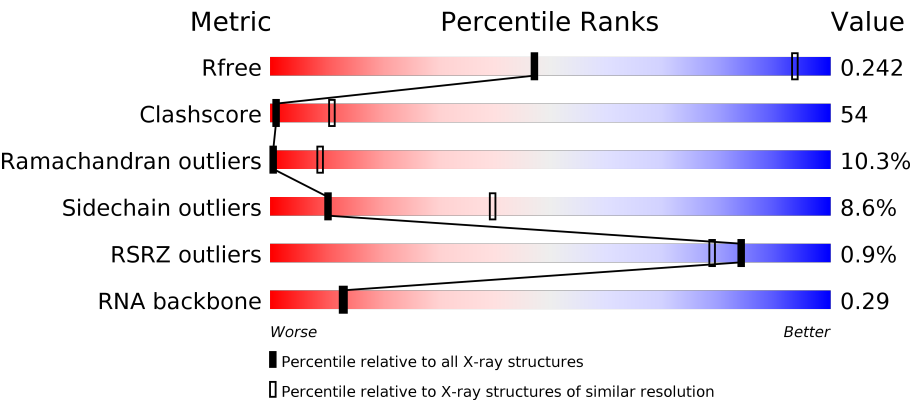
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1212 (4.00-3.60)                                      |
| Clashscore            | 141614                      | 1288 (4.00-3.60)                                      |
| Ramachandran outliers | 138981                      | 1243 (4.00-3.60)                                      |
| Sidechain outliers    | 138945                      | 1237 (4.00-3.60)                                      |
| RSRZ outliers         | 127900                      | 1121 (4.00-3.60)                                      |
| RNA backbone          | 3102                        | 1036 (4.60-3.00)                                      |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 1733   | <div><div>%</div><div><div></div><div>25%</div><div>46%</div><div>10%</div><div>•</div><div>18%</div></div></div> |
| 2   | B     | 1224   | <div><div>%</div><div><div></div><div>28%</div><div>52%</div><div>11%</div><div>9%</div></div></div>              |
| 3   | C     | 318    | <div><div></div><div><div></div><div>22%</div><div>51%</div><div>10%</div><div>•</div><div>16%</div></div></div>  |
| 4   | D     | 221    | <div><div>%</div><div><div></div><div>27%</div><div>40%</div><div>12%</div><div>•</div><div>20%</div></div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | E     | 215    |                  |
| 6   | F     | 155    |                  |
| 7   | G     | 171    |                  |
| 8   | H     | 146    |                  |
| 9   | I     | 122    |                  |
| 10  | J     | 70     |                  |
| 11  | K     | 120    |                  |
| 12  | L     | 70     |                  |
| 13  | N     | 14     |                  |
| 14  | P     | 11     |                  |
| 15  | T     | 25     |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 15  | TT   | T     | 19  | -         | -        | X       | -                |

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32000 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II LARGEST SUB-UNIT.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1421     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 11186 | 7048 | 1958 | 2118 | 62 |         |         |       |

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | B     | 1115     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8866  | 5614 | 1553 | 1644 | 55 |         |         |       |

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 267      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2101  | 1320 | 349 | 419 | 13 |         |         |       |

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1427  | 882 | 256 | 287 | 2 |         |         |       |

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 5   | E     | 214      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1752  | 1111 | 309 | 321 | 11 |         |         |       |

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 23

## KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 451 | 119 | 132 | 3 |         |         |       |

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | G     | 171      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1340  | 861 | 222 | 249 | 8 |         |         |       |

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1084  | 683 | 183 | 214 | 4 |         |         |       |

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 9   | I     | 116      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 944   | 581 | 172 | 181 | 10 |         |         |       |

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | J     | 65       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 532   | 339 | 93 | 94 | 6 |         |         |       |

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | K     | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 919   | 590 | 156 | 171 | 2 |         |         |       |

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | L     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 364   | 224 | 72 | 64 | 4 |         |         |       |

- Molecule 13 is a DNA chain called 5'-D(\*TP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 13  | N     | 8        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 161   | 79 | 29 | 46 | 7 |         |         |       |

- Molecule 14 is a RNA chain called 5'-R(\*UP\*UP\*CP\*GP\*AP\*CP\*CP\*AP\*GP\*AP\*UP)-3'.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 14  | P     | 10       | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 209   | 95 | 38 | 67 | 9 |         |         |       |

- Molecule 15 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*TP\*TP\*TTP\*CP\*BRUP\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'.

| Mol | Chain | Residues | Atoms |    |     |    |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|-----|----|-----|---------|---------|-------|
| 15  | T     | 19       | Total | Br | C   | N  | O   | P       | 0       | 0     |
|     |       |          | 401   | 1  | 197 | 61 | 124 | 18      |         |       |

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16  | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

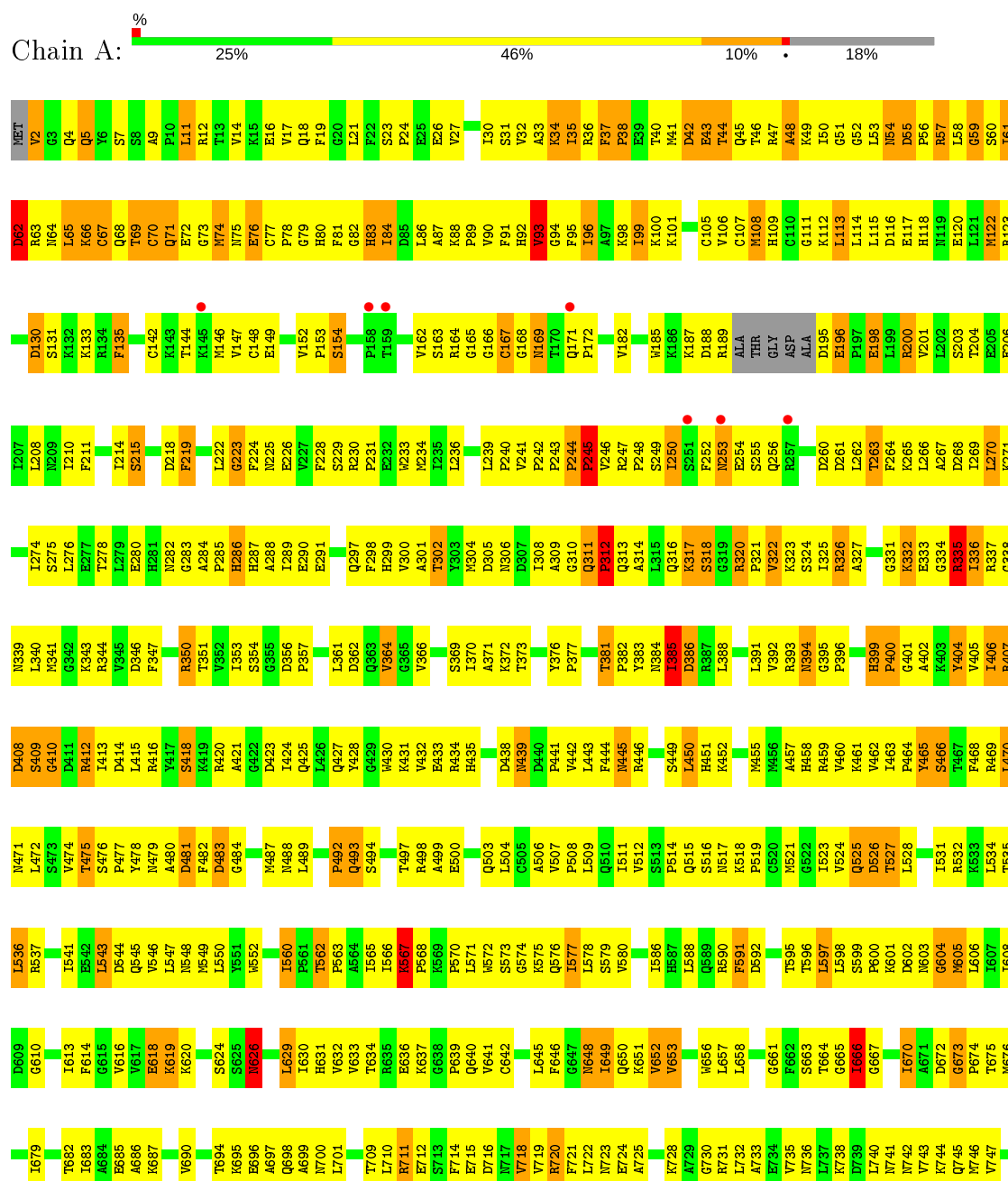
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 17  | A     | 8        | Total | Zn | 0       | 0       |
|     |       |          | 8     | 8  |         |         |

### 3 Residue-property plots

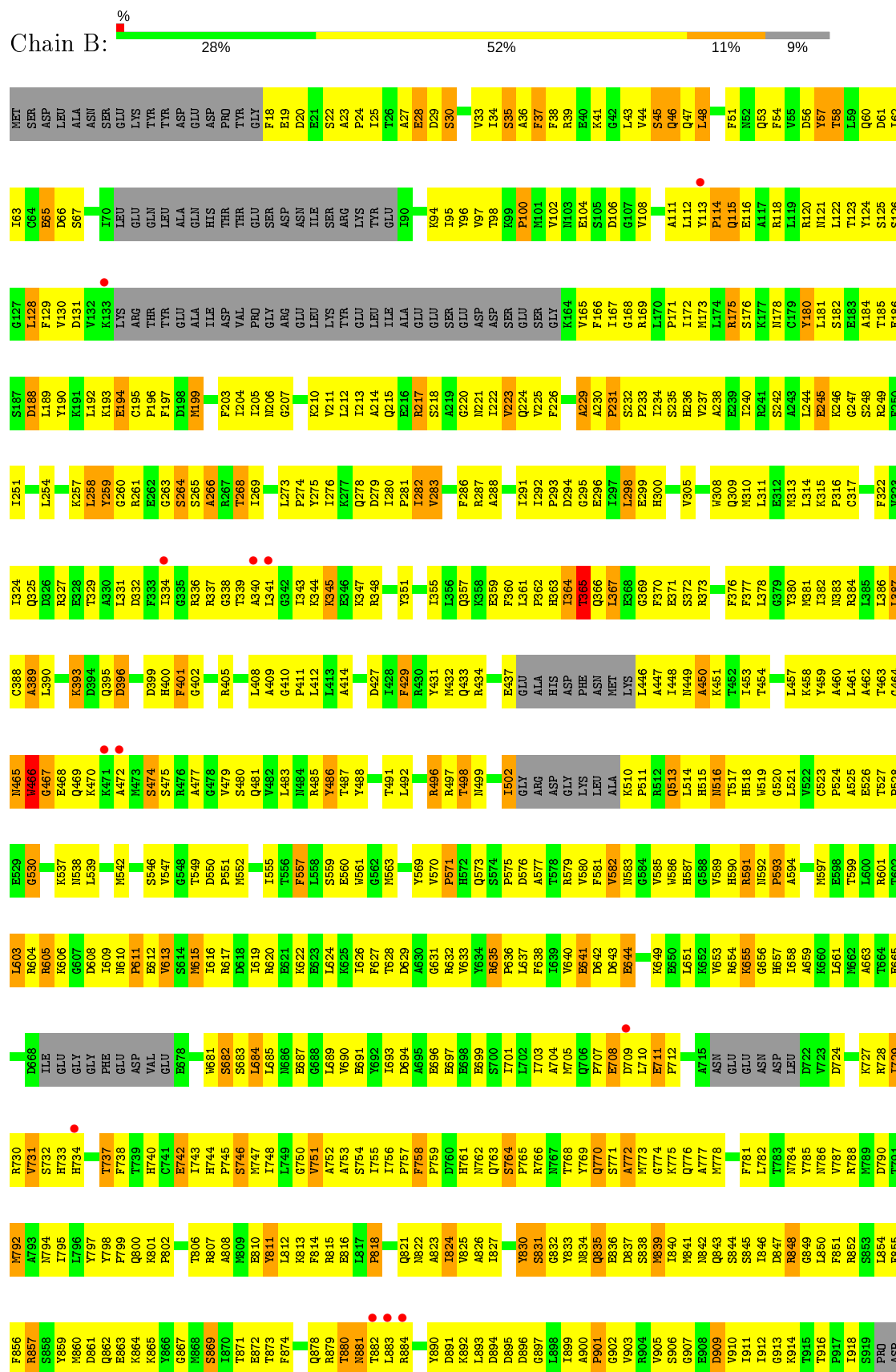
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

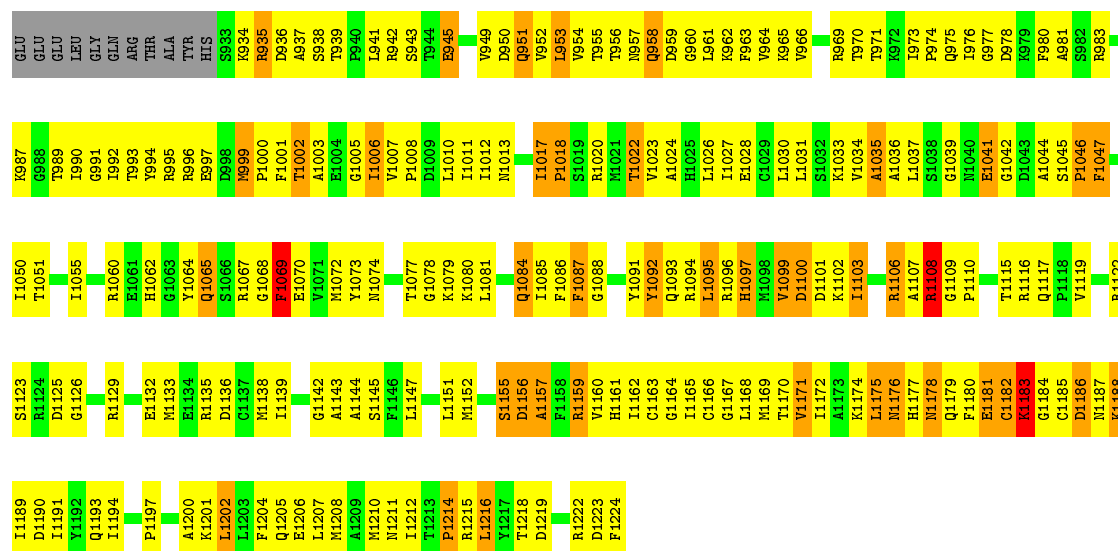
#### • Molecule 1: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT

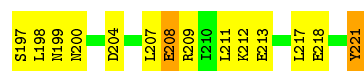


● Molecule 2: DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE

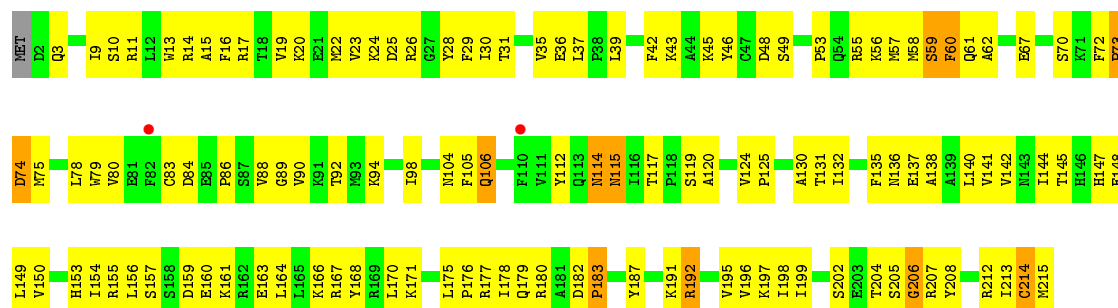




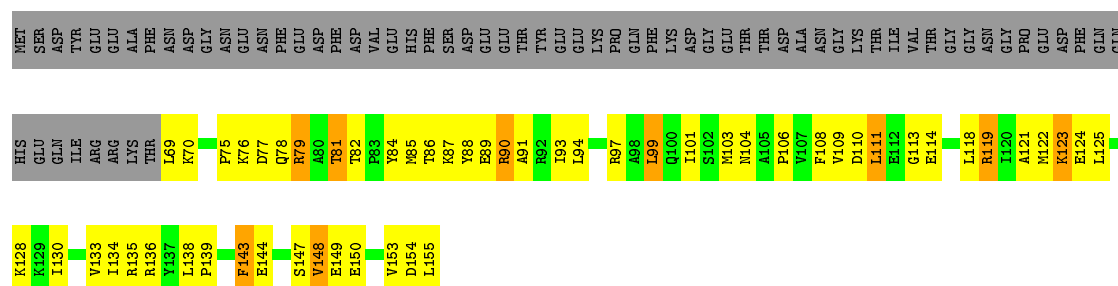
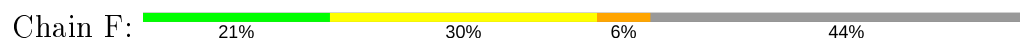




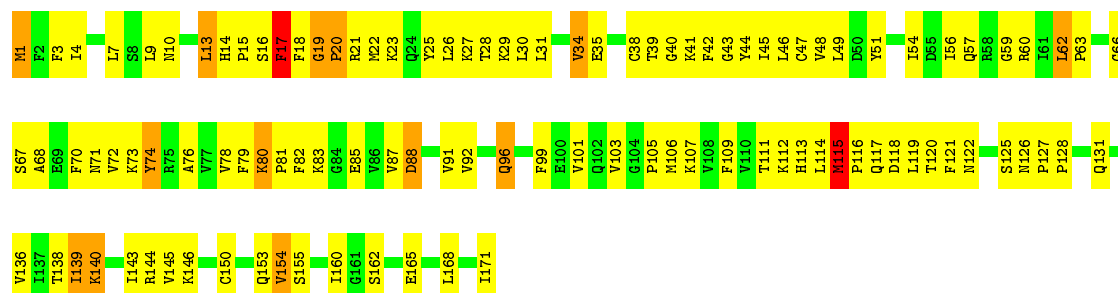
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE



- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III 23 KDA POLYPEPTIDE

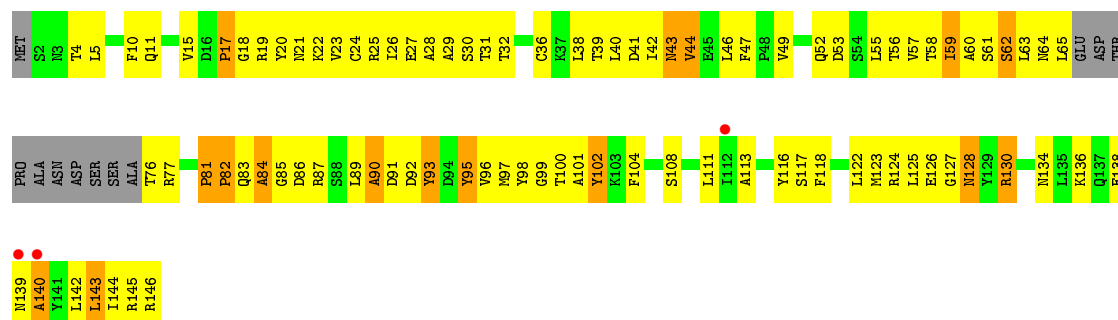


- Molecule 7: DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE

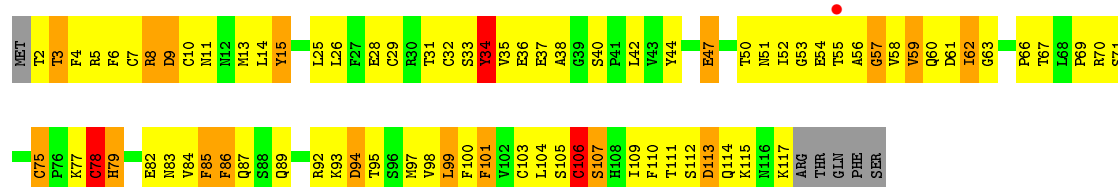


- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE

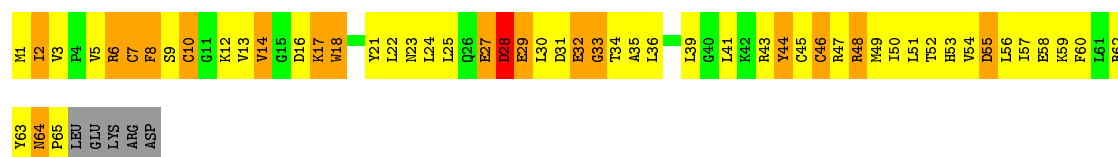
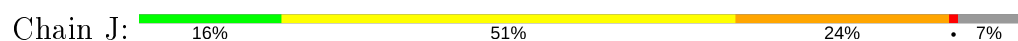




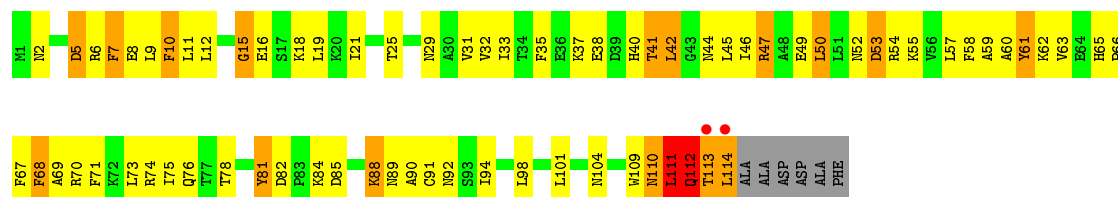
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9



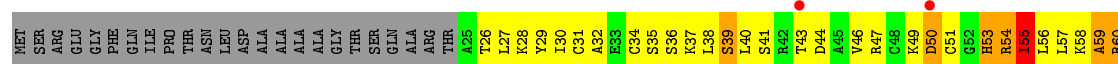
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10

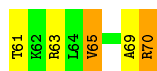


• Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE

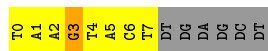
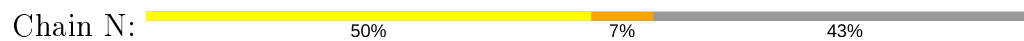


• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE

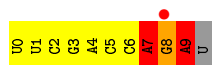




- Molecule 13: 5'-D(\*TP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*GP \*AP\*GP\*CP\*T)-3'



- Molecule 14: 5'-R(\*UP\*UP\*CP\*GP\*AP\*CP\*CP\*AP\*GP\*AP\*UP)-3'



- Molecule 15: 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP \*CP\*TP\*TP\*TP\*TP\*TTP\*CP \*BRUP\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 2 2 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 222.64Å 392.85Å 282.89Å<br>90.00° 90.00° 90.00°                               | Depositor        |
| Resolution (Å)  | 50.00 – 3.80<br>48.85 – 3.80  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.2 (50.00-3.80)<br>99.9 (48.85-3.80)  | Depositor<br>EDS |
| $R_{merge}$   | 0.08  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.30 (at 3.77Å)   | Xtriage          |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.269 , 0.288<br>0.210 , 0.242  | Depositor<br>DCC |
| $R_{free}$ test set   | 4685 reflections (1.99%)  | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 110.0   | Xtriage          |
| Anisotropy  | 0.478   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 70.5   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$                   | Xtriage          |
| Estimated twinning fraction   | 0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l<br>0.023 for 1/2*h+1/2*k,3/2*h-1/2*k,-l | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 32000   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 95.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 0.46         | 0/11385        | 0.73        | 1/15393 (0.0%)  |
| 2   | B     | 0.45         | 0/9037         | 0.71        | 2/12181 (0.0%)  |
| 3   | C     | 0.48         | 0/2138         | 0.71        | 0/2896          |
| 4   | D     | 0.42         | 0/1437         | 0.67        | 0/1925          |
| 5   | E     | 0.43         | 1/1788 (0.1%)  | 0.62        | 0/2406          |
| 6   | F     | 0.53         | 0/716          | 0.77        | 0/964           |
| 7   | G     | 0.49         | 0/1368         | 0.73        | 0/1844          |
| 8   | H     | 0.38         | 0/1102         | 0.65        | 0/1492          |
| 9   | I     | 0.39         | 0/962          | 0.68        | 0/1295          |
| 10  | J     | 0.48         | 0/541          | 0.80        | 0/727           |
| 11  | K     | 0.67         | 3/937 (0.3%)   | 0.86        | 4/1265 (0.3%)   |
| 12  | L     | 0.41         | 0/366          | 0.68        | 0/485           |
| 13  | N     | 1.21         | 1/180 (0.6%)   | 1.08        | 0/276           |
| 14  | P     | 0.85         | 0/233          | 1.41        | 2/361 (0.6%)    |
| 15  | T     | 1.12         | 2/380 (0.5%)   | 1.39        | 3/580 (0.5%)    |
| All | All   | 0.49         | 7/32570 (0.0%) | 0.74        | 12/44090 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 1                   |
| 15  | T     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 11  | K     | 113 | THR  | N-CA  | 5.90 | 1.58        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11  | K     | 113 | THR  | CA-C  | 5.73  | 1.67        | 1.52     |
| 15  | T     | 12  | DT   | N1-C2 | 5.38  | 1.42        | 1.38     |
| 5   | E     | 214 | CYS  | CB-SG | -5.28 | 1.73        | 1.81     |
| 11  | K     | 114 | LEU  | N-CA  | 5.10  | 1.56        | 1.46     |
| 15  | T     | 14  | DC   | N1-C2 | 5.10  | 1.45        | 1.40     |
| 13  | N     | 3   | DG   | N9-C4 | 5.03  | 1.42        | 1.38     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | K     | 113  | THR  | N-CA-C      | 9.56  | 136.81      | 111.00   |
| 15  | T     | 24   | DG   | O4'-C1'-N9  | 7.22  | 113.06      | 108.00   |
| 15  | T     | 21   | DC   | O5'-P-OP1   | 7.09  | 119.21      | 110.70   |
| 14  | P     | 9    | A    | C2'-C3'-O3' | 7.01  | 124.92      | 109.50   |
| 14  | P     | 7    | A    | N9-C1'-C2'  | -6.77 | 104.56      | 112.00   |
| 11  | K     | 111  | LEU  | N-CA-C      | 6.32  | 128.07      | 111.00   |
| 11  | K     | 114  | LEU  | N-CA-C      | 5.93  | 127.00      | 111.00   |
| 2   | B     | 111  | ALA  | N-CA-C      | -5.85 | 95.21       | 111.00   |
| 11  | K     | 113  | THR  | C-N-CA      | 5.83  | 136.26      | 121.70   |
| 15  | T     | 10   | DA   | OP2-P-O3'   | 5.60  | 117.52      | 105.20   |
| 2   | B     | 1185 | CYS  | N-CA-C      | -5.06 | 97.34       | 111.00   |
| 1   | A     | 567  | LYS  | C-N-CD      | 5.02  | 138.93      | 128.40   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | B     | 486 | TYR  | Sidechain |
| 15  | T     | 13  | 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   | A     | 11186 | 0        | 11266    | 1310    | 0            |
| 2   | B     | 8866  | 0        | 8898     | 1015    | 0            |
| 3   | C     | 2101  | 0        | 2055     | 265     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | D     | 1427  | 0        | 1451     | 139     | 0            |
| 5   | E     | 1752  | 0        | 1776     | 134     | 0            |
| 6   | F     | 705   | 0        | 730      | 89      | 0            |
| 7   | G     | 1340  | 0        | 1357     | 173     | 0            |
| 8   | H     | 1084  | 0        | 1057     | 127     | 0            |
| 9   | I     | 944   | 0        | 900      | 110     | 0            |
| 10  | J     | 532   | 0        | 542      | 99      | 0            |
| 11  | K     | 919   | 0        | 929      | 107     | 0            |
| 12  | L     | 364   | 0        | 386      | 47      | 0            |
| 13  | N     | 161   | 0        | 93       | 17      | 0            |
| 14  | P     | 209   | 0        | 109      | 28      | 0            |
| 15  | T     | 401   | 0        | 231      | 64      | 0            |
| 16  | A     | 1     | 0        | 0        | 0       | 0            |
| 17  | A     | 8     | 0        | 0        | 0       | 0            |
| All | All   | 32000 | 0        | 31780    | 3425    | 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 54.

All (3425) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:53:LEU:HD23  | 1:A:54:ASN:N      | 1.61                     | 1.13              |
| 1:A:855:THR:HG21 | 1:A:857:ARG:HE    | 1.10                     | 1.11              |
| 7:G:14:HIS:CD2   | 7:G:16:SER:HB2    | 1.87                     | 1.10              |
| 15:T:19:TT:C1'   | 15:T:19:TT:H5R1   | 1.83                     | 1.09              |
| 1:A:1445:ILE:H   | 1:A:1445:ILE:HD12 | 1.16                     | 1.09              |
| 15:T:17:DT:H2''  | 15:T:18:DT:H5'    | 1.32                     | 1.08              |
| 2:B:343:ILE:HG23 | 2:B:347:LYS:HB2   | 1.16                     | 1.08              |
| 2:B:273:LEU:HB2  | 2:B:276:ILE:HD12  | 1.36                     | 1.08              |
| 15:T:19:TT:H5R1  | 15:T:19:TT:H1'    | 1.23                     | 1.07              |
| 5:E:22:MET:HE3   | 5:E:26:ARG:HH21   | 1.15                     | 1.07              |
| 2:B:336:ARG:HG2  | 2:B:348:ARG:HD3   | 1.31                     | 1.07              |
| 7:G:138:THR:HG22 | 7:G:139:ILE:H     | 1.20                     | 1.07              |
| 15:T:17:DT:C2'   | 15:T:18:DT:H5'    | 1.83                     | 1.06              |
| 1:A:34:LYS:HD3   | 1:A:57:ARG:HH22   | 0.92                     | 1.04              |
| 4:D:40:HIS:HB3   | 7:G:73:LYS:HZ3    | 1.16                     | 1.04              |
| 11:K:47:ARG:HB3  | 11:K:47:ARG:HH11  | 1.17                     | 1.03              |
| 2:B:882:THR:HG22 | 2:B:884:ARG:H     | 1.20                     | 1.03              |
| 1:A:40:THR:HG22  | 1:A:41:MET:HG3    | 1.39                     | 1.03              |
| 1:A:913:LEU:HD12 | 1:A:914:GLU:H     | 1.24                     | 1.02              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:58:LEU:HD12   | 1:A:59:GLY:H      | 1.23                     | 1.01              |
| 1:A:53:LEU:HD23   | 1:A:54:ASN:H      | 0.84                     | 1.01              |
| 2:B:589:VAL:HG12  | 2:B:590:HIS:H     | 1.24                     | 1.01              |
| 1:A:1402:PHE:CE1  | 1:A:1403:GLU:HG3  | 1.94                     | 1.01              |
| 10:J:5:VAL:HG12   | 10:J:6:ARG:HG3    | 1.42                     | 1.01              |
| 11:K:111:LEU:C    | 11:K:112:GLN:HG2  | 1.76                     | 1.01              |
| 1:A:868:TYR:CE1   | 1:A:1064:VAL:HG11 | 1.96                     | 1.00              |
| 3:C:166:GLU:HG3   | 11:K:10:PHE:HZ    | 1.27                     | 1.00              |
| 7:G:13:LEU:HD21   | 7:G:17:PHE:HB2    | 1.38                     | 1.00              |
| 1:A:34:LYS:HD3    | 1:A:57:ARG:NH2    | 1.77                     | 1.00              |
| 1:A:1017:LEU:HB2  | 5:E:206:GLY:H     | 1.25                     | 0.99              |
| 1:A:567:LYS:CG    | 1:A:568:PRO:HD2   | 1.91                     | 0.98              |
| 1:A:53:LEU:CD2    | 1:A:54:ASN:H      | 1.74                     | 0.98              |
| 2:B:65:GLU:HG3    | 2:B:66:ASP:H      | 1.27                     | 0.98              |
| 3:C:57:VAL:HG11   | 10:J:60:PHE:HB3   | 1.43                     | 0.98              |
| 3:C:43:THR:HG22   | 3:C:44:LEU:H      | 1.29                     | 0.97              |
| 10:J:3:VAL:HG21   | 10:J:18:TRP:HB2   | 1.45                     | 0.97              |
| 2:B:214:ALA:HB3   | 2:B:498:THR:HA    | 1.46                     | 0.97              |
| 2:B:510:LYS:CG    | 2:B:511:PRO:HD3   | 1.94                     | 0.96              |
| 10:J:1:MET:N      | 10:J:57:ILE:H     | 1.63                     | 0.96              |
| 2:B:1187:ASN:O    | 2:B:1188:LYS:HB2  | 1.65                     | 0.96              |
| 2:B:806:THR:HG22  | 2:B:808:ALA:H     | 1.29                     | 0.96              |
| 1:A:709:THR:HG23  | 9:I:94:ASP:HA     | 1.46                     | 0.96              |
| 1:A:590:ARG:HH21  | 1:A:620:LYS:HB3   | 1.31                     | 0.96              |
| 1:A:590:ARG:NH2   | 1:A:620:LYS:HB3   | 1.80                     | 0.96              |
| 15:T:19:TT:H1'    | 15:T:19:TT:C5R    | 1.96                     | 0.96              |
| 1:A:225:ASN:HD22  | 1:A:228:PHE:H     | 1.03                     | 0.95              |
| 15:T:18:DT:C2'    | 15:T:19:TT:H5'1   | 1.94                     | 0.95              |
| 1:A:1394:THR:HG21 | 1:A:1398:MET:SD   | 2.06                     | 0.95              |
| 2:B:516:ASN:N     | 2:B:516:ASN:HD22  | 1.64                     | 0.94              |
| 5:E:94:LYS:HE2    | 5:E:98:ILE:HD11   | 1.48                     | 0.94              |
| 4:D:144:THR:O     | 4:D:148:LEU:HB2   | 1.67                     | 0.94              |
| 2:B:217:ARG:HE    | 2:B:405:ARG:HB2   | 1.28                     | 0.94              |
| 2:B:502:ILE:HD12  | 2:B:502:ILE:H     | 1.31                     | 0.94              |
| 1:A:567:LYS:HB3   | 8:H:96:VAL:H      | 1.33                     | 0.94              |
| 15:T:17:DT:H2''   | 15:T:18:DT:C5'    | 1.97                     | 0.94              |
| 9:I:8:ARG:HG3     | 9:I:34:TYR:HE1    | 1.30                     | 0.94              |
| 1:A:34:LYS:HE3    | 1:A:57:ARG:HH12   | 1.30                     | 0.94              |
| 2:B:168:GLY:H     | 2:B:450:ALA:HB1   | 1.32                     | 0.94              |
| 11:K:110:ASN:O    | 11:K:111:LEU:HD23 | 1.68                     | 0.94              |
| 2:B:1201:LYS:HE2  | 2:B:1205:GLN:OE1  | 1.65                     | 0.93              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:486:TYR:OH    | 2:B:1096:ARG:HB3 | 1.66                     | 0.93              |
| 15:T:19:TT:H5M1   | 15:T:21:DC:C5    | 2.03                     | 0.93              |
| 1:A:58:LEU:HD21   | 1:A:243:PRO:HA   | 1.47                     | 0.93              |
| 10:J:1:MET:H1     | 10:J:57:ILE:N    | 1.66                     | 0.93              |
| 11:K:65:HIS:HD2   | 11:K:67:PHE:H    | 1.10                     | 0.93              |
| 1:A:58:LEU:CD1    | 1:A:59:GLY:H     | 1.82                     | 0.93              |
| 1:A:34:LYS:CD     | 1:A:57:ARG:HH22  | 1.82                     | 0.93              |
| 1:A:754:SER:H     | 1:A:757:ASN:HD22 | 1.11                     | 0.93              |
| 2:B:336:ARG:HH22  | 2:B:345:LYS:HE2  | 1.33                     | 0.92              |
| 10:J:48:ARG:HE    | 10:J:49:MET:HE2  | 1.31                     | 0.92              |
| 15:T:17:DT:C1'    | 15:T:18:DT:H5'   | 1.99                     | 0.92              |
| 2:B:232:SER:HB3   | 2:B:261:ARG:HH21 | 1.32                     | 0.92              |
| 3:C:66:ARG:NH1    | 10:J:2:ILE:HG21  | 1.82                     | 0.92              |
| 3:C:6:PRO:HB3     | 3:C:25:VAL:HG12  | 1.50                     | 0.92              |
| 1:A:524:VAL:HG12  | 1:A:525:GLN:H    | 1.32                     | 0.92              |
| 3:C:6:PRO:HB3     | 3:C:25:VAL:CG1   | 1.99                     | 0.92              |
| 1:A:254:GLU:HB2   | 2:B:935:ARG:HH12 | 1.34                     | 0.92              |
| 2:B:515:HIS:H     | 2:B:518:HIS:HD2  | 1.16                     | 0.92              |
| 6:F:111:LEU:HD12  | 6:F:111:LEU:H    | 1.35                     | 0.91              |
| 1:A:563:PRO:HG3   | 1:A:572:TRP:CZ2  | 2.05                     | 0.91              |
| 14:P:5:C:H2'      | 14:P:6:C:O4'     | 1.70                     | 0.91              |
| 7:G:15:PRO:HA     | 7:G:18:PHE:CD1   | 2.04                     | 0.91              |
| 1:A:399:HIS:HB3   | 1:A:400:PRO:HD3  | 1.51                     | 0.91              |
| 8:H:4:THR:HA      | 8:H:60:ALA:HB2   | 1.53                     | 0.91              |
| 2:B:577:ALA:HB1   | 2:B:589:VAL:HG11 | 1.53                     | 0.91              |
| 6:F:93:ILE:HD11   | 6:F:134:ILE:HD11 | 1.53                     | 0.91              |
| 9:I:85:PHE:H      | 9:I:85:PHE:HD2   | 1.18                     | 0.91              |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:H   | 1.36                     | 0.91              |
| 4:D:40:HIS:HB3    | 7:G:73:LYS:NZ    | 1.84                     | 0.90              |
| 1:A:1420:ASP:HB3  | 1:A:1422:ARG:HG3 | 1.53                     | 0.90              |
| 8:H:100:THR:HG23  | 8:H:138:GLU:HA   | 1.49                     | 0.90              |
| 1:A:382:PRO:HB3   | 1:A:428:TYR:HE2  | 1.34                     | 0.90              |
| 1:A:285:PRO:HG2   | 1:A:288:ALA:HB3  | 1.52                     | 0.90              |
| 15:T:22:BRU:H2'   | 15:T:23:DG:C8    | 2.07                     | 0.90              |
| 1:A:1094:VAL:HG12 | 1:A:1095:THR:H   | 1.34                     | 0.90              |
| 8:H:84:ALA:HA     | 8:H:87:ARG:HB2   | 1.53                     | 0.90              |
| 1:A:855:THR:HG21  | 1:A:857:ARG:NE   | 1.86                     | 0.90              |
| 1:A:567:LYS:CD    | 1:A:568:PRO:HD2  | 2.02                     | 0.89              |
| 2:B:549:THR:HG22  | 2:B:550:ASP:H    | 1.36                     | 0.89              |
| 1:A:836:TYR:CD2   | 1:A:840:ARG:HD2  | 2.08                     | 0.89              |
| 15:T:17:DT:H1'    | 15:T:18:DT:H5'   | 1.53                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:T:19:TT:H2'1   | 15:T:19:TT:H2R2   | 1.55                     | 0.89              |
| 1:A:779:PHE:HE1   | 1:A:785:PRO:HD3   | 1.38                     | 0.89              |
| 15:T:19:TT:C2'    | 15:T:19:TT:H5R1   | 2.02                     | 0.88              |
| 15:T:15:DT:H1'    | 15:T:16:DT:H5'    | 1.53                     | 0.88              |
| 2:B:1072:MET:CE   | 2:B:1085:ILE:HB   | 2.03                     | 0.88              |
| 2:B:661:LEU:HD11  | 2:B:684:LEU:HD11  | 1.56                     | 0.88              |
| 1:A:901:LEU:H     | 1:A:926:GLN:NE2   | 1.71                     | 0.88              |
| 2:B:842:ASN:ND2   | 2:B:845:SER:H     | 1.72                     | 0.88              |
| 1:A:783:THR:HG21  | 1:A:815:PHE:CZ    | 2.08                     | 0.88              |
| 2:B:824:ILE:HG22  | 2:B:1087:PHE:HE2  | 1.35                     | 0.88              |
| 2:B:393:LYS:HA    | 2:B:393:LYS:HE3   | 1.56                     | 0.88              |
| 1:A:534:LEU:O     | 1:A:574:GLY:HA3   | 1.74                     | 0.87              |
| 1:A:768:GLN:HG2   | 1:A:816:HIS:HA    | 1.54                     | 0.87              |
| 1:A:58:LEU:HD11   | 1:A:243:PRO:HB3   | 1.56                     | 0.87              |
| 2:B:1002:THR:HG21 | 2:B:1006:ILE:HD12 | 1.55                     | 0.87              |
| 1:A:93:VAL:HG13   | 1:A:301:ALA:HB1   | 1.55                     | 0.86              |
| 2:B:364:ILE:HG12  | 2:B:585:VAL:HG13  | 1.57                     | 0.86              |
| 9:I:26:LEU:HD23   | 9:I:37:GLU:HA     | 1.56                     | 0.86              |
| 1:A:323:LYS:HZ3   | 14:P:1:U:H4'      | 1.39                     | 0.86              |
| 2:B:942:ARG:HH22  | 15:T:25:DT:P      | 1.98                     | 0.86              |
| 2:B:800:GLN:HB3   | 10:J:52:THR:HG21  | 1.56                     | 0.86              |
| 2:B:510:LYS:HG2   | 2:B:511:PRO:HD3   | 1.58                     | 0.86              |
| 3:C:43:THR:HG22   | 3:C:44:LEU:N      | 1.89                     | 0.86              |
| 1:A:70:CYS:O      | 1:A:72:GLU:HG2    | 1.75                     | 0.85              |
| 1:A:828:ALA:CB    | 2:B:530:GLY:HA2   | 2.06                     | 0.85              |
| 1:A:646:PHE:O     | 1:A:650:GLN:HG3   | 1.76                     | 0.85              |
| 2:B:343:ILE:HG21  | 2:B:348:ARG:HG3   | 1.58                     | 0.85              |
| 5:E:19:VAL:O      | 5:E:23:VAL:HG23   | 1.76                     | 0.85              |
| 9:I:8:ARG:HG3     | 9:I:34:TYR:CE1    | 2.11                     | 0.85              |
| 2:B:770:GLN:OE1   | 2:B:983:ARG:HA    | 1.76                     | 0.85              |
| 6:F:86:THR:OG1    | 6:F:89:GLU:HG3    | 1.77                     | 0.85              |
| 8:H:40:LEU:HD13   | 8:H:123:MET:HB2   | 1.59                     | 0.85              |
| 9:I:115:LYS:HD3   | 9:I:117:LYS:HE3   | 1.57                     | 0.85              |
| 2:B:343:ILE:CG2   | 2:B:348:ARG:HG3   | 2.05                     | 0.85              |
| 3:C:47:ASP:HA     | 12:L:69:ALA:HB3   | 1.58                     | 0.85              |
| 11:K:21:ILE:HG12  | 11:K:33:ILE:HG12  | 1.57                     | 0.85              |
| 2:B:172:ILE:HD13  | 2:B:178:ASN:HB3   | 1.59                     | 0.85              |
| 1:A:320:ARG:HH22  | 14:P:1:U:H1'      | 1.40                     | 0.85              |
| 1:A:321:PRO:O     | 1:A:322:VAL:HB    | 1.76                     | 0.84              |
| 2:B:46:GLN:HG3    | 2:B:47:GLN:H      | 1.41                     | 0.84              |
| 11:K:65:HIS:CD2   | 11:K:67:PHE:H     | 1.94                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:34:VAL:HG12   | 7:G:45:ILE:HG21   | 1.59                     | 0.84              |
| 1:A:225:ASN:ND2   | 1:A:228:PHE:H     | 1.76                     | 0.84              |
| 1:A:855:THR:CG2   | 1:A:857:ARG:HE    | 1.90                     | 0.84              |
| 2:B:847:ASP:HB3   | 3:C:167:HIS:NE2   | 1.92                     | 0.84              |
| 1:A:535:THR:HG21  | 1:A:616:VAL:HA    | 1.60                     | 0.84              |
| 2:B:343:ILE:HG21  | 2:B:348:ARG:N     | 1.92                     | 0.84              |
| 1:A:567:LYS:HD2   | 1:A:568:PRO:HD2   | 1.59                     | 0.84              |
| 14:P:6:C:H2'      | 14:P:7:A:C8       | 2.12                     | 0.84              |
| 2:B:98:THR:O      | 2:B:126:SER:HB2   | 1.78                     | 0.84              |
| 6:F:69:LEU:HA     | 6:F:70:LYS:N      | 1.91                     | 0.84              |
| 1:A:1424:VAL:HG13 | 1:A:1436:ILE:HD11 | 1.60                     | 0.83              |
| 3:C:32:SER:O      | 3:C:36:VAL:HG23   | 1.78                     | 0.83              |
| 1:A:215:SER:HB3   | 1:A:218:ASP:OD2   | 1.77                     | 0.83              |
| 1:A:853:ASP:OD1   | 1:A:855:THR:HB    | 1.77                     | 0.83              |
| 1:A:1094:VAL:HG12 | 1:A:1095:THR:N    | 1.93                     | 0.83              |
| 1:A:340:LEU:HD13  | 1:A:1429:ILE:HG23 | 1.59                     | 0.83              |
| 1:A:58:LEU:HD12   | 1:A:59:GLY:N      | 1.94                     | 0.83              |
| 1:A:913:LEU:HD12  | 1:A:914:GLU:N     | 1.94                     | 0.83              |
| 1:A:1325:THR:O    | 5:E:148:GLU:HB2   | 1.79                     | 0.83              |
| 1:A:741:ASN:HD22  | 1:A:744:LYS:H     | 1.27                     | 0.82              |
| 7:G:7:LEU:HB2     | 7:G:74:TYR:CE2    | 2.14                     | 0.82              |
| 1:A:709:THR:HG22  | 1:A:711:ARG:H     | 1.44                     | 0.82              |
| 2:B:642:ASP:HA    | 2:B:649:LYS:HA    | 1.59                     | 0.82              |
| 2:B:363:HIS:O     | 2:B:364:ILE:HB    | 1.76                     | 0.82              |
| 1:A:903:ASN:HD22  | 1:A:904:THR:N     | 1.77                     | 0.82              |
| 1:A:84:ILE:HD11   | 1:A:270:LEU:HD13  | 1.60                     | 0.82              |
| 1:A:590:ARG:HG3   | 1:A:590:ARG:NH1   | 1.94                     | 0.82              |
| 8:H:59:ILE:HG22   | 8:H:60:ALA:N      | 1.93                     | 0.82              |
| 9:I:34:TYR:CD2    | 9:I:35:VAL:N      | 2.48                     | 0.82              |
| 1:A:472:LEU:O     | 1:A:475:THR:HB    | 1.79                     | 0.82              |
| 2:B:955:THR:HG22  | 2:B:956:THR:H     | 1.44                     | 0.82              |
| 1:A:1100:ARG:HH21 | 1:A:1351:GLU:HG2  | 1.44                     | 0.81              |
| 9:I:105:SER:O     | 9:I:106:CYS:HB3   | 1.77                     | 0.81              |
| 1:A:779:PHE:CE1   | 1:A:785:PRO:HD3   | 2.15                     | 0.81              |
| 2:B:365:THR:HG23  | 2:B:367:LEU:H     | 1.45                     | 0.81              |
| 4:D:47:LEU:HD11   | 7:G:3:PHE:CD2     | 2.14                     | 0.81              |
| 11:K:47:ARG:NH1   | 11:K:47:ARG:HB3   | 1.96                     | 0.81              |
| 2:B:336:ARG:HD3   | 2:B:348:ARG:HH11  | 1.46                     | 0.81              |
| 2:B:521:LEU:HD22  | 2:B:633:VAL:HG12  | 1.62                     | 0.81              |
| 7:G:80:LYS:HD3    | 7:G:80:LYS:H      | 1.45                     | 0.81              |
| 7:G:80:LYS:HD3    | 7:G:80:LYS:N      | 1.96                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:T:18:DT:C3'    | 15:T:19:TT:H4'    | 2.11                     | 0.81              |
| 1:A:1004:ASN:ND2  | 5:E:167:ARG:HD2   | 1.96                     | 0.81              |
| 7:G:128:PRO:O     | 7:G:138:THR:HG23  | 1.81                     | 0.81              |
| 1:A:356:ASP:HB2   | 1:A:469:ARG:NH1   | 1.96                     | 0.81              |
| 1:A:49:LYS:HE2    | 1:A:61:ILE:HD12   | 1.62                     | 0.81              |
| 2:B:1007:VAL:HG22 | 2:B:1008:PRO:HD2  | 1.63                     | 0.81              |
| 2:B:879:ARG:HH11  | 2:B:883:LEU:HD22  | 1.44                     | 0.81              |
| 15:T:18:DT:H2''   | 15:T:19:TT:C5'    | 2.11                     | 0.81              |
| 5:E:16:PHE:CZ     | 5:E:20:LYS:HE2    | 2.16                     | 0.80              |
| 10:J:7:CYS:HB2    | 10:J:46:CYS:HB3   | 1.63                     | 0.80              |
| 15:T:18:DT:H2'    | 15:T:19:TT:H5'1   | 1.62                     | 0.80              |
| 1:A:427:GLN:HG3   | 1:A:430:TRP:CZ2   | 2.16                     | 0.80              |
| 1:A:743:VAL:O     | 1:A:747:VAL:HG23  | 1.82                     | 0.80              |
| 5:E:192:ARG:HG3   | 5:E:192:ARG:HH11  | 1.45                     | 0.80              |
| 3:C:244:VAL:O     | 3:C:248:ILE:HG13  | 1.82                     | 0.80              |
| 2:B:189:LEU:O     | 2:B:192:LEU:N     | 2.14                     | 0.80              |
| 2:B:467:GLY:H     | 2:B:475:SER:HB3   | 1.46                     | 0.80              |
| 1:A:1116:LEU:N    | 1:A:1308:THR:HG22 | 1.97                     | 0.80              |
| 10:J:64:ASN:HB3   | 10:J:65:PRO:HD3   | 1.64                     | 0.80              |
| 4:D:22:GLU:H      | 4:D:22:GLU:CD     | 1.85                     | 0.80              |
| 9:I:34:TYR:HD2    | 9:I:35:VAL:N      | 1.80                     | 0.80              |
| 1:A:767:GLN:NE2   | 1:A:774:ARG:HB3   | 1.96                     | 0.79              |
| 5:E:22:MET:HE3    | 5:E:26:ARG:NH2    | 1.96                     | 0.79              |
| 10:J:64:ASN:HB3   | 10:J:65:PRO:CD    | 2.12                     | 0.79              |
| 15:T:18:DT:H2''   | 15:T:19:TT:O5'    | 1.82                     | 0.79              |
| 10:J:8:PHE:H      | 10:J:49:MET:HE1   | 1.46                     | 0.79              |
| 1:A:107:CYS:SG    | 1:A:171:GLN:HG2   | 2.21                     | 0.79              |
| 1:A:821:ARG:HB2   | 1:A:821:ARG:HH11  | 1.45                     | 0.79              |
| 1:A:886:ILE:HG22  | 1:A:887:GLY:N     | 1.96                     | 0.79              |
| 2:B:483:LEU:HD11  | 2:B:491:THR:HG23  | 1.63                     | 0.79              |
| 15:T:18:DT:C2'    | 15:T:19:TT:C5'    | 2.60                     | 0.79              |
| 2:B:171:PRO:HD2   | 2:B:457:LEU:HD13  | 1.62                     | 0.79              |
| 2:B:467:GLY:N     | 2:B:475:SER:HB3   | 1.98                     | 0.79              |
| 1:A:567:LYS:HE3   | 8:H:46:LEU:HB2    | 1.64                     | 0.79              |
| 1:A:768:GLN:CG    | 1:A:816:HIS:HA    | 2.12                     | 0.79              |
| 8:H:81:PRO:HB2    | 8:H:82:PRO:HD2    | 1.65                     | 0.79              |
| 1:A:590:ARG:HG3   | 1:A:590:ARG:HH11  | 1.47                     | 0.79              |
| 2:B:1096:ARG:O    | 2:B:1097:HIS:HB2  | 1.82                     | 0.79              |
| 2:B:244:LEU:HD21  | 2:B:366:GLN:NE2   | 1.97                     | 0.79              |
| 2:B:112:LEU:HD12  | 2:B:113:TYR:H     | 1.48                     | 0.79              |
| 2:B:1202:LEU:O    | 2:B:1206:GLU:HG3  | 1.82                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:34:TYR:HE2    | 9:I:36:GLU:HB3    | 1.48                     | 0.79              |
| 1:A:1030:ARG:HG3  | 1:A:1034:GLU:OE2  | 1.83                     | 0.78              |
| 1:A:963:ILE:HD11  | 1:A:1048:ASN:HB3  | 1.63                     | 0.78              |
| 1:A:1312:ASN:O    | 1:A:1316:VAL:HG23 | 1.83                     | 0.78              |
| 1:A:567:LYS:HB3   | 8:H:95:TYR:HA     | 1.64                     | 0.78              |
| 1:A:1206:ASP:HB3  | 1:A:1274:ARG:HH12 | 1.47                     | 0.78              |
| 1:A:63:ARG:HA     | 1:A:74:MET:SD     | 2.24                     | 0.78              |
| 1:A:93:VAL:HG22   | 1:A:301:ALA:HA    | 1.66                     | 0.78              |
| 2:B:613:VAL:HG13  | 2:B:627:PHE:O     | 1.83                     | 0.78              |
| 3:C:147:LEU:HB2   | 3:C:151:GLN:HB2   | 1.65                     | 0.78              |
| 2:B:580:VAL:HG22  | 2:B:624:LEU:HB3   | 1.66                     | 0.78              |
| 2:B:758:PHE:CE2   | 2:B:1044:ALA:HA   | 2.18                     | 0.78              |
| 3:C:174:ALA:HB2   | 3:C:235:VAL:HG22  | 1.65                     | 0.78              |
| 1:A:34:LYS:CE     | 1:A:57:ARG:HH12   | 1.95                     | 0.78              |
| 4:D:153:ARG:NH2   | 4:D:184:ALA:HA    | 1.99                     | 0.78              |
| 8:H:59:ILE:HG22   | 8:H:60:ALA:H      | 1.48                     | 0.78              |
| 2:B:169:ARG:HB2   | 2:B:454:THR:HG23  | 1.66                     | 0.78              |
| 5:E:213:ILE:HG12  | 5:E:214:CYS:H     | 1.48                     | 0.78              |
| 1:A:346:ASP:HB3   | 2:B:1108:ARG:H    | 1.49                     | 0.78              |
| 2:B:882:THR:HG22  | 2:B:884:ARG:N     | 1.99                     | 0.78              |
| 3:C:35:ARG:NH1    | 11:K:41:THR:H     | 1.80                     | 0.78              |
| 7:G:111:THR:HG22  | 7:G:113:HIS:H     | 1.49                     | 0.78              |
| 9:I:55:THR:HG21   | 9:I:109:ILE:HD13  | 1.66                     | 0.78              |
| 1:A:1028:THR:O    | 1:A:1032:LEU:HD12 | 1.84                     | 0.78              |
| 2:B:654:ARG:H     | 2:B:657:HIS:HD2   | 1.28                     | 0.78              |
| 1:A:1341:ILE:HD12 | 1:A:1379:GLY:O    | 1.84                     | 0.77              |
| 1:A:351:THR:HG22  | 2:B:1103:ILE:HA   | 1.64                     | 0.77              |
| 8:H:17:PRO:HB3    | 8:H:24:CYS:SG     | 2.24                     | 0.77              |
| 12:L:53:HIS:HB3   | 12:L:55:ILE:HD11  | 1.66                     | 0.77              |
| 1:A:528:LEU:O     | 1:A:531:ILE:HG22  | 1.84                     | 0.77              |
| 1:A:14:VAL:HG21   | 2:B:1216:LEU:HD13 | 1.66                     | 0.77              |
| 1:A:596:THR:O     | 1:A:598:LEU:N     | 2.18                     | 0.77              |
| 1:A:308:ILE:HG22  | 1:A:309:ALA:H     | 1.48                     | 0.77              |
| 2:B:1095:LEU:HD12 | 2:B:1095:LEU:H    | 1.49                     | 0.77              |
| 2:B:65:GLU:HG3    | 2:B:66:ASP:N      | 1.97                     | 0.77              |
| 2:B:1224:PHE:HE2  | 5:E:171:LYS:HG3   | 1.49                     | 0.77              |
| 6:F:82:THR:HG22   | 6:F:84:TYR:H      | 1.49                     | 0.77              |
| 1:A:49:LYS:NZ     | 1:A:61:ILE:HG13   | 2.00                     | 0.77              |
| 1:A:794:PRO:HG2   | 1:A:795:GLU:OE2   | 1.85                     | 0.77              |
| 1:A:1036:ARG:HH11 | 1:A:1036:ARG:HG2  | 1.49                     | 0.77              |
| 1:A:567:LYS:HG3   | 1:A:568:PRO:HD2   | 1.66                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:906:SER:O     | 2:B:941:LEU:HD23  | 1.85                     | 0.77              |
| 1:A:866:PHE:C     | 1:A:867:ILE:HD12  | 2.05                     | 0.77              |
| 12:L:32:ALA:HB3   | 12:L:55:ILE:HD12  | 1.67                     | 0.77              |
| 1:A:836:TYR:CD1   | 15:T:18:DT:H5''   | 2.19                     | 0.77              |
| 1:A:903:ASN:ND2   | 1:A:905:ASP:H     | 1.83                     | 0.77              |
| 7:G:138:THR:HG22  | 7:G:139:ILE:N     | 1.99                     | 0.77              |
| 13:N:5:DA:H1'     | 13:N:6:DC:O5'     | 1.85                     | 0.77              |
| 1:A:269:ILE:HD13  | 1:A:300:VAL:HG22  | 1.67                     | 0.76              |
| 1:A:323:LYS:NZ    | 14:P:1:U:H4'      | 1.99                     | 0.76              |
| 2:B:340:ALA:HB2   | 2:B:343:ILE:HD12  | 1.67                     | 0.76              |
| 2:B:737:THR:HG21  | 9:I:66:PRO:HA     | 1.67                     | 0.76              |
| 4:D:40:HIS:CE1    | 4:D:41:GLN:HG3    | 2.21                     | 0.76              |
| 14:P:9:A:N1       | 15:T:19:TT:O4T    | 2.17                     | 0.76              |
| 1:A:868:TYR:HD2   | 1:A:1058:VAL:HG21 | 1.48                     | 0.76              |
| 2:B:778:MET:CE    | 2:B:1094:ARG:HD3  | 2.16                     | 0.76              |
| 2:B:821:GLN:HE22  | 2:B:851:PHE:HA    | 1.50                     | 0.76              |
| 4:D:47:LEU:HD13   | 4:D:48:ILE:H      | 1.49                     | 0.76              |
| 8:H:61:SER:O      | 8:H:62:SER:HB3    | 1.85                     | 0.76              |
| 1:A:466:SER:O     | 2:B:1103:ILE:HD11 | 1.85                     | 0.76              |
| 2:B:859:TYR:OH    | 2:B:941:LEU:HD12  | 1.85                     | 0.76              |
| 1:A:106:VAL:HG13  | 1:A:112:LYS:O     | 1.85                     | 0.76              |
| 1:A:21:LEU:HD11   | 1:A:1414:ALA:HA   | 1.68                     | 0.76              |
| 2:B:114:PRO:HG2   | 2:B:115:GLN:H     | 1.51                     | 0.76              |
| 13:N:3:DG:H1'     | 13:N:4:DT:H5'     | 1.68                     | 0.76              |
| 1:A:1171:GLN:HA   | 1:A:1174:PHE:CE1  | 2.21                     | 0.76              |
| 1:A:1372:VAL:O    | 1:A:1376:THR:HG22 | 1.84                     | 0.76              |
| 2:B:217:ARG:NE    | 2:B:405:ARG:HB2   | 2.01                     | 0.76              |
| 2:B:44:VAL:HG11   | 2:B:199:MET:HG2   | 1.66                     | 0.76              |
| 3:C:213:PRO:O     | 3:C:214:ASN:HB2   | 1.84                     | 0.76              |
| 1:A:1332:PHE:H    | 1:A:1332:PHE:HD2  | 1.32                     | 0.76              |
| 3:C:73:GLN:HE21   | 3:C:75:MET:N      | 1.84                     | 0.76              |
| 8:H:36:CYS:HA     | 8:H:126:GLU:O     | 1.84                     | 0.76              |
| 1:A:16:GLU:HB3    | 1:A:1418:LEU:HD11 | 1.66                     | 0.75              |
| 1:A:982:THR:HB    | 1:A:985:ASP:H     | 1.49                     | 0.75              |
| 1:A:868:TYR:HE1   | 1:A:1064:VAL:HG11 | 1.48                     | 0.75              |
| 2:B:708:GLU:O     | 2:B:710:LEU:N     | 2.20                     | 0.75              |
| 6:F:90:ARG:HD3    | 6:F:155:LEU:HD11  | 1.67                     | 0.75              |
| 1:A:986:ILE:HG22  | 1:A:987:VAL:N     | 2.00                     | 0.75              |
| 2:B:1162:ILE:HD11 | 2:B:1194:ILE:HD13 | 1.68                     | 0.75              |
| 2:B:510:LYS:HG3   | 2:B:511:PRO:HD3   | 1.67                     | 0.75              |
| 1:A:1329:THR:HG22 | 1:A:1331:SER:H    | 1.51                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:657:LEU:HD12  | 1:A:657:LEU:O     | 1.86                     | 0.75              |
| 1:A:885:THR:O     | 1:A:940:ARG:HD2   | 1.87                     | 0.75              |
| 1:A:666:ILE:HD12  | 1:A:667:GLY:H     | 1.51                     | 0.75              |
| 1:A:1424:VAL:HG13 | 1:A:1436:ILE:CD1  | 2.16                     | 0.75              |
| 1:A:230:ARG:H     | 1:A:233:TRP:HE3   | 1.35                     | 0.75              |
| 1:A:351:THR:HB    | 2:B:1103:ILE:HD12 | 1.69                     | 0.75              |
| 1:A:385:ILE:HG22  | 1:A:386:ASP:N     | 2.01                     | 0.75              |
| 1:A:512:VAL:HA    | 1:A:519:PRO:HA    | 1.68                     | 0.75              |
| 1:A:852:TYR:CD2   | 1:A:1060:PRO:HB2  | 2.22                     | 0.75              |
| 3:C:73:GLN:HE21   | 3:C:75:MET:H      | 1.31                     | 0.75              |
| 2:B:361:LEU:HD21  | 2:B:377:PHE:CD2   | 2.21                     | 0.75              |
| 2:B:516:ASN:ND2   | 2:B:516:ASN:N     | 2.35                     | 0.75              |
| 2:B:637:LEU:HD12  | 2:B:693:ILE:HD12  | 1.69                     | 0.75              |
| 11:K:12:LEU:HD12  | 11:K:12:LEU:H     | 1.50                     | 0.75              |
| 1:A:855:THR:HG23  | 1:A:857:ARG:HG3   | 1.68                     | 0.75              |
| 4:D:47:LEU:HD11   | 7:G:3:PHE:HD2     | 1.50                     | 0.75              |
| 1:A:87:ALA:CB     | 1:A:276:LEU:HD23  | 2.17                     | 0.74              |
| 1:A:92:HIS:O      | 1:A:94:GLY:N      | 2.20                     | 0.74              |
| 2:B:701:ILE:HD11  | 2:B:703:ILE:HD11  | 1.67                     | 0.74              |
| 7:G:81:PRO:HG3    | 7:G:106:MET:SD    | 2.26                     | 0.74              |
| 11:K:47:ARG:HH11  | 11:K:47:ARG:CB    | 1.98                     | 0.74              |
| 1:A:1387:HIS:CE1  | 13:N:4:DT:H4'     | 2.21                     | 0.74              |
| 7:G:39:THR:HG22   | 7:G:41:LYS:H      | 1.52                     | 0.74              |
| 1:A:1063:MET:SD   | 1:A:1436:ILE:HG12 | 2.28                     | 0.74              |
| 1:A:1100:ARG:HH21 | 1:A:1351:GLU:CG   | 2.00                     | 0.74              |
| 1:A:335:ARG:HA    | 1:A:339:ASN:HB2   | 1.68                     | 0.74              |
| 1:A:754:SER:H     | 1:A:757:ASN:ND2   | 1.86                     | 0.74              |
| 2:B:830:TYR:O     | 2:B:832:GLY:N     | 2.20                     | 0.74              |
| 3:C:212:PRO:HB3   | 3:C:213:PRO:HD2   | 1.69                     | 0.74              |
| 7:G:59:GLY:HA3    | 7:G:70:PHE:CD2    | 2.23                     | 0.74              |
| 2:B:189:LEU:HA    | 2:B:192:LEU:HD12  | 1.68                     | 0.74              |
| 2:B:434:ARG:O     | 2:B:437:GLU:HB2   | 1.86                     | 0.74              |
| 2:B:515:HIS:HD2   | 2:B:517:THR:H     | 1.35                     | 0.74              |
| 2:B:526:GLU:HG2   | 2:B:538:ASN:HD22  | 1.52                     | 0.74              |
| 12:L:30:ILE:O     | 12:L:56:LEU:HA    | 1.87                     | 0.74              |
| 1:A:567:LYS:HD3   | 8:H:95:TYR:CG     | 2.23                     | 0.74              |
| 2:B:549:THR:H     | 2:B:628:THR:HG23  | 1.52                     | 0.74              |
| 3:C:43:THR:CG2    | 3:C:44:LEU:H      | 2.01                     | 0.74              |
| 5:E:157:SER:OG    | 5:E:160:GLU:HG3   | 1.87                     | 0.74              |
| 1:A:858:ASN:HD22  | 1:A:858:ASN:C     | 1.91                     | 0.74              |
| 2:B:1034:VAL:HG12 | 2:B:1035:ALA:N    | 2.03                     | 0.74              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:899:ILE:HD11 | 2:B:911:ILE:HA    | 1.70                     | 0.74              |
| 1:A:798:GLY:HA2  | 1:A:815:PHE:CD1   | 2.22                     | 0.73              |
| 7:G:14:HIS:ND1   | 7:G:15:PRO:HD2    | 2.03                     | 0.73              |
| 1:A:1189:SER:O   | 1:A:1241:ARG:HD3  | 1.87                     | 0.73              |
| 1:A:353:ILE:HG21 | 1:A:487:MET:HG3   | 1.69                     | 0.73              |
| 2:B:1180:PHE:HB3 | 2:B:1191:ILE:HD12 | 1.68                     | 0.73              |
| 12:L:38:LEU:O    | 12:L:39:SER:HB3   | 1.88                     | 0.73              |
| 2:B:332:ASP:O    | 2:B:336:ARG:HG3   | 1.86                     | 0.73              |
| 4:D:153:ARG:HB3  | 4:D:154:PHE:CE1   | 2.23                     | 0.73              |
| 7:G:39:THR:HG22  | 7:G:40:GLY:H      | 1.54                     | 0.73              |
| 1:A:35:ILE:O     | 1:A:35:ILE:HG22   | 1.89                     | 0.73              |
| 1:A:63:ARG:HA    | 1:A:74:MET:CE     | 2.19                     | 0.73              |
| 7:G:14:HIS:HD2   | 7:G:16:SER:HB2    | 1.49                     | 0.73              |
| 3:C:166:GLU:HG3  | 11:K:10:PHE:CZ    | 2.18                     | 0.73              |
| 1:A:384:ASN:OD1  | 1:A:388:LEU:HD12  | 1.89                     | 0.73              |
| 1:A:53:LEU:HD22  | 1:A:54:ASN:HD22   | 1.54                     | 0.73              |
| 2:B:1072:MET:HE1 | 2:B:1085:ILE:HB   | 1.68                     | 0.73              |
| 4:D:66:ARG:HD2   | 4:D:133:THR:HB    | 1.71                     | 0.73              |
| 1:A:254:GLU:HB2  | 2:B:935:ARG:NH1   | 2.03                     | 0.73              |
| 2:B:232:SER:HB3  | 2:B:261:ARG:NH2   | 2.04                     | 0.73              |
| 1:A:249:SER:O    | 1:A:250:ILE:HG13  | 1.87                     | 0.73              |
| 1:A:567:LYS:HB3  | 8:H:96:VAL:N      | 2.03                     | 0.73              |
| 1:A:547:LEU:HD22 | 11:K:58:PHE:CD1   | 2.24                     | 0.72              |
| 3:C:47:ASP:HA    | 12:L:69:ALA:CB    | 2.19                     | 0.72              |
| 1:A:845:LEU:HB3  | 1:A:848:ILE:HD12  | 1.71                     | 0.72              |
| 2:B:589:VAL:HG12 | 2:B:590:HIS:N     | 2.03                     | 0.72              |
| 4:D:130:LEU:O    | 4:D:132:GLN:N     | 2.21                     | 0.72              |
| 3:C:167:HIS:HD2  | 3:C:168:ALA:N     | 1.85                     | 0.72              |
| 9:I:7:CYS:HB3    | 9:I:14:LEU:HD21   | 1.71                     | 0.72              |
| 1:A:337:ARG:HD3  | 2:B:1132:GLU:OE1  | 1.89                     | 0.72              |
| 1:A:67:CYS:O     | 1:A:70:CYS:HB3    | 1.89                     | 0.72              |
| 2:B:778:MET:HE3  | 2:B:1094:ARG:HD3  | 1.71                     | 0.72              |
| 3:C:174:ALA:HB2  | 3:C:235:VAL:CG2   | 2.19                     | 0.72              |
| 1:A:51:GLY:HA2   | 1:A:56:PRO:HA     | 1.70                     | 0.72              |
| 2:B:336:ARG:NH2  | 2:B:345:LYS:HG2   | 2.05                     | 0.72              |
| 2:B:879:ARG:NH1  | 2:B:883:LEU:HD22  | 2.03                     | 0.72              |
| 6:F:103:MET:HE2  | 7:G:66:GLY:H      | 1.54                     | 0.72              |
| 9:I:111:THR:HG22 | 9:I:112:SER:N     | 2.04                     | 0.72              |
| 5:E:124:VAL:HG13 | 5:E:132:ILE:HB    | 1.71                     | 0.72              |
| 1:A:115:LEU:O    | 1:A:122:MET:HE2   | 1.90                     | 0.72              |
| 1:A:62:ASP:HB3   | 1:A:64:ASN:ND2    | 2.05                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1138:MET:HA   | 2:B:1138:MET:HE3  | 1.72                     | 0.72              |
| 2:B:343:ILE:CG2   | 2:B:347:LYS:HB2   | 2.07                     | 0.72              |
| 2:B:569:TYR:CE1   | 2:B:589:VAL:HG21  | 2.24                     | 0.72              |
| 2:B:800:GLN:HB3   | 10:J:52:THR:CG2   | 2.19                     | 0.72              |
| 4:D:29:LEU:HD22   | 7:G:82:PHE:CE2    | 2.25                     | 0.72              |
| 1:A:537:ARG:HD2   | 8:H:20:TYR:HE1    | 1.55                     | 0.72              |
| 2:B:622:LYS:HE2   | 9:I:59:VAL:HG22   | 1.71                     | 0.72              |
| 1:A:58:LEU:HD13   | 1:A:80:HIS:O      | 1.90                     | 0.72              |
| 2:B:1197:PRO:HG2  | 2:B:1200:ALA:HB2  | 1.72                     | 0.72              |
| 2:B:336:ARG:CG    | 2:B:348:ARG:HD3   | 2.15                     | 0.72              |
| 2:B:999:MET:HG3   | 2:B:1000:PRO:HD2  | 1.71                     | 0.72              |
| 15:T:24:DG:H2''   | 15:T:25:DT:O5'    | 1.89                     | 0.72              |
| 2:B:1087:PHE:HD2  | 2:B:1088:GLY:N    | 1.86                     | 0.72              |
| 1:A:993:LEU:HD22  | 1:A:1046:LEU:HD22 | 1.71                     | 0.71              |
| 10:J:1:MET:H1     | 10:J:57:ILE:H     | 0.80                     | 0.71              |
| 1:A:567:LYS:HD3   | 8:H:95:TYR:CD2    | 2.24                     | 0.71              |
| 4:D:134:THR:HG22  | 4:D:136:GLY:H     | 1.55                     | 0.71              |
| 5:E:180:ARG:HH21  | 5:E:192:ARG:HB2   | 1.54                     | 0.71              |
| 1:A:858:ASN:ND2   | 1:A:860:LEU:H     | 1.88                     | 0.71              |
| 1:A:325:ILE:HG21  | 2:B:1210:MET:HG3  | 1.72                     | 0.71              |
| 2:B:516:ASN:H     | 2:B:516:ASN:HD22  | 1.37                     | 0.71              |
| 14:P:5:C:O2'      | 14:P:6:C:H5'      | 1.91                     | 0.71              |
| 1:A:1015:VAL:HG12 | 1:A:1019:CYS:SG   | 2.31                     | 0.71              |
| 1:A:1171:GLN:HA   | 1:A:1174:PHE:CD1  | 2.26                     | 0.71              |
| 2:B:815:ARG:HD3   | 2:B:1041:GLU:OE2  | 1.91                     | 0.71              |
| 4:D:176:GLU:C     | 4:D:178:ALA:H     | 1.94                     | 0.71              |
| 13:N:6:DC:H2''    | 13:N:7:DT:OP2     | 1.89                     | 0.71              |
| 15:T:19:TT:C2'    | 15:T:19:TT:H2R2   | 2.19                     | 0.71              |
| 2:B:336:ARG:HH22  | 2:B:345:LYS:CE    | 2.03                     | 0.71              |
| 2:B:310:MET:HE3   | 2:B:387:LEU:HD12  | 1.70                     | 0.71              |
| 3:C:39:ALA:HA     | 3:C:164:ALA:HB3   | 1.72                     | 0.71              |
| 2:B:336:ARG:HD3   | 2:B:348:ARG:NH1   | 2.05                     | 0.71              |
| 2:B:226:PHE:HA    | 2:B:395:GLN:HG3   | 1.73                     | 0.71              |
| 2:B:515:HIS:H     | 2:B:518:HIS:CD2   | 2.04                     | 0.71              |
| 2:B:35:SER:HA     | 2:B:811:TYR:HE2   | 1.56                     | 0.71              |
| 3:C:208:GLU:O     | 3:C:210:GLU:N     | 2.24                     | 0.71              |
| 8:H:56:THR:HB     | 8:H:145:ARG:HG2   | 1.72                     | 0.71              |
| 1:A:960:ILE:O     | 1:A:963:ILE:HG22  | 1.89                     | 0.71              |
| 2:B:839:MET:HE3   | 2:B:1010:LEU:HD21 | 1.72                     | 0.71              |
| 1:A:254:GLU:CB    | 2:B:935:ARG:HH12  | 2.04                     | 0.71              |
| 3:C:67:LEU:HD11   | 3:C:155:LEU:CD1   | 2.20                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:807:ARG:HG2   | 2:B:1045:SER:OG   | 1.89                     | 0.71              |
| 5:E:135:PHE:HD2   | 5:E:140:LEU:HD21  | 1.54                     | 0.71              |
| 1:A:1341:ILE:HG23 | 1:A:1342:GLU:N    | 2.05                     | 0.71              |
| 1:A:382:PRO:HB3   | 1:A:428:TYR:CE2   | 2.23                     | 0.71              |
| 10:J:43:ARG:HG3   | 10:J:45:CYS:SG    | 2.30                     | 0.71              |
| 10:J:64:ASN:HD22  | 10:J:65:PRO:HD3   | 1.55                     | 0.71              |
| 2:B:955:THR:HG22  | 2:B:956:THR:N     | 2.05                     | 0.71              |
| 2:B:953:LEU:CD2   | 2:B:965:LYS:HB2   | 2.20                     | 0.71              |
| 3:C:186:LEU:HD21  | 3:C:224:GLN:O     | 1.90                     | 0.71              |
| 3:C:35:ARG:NH1    | 11:K:41:THR:N     | 2.38                     | 0.71              |
| 1:A:1348:LEU:HG   | 1:A:1372:VAL:CG2  | 2.21                     | 0.70              |
| 1:A:1437:GLY:O    | 1:A:1439:GLY:N    | 2.23                     | 0.70              |
| 1:A:326:ARG:HH22  | 1:A:1407:GLU:HG3  | 1.53                     | 0.70              |
| 1:A:69:THR:O      | 1:A:71:GLN:N      | 2.23                     | 0.70              |
| 4:D:134:THR:HG22  | 4:D:135:GLY:N     | 2.06                     | 0.70              |
| 1:A:541:ILE:HD13  | 1:A:549:MET:CE    | 2.21                     | 0.70              |
| 2:B:280:ILE:HD13  | 2:B:334:ILE:HG12  | 1.71                     | 0.70              |
| 2:B:359:GLU:O     | 2:B:362:PRO:HD3   | 1.92                     | 0.70              |
| 1:A:546:VAL:O     | 1:A:550:LEU:HG    | 1.92                     | 0.70              |
| 1:A:901:LEU:HG    | 1:A:926:GLN:HE21  | 1.55                     | 0.70              |
| 4:D:130:LEU:C     | 4:D:132:GLN:H     | 1.94                     | 0.70              |
| 5:E:117:THR:HG22  | 5:E:119:SER:H     | 1.56                     | 0.70              |
| 9:I:111:THR:HG22  | 9:I:112:SER:H     | 1.56                     | 0.70              |
| 1:A:567:LYS:CB    | 8:H:95:TYR:HA     | 2.21                     | 0.70              |
| 1:A:741:ASN:HD21  | 1:A:743:VAL:HB    | 1.55                     | 0.70              |
| 3:C:226:ASP:O     | 3:C:227:THR:HB    | 1.90                     | 0.70              |
| 8:H:40:LEU:CD1    | 8:H:123:MET:HB2   | 2.22                     | 0.70              |
| 15:T:18:DT:O3'    | 15:T:19:TT:H4'    | 1.90                     | 0.70              |
| 1:A:34:LYS:HB2    | 1:A:36:ARG:HH21   | 1.57                     | 0.70              |
| 2:B:1172:ILE:O    | 2:B:1172:ILE:HG22 | 1.90                     | 0.70              |
| 1:A:18:GLN:HB2    | 2:B:1215:ARG:HB2  | 1.73                     | 0.70              |
| 7:G:39:THR:HG22   | 7:G:40:GLY:N      | 2.06                     | 0.70              |
| 1:A:58:LEU:HD11   | 1:A:243:PRO:CB    | 2.21                     | 0.70              |
| 1:A:55:ASP:N      | 1:A:56:PRO:HD3    | 2.04                     | 0.70              |
| 2:B:615:MET:C     | 2:B:616:ILE:HD12  | 2.12                     | 0.70              |
| 10:J:7:CYS:CB     | 10:J:46:CYS:HB3   | 2.21                     | 0.70              |
| 1:A:963:ILE:HD11  | 1:A:1048:ASN:CB   | 2.21                     | 0.70              |
| 1:A:438:ASP:O     | 1:A:439:ASN:HB2   | 1.90                     | 0.70              |
| 4:D:7:THR:HG21    | 4:D:32:GLU:CD     | 2.11                     | 0.70              |
| 4:D:8:PHE:CE2     | 4:D:40:HIS:HA     | 2.25                     | 0.70              |
| 7:G:15:PRO:HA     | 7:G:18:PHE:CE1    | 2.25                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1329:THR:HG22 | 1:A:1331:SER:N    | 2.06                     | 0.70              |
| 1:A:1348:LEU:HG   | 1:A:1372:VAL:HG23 | 1.73                     | 0.70              |
| 2:B:175:ARG:HH11  | 2:B:175:ARG:HG2   | 1.55                     | 0.70              |
| 2:B:336:ARG:HG2   | 2:B:348:ARG:CD    | 2.17                     | 0.70              |
| 1:A:1332:PHE:N    | 1:A:1332:PHE:CD2  | 2.60                     | 0.70              |
| 1:A:265:LYS:HD2   | 1:A:265:LYS:N     | 2.06                     | 0.70              |
| 1:A:34:LYS:H      | 1:A:57:ARG:NH2    | 1.90                     | 0.70              |
| 8:H:123:MET:HG2   | 8:H:124:ARG:N     | 2.07                     | 0.70              |
| 1:A:637:LYS:HB3   | 1:A:641:VAL:HG11  | 1.73                     | 0.69              |
| 2:B:38:PHE:HD1    | 2:B:811:TYR:CD2   | 2.09                     | 0.69              |
| 1:A:1035:TYR:O    | 1:A:1037:LEU:N    | 2.25                     | 0.69              |
| 1:A:996:ASN:O     | 1:A:998:LEU:HD12  | 1.91                     | 0.69              |
| 2:B:1069:PHE:HD1  | 2:B:1069:PHE:H    | 1.39                     | 0.69              |
| 2:B:336:ARG:CD    | 2:B:348:ARG:HH11  | 2.04                     | 0.69              |
| 2:B:824:ILE:CG2   | 2:B:1087:PHE:HE2  | 2.05                     | 0.69              |
| 4:D:40:HIS:CB     | 7:G:73:LYS:NZ     | 2.54                     | 0.69              |
| 1:A:1149:ALA:HB2  | 9:I:47:GLU:HA     | 1.74                     | 0.69              |
| 4:D:34:GLN:O      | 4:D:47:LEU:HD23   | 1.92                     | 0.69              |
| 6:F:111:LEU:N     | 6:F:111:LEU:HD12  | 2.06                     | 0.69              |
| 6:F:90:ARG:HD3    | 6:F:155:LEU:CD1   | 2.22                     | 0.69              |
| 12:L:53:HIS:HB3   | 12:L:55:ILE:CD1   | 2.22                     | 0.69              |
| 1:A:347:PHE:H     | 2:B:1107:ALA:HA   | 1.57                     | 0.69              |
| 1:A:471:ASN:OD1   | 1:A:472:LEU:N     | 2.25                     | 0.69              |
| 15:T:26:DC:H2''   | 15:T:27:DA:H5'    | 1.74                     | 0.69              |
| 1:A:541:ILE:HG21  | 1:A:549:MET:HE3   | 1.74                     | 0.69              |
| 3:C:70:ILE:HG12   | 3:C:142:VAL:HG11  | 1.74                     | 0.69              |
| 8:H:100:THR:OG1   | 8:H:138:GLU:HG3   | 1.92                     | 0.69              |
| 2:B:1017:ILE:HB   | 2:B:1018:PRO:HD3  | 1.75                     | 0.69              |
| 2:B:847:ASP:HB3   | 3:C:167:HIS:HE2   | 1.54                     | 0.69              |
| 1:A:114:LEU:HD13  | 1:A:171:GLN:HE22  | 1.56                     | 0.69              |
| 2:B:745:PRO:O     | 2:B:748:ILE:HG12  | 1.93                     | 0.69              |
| 2:B:842:ASN:HD22  | 2:B:845:SER:CB    | 2.06                     | 0.69              |
| 2:B:857:ARG:HD2   | 2:B:945:GLU:OE1   | 1.93                     | 0.69              |
| 4:D:213:GLU:O     | 4:D:217:LEU:HG    | 1.93                     | 0.69              |
| 1:A:463:ILE:HB    | 1:A:464:PRO:HD2   | 1.74                     | 0.69              |
| 2:B:287:ARG:HG2   | 2:B:292:ILE:HA    | 1.73                     | 0.69              |
| 2:B:411:PRO:O     | 2:B:414:ALA:HB3   | 1.93                     | 0.69              |
| 2:B:642:ASP:O     | 2:B:644:GLU:N     | 2.26                     | 0.69              |
| 7:G:23:LYS:HG3    | 7:G:56:ILE:HD11   | 1.75                     | 0.69              |
| 1:A:836:TYR:HD1   | 15:T:18:DT:H5''   | 1.57                     | 0.69              |
| 1:A:265:LYS:NZ    | 1:A:322:VAL:HG22  | 2.08                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1115:THR:O    | 2:B:1116:ARG:HB2  | 1.92                     | 0.69              |
| 2:B:975:GLN:HG2   | 2:B:976:ILE:H     | 1.58                     | 0.69              |
| 1:A:701:LEU:HA    | 9:I:115:LYS:HE3   | 1.75                     | 0.69              |
| 10:J:14:VAL:HG12  | 10:J:14:VAL:O     | 1.92                     | 0.69              |
| 1:A:19:PHE:O      | 1:A:1416:ALA:HA   | 1.93                     | 0.69              |
| 1:A:441:PRO:HD2   | 1:A:498:ARG:NH2   | 2.08                     | 0.69              |
| 2:B:1065:GLN:HG3  | 2:B:1067:ARG:H    | 1.57                     | 0.69              |
| 5:E:198:ILE:CD1   | 5:E:212:ARG:HG3   | 2.23                     | 0.69              |
| 8:H:4:THR:HA      | 8:H:60:ALA:CB     | 2.22                     | 0.69              |
| 1:A:1332:PHE:HD2  | 1:A:1332:PHE:N    | 1.90                     | 0.69              |
| 1:A:382:PRO:HD3   | 1:A:428:TYR:CD2   | 2.28                     | 0.69              |
| 1:A:901:LEU:HB2   | 1:A:926:GLN:HG2   | 1.74                     | 0.69              |
| 1:A:870:GLU:HG2   | 5:E:208:TYR:CG    | 2.28                     | 0.69              |
| 7:G:23:LYS:HG3    | 7:G:56:ILE:CD1    | 2.23                     | 0.69              |
| 15:T:18:DT:H3'    | 15:T:19:TT:H4'    | 1.73                     | 0.69              |
| 2:B:39:ARG:NH2    | 2:B:665:GLU:HG2   | 2.08                     | 0.68              |
| 1:A:598:LEU:HA    | 8:H:122:LEU:HD13  | 1.75                     | 0.68              |
| 11:K:6:ARG:O      | 11:K:9:LEU:HG     | 1.93                     | 0.68              |
| 1:A:1029:ARG:HG3  | 1:A:1029:ARG:HH11 | 1.58                     | 0.68              |
| 1:A:896:ARG:HD3   | 1:A:897:TYR:CE1   | 2.28                     | 0.68              |
| 2:B:180:TYR:HD1   | 2:B:180:TYR:H     | 1.41                     | 0.68              |
| 2:B:1006:ILE:HD13 | 10:J:44:TYR:CE2   | 2.28                     | 0.68              |
| 1:A:549:MET:SD    | 1:A:577:ILE:HD11  | 2.33                     | 0.68              |
| 1:A:856:THR:HB    | 1:A:865:GLN:HB2   | 1.75                     | 0.68              |
| 2:B:273:LEU:CB    | 2:B:276:ILE:HD12  | 2.19                     | 0.68              |
| 2:B:53:GLN:HG2    | 2:B:547:VAL:HG22  | 1.75                     | 0.68              |
| 11:K:53:ASP:OD1   | 11:K:55:LYS:HB2   | 1.93                     | 0.68              |
| 2:B:1223:ASP:O    | 2:B:1224:PHE:HB2  | 1.92                     | 0.68              |
| 4:D:33:PHE:CE1    | 7:G:80:LYS:HE3    | 2.29                     | 0.68              |
| 6:F:76:LYS:O      | 6:F:79:ARG:HD3    | 1.94                     | 0.68              |
| 1:A:1445:ILE:HG12 | 7:G:18:PHE:CE2    | 2.28                     | 0.68              |
| 8:H:102:TYR:OH    | 8:H:122:LEU:HD22  | 1.94                     | 0.68              |
| 1:A:1057:VAL:HG12 | 1:A:1058:VAL:H    | 1.59                     | 0.68              |
| 1:A:1345:ARG:HG3  | 1:A:1376:THR:HG21 | 1.74                     | 0.68              |
| 4:D:118:THR:HB    | 4:D:121:LYS:HB2   | 1.76                     | 0.68              |
| 4:D:189:ASP:O     | 4:D:193:THR:HB    | 1.92                     | 0.68              |
| 5:E:78:LEU:HD21   | 5:E:80:VAL:HG23   | 1.76                     | 0.68              |
| 2:B:121:ASN:HA    | 2:B:207:GLY:CA    | 2.23                     | 0.68              |
| 2:B:863:GLU:OE2   | 2:B:873:THR:HA    | 1.94                     | 0.68              |
| 2:B:882:THR:HB    | 2:B:934:LYS:O     | 1.94                     | 0.68              |
| 6:F:103:MET:O     | 6:F:104:ASN:HB2   | 1.93                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:537:ARG:HD2   | 8:H:20:TYR:CE1    | 2.29                     | 0.68              |
| 11:K:31:VAL:HG12  | 11:K:32:VAL:N     | 2.09                     | 0.68              |
| 15:T:19:TT:C2R    | 15:T:19:TT:H2'1   | 2.23                     | 0.68              |
| 1:A:1436:ILE:O    | 1:A:1437:GLY:C    | 2.33                     | 0.68              |
| 5:E:198:ILE:HD11  | 5:E:212:ARG:HG3   | 1.74                     | 0.68              |
| 8:H:84:ALA:CA     | 8:H:87:ARG:HB2    | 2.22                     | 0.68              |
| 1:A:552:TRP:HE3   | 1:A:651:LYS:HB3   | 1.60                     | 0.68              |
| 2:B:1180:PHE:HB3  | 2:B:1191:ILE:CD1  | 2.24                     | 0.68              |
| 2:B:232:SER:CB    | 2:B:261:ARG:HH21  | 2.06                     | 0.68              |
| 5:E:157:SER:C     | 5:E:159:ASP:H     | 1.97                     | 0.68              |
| 1:A:58:LEU:HD21   | 1:A:243:PRO:CA    | 2.23                     | 0.67              |
| 2:B:1099:VAL:CG1  | 2:B:1100:ASP:N    | 2.56                     | 0.67              |
| 8:H:130:ARG:H     | 8:H:130:ARG:HD2   | 1.59                     | 0.67              |
| 1:A:42:ASP:HB3    | 1:A:45:GLN:H      | 1.59                     | 0.67              |
| 1:A:903:ASN:HD22  | 1:A:903:ASN:C     | 1.96                     | 0.67              |
| 1:A:1313:LEU:HD23 | 1:A:1338:VAL:HG21 | 1.75                     | 0.67              |
| 2:B:351:TYR:O     | 2:B:355:ILE:HG13  | 1.95                     | 0.67              |
| 2:B:983:ARG:HD2   | 2:B:1091:TYR:HD2  | 1.59                     | 0.67              |
| 3:C:232:VAL:HG21  | 3:C:244:VAL:HG22  | 1.77                     | 0.67              |
| 3:C:35:ARG:HH12   | 11:K:41:THR:H     | 1.40                     | 0.67              |
| 6:F:130:ILE:O     | 6:F:148:VAL:HG21  | 1.93                     | 0.67              |
| 7:G:13:LEU:CD2    | 7:G:17:PHE:HB2    | 2.19                     | 0.67              |
| 1:A:1002:GLY:HA3  | 1:A:1007:ILE:HG21 | 1.75                     | 0.67              |
| 1:A:868:TYR:CD2   | 1:A:1058:VAL:HG21 | 2.29                     | 0.67              |
| 1:A:1120:LEU:N    | 1:A:1120:LEU:HD12 | 2.09                     | 0.67              |
| 1:A:567:LYS:HB2   | 1:A:568:PRO:CD    | 2.25                     | 0.67              |
| 1:A:901:LEU:H     | 1:A:926:GLN:HE21  | 1.40                     | 0.67              |
| 2:B:953:LEU:O     | 2:B:953:LEU:HD23  | 1.94                     | 0.67              |
| 5:E:153:HIS:HB3   | 5:E:196:VAL:CG1   | 2.24                     | 0.67              |
| 1:A:34:LYS:HE3    | 1:A:57:ARG:NH1    | 2.08                     | 0.67              |
| 10:J:1:MET:H3     | 10:J:56:LEU:N     | 1.91                     | 0.67              |
| 1:A:68:GLN:C      | 1:A:70:CYS:H      | 1.97                     | 0.67              |
| 1:A:69:THR:C      | 1:A:71:GLN:H      | 1.96                     | 0.67              |
| 2:B:1174:LYS:O    | 2:B:1176:ASN:N    | 2.28                     | 0.67              |
| 2:B:871:THR:HG22  | 2:B:872:GLU:O     | 1.94                     | 0.67              |
| 3:C:56:THR:HG22   | 3:C:57:VAL:H      | 1.60                     | 0.67              |
| 5:E:94:LYS:CE     | 5:E:98:ILE:HD11   | 2.23                     | 0.67              |
| 8:H:143:LEU:N     | 8:H:143:LEU:HD12  | 2.08                     | 0.67              |
| 15:T:19:TT:H5M1   | 15:T:21:DC:C4     | 2.29                     | 0.67              |
| 1:A:1121:GLU:HG2  | 1:A:1122:PRO:HD2  | 1.75                     | 0.67              |
| 1:A:1424:VAL:HG11 | 2:B:1139:ILE:HD13 | 1.77                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:384:ASN:O     | 1:A:385:ILE:C     | 2.33                     | 0.67              |
| 2:B:1159:ARG:HD3  | 2:B:1193:GLN:HG3  | 1.76                     | 0.67              |
| 1:A:253:ASN:HB3   | 2:B:935:ARG:CZ    | 2.25                     | 0.67              |
| 9:I:8:ARG:CG      | 9:I:34:TYR:HE1    | 2.06                     | 0.67              |
| 1:A:407:ARG:HB3   | 1:A:430:TRP:CE2   | 2.29                     | 0.67              |
| 1:A:450:LEU:HD12  | 1:A:450:LEU:H     | 1.60                     | 0.67              |
| 1:A:527:THR:CG2   | 1:A:650:GLN:HA    | 2.25                     | 0.67              |
| 5:E:192:ARG:NH1   | 5:E:192:ARG:HG3   | 2.09                     | 0.67              |
| 8:H:58:THR:HG22   | 8:H:59:ILE:H      | 1.60                     | 0.67              |
| 1:A:252:PHE:O     | 1:A:253:ASN:HB2   | 1.95                     | 0.66              |
| 2:B:1072:MET:HE3  | 2:B:1085:ILE:HB   | 1.75                     | 0.66              |
| 3:C:238:ILE:CG2   | 3:C:242:GLN:HB2   | 2.25                     | 0.66              |
| 8:H:44:VAL:O      | 8:H:44:VAL:HG12   | 1.96                     | 0.66              |
| 2:B:516:ASN:ND2   | 2:B:516:ASN:H     | 1.92                     | 0.66              |
| 1:A:1438:THR:HB   | 2:B:1144:ALA:HB3  | 1.78                     | 0.66              |
| 1:A:1450:LEU:HG   | 1:A:1450:LEU:O    | 1.96                     | 0.66              |
| 1:A:268:ASP:HB3   | 1:A:299:HIS:CE1   | 2.31                     | 0.66              |
| 2:B:1085:ILE:HD12 | 2:B:1085:ILE:N    | 2.10                     | 0.66              |
| 8:H:41:ASP:O      | 8:H:42:ILE:HG13   | 1.95                     | 0.66              |
| 1:A:881:GLN:NE2   | 1:A:958:VAL:O     | 2.28                     | 0.66              |
| 2:B:1106:ARG:NH1  | 2:B:1110:PRO:HG2  | 2.11                     | 0.66              |
| 2:B:1169:MET:HE1  | 2:B:1201:LYS:HA   | 1.77                     | 0.66              |
| 3:C:167:HIS:CD2   | 3:C:168:ALA:N     | 2.64                     | 0.66              |
| 3:C:43:THR:CG2    | 3:C:44:LEU:N      | 2.58                     | 0.66              |
| 6:F:109:VAL:HG11  | 6:F:123:LYS:HD3   | 1.78                     | 0.66              |
| 9:I:75:CYS:SG     | 9:I:79:HIS:N      | 2.68                     | 0.66              |
| 2:B:1039:GLY:HA2  | 10:J:51:LEU:CD2   | 2.24                     | 0.66              |
| 15:T:18:DT:H2"    | 15:T:19:TT:H5'1   | 1.72                     | 0.66              |
| 1:A:1279:ILE:O    | 1:A:1279:ILE:HG22 | 1.96                     | 0.66              |
| 2:B:378:LEU:O     | 2:B:382:ILE:HG13  | 1.95                     | 0.66              |
| 2:B:464:GLY:HA2   | 2:B:479:VAL:O     | 1.96                     | 0.66              |
| 1:A:1127:ASP:HB3  | 1:A:1130:GLN:HB3  | 1.78                     | 0.66              |
| 1:A:1362:TYR:CD1  | 1:A:1363:VAL:N    | 2.64                     | 0.66              |
| 2:B:18:PHE:N      | 2:B:19:GLU:N      | 2.44                     | 0.66              |
| 2:B:825:VAL:CG1   | 2:B:826:ALA:N     | 2.58                     | 0.66              |
| 1:A:1011:GLN:NE2  | 1:A:1015:VAL:HG21 | 2.11                     | 0.66              |
| 1:A:896:ARG:NH2   | 1:A:1030:ARG:HH21 | 1.93                     | 0.66              |
| 2:B:217:ARG:C     | 2:B:217:ARG:HD2   | 2.15                     | 0.66              |
| 2:B:563:MET:HE3   | 2:B:580:VAL:HB    | 1.78                     | 0.66              |
| 2:B:794:ASN:O     | 2:B:795:ILE:HD12  | 1.95                     | 0.66              |
| 2:B:847:ASP:HB3   | 3:C:167:HIS:CD2   | 2.31                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:176:GLU:O     | 4:D:178:ALA:N     | 2.29                     | 0.66              |
| 11:K:46:ILE:O     | 11:K:46:ILE:HG22  | 1.96                     | 0.66              |
| 2:B:224:GLN:O     | 2:B:238:ALA:HA    | 1.95                     | 0.66              |
| 2:B:840:ILE:HB    | 2:B:1011:ILE:HB   | 1.77                     | 0.66              |
| 1:A:356:ASP:HB2   | 1:A:469:ARG:HH11  | 1.60                     | 0.66              |
| 1:A:84:ILE:HG23   | 1:A:84:ILE:O      | 1.96                     | 0.66              |
| 2:B:842:ASN:ND2   | 2:B:845:SER:OG    | 2.29                     | 0.66              |
| 10:J:64:ASN:ND2   | 10:J:65:PRO:HD3   | 2.11                     | 0.66              |
| 14:P:1:U:O2'      | 14:P:2:C:H5'      | 1.96                     | 0.66              |
| 1:A:768:GLN:HG2   | 1:A:816:HIS:CA    | 2.26                     | 0.65              |
| 2:B:1197:PRO:HG2  | 2:B:1200:ALA:CB   | 2.25                     | 0.65              |
| 1:A:1100:ARG:NH2  | 1:A:1351:GLU:HG2  | 2.11                     | 0.65              |
| 1:A:728:LYS:O     | 1:A:732:LEU:HG    | 1.97                     | 0.65              |
| 2:B:710:LEU:HA    | 2:B:733:HIS:HB3   | 1.78                     | 0.65              |
| 2:B:824:ILE:HG22  | 2:B:1087:PHE:CE2  | 2.26                     | 0.65              |
| 1:A:982:THR:H     | 1:A:985:ASP:HB2   | 1.61                     | 0.65              |
| 1:A:984:LYS:O     | 1:A:988:LEU:HB2   | 1.97                     | 0.65              |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:H    | 1.44                     | 0.65              |
| 2:B:1069:PHE:HA   | 2:B:1085:ILE:O    | 1.96                     | 0.65              |
| 2:B:593:PRO:HG2   | 2:B:617:ARG:NH2   | 2.11                     | 0.65              |
| 3:C:66:ARG:NH2    | 10:J:3:VAL:O      | 2.29                     | 0.65              |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:N    | 2.08                     | 0.65              |
| 1:A:1057:VAL:HG12 | 1:A:1058:VAL:N    | 2.12                     | 0.65              |
| 1:A:164:ARG:HG3   | 1:A:165:GLY:N     | 2.11                     | 0.65              |
| 1:A:335:ARG:NH1   | 2:B:1202:LEU:HD13 | 2.11                     | 0.65              |
| 1:A:541:ILE:HG22  | 1:A:546:VAL:HG23  | 1.78                     | 0.65              |
| 2:B:557:PHE:C     | 2:B:557:PHE:CD2   | 2.70                     | 0.65              |
| 11:K:61:TYR:CD2   | 11:K:61:TYR:C     | 2.69                     | 0.65              |
| 1:A:320:ARG:NH2   | 14:P:1:U:O2'      | 2.29                     | 0.65              |
| 1:A:50:ILE:C      | 1:A:52:GLY:H      | 2.00                     | 0.65              |
| 1:A:899:VAL:HB    | 1:A:929:LEU:CD1   | 2.27                     | 0.65              |
| 2:B:35:SER:O      | 2:B:39:ARG:HG3    | 1.97                     | 0.65              |
| 2:B:911:ILE:HD11  | 2:B:941:LEU:HD13  | 1.79                     | 0.65              |
| 3:C:167:HIS:HD2   | 3:C:168:ALA:H     | 1.43                     | 0.65              |
| 8:H:11:GLN:HA     | 8:H:53:ASP:O      | 1.96                     | 0.65              |
| 1:A:1005:GLU:O    | 1:A:1009:ASN:HB2  | 1.97                     | 0.65              |
| 1:A:714:PHE:O     | 1:A:718:VAL:HG23  | 1.97                     | 0.65              |
| 2:B:1165:ILE:HG22 | 2:B:1166:CYS:N    | 2.11                     | 0.65              |
| 2:B:850:LEU:HD12  | 2:B:851:PHE:N     | 2.11                     | 0.65              |
| 4:D:71:LYS:HA     | 4:D:74:GLN:HB2    | 1.78                     | 0.65              |
| 5:E:22:MET:CE     | 5:E:26:ARG:HH21   | 2.02                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:152:VAL:CG1   | 1:A:153:PRO:HD2   | 2.26                     | 0.65              |
| 1:A:886:ILE:HD11  | 1:A:943:LEU:HB3   | 1.77                     | 0.65              |
| 1:A:828:ALA:HB2   | 2:B:530:GLY:HA2   | 1.79                     | 0.65              |
| 2:B:308:TRP:HA    | 2:B:311:LEU:HD12  | 1.78                     | 0.65              |
| 8:H:89:LEU:HB3    | 8:H:91:ASP:OD1    | 1.97                     | 0.65              |
| 1:A:69:THR:C      | 1:A:71:GLN:N      | 2.49                     | 0.65              |
| 5:E:114:ASN:O     | 5:E:115:ASN:HB3   | 1.97                     | 0.65              |
| 1:A:547:LEU:HD22  | 11:K:58:PHE:HD1   | 1.60                     | 0.65              |
| 1:A:372:LYS:HA    | 1:A:435:HIS:ND1   | 2.11                     | 0.64              |
| 2:B:770:GLN:HG2   | 2:B:983:ARG:O     | 1.97                     | 0.64              |
| 2:B:782:LEU:HD12  | 2:B:788:ARG:HH11  | 1.62                     | 0.64              |
| 3:C:101:LEU:HD13  | 3:C:118:LEU:HD23  | 1.78                     | 0.64              |
| 4:D:192:LYS:HE3   | 4:D:204:ASP:OD1   | 1.97                     | 0.64              |
| 4:D:47:LEU:HD13   | 4:D:48:ILE:N      | 2.11                     | 0.64              |
| 1:A:852:TYR:CE2   | 1:A:1060:PRO:HB2  | 2.33                     | 0.64              |
| 1:A:1445:ILE:HD12 | 1:A:1445:ILE:N    | 1.98                     | 0.64              |
| 1:A:392:VAL:HG13  | 1:A:415:LEU:HD11  | 1.79                     | 0.64              |
| 1:A:450:LEU:N     | 1:A:450:LEU:HD12  | 2.13                     | 0.64              |
| 2:B:589:VAL:CG1   | 2:B:590:HIS:H     | 2.07                     | 0.64              |
| 5:E:153:HIS:HB3   | 5:E:196:VAL:HG11  | 1.77                     | 0.64              |
| 15:T:13:DA:H1'    | 15:T:14:DC:H5'    | 1.78                     | 0.64              |
| 1:A:105:CYS:O     | 1:A:114:LEU:HG    | 1.97                     | 0.64              |
| 1:A:591:PHE:HA    | 1:A:595:THR:HG21  | 1.80                     | 0.64              |
| 1:A:979:SER:OG    | 1:A:980:ASP:N     | 2.29                     | 0.64              |
| 2:B:185:THR:H     | 2:B:188:ASP:HB2   | 1.62                     | 0.64              |
| 2:B:467:GLY:H     | 2:B:475:SER:CB    | 2.10                     | 0.64              |
| 2:B:744:HIS:HD2   | 2:B:746:SER:OG    | 1.80                     | 0.64              |
| 1:A:14:VAL:H      | 1:A:1432:GLN:HE22 | 1.45                     | 0.64              |
| 1:A:265:LYS:HE2   | 1:A:322:VAL:CG1   | 2.27                     | 0.64              |
| 1:A:414:ASP:OD1   | 1:A:416:ARG:HG2   | 1.97                     | 0.64              |
| 1:A:93:VAL:CG2    | 1:A:301:ALA:HA    | 2.27                     | 0.64              |
| 2:B:1161:HIS:NE2  | 2:B:1175:LEU:HD21 | 2.11                     | 0.64              |
| 2:B:247:GLY:C     | 2:B:249:ARG:H     | 1.99                     | 0.64              |
| 3:C:183:TRP:O     | 3:C:185:LYS:N     | 2.30                     | 0.64              |
| 5:E:46:TYR:CD2    | 5:E:58:MET:HG2    | 2.32                     | 0.64              |
| 2:B:776:GLN:HE22  | 14:P:8:G:H5'      | 1.62                     | 0.64              |
| 1:A:1006:ILE:HD12 | 5:E:163:GLU:HG3   | 1.78                     | 0.64              |
| 1:A:35:ILE:HA     | 1:A:52:GLY:O      | 1.97                     | 0.64              |
| 1:A:458:HIS:CE1   | 1:A:507:VAL:HG21  | 2.33                     | 0.64              |
| 2:B:918:ILE:HB    | 2:B:935:ARG:HD2   | 1.80                     | 0.64              |
| 5:E:9:ILE:HD11    | 5:E:53:PRO:HD3    | 1.78                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:127:PRO:HG2  | 7:G:138:THR:HG21  | 1.79                     | 0.64              |
| 1:A:1094:VAL:CG1 | 1:A:1095:THR:H    | 2.06                     | 0.64              |
| 1:A:1134:ILE:O   | 1:A:1138:ILE:HG13 | 1.98                     | 0.64              |
| 2:B:1159:ARG:HB3 | 2:B:1159:ARG:HH11 | 1.62                     | 0.64              |
| 2:B:745:PRO:O    | 2:B:747:MET:N     | 2.31                     | 0.64              |
| 4:D:56:ARG:HB2   | 4:D:148:LEU:HD22  | 1.80                     | 0.64              |
| 10:J:57:ILE:HA   | 10:J:60:PHE:HD2   | 1.61                     | 0.64              |
| 1:A:1155:ASP:OD2 | 1:A:1161:THR:HG23 | 1.98                     | 0.64              |
| 1:A:853:ASP:OD1  | 1:A:855:THR:CB    | 2.45                     | 0.64              |
| 3:C:133:ILE:HD11 | 3:C:237:SER:HA    | 1.80                     | 0.64              |
| 1:A:1063:MET:CG  | 1:A:1436:ILE:HG23 | 2.28                     | 0.64              |
| 1:A:254:GLU:O    | 1:A:256:GLN:N     | 2.30                     | 0.64              |
| 1:A:388:LEU:O    | 1:A:392:VAL:HG23  | 1.98                     | 0.64              |
| 2:B:29:ASP:HB3   | 2:B:658:ILE:CD1   | 2.28                     | 0.64              |
| 2:B:842:ASN:O    | 2:B:846:ILE:HG13  | 1.98                     | 0.64              |
| 3:C:36:VAL:HG21  | 3:C:251:LEU:HB2   | 1.79                     | 0.64              |
| 6:F:99:LEU:O     | 6:F:103:MET:HG2   | 1.97                     | 0.64              |
| 6:F:93:ILE:HD11  | 6:F:134:ILE:CD1   | 2.26                     | 0.64              |
| 1:A:1444:MET:CG  | 7:G:60:ARG:HA     | 2.28                     | 0.64              |
| 8:H:81:PRO:CB    | 8:H:82:PRO:CD     | 2.75                     | 0.64              |
| 12:L:47:ARG:HH21 | 12:L:54:ARG:HH21  | 1.44                     | 0.64              |
| 1:A:34:LYS:CE    | 1:A:57:ARG:NH1    | 2.61                     | 0.64              |
| 2:B:860:MET:HG2  | 2:B:861:ASP:H     | 1.63                     | 0.64              |
| 2:B:859:TYR:CZ   | 2:B:941:LEU:HD12  | 2.33                     | 0.64              |
| 11:K:111:LEU:C   | 11:K:112:GLN:CG   | 2.59                     | 0.64              |
| 2:B:1001:PHE:CE1 | 2:B:1073:TYR:HB2  | 2.33                     | 0.63              |
| 2:B:39:ARG:HH21  | 2:B:665:GLU:CD    | 2.01                     | 0.63              |
| 2:B:806:THR:HG22 | 2:B:808:ALA:N     | 2.07                     | 0.63              |
| 15:T:22:BRU:C2'  | 15:T:23:DG:O4'    | 2.46                     | 0.63              |
| 1:A:144:THR:O    | 1:A:146:MET:HG3   | 1.98                     | 0.63              |
| 1:A:567:LYS:CB   | 1:A:568:PRO:HD2   | 2.28                     | 0.63              |
| 2:B:339:THR:HG22 | 2:B:339:THR:O     | 1.98                     | 0.63              |
| 2:B:601:ARG:O    | 2:B:605:ARG:HG3   | 1.98                     | 0.63              |
| 2:B:637:LEU:O    | 2:B:690:VAL:HG13  | 1.99                     | 0.63              |
| 3:C:133:ILE:CD1  | 3:C:237:SER:HA    | 2.28                     | 0.63              |
| 1:A:79:GLY:HA3   | 1:A:243:PRO:HG3   | 1.79                     | 0.63              |
| 1:A:477:PRO:CG   | 1:A:521:MET:HG2   | 2.29                     | 0.63              |
| 1:A:675:THR:O    | 1:A:679:ILE:HG13  | 1.98                     | 0.63              |
| 2:B:1084:GLN:NE2 | 2:B:1084:GLN:N    | 2.46                     | 0.63              |
| 2:B:211:VAL:O    | 2:B:480:SER:HA    | 1.99                     | 0.63              |
| 2:B:336:ARG:HH21 | 2:B:345:LYS:HG2   | 1.63                     | 0.63              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:J:23:ASN:C     | 10:J:25:LEU:H    | 1.99                     | 0.63              |
| 10:J:28:ASP:O     | 10:J:30:LEU:HG   | 1.99                     | 0.63              |
| 1:A:326:ARG:NH2   | 1:A:1407:GLU:HG3 | 2.13                     | 0.63              |
| 1:A:535:THR:HG23  | 1:A:575:LYS:HE2  | 1.81                     | 0.63              |
| 2:B:799:PRO:HB3   | 2:B:818:PRO:HG2  | 1.80                     | 0.63              |
| 1:A:265:LYS:HD2   | 1:A:265:LYS:H    | 1.64                     | 0.63              |
| 1:A:518:LYS:HE2   | 1:A:624:SER:O    | 1.97                     | 0.63              |
| 2:B:125:SER:HA    | 2:B:171:PRO:HA   | 1.80                     | 0.63              |
| 2:B:121:ASN:HA    | 2:B:207:GLY:HA2  | 1.78                     | 0.63              |
| 2:B:23:ALA:HB1    | 2:B:24:PRO:HD2   | 1.80                     | 0.63              |
| 2:B:642:ASP:HB3   | 2:B:649:LYS:CD   | 2.28                     | 0.63              |
| 2:B:957:ASN:O     | 2:B:959:ASP:N    | 2.31                     | 0.63              |
| 3:C:263:THR:C     | 3:C:265:MET:H    | 2.02                     | 0.63              |
| 4:D:52:LEU:O      | 4:D:54:GLU:N     | 2.32                     | 0.63              |
| 7:G:79:PHE:CZ     | 7:G:106:MET:HE1  | 2.33                     | 0.63              |
| 6:F:69:LEU:CA     | 6:F:70:LYS:N     | 2.60                     | 0.63              |
| 1:A:598:LEU:HD22  | 8:H:25:ARG:NH1   | 2.14                     | 0.63              |
| 1:A:588:LEU:O     | 1:A:606:LEU:HA   | 1.99                     | 0.63              |
| 1:A:61:ILE:HG22   | 1:A:62:ASP:H     | 1.64                     | 0.63              |
| 2:B:365:THR:HG23  | 2:B:367:LEU:HG   | 1.79                     | 0.63              |
| 2:B:975:GLN:O     | 2:B:990:ILE:HD12 | 1.99                     | 0.63              |
| 3:C:189:THR:HG22  | 3:C:190:ASP:N    | 2.14                     | 0.63              |
| 7:G:17:PHE:N      | 7:G:17:PHE:CD2   | 2.66                     | 0.63              |
| 8:H:93:TYR:HB3    | 8:H:144:ILE:O    | 1.99                     | 0.63              |
| 1:A:321:PRO:O     | 1:A:322:VAL:CB   | 2.46                     | 0.63              |
| 2:B:315:LYS:N     | 2:B:316:PRO:HD2  | 2.13                     | 0.63              |
| 2:B:916:THR:O     | 2:B:935:ARG:HG3  | 1.99                     | 0.63              |
| 6:F:138:LEU:HB3   | 6:F:139:PRO:HD2  | 1.80                     | 0.63              |
| 4:D:7:THR:HB      | 7:G:42:PHE:CE2   | 2.34                     | 0.63              |
| 1:A:1299:VAL:HG12 | 1:A:1300:LYS:N   | 2.14                     | 0.62              |
| 2:B:705:MET:H     | 2:B:710:LEU:HD12 | 1.63                     | 0.62              |
| 1:A:49:LYS:HZ1    | 1:A:61:ILE:HG13  | 1.64                     | 0.62              |
| 1:A:57:ARG:O      | 1:A:68:GLN:HG3   | 1.99                     | 0.62              |
| 1:A:87:ALA:HB1    | 1:A:276:LEU:HD23 | 1.80                     | 0.62              |
| 9:I:34:TYR:CE2    | 9:I:36:GLU:HB3   | 2.34                     | 0.62              |
| 1:A:730:GLY:O     | 1:A:732:LEU:N    | 2.32                     | 0.62              |
| 1:A:979:SER:OG    | 1:A:981:LEU:HG   | 1.99                     | 0.62              |
| 2:B:731:VAL:HG12  | 2:B:732:SER:H    | 1.64                     | 0.62              |
| 4:D:159:THR:O     | 4:D:163:VAL:HG23 | 1.99                     | 0.62              |
| 7:G:145:VAL:HG12  | 7:G:146:LYS:N    | 2.14                     | 0.62              |
| 10:J:12:LYS:O     | 10:J:14:VAL:HG23 | 1.99                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:T:15:DT:C1'    | 15:T:16:DT:H5'    | 2.29                     | 0.62              |
| 1:A:335:ARG:HA    | 1:A:339:ASN:HD22  | 1.63                     | 0.62              |
| 2:B:1034:VAL:O    | 2:B:1037:LEU:N    | 2.30                     | 0.62              |
| 2:B:120:ARG:HG2   | 2:B:955:THR:HG21  | 1.80                     | 0.62              |
| 2:B:563:MET:CE    | 2:B:580:VAL:HB    | 2.29                     | 0.62              |
| 2:B:999:MET:HE2   | 2:B:1000:PRO:HD2  | 1.80                     | 0.62              |
| 3:C:100:THR:OG1   | 3:C:121:VAL:HG21  | 1.99                     | 0.62              |
| 3:C:104:PHE:HD2   | 3:C:105:GLY:H     | 1.47                     | 0.62              |
| 8:H:81:PRO:CB     | 8:H:82:PRO:HD2    | 2.28                     | 0.62              |
| 9:I:61:ASP:C      | 9:I:63:GLY:H      | 2.03                     | 0.62              |
| 1:A:332:LYS:HG3   | 1:A:333:GLU:HG2   | 1.81                     | 0.62              |
| 1:A:567:LYS:CB    | 1:A:568:PRO:CD    | 2.77                     | 0.62              |
| 2:B:616:ILE:HD12  | 2:B:616:ILE:N     | 2.14                     | 0.62              |
| 3:C:35:ARG:HH11   | 11:K:41:THR:CA    | 2.12                     | 0.62              |
| 9:I:55:THR:HG22   | 9:I:58:VAL:HG21   | 1.79                     | 0.62              |
| 10:J:16:ASP:OD1   | 10:J:17:LYS:HD2   | 1.99                     | 0.62              |
| 1:A:1149:ALA:CB   | 9:I:47:GLU:HA     | 2.29                     | 0.62              |
| 1:A:1209:MET:SD   | 1:A:1236:LEU:HD22 | 2.39                     | 0.62              |
| 1:A:1412:ALA:HA   | 1:A:1417:GLU:OE2  | 1.98                     | 0.62              |
| 1:A:741:ASN:ND2   | 1:A:744:LYS:H     | 1.98                     | 0.62              |
| 1:A:763:ALA:O     | 1:A:803:SER:HB3   | 2.00                     | 0.62              |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:N    | 1.98                     | 0.62              |
| 2:B:842:ASN:HB3   | 2:B:845:SER:OG    | 1.99                     | 0.62              |
| 11:K:10:PHE:CD2   | 11:K:10:PHE:N     | 2.68                     | 0.62              |
| 11:K:45:LEU:HG    | 11:K:94:ILE:HD13  | 1.81                     | 0.62              |
| 1:A:1279:ILE:HD11 | 1:A:1316:VAL:HG21 | 1.80                     | 0.62              |
| 1:A:524:VAL:HG12  | 1:A:525:GLN:N     | 2.12                     | 0.62              |
| 1:A:58:LEU:CG     | 1:A:59:GLY:H      | 2.11                     | 0.62              |
| 1:A:844:ALA:C     | 1:A:845:LEU:HD23  | 2.20                     | 0.62              |
| 2:B:465:ASN:HD22  | 2:B:465:ASN:N     | 1.98                     | 0.62              |
| 3:C:39:ALA:CA     | 3:C:164:ALA:HB3   | 2.30                     | 0.62              |
| 5:E:39:LEU:O      | 5:E:42:PHE:HB3    | 2.00                     | 0.62              |
| 5:E:48:ASP:CG     | 5:E:49:SER:H      | 2.03                     | 0.62              |
| 6:F:97:ARG:O      | 6:F:101:ILE:HG13  | 1.99                     | 0.62              |
| 11:K:67:PHE:C     | 11:K:68:PHE:HD2   | 2.03                     | 0.62              |
| 2:B:1007:VAL:CG2  | 2:B:1008:PRO:HD2  | 2.29                     | 0.62              |
| 2:B:525:ALA:O     | 2:B:768:THR:HA    | 2.00                     | 0.62              |
| 3:C:112:ASN:HB2   | 3:C:114:TYR:CE1   | 2.34                     | 0.62              |
| 3:C:253:LYS:O     | 3:C:256:ALA:HB3   | 2.00                     | 0.62              |
| 4:D:8:PHE:CZ      | 4:D:40:HIS:HA     | 2.35                     | 0.62              |
| 5:E:202:SER:OG    | 5:E:204:THR:HG22  | 2.00                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:90:ARG:HG3   | 6:F:91:ALA:N     | 2.14                     | 0.62              |
| 1:A:997:LEU:HD13 | 1:A:1018:PHE:CE2 | 2.34                     | 0.62              |
| 1:A:53:LEU:CD2   | 1:A:54:ASN:HD22  | 2.13                     | 0.62              |
| 2:B:1182:CYS:O   | 2:B:1182:CYS:SG  | 2.57                     | 0.62              |
| 2:B:446:LEU:O    | 2:B:447:ALA:HB3  | 1.99                     | 0.62              |
| 2:B:797:TYR:HE1  | 2:B:854:LEU:HD23 | 1.65                     | 0.62              |
| 2:B:822:ASN:O    | 10:J:48:ARG:NH1  | 2.33                     | 0.62              |
| 13:N:5:DA:C2     | 15:T:13:DA:C2    | 2.88                     | 0.62              |
| 1:A:1244:ARG:HB3 | 1:A:1245:PRO:HD2 | 1.80                     | 0.62              |
| 1:A:1441:PHE:CZ  | 6:F:89:GLU:HA    | 2.34                     | 0.62              |
| 2:B:751:VAL:HG13 | 2:B:812:LEU:HD22 | 1.80                     | 0.62              |
| 1:A:567:LYS:CE   | 8:H:46:LEU:HB2   | 2.29                     | 0.62              |
| 1:A:107:CYS:N    | 1:A:114:LEU:HD21 | 2.15                     | 0.61              |
| 1:A:849:MET:CE   | 1:A:1061:GLY:HA2 | 2.30                     | 0.61              |
| 2:B:36:ALA:HA    | 2:B:39:ARG:HD2   | 1.81                     | 0.61              |
| 2:B:433:GLN:O    | 2:B:437:GLU:HG3  | 1.99                     | 0.61              |
| 2:B:269:ILE:HD11 | 2:B:386:LEU:HD21 | 1.81                     | 0.61              |
| 3:C:44:LEU:HB2   | 3:C:77:ILE:HD11  | 1.82                     | 0.61              |
| 1:A:477:PRO:HG2  | 1:A:521:MET:HG2  | 1.82                     | 0.61              |
| 1:A:901:LEU:N    | 1:A:926:GLN:NE2  | 2.47                     | 0.61              |
| 2:B:464:GLY:O    | 2:B:477:ALA:HA   | 2.00                     | 0.61              |
| 10:J:64:ASN:CB   | 10:J:65:PRO:HD3  | 2.30                     | 0.61              |
| 2:B:336:ARG:NH2  | 2:B:345:LYS:HE2  | 2.10                     | 0.61              |
| 2:B:498:THR:HB   | 2:B:537:LYS:O    | 2.00                     | 0.61              |
| 3:C:70:ILE:HD11  | 3:C:144:ILE:HG12 | 1.82                     | 0.61              |
| 7:G:34:VAL:CG1   | 7:G:45:ILE:HG21  | 2.29                     | 0.61              |
| 10:J:44:TYR:HA   | 10:J:47:ARG:CB   | 2.30                     | 0.61              |
| 10:J:8:PHE:H     | 10:J:49:MET:CE   | 2.12                     | 0.61              |
| 1:A:1066:VAL:O   | 1:A:1070:GLN:HG3 | 2.01                     | 0.61              |
| 2:B:168:GLY:N    | 2:B:450:ALA:HB1  | 2.12                     | 0.61              |
| 2:B:616:ILE:CG1  | 2:B:697:GLU:HA   | 2.31                     | 0.61              |
| 2:B:622:LYS:CE   | 9:I:59:VAL:HG22  | 2.30                     | 0.61              |
| 3:C:123:ASN:HD22 | 3:C:125:MET:HG2  | 1.66                     | 0.61              |
| 1:A:971:PHE:CE2  | 1:A:1040:GLN:HG2 | 2.34                     | 0.61              |
| 1:A:907:THR:CG2  | 1:A:908:LEU:N    | 2.63                     | 0.61              |
| 7:G:143:ILE:HG22 | 7:G:144:ARG:N    | 2.15                     | 0.61              |
| 3:C:164:ALA:HA   | 3:C:167:HIS:O    | 2.00                     | 0.61              |
| 1:A:450:LEU:HB3  | 1:A:838:GLN:NE2  | 2.15                     | 0.61              |
| 2:B:278:GLN:HE22 | 2:B:337:ARG:HH21 | 1.47                     | 0.61              |
| 2:B:520:GLY:H    | 2:B:748:ILE:HG22 | 1.64                     | 0.61              |
| 3:C:104:PHE:HD2  | 3:C:105:GLY:N    | 1.99                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:142:VAL:H    | 10:J:16:ASP:HB3   | 1.66                     | 0.61              |
| 3:C:69:LEU:HD12  | 3:C:69:LEU:N      | 2.16                     | 0.61              |
| 8:H:24:CYS:HB2   | 8:H:44:VAL:HG21   | 1.82                     | 0.61              |
| 8:H:42:ILE:HG23  | 8:H:95:TYR:HE1    | 1.64                     | 0.61              |
| 1:A:382:PRO:HD3  | 1:A:428:TYR:HD2   | 1.65                     | 0.61              |
| 1:A:353:ILE:HD13 | 1:A:487:MET:HE2   | 1.81                     | 0.61              |
| 3:C:34:ARG:O     | 3:C:38:ILE:HG13   | 2.01                     | 0.61              |
| 2:B:1177:HIS:HB2 | 2:B:1179:GLN:HE21 | 1.65                     | 0.61              |
| 2:B:579:ARG:HB2  | 2:B:586:TRP:NE1   | 2.16                     | 0.61              |
| 3:C:77:ILE:HG23  | 3:C:161:LYS:HE3   | 1.81                     | 0.61              |
| 3:C:20:PHE:HE1   | 3:C:22:LEU:HD12   | 1.66                     | 0.61              |
| 3:C:238:ILE:HG23 | 3:C:242:GLN:HB2   | 1.83                     | 0.61              |
| 5:E:29:PHE:O     | 5:E:30:ILE:HG13   | 2.00                     | 0.61              |
| 8:H:25:ARG:HA    | 8:H:41:ASP:HA     | 1.83                     | 0.61              |
| 8:H:47:PHE:CD2   | 8:H:95:TYR:HD1    | 2.19                     | 0.61              |
| 1:A:427:GLN:HG3  | 1:A:430:TRP:CE2   | 2.34                     | 0.60              |
| 1:A:590:ARG:HH11 | 1:A:590:ARG:CG    | 2.10                     | 0.60              |
| 2:B:1084:GLN:NE2 | 2:B:1084:GLN:H    | 1.99                     | 0.60              |
| 2:B:811:TYR:N    | 2:B:811:TYR:CD1   | 2.68                     | 0.60              |
| 6:F:103:MET:CE   | 7:G:66:GLY:H      | 2.13                     | 0.60              |
| 10:J:3:VAL:HG21  | 10:J:18:TRP:CB    | 2.24                     | 0.60              |
| 10:J:48:ARG:HE   | 10:J:49:MET:CE    | 2.10                     | 0.60              |
| 13:N:1:DA:H2"    | 13:N:2:DA:OP2     | 2.00                     | 0.60              |
| 1:A:997:LEU:HD13 | 1:A:1018:PHE:HE2  | 1.66                     | 0.60              |
| 2:B:882:THR:CG2  | 2:B:884:ARG:HB2   | 2.31                     | 0.60              |
| 4:D:5:THR:O      | 4:D:5:THR:HG23    | 2.01                     | 0.60              |
| 11:K:114:LEU:C   | 11:K:114:LEU:HD13 | 2.20                     | 0.60              |
| 11:K:7:PHE:HA    | 11:K:10:PHE:CE2   | 2.36                     | 0.60              |
| 1:A:320:ARG:NH2  | 14:P:1:U:H1'      | 2.15                     | 0.60              |
| 1:A:1095:THR:O   | 1:A:1096:SER:HB2  | 1.99                     | 0.60              |
| 1:A:79:GLY:HA3   | 1:A:243:PRO:CG    | 2.31                     | 0.60              |
| 1:A:899:VAL:HB   | 1:A:929:LEU:HD12  | 1.83                     | 0.60              |
| 13:N:0:DT:H2"    | 13:N:1:DA:O5'     | 2.01                     | 0.60              |
| 1:A:886:ILE:CG2  | 1:A:887:GLY:N     | 2.64                     | 0.60              |
| 2:B:1096:ARG:O   | 2:B:1097:HIS:CB   | 2.49                     | 0.60              |
| 2:B:100:PRO:HD2  | 2:B:180:TYR:HE1   | 1.66                     | 0.60              |
| 2:B:770:GLN:CD   | 2:B:983:ARG:HA    | 2.21                     | 0.60              |
| 3:C:147:LEU:N    | 3:C:147:LEU:HD23  | 2.16                     | 0.60              |
| 10:J:1:MET:N     | 10:J:56:LEU:N     | 2.48                     | 0.60              |
| 2:B:112:LEU:HD12 | 2:B:113:TYR:N     | 2.15                     | 0.60              |
| 2:B:1163:CYS:SG  | 2:B:1165:ILE:HB   | 2.41                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:K:65:HIS:HD2  | 11:K:67:PHE:N    | 1.92                     | 0.60              |
| 1:A:407:ARG:HG2  | 1:A:430:TRP:CH2  | 2.36                     | 0.60              |
| 1:A:663:SER:OG   | 1:A:664:THR:N    | 2.33                     | 0.60              |
| 1:A:694:THR:O    | 1:A:698:GLN:HG3  | 2.00                     | 0.60              |
| 1:A:836:TYR:CE2  | 1:A:840:ARG:HD2  | 2.36                     | 0.60              |
| 2:B:834:ASN:HB3  | 2:B:840:ILE:HG13 | 1.82                     | 0.60              |
| 6:F:130:ILE:O    | 6:F:148:VAL:CG2  | 2.49                     | 0.60              |
| 6:F:79:ARG:HG3   | 6:F:144:GLU:OE1  | 2.02                     | 0.60              |
| 7:G:153:GLN:HG2  | 7:G:154:VAL:HG23 | 1.83                     | 0.60              |
| 9:I:86:PHE:CE1   | 9:I:100:PHE:HB2  | 2.36                     | 0.60              |
| 11:K:42:LEU:O    | 11:K:46:ILE:HG13 | 2.02                     | 0.60              |
| 1:A:356:ASP:OD2  | 11:K:65:HIS:HE1  | 1.83                     | 0.60              |
| 1:A:1333:ILE:O   | 1:A:1337:GLU:HG3 | 2.02                     | 0.60              |
| 1:A:353:ILE:HG21 | 1:A:487:MET:HE3  | 1.82                     | 0.60              |
| 3:C:165:LYS:O    | 11:K:6:ARG:NH1   | 2.35                     | 0.60              |
| 1:A:1289:ARG:HD2 | 1:A:1303:GLU:OE2 | 2.02                     | 0.60              |
| 1:A:382:PRO:CB   | 1:A:428:TYR:HE2  | 2.12                     | 0.60              |
| 1:A:783:THR:HG22 | 1:A:784:LEU:HG   | 1.84                     | 0.60              |
| 1:A:821:ARG:HD2  | 1:A:825:ILE:HD11 | 1.83                     | 0.60              |
| 1:A:351:THR:HB   | 2:B:1103:ILE:CD1 | 2.32                     | 0.60              |
| 2:B:515:HIS:CD2  | 2:B:517:THR:H    | 2.17                     | 0.60              |
| 2:B:830:TYR:CE2  | 2:B:1000:PRO:HD3 | 2.37                     | 0.60              |
| 1:A:268:ASP:HB3  | 1:A:299:HIS:ND1  | 2.17                     | 0.60              |
| 1:A:901:LEU:HA   | 1:A:907:THR:OG1  | 2.02                     | 0.60              |
| 2:B:1001:PHE:CD2 | 3:C:34:ARG:NH2   | 2.70                     | 0.60              |
| 2:B:798:TYR:HE2  | 3:C:62:PHE:CZ    | 2.20                     | 0.60              |
| 3:C:100:THR:HG22 | 3:C:101:LEU:N    | 2.16                     | 0.60              |
| 4:D:138:ASN:OD1  | 4:D:141:LEU:HB2  | 2.02                     | 0.60              |
| 7:G:1:MET:SD     | 7:G:79:PHE:CD1   | 2.95                     | 0.60              |
| 11:K:68:PHE:N    | 11:K:68:PHE:CD2  | 2.67                     | 0.60              |
| 15:T:22:BRU:H2'  | 15:T:23:DG:O4'   | 2.01                     | 0.60              |
| 3:C:179:GLU:HG2  | 3:C:180:TYR:N    | 2.17                     | 0.60              |
| 4:D:4:SER:OG     | 4:D:5:THR:N      | 2.34                     | 0.60              |
| 6:F:77:ASP:C     | 6:F:79:ARG:H     | 2.06                     | 0.60              |
| 7:G:80:LYS:HG2   | 7:G:80:LYS:O     | 2.02                     | 0.60              |
| 12:L:32:ALA:HB3  | 12:L:55:ILE:CD1  | 2.31                     | 0.60              |
| 1:A:12:ARG:HD2   | 2:B:1218:THR:HB  | 1.84                     | 0.59              |
| 2:B:880:THR:O    | 2:B:881:ASN:HB2  | 2.01                     | 0.59              |
| 3:C:2:SER:N      | 3:C:3:GLU:N      | 2.50                     | 0.59              |
| 3:C:66:ARG:NH2   | 10:J:5:VAL:HG23  | 2.15                     | 0.59              |
| 1:A:1017:LEU:HB3 | 5:E:205:SER:HA   | 1.83                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:111:LEU:C     | 6:F:113:GLY:H     | 2.05                     | 0.59              |
| 7:G:119:LEU:HD12  | 7:G:131:GLN:O     | 2.01                     | 0.59              |
| 1:A:1120:LEU:HD13 | 1:A:1304:TRP:O    | 2.01                     | 0.59              |
| 1:A:1451:VAL:O    | 1:A:1454:MET:HG2  | 2.02                     | 0.59              |
| 1:A:384:ASN:O     | 1:A:386:ASP:N     | 2.34                     | 0.59              |
| 1:A:463:ILE:HD12  | 1:A:469:ARG:HD2   | 1.84                     | 0.59              |
| 2:B:240:ILE:CG2   | 2:B:254:LEU:HB3   | 2.32                     | 0.59              |
| 2:B:603:LEU:HD13  | 2:B:608:ASP:HB2   | 1.83                     | 0.59              |
| 2:B:995:ARG:HH12  | 3:C:165:LYS:HG2   | 1.66                     | 0.59              |
| 3:C:147:LEU:HD12  | 3:C:151:GLN:O     | 2.02                     | 0.59              |
| 7:G:49:LEU:HG     | 7:G:76:ALA:HA     | 1.82                     | 0.59              |
| 8:H:127:GLY:O     | 8:H:128:ASN:HB2   | 2.02                     | 0.59              |
| 3:C:66:ARG:CZ     | 10:J:2:ILE:HG21   | 2.31                     | 0.59              |
| 15:T:22:BRU:H2'   | 15:T:23:DG:H8     | 1.62                     | 0.59              |
| 1:A:1323:ASP:OD1  | 1:A:1325:THR:HB   | 2.02                     | 0.59              |
| 1:A:720:ARG:O     | 1:A:724:GLU:HB2   | 2.02                     | 0.59              |
| 15:T:17:DT:C2'    | 15:T:18:DT:C5'    | 2.65                     | 0.59              |
| 1:A:1063:MET:HG3  | 1:A:1436:ILE:HG23 | 1.83                     | 0.59              |
| 1:A:590:ARG:O     | 1:A:591:PHE:HB2   | 2.01                     | 0.59              |
| 1:A:809:THR:H     | 1:A:812:GLU:HB2   | 1.66                     | 0.59              |
| 1:A:901:LEU:HD22  | 1:A:919:ILE:CG2   | 2.32                     | 0.59              |
| 2:B:1079:LYS:HA   | 3:C:27:LEU:HD21   | 1.83                     | 0.59              |
| 2:B:899:ILE:HD13  | 2:B:905:VAL:HG11  | 1.82                     | 0.59              |
| 2:B:980:PHE:HD2   | 2:B:1094:ARG:HA   | 1.68                     | 0.59              |
| 5:E:94:LYS:HE2    | 5:E:98:ILE:CD1    | 2.30                     | 0.59              |
| 4:D:40:HIS:CB     | 7:G:73:LYS:HZ3    | 2.02                     | 0.59              |
| 8:H:40:LEU:HD12   | 8:H:122:LEU:O     | 2.03                     | 0.59              |
| 1:A:1261:LYS:O    | 1:A:1264:GLU:HB3  | 2.03                     | 0.59              |
| 1:A:23:SER:HA     | 1:A:233:TRP:CD1   | 2.38                     | 0.59              |
| 1:A:289:ILE:C     | 1:A:291:GLU:H     | 2.03                     | 0.59              |
| 1:A:405:VAL:HG22  | 1:A:432:VAL:HG13  | 1.85                     | 0.59              |
| 1:A:55:ASP:C      | 1:A:57:ARG:H      | 2.04                     | 0.59              |
| 1:A:49:LYS:HZ3    | 1:A:61:ILE:HG13   | 1.67                     | 0.59              |
| 1:A:738:LYS:HD2   | 1:A:740:LEU:HD21  | 1.84                     | 0.59              |
| 2:B:1103:ILE:O    | 2:B:1122:ARG:NH1  | 2.35                     | 0.59              |
| 2:B:401:PHE:HD2   | 2:B:521:LEU:HD12  | 1.66                     | 0.59              |
| 2:B:579:ARG:HH11  | 2:B:579:ARG:HG2   | 1.66                     | 0.59              |
| 2:B:603:LEU:HD12  | 2:B:609:ILE:HG13  | 1.82                     | 0.59              |
| 2:B:942:ARG:NH2   | 15:T:25:DT:P      | 2.75                     | 0.59              |
| 1:A:1291:VAL:HG13 | 1:A:1292:PRO:HD2  | 1.84                     | 0.59              |
| 1:A:665:GLY:O     | 1:A:667:GLY:N     | 2.35                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:185:THR:H     | 2:B:188:ASP:CB   | 2.14                     | 0.59              |
| 2:B:611:PRO:HB3   | 2:B:685:LEU:HD11 | 1.84                     | 0.59              |
| 2:B:731:VAL:HG12  | 2:B:732:SER:N    | 2.17                     | 0.59              |
| 5:E:177:ARG:C     | 5:E:212:ARG:HD3  | 2.22                     | 0.59              |
| 10:J:44:TYR:HD2   | 10:J:44:TYR:H    | 1.48                     | 0.59              |
| 1:A:1283:VAL:HG12 | 1:A:1284:MET:N   | 2.18                     | 0.59              |
| 1:A:269:ILE:HD11  | 1:A:300:VAL:HA   | 1.83                     | 0.59              |
| 1:A:596:THR:C     | 1:A:598:LEU:H    | 2.05                     | 0.59              |
| 2:B:616:ILE:HG13  | 2:B:697:GLU:HA   | 1.85                     | 0.59              |
| 6:F:119:ARG:HH11  | 6:F:119:ARG:HG3  | 1.67                     | 0.59              |
| 10:J:36:LEU:HD22  | 10:J:41:LEU:HD12 | 1.83                     | 0.59              |
| 1:A:1107:VAL:HG12 | 1:A:1107:VAL:O   | 2.02                     | 0.59              |
| 1:A:1385:THR:O    | 1:A:1387:HIS:N   | 2.36                     | 0.59              |
| 3:C:124:LEU:O     | 3:C:127:ARG:HG2  | 2.03                     | 0.59              |
| 2:B:1005:GLY:HA2  | 3:C:176:ILE:O    | 2.02                     | 0.59              |
| 15:T:26:DC:H2''   | 15:T:27:DA:C5'   | 2.32                     | 0.59              |
| 1:A:1224:LEU:HD12 | 1:A:1241:ARG:O   | 2.02                     | 0.59              |
| 1:A:765:VAL:HG23  | 1:A:802:ASN:O    | 2.03                     | 0.59              |
| 4:D:13:ARG:HB2    | 4:D:17:LYS:HZ2   | 1.67                     | 0.59              |
| 5:E:15:ALA:O      | 5:E:19:VAL:HG23  | 2.03                     | 0.59              |
| 8:H:43:ASN:OD1    | 8:H:46:LEU:HG    | 2.03                     | 0.59              |
| 1:A:75:ASN:O      | 1:A:76:GLU:CB    | 2.51                     | 0.59              |
| 2:B:229:ALA:HB1   | 2:B:231:PRO:HD2  | 1.85                     | 0.59              |
| 2:B:483:LEU:HD11  | 2:B:491:THR:CG2  | 2.33                     | 0.59              |
| 2:B:57:TYR:N      | 2:B:57:TYR:HD1   | 2.01                     | 0.59              |
| 2:B:745:PRO:C     | 2:B:747:MET:H    | 2.06                     | 0.59              |
| 2:B:431:TYR:CZ    | 2:B:447:ALA:HB2  | 2.38                     | 0.58              |
| 2:B:594:ALA:HA    | 2:B:617:ARG:NH1  | 2.18                     | 0.58              |
| 5:E:156:LEU:HD12  | 5:E:195:VAL:HB   | 1.84                     | 0.58              |
| 8:H:15:VAL:HG22   | 8:H:26:ILE:HG12  | 1.85                     | 0.58              |
| 1:A:630:ILE:HD13  | 1:A:646:PHE:CZ   | 2.38                     | 0.58              |
| 1:A:914:GLU:HB2   | 1:A:979:SER:O    | 2.03                     | 0.58              |
| 4:D:52:LEU:C      | 4:D:54:GLU:H     | 2.05                     | 0.58              |
| 5:E:157:SER:HG    | 5:E:160:GLU:HG3  | 1.68                     | 0.58              |
| 7:G:1:MET:SD      | 7:G:1:MET:O      | 2.61                     | 0.58              |
| 2:B:1039:GLY:HA2  | 10:J:51:LEU:HD22 | 1.84                     | 0.58              |
| 10:J:64:ASN:CB    | 10:J:65:PRO:CD   | 2.81                     | 0.58              |
| 1:A:1116:LEU:HB2  | 1:A:1329:THR:OG1 | 2.03                     | 0.58              |
| 1:A:1120:LEU:O    | 1:A:1323:ASP:HB2 | 2.03                     | 0.58              |
| 1:A:33:ALA:HA     | 1:A:57:ARG:NH2   | 2.18                     | 0.58              |
| 1:A:528:LEU:HD12  | 1:A:528:LEU:C    | 2.23                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:666:ILE:CD1   | 1:A:667:GLY:H     | 2.17                     | 0.58              |
| 1:A:832:ALA:O     | 1:A:833:GLU:C     | 2.42                     | 0.58              |
| 8:H:38:LEU:HD12   | 8:H:124:ARG:O     | 2.03                     | 0.58              |
| 15:T:14:DC:H1'    | 15:T:15:DT:H5'    | 1.86                     | 0.58              |
| 1:A:444:PHE:HB2   | 1:A:458:HIS:HD2   | 1.68                     | 0.58              |
| 2:B:225:VAL:HA    | 2:B:237:VAL:O     | 2.03                     | 0.58              |
| 2:B:343:ILE:HG22  | 2:B:345:LYS:H     | 1.66                     | 0.58              |
| 3:C:174:ALA:O     | 3:C:175:ALA:HB2   | 2.04                     | 0.58              |
| 4:D:160:VAL:O     | 4:D:164:ILE:HG13  | 2.03                     | 0.58              |
| 1:A:1118:VAL:CG2  | 1:A:1306:LEU:HB2  | 2.33                     | 0.58              |
| 1:A:982:THR:O     | 1:A:985:ASP:HB2   | 2.04                     | 0.58              |
| 2:B:57:TYR:CD1    | 2:B:57:TYR:N      | 2.70                     | 0.58              |
| 2:B:864:LYS:N     | 2:B:872:GLU:OE1   | 2.37                     | 0.58              |
| 5:E:178:ILE:HG22  | 5:E:213:ILE:O     | 2.04                     | 0.58              |
| 6:F:111:LEU:H     | 6:F:111:LEU:CD1   | 2.13                     | 0.58              |
| 2:B:309:GLN:OE1   | 9:I:52:ILE:HD11   | 2.04                     | 0.58              |
| 1:A:224:PHE:HD2   | 1:A:229:SER:O     | 1.86                     | 0.58              |
| 1:A:399:HIS:O     | 1:A:401:GLY:N     | 2.36                     | 0.58              |
| 1:A:444:PHE:CB    | 1:A:458:HIS:HD2   | 2.15                     | 0.58              |
| 2:B:486:TYR:HH    | 2:B:1096:ARG:HB3  | 1.68                     | 0.58              |
| 2:B:344:LYS:O     | 2:B:345:LYS:HB2   | 2.03                     | 0.58              |
| 2:B:777:ALA:HA    | 2:B:1095:LEU:HA   | 1.85                     | 0.58              |
| 4:D:53:SER:HB3    | 4:D:153:ARG:H     | 1.67                     | 0.58              |
| 4:D:66:ARG:O      | 4:D:70:PHE:HB2    | 2.04                     | 0.58              |
| 7:G:48:VAL:HG13   | 7:G:74:TYR:HD1    | 1.68                     | 0.58              |
| 1:A:1313:LEU:HD23 | 1:A:1338:VAL:CG2  | 2.33                     | 0.58              |
| 1:A:1402:PHE:CD1  | 1:A:1403:GLU:HG3  | 2.38                     | 0.58              |
| 1:A:34:LYS:HB3    | 1:A:36:ARG:HE     | 1.69                     | 0.58              |
| 1:A:49:LYS:HZ1    | 1:A:61:ILE:N      | 2.01                     | 0.58              |
| 1:A:783:THR:HG21  | 1:A:815:PHE:CE2   | 2.39                     | 0.58              |
| 1:A:964:ILE:O     | 1:A:967:ALA:N     | 2.37                     | 0.58              |
| 2:B:1084:GLN:HE21 | 2:B:1084:GLN:H    | 1.50                     | 0.58              |
| 2:B:1159:ARG:HE   | 2:B:1193:GLN:HE21 | 1.51                     | 0.58              |
| 2:B:990:ILE:HG22  | 2:B:991:GLY:N     | 2.19                     | 0.58              |
| 5:E:23:VAL:O      | 5:E:28:TYR:HB2    | 2.04                     | 0.58              |
| 8:H:81:PRO:HB2    | 8:H:82:PRO:CD     | 2.34                     | 0.58              |
| 1:A:606:LEU:HB3   | 1:A:614:PHE:CE2   | 2.39                     | 0.58              |
| 2:B:981:ALA:HB2   | 2:B:987:LYS:HA    | 1.86                     | 0.58              |
| 4:D:192:LYS:HB3   | 4:D:192:LYS:HZ3   | 1.69                     | 0.58              |
| 9:I:25:LEU:HB3    | 9:I:38:ALA:HB2    | 1.84                     | 0.58              |
| 1:A:1001:ARG:O    | 1:A:1002:GLY:O    | 2.22                     | 0.58              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:475:THR:CG2   | 1:A:476:SER:N    | 2.66                     | 0.58              |
| 1:A:492:PRO:O     | 1:A:493:GLN:NE2  | 2.36                     | 0.58              |
| 1:A:457:ALA:HB3   | 1:A:506:ALA:HA   | 1.85                     | 0.58              |
| 1:A:648:ASN:O     | 1:A:649:ILE:C    | 2.41                     | 0.58              |
| 2:B:1159:ARG:NH1  | 2:B:1159:ARG:HB3 | 2.18                     | 0.58              |
| 2:B:265:SER:O     | 2:B:266:ALA:HB3  | 2.04                     | 0.58              |
| 2:B:778:MET:CE    | 2:B:1094:ARG:CD  | 2.82                     | 0.58              |
| 3:C:18:VAL:HG23   | 3:C:240:VAL:CG1  | 2.34                     | 0.58              |
| 4:D:144:THR:HG21  | 7:G:46:LEU:HD13  | 1.85                     | 0.58              |
| 6:F:99:LEU:C      | 6:F:99:LEU:HD12  | 2.24                     | 0.58              |
| 11:K:111:LEU:O    | 11:K:112:GLN:HG2 | 2.03                     | 0.58              |
| 15:T:19:TT:H2'1   | 15:T:19:TT:H5R1  | 1.83                     | 0.58              |
| 3:C:184:ASN:ND2   | 3:C:187:LYS:HA   | 2.19                     | 0.58              |
| 4:D:53:SER:HB3    | 4:D:152:SER:CB   | 2.33                     | 0.58              |
| 6:F:75:PRO:O      | 6:F:77:ASP:O     | 2.22                     | 0.58              |
| 1:A:1017:LEU:HB2  | 5:E:206:GLY:N    | 2.07                     | 0.57              |
| 1:A:1305:VAL:HG12 | 1:A:1306:LEU:N   | 2.19                     | 0.57              |
| 1:A:58:LEU:CG     | 1:A:59:GLY:N     | 2.66                     | 0.57              |
| 1:A:699:ALA:CB    | 1:A:701:LEU:HG   | 2.34                     | 0.57              |
| 3:C:214:ASN:HB3   | 3:C:217:ASP:OD2  | 2.03                     | 0.57              |
| 4:D:51:ASN:O      | 4:D:52:LEU:O     | 2.22                     | 0.57              |
| 5:E:207:ARG:CB    | 5:E:207:ARG:HH11 | 2.16                     | 0.57              |
| 1:A:1293:SER:OG   | 1:A:1294:PRO:HD2 | 2.03                     | 0.57              |
| 1:A:399:HIS:CB    | 1:A:400:PRO:HD3  | 2.29                     | 0.57              |
| 2:B:229:ALA:CB    | 2:B:231:PRO:HD2  | 2.34                     | 0.57              |
| 2:B:370:PHE:HD2   | 2:B:373:ARG:HD2  | 1.69                     | 0.57              |
| 4:D:134:THR:CG2   | 4:D:135:GLY:N    | 2.66                     | 0.57              |
| 4:D:167:LEU:HB3   | 4:D:177:VAL:HG13 | 1.85                     | 0.57              |
| 7:G:3:PHE:CE1     | 7:G:80:LYS:HE2   | 2.38                     | 0.57              |
| 12:L:39:SER:O     | 12:L:40:LEU:HG   | 2.03                     | 0.57              |
| 1:A:1341:ILE:CG2  | 1:A:1342:GLU:N   | 2.67                     | 0.57              |
| 1:A:471:ASN:O     | 1:A:474:VAL:HG12 | 2.04                     | 0.57              |
| 2:B:792:MET:HG3   | 2:B:855:PHE:HE1  | 1.69                     | 0.57              |
| 2:B:910:VAL:HG12  | 2:B:912:ILE:H    | 1.69                     | 0.57              |
| 5:E:213:ILE:HG12  | 5:E:214:CYS:N    | 2.19                     | 0.57              |
| 1:A:699:ALA:HB1   | 1:A:701:LEU:HG   | 1.85                     | 0.57              |
| 1:A:754:SER:N     | 1:A:757:ASN:HD22 | 1.92                     | 0.57              |
| 2:B:167:ILE:HG22  | 2:B:453:ILE:HD12 | 1.86                     | 0.57              |
| 1:A:1373:ASP:HA   | 1:A:1376:THR:CG2 | 2.34                     | 0.57              |
| 1:A:37:PHE:N      | 1:A:37:PHE:CD1   | 2.72                     | 0.57              |
| 1:A:567:LYS:CG    | 1:A:568:PRO:CD   | 2.76                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:486:TYR:CZ    | 2:B:1096:ARG:HB3  | 2.39                     | 0.57              |
| 2:B:996:ARG:NH2   | 3:C:175:ALA:HA    | 2.20                     | 0.57              |
| 4:D:18:VAL:O      | 4:D:18:VAL:HG13   | 2.05                     | 0.57              |
| 7:G:145:VAL:CG1   | 7:G:146:LYS:N     | 2.67                     | 0.57              |
| 9:I:103:CYS:HB3   | 9:I:106:CYS:SG    | 2.45                     | 0.57              |
| 14:P:4:A:O2'      | 14:P:5:C:H5'      | 2.05                     | 0.57              |
| 1:A:42:ASP:HB3    | 1:A:45:GLN:N      | 2.19                     | 0.57              |
| 1:A:482:PHE:C     | 1:A:484:GLY:H     | 2.07                     | 0.57              |
| 1:A:683:ILE:HD13  | 1:A:801:GLU:HG3   | 1.86                     | 0.57              |
| 1:A:709:THR:HG21  | 9:I:93:LYS:O      | 2.05                     | 0.57              |
| 2:B:1033:LYS:NZ   | 2:B:1070:GLU:OE1  | 2.36                     | 0.57              |
| 2:B:1159:ARG:HD3  | 2:B:1193:GLN:CG   | 2.35                     | 0.57              |
| 2:B:1219:ASP:O    | 2:B:1219:ASP:OD1  | 2.23                     | 0.57              |
| 2:B:521:LEU:HB3   | 2:B:633:VAL:HG11  | 1.86                     | 0.57              |
| 2:B:580:VAL:HG22  | 2:B:624:LEU:CB    | 2.35                     | 0.57              |
| 3:C:46:ILE:HG23   | 3:C:157:CYS:HB3   | 1.86                     | 0.57              |
| 5:E:124:VAL:HB    | 5:E:125:PRO:HD3   | 1.87                     | 0.57              |
| 12:L:58:LYS:HG2   | 12:L:58:LYS:O     | 2.03                     | 0.57              |
| 1:A:1116:LEU:HB3  | 1:A:1308:THR:HG21 | 1.87                     | 0.57              |
| 2:B:1023:VAL:O    | 2:B:1026:LEU:N    | 2.38                     | 0.57              |
| 2:B:195:CYS:SG    | 2:B:197:PHE:HB2   | 2.45                     | 0.57              |
| 1:A:1332:PHE:CE1  | 1:A:1348:LEU:HD13 | 2.39                     | 0.57              |
| 1:A:58:LEU:CD1    | 1:A:243:PRO:HB3   | 2.33                     | 0.57              |
| 1:A:699:ALA:O     | 1:A:700:ASN:HB3   | 2.04                     | 0.57              |
| 2:B:332:ASP:OD1   | 2:B:336:ARG:NE    | 2.38                     | 0.57              |
| 2:B:340:ALA:CB    | 2:B:343:ILE:HD12  | 2.35                     | 0.57              |
| 7:G:154:VAL:HG12  | 7:G:155:SER:N     | 2.20                     | 0.57              |
| 1:A:1226:VAL:HG13 | 1:A:1240:CYS:HB3  | 1.87                     | 0.57              |
| 2:B:1106:ARG:HG3  | 2:B:1107:ALA:N    | 2.18                     | 0.57              |
| 2:B:496:ARG:HH11  | 2:B:496:ARG:HB3   | 1.69                     | 0.57              |
| 2:B:744:HIS:HD2   | 2:B:746:SER:CB    | 2.16                     | 0.57              |
| 2:B:874:PHE:HA    | 2:B:913:GLY:O     | 2.05                     | 0.57              |
| 3:C:46:ILE:HG13   | 3:C:72:LEU:HD11   | 1.87                     | 0.57              |
| 4:D:4:SER:O       | 4:D:5:THR:HB      | 2.03                     | 0.57              |
| 1:A:1095:THR:OG1  | 1:A:1113:THR:HB   | 2.05                     | 0.57              |
| 1:A:1127:ASP:HB3  | 1:A:1130:GLN:CB   | 2.34                     | 0.57              |
| 1:A:35:ILE:HD12   | 1:A:241:VAL:HG21  | 1.85                     | 0.57              |
| 10:J:44:TYR:HA    | 10:J:47:ARG:HB3   | 1.87                     | 0.57              |
| 1:A:406:ILE:HG13  | 1:A:431:LYS:HB2   | 1.87                     | 0.56              |
| 1:A:600:PRO:HG2   | 1:A:601:LYS:H     | 1.70                     | 0.56              |
| 1:A:709:THR:HB    | 1:A:712:GLU:HG3   | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:176:SER:O     | 2:B:182:SER:HB3   | 2.04                     | 0.56              |
| 2:B:386:LEU:O     | 2:B:388:CYS:N     | 2.37                     | 0.56              |
| 3:C:11:ARG:HD3    | 3:C:209:TYR:CE2   | 2.39                     | 0.56              |
| 3:C:212:PRO:CB    | 3:C:213:PRO:HD2   | 2.35                     | 0.56              |
| 5:E:90:VAL:HA     | 5:E:120:ALA:HB2   | 1.86                     | 0.56              |
| 7:G:88:ASP:OD2    | 7:G:88:ASP:N      | 2.37                     | 0.56              |
| 9:I:15:TYR:CD1    | 9:I:15:TYR:N      | 2.73                     | 0.56              |
| 11:K:47:ARG:HD2   | 11:K:47:ARG:O     | 2.05                     | 0.56              |
| 1:A:1446:ASP:HB3  | 1:A:1449:SER:OG   | 2.05                     | 0.56              |
| 1:A:1450:LEU:HD21 | 7:G:18:PHE:O      | 2.04                     | 0.56              |
| 1:A:853:ASP:OD1   | 1:A:855:THR:N     | 2.38                     | 0.56              |
| 1:A:982:THR:N     | 1:A:985:ASP:HB2   | 2.20                     | 0.56              |
| 2:B:1176:ASN:C    | 2:B:1178:ASN:H    | 2.08                     | 0.56              |
| 2:B:288:ALA:HA    | 2:B:331:LEU:HD12  | 1.87                     | 0.56              |
| 2:B:199:MET:HE2   | 2:B:492:LEU:HD23  | 1.87                     | 0.56              |
| 3:C:20:PHE:CE1    | 3:C:22:LEU:HD12   | 2.40                     | 0.56              |
| 3:C:241:ASP:O     | 3:C:245:VAL:HG23  | 2.05                     | 0.56              |
| 6:F:81:THR:HG23   | 6:F:144:GLU:OE2   | 2.06                     | 0.56              |
| 7:G:51:TYR:C      | 7:G:51:TYR:CD2    | 2.79                     | 0.56              |
| 9:I:62:ILE:HG12   | 9:I:62:ILE:O      | 2.05                     | 0.56              |
| 1:A:1356:ILE:HD12 | 1:A:1368:MET:SD   | 2.45                     | 0.56              |
| 1:A:1428:VAL:HG13 | 2:B:1151:LEU:CD2  | 2.36                     | 0.56              |
| 1:A:709:THR:HG22  | 1:A:710:LEU:N     | 2.20                     | 0.56              |
| 1:A:866:PHE:O     | 1:A:867:ILE:HD12  | 2.06                     | 0.56              |
| 2:B:1050:ILE:HG22 | 2:B:1051:THR:N    | 2.19                     | 0.56              |
| 1:A:412:ARG:NH2   | 2:B:1108:ARG:NH1  | 2.54                     | 0.56              |
| 2:B:1155:SER:OG   | 2:B:1156:ASP:N    | 2.37                     | 0.56              |
| 3:C:98:VAL:C      | 3:C:99:LEU:HD23   | 2.26                     | 0.56              |
| 5:E:168:TYR:HB2   | 5:E:170:LEU:HG    | 1.86                     | 0.56              |
| 9:I:82:GLU:O      | 9:I:104:LEU:HG    | 2.05                     | 0.56              |
| 1:A:1072:ILE:O    | 1:A:1075:PRO:HD2  | 2.05                     | 0.56              |
| 1:A:1162:VAL:HG12 | 1:A:1162:VAL:O    | 2.06                     | 0.56              |
| 1:A:1279:ILE:CD1  | 1:A:1316:VAL:HG21 | 2.35                     | 0.56              |
| 1:A:222:LEU:O     | 1:A:224:PHE:N     | 2.38                     | 0.56              |
| 1:A:244:PRO:HG2   | 1:A:245:PRO:HD3   | 1.86                     | 0.56              |
| 1:A:500:GLU:OE1   | 2:B:1143:ALA:C    | 2.44                     | 0.56              |
| 1:A:525:GLN:HG3   | 2:B:835:GLN:HG2   | 1.86                     | 0.56              |
| 1:A:711:ARG:NH2   | 9:I:87:GLN:OE1    | 2.39                     | 0.56              |
| 1:A:31:SER:OG     | 1:A:82:GLY:HA2    | 2.04                     | 0.56              |
| 1:A:858:ASN:ND2   | 1:A:858:ASN:C     | 2.59                     | 0.56              |
| 1:A:869:GLY:O     | 5:E:204:THR:HG21  | 2.04                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:295:GLY:H     | 2:B:298:LEU:HD23  | 1.69                     | 0.56              |
| 6:F:89:GLU:OE2    | 6:F:134:ILE:HG21  | 2.05                     | 0.56              |
| 7:G:114:LEU:HG    | 7:G:162:SER:HB3   | 1.87                     | 0.56              |
| 2:B:1006:ILE:HG22 | 10:J:45:CYS:HB3   | 1.87                     | 0.56              |
| 1:A:968:GLN:O     | 1:A:970:THR:N     | 2.38                     | 0.56              |
| 2:B:758:PHE:CE1   | 2:B:1027:ILE:HG22 | 2.41                     | 0.56              |
| 2:B:310:MET:HE3   | 2:B:387:LEU:CD1   | 2.34                     | 0.56              |
| 2:B:527:THR:OG1   | 2:B:528:PRO:HD2   | 2.04                     | 0.56              |
| 3:C:77:ILE:O      | 3:C:79:GLN:N      | 2.39                     | 0.56              |
| 8:H:61:SER:O      | 8:H:62:SER:CB     | 2.54                     | 0.56              |
| 8:H:91:ASP:C      | 8:H:93:TYR:H      | 2.08                     | 0.56              |
| 10:J:44:TYR:N     | 10:J:44:TYR:CD2   | 2.73                     | 0.56              |
| 2:B:1039:GLY:HA2  | 10:J:51:LEU:HD21  | 1.87                     | 0.56              |
| 3:C:58:LEU:HD21   | 10:J:57:ILE:HD12  | 1.88                     | 0.56              |
| 1:A:1124:HIS:HB3  | 1:A:1130:GLN:HG2  | 1.87                     | 0.56              |
| 1:A:154:SER:HB3   | 1:A:162:VAL:HG21  | 1.88                     | 0.56              |
| 1:A:626:ASN:O     | 1:A:631:HIS:CD2   | 2.59                     | 0.56              |
| 2:B:344:LYS:O     | 2:B:345:LYS:CB    | 2.53                     | 0.56              |
| 2:B:831:SER:HB3   | 2:B:994:TYR:OH    | 2.05                     | 0.56              |
| 8:H:113:ALA:HB2   | 8:H:126:GLU:HG3   | 1.88                     | 0.56              |
| 9:I:55:THR:CG2    | 9:I:58:VAL:HG21   | 2.36                     | 0.56              |
| 9:I:92:ARG:HB3    | 9:I:95:THR:OG1    | 2.05                     | 0.56              |
| 12:L:58:LYS:O     | 12:L:59:ALA:O     | 2.24                     | 0.56              |
| 1:A:384:ASN:CG    | 1:A:388:LEU:HD12  | 2.25                     | 0.56              |
| 1:A:730:GLY:C     | 1:A:732:LEU:H     | 2.09                     | 0.56              |
| 1:A:867:ILE:HG22  | 1:A:872:GLY:N     | 2.21                     | 0.56              |
| 2:B:758:PHE:CE1   | 2:B:1027:ILE:CG2  | 2.88                     | 0.56              |
| 1:A:1436:ILE:HD13 | 2:B:1139:ILE:HG23 | 1.87                     | 0.56              |
| 2:B:776:GLN:O     | 2:B:1095:LEU:HA   | 2.06                     | 0.56              |
| 6:F:99:LEU:HD12   | 6:F:99:LEU:O      | 2.05                     | 0.56              |
| 7:G:111:THR:HG22  | 7:G:113:HIS:N     | 2.17                     | 0.56              |
| 8:H:100:THR:HG22  | 8:H:101:ALA:N     | 2.20                     | 0.56              |
| 8:H:39:THR:O      | 8:H:123:MET:HA    | 2.06                     | 0.56              |
| 10:J:44:TYR:HD2   | 10:J:44:TYR:N     | 2.03                     | 0.56              |
| 14:P:3:G:H2'      | 14:P:4:A:C8       | 2.41                     | 0.56              |
| 1:A:528:LEU:O     | 1:A:528:LEU:HD12  | 2.05                     | 0.56              |
| 1:A:806:ARG:HH12  | 2:B:729:ILE:CD1   | 2.18                     | 0.56              |
| 1:A:89:PRO:HB2    | 1:A:204:THR:HG22  | 1.87                     | 0.56              |
| 2:B:521:LEU:HD13  | 2:B:633:VAL:HB    | 1.86                     | 0.56              |
| 2:B:557:PHE:C     | 2:B:557:PHE:HD2   | 2.09                     | 0.56              |
| 3:C:176:ILE:HG22  | 3:C:177:GLU:N     | 2.21                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:902:LEU:HG    | 1:A:926:GLN:HG3   | 1.86                     | 0.56              |
| 2:B:1002:THR:HG23 | 2:B:1006:ILE:HG13 | 1.88                     | 0.56              |
| 2:B:343:ILE:HG21  | 2:B:348:ARG:H     | 1.70                     | 0.56              |
| 2:B:357:GLN:O     | 2:B:366:GLN:HA    | 2.04                     | 0.56              |
| 2:B:635:ARG:NH2   | 2:B:742:GLU:OE2   | 2.37                     | 0.56              |
| 2:B:658:ILE:HG22  | 2:B:659:ALA:N     | 2.21                     | 0.56              |
| 8:H:128:ASN:CG    | 8:H:128:ASN:O     | 2.44                     | 0.56              |
| 10:J:36:LEU:O     | 10:J:39:LEU:N     | 2.37                     | 0.56              |
| 14:P:7:A:H2'      | 14:P:8:G:C1'      | 2.36                     | 0.56              |
| 1:A:1387:HIS:NE2  | 13:N:4:DT:H5''    | 2.21                     | 0.56              |
| 1:A:442:VAL:HB    | 1:A:489:LEU:HD11  | 1.87                     | 0.56              |
| 1:A:590:ARG:HB3   | 1:A:605:MET:N     | 2.20                     | 0.56              |
| 1:A:596:THR:C     | 1:A:598:LEU:N     | 2.58                     | 0.56              |
| 1:A:95:PHE:O      | 1:A:96:ILE:C      | 2.44                     | 0.56              |
| 1:A:1410:PHE:HA   | 2:B:1212:ILE:CD1  | 2.35                     | 0.56              |
| 2:B:466:TRP:HA    | 2:B:466:TRP:CE3   | 2.41                     | 0.56              |
| 2:B:705:MET:H     | 2:B:710:LEU:CD1   | 2.19                     | 0.56              |
| 2:B:843:GLN:O     | 2:B:846:ILE:HB    | 2.06                     | 0.56              |
| 2:B:882:THR:HG21  | 2:B:935:ARG:HA    | 1.87                     | 0.56              |
| 5:E:105:PHE:O     | 5:E:106:GLN:HB2   | 2.06                     | 0.56              |
| 1:A:1444:MET:HG3  | 7:G:60:ARG:HA     | 1.88                     | 0.56              |
| 8:H:61:SER:HB2    | 8:H:139:ASN:HB3   | 1.87                     | 0.56              |
| 11:K:18:LYS:HZ3   | 11:K:38:GLU:HG2   | 1.70                     | 0.56              |
| 1:A:364:VAL:O     | 1:A:364:VAL:HG13  | 2.06                     | 0.56              |
| 1:A:920:LEU:HD23  | 1:A:921:GLY:N     | 2.20                     | 0.56              |
| 1:A:929:LEU:HD23  | 1:A:983:ILE:HG21  | 1.88                     | 0.56              |
| 1:A:942:PHE:HD2   | 1:A:943:LEU:HD23  | 1.70                     | 0.56              |
| 1:A:98:LYS:O      | 1:A:99:ILE:C      | 2.44                     | 0.56              |
| 4:D:17:LYS:CA     | 4:D:17:LYS:HE3    | 2.35                     | 0.56              |
| 11:K:49:GLU:HG3   | 11:K:94:ILE:HG12  | 1.87                     | 0.56              |
| 1:A:108:MET:N     | 1:A:108:MET:SD    | 2.79                     | 0.55              |
| 1:A:1397:LEU:HB2  | 1:A:1426:GLU:OE1  | 2.05                     | 0.55              |
| 1:A:239:LEU:HD12  | 1:A:240:PRO:HD2   | 1.87                     | 0.55              |
| 1:A:87:ALA:HB3    | 1:A:276:LEU:HD23  | 1.86                     | 0.55              |
| 1:A:446:ARG:HB2   | 1:A:487:MET:SD    | 2.47                     | 0.55              |
| 2:B:1166:CYS:O    | 2:B:1166:CYS:SG   | 2.63                     | 0.55              |
| 2:B:53:GLN:HG2    | 2:B:547:VAL:CG2   | 2.35                     | 0.55              |
| 3:C:243:VAL:HG12  | 3:C:243:VAL:O     | 2.05                     | 0.55              |
| 5:E:78:LEU:HD23   | 5:E:78:LEU:C      | 2.26                     | 0.55              |
| 4:D:47:LEU:HD11   | 7:G:3:PHE:CE2     | 2.40                     | 0.55              |
| 1:A:883:LEU:HD11  | 1:A:1017:LEU:HD11 | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1377:THR:O   | 1:A:1379:GLY:N   | 2.39                     | 0.55              |
| 1:A:93:VAL:CG1   | 1:A:301:ALA:HB1  | 2.33                     | 0.55              |
| 1:A:302:THR:HA   | 1:A:305:ASP:O    | 2.05                     | 0.55              |
| 1:A:449:SER:O    | 2:B:1133:MET:HB3 | 2.06                     | 0.55              |
| 1:A:981:LEU:CD2  | 1:A:1039:LYS:HA  | 2.35                     | 0.55              |
| 2:B:114:PRO:O    | 2:B:116:GLU:N    | 2.39                     | 0.55              |
| 2:B:293:PRO:HG2  | 2:B:296:GLU:CB   | 2.36                     | 0.55              |
| 2:B:51:PHE:O     | 2:B:54:PHE:HB3   | 2.06                     | 0.55              |
| 3:C:18:VAL:O     | 3:C:20:PHE:HD2   | 1.90                     | 0.55              |
| 6:F:118:LEU:O    | 6:F:122:MET:HG3  | 2.06                     | 0.55              |
| 9:I:106:CYS:O    | 9:I:107:SER:HB2  | 2.07                     | 0.55              |
| 11:K:110:ASN:O   | 11:K:111:LEU:CD2 | 2.50                     | 0.55              |
| 1:A:42:ASP:HB3   | 1:A:45:GLN:HA    | 1.88                     | 0.55              |
| 1:A:785:PRO:HG2  | 1:A:786:HIS:HD2  | 1.71                     | 0.55              |
| 1:A:898:ARG:HB2  | 1:A:933:TYR:CE1  | 2.41                     | 0.55              |
| 3:C:183:TRP:CZ2  | 3:C:207:CYS:HB3  | 2.41                     | 0.55              |
| 4:D:137:ASN:HD22 | 4:D:137:ASN:C    | 2.10                     | 0.55              |
| 4:D:52:LEU:HD21  | 4:D:147:TYR:HE2  | 1.71                     | 0.55              |
| 6:F:89:GLU:HB3   | 6:F:134:ILE:CD1  | 2.35                     | 0.55              |
| 7:G:83:LYS:HE2   | 7:G:150:CYS:H    | 1.72                     | 0.55              |
| 8:H:4:THR:CA     | 8:H:60:ALA:HB2   | 2.32                     | 0.55              |
| 8:H:64:ASN:O     | 8:H:65:LEU:HB2   | 2.05                     | 0.55              |
| 8:H:83:GLN:C     | 8:H:85:GLY:H     | 2.09                     | 0.55              |
| 8:H:84:ALA:CB    | 8:H:87:ARG:HB2   | 2.36                     | 0.55              |
| 15:T:10:DA:H2"   | 15:T:11:DG:OP2   | 2.06                     | 0.55              |
| 1:A:1076:ALA:HA  | 1:A:1079:MET:CE  | 2.36                     | 0.55              |
| 1:A:595:THR:O    | 1:A:596:THR:HG23 | 2.05                     | 0.55              |
| 1:A:852:TYR:CD2  | 1:A:1060:PRO:CB  | 2.89                     | 0.55              |
| 4:D:128:VAL:O    | 4:D:132:GLN:HG3  | 2.06                     | 0.55              |
| 5:E:55:ARG:C     | 5:E:57:MET:H     | 2.08                     | 0.55              |
| 7:G:47:CYS:O     | 7:G:76:ALA:HB1   | 2.06                     | 0.55              |
| 8:H:40:LEU:HD22  | 8:H:123:MET:HE2  | 1.87                     | 0.55              |
| 8:H:82:PRO:C     | 8:H:84:ALA:H     | 2.09                     | 0.55              |
| 9:I:86:PHE:HE1   | 9:I:100:PHE:HB2  | 1.71                     | 0.55              |
| 3:C:35:ARG:NH1   | 11:K:41:THR:OG1  | 2.40                     | 0.55              |
| 1:A:896:ARG:NH2  | 1:A:1030:ARG:NH2 | 2.54                     | 0.55              |
| 1:A:1114:PRO:O   | 1:A:1115:SER:O   | 2.24                     | 0.55              |
| 1:A:38:PRO:HA    | 1:A:270:LEU:HD23 | 1.88                     | 0.55              |
| 1:A:427:GLN:HB2  | 1:A:430:TRP:CD1  | 2.42                     | 0.55              |
| 1:A:42:ASP:HB3   | 1:A:45:GLN:CA    | 2.36                     | 0.55              |
| 1:A:61:ILE:O     | 1:A:63:ARG:N     | 2.40                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:742:ASN:O     | 1:A:745:GLN:HB2   | 2.05                     | 0.55              |
| 1:A:670:ILE:HG23  | 1:A:805:LEU:HD21  | 1.86                     | 0.55              |
| 2:B:254:LEU:HD23  | 2:B:381:MET:CE    | 2.37                     | 0.55              |
| 3:C:67:LEU:HD11   | 3:C:155:LEU:HD13  | 1.89                     | 0.55              |
| 4:D:7:THR:O       | 4:D:9:GLN:N       | 2.40                     | 0.55              |
| 5:E:157:SER:C     | 5:E:159:ASP:N     | 2.57                     | 0.55              |
| 6:F:125:LEU:O     | 6:F:125:LEU:HG    | 2.07                     | 0.55              |
| 6:F:69:LEU:N      | 6:F:70:LYS:CA     | 2.69                     | 0.55              |
| 8:H:55:LEU:HD22   | 8:H:144:ILE:CG2   | 2.36                     | 0.55              |
| 1:A:1191:TRP:CD1  | 1:A:1256:GLU:HB2  | 2.42                     | 0.55              |
| 2:B:1002:THR:HG21 | 2:B:1006:ILE:CD1  | 2.30                     | 0.55              |
| 2:B:217:ARG:O     | 2:B:217:ARG:HD2   | 2.07                     | 0.55              |
| 2:B:466:TRP:O     | 2:B:468:GLU:N     | 2.39                     | 0.55              |
| 3:C:167:HIS:CD2   | 3:C:168:ALA:H     | 2.23                     | 0.55              |
| 9:I:52:ILE:HG13   | 9:I:52:ILE:O      | 2.06                     | 0.55              |
| 11:K:69:ALA:O     | 11:K:70:ARG:HB3   | 2.06                     | 0.55              |
| 1:A:311:GLN:O     | 1:A:312:PRO:C     | 2.45                     | 0.55              |
| 2:B:1087:PHE:HD2  | 2:B:1088:GLY:H    | 1.50                     | 0.55              |
| 1:A:17:VAL:HA     | 2:B:1215:ARG:O    | 2.06                     | 0.55              |
| 2:B:729:ILE:HG22  | 2:B:729:ILE:O     | 2.04                     | 0.55              |
| 2:B:792:MET:HA    | 2:B:856:PHE:O     | 2.06                     | 0.55              |
| 2:B:971:THR:OG1   | 3:C:61:GLU:HG3    | 2.06                     | 0.55              |
| 7:G:10:ASN:OD1    | 7:G:71:ASN:HA     | 2.07                     | 0.55              |
| 7:G:20:PRO:HG2    | 7:G:21:ARG:H      | 1.70                     | 0.55              |
| 15:T:17:DT:H1'    | 15:T:18:DT:C5'    | 2.33                     | 0.55              |
| 1:A:1039:LYS:HE3  | 1:A:1043:ASP:OD2  | 2.07                     | 0.55              |
| 1:A:1215:ARG:HA   | 1:A:1218:GLN:HG2  | 1.89                     | 0.55              |
| 1:A:683:ILE:HG21  | 1:A:801:GLU:HG3   | 1.88                     | 0.55              |
| 1:A:687:LYS:O     | 1:A:690:VAL:HB    | 2.06                     | 0.55              |
| 1:A:68:GLN:O      | 1:A:70:CYS:N      | 2.39                     | 0.55              |
| 2:B:1106:ARG:HD3  | 2:B:1126:GLY:C    | 2.27                     | 0.55              |
| 1:A:14:VAL:CG2    | 2:B:1216:LEU:HD13 | 2.34                     | 0.55              |
| 2:B:130:VAL:HB    | 2:B:167:ILE:CD1   | 2.36                     | 0.55              |
| 3:C:90:ASP:O      | 3:C:91:HIS:HB3    | 2.05                     | 0.55              |
| 1:A:1450:LEU:HD11 | 6:F:108:PHE:CZ    | 2.41                     | 0.55              |
| 1:A:1151:GLU:HA   | 9:I:44:TYR:O      | 2.07                     | 0.55              |
| 10:J:48:ARG:HD2   | 10:J:49:MET:N     | 2.21                     | 0.55              |
| 14:P:6:C:H2'      | 14:P:7:A:H8       | 1.68                     | 0.55              |
| 1:A:115:LEU:HB2   | 1:A:122:MET:HE2   | 1.89                     | 0.55              |
| 1:A:353:ILE:CD1   | 1:A:487:MET:HE2   | 2.37                     | 0.55              |
| 1:A:341:MET:CE    | 2:B:1135:ARG:NH1  | 2.70                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:13:TRP:O      | 5:E:16:PHE:HB3    | 2.07                     | 0.55              |
| 2:B:1077:THR:HG22 | 11:K:44:ASN:HD21  | 1.71                     | 0.55              |
| 11:K:55:LYS:HB3   | 11:K:81:TYR:CD1   | 2.42                     | 0.55              |
| 1:A:1364:ASN:HD22 | 1:A:1365:TYR:N    | 2.05                     | 0.55              |
| 1:A:47:ARG:HH12   | 1:A:254:GLU:HG2   | 1.72                     | 0.55              |
| 2:B:129:PHE:HA    | 2:B:165:VAL:O     | 2.07                     | 0.55              |
| 2:B:343:ILE:CG2   | 2:B:348:ARG:N     | 2.66                     | 0.55              |
| 2:B:654:ARG:H     | 2:B:657:HIS:CD2   | 2.17                     | 0.55              |
| 2:B:745:PRO:C     | 2:B:747:MET:N     | 2.60                     | 0.55              |
| 4:D:176:GLU:C     | 4:D:178:ALA:N     | 2.60                     | 0.55              |
| 4:D:7:THR:HB      | 7:G:42:PHE:HE2    | 1.72                     | 0.55              |
| 1:A:1120:LEU:CD1  | 1:A:1120:LEU:N    | 2.69                     | 0.54              |
| 1:A:265:LYS:HZ3   | 1:A:322:VAL:HG13  | 1.71                     | 0.54              |
| 1:A:548:ASN:HA    | 11:K:60:ALA:HB1   | 1.89                     | 0.54              |
| 2:B:758:PHE:HE1   | 2:B:1027:ILE:HG22 | 1.72                     | 0.54              |
| 2:B:911:ILE:O     | 2:B:912:ILE:HG13  | 2.07                     | 0.54              |
| 3:C:189:THR:HG22  | 3:C:190:ASP:H     | 1.71                     | 0.54              |
| 7:G:18:PHE:HA     | 7:G:22:MET:CE     | 2.36                     | 0.54              |
| 1:A:1308:THR:HG23 | 1:A:1309:ASP:N    | 2.22                     | 0.54              |
| 1:A:1348:LEU:O    | 1:A:1352:VAL:HG23 | 2.07                     | 0.54              |
| 1:A:1424:VAL:CG1  | 1:A:1436:ILE:HD11 | 2.34                     | 0.54              |
| 1:A:182:VAL:HG22  | 1:A:201:VAL:HA    | 1.89                     | 0.54              |
| 1:A:265:LYS:HE2   | 1:A:322:VAL:HG11  | 1.89                     | 0.54              |
| 3:C:97:VAL:HG12   | 3:C:99:LEU:CD2    | 2.37                     | 0.54              |
| 4:D:48:ILE:HG21   | 7:G:4:ILE:HB      | 1.89                     | 0.54              |
| 4:D:63:LEU:HD13   | 4:D:133:THR:OG1   | 2.07                     | 0.54              |
| 9:I:50:THR:HG22   | 9:I:52:ILE:H      | 1.72                     | 0.54              |
| 1:A:1227:ILE:HG22 | 1:A:1228:TRP:N    | 2.22                     | 0.54              |
| 2:B:1165:ILE:HG12 | 4:D:17:LYS:HD2    | 1.89                     | 0.54              |
| 2:B:38:PHE:CD1    | 2:B:811:TYR:CD2   | 2.94                     | 0.54              |
| 2:B:834:ASN:HA    | 2:B:838:SER:O     | 2.06                     | 0.54              |
| 4:D:185:CYS:HB2   | 4:D:211:LEU:HD22  | 1.88                     | 0.54              |
| 1:A:1343:ALA:HB2  | 5:E:150:VAL:HG22  | 1.88                     | 0.54              |
| 5:E:35:VAL:C      | 5:E:37:LEU:H      | 2.10                     | 0.54              |
| 1:A:1445:ILE:HD11 | 7:G:68:ALA:HB1    | 1.90                     | 0.54              |
| 1:A:873:MET:C     | 1:A:1058:VAL:HG23 | 2.27                     | 0.54              |
| 1:A:44:THR:O      | 1:A:45:GLN:HB2    | 2.07                     | 0.54              |
| 1:A:527:THR:HG23  | 1:A:650:GLN:HA    | 1.89                     | 0.54              |
| 2:B:1187:ASN:O    | 2:B:1188:LYS:CB   | 2.49                     | 0.54              |
| 2:B:129:PHE:HE2   | 2:B:166:PHE:HD1   | 1.56                     | 0.54              |
| 2:B:479:VAL:O     | 2:B:480:SER:HB3   | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:496:ARG:NH1  | 2:B:539:LEU:HB2  | 2.22                     | 0.54              |
| 2:B:542:MET:HG2  | 2:B:747:MET:HB3  | 1.89                     | 0.54              |
| 2:B:841:MET:O    | 2:B:993:THR:HA   | 2.08                     | 0.54              |
| 2:B:879:ARG:HH11 | 2:B:883:LEU:CD2  | 2.17                     | 0.54              |
| 7:G:143:ILE:CG2  | 7:G:144:ARG:N    | 2.71                     | 0.54              |
| 8:H:116:TYR:HE2  | 8:H:140:ALA:CB   | 2.19                     | 0.54              |
| 9:I:101:PHE:N    | 9:I:101:PHE:CD1  | 2.76                     | 0.54              |
| 1:A:306:ASN:HB2  | 1:A:324:SER:HB3  | 1.90                     | 0.54              |
| 1:A:18:GLN:CB    | 2:B:1215:ARG:HB2 | 2.38                     | 0.54              |
| 2:B:287:ARG:NH1  | 2:B:324:ILE:O    | 2.41                     | 0.54              |
| 2:B:305:VAL:HG12 | 2:B:305:VAL:O    | 2.07                     | 0.54              |
| 2:B:865:LYS:NZ   | 2:B:869:SER:HA   | 2.23                     | 0.54              |
| 2:B:872:GLU:CD   | 2:B:914:LYS:HE2  | 2.28                     | 0.54              |
| 5:E:55:ARG:C     | 5:E:57:MET:N     | 2.61                     | 0.54              |
| 10:J:32:GLU:CD   | 10:J:32:GLU:H    | 2.10                     | 0.54              |
| 1:A:340:LEU:HD21 | 2:B:1200:ALA:N   | 2.23                     | 0.54              |
| 1:A:695:LYS:C    | 1:A:697:ALA:H    | 2.10                     | 0.54              |
| 1:A:814:PHE:O    | 1:A:817:ALA:HB3  | 2.08                     | 0.54              |
| 2:B:372:SER:O    | 2:B:376:PHE:HD1  | 1.90                     | 0.54              |
| 3:C:100:THR:HG22 | 3:C:101:LEU:H    | 1.71                     | 0.54              |
| 14:P:7:A:H2'     | 14:P:8:G:O4'     | 2.08                     | 0.54              |
| 1:A:381:THR:HG21 | 1:A:383:TYR:CD1  | 2.43                     | 0.54              |
| 2:B:25:ILE:HD11  | 2:B:653:VAL:O    | 2.08                     | 0.54              |
| 3:C:70:ILE:HD11  | 3:C:144:ILE:CG1  | 2.38                     | 0.54              |
| 6:F:69:LEU:N     | 6:F:70:LYS:N     | 2.56                     | 0.54              |
| 7:G:111:THR:HB   | 7:G:114:LEU:HB2  | 1.90                     | 0.54              |
| 8:H:58:THR:HG22  | 8:H:59:ILE:N     | 2.22                     | 0.54              |
| 1:A:399:HIS:HB3  | 1:A:400:PRO:CD   | 2.29                     | 0.54              |
| 1:A:4:GLN:O      | 1:A:5:GLN:HB2    | 2.07                     | 0.54              |
| 2:B:1001:PHE:CE2 | 3:C:34:ARG:CZ    | 2.90                     | 0.54              |
| 2:B:1023:VAL:O   | 2:B:1026:LEU:HB2 | 2.08                     | 0.54              |
| 2:B:687:GLU:O    | 2:B:689:LEU:HG   | 2.08                     | 0.54              |
| 2:B:705:MET:N    | 2:B:710:LEU:HD12 | 2.23                     | 0.54              |
| 2:B:850:LEU:HD12 | 2:B:851:PHE:H    | 1.72                     | 0.54              |
| 2:B:899:ILE:CG2  | 2:B:949:VAL:HG21 | 2.38                     | 0.54              |
| 2:B:977:GLY:HA3  | 2:B:1099:VAL:HB  | 1.90                     | 0.54              |
| 3:C:235:VAL:HG13 | 10:J:13:VAL:CG2  | 2.37                     | 0.54              |
| 11:K:18:LYS:NZ   | 11:K:38:GLU:HG2  | 2.23                     | 0.54              |
| 1:A:71:GLN:O     | 1:A:73:GLY:N     | 2.37                     | 0.54              |
| 2:B:63:ILE:O     | 2:B:67:SER:HB3   | 2.08                     | 0.54              |
| 2:B:942:ARG:NH2  | 15:T:25:DT:OP2   | 2.39                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:969:ARG:HD2   | 3:C:61:GLU:OE2    | 2.08                     | 0.54              |
| 9:I:26:LEU:CD2    | 9:I:37:GLU:HA     | 2.33                     | 0.54              |
| 10:J:57:ILE:HA    | 10:J:60:PHE:CD2   | 2.41                     | 0.54              |
| 11:K:31:VAL:CG1   | 11:K:32:VAL:N     | 2.71                     | 0.54              |
| 1:A:1171:GLN:HA   | 1:A:1174:PHE:HE1  | 1.71                     | 0.54              |
| 1:A:164:ARG:HG3   | 1:A:165:GLY:H     | 1.72                     | 0.54              |
| 1:A:535:THR:CG2   | 1:A:616:VAL:HA    | 2.35                     | 0.54              |
| 1:A:787:PHE:CE1   | 1:A:796:SER:HA    | 2.43                     | 0.54              |
| 1:A:821:ARG:HB2   | 1:A:821:ARG:NH1   | 2.18                     | 0.54              |
| 1:A:863:VAL:HG11  | 1:A:866:PHE:CD2   | 2.42                     | 0.54              |
| 2:B:502:ILE:CD1   | 2:B:502:ILE:H     | 2.07                     | 0.54              |
| 2:B:860:MET:HG2   | 2:B:861:ASP:N     | 2.23                     | 0.54              |
| 1:A:857:ARG:NH1   | 6:F:139:PRO:HB2   | 2.23                     | 0.54              |
| 11:K:47:ARG:HD3   | 11:K:59:ALA:O     | 2.07                     | 0.54              |
| 11:K:55:LYS:HB2   | 11:K:81:TYR:HE1   | 1.73                     | 0.54              |
| 1:A:1369:ALA:O    | 1:A:1372:VAL:HG12 | 2.08                     | 0.53              |
| 1:A:187:LYS:HE3   | 1:A:198:GLU:OE2   | 2.08                     | 0.53              |
| 2:B:1073:TYR:CE2  | 2:B:1080:LYS:HG2  | 2.43                     | 0.53              |
| 1:A:500:GLU:OE2   | 2:B:1145:SER:HB2  | 2.08                     | 0.53              |
| 2:B:549:THR:HG22  | 2:B:550:ASP:N     | 2.15                     | 0.53              |
| 2:B:642:ASP:HB3   | 2:B:649:LYS:HD2   | 1.89                     | 0.53              |
| 2:B:952:VAL:HG22  | 2:B:966:VAL:HG13  | 1.90                     | 0.53              |
| 1:A:1313:LEU:O    | 1:A:1315:GLU:N    | 2.41                     | 0.53              |
| 1:A:590:ARG:HB2   | 1:A:605:MET:HB3   | 1.90                     | 0.53              |
| 2:B:1189:ILE:HG22 | 2:B:1190:ASP:N    | 2.22                     | 0.53              |
| 2:B:327:ARG:O     | 2:B:331:LEU:HD13  | 2.07                     | 0.53              |
| 2:B:582:VAL:HG23  | 2:B:626:ILE:HB    | 1.90                     | 0.53              |
| 3:C:73:GLN:HB3    | 3:C:131:HIS:H     | 1.73                     | 0.53              |
| 12:L:31:CYS:HB3   | 12:L:34:CYS:C     | 2.28                     | 0.53              |
| 1:A:886:ILE:HG13  | 1:A:943:LEU:HD12  | 1.89                     | 0.53              |
| 2:B:1077:THR:HG22 | 11:K:44:ASN:ND2   | 2.23                     | 0.53              |
| 3:C:123:ASN:ND2   | 3:C:125:MET:HG2   | 2.23                     | 0.53              |
| 7:G:138:THR:CG2   | 7:G:139:ILE:H     | 2.00                     | 0.53              |
| 11:K:109:TRP:O    | 11:K:111:LEU:N    | 2.39                     | 0.53              |
| 11:K:63:VAL:O     | 11:K:63:VAL:HG23  | 2.09                     | 0.53              |
| 12:L:32:ALA:CB    | 12:L:55:ILE:HD12  | 2.39                     | 0.53              |
| 1:A:1102:LYS:O    | 1:A:1106:ASN:ND2  | 2.42                     | 0.53              |
| 1:A:42:ASP:C      | 1:A:44:THR:H      | 2.09                     | 0.53              |
| 1:A:761:MET:HA    | 1:A:804:TYR:HB2   | 1.89                     | 0.53              |
| 1:A:958:VAL:O     | 1:A:958:VAL:HG12  | 2.08                     | 0.53              |
| 2:B:830:TYR:O     | 2:B:831:SER:C     | 2.47                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:177:GLU:HG3   | 3:C:231:ASN:HD22  | 1.73                     | 0.53              |
| 1:A:1339:LEU:HD13 | 5:E:147:HIS:CD2   | 2.43                     | 0.53              |
| 11:K:55:LYS:CB    | 11:K:81:TYR:HE1   | 2.21                     | 0.53              |
| 1:A:1120:LEU:CD1  | 1:A:1120:LEU:H    | 2.21                     | 0.53              |
| 4:D:198:LEU:O     | 4:D:200:ASN:N     | 2.42                     | 0.53              |
| 5:E:207:ARG:HB2   | 5:E:207:ARG:NH1   | 2.23                     | 0.53              |
| 7:G:35:GLU:OE2    | 7:G:48:VAL:HG23   | 2.08                     | 0.53              |
| 1:A:53:LEU:CD2    | 1:A:54:ASN:N      | 2.51                     | 0.53              |
| 1:A:666:ILE:HD12  | 1:A:666:ILE:N     | 2.23                     | 0.53              |
| 1:A:816:HIS:CD2   | 2:B:764:SER:HB2   | 2.43                     | 0.53              |
| 1:A:90:VAL:HG13   | 1:A:297:GLN:HA    | 1.90                     | 0.53              |
| 1:A:982:THR:HB    | 1:A:985:ASP:N     | 2.23                     | 0.53              |
| 2:B:412:LEU:HB3   | 2:B:466:TRP:CZ2   | 2.43                     | 0.53              |
| 7:G:91:VAL:HB     | 7:G:139:ILE:O     | 2.08                     | 0.53              |
| 1:A:1341:ILE:HG23 | 1:A:1342:GLU:H    | 1.74                     | 0.53              |
| 1:A:446:ARG:CD    | 1:A:480:ALA:HB2   | 2.39                     | 0.53              |
| 1:A:351:THR:HG21  | 2:B:1103:ILE:HG13 | 1.91                     | 0.53              |
| 2:B:408:LEU:HG    | 2:B:409:ALA:H     | 1.74                     | 0.53              |
| 4:D:56:ARG:HD3    | 4:D:149:THR:HA    | 1.91                     | 0.53              |
| 5:E:163:GLU:O     | 5:E:164:LEU:C     | 2.47                     | 0.53              |
| 1:A:288:ALA:HA    | 1:A:291:GLU:OE2   | 2.09                     | 0.53              |
| 1:A:407:ARG:HG2   | 1:A:430:TRP:CZ3   | 2.44                     | 0.53              |
| 1:A:478:TYR:O     | 1:A:479:ASN:HB3   | 2.08                     | 0.53              |
| 2:B:1166:CYS:O    | 2:B:1168:LEU:N    | 2.41                     | 0.53              |
| 2:B:1180:PHE:O    | 2:B:1181:GLU:O    | 2.27                     | 0.53              |
| 2:B:343:ILE:CB    | 2:B:348:ARG:HG3   | 2.37                     | 0.53              |
| 3:C:239:PRO:HB2   | 3:C:241:ASP:OD1   | 2.08                     | 0.53              |
| 4:D:53:SER:HB3    | 4:D:152:SER:HB2   | 1.91                     | 0.53              |
| 6:F:124:GLU:HB3   | 6:F:130:ILE:HG12  | 1.90                     | 0.53              |
| 2:B:39:ARG:HG2    | 2:B:39:ARG:HH11   | 1.74                     | 0.53              |
| 2:B:54:PHE:O      | 2:B:58:THR:HB     | 2.09                     | 0.53              |
| 2:B:899:ILE:CD1   | 2:B:911:ILE:HA    | 2.39                     | 0.53              |
| 3:C:120:ILE:HD13  | 3:C:124:LEU:HD21  | 1.91                     | 0.53              |
| 9:I:111:THR:CG2   | 9:I:112:SER:N     | 2.72                     | 0.53              |
| 9:I:112:SER:O     | 9:I:114:GLN:N     | 2.42                     | 0.53              |
| 12:L:70:ARG:HG2   | 12:L:70:ARG:HH11  | 1.73                     | 0.53              |
| 14:P:1:U:H2'      | 14:P:2:C:C6       | 2.43                     | 0.53              |
| 15:T:22:BRU:H2''  | 15:T:23:DG:O4'    | 2.09                     | 0.53              |
| 1:A:1369:ALA:O    | 1:A:1370:LEU:C    | 2.46                     | 0.53              |
| 1:A:317:LYS:O     | 1:A:318:SER:HB3   | 2.09                     | 0.53              |
| 1:A:353:ILE:HD12  | 1:A:470:LEU:HD21  | 1.91                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:608:ILE:C    | 1:A:610:GLY:N     | 2.63                     | 0.53              |
| 1:A:645:LEU:HD11 | 1:A:649:ILE:HD11  | 1.91                     | 0.53              |
| 2:B:839:MET:CE   | 2:B:1010:LEU:HD21 | 2.38                     | 0.53              |
| 2:B:683:SER:C    | 2:B:685:LEU:N     | 2.62                     | 0.53              |
| 2:B:756:ILE:O    | 2:B:759:PRO:HD3   | 2.08                     | 0.53              |
| 3:C:263:THR:C    | 3:C:265:MET:N     | 2.63                     | 0.53              |
| 4:D:208:GLU:O    | 4:D:212:LYS:HG3   | 2.08                     | 0.53              |
| 6:F:86:THR:HG23  | 6:F:89:GLU:OE1    | 2.09                     | 0.53              |
| 7:G:44:TYR:CD2   | 7:G:105:PRO:HB2   | 2.44                     | 0.53              |
| 1:A:1444:MET:HG2 | 7:G:60:ARG:HA     | 1.91                     | 0.53              |
| 1:A:1153:TYR:CE1 | 9:I:42:LEU:HD13   | 2.44                     | 0.53              |
| 13:N:0:DT:H1'    | 13:N:1:DA:H5'     | 1.90                     | 0.53              |
| 1:A:1214:GLU:O   | 1:A:1218:GLN:HG2  | 2.10                     | 0.52              |
| 1:A:282:ASN:O    | 1:A:284:ALA:N     | 2.42                     | 0.52              |
| 1:A:563:PRO:HG3  | 1:A:572:TRP:CE2   | 2.42                     | 0.52              |
| 1:A:828:ALA:HB1  | 2:B:530:GLY:HA2   | 1.88                     | 0.52              |
| 2:B:412:LEU:HB3  | 2:B:466:TRP:HZ2   | 1.74                     | 0.52              |
| 2:B:654:ARG:C    | 2:B:656:GLY:H     | 2.11                     | 0.52              |
| 3:C:87:PHE:HD1   | 3:C:87:PHE:H      | 1.56                     | 0.52              |
| 4:D:19:GLU:O     | 4:D:21:GLU:N      | 2.42                     | 0.52              |
| 9:I:99:LEU:O     | 9:I:111:THR:HG23  | 2.09                     | 0.52              |
| 9:I:115:LYS:CD   | 9:I:117:LYS:HE3   | 2.35                     | 0.52              |
| 11:K:60:ALA:O    | 11:K:73:LEU:HD12  | 2.09                     | 0.52              |
| 14:P:8:G:H8      | 14:P:8:G:OP2      | 1.91                     | 0.52              |
| 1:A:1187:GLN:O   | 1:A:1243:VAL:HG13 | 2.09                     | 0.52              |
| 1:A:19:PHE:HB3   | 1:A:1413:GLY:HA2  | 1.90                     | 0.52              |
| 1:A:541:ILE:HD13 | 1:A:549:MET:HE1   | 1.91                     | 0.52              |
| 1:A:897:TYR:CD2  | 1:A:936:LEU:HD13  | 2.44                     | 0.52              |
| 1:A:903:ASN:ND2  | 1:A:903:ASN:C     | 2.63                     | 0.52              |
| 2:B:1183:LYS:CE  | 2:B:1183:LYS:N    | 2.72                     | 0.52              |
| 2:B:550:ASP:OD1  | 2:B:551:PRO:HD2   | 2.09                     | 0.52              |
| 3:C:263:THR:O    | 3:C:265:MET:N     | 2.43                     | 0.52              |
| 5:E:168:TYR:CB   | 5:E:170:LEU:HG    | 2.38                     | 0.52              |
| 7:G:138:THR:HG22 | 7:G:139:ILE:HG13  | 1.90                     | 0.52              |
| 7:G:1:MET:O      | 7:G:3:PHE:CE1     | 2.63                     | 0.52              |
| 2:B:954:VAL:O    | 12:L:55:ILE:O     | 2.28                     | 0.52              |
| 1:A:963:ILE:HD13 | 1:A:1049:ILE:HG13 | 1.90                     | 0.52              |
| 1:A:89:PRO:HB2   | 1:A:204:THR:CG2   | 2.39                     | 0.52              |
| 1:A:54:ASN:HB3   | 1:A:247:ARG:HH22  | 1.74                     | 0.52              |
| 1:A:682:THR:HG23 | 1:A:728:LYS:HE3   | 1.91                     | 0.52              |
| 2:B:102:VAL:CG2  | 2:B:112:LEU:HD22  | 2.39                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:95:ILE:HG13   | 2:B:129:PHE:O    | 2.08                     | 0.52              |
| 2:B:546:SER:OG    | 2:B:631:GLY:N    | 2.39                     | 0.52              |
| 4:D:29:LEU:HD22   | 7:G:82:PHE:CD2   | 2.44                     | 0.52              |
| 5:E:78:LEU:HD23   | 5:E:79:TRP:N     | 2.24                     | 0.52              |
| 6:F:85:MET:HE1    | 6:F:148:VAL:HG12 | 1.89                     | 0.52              |
| 1:A:108:MET:HB3   | 1:A:210:ILE:CD1  | 2.39                     | 0.52              |
| 1:A:722:LEU:HD22  | 1:A:799:PHE:CD1  | 2.44                     | 0.52              |
| 2:B:223:VAL:HG21  | 2:B:380:TYR:HE2  | 1.75                     | 0.52              |
| 2:B:525:ALA:O     | 2:B:768:THR:HG23 | 2.09                     | 0.52              |
| 2:B:787:VAL:HG12  | 2:B:787:VAL:O    | 2.09                     | 0.52              |
| 2:B:980:PHE:CD2   | 2:B:1094:ARG:HA  | 2.44                     | 0.52              |
| 6:F:94:LEU:HD21   | 6:F:122:MET:HA   | 1.92                     | 0.52              |
| 7:G:115:MET:HB3   | 7:G:116:PRO:HD2  | 1.91                     | 0.52              |
| 7:G:51:TYR:O      | 7:G:54:ILE:HG13  | 2.10                     | 0.52              |
| 1:A:1095:THR:O    | 1:A:1096:SER:CB  | 2.57                     | 0.52              |
| 1:A:475:THR:HG23  | 1:A:476:SER:N    | 2.25                     | 0.52              |
| 1:A:60:SER:C      | 1:A:61:ILE:HG13  | 2.29                     | 0.52              |
| 1:A:92:HIS:O      | 1:A:95:PHE:N     | 2.36                     | 0.52              |
| 2:B:1201:LYS:O    | 2:B:1204:PHE:HB2 | 2.09                     | 0.52              |
| 2:B:274:PRO:O     | 2:B:275:TYR:HB2  | 2.09                     | 0.52              |
| 2:B:434:ARG:HA    | 2:B:437:GLU:CD   | 2.29                     | 0.52              |
| 2:B:657:HIS:CE1   | 2:B:689:LEU:HD11 | 2.45                     | 0.52              |
| 3:C:76:ASP:OD2    | 3:C:128:ASN:N    | 2.41                     | 0.52              |
| 8:H:102:TYR:N     | 8:H:102:TYR:CD2  | 2.77                     | 0.52              |
| 13:N:3:DG:C1'     | 13:N:4:DT:H5'    | 2.38                     | 0.52              |
| 1:A:115:LEU:HB2   | 1:A:122:MET:CE   | 2.39                     | 0.52              |
| 1:A:244:PRO:O     | 1:A:246:VAL:N    | 2.43                     | 0.52              |
| 1:A:407:ARG:HD2   | 1:A:413:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:78:PRO:HA     | 2:B:1201:LYS:NZ  | 2.24                     | 0.52              |
| 1:A:838:GLN:O     | 1:A:842:VAL:HG23 | 2.09                     | 0.52              |
| 1:A:840:ARG:O     | 1:A:841:LEU:C    | 2.47                     | 0.52              |
| 1:A:897:TYR:HD2   | 1:A:936:LEU:HD13 | 1.74                     | 0.52              |
| 3:C:66:ARG:NH1    | 3:C:144:ILE:O    | 2.43                     | 0.52              |
| 4:D:130:LEU:C     | 4:D:132:GLN:N    | 2.62                     | 0.52              |
| 1:A:567:LYS:HE3   | 8:H:46:LEU:HD12  | 1.91                     | 0.52              |
| 1:A:836:TYR:HB2   | 15:T:18:DT:H4'   | 1.92                     | 0.52              |
| 1:A:1394:THR:CG2  | 1:A:1398:MET:SD  | 2.89                     | 0.52              |
| 1:A:317:LYS:O     | 1:A:318:SER:CB   | 2.57                     | 0.52              |
| 1:A:881:GLN:O     | 1:A:953:ASN:HA   | 2.10                     | 0.52              |
| 2:B:1095:LEU:HD12 | 2:B:1095:LEU:N   | 2.21                     | 0.52              |
| 1:A:341:MET:HE1   | 2:B:1135:ARG:NH1 | 2.24                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:34:ILE:O      | 2:B:37:PHE:N      | 2.41                     | 0.52              |
| 2:B:953:LEU:HD21  | 2:B:965:LYS:HB2   | 1.91                     | 0.52              |
| 7:G:1:MET:HG3     | 7:G:85:GLU:OE2    | 2.10                     | 0.52              |
| 8:H:4:THR:O       | 8:H:5:LEU:HD23    | 2.09                     | 0.52              |
| 10:J:23:ASN:C     | 10:J:25:LEU:N     | 2.61                     | 0.52              |
| 1:A:40:THR:HG22   | 1:A:41:MET:CG     | 2.28                     | 0.52              |
| 1:A:774:ARG:O     | 1:A:775:ILE:C     | 2.47                     | 0.52              |
| 1:A:956:LEU:HD23  | 1:A:957:PRO:HD2   | 1.92                     | 0.52              |
| 2:B:1022:THR:HG23 | 2:B:1022:THR:O    | 2.09                     | 0.52              |
| 2:B:1099:VAL:HG12 | 2:B:1100:ASP:N    | 2.24                     | 0.52              |
| 2:B:1177:HIS:O    | 2:B:1179:GLN:N    | 2.42                     | 0.52              |
| 1:A:1410:PHE:HA   | 2:B:1212:ILE:HD11 | 1.91                     | 0.52              |
| 2:B:496:ARG:HH12  | 2:B:539:LEU:HB2   | 1.75                     | 0.52              |
| 2:B:654:ARG:N     | 2:B:657:HIS:HD2   | 2.04                     | 0.52              |
| 2:B:899:ILE:O     | 2:B:952:VAL:HG21  | 2.09                     | 0.52              |
| 3:C:167:HIS:CD2   | 3:C:169:LYS:H     | 2.27                     | 0.52              |
| 3:C:256:ALA:O     | 3:C:259:LEU:N     | 2.42                     | 0.52              |
| 5:E:17:ARG:O      | 5:E:20:LYS:HB2    | 2.10                     | 0.52              |
| 6:F:125:LEU:N     | 6:F:130:ILE:HD11  | 2.23                     | 0.52              |
| 7:G:30:LEU:HD22   | 7:G:72:VAL:HG11   | 1.92                     | 0.52              |
| 8:H:84:ALA:HA     | 8:H:87:ARG:CB     | 2.34                     | 0.52              |
| 9:I:13:MET:HG3    | 9:I:14:LEU:N      | 2.23                     | 0.52              |
| 1:A:114:LEU:HD13  | 1:A:171:GLN:NE2   | 2.25                     | 0.52              |
| 1:A:1428:VAL:HG13 | 2:B:1151:LEU:HD21 | 1.91                     | 0.52              |
| 1:A:30:ILE:HD11   | 2:B:1168:LEU:HD13 | 1.92                     | 0.52              |
| 1:A:672:ASP:HB2   | 1:A:736:ASN:OD1   | 2.09                     | 0.52              |
| 1:A:886:ILE:HG13  | 1:A:943:LEU:CD1   | 2.40                     | 0.52              |
| 2:B:936:ASP:OD1   | 2:B:938:SER:N     | 2.39                     | 0.52              |
| 4:D:53:SER:CB     | 4:D:153:ARG:H     | 2.22                     | 0.52              |
| 8:H:62:SER:C      | 8:H:64:ASN:H      | 2.13                     | 0.52              |
| 11:K:55:LYS:HB3   | 11:K:81:TYR:CE1   | 2.45                     | 0.52              |
| 1:A:58:LEU:CD1    | 1:A:80:HIS:H      | 2.23                     | 0.52              |
| 1:A:67:CYS:O      | 1:A:68:GLN:HB2    | 2.09                     | 0.52              |
| 2:B:337:ARG:C     | 2:B:338:GLY:N     | 2.64                     | 0.52              |
| 2:B:33:VAL:HG21   | 2:B:638:PHE:HZ    | 1.75                     | 0.52              |
| 2:B:640:VAL:O     | 2:B:641:GLU:C     | 2.47                     | 0.52              |
| 3:C:33:LEU:O      | 3:C:34:ARG:C      | 2.48                     | 0.52              |
| 5:E:177:ARG:HD3   | 5:E:215:MET:CG    | 2.40                     | 0.52              |
| 1:A:1441:PHE:HZ   | 6:F:89:GLU:HA     | 1.74                     | 0.52              |
| 7:G:79:PHE:HZ     | 7:G:106:MET:HE1   | 1.71                     | 0.52              |
| 7:G:3:PHE:CD1     | 7:G:80:LYS:NZ     | 2.68                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:26:ILE:HD13   | 8:H:49:VAL:HG11   | 1.92                     | 0.52              |
| 9:I:2:THR:O       | 9:I:3:THR:C       | 2.47                     | 0.52              |
| 9:I:61:ASP:O      | 9:I:63:GLY:N      | 2.43                     | 0.52              |
| 11:K:55:LYS:CB    | 11:K:81:TYR:CE1   | 2.93                     | 0.52              |
| 1:A:1118:VAL:HG12 | 1:A:1327:ILE:HG13 | 1.92                     | 0.51              |
| 1:A:84:ILE:HG22   | 1:A:239:LEU:HB3   | 1.91                     | 0.51              |
| 1:A:264:PHE:O     | 1:A:267:ALA:HB3   | 2.10                     | 0.51              |
| 1:A:350:ARG:HB2   | 1:A:488:ASN:OD1   | 2.09                     | 0.51              |
| 1:A:381:THR:CG2   | 1:A:383:TYR:H     | 2.23                     | 0.51              |
| 1:A:613:ILE:O     | 1:A:614:PHE:HB3   | 2.09                     | 0.51              |
| 1:A:715:GLU:OE2   | 1:A:774:ARG:NH1   | 2.43                     | 0.51              |
| 1:A:896:ARG:HD3   | 1:A:897:TYR:HE1   | 1.72                     | 0.51              |
| 1:A:965:GLN:O     | 1:A:968:GLN:HB2   | 2.10                     | 0.51              |
| 2:B:1162:ILE:HG22 | 2:B:1163:CYS:H    | 1.75                     | 0.51              |
| 2:B:184:ALA:HB1   | 2:B:188:ASP:HB3   | 1.92                     | 0.51              |
| 2:B:278:GLN:HG2   | 2:B:279:ASP:H     | 1.74                     | 0.51              |
| 2:B:376:PHE:CE2   | 2:B:569:TYR:HD2   | 2.27                     | 0.51              |
| 2:B:825:VAL:HG13  | 2:B:826:ALA:N     | 2.25                     | 0.51              |
| 7:G:139:ILE:HG22  | 7:G:140:LYS:N     | 2.24                     | 0.51              |
| 9:I:14:LEU:HA     | 9:I:28:GLU:O      | 2.10                     | 0.51              |
| 9:I:50:THR:CG2    | 9:I:52:ILE:HG12   | 2.40                     | 0.51              |
| 1:A:168:GLY:O     | 1:A:169:ASN:C     | 2.47                     | 0.51              |
| 1:A:974:ASP:C     | 1:A:976:THR:H     | 2.13                     | 0.51              |
| 2:B:343:ILE:CG2   | 2:B:348:ARG:H     | 2.22                     | 0.51              |
| 1:A:822:GLU:HG3   | 2:B:513:GLN:NE2   | 2.26                     | 0.51              |
| 3:C:83:SER:OG     | 3:C:160:LYS:HD3   | 2.10                     | 0.51              |
| 4:D:167:LEU:O     | 4:D:170:THR:OG1   | 2.24                     | 0.51              |
| 4:D:17:LYS:HA     | 4:D:17:LYS:HE3    | 1.92                     | 0.51              |
| 5:E:61:GLN:HG2    | 5:E:62:ALA:N      | 2.24                     | 0.51              |
| 1:A:107:CYS:H     | 1:A:114:LEU:HD21  | 1.74                     | 0.51              |
| 1:A:1376:THR:O    | 1:A:1377:THR:C    | 2.48                     | 0.51              |
| 1:A:152:VAL:HG13  | 1:A:153:PRO:HD2   | 1.91                     | 0.51              |
| 1:A:211:PHE:HA    | 1:A:214:ILE:HG13  | 1.92                     | 0.51              |
| 1:A:826:ASP:HB2   | 1:A:830:LYS:HD3   | 1.91                     | 0.51              |
| 2:B:281:PRO:O     | 2:B:283:VAL:N     | 2.43                     | 0.51              |
| 2:B:278:GLN:NE2   | 2:B:337:ARG:HH21  | 2.08                     | 0.51              |
| 2:B:449:ASN:C     | 2:B:451:LYS:H     | 2.13                     | 0.51              |
| 2:B:693:ILE:HD13  | 2:B:701:ILE:HD13  | 1.93                     | 0.51              |
| 3:C:226:ASP:O     | 3:C:227:THR:CB    | 2.58                     | 0.51              |
| 4:D:191:ALA:C     | 4:D:193:THR:H     | 2.12                     | 0.51              |
| 4:D:29:LEU:HD13   | 7:G:82:PHE:CZ     | 2.45                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1409:LEU:HD13 | 2:B:1207:LEU:HD11 | 1.92                     | 0.51              |
| 1:A:500:GLU:OE2   | 1:A:1438:THR:HG21 | 2.10                     | 0.51              |
| 1:A:567:LYS:HB3   | 8:H:95:TYR:CA     | 2.38                     | 0.51              |
| 1:A:72:GLU:OE2    | 2:B:1175:LEU:HB2  | 2.11                     | 0.51              |
| 1:A:738:LYS:HB2   | 1:A:740:LEU:HG    | 1.91                     | 0.51              |
| 2:B:388:CYS:C     | 2:B:390:LEU:H     | 2.13                     | 0.51              |
| 2:B:37:PHE:HD2    | 2:B:542:MET:SD    | 2.33                     | 0.51              |
| 2:B:882:THR:O     | 2:B:883:LEU:HB2   | 2.10                     | 0.51              |
| 2:B:899:ILE:HG21  | 2:B:949:VAL:HG21  | 1.93                     | 0.51              |
| 2:B:995:ARG:HB3   | 2:B:997:GLU:OE2   | 2.10                     | 0.51              |
| 4:D:50:LEU:HD13   | 4:D:55:ALA:HA     | 1.93                     | 0.51              |
| 2:B:902:GLY:O     | 12:L:65:VAL:HG11  | 2.11                     | 0.51              |
| 13:N:0:DT:H71     | 13:N:1:DA:N6      | 2.24                     | 0.51              |
| 1:A:1453:TYR:O    | 1:A:1454:MET:HB3  | 2.10                     | 0.51              |
| 1:A:90:VAL:CG1    | 1:A:297:GLN:HA    | 2.40                     | 0.51              |
| 1:A:982:THR:HG22  | 1:A:984:LYS:H     | 1.75                     | 0.51              |
| 2:B:37:PHE:CD1    | 2:B:41:LYS:HG3    | 2.45                     | 0.51              |
| 2:B:483:LEU:CD1   | 2:B:491:THR:HG23  | 2.39                     | 0.51              |
| 3:C:56:THR:HG21   | 3:C:145:CYS:SG    | 2.51                     | 0.51              |
| 7:G:16:SER:HB3    | 7:G:17:PHE:CD2    | 2.46                     | 0.51              |
| 2:B:852:ARG:NH2   | 12:L:70:ARG:OXT   | 2.37                     | 0.51              |
| 1:A:2:VAL:HG21    | 2:B:1157:ALA:C    | 2.31                     | 0.51              |
| 1:A:55:ASP:CG     | 1:A:55:ASP:O      | 2.46                     | 0.51              |
| 2:B:100:PRO:HD2   | 2:B:180:TYR:CE1   | 2.46                     | 0.51              |
| 2:B:46:GLN:HG3    | 2:B:47:GLN:N      | 2.18                     | 0.51              |
| 2:B:606:LYS:HD2   | 2:B:608:ASP:OD2   | 2.11                     | 0.51              |
| 3:C:238:ILE:HG22  | 3:C:243:VAL:HG23  | 1.92                     | 0.51              |
| 1:A:626:ASN:O     | 1:A:631:HIS:HD2   | 1.93                     | 0.51              |
| 1:A:527:THR:HG21  | 1:A:650:GLN:HA    | 1.91                     | 0.51              |
| 1:A:834:THR:O     | 1:A:837:ILE:HB    | 2.10                     | 0.51              |
| 2:B:226:PHE:HA    | 2:B:395:GLN:CG    | 2.40                     | 0.51              |
| 2:B:769:TYR:C     | 2:B:771:SER:N     | 2.62                     | 0.51              |
| 8:H:58:THR:HB     | 8:H:143:LEU:HD13  | 1.93                     | 0.51              |
| 1:A:899:VAL:CG2   | 1:A:1029:ARG:HG2  | 2.41                     | 0.51              |
| 1:A:1121:GLU:CG   | 1:A:1122:PRO:HD2  | 2.41                     | 0.51              |
| 1:A:332:LYS:HG3   | 1:A:333:GLU:N     | 2.26                     | 0.51              |
| 1:A:730:GLY:C     | 1:A:732:LEU:N     | 2.62                     | 0.51              |
| 2:B:778:MET:HE2   | 2:B:1094:ARG:HG2  | 1.91                     | 0.51              |
| 2:B:360:PHE:CD2   | 2:B:360:PHE:C     | 2.84                     | 0.51              |
| 2:B:434:ARG:HA    | 2:B:437:GLU:OE2   | 2.10                     | 0.51              |
| 2:B:711:GLU:H     | 2:B:712:PRO:HD2   | 1.75                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:825:VAL:HG13  | 2:B:826:ALA:H    | 1.76                     | 0.51              |
| 3:C:174:ALA:O     | 10:J:10:CYS:O    | 2.29                     | 0.51              |
| 10:J:36:LEU:HA    | 10:J:39:LEU:HD12 | 1.91                     | 0.51              |
| 1:A:1242:VAL:HG12 | 1:A:1243:VAL:N   | 2.26                     | 0.51              |
| 1:A:84:ILE:CG2    | 1:A:84:ILE:O     | 2.58                     | 0.51              |
| 2:B:27:ALA:O      | 2:B:29:ASP:N     | 2.44                     | 0.51              |
| 2:B:310:MET:CE    | 2:B:387:LEU:HD12 | 2.37                     | 0.51              |
| 2:B:616:ILE:HG13  | 2:B:697:GLU:HG3  | 1.92                     | 0.51              |
| 2:B:604:ARG:NH1   | 2:B:691:GLU:OE2  | 2.43                     | 0.51              |
| 2:B:896:ASP:OD2   | 12:L:58:LYS:HE3  | 2.11                     | 0.51              |
| 3:C:77:ILE:HG22   | 3:C:78:GLU:N     | 2.26                     | 0.51              |
| 8:H:89:LEU:C      | 8:H:91:ASP:H     | 2.13                     | 0.51              |
| 9:I:5:ARG:HD3     | 9:I:36:GLU:OE2   | 2.11                     | 0.51              |
| 1:A:1362:TYR:HD1  | 1:A:1363:VAL:N   | 2.08                     | 0.51              |
| 1:A:1420:ASP:O    | 1:A:1421:CYS:HB2 | 2.11                     | 0.51              |
| 1:A:33:ALA:O      | 1:A:83:HIS:HD2   | 1.93                     | 0.51              |
| 2:B:955:THR:CG2   | 2:B:956:THR:H    | 2.19                     | 0.51              |
| 4:D:177:VAL:O     | 4:D:177:VAL:HG12 | 2.11                     | 0.51              |
| 5:E:9:ILE:CD1     | 5:E:53:PRO:HD3   | 2.40                     | 0.51              |
| 10:J:44:TYR:HA    | 10:J:47:ARG:HB2  | 1.93                     | 0.51              |
| 1:A:23:SER:O      | 1:A:24:PRO:C     | 2.48                     | 0.50              |
| 1:A:244:PRO:CB    | 1:A:245:PRO:HD3  | 2.41                     | 0.50              |
| 1:A:366:VAL:HG21  | 1:A:460:VAL:HG22 | 1.93                     | 0.50              |
| 2:B:123:THR:O     | 2:B:125:SER:N    | 2.44                     | 0.50              |
| 2:B:190:TYR:CE1   | 2:B:196:PRO:HG3  | 2.45                     | 0.50              |
| 2:B:552:MET:HA    | 2:B:555:ILE:HB   | 1.93                     | 0.50              |
| 7:G:1:MET:O       | 7:G:3:PHE:CD1    | 2.65                     | 0.50              |
| 7:G:1:MET:SD      | 7:G:1:MET:C      | 2.89                     | 0.50              |
| 11:K:68:PHE:N     | 11:K:68:PHE:HD2  | 2.08                     | 0.50              |
| 1:A:284:ALA:O     | 1:A:286:HIS:N    | 2.36                     | 0.50              |
| 1:A:464:PRO:O     | 1:A:465:TYR:O    | 2.29                     | 0.50              |
| 1:A:608:ILE:HD12  | 1:A:613:ILE:CD1  | 2.42                     | 0.50              |
| 1:A:64:ASN:O      | 1:A:65:LEU:C     | 2.50                     | 0.50              |
| 2:B:778:MET:HE2   | 2:B:1094:ARG:CD  | 2.41                     | 0.50              |
| 2:B:43:LEU:HD13   | 2:B:812:LEU:HD23 | 1.93                     | 0.50              |
| 4:D:56:ARG:HA     | 4:D:148:LEU:HD13 | 1.93                     | 0.50              |
| 6:F:77:ASP:O      | 6:F:78:GLN:HB2   | 2.11                     | 0.50              |
| 7:G:27:LYS:HE2    | 7:G:54:ILE:HB    | 1.93                     | 0.50              |
| 7:G:13:LEU:O      | 7:G:67:SER:HA    | 2.12                     | 0.50              |
| 8:H:40:LEU:HD22   | 8:H:123:MET:CE   | 2.40                     | 0.50              |
| 8:H:26:ILE:CD1    | 8:H:49:VAL:HG11  | 2.41                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:737:THR:CG2   | 9:I:66:PRO:HA     | 2.38                     | 0.50              |
| 1:A:1135:ARG:HH21 | 1:A:1284:MET:HG3  | 1.77                     | 0.50              |
| 1:A:316:GLN:O     | 1:A:317:LYS:C     | 2.49                     | 0.50              |
| 1:A:362:ASP:OD2   | 1:A:459:ARG:HD3   | 2.10                     | 0.50              |
| 1:A:919:ILE:O     | 1:A:920:LEU:C     | 2.50                     | 0.50              |
| 2:B:1099:VAL:O    | 2:B:1101:ASP:N    | 2.44                     | 0.50              |
| 2:B:654:ARG:O     | 2:B:656:GLY:N     | 2.45                     | 0.50              |
| 2:B:955:THR:CG2   | 2:B:956:THR:N     | 2.74                     | 0.50              |
| 5:E:35:VAL:O      | 5:E:37:LEU:N      | 2.44                     | 0.50              |
| 9:I:111:THR:CG2   | 9:I:112:SER:H     | 2.22                     | 0.50              |
| 1:A:1283:VAL:HG12 | 1:A:1284:MET:H    | 1.76                     | 0.50              |
| 1:A:244:PRO:O     | 1:A:247:ARG:N     | 2.43                     | 0.50              |
| 1:A:252:PHE:HB2   | 1:A:256:GLN:NE2   | 2.27                     | 0.50              |
| 1:A:262:LEU:O     | 1:A:264:PHE:N     | 2.45                     | 0.50              |
| 1:A:90:VAL:HG13   | 1:A:297:GLN:CD    | 2.32                     | 0.50              |
| 1:A:710:LEU:HD12  | 1:A:710:LEU:N     | 2.27                     | 0.50              |
| 1:A:786:HIS:CD2   | 1:A:786:HIS:N     | 2.79                     | 0.50              |
| 2:B:1020:ARG:HB2  | 2:B:1022:THR:HG22 | 1.93                     | 0.50              |
| 2:B:1085:ILE:HG22 | 2:B:1086:PHE:N    | 2.27                     | 0.50              |
| 2:B:515:HIS:N     | 2:B:518:HIS:HD2   | 1.98                     | 0.50              |
| 3:C:179:GLU:HG2   | 3:C:180:TYR:H     | 1.77                     | 0.50              |
| 3:C:89:GLU:O      | 3:C:90:ASP:HB3    | 2.11                     | 0.50              |
| 4:D:51:ASN:O      | 4:D:54:GLU:HB3    | 2.10                     | 0.50              |
| 1:A:1324:PRO:HB2  | 5:E:142:VAL:HG11  | 1.93                     | 0.50              |
| 9:I:61:ASP:C      | 9:I:63:GLY:N      | 2.63                     | 0.50              |
| 11:K:47:ARG:HD2   | 11:K:47:ARG:C     | 2.32                     | 0.50              |
| 1:A:23:SER:HA     | 1:A:233:TRP:NE1   | 2.27                     | 0.50              |
| 1:A:54:ASN:HB3    | 1:A:247:ARG:HH12  | 1.76                     | 0.50              |
| 1:A:798:GLY:HA2   | 1:A:815:PHE:HD1   | 1.73                     | 0.50              |
| 2:B:1102:LYS:O    | 2:B:1103:ILE:C    | 2.49                     | 0.50              |
| 2:B:298:LEU:HD13  | 2:B:314:LEU:HD13  | 1.92                     | 0.50              |
| 2:B:44:VAL:O      | 2:B:45:SER:C      | 2.49                     | 0.50              |
| 2:B:653:VAL:CG2   | 2:B:689:LEU:HB3   | 2.40                     | 0.50              |
| 3:C:112:ASN:N     | 3:C:112:ASN:HD22  | 2.07                     | 0.50              |
| 3:C:140:ASN:O     | 3:C:141:GLY:O     | 2.29                     | 0.50              |
| 4:D:27:LEU:HD22   | 4:D:173:HIS:CD2   | 2.46                     | 0.50              |
| 6:F:114:GLU:OE2   | 6:F:119:ARG:HG2   | 2.12                     | 0.50              |
| 6:F:82:THR:HG22   | 6:F:84:TYR:N      | 2.23                     | 0.50              |
| 1:A:310:GLY:O     | 1:A:312:PRO:HD2   | 2.12                     | 0.50              |
| 1:A:432:VAL:O     | 1:A:433:GLU:C     | 2.49                     | 0.50              |
| 1:A:34:LYS:NZ     | 1:A:57:ARG:NH1    | 2.60                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:774:ARG:NH2   | 1:A:797:LYS:HG3  | 2.27                     | 0.50              |
| 1:A:58:LEU:HD11   | 1:A:80:HIS:H     | 1.76                     | 0.50              |
| 1:A:809:THR:OG1   | 1:A:812:GLU:HG3  | 2.11                     | 0.50              |
| 1:A:960:ILE:O     | 1:A:961:ARG:C    | 2.50                     | 0.50              |
| 2:B:192:LEU:O     | 2:B:193:LYS:HB2  | 2.12                     | 0.50              |
| 2:B:510:LYS:HG3   | 2:B:511:PRO:CD   | 2.38                     | 0.50              |
| 3:C:69:LEU:HD12   | 3:C:69:LEU:H     | 1.76                     | 0.50              |
| 4:D:24:ALA:C      | 4:D:26:THR:H     | 2.15                     | 0.50              |
| 5:E:131:THR:HG21  | 5:E:191:LYS:NZ   | 2.26                     | 0.50              |
| 7:G:96:GLN:HB3    | 7:G:121:PHE:CE2  | 2.47                     | 0.50              |
| 7:G:88:ASP:HA     | 7:G:144:ARG:HA   | 1.92                     | 0.50              |
| 1:A:1341:ILE:CG2  | 1:A:1342:GLU:H   | 2.24                     | 0.50              |
| 1:A:269:ILE:CD1   | 1:A:300:VAL:HA   | 2.41                     | 0.50              |
| 1:A:350:ARG:HA    | 1:A:468:PHE:HE1  | 1.77                     | 0.50              |
| 1:A:55:ASP:HA     | 1:A:58:LEU:HB3   | 1.94                     | 0.50              |
| 2:B:233:PRO:HG2   | 2:B:234:ILE:CD1  | 2.42                     | 0.50              |
| 2:B:329:THR:O     | 2:B:332:ASP:HB3  | 2.12                     | 0.50              |
| 2:B:497:ARG:NH2   | 2:B:775:LYS:NZ   | 2.59                     | 0.50              |
| 6:F:69:LEU:N      | 6:F:70:LYS:HA    | 2.26                     | 0.50              |
| 1:A:1118:VAL:HG23 | 1:A:1118:VAL:O   | 2.11                     | 0.50              |
| 1:A:130:ASP:O     | 1:A:131:SER:C    | 2.50                     | 0.50              |
| 1:A:95:PHE:CZ     | 1:A:1414:ALA:HB2 | 2.47                     | 0.50              |
| 1:A:195:ASP:O     | 1:A:196:GLU:HB3  | 2.12                     | 0.50              |
| 1:A:265:LYS:HZ3   | 1:A:322:VAL:HG22 | 1.75                     | 0.50              |
| 1:A:567:LYS:HG3   | 1:A:568:PRO:CD   | 2.39                     | 0.50              |
| 2:B:746:SER:HB2   | 2:B:1046:PRO:HG2 | 1.93                     | 0.50              |
| 2:B:213:ILE:HD12  | 2:B:497:ARG:HB3  | 1.94                     | 0.50              |
| 2:B:233:PRO:HG2   | 2:B:234:ILE:HD12 | 1.92                     | 0.50              |
| 3:C:22:LEU:HD13   | 3:C:230:MET:CE   | 2.42                     | 0.50              |
| 4:D:64:VAL:C      | 4:D:66:ARG:H     | 2.14                     | 0.50              |
| 7:G:18:PHE:HA     | 7:G:22:MET:HE2   | 1.93                     | 0.50              |
| 12:L:55:ILE:O     | 12:L:56:LEU:HB2  | 2.11                     | 0.50              |
| 1:A:250:ILE:CD1   | 14:P:0:U:H1'     | 2.41                     | 0.50              |
| 1:A:58:LEU:HG     | 1:A:59:GLY:N     | 2.26                     | 0.50              |
| 1:A:853:ASP:C     | 1:A:853:ASP:OD1  | 2.50                     | 0.50              |
| 2:B:1033:LYS:NZ   | 2:B:1068:GLY:O   | 2.45                     | 0.50              |
| 2:B:847:ASP:C     | 2:B:849:GLY:H    | 2.14                     | 0.50              |
| 15:T:19:TT:H2'1   | 15:T:19:TT:C5R   | 2.42                     | 0.50              |
| 1:A:116:ASP:C     | 1:A:118:HIS:N    | 2.66                     | 0.49              |
| 1:A:1198:ASP:O    | 1:A:1202:MET:HG2 | 2.12                     | 0.49              |
| 1:A:90:VAL:HG13   | 1:A:297:GLN:OE1  | 2.11                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:37:PHE:HB2    | 1:A:52:GLY:HA3   | 1.94                     | 0.49              |
| 2:B:122:LEU:O     | 2:B:206:ASN:HA   | 2.12                     | 0.49              |
| 2:B:220:GLY:O     | 2:B:222:ILE:HG13 | 2.12                     | 0.49              |
| 2:B:365:THR:HG23  | 2:B:367:LEU:N    | 2.21                     | 0.49              |
| 2:B:549:THR:N     | 2:B:628:THR:HG23 | 2.25                     | 0.49              |
| 2:B:899:ILE:CG2   | 2:B:903:VAL:HB   | 2.42                     | 0.49              |
| 4:D:195:ILE:HG22  | 4:D:198:LEU:HG   | 1.93                     | 0.49              |
| 7:G:59:GLY:CA     | 7:G:70:PHE:CD2   | 2.94                     | 0.49              |
| 1:A:1329:THR:CG2  | 1:A:1331:SER:H   | 2.22                     | 0.49              |
| 1:A:152:VAL:HG12  | 1:A:153:PRO:HD2  | 1.93                     | 0.49              |
| 1:A:541:ILE:HG21  | 1:A:549:MET:CE   | 2.39                     | 0.49              |
| 1:A:608:ILE:HB    | 1:A:613:ILE:HD11 | 1.94                     | 0.49              |
| 1:A:867:ILE:CG2   | 1:A:872:GLY:N    | 2.75                     | 0.49              |
| 2:B:259:TYR:HB2   | 2:B:268:THR:HG23 | 1.93                     | 0.49              |
| 2:B:549:THR:H     | 2:B:628:THR:CG2  | 2.22                     | 0.49              |
| 3:C:74:SER:HB2    | 3:C:77:ILE:HG12  | 1.93                     | 0.49              |
| 5:E:145:THR:HG21  | 5:E:187:TYR:CE2  | 2.47                     | 0.49              |
| 8:H:116:TYR:HE2   | 8:H:140:ALA:HB1  | 1.76                     | 0.49              |
| 9:I:58:VAL:HG12   | 9:I:58:VAL:O     | 2.11                     | 0.49              |
| 14:P:5:C:C2'      | 14:P:6:C:H5'     | 2.41                     | 0.49              |
| 1:A:1291:VAL:HG13 | 1:A:1292:PRO:CD  | 2.42                     | 0.49              |
| 1:A:244:PRO:HB2   | 1:A:245:PRO:HD3  | 1.93                     | 0.49              |
| 1:A:947:PHE:CD2   | 1:A:954:TRP:CE2  | 3.00                     | 0.49              |
| 2:B:199:MET:CE    | 2:B:492:LEU:HD23 | 2.43                     | 0.49              |
| 2:B:792:MET:HG3   | 2:B:855:PHE:CE1  | 2.47                     | 0.49              |
| 4:D:14:ARG:N      | 4:D:17:LYS:HZ3   | 2.10                     | 0.49              |
| 4:D:40:HIS:CG     | 4:D:41:GLN:N     | 2.80                     | 0.49              |
| 4:D:57:LEU:O      | 4:D:61:GLU:HB2   | 2.12                     | 0.49              |
| 6:F:143:PHE:C     | 6:F:143:PHE:CD1  | 2.85                     | 0.49              |
| 7:G:9:LEU:HD12    | 7:G:10:ASN:H     | 1.77                     | 0.49              |
| 11:K:21:ILE:HG23  | 11:K:31:VAL:CG1  | 2.42                     | 0.49              |
| 15:T:19:TT:H2'1   | 15:T:19:TT:C3R   | 2.42                     | 0.49              |
| 1:A:1115:SER:OG   | 1:A:1116:LEU:N   | 2.45                     | 0.49              |
| 1:A:1164:PRO:HG2  | 1:A:1165:GLU:H   | 1.78                     | 0.49              |
| 1:A:767:GLN:HA    | 1:A:799:PHE:HA   | 1.94                     | 0.49              |
| 2:B:1159:ARG:HD2  | 2:B:1159:ARG:C   | 2.33                     | 0.49              |
| 2:B:797:TYR:HE1   | 2:B:854:LEU:CD2  | 2.24                     | 0.49              |
| 2:B:980:PHE:HE2   | 2:B:1094:ARG:HB2 | 1.78                     | 0.49              |
| 3:C:123:ASN:HD21  | 3:C:125:MET:HA   | 1.78                     | 0.49              |
| 3:C:254:LYS:O     | 3:C:256:ALA:N    | 2.45                     | 0.49              |
| 5:E:55:ARG:O      | 5:E:57:MET:N     | 2.46                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:26:LEU:O     | 7:G:27:LYS:C      | 2.50                     | 0.49              |
| 7:G:4:ILE:O      | 7:G:4:ILE:HG22    | 2.12                     | 0.49              |
| 10:J:7:CYS:SG    | 10:J:8:PHE:N      | 2.85                     | 0.49              |
| 11:K:12:LEU:HD12 | 11:K:12:LEU:N     | 2.22                     | 0.49              |
| 12:L:34:CYS:O    | 12:L:36:SER:N     | 2.46                     | 0.49              |
| 1:A:1370:LEU:O   | 1:A:1374:VAL:HG23 | 2.11                     | 0.49              |
| 1:A:601:LYS:HB2  | 1:A:603:ASN:ND2   | 2.27                     | 0.49              |
| 1:A:335:ARG:HH11 | 2:B:1202:LEU:HD13 | 1.76                     | 0.49              |
| 2:B:190:TYR:CE2  | 10:J:62:ARG:HB3   | 2.47                     | 0.49              |
| 2:B:973:ILE:HG23 | 2:B:974:PRO:HD2   | 1.95                     | 0.49              |
| 3:C:241:ASP:OD1  | 3:C:242:GLN:N     | 2.39                     | 0.49              |
| 3:C:73:GLN:NE2   | 3:C:75:MET:N      | 2.57                     | 0.49              |
| 4:D:176:GLU:HB3  | 4:D:198:LEU:HD21  | 1.94                     | 0.49              |
| 4:D:59:ILE:O     | 4:D:60:LYS:C      | 2.50                     | 0.49              |
| 6:F:119:ARG:HG3  | 6:F:119:ARG:NH1   | 2.26                     | 0.49              |
| 7:G:15:PRO:O     | 7:G:16:SER:C      | 2.50                     | 0.49              |
| 8:H:123:MET:HE3  | 8:H:142:LEU:CD2   | 2.42                     | 0.49              |
| 8:H:18:GLY:O     | 8:H:19:ARG:HB2    | 2.12                     | 0.49              |
| 9:I:84:VAL:HG13  | 9:I:84:VAL:O      | 2.13                     | 0.49              |
| 12:L:38:LEU:O    | 12:L:39:SER:CB    | 2.60                     | 0.49              |
| 1:A:1139:GLU:O   | 1:A:1275:GLY:HA3  | 2.12                     | 0.49              |
| 1:A:224:PHE:CZ   | 1:A:234:MET:HE2   | 2.47                     | 0.49              |
| 1:A:93:VAL:HG21  | 1:A:301:ALA:O     | 2.13                     | 0.49              |
| 1:A:534:LEU:HG   | 1:A:534:LEU:O     | 2.11                     | 0.49              |
| 1:A:901:LEU:HD22 | 1:A:919:ILE:HG22  | 1.94                     | 0.49              |
| 2:B:294:ASP:O    | 2:B:296:GLU:N     | 2.43                     | 0.49              |
| 4:D:156:ASP:C    | 4:D:158:GLU:H     | 2.15                     | 0.49              |
| 5:E:156:LEU:HD12 | 5:E:195:VAL:CG1   | 2.42                     | 0.49              |
| 1:A:1017:LEU:CB  | 5:E:205:SER:HA    | 2.42                     | 0.49              |
| 2:B:309:GLN:HG3  | 9:I:52:ILE:HD11   | 1.94                     | 0.49              |
| 3:C:66:ARG:HH12  | 10:J:2:ILE:HG21   | 1.75                     | 0.49              |
| 11:K:21:ILE:HG23 | 11:K:31:VAL:HG11  | 1.95                     | 0.49              |
| 15:T:17:DT:H2''  | 15:T:18:DT:O5'    | 2.12                     | 0.49              |
| 1:A:1032:LEU:O   | 1:A:1036:ARG:HD3  | 2.12                     | 0.49              |
| 1:A:1364:ASN:O   | 1:A:1365:TYR:C    | 2.51                     | 0.49              |
| 1:A:147:VAL:O    | 1:A:149:GLU:N     | 2.46                     | 0.49              |
| 1:A:381:THR:HG23 | 1:A:383:TYR:H     | 1.78                     | 0.49              |
| 1:A:441:PRO:HD2  | 1:A:498:ARG:CZ    | 2.43                     | 0.49              |
| 1:A:837:ILE:HA   | 1:A:840:ARG:HD3   | 1.95                     | 0.49              |
| 2:B:1068:GLY:O   | 2:B:1069:PHE:O    | 2.31                     | 0.49              |
| 2:B:118:ARG:HH22 | 2:B:194:GLU:CD    | 2.15                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:259:TYR:HD1   | 2:B:259:TYR:H     | 1.60                     | 0.49              |
| 1:A:658:LEU:HD13  | 2:B:831:SER:N     | 2.27                     | 0.49              |
| 2:B:995:ARG:NH1   | 3:C:165:LYS:HG2   | 2.27                     | 0.49              |
| 3:C:175:ALA:HB3   | 10:J:43:ARG:NH2   | 2.28                     | 0.49              |
| 4:D:53:SER:HB3    | 4:D:152:SER:CA    | 2.42                     | 0.49              |
| 1:A:1029:ARG:HG3  | 1:A:1029:ARG:NH1  | 2.24                     | 0.49              |
| 1:A:1342:GLU:OE2  | 5:E:212:ARG:NH1   | 2.45                     | 0.49              |
| 1:A:166:GLY:O     | 1:A:167:CYS:CB    | 2.60                     | 0.49              |
| 1:A:966:ASN:O     | 1:A:967:ALA:C     | 2.51                     | 0.49              |
| 2:B:1010:LEU:HD23 | 2:B:1092:TYR:CD1  | 2.47                     | 0.49              |
| 2:B:1084:GLN:HE21 | 2:B:1084:GLN:N    | 2.10                     | 0.49              |
| 2:B:472:ALA:C     | 2:B:474:SER:H     | 2.14                     | 0.49              |
| 2:B:46:GLN:CG     | 2:B:47:GLN:H      | 2.20                     | 0.49              |
| 2:B:758:PHE:N     | 2:B:759:PRO:CD    | 2.76                     | 0.49              |
| 2:B:769:TYR:C     | 2:B:771:SER:H     | 2.16                     | 0.49              |
| 3:C:129:ILE:HG23  | 3:C:130:GLY:N     | 2.26                     | 0.49              |
| 3:C:161:LYS:O     | 3:C:170:TRP:NE1   | 2.46                     | 0.49              |
| 3:C:254:LYS:C     | 3:C:256:ALA:H     | 2.16                     | 0.49              |
| 1:A:1334:ASP:O    | 1:A:1336:MET:N    | 2.46                     | 0.49              |
| 1:A:1389:PHE:CD1  | 1:A:1390:ASN:N    | 2.81                     | 0.49              |
| 1:A:401:GLY:C     | 1:A:435:HIS:CD2   | 2.86                     | 0.49              |
| 1:A:50:ILE:C      | 1:A:52:GLY:N      | 2.65                     | 0.49              |
| 1:A:50:ILE:O      | 1:A:52:GLY:N      | 2.45                     | 0.49              |
| 1:A:699:ALA:O     | 1:A:700:ASN:CB    | 2.60                     | 0.49              |
| 1:A:894:GLU:HG3   | 1:A:933:TYR:OH    | 2.12                     | 0.49              |
| 2:B:180:TYR:N     | 2:B:180:TYR:CD1   | 2.81                     | 0.49              |
| 2:B:23:ALA:H      | 2:B:654:ARG:HB3   | 1.78                     | 0.49              |
| 2:B:801:LYS:O     | 10:J:52:THR:HG23  | 2.13                     | 0.49              |
| 2:B:843:GLN:O     | 2:B:844:SER:C     | 2.50                     | 0.49              |
| 2:B:843:GLN:O     | 2:B:846:ILE:N     | 2.45                     | 0.49              |
| 2:B:910:VAL:HG12  | 2:B:911:ILE:N     | 2.28                     | 0.49              |
| 3:C:191:TYR:CD2   | 3:C:201:TRP:CD1   | 3.01                     | 0.49              |
| 3:C:208:GLU:C     | 3:C:210:GLU:H     | 2.15                     | 0.49              |
| 4:D:135:GLY:C     | 4:D:137:ASN:H     | 2.15                     | 0.49              |
| 1:A:1446:ASP:HB2  | 6:F:133:VAL:CG2   | 2.43                     | 0.49              |
| 10:J:27:GLU:O     | 10:J:29:GLU:N     | 2.40                     | 0.49              |
| 1:A:1329:THR:H    | 1:A:1335:ILE:HD11 | 1.78                     | 0.49              |
| 1:A:18:GLN:HB3    | 2:B:1215:ARG:HG3  | 1.94                     | 0.49              |
| 1:A:577:ILE:HG13  | 1:A:578:LEU:N     | 2.27                     | 0.49              |
| 1:A:901:LEU:HD22  | 1:A:919:ILE:HG21  | 1.95                     | 0.49              |
| 2:B:1142:GLY:HA3  | 6:F:88:TYR:HE2    | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1214:PRO:O    | 2:B:1214:PRO:HG2  | 2.13                     | 0.49              |
| 2:B:222:ILE:O     | 2:B:240:ILE:HA    | 2.13                     | 0.49              |
| 2:B:386:LEU:O     | 2:B:387:LEU:C     | 2.50                     | 0.49              |
| 2:B:1084:GLN:OE1  | 3:C:189:THR:CG2   | 2.61                     | 0.49              |
| 4:D:173:HIS:ND1   | 4:D:174:PRO:HD2   | 2.28                     | 0.49              |
| 5:E:124:VAL:HG13  | 5:E:132:ILE:CB    | 2.41                     | 0.49              |
| 11:K:52:ASN:O     | 11:K:53:ASP:C     | 2.51                     | 0.49              |
| 1:A:862:ASN:O     | 1:A:864:ILE:HG13  | 2.12                     | 0.48              |
| 1:A:958:VAL:HG22  | 1:A:1052:GLN:HB3  | 1.95                     | 0.48              |
| 2:B:167:ILE:HG22  | 2:B:453:ILE:CD1   | 2.42                     | 0.48              |
| 2:B:29:ASP:HB3    | 2:B:658:ILE:HD13  | 1.95                     | 0.48              |
| 2:B:763:GLN:HG2   | 2:B:765:PRO:HD2   | 1.94                     | 0.48              |
| 2:B:863:GLU:O     | 2:B:961:LEU:HD22  | 2.12                     | 0.48              |
| 3:C:245:VAL:HA    | 3:C:248:ILE:HD12  | 1.94                     | 0.48              |
| 5:E:136:ASN:OD1   | 5:E:137:GLU:N     | 2.46                     | 0.48              |
| 9:I:60:GLN:NE2    | 9:I:107:SER:OG    | 2.46                     | 0.48              |
| 3:C:35:ARG:HH11   | 11:K:41:THR:N     | 2.10                     | 0.48              |
| 12:L:31:CYS:SG    | 12:L:34:CYS:N     | 2.84                     | 0.48              |
| 1:A:1115:SER:HB3  | 1:A:1330:ASN:HD21 | 1.78                     | 0.48              |
| 1:A:1219:THR:HG21 | 1:A:1271:ILE:CD1  | 2.43                     | 0.48              |
| 1:A:1349:TYR:CA   | 1:A:1372:VAL:HG21 | 2.43                     | 0.48              |
| 1:A:388:LEU:CD2   | 1:A:432:VAL:HB    | 2.43                     | 0.48              |
| 1:A:710:LEU:HD12  | 1:A:710:LEU:H     | 1.78                     | 0.48              |
| 1:A:961:ARG:HG2   | 1:A:965:GLN:HE21  | 1.78                     | 0.48              |
| 1:A:993:LEU:HD23  | 1:A:1022:LEU:HD21 | 1.95                     | 0.48              |
| 2:B:1070:GLU:OE1  | 10:J:44:TYR:OH    | 2.30                     | 0.48              |
| 2:B:1095:LEU:CD1  | 2:B:1095:LEU:H    | 2.16                     | 0.48              |
| 2:B:1182:CYS:O    | 2:B:1183:LYS:C    | 2.51                     | 0.48              |
| 2:B:203:PHE:N     | 2:B:203:PHE:CD1   | 2.81                     | 0.48              |
| 2:B:33:VAL:O      | 2:B:36:ALA:HB3    | 2.13                     | 0.48              |
| 2:B:344:LYS:O     | 2:B:345:LYS:HG3   | 2.13                     | 0.48              |
| 2:B:799:PRO:CB    | 2:B:818:PRO:HG2   | 2.43                     | 0.48              |
| 2:B:978:ASP:O     | 2:B:989:THR:HB    | 2.12                     | 0.48              |
| 3:C:45:ALA:HA     | 3:C:72:LEU:HD12   | 1.94                     | 0.48              |
| 5:E:124:VAL:HA    | 5:E:132:ILE:HD12  | 1.95                     | 0.48              |
| 5:E:10:SER:O      | 5:E:14:ARG:HG3    | 2.11                     | 0.48              |
| 9:I:69:PRO:HB2    | 9:I:85:PHE:CE2    | 2.48                     | 0.48              |
| 1:A:1059:HIS:O    | 1:A:1060:PRO:C    | 2.52                     | 0.48              |
| 1:A:35:ILE:CD1    | 1:A:241:VAL:HG11  | 2.42                     | 0.48              |
| 1:A:300:VAL:O     | 1:A:300:VAL:HG12  | 2.11                     | 0.48              |
| 1:A:767:GLN:HE21  | 1:A:774:ARG:HB3   | 1.74                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:947:PHE:CD2   | 1:A:954:TRP:CZ2   | 3.02                     | 0.48              |
| 2:B:1156:ASP:HB3  | 2:B:1197:PRO:HA   | 1.95                     | 0.48              |
| 2:B:254:LEU:HD23  | 2:B:381:MET:HE3   | 1.94                     | 0.48              |
| 2:B:343:ILE:HB    | 2:B:348:ARG:HG3   | 1.95                     | 0.48              |
| 8:H:11:GLN:O      | 8:H:28:ALA:HB1    | 2.13                     | 0.48              |
| 10:J:14:VAL:HG12  | 10:J:50:ILE:HD11  | 1.95                     | 0.48              |
| 12:L:47:ARG:HH21  | 12:L:54:ARG:NH2   | 2.11                     | 0.48              |
| 13:N:5:DA:H2"     | 13:N:6:DC:OP2     | 2.12                     | 0.48              |
| 1:A:108:MET:SD    | 1:A:210:ILE:HD13  | 2.53                     | 0.48              |
| 1:A:718:VAL:O     | 1:A:721:PHE:HB2   | 2.12                     | 0.48              |
| 1:A:913:LEU:CD1   | 1:A:914:GLU:N     | 2.71                     | 0.48              |
| 2:B:1007:VAL:HG22 | 2:B:1008:PRO:CD   | 2.41                     | 0.48              |
| 2:B:363:HIS:O     | 2:B:364:ILE:CB    | 2.55                     | 0.48              |
| 2:B:429:PHE:HA    | 2:B:432:MET:HE3   | 1.96                     | 0.48              |
| 2:B:604:ARG:O     | 2:B:606:LYS:N     | 2.46                     | 0.48              |
| 2:B:603:LEU:HB3   | 2:B:609:ILE:HG13  | 1.93                     | 0.48              |
| 2:B:758:PHE:CE2   | 2:B:1044:ALA:CA   | 2.92                     | 0.48              |
| 7:G:117:GLN:C     | 7:G:119:LEU:H     | 2.17                     | 0.48              |
| 7:G:80:LYS:CD     | 7:G:80:LYS:N      | 2.73                     | 0.48              |
| 1:A:701:LEU:HD23  | 9:I:115:LYS:HG3   | 1.95                     | 0.48              |
| 1:A:1208:THR:HG22 | 1:A:1210:GLY:H    | 1.78                     | 0.48              |
| 1:A:1299:VAL:CG1  | 1:A:1300:LYS:N    | 2.76                     | 0.48              |
| 1:A:43:GLU:O      | 1:A:44:THR:CB     | 2.61                     | 0.48              |
| 1:A:936:LEU:O     | 1:A:939:ASP:HB2   | 2.13                     | 0.48              |
| 2:B:34:ILE:O      | 2:B:35:SER:C      | 2.52                     | 0.48              |
| 2:B:37:PHE:HE1    | 2:B:41:LYS:CD     | 2.26                     | 0.48              |
| 2:B:810:GLU:HB3   | 2:B:811:TYR:CE1   | 2.48                     | 0.48              |
| 2:B:899:ILE:HD13  | 2:B:905:VAL:CG1   | 2.43                     | 0.48              |
| 3:C:209:TYR:H     | 3:C:209:TYR:HD1   | 1.58                     | 0.48              |
| 7:G:20:PRO:CG     | 7:G:21:ARG:H      | 2.26                     | 0.48              |
| 1:A:1225:PHE:CE2  | 1:A:1227:ILE:HD11 | 2.49                     | 0.48              |
| 1:A:399:HIS:CB    | 1:A:400:PRO:CD    | 2.88                     | 0.48              |
| 1:A:420:ARG:O     | 1:A:421:ALA:C     | 2.50                     | 0.48              |
| 1:A:446:ARG:HD2   | 1:A:480:ALA:HB2   | 1.95                     | 0.48              |
| 1:A:535:THR:HG22  | 1:A:536:LEU:N     | 2.27                     | 0.48              |
| 1:A:603:ASN:O     | 1:A:604:GLY:C     | 2.51                     | 0.48              |
| 2:B:128:LEU:HB2   | 2:B:168:GLY:O     | 2.13                     | 0.48              |
| 2:B:197:PHE:HZ    | 2:B:816:GLU:HG2   | 1.78                     | 0.48              |
| 2:B:769:TYR:O     | 2:B:771:SER:N     | 2.47                     | 0.48              |
| 9:I:71:SER:OG     | 9:I:83:ASN:HB2    | 2.13                     | 0.48              |
| 1:A:1030:ARG:NH1  | 1:A:1035:TYR:OH   | 2.47                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:504:LEU:HD12 | 1:A:504:LEU:N     | 2.28                     | 0.48              |
| 1:A:868:TYR:CE1  | 1:A:1064:VAL:CG1  | 2.84                     | 0.48              |
| 2:B:1001:PHE:CZ  | 2:B:1073:TYR:HB2  | 2.49                     | 0.48              |
| 2:B:213:ILE:O    | 2:B:215:GLN:HG2   | 2.13                     | 0.48              |
| 2:B:39:ARG:HG2   | 2:B:39:ARG:NH1    | 2.29                     | 0.48              |
| 2:B:579:ARG:HB2  | 2:B:586:TRP:HE1   | 1.78                     | 0.48              |
| 2:B:911:ILE:CG2  | 2:B:966:VAL:HG11  | 2.44                     | 0.48              |
| 3:C:215:GLU:O    | 3:C:216:GLY:C     | 2.51                     | 0.48              |
| 3:C:88:CYS:SG    | 3:C:91:HIS:HA     | 2.53                     | 0.48              |
| 6:F:85:MET:CE    | 6:F:93:ILE:HD12   | 2.44                     | 0.48              |
| 7:G:20:PRO:HG2   | 7:G:21:ARG:N      | 2.28                     | 0.48              |
| 8:H:63:LEU:HD22  | 8:H:90:ALA:HB3    | 1.96                     | 0.48              |
| 9:I:85:PHE:N     | 9:I:85:PHE:CD2    | 2.68                     | 0.48              |
| 1:A:1076:ALA:HA  | 1:A:1079:MET:HE2  | 1.95                     | 0.48              |
| 1:A:1259:MET:C   | 1:A:1261:LYS:H    | 2.16                     | 0.48              |
| 1:A:844:ALA:O    | 1:A:845:LEU:HD23  | 2.13                     | 0.48              |
| 1:A:852:TYR:HA   | 1:A:1060:PRO:HB3  | 1.96                     | 0.48              |
| 1:A:863:VAL:HG11 | 1:A:866:PHE:CE2   | 2.49                     | 0.48              |
| 2:B:683:SER:C    | 2:B:685:LEU:H     | 2.15                     | 0.48              |
| 1:A:701:LEU:HD23 | 9:I:115:LYS:CG    | 2.44                     | 0.48              |
| 1:A:1036:ARG:HG2 | 1:A:1036:ARG:NH1  | 2.21                     | 0.48              |
| 1:A:1373:ASP:O   | 1:A:1376:THR:HG23 | 2.14                     | 0.48              |
| 1:A:218:ASP:O    | 1:A:219:PHE:O     | 2.32                     | 0.48              |
| 1:A:353:ILE:HB   | 1:A:470:LEU:CD2   | 2.43                     | 0.48              |
| 1:A:427:GLN:O    | 1:A:428:TYR:C     | 2.52                     | 0.48              |
| 1:A:618:GLU:O    | 1:A:619:LYS:C     | 2.52                     | 0.48              |
| 1:A:666:ILE:HD12 | 1:A:667:GLY:N     | 2.25                     | 0.48              |
| 1:A:71:GLN:C     | 1:A:73:GLY:H      | 2.16                     | 0.48              |
| 1:A:954:TRP:HB3  | 1:A:955:PRO:HD2   | 1.95                     | 0.48              |
| 2:B:175:ARG:NH1  | 2:B:175:ARG:HG2   | 2.27                     | 0.48              |
| 2:B:575:PRO:HG2  | 2:B:576:ASP:H     | 1.79                     | 0.48              |
| 2:B:970:THR:HG22 | 2:B:971:THR:N     | 2.28                     | 0.48              |
| 3:C:82:TYR:O     | 3:C:83:SER:C      | 2.51                     | 0.48              |
| 7:G:122:ASN:ND2  | 7:G:125:SER:HB3   | 2.29                     | 0.48              |
| 11:K:110:ASN:C   | 11:K:111:LEU:HG   | 2.34                     | 0.48              |
| 1:A:130:ASP:O    | 1:A:133:LYS:N     | 2.38                     | 0.48              |
| 1:A:1325:THR:CG2 | 1:A:1325:THR:O    | 2.61                     | 0.48              |
| 1:A:21:LEU:HG    | 1:A:1413:GLY:O    | 2.14                     | 0.48              |
| 1:A:1445:ILE:N   | 1:A:1445:ILE:CD1  | 2.68                     | 0.48              |
| 2:B:259:TYR:N    | 2:B:259:TYR:CD1   | 2.82                     | 0.48              |
| 2:B:236:HIS:CE1  | 2:B:389:ALA:HA    | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:446:LEU:O     | 2:B:447:ALA:CB    | 2.62                     | 0.48              |
| 2:B:515:HIS:CD2   | 2:B:517:THR:HG23  | 2.49                     | 0.48              |
| 2:B:653:VAL:HG22  | 2:B:689:LEU:HD13  | 1.95                     | 0.48              |
| 2:B:899:ILE:HD12  | 2:B:911:ILE:HG23  | 1.95                     | 0.48              |
| 3:C:235:VAL:HG13  | 10:J:13:VAL:HG23  | 1.95                     | 0.48              |
| 5:E:161:LYS:HD2   | 5:E:195:VAL:HG23  | 1.95                     | 0.48              |
| 5:E:180:ARG:NH2   | 5:E:192:ARG:HB2   | 2.25                     | 0.48              |
| 1:A:1446:ASP:HB2  | 6:F:133:VAL:HG23  | 1.96                     | 0.48              |
| 8:H:111:LEU:HD23  | 8:H:127:GLY:O     | 2.14                     | 0.48              |
| 10:J:23:ASN:O     | 10:J:25:LEU:N     | 2.47                     | 0.48              |
| 2:B:992:ILE:HD11  | 11:K:66:PRO:HB2   | 1.96                     | 0.48              |
| 1:A:1387:HIS:CE1  | 13:N:4:DT:H5"     | 2.48                     | 0.48              |
| 1:A:1377:THR:HA   | 5:E:212:ARG:HH21  | 1.79                     | 0.47              |
| 1:A:1377:THR:O    | 1:A:1378:GLN:C    | 2.52                     | 0.47              |
| 1:A:1397:LEU:O    | 1:A:1400:CYS:HB3  | 2.13                     | 0.47              |
| 1:A:541:ILE:HD13  | 1:A:549:MET:HE3   | 1.93                     | 0.47              |
| 2:B:1047:PHE:N    | 2:B:1047:PHE:CD1  | 2.76                     | 0.47              |
| 2:B:1099:VAL:HG12 | 2:B:1100:ASP:H    | 1.79                     | 0.47              |
| 2:B:247:GLY:C     | 2:B:249:ARG:N     | 2.67                     | 0.47              |
| 2:B:310:MET:O     | 2:B:313:MET:HB2   | 2.14                     | 0.47              |
| 2:B:579:ARG:N     | 2:B:589:VAL:HG13  | 2.29                     | 0.47              |
| 2:B:30:SER:HB3    | 2:B:743:ILE:O     | 2.14                     | 0.47              |
| 3:C:31:ASN:O      | 3:C:34:ARG:HB3    | 2.14                     | 0.47              |
| 7:G:35:GLU:CG     | 7:G:48:VAL:HG23   | 2.44                     | 0.47              |
| 1:A:789:LYS:HE3   | 9:I:67:THR:OG1    | 2.14                     | 0.47              |
| 11:K:19:LEU:HD22  | 11:K:33:ILE:CG2   | 2.43                     | 0.47              |
| 3:C:29:MET:HE1    | 11:K:98:LEU:HG    | 1.95                     | 0.47              |
| 1:A:224:PHE:CE2   | 1:A:231:PRO:HA    | 2.49                     | 0.47              |
| 1:A:401:GLY:C     | 1:A:435:HIS:HD2   | 2.16                     | 0.47              |
| 1:A:600:PRO:C     | 1:A:602:ASP:H     | 2.16                     | 0.47              |
| 2:B:1050:ILE:HG22 | 2:B:1051:THR:H    | 1.79                     | 0.47              |
| 1:A:466:SER:HB2   | 2:B:1099:VAL:HG11 | 1.96                     | 0.47              |
| 2:B:118:ARG:HG2   | 2:B:204:ILE:HD13  | 1.94                     | 0.47              |
| 2:B:185:THR:O     | 2:B:188:ASP:HB2   | 2.13                     | 0.47              |
| 2:B:205:ILE:N     | 2:B:205:ILE:HD12  | 2.28                     | 0.47              |
| 2:B:459:TYR:CD2   | 2:B:459:TYR:C     | 2.88                     | 0.47              |
| 3:C:114:TYR:CD2   | 3:C:140:ASN:HB2   | 2.49                     | 0.47              |
| 3:C:31:ASN:O      | 3:C:32:SER:C      | 2.51                     | 0.47              |
| 1:A:381:THR:HG23  | 1:A:382:PRO:HD2   | 1.95                     | 0.47              |
| 1:A:399:HIS:CG    | 1:A:400:PRO:N     | 2.81                     | 0.47              |
| 1:A:722:LEU:O     | 1:A:725:ALA:HB3   | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1033:LYS:CE   | 2:B:1070:GLU:OE1  | 2.62                     | 0.47              |
| 2:B:1031:LEU:HA   | 2:B:1055:ILE:HD13 | 1.96                     | 0.47              |
| 2:B:1147:LEU:HD23 | 2:B:1147:LEU:C    | 2.35                     | 0.47              |
| 2:B:100:PRO:HD3   | 2:B:172:ILE:HD12  | 1.96                     | 0.47              |
| 2:B:197:PHE:CZ    | 2:B:816:GLU:HG2   | 2.49                     | 0.47              |
| 2:B:882:THR:CB    | 2:B:934:LYS:O     | 2.62                     | 0.47              |
| 3:C:177:GLU:HB2   | 3:C:231:ASN:HB3   | 1.95                     | 0.47              |
| 3:C:242:GLN:C     | 3:C:244:VAL:H     | 2.16                     | 0.47              |
| 3:C:36:VAL:HG11   | 3:C:251:LEU:HB2   | 1.96                     | 0.47              |
| 7:G:115:MET:CB    | 7:G:116:PRO:HD2   | 2.44                     | 0.47              |
| 7:G:154:VAL:HG12  | 7:G:155:SER:H     | 1.79                     | 0.47              |
| 7:G:25:TYR:O      | 7:G:28:THR:HB     | 2.14                     | 0.47              |
| 8:H:26:ILE:CG2    | 8:H:27:GLU:N      | 2.77                     | 0.47              |
| 8:H:31:THR:O      | 8:H:31:THR:HG22   | 2.13                     | 0.47              |
| 1:A:325:ILE:O     | 1:A:326:ARG:C     | 2.52                     | 0.47              |
| 1:A:500:GLU:O     | 1:A:504:LEU:HD13  | 2.14                     | 0.47              |
| 1:A:735:VAL:HG12  | 1:A:735:VAL:O     | 2.14                     | 0.47              |
| 1:A:770:VAL:HA    | 1:A:822:GLU:OE1   | 2.14                     | 0.47              |
| 2:B:1099:VAL:HG13 | 2:B:1100:ASP:N    | 2.27                     | 0.47              |
| 2:B:1110:PRO:HB2  | 2:B:1119:VAL:HG21 | 1.96                     | 0.47              |
| 2:B:1162:ILE:C    | 2:B:1171:VAL:HG21 | 2.34                     | 0.47              |
| 2:B:298:LEU:N     | 2:B:298:LEU:CD2   | 2.77                     | 0.47              |
| 2:B:696:GLU:O     | 2:B:699:GLU:HB2   | 2.14                     | 0.47              |
| 3:C:242:GLN:HB3   | 3:C:246:ARG:HG3   | 1.97                     | 0.47              |
| 3:C:254:LYS:C     | 3:C:256:ALA:N     | 2.67                     | 0.47              |
| 7:G:34:VAL:HG12   | 7:G:45:ILE:CG2    | 2.39                     | 0.47              |
| 11:K:40:HIS:O     | 11:K:41:THR:C     | 2.53                     | 0.47              |
| 1:A:1111:MET:HE1  | 1:A:1330:ASN:OD1  | 2.13                     | 0.47              |
| 1:A:326:ARG:HG2   | 1:A:327:ALA:N     | 2.30                     | 0.47              |
| 1:A:567:LYS:NZ    | 8:H:46:LEU:HB2    | 2.30                     | 0.47              |
| 1:A:921:GLY:O     | 1:A:922:ASP:C     | 2.52                     | 0.47              |
| 2:B:579:ARG:HG2   | 2:B:579:ARG:NH1   | 2.29                     | 0.47              |
| 2:B:841:MET:SD    | 2:B:846:ILE:HD11  | 2.54                     | 0.47              |
| 14:P:7:A:C2'      | 14:P:8:G:O4'      | 2.62                     | 0.47              |
| 1:A:1166:ASP:OD2  | 1:A:1239:ARG:HD2  | 2.14                     | 0.47              |
| 1:A:1356:ILE:O    | 1:A:1356:ILE:HG22 | 2.14                     | 0.47              |
| 1:A:88:LYS:HE3    | 1:A:280:GLU:OE2   | 2.15                     | 0.47              |
| 1:A:331:GLY:O     | 1:A:332:LYS:HB3   | 2.15                     | 0.47              |
| 1:A:369:SER:HB2   | 11:K:2:ASN:OD1    | 2.15                     | 0.47              |
| 1:A:867:ILE:HG22  | 1:A:872:GLY:H     | 1.79                     | 0.47              |
| 2:B:1064:TYR:O    | 2:B:1065:GLN:C    | 2.53                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:115:GLN:HG2   | 2:B:193:LYS:HB2   | 1.96                     | 0.47              |
| 2:B:386:LEU:O     | 2:B:389:ALA:N     | 2.47                     | 0.47              |
| 2:B:794:ASN:C     | 2:B:795:ILE:HD12  | 2.35                     | 0.47              |
| 6:F:135:ARG:HD3   | 6:F:143:PHE:CD2   | 2.50                     | 0.47              |
| 7:G:3:PHE:CG      | 7:G:80:LYS:NZ     | 2.73                     | 0.47              |
| 8:H:142:LEU:C     | 8:H:143:LEU:HD12  | 2.35                     | 0.47              |
| 9:I:33:SER:O      | 9:I:34:TYR:O      | 2.32                     | 0.47              |
| 10:J:36:LEU:HD12  | 10:J:47:ARG:NH1   | 2.30                     | 0.47              |
| 12:L:30:ILE:HG22  | 12:L:31:CYS:N     | 2.29                     | 0.47              |
| 12:L:61:THR:HG22  | 12:L:63:ARG:HG2   | 1.96                     | 0.47              |
| 1:A:243:PRO:O     | 1:A:244:PRO:C     | 2.53                     | 0.47              |
| 1:A:298:PHE:O     | 1:A:301:ALA:HB3   | 2.13                     | 0.47              |
| 1:A:339:ASN:O     | 1:A:343:LYS:HG2   | 2.14                     | 0.47              |
| 1:A:350:ARG:HG3   | 1:A:350:ARG:HH11  | 1.79                     | 0.47              |
| 1:A:41:MET:HB3    | 1:A:48:ALA:O      | 2.15                     | 0.47              |
| 1:A:888:GLY:O     | 1:A:940:ARG:NH2   | 2.48                     | 0.47              |
| 2:B:757:PRO:HG3   | 2:B:1028:GLU:OE2  | 2.14                     | 0.47              |
| 3:C:73:GLN:NE2    | 3:C:75:MET:HB2    | 2.30                     | 0.47              |
| 4:D:119:ARG:HG2   | 4:D:120:GLU:N     | 2.29                     | 0.47              |
| 4:D:134:THR:CG2   | 4:D:135:GLY:H     | 2.26                     | 0.47              |
| 4:D:191:ALA:O     | 4:D:193:THR:N     | 2.47                     | 0.47              |
| 8:H:93:TYR:N      | 8:H:93:TYR:CD1    | 2.82                     | 0.47              |
| 1:A:1151:GLU:HB3  | 1:A:1153:TYR:HE1  | 1.79                     | 0.47              |
| 1:A:1144:LYS:HB2  | 1:A:1268:LEU:O    | 2.13                     | 0.47              |
| 1:A:1313:LEU:HD23 | 1:A:1338:VAL:CB   | 2.45                     | 0.47              |
| 1:A:402:ALA:CB    | 1:A:434:ARG:HA    | 2.45                     | 0.47              |
| 1:A:565:ILE:O     | 1:A:570:PRO:HA    | 2.14                     | 0.47              |
| 1:A:829:VAL:C     | 1:A:831:THR:N     | 2.68                     | 0.47              |
| 1:A:899:VAL:HB    | 1:A:929:LEU:HD11  | 1.97                     | 0.47              |
| 1:A:982:THR:H     | 1:A:985:ASP:CB    | 2.27                     | 0.47              |
| 2:B:839:MET:HB3   | 2:B:1012:ILE:HG22 | 1.96                     | 0.47              |
| 2:B:168:GLY:HA2   | 2:B:454:THR:OG1   | 2.15                     | 0.47              |
| 2:B:37:PHE:CD2    | 2:B:542:MET:SD    | 3.08                     | 0.47              |
| 2:B:653:VAL:HG23  | 2:B:689:LEU:HB3   | 1.97                     | 0.47              |
| 2:B:950:ASP:O     | 2:B:951:GLN:HB2   | 2.15                     | 0.47              |
| 5:E:31:THR:O      | 5:E:35:VAL:HG23   | 2.13                     | 0.47              |
| 5:E:84:ASP:O      | 5:E:86:PRO:HD3    | 2.15                     | 0.47              |
| 6:F:88:TYR:N      | 6:F:88:TYR:CD1    | 2.83                     | 0.47              |
| 1:A:504:LEU:HD11  | 6:F:91:ALA:HB1    | 1.95                     | 0.47              |
| 8:H:128:ASN:O     | 8:H:128:ASN:OD1   | 2.32                     | 0.47              |
| 8:H:55:LEU:HD22   | 8:H:144:ILE:HG21  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:52:ASN:O     | 11:K:54:ARG:N     | 2.48                     | 0.47              |
| 11:K:89:ASN:O     | 11:K:92:ASN:N     | 2.48                     | 0.47              |
| 1:A:1105:LEU:HD22 | 1:A:1384:VAL:HG21 | 1.97                     | 0.47              |
| 1:A:1323:ASP:C    | 1:A:1325:THR:H    | 2.18                     | 0.47              |
| 1:A:37:PHE:HD1    | 1:A:37:PHE:N      | 2.13                     | 0.47              |
| 1:A:534:LEU:HD13  | 1:A:656:TRP:CG    | 2.50                     | 0.47              |
| 1:A:632:VAL:O     | 1:A:633:VAL:C     | 2.53                     | 0.47              |
| 1:A:63:ARG:HA     | 1:A:74:MET:HE2    | 1.95                     | 0.47              |
| 1:A:774:ARG:H     | 1:A:774:ARG:HG2   | 1.42                     | 0.47              |
| 2:B:361:LEU:HD21  | 2:B:377:PHE:HD2   | 1.72                     | 0.47              |
| 2:B:949:VAL:HG12  | 2:B:950:ASP:N     | 2.29                     | 0.47              |
| 4:D:20:GLU:HA     | 4:D:20:GLU:OE2    | 2.14                     | 0.47              |
| 5:E:175:LEU:HD23  | 5:E:176:PRO:HD2   | 1.95                     | 0.47              |
| 7:G:1:MET:SD      | 7:G:79:PHE:CE1    | 3.08                     | 0.47              |
| 10:J:7:CYS:SG     | 10:J:49:MET:HE3   | 2.54                     | 0.47              |
| 11:K:12:LEU:H     | 11:K:12:LEU:CD1   | 2.24                     | 0.47              |
| 12:L:60:ARG:HG2   | 12:L:61:THR:H     | 1.80                     | 0.47              |
| 1:A:42:ASP:HA     | 1:A:46:THR:O      | 2.15                     | 0.47              |
| 1:A:853:ASP:O     | 1:A:854:ASN:HB2   | 2.15                     | 0.47              |
| 1:A:901:LEU:N     | 1:A:926:GLN:HE21  | 2.08                     | 0.47              |
| 2:B:983:ARG:HH11  | 2:B:1091:TYR:HB3  | 1.80                     | 0.47              |
| 2:B:1107:ALA:O    | 2:B:1108:ARG:HG2  | 2.15                     | 0.47              |
| 2:B:431:TYR:CE2   | 2:B:447:ALA:HB2   | 2.50                     | 0.47              |
| 2:B:582:VAL:HA    | 2:B:626:ILE:O     | 2.15                     | 0.47              |
| 2:B:730:ARG:O     | 2:B:731:VAL:O     | 2.33                     | 0.47              |
| 2:B:758:PHE:HB3   | 2:B:761:HIS:CD2   | 2.50                     | 0.47              |
| 3:C:168:ALA:O     | 3:C:170:TRP:N     | 2.48                     | 0.47              |
| 7:G:25:TYR:HE2    | 7:G:29:LYS:HD2    | 1.80                     | 0.47              |
| 11:K:101:LEU:HD23 | 11:K:101:LEU:O    | 2.15                     | 0.47              |
| 1:A:1280:GLU:O    | 1:A:1281:ARG:O    | 2.33                     | 0.47              |
| 1:A:236:LEU:HD11  | 1:A:304:MET:HE1   | 1.96                     | 0.47              |
| 1:A:427:GLN:HB2   | 1:A:430:TRP:NE1   | 2.30                     | 0.47              |
| 1:A:43:GLU:O      | 1:A:44:THR:HB     | 2.15                     | 0.47              |
| 1:A:588:LEU:O     | 1:A:606:LEU:HD12  | 2.14                     | 0.47              |
| 1:A:1410:PHE:HD2  | 2:B:1212:ILE:HD12 | 1.80                     | 0.47              |
| 2:B:388:CYS:C     | 2:B:390:LEU:N     | 2.67                     | 0.47              |
| 2:B:37:PHE:CE1    | 2:B:41:LYS:HG3    | 2.51                     | 0.47              |
| 2:B:461:LEU:N     | 2:B:461:LEU:HD12  | 2.29                     | 0.47              |
| 5:E:205:SER:O     | 5:E:206:GLY:C     | 2.52                     | 0.47              |
| 7:G:23:LYS:HG3    | 7:G:56:ILE:HD12   | 1.96                     | 0.47              |
| 11:K:111:LEU:O    | 11:K:112:GLN:CG   | 2.62                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:278:THR:O     | 1:A:278:THR:HG22  | 2.15                     | 0.46              |
| 2:B:118:ARG:HH11  | 2:B:204:ILE:HD11  | 1.80                     | 0.46              |
| 2:B:640:VAL:HG12  | 2:B:640:VAL:O     | 2.16                     | 0.46              |
| 2:B:999:MET:HA    | 2:B:999:MET:CE    | 2.45                     | 0.46              |
| 3:C:146:LYS:C     | 3:C:147:LEU:HD23  | 2.36                     | 0.46              |
| 3:C:256:ALA:C     | 3:C:258:ILE:N     | 2.68                     | 0.46              |
| 4:D:7:THR:HG21    | 4:D:32:GLU:OE2    | 2.15                     | 0.46              |
| 7:G:39:THR:CG2    | 7:G:40:GLY:H      | 2.26                     | 0.46              |
| 4:D:48:ILE:CG2    | 7:G:4:ILE:HB      | 2.45                     | 0.46              |
| 8:H:42:ILE:O      | 8:H:44:VAL:HG23   | 2.15                     | 0.46              |
| 1:A:698:GLN:HA    | 9:I:97:MET:O      | 2.14                     | 0.46              |
| 1:A:1027:ALA:O    | 1:A:1031:VAL:HG23 | 2.15                     | 0.46              |
| 1:A:1072:ILE:HD11 | 1:A:1368:MET:HA   | 1.98                     | 0.46              |
| 1:A:224:PHE:HZ    | 1:A:234:MET:CE    | 2.27                     | 0.46              |
| 1:A:353:ILE:HG21  | 1:A:487:MET:CG    | 2.41                     | 0.46              |
| 1:A:586:ILE:CD1   | 1:A:633:VAL:HG22  | 2.45                     | 0.46              |
| 2:B:1109:GLY:O    | 2:B:1110:PRO:C    | 2.54                     | 0.46              |
| 2:B:1115:THR:CG2  | 2:B:1117:GLN:HG3  | 2.45                     | 0.46              |
| 2:B:212:LEU:HD23  | 2:B:480:SER:HB2   | 1.97                     | 0.46              |
| 2:B:823:ALA:O     | 2:B:825:VAL:N     | 2.48                     | 0.46              |
| 2:B:865:LYS:HE2   | 2:B:871:THR:OG1   | 2.15                     | 0.46              |
| 1:A:253:ASN:HB3   | 2:B:935:ARG:NH1   | 2.30                     | 0.46              |
| 6:F:123:LYS:O     | 6:F:124:GLU:C     | 2.54                     | 0.46              |
| 8:H:4:THR:HG22    | 8:H:5:LEU:N       | 2.29                     | 0.46              |
| 10:J:16:ASP:O     | 10:J:18:TRP:N     | 2.48                     | 0.46              |
| 11:K:42:LEU:HD21  | 11:K:46:ILE:HD11  | 1.96                     | 0.46              |
| 1:A:547:LEU:HD22  | 11:K:58:PHE:CE1   | 2.50                     | 0.46              |
| 15:T:11:DG:H2"    | 15:T:12:DT:OP2    | 2.15                     | 0.46              |
| 1:A:1175:SER:O    | 1:A:1176:LEU:HB2  | 2.15                     | 0.46              |
| 1:A:1239:ARG:HB3  | 1:A:1239:ARG:NH1  | 2.30                     | 0.46              |
| 1:A:1193:LEU:HD22 | 1:A:1260:LEU:HD11 | 1.97                     | 0.46              |
| 1:A:1219:THR:HG21 | 1:A:1271:ILE:HD11 | 1.96                     | 0.46              |
| 1:A:224:PHE:CE2   | 1:A:231:PRO:HG3   | 2.50                     | 0.46              |
| 1:A:289:ILE:C     | 1:A:291:GLU:N     | 2.68                     | 0.46              |
| 1:A:438:ASP:OD1   | 1:A:461:LYS:HA    | 2.15                     | 0.46              |
| 1:A:634:THR:HG1   | 1:A:642:CYS:HG    | 1.63                     | 0.46              |
| 1:A:967:ALA:O     | 1:A:968:GLN:O     | 2.33                     | 0.46              |
| 1:A:343:LYS:NZ    | 2:B:1151:LEU:O    | 2.40                     | 0.46              |
| 2:B:185:THR:N     | 2:B:188:ASP:HB2   | 2.27                     | 0.46              |
| 2:B:230:ALA:N     | 2:B:231:PRO:CD    | 2.78                     | 0.46              |
| 2:B:467:GLY:N     | 2:B:475:SER:CB    | 2.71                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:821:GLN:NE2   | 2:B:851:PHE:HA    | 2.23                     | 0.46              |
| 2:B:861:ASP:OD1   | 2:B:862:GLN:N     | 2.48                     | 0.46              |
| 3:C:141:GLY:HA2   | 10:J:16:ASP:HB3   | 1.97                     | 0.46              |
| 3:C:47:ASP:HA     | 3:C:169:LYS:NZ    | 2.30                     | 0.46              |
| 4:D:156:ASP:C     | 4:D:158:GLU:N     | 2.69                     | 0.46              |
| 4:D:54:GLU:O      | 4:D:58:VAL:HG23   | 2.14                     | 0.46              |
| 7:G:1:MET:CE      | 7:G:1:MET:O       | 2.64                     | 0.46              |
| 9:I:98:VAL:HG11   | 9:I:113:ASP:OD1   | 2.15                     | 0.46              |
| 1:A:1219:THR:HG21 | 1:A:1271:ILE:HG13 | 1.97                     | 0.46              |
| 1:A:261:ASP:O     | 1:A:264:PHE:HB2   | 2.15                     | 0.46              |
| 1:A:393:ARG:O     | 1:A:395:GLY:N     | 2.49                     | 0.46              |
| 1:A:42:ASP:C      | 1:A:44:THR:N      | 2.68                     | 0.46              |
| 1:A:499:ALA:O     | 1:A:503:GLN:HG2   | 2.15                     | 0.46              |
| 1:A:871:ASP:OD2   | 1:A:873:MET:HB2   | 2.15                     | 0.46              |
| 2:B:383:ASN:O     | 2:B:384:ARG:C     | 2.53                     | 0.46              |
| 2:B:39:ARG:CZ     | 2:B:665:GLU:HG2   | 2.45                     | 0.46              |
| 2:B:547:VAL:HG12  | 2:B:612:GLU:OE2   | 2.14                     | 0.46              |
| 2:B:683:SER:O     | 2:B:685:LEU:N     | 2.48                     | 0.46              |
| 2:B:990:ILE:CG2   | 2:B:991:GLY:N     | 2.78                     | 0.46              |
| 3:C:123:ASN:ND2   | 3:C:125:MET:SD    | 2.89                     | 0.46              |
| 4:D:10:THR:O      | 4:D:10:THR:HG23   | 2.16                     | 0.46              |
| 4:D:151:PHE:N     | 4:D:151:PHE:CD1   | 2.83                     | 0.46              |
| 5:E:16:PHE:HZ     | 5:E:20:LYS:HE2    | 1.77                     | 0.46              |
| 5:E:67:GLU:O      | 5:E:70:SER:HB3    | 2.15                     | 0.46              |
| 9:I:82:GLU:HB3    | 9:I:104:LEU:HD12  | 1.97                     | 0.46              |
| 11:K:10:PHE:CD1   | 11:K:11:LEU:CD2   | 2.99                     | 0.46              |
| 1:A:1118:VAL:HG23 | 1:A:1306:LEU:HB2  | 1.96                     | 0.46              |
| 1:A:114:LEU:O     | 1:A:115:LEU:HG    | 2.14                     | 0.46              |
| 1:A:1111:MET:CE   | 1:A:1330:ASN:OD1  | 2.64                     | 0.46              |
| 1:A:167:CYS:SG    | 1:A:167:CYS:O     | 2.73                     | 0.46              |
| 1:A:224:PHE:CD2   | 1:A:231:PRO:HG3   | 2.50                     | 0.46              |
| 1:A:34:LYS:HB3    | 1:A:36:ARG:NE     | 2.31                     | 0.46              |
| 1:A:445:ASN:HB2   | 1:A:455:MET:HG2   | 1.98                     | 0.46              |
| 1:A:470:LEU:HD22  | 1:A:487:MET:CE    | 2.46                     | 0.46              |
| 1:A:637:LYS:CB    | 1:A:641:VAL:HG11  | 2.45                     | 0.46              |
| 2:B:388:CYS:O     | 2:B:390:LEU:N     | 2.49                     | 0.46              |
| 2:B:604:ARG:C     | 2:B:606:LYS:H     | 2.18                     | 0.46              |
| 2:B:520:GLY:N     | 2:B:748:ILE:HG22  | 2.29                     | 0.46              |
| 3:C:112:ASN:CB    | 3:C:114:TYR:CE1   | 2.98                     | 0.46              |
| 3:C:152:GLU:OE2   | 3:C:154:LYS:HE3   | 2.15                     | 0.46              |
| 8:H:123:MET:HE3   | 8:H:142:LEU:HD22  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 9:I:51:ASN:O      | 9:I:54:GLU:HG3   | 2.16                     | 0.46              |
| 1:A:1053:PHE:O    | 1:A:1055:ARG:N   | 2.49                     | 0.46              |
| 1:A:560:ILE:HG12  | 1:A:560:ILE:H    | 1.46                     | 0.46              |
| 1:A:767:GLN:HB2   | 1:A:799:PHE:HD1  | 1.80                     | 0.46              |
| 2:B:95:ILE:CG1    | 2:B:130:VAL:HG22 | 2.46                     | 0.46              |
| 2:B:293:PRO:HG2   | 2:B:296:GLU:HB2  | 1.97                     | 0.46              |
| 2:B:39:ARG:NH2    | 2:B:665:GLU:CG   | 2.76                     | 0.46              |
| 2:B:763:GLN:C     | 2:B:765:PRO:HD2  | 2.36                     | 0.46              |
| 2:B:814:PHE:C     | 2:B:816:GLU:N    | 2.69                     | 0.46              |
| 3:C:115:SER:HB3   | 3:C:142:VAL:HB   | 1.98                     | 0.46              |
| 3:C:168:ALA:C     | 3:C:170:TRP:N    | 2.68                     | 0.46              |
| 3:C:87:PHE:CD1    | 3:C:87:PHE:N     | 2.84                     | 0.46              |
| 3:C:99:LEU:HD12   | 3:C:118:LEU:HB3  | 1.96                     | 0.46              |
| 5:E:207:ARG:CB    | 5:E:207:ARG:NH1  | 2.78                     | 0.46              |
| 7:G:138:THR:CG2   | 7:G:139:ILE:N    | 2.68                     | 0.46              |
| 4:D:175:PHE:HZ    | 7:G:85:GLU:HG3   | 1.79                     | 0.46              |
| 3:C:175:ALA:HB3   | 10:J:43:ARG:HH22 | 1.81                     | 0.46              |
| 11:K:85:ASP:O     | 11:K:88:LYS:HB2  | 2.15                     | 0.46              |
| 1:A:23:SER:CB     | 1:A:233:TRP:NE1  | 2.79                     | 0.46              |
| 1:A:34:LYS:NZ     | 1:A:57:ARG:CZ    | 2.79                     | 0.46              |
| 1:A:566:ILE:O     | 1:A:567:LYS:O    | 2.34                     | 0.46              |
| 1:A:826:ASP:O     | 1:A:827:THR:C    | 2.52                     | 0.46              |
| 2:B:244:LEU:C     | 2:B:246:LYS:N    | 2.68                     | 0.46              |
| 2:B:360:PHE:O     | 2:B:361:LEU:C    | 2.54                     | 0.46              |
| 2:B:801:LYS:O     | 10:J:52:THR:CG2  | 2.64                     | 0.46              |
| 2:B:859:TYR:OH    | 2:B:941:LEU:CD1  | 2.60                     | 0.46              |
| 3:C:114:TYR:HB3   | 3:C:140:ASN:O    | 2.16                     | 0.46              |
| 9:I:115:LYS:HD3   | 9:I:117:LYS:CE   | 2.38                     | 0.46              |
| 9:I:55:THR:HG22   | 9:I:58:VAL:CG2   | 2.45                     | 0.46              |
| 10:J:27:GLU:C     | 10:J:29:GLU:H    | 2.17                     | 0.46              |
| 1:A:1385:THR:O    | 1:A:1388:GLY:N   | 2.46                     | 0.46              |
| 1:A:1418:LEU:HD12 | 1:A:1419:ASP:N   | 2.30                     | 0.46              |
| 1:A:262:LEU:C     | 1:A:264:PHE:N    | 2.69                     | 0.46              |
| 1:A:49:LYS:NZ     | 1:A:61:ILE:CG1   | 2.74                     | 0.46              |
| 1:A:652:VAL:O     | 1:A:653:VAL:C    | 2.55                     | 0.46              |
| 1:A:7:SER:C       | 1:A:9:ALA:H      | 2.19                     | 0.46              |
| 1:A:835:GLY:HA3   | 15:T:19:TT:O1P   | 2.16                     | 0.46              |
| 2:B:911:ILE:HD11  | 2:B:941:LEU:CD1  | 2.43                     | 0.46              |
| 4:D:64:VAL:O      | 4:D:66:ARG:N     | 2.49                     | 0.46              |
| 5:E:145:THR:HG21  | 5:E:187:TYR:CD2  | 2.50                     | 0.46              |
| 7:G:106:MET:CG    | 7:G:107:LYS:N    | 2.77                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:29:LEU:HB3    | 7:G:82:PHE:HE2   | 1.81                     | 0.46              |
| 1:A:1152:ILE:HG13 | 9:I:44:TYR:HD2   | 1.81                     | 0.46              |
| 2:B:900:ALA:HB3   | 12:L:61:THR:OG1  | 2.15                     | 0.46              |
| 1:A:172:PRO:HG3   | 1:A:185:TRP:CZ2  | 2.51                     | 0.46              |
| 1:A:172:PRO:HB3   | 1:A:185:TRP:CE2  | 2.51                     | 0.46              |
| 1:A:494:SER:O     | 1:A:497:THR:N    | 2.49                     | 0.46              |
| 1:A:883:LEU:CD2   | 1:A:1021:LEU:HB2 | 2.46                     | 0.46              |
| 2:B:1110:PRO:HG3  | 2:B:1125:ASP:HB3 | 1.98                     | 0.46              |
| 1:A:343:LYS:HZ3   | 2:B:1197:PRO:HB3 | 1.81                     | 0.46              |
| 14:P:8:G:H2'      | 14:P:9:A:C8      | 2.51                     | 0.46              |
| 1:A:1222:ASN:O    | 1:A:1223:ASP:HB3 | 2.16                     | 0.46              |
| 1:A:1224:LEU:HD11 | 1:A:1240:CYS:HB2 | 1.97                     | 0.46              |
| 1:A:1445:ILE:HD12 | 7:G:59:GLY:O     | 2.15                     | 0.46              |
| 1:A:18:GLN:O      | 2:B:1215:ARG:HG2 | 2.16                     | 0.46              |
| 1:A:241:VAL:HG13  | 1:A:266:LEU:HD13 | 1.97                     | 0.46              |
| 1:A:474:VAL:C     | 1:A:477:PRO:HD2  | 2.36                     | 0.46              |
| 1:A:639:PRO:HG2   | 1:A:640:GLN:H    | 1.81                     | 0.46              |
| 1:A:818:MET:HA    | 2:B:514:LEU:HB3  | 1.98                     | 0.46              |
| 1:A:857:ARG:HG2   | 1:A:863:VAL:HA   | 1.98                     | 0.46              |
| 2:B:1045:SER:O    | 2:B:1046:PRO:O   | 2.34                     | 0.46              |
| 2:B:244:LEU:O     | 2:B:246:LYS:N    | 2.49                     | 0.46              |
| 2:B:210:LYS:HG3   | 2:B:461:LEU:O    | 2.16                     | 0.46              |
| 2:B:510:LYS:CG    | 2:B:511:PRO:CD   | 2.82                     | 0.46              |
| 3:C:112:ASN:HB2   | 3:C:114:TYR:HE1  | 1.80                     | 0.46              |
| 3:C:186:LEU:HB3   | 3:C:188:HIS:CD2  | 2.51                     | 0.46              |
| 8:H:38:LEU:HD13   | 8:H:125:LEU:HD13 | 1.98                     | 0.46              |
| 12:L:49:LYS:O     | 12:L:50:ASP:CB   | 2.63                     | 0.46              |
| 1:A:332:LYS:NZ    | 15:T:19:TT:H7C2  | 2.31                     | 0.46              |
| 1:A:244:PRO:HG2   | 1:A:245:PRO:CD   | 2.46                     | 0.45              |
| 1:A:695:LYS:C     | 1:A:697:ALA:N    | 2.69                     | 0.45              |
| 1:A:675:THR:OG1   | 1:A:736:ASN:ND2  | 2.49                     | 0.45              |
| 1:A:846:GLU:OE1   | 1:A:1425:SER:OG  | 2.33                     | 0.45              |
| 1:A:514:PRO:CB    | 1:A:875:ALA:HB3  | 2.47                     | 0.45              |
| 1:A:981:LEU:HD21  | 1:A:1038:THR:C   | 2.36                     | 0.45              |
| 2:B:1162:ILE:HG22 | 2:B:1163:CYS:N   | 2.30                     | 0.45              |
| 2:B:37:PHE:HE2    | 2:B:542:MET:HA   | 1.81                     | 0.45              |
| 3:C:44:LEU:HD21   | 3:C:159:ALA:CB   | 2.46                     | 0.45              |
| 3:C:41:ILE:HD11   | 3:C:247:GLY:CA   | 2.46                     | 0.45              |
| 3:C:73:GLN:NE2    | 3:C:74:SER:H     | 2.14                     | 0.45              |
| 12:L:40:LEU:HB3   | 12:L:41:SER:H    | 1.68                     | 0.45              |
| 12:L:55:ILE:H     | 12:L:55:ILE:HG12 | 1.32                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1004:ASN:O    | 1:A:1008:GLN:HB2  | 2.16                     | 0.45              |
| 1:A:1445:ILE:HG12 | 7:G:18:PHE:HE2    | 1.78                     | 0.45              |
| 1:A:409:SER:O     | 1:A:410:GLY:C     | 2.54                     | 0.45              |
| 1:A:800:VAL:HA    | 1:A:812:GLU:OE2   | 2.16                     | 0.45              |
| 1:A:874:ASP:O     | 1:A:876:ALA:N     | 2.49                     | 0.45              |
| 2:B:102:VAL:HG12  | 2:B:104:GLU:HG2   | 1.98                     | 0.45              |
| 2:B:1084:GLN:C    | 2:B:1085:ILE:HD12 | 2.37                     | 0.45              |
| 2:B:240:ILE:HG22  | 2:B:254:LEU:HB3   | 1.97                     | 0.45              |
| 3:C:167:HIS:ND1   | 12:L:70:ARG:HB3   | 2.31                     | 0.45              |
| 2:B:798:TYR:CE2   | 3:C:62:PHE:CZ     | 3.04                     | 0.45              |
| 4:D:119:ARG:HD3   | 4:D:221:TYR:CE2   | 2.51                     | 0.45              |
| 4:D:52:LEU:C      | 4:D:54:GLU:N      | 2.69                     | 0.45              |
| 7:G:22:MET:O      | 7:G:23:LYS:C      | 2.54                     | 0.45              |
| 7:G:39:THR:O      | 7:G:43:GLY:HA2    | 2.15                     | 0.45              |
| 14:P:2:C:O2'      | 14:P:3:G:H5'      | 2.16                     | 0.45              |
| 1:A:1319:VAL:HG13 | 1:A:1320:PRO:HD2  | 1.98                     | 0.45              |
| 1:A:1381:LEU:HA   | 1:A:1381:LEU:HD23 | 1.77                     | 0.45              |
| 1:A:332:LYS:C     | 1:A:334:GLY:H     | 2.20                     | 0.45              |
| 1:A:500:GLU:OE2   | 2:B:1145:SER:N    | 2.49                     | 0.45              |
| 1:A:526:ASP:OD1   | 2:B:1013:ASN:ND2  | 2.48                     | 0.45              |
| 1:A:71:GLN:HG3    | 1:A:72:GLU:N      | 2.31                     | 0.45              |
| 1:A:730:GLY:O     | 1:A:733:ALA:N     | 2.49                     | 0.45              |
| 1:A:843:LYS:HD3   | 1:A:846:GLU:OE2   | 2.16                     | 0.45              |
| 2:B:758:PHE:HZ    | 2:B:1031:LEU:HD22 | 1.82                     | 0.45              |
| 1:A:1021:LEU:O    | 1:A:1024:SER:HB3  | 2.16                     | 0.45              |
| 1:A:1171:GLN:HA   | 1:A:1174:PHE:HD1  | 1.80                     | 0.45              |
| 1:A:1394:THR:O    | 1:A:1395:GLY:O    | 2.34                     | 0.45              |
| 1:A:361:LEU:HA    | 1:A:471:ASN:ND2   | 2.31                     | 0.45              |
| 1:A:370:ILE:O     | 1:A:371:ALA:C     | 2.52                     | 0.45              |
| 1:A:915:SER:O     | 1:A:919:ILE:HG13  | 2.16                     | 0.45              |
| 1:A:963:ILE:HD13  | 1:A:1049:ILE:CG1  | 2.47                     | 0.45              |
| 2:B:1184:GLY:C    | 2:B:1186:ASP:H    | 2.16                     | 0.45              |
| 2:B:96:TYR:HE1    | 2:B:131:ASP:OD2   | 1.99                     | 0.45              |
| 2:B:570:VAL:HG23  | 2:B:573:GLN:HB3   | 1.97                     | 0.45              |
| 2:B:364:ILE:CG1   | 2:B:585:VAL:HG13  | 2.38                     | 0.45              |
| 2:B:825:VAL:HG21  | 2:B:1092:TYR:HE1  | 1.80                     | 0.45              |
| 3:C:184:ASN:HD21  | 3:C:187:LYS:HA    | 1.80                     | 0.45              |
| 1:A:667:GLY:HA3   | 3:C:192:TRP:CH2   | 2.51                     | 0.45              |
| 2:B:1065:GLN:HB2  | 3:C:201:TRP:CZ3   | 2.51                     | 0.45              |
| 9:I:29:CYS:SG     | 9:I:31:THR:N      | 2.86                     | 0.45              |
| 10:J:45:CYS:O     | 10:J:48:ARG:HG3   | 2.17                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 13:N:6:DC:H1'     | 13:N:7:DT:H5'    | 1.97                     | 0.45              |
| 1:A:1111:MET:HE3  | 1:A:1113:THR:O   | 2.16                     | 0.45              |
| 1:A:396:PRO:HG3   | 1:A:416:ARG:HB3  | 1.97                     | 0.45              |
| 1:A:885:THR:O     | 1:A:885:THR:HG22 | 2.16                     | 0.45              |
| 2:B:1182:CYS:O    | 2:B:1183:LYS:O   | 2.35                     | 0.45              |
| 3:C:113:VAL:CG2   | 3:C:147:LEU:HD21 | 2.47                     | 0.45              |
| 3:C:22:LEU:HD13   | 3:C:230:MET:HE1  | 1.99                     | 0.45              |
| 3:C:242:GLN:C     | 3:C:244:VAL:N    | 2.70                     | 0.45              |
| 4:D:29:LEU:HB3    | 7:G:82:PHE:CE2   | 2.52                     | 0.45              |
| 5:E:156:LEU:HD12  | 5:E:195:VAL:CB   | 2.47                     | 0.45              |
| 8:H:40:LEU:HB2    | 8:H:123:MET:HG3  | 1.99                     | 0.45              |
| 11:K:11:LEU:N     | 11:K:11:LEU:HD22 | 2.32                     | 0.45              |
| 11:K:65:HIS:CG    | 11:K:66:PRO:HD2  | 2.51                     | 0.45              |
| 2:B:833:TYR:CZ    | 11:K:66:PRO:HG3  | 2.51                     | 0.45              |
| 12:L:27:LEU:N     | 12:L:27:LEU:HD23 | 2.32                     | 0.45              |
| 1:A:11:LEU:HB2    | 2:B:1193:GLN:OE1 | 2.16                     | 0.45              |
| 1:A:172:PRO:HB3   | 1:A:185:TRP:CD2  | 2.52                     | 0.45              |
| 1:A:381:THR:HG23  | 1:A:382:PRO:CD   | 2.47                     | 0.45              |
| 1:A:32:VAL:HG21   | 1:A:68:GLN:NE2   | 2.32                     | 0.45              |
| 1:A:898:ARG:O     | 1:A:1029:ARG:NH1 | 2.50                     | 0.45              |
| 2:B:502:ILE:CD1   | 2:B:502:ILE:N    | 2.78                     | 0.45              |
| 2:B:854:LEU:HB3   | 2:B:856:PHE:HE1  | 1.80                     | 0.45              |
| 3:C:123:ASN:ND2   | 3:C:125:MET:CG   | 2.79                     | 0.45              |
| 3:C:176:ILE:CG2   | 3:C:177:GLU:N    | 2.79                     | 0.45              |
| 3:C:190:ASP:O     | 3:C:191:TYR:C    | 2.55                     | 0.45              |
| 3:C:191:TYR:HD2   | 3:C:201:TRP:CD1  | 2.34                     | 0.45              |
| 3:C:20:PHE:HE1    | 3:C:22:LEU:CD1   | 2.30                     | 0.45              |
| 5:E:167:ARG:HD3   | 5:E:167:ARG:HA   | 1.84                     | 0.45              |
| 8:H:99:GLY:HA3    | 8:H:117:SER:O    | 2.17                     | 0.45              |
| 10:J:43:ARG:O     | 10:J:47:ARG:HB2  | 2.17                     | 0.45              |
| 1:A:1064:VAL:HG12 | 1:A:1064:VAL:O   | 2.16                     | 0.45              |
| 1:A:19:PHE:HE1    | 1:A:1396:ALA:HB3 | 1.82                     | 0.45              |
| 1:A:23:SER:O      | 1:A:26:GLU:N     | 2.49                     | 0.45              |
| 2:B:1060:ARG:C    | 2:B:1062:HIS:H   | 2.19                     | 0.45              |
| 2:B:282:ILE:HD12  | 2:B:382:ILE:HD13 | 1.99                     | 0.45              |
| 2:B:58:THR:O      | 2:B:62:ILE:HG13  | 2.17                     | 0.45              |
| 2:B:999:MET:HE2   | 2:B:1000:PRO:CD  | 2.47                     | 0.45              |
| 8:H:4:THR:HG22    | 8:H:5:LEU:H      | 1.81                     | 0.45              |
| 9:I:69:PRO:HG2    | 9:I:85:PHE:CD2   | 2.52                     | 0.45              |
| 11:K:15:GLY:O     | 11:K:16:GLU:HG3  | 2.17                     | 0.45              |
| 1:A:166:GLY:O     | 1:A:167:CYS:SG   | 2.74                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:244:PRO:CG    | 1:A:245:PRO:HD3   | 2.47                     | 0.45              |
| 2:B:1006:ILE:HD13 | 10:J:44:TYR:CZ    | 2.51                     | 0.45              |
| 2:B:1031:LEU:HD11 | 2:B:1042:GLY:HA3  | 1.99                     | 0.45              |
| 2:B:223:VAL:HG21  | 2:B:380:TYR:CE2   | 2.51                     | 0.45              |
| 2:B:704:ALA:HB2   | 2:B:738:PHE:CD2   | 2.52                     | 0.45              |
| 2:B:800:GLN:O     | 2:B:801:LYS:C     | 2.55                     | 0.45              |
| 2:B:839:MET:HE3   | 2:B:1010:LEU:CD2  | 2.44                     | 0.45              |
| 2:B:860:MET:CG    | 2:B:861:ASP:N     | 2.80                     | 0.45              |
| 3:C:99:LEU:HD23   | 3:C:99:LEU:N      | 2.32                     | 0.45              |
| 5:E:124:VAL:HB    | 5:E:125:PRO:CD    | 2.47                     | 0.45              |
| 12:L:36:SER:O     | 12:L:37:LYS:C     | 2.54                     | 0.45              |
| 1:A:1146:VAL:HG11 | 1:A:1207:LEU:HD12 | 1.99                     | 0.45              |
| 1:A:120:GLU:HA    | 1:A:123:ARG:HG3   | 1.99                     | 0.45              |
| 1:A:1211:GLN:O    | 1:A:1212:VAL:C    | 2.55                     | 0.45              |
| 1:A:185:TRP:CZ3   | 1:A:200:ARG:HG2   | 2.52                     | 0.45              |
| 1:A:482:PHE:O     | 1:A:484:GLY:N     | 2.49                     | 0.45              |
| 1:A:508:PRO:O     | 1:A:511:ILE:HG13  | 2.16                     | 0.45              |
| 1:A:549:MET:SD    | 1:A:577:ILE:CD1   | 3.04                     | 0.45              |
| 1:A:666:ILE:CD1   | 1:A:667:GLY:N     | 2.80                     | 0.45              |
| 2:B:244:LEU:HD11  | 2:B:366:GLN:HE22  | 1.81                     | 0.45              |
| 2:B:360:PHE:CD2   | 2:B:361:LEU:HB2   | 2.51                     | 0.45              |
| 2:B:582:VAL:HG12  | 2:B:587:HIS:NE2   | 2.32                     | 0.45              |
| 2:B:802:PRO:HB3   | 2:B:1091:TYR:CD2  | 2.51                     | 0.45              |
| 2:B:911:ILE:O     | 2:B:911:ILE:HG22  | 2.17                     | 0.45              |
| 2:B:954:VAL:HA    | 2:B:964:VAL:HG22  | 1.98                     | 0.45              |
| 5:E:60:PHE:CE2    | 5:E:80:VAL:HB     | 2.51                     | 0.45              |
| 9:I:34:TYR:O      | 9:I:35:VAL:HG23   | 2.17                     | 0.45              |
| 9:I:70:ARG:HH11   | 9:I:84:VAL:HB     | 1.81                     | 0.45              |
| 11:K:82:ASP:O     | 11:K:85:ASP:HB2   | 2.17                     | 0.45              |
| 12:L:28:LYS:HB2   | 12:L:39:SER:HB2   | 1.99                     | 0.45              |
| 1:A:1220:PHE:O    | 1:A:1221:LYS:HB2  | 2.17                     | 0.45              |
| 1:A:1333:ILE:HG22 | 1:A:1334:ASP:N    | 2.32                     | 0.45              |
| 1:A:313:GLN:O     | 1:A:314:ALA:HB3   | 2.17                     | 0.45              |
| 1:A:427:GLN:HB2   | 1:A:430:TRP:CE2   | 2.52                     | 0.45              |
| 1:A:567:LYS:HD2   | 1:A:568:PRO:CD    | 2.38                     | 0.45              |
| 1:A:710:LEU:HD13  | 9:I:94:ASP:O      | 2.16                     | 0.45              |
| 2:B:1164:GLY:HA3  | 2:B:1190:ASP:OD2  | 2.16                     | 0.45              |
| 2:B:19:GLU:O      | 2:B:20:ASP:C      | 2.55                     | 0.45              |
| 2:B:405:ARG:HA    | 2:B:631:GLY:O     | 2.16                     | 0.45              |
| 3:C:215:GLU:O     | 3:C:217:ASP:N     | 2.50                     | 0.45              |
| 3:C:27:LEU:HD13   | 3:C:228:PHE:HE2   | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:24:LYS:CG    | 5:E:25:ASP:N     | 2.79                     | 0.45              |
| 5:E:29:PHE:C     | 5:E:30:ILE:HG13  | 2.37                     | 0.45              |
| 7:G:20:PRO:CG    | 7:G:21:ARG:N     | 2.80                     | 0.45              |
| 8:H:10:PHE:CE1   | 8:H:57:VAL:HB    | 2.52                     | 0.45              |
| 8:H:138:GLU:O    | 8:H:139:ASN:C    | 2.54                     | 0.45              |
| 11:K:31:VAL:O    | 11:K:74:ARG:HA   | 2.17                     | 0.45              |
| 1:A:1206:ASP:O   | 1:A:1274:ARG:NH1 | 2.51                     | 0.44              |
| 2:B:1138:MET:HA  | 2:B:1138:MET:CE  | 2.38                     | 0.44              |
| 2:B:118:ARG:CG   | 2:B:204:ILE:HD13 | 2.47                     | 0.44              |
| 2:B:295:GLY:O    | 2:B:299:GLU:HG3  | 2.18                     | 0.44              |
| 2:B:280:ILE:CD1  | 2:B:334:ILE:HG12 | 2.44                     | 0.44              |
| 2:B:364:ILE:HG12 | 2:B:585:VAL:CG1  | 2.38                     | 0.44              |
| 2:B:96:TYR:HB2   | 2:B:129:PHE:HB2  | 1.99                     | 0.44              |
| 3:C:35:ARG:HH11  | 11:K:41:THR:HA   | 1.81                     | 0.44              |
| 4:D:33:PHE:CZ    | 7:G:80:LYS:HE3   | 2.53                     | 0.44              |
| 5:E:112:TYR:CZ   | 5:E:136:ASN:HB2  | 2.52                     | 0.44              |
| 5:E:163:GLU:O    | 5:E:166:LYS:N    | 2.50                     | 0.44              |
| 6:F:109:VAL:HG12 | 6:F:110:ASP:N    | 2.31                     | 0.44              |
| 7:G:7:LEU:O      | 7:G:73:LYS:HD2   | 2.17                     | 0.44              |
| 7:G:87:VAL:HG23  | 7:G:103:VAL:HG21 | 1.99                     | 0.44              |
| 7:G:9:LEU:HD23   | 7:G:30:LEU:HD12  | 2.00                     | 0.44              |
| 10:J:56:LEU:O    | 10:J:59:LYS:N    | 2.44                     | 0.44              |
| 11:K:35:PHE:CD1  | 11:K:71:PHE:CE1  | 3.05                     | 0.44              |
| 15:T:16:DT:H1'   | 15:T:17:DT:H5'   | 1.98                     | 0.44              |
| 1:A:1213:GLY:O   | 1:A:1214:GLU:C   | 2.56                     | 0.44              |
| 1:A:1265:ASN:O   | 1:A:1268:LEU:N   | 2.47                     | 0.44              |
| 1:A:285:PRO:O    | 1:A:287:HIS:N    | 2.50                     | 0.44              |
| 1:A:34:LYS:CB    | 1:A:36:ARG:HE    | 2.28                     | 0.44              |
| 1:A:469:ARG:NH2  | 2:B:991:GLY:O    | 2.50                     | 0.44              |
| 1:A:567:LYS:HE3  | 8:H:46:LEU:CB    | 2.42                     | 0.44              |
| 1:A:572:TRP:HA   | 1:A:576:GLN:OE1  | 2.17                     | 0.44              |
| 1:A:67:CYS:O     | 1:A:68:GLN:CB    | 2.65                     | 0.44              |
| 1:A:75:ASN:O     | 1:A:76:GLU:HB2   | 2.17                     | 0.44              |
| 2:B:283:VAL:O    | 2:B:286:PHE:N    | 2.50                     | 0.44              |
| 2:B:25:ILE:HD11  | 2:B:653:VAL:C    | 2.37                     | 0.44              |
| 5:E:30:ILE:HG22  | 5:E:31:THR:N     | 2.31                     | 0.44              |
| 6:F:90:ARG:CG    | 6:F:91:ALA:N     | 2.81                     | 0.44              |
| 8:H:143:LEU:N    | 8:H:143:LEU:CD1  | 2.79                     | 0.44              |
| 8:H:91:ASP:O     | 8:H:93:TYR:N     | 2.50                     | 0.44              |
| 11:K:6:ARG:O     | 11:K:8:GLU:N     | 2.50                     | 0.44              |
| 2:B:776:GLN:NE2  | 14:P:8:G:H5'     | 2.30                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:337:ARG:HH12  | 15:T:18:DT:P      | 2.39                     | 0.44              |
| 1:A:1265:ASN:C    | 1:A:1267:MET:N    | 2.69                     | 0.44              |
| 1:A:524:VAL:HG12  | 1:A:525:GLN:HE21  | 1.81                     | 0.44              |
| 2:B:744:HIS:CG    | 2:B:745:PRO:HD2   | 2.52                     | 0.44              |
| 2:B:847:ASP:C     | 2:B:849:GLY:N     | 2.71                     | 0.44              |
| 2:B:848:ARG:HD2   | 10:J:7:CYS:O      | 2.18                     | 0.44              |
| 2:B:893:LEU:HD22  | 2:B:897:GLY:C     | 2.38                     | 0.44              |
| 3:C:45:ALA:HA     | 3:C:72:LEU:CD1    | 2.47                     | 0.44              |
| 5:E:147:HIS:CD2   | 5:E:149:LEU:H     | 2.35                     | 0.44              |
| 5:E:180:ARG:HB2   | 5:E:215:MET:OXT   | 2.17                     | 0.44              |
| 6:F:77:ASP:C      | 6:F:79:ARG:N      | 2.70                     | 0.44              |
| 7:G:106:MET:HG2   | 7:G:107:LYS:N     | 2.31                     | 0.44              |
| 7:G:117:GLN:C     | 7:G:119:LEU:N     | 2.71                     | 0.44              |
| 7:G:1:MET:SD      | 7:G:79:PHE:HD1    | 2.40                     | 0.44              |
| 8:H:104:PHE:CZ    | 8:H:136:LYS:HA    | 2.52                     | 0.44              |
| 9:I:78:CYS:HB3    | 9:I:106:CYS:SG    | 2.58                     | 0.44              |
| 9:I:55:THR:O      | 9:I:55:THR:HG22   | 2.18                     | 0.44              |
| 10:J:56:LEU:O     | 10:J:57:ILE:C     | 2.54                     | 0.44              |
| 10:J:57:ILE:HA    | 10:J:60:PHE:HB2   | 1.98                     | 0.44              |
| 15:T:15:DT:H6     | 15:T:15:DT:H2'    | 1.61                     | 0.44              |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:HG13 | 1.99                     | 0.44              |
| 1:A:1334:ASP:O    | 1:A:1337:GLU:N    | 2.50                     | 0.44              |
| 1:A:1389:PHE:C    | 1:A:1389:PHE:CD1  | 2.90                     | 0.44              |
| 1:A:260:ASP:O     | 1:A:261:ASP:C     | 2.56                     | 0.44              |
| 1:A:42:ASP:O      | 1:A:44:THR:N      | 2.38                     | 0.44              |
| 1:A:606:LEU:HB3   | 1:A:614:PHE:CD2   | 2.52                     | 0.44              |
| 1:A:825:ILE:O     | 1:A:826:ASP:C     | 2.55                     | 0.44              |
| 2:B:1223:ASP:HB3  | 2:B:1224:PHE:H    | 1.58                     | 0.44              |
| 2:B:240:ILE:O     | 2:B:240:ILE:HG23  | 2.17                     | 0.44              |
| 3:C:239:PRO:O     | 3:C:240:VAL:C     | 2.55                     | 0.44              |
| 3:C:3:GLU:O       | 3:C:4:GLU:HG3     | 2.18                     | 0.44              |
| 4:D:7:THR:HG23    | 4:D:7:THR:O       | 2.17                     | 0.44              |
| 7:G:91:VAL:HG12   | 7:G:92:VAL:N      | 2.32                     | 0.44              |
| 9:I:50:THR:HG22   | 9:I:51:ASN:N      | 2.32                     | 0.44              |
| 1:A:1435:PRO:HA   | 1:A:1439:GLY:O    | 2.17                     | 0.44              |
| 1:A:401:GLY:O     | 1:A:435:HIS:CD2   | 2.71                     | 0.44              |
| 1:A:404:TYR:CE2   | 1:A:414:ASP:HA    | 2.53                     | 0.44              |
| 1:A:415:LEU:HA    | 1:A:415:LEU:HD23  | 1.69                     | 0.44              |
| 1:A:452:LYS:HB3   | 1:A:452:LYS:HE2   | 1.71                     | 0.44              |
| 1:A:506:ALA:O     | 1:A:509:LEU:HB2   | 2.17                     | 0.44              |
| 1:A:806:ARG:NH1   | 2:B:729:ILE:HG13  | 2.32                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:829:VAL:C    | 1:A:831:THR:H     | 2.20                     | 0.44              |
| 1:A:979:SER:HG   | 1:A:981:LEU:HG    | 1.80                     | 0.44              |
| 1:A:929:LEU:CD2  | 1:A:983:ILE:HG21  | 2.48                     | 0.44              |
| 1:A:996:ASN:C    | 1:A:998:LEU:HD12  | 2.36                     | 0.44              |
| 2:B:1099:VAL:C   | 2:B:1101:ASP:H    | 2.21                     | 0.44              |
| 2:B:1152:MET:HE1 | 2:B:1157:ALA:HA   | 1.99                     | 0.44              |
| 2:B:313:MET:HE2  | 2:B:386:LEU:HD22  | 2.00                     | 0.44              |
| 2:B:43:LEU:HD11  | 2:B:811:TYR:O     | 2.17                     | 0.44              |
| 2:B:210:LYS:HA   | 2:B:481:GLN:O     | 2.18                     | 0.44              |
| 2:B:487:THR:CG2  | 2:B:488:TYR:N     | 2.81                     | 0.44              |
| 2:B:560:GLU:O    | 2:B:561:TRP:CD1   | 2.71                     | 0.44              |
| 3:C:18:VAL:O     | 3:C:20:PHE:CD2    | 2.70                     | 0.44              |
| 3:C:27:LEU:HA    | 3:C:228:PHE:CZ    | 2.53                     | 0.44              |
| 4:D:146:GLN:O    | 4:D:149:THR:HG22  | 2.17                     | 0.44              |
| 4:D:27:LEU:HG    | 4:D:197:SER:HB2   | 1.98                     | 0.44              |
| 5:E:161:LYS:C    | 5:E:163:GLU:N     | 2.69                     | 0.44              |
| 5:E:23:VAL:HG13  | 5:E:78:LEU:HD13   | 2.00                     | 0.44              |
| 5:E:48:ASP:CG    | 5:E:49:SER:N      | 2.69                     | 0.44              |
| 7:G:73:LYS:HE2   | 7:G:74:TYR:O      | 2.18                     | 0.44              |
| 11:K:82:ASP:OD1  | 11:K:84:LYS:N     | 2.46                     | 0.44              |
| 1:A:1098:VAL:N   | 1:A:1099:PRO:HD2  | 2.32                     | 0.44              |
| 1:A:1102:LYS:HG2 | 1:A:1106:ASN:HD21 | 1.82                     | 0.44              |
| 1:A:172:PRO:HD3  | 1:A:185:TRP:NE1   | 2.33                     | 0.44              |
| 1:A:35:ILE:HD13  | 1:A:241:VAL:HG11  | 1.99                     | 0.44              |
| 1:A:56:PRO:O     | 1:A:57:ARG:HG3    | 2.18                     | 0.44              |
| 1:A:664:THR:CG2  | 1:A:665:GLY:N     | 2.80                     | 0.44              |
| 1:A:68:GLN:C     | 1:A:70:CYS:N      | 2.66                     | 0.44              |
| 1:A:816:HIS:CD2  | 2:B:764:SER:H     | 2.36                     | 0.44              |
| 1:A:986:ILE:HD12 | 1:A:1032:LEU:HD11 | 1.98                     | 0.44              |
| 2:B:223:VAL:CG1  | 2:B:381:MET:HG2   | 2.48                     | 0.44              |
| 2:B:314:LEU:O    | 2:B:317:CYS:HB3   | 2.17                     | 0.44              |
| 2:B:610:ASN:HA   | 2:B:611:PRO:HD3   | 1.89                     | 0.44              |
| 2:B:782:LEU:CD1  | 2:B:788:ARG:HH11  | 2.29                     | 0.44              |
| 3:C:44:LEU:HD21  | 3:C:159:ALA:HB1   | 1.99                     | 0.44              |
| 3:C:77:ILE:C     | 3:C:79:GLN:H      | 2.21                     | 0.44              |
| 7:G:48:VAL:HA    | 7:G:76:ALA:HB2    | 1.99                     | 0.44              |
| 11:K:18:LYS:NZ   | 11:K:37:LYS:O     | 2.51                     | 0.44              |
| 1:A:1062:GLU:OE2 | 6:F:88:TYR:OH     | 2.35                     | 0.44              |
| 1:A:577:ILE:O    | 1:A:578:LEU:C     | 2.52                     | 0.44              |
| 1:A:673:GLY:O    | 1:A:676:MET:HB2   | 2.17                     | 0.44              |
| 1:A:709:THR:CG2  | 1:A:710:LEU:N     | 2.81                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:71:GLN:C     | 1:A:73:GLY:N     | 2.71                     | 0.44              |
| 2:B:293:PRO:HG2  | 2:B:296:GLU:HB3  | 2.00                     | 0.44              |
| 2:B:591:ARG:O    | 2:B:592:ASN:C    | 2.55                     | 0.44              |
| 2:B:682:SER:O    | 2:B:685:LEU:HB3  | 2.17                     | 0.44              |
| 2:B:806:THR:HG22 | 2:B:808:ALA:HB3  | 1.99                     | 0.44              |
| 2:B:980:PHE:HE1  | 2:B:990:ILE:HD11 | 1.81                     | 0.44              |
| 3:C:238:ILE:HD11 | 3:C:246:ARG:NH1  | 2.33                     | 0.44              |
| 3:C:259:LEU:CD1  | 11:K:91:CYS:HB2  | 2.47                     | 0.44              |
| 5:E:90:VAL:O     | 5:E:90:VAL:HG22  | 2.17                     | 0.44              |
| 6:F:89:GLU:HB3   | 6:F:134:ILE:HD13 | 2.00                     | 0.44              |
| 7:G:29:LYS:O     | 7:G:30:LEU:C     | 2.54                     | 0.44              |
| 9:I:15:TYR:HD1   | 9:I:15:TYR:N     | 2.14                     | 0.44              |
| 9:I:32:CYS:SG    | 9:I:33:SER:N     | 2.90                     | 0.44              |
| 9:I:70:ARG:NH1   | 9:I:84:VAL:HB    | 2.33                     | 0.44              |
| 14:P:4:A:C2'     | 14:P:5:C:H5'     | 2.47                     | 0.44              |
| 15:T:18:DT:C3'   | 15:T:19:TT:C5'   | 2.96                     | 0.44              |
| 1:A:1094:VAL:CG1 | 1:A:1095:THR:N   | 2.63                     | 0.44              |
| 1:A:113:LEU:HG   | 1:A:218:ASP:OD1  | 2.17                     | 0.44              |
| 1:A:719:VAL:O    | 1:A:721:PHE:N    | 2.51                     | 0.44              |
| 1:A:760:GLN:HG2  | 1:A:765:VAL:O    | 2.17                     | 0.44              |
| 2:B:1087:PHE:CD2 | 2:B:1088:GLY:N   | 2.76                     | 0.44              |
| 2:B:113:TYR:HB3  | 2:B:114:PRO:HD2  | 1.99                     | 0.44              |
| 2:B:259:TYR:HD1  | 2:B:259:TYR:N    | 2.16                     | 0.44              |
| 1:A:1006:ILE:CD1 | 5:E:163:GLU:HG3  | 2.45                     | 0.44              |
| 5:E:197:LYS:HE2  | 5:E:199:ILE:HD11 | 2.00                     | 0.44              |
| 7:G:125:SER:OG   | 7:G:128:PRO:HA   | 2.18                     | 0.44              |
| 9:I:110:PHE:H    | 9:I:110:PHE:HD2  | 1.66                     | 0.44              |
| 1:A:548:ASN:OD1  | 11:K:60:ALA:HB1  | 2.18                     | 0.44              |
| 13:N:3:DG:H2''   | 13:N:4:DT:OP2    | 2.18                     | 0.44              |
| 1:A:1385:THR:C   | 1:A:1387:HIS:N   | 2.70                     | 0.44              |
| 1:A:34:LYS:H     | 1:A:57:ARG:HH21  | 1.66                     | 0.44              |
| 1:A:388:LEU:HD22 | 1:A:432:VAL:HG21 | 2.00                     | 0.44              |
| 1:A:523:ILE:HG22 | 1:A:528:LEU:HB2  | 2.00                     | 0.44              |
| 1:A:34:LYS:HZ1   | 1:A:57:ARG:NH1   | 2.15                     | 0.44              |
| 1:A:773:LYS:HG3  | 1:A:773:LYS:H    | 1.49                     | 0.44              |
| 1:A:82:GLY:O     | 1:A:241:VAL:N    | 2.37                     | 0.44              |
| 2:B:1135:ARG:O   | 2:B:1136:ASP:C   | 2.56                     | 0.44              |
| 2:B:1183:LYS:HE3 | 2:B:1183:LYS:O   | 2.17                     | 0.44              |
| 2:B:212:LEU:HD21 | 2:B:466:TRP:CH2  | 2.53                     | 0.44              |
| 2:B:343:ILE:HG21 | 2:B:348:ARG:CA   | 2.47                     | 0.44              |
| 2:B:770:GLN:OE1  | 2:B:983:ARG:CA   | 2.58                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:806:THR:CG2  | 2:B:808:ALA:HB3  | 2.48                     | 0.44              |
| 3:C:36:VAL:HG21  | 3:C:251:LEU:HD22 | 2.00                     | 0.44              |
| 3:C:255:VAL:O    | 3:C:255:VAL:HG12 | 2.18                     | 0.44              |
| 3:C:70:ILE:HG22  | 3:C:70:ILE:O     | 2.17                     | 0.44              |
| 6:F:128:LYS:HD3  | 6:F:149:GLU:O    | 2.18                     | 0.44              |
| 7:G:131:GLN:HG2  | 7:G:136:VAL:HG22 | 1.99                     | 0.44              |
| 7:G:31:LEU:CD2   | 7:G:48:VAL:HG21  | 2.48                     | 0.44              |
| 7:G:39:THR:CG2   | 7:G:40:GLY:N     | 2.76                     | 0.44              |
| 8:H:40:LEU:HG    | 8:H:41:ASP:O     | 2.18                     | 0.44              |
| 14:P:5:C:C2'     | 14:P:6:C:O4'     | 2.55                     | 0.44              |
| 1:A:230:ARG:N    | 1:A:233:TRP:CE3  | 2.65                     | 0.43              |
| 1:A:242:PRO:HA   | 1:A:243:PRO:HD2  | 1.75                     | 0.43              |
| 1:A:265:LYS:CE   | 1:A:322:VAL:HG13 | 2.47                     | 0.43              |
| 1:A:37:PHE:H     | 1:A:37:PHE:HD1   | 1.65                     | 0.43              |
| 1:A:783:THR:CG2  | 1:A:815:PHE:CE2  | 3.00                     | 0.43              |
| 1:A:935:GLN:O    | 1:A:936:LEU:C    | 2.56                     | 0.43              |
| 2:B:1183:LYS:HE3 | 2:B:1183:LYS:N   | 2.33                     | 0.43              |
| 2:B:377:PHE:CD2  | 2:B:381:MET:HE2  | 2.53                     | 0.43              |
| 2:B:465:ASN:N    | 2:B:465:ASN:ND2  | 2.64                     | 0.43              |
| 2:B:640:VAL:HB   | 2:B:738:PHE:O    | 2.19                     | 0.43              |
| 3:C:107:SER:C    | 3:C:109:SER:H    | 2.21                     | 0.43              |
| 2:B:798:TYR:CE2  | 3:C:62:PHE:CE2   | 3.06                     | 0.43              |
| 2:B:798:TYR:HE2  | 3:C:62:PHE:HZ    | 1.63                     | 0.43              |
| 4:D:18:VAL:O     | 4:D:19:GLU:HB3   | 2.18                     | 0.43              |
| 5:E:157:SER:O    | 5:E:159:ASP:N    | 2.51                     | 0.43              |
| 6:F:75:PRO:HG2   | 6:F:78:GLN:HB2   | 2.00                     | 0.43              |
| 7:G:18:PHE:HZ    | 7:G:68:ALA:HB2   | 1.83                     | 0.43              |
| 7:G:80:LYS:O     | 7:G:82:PHE:CE1   | 2.71                     | 0.43              |
| 1:A:1350:LYS:O   | 1:A:1354:ASN:ND2 | 2.47                     | 0.43              |
| 1:A:442:VAL:O    | 1:A:457:ALA:HA   | 2.17                     | 0.43              |
| 1:A:474:VAL:HG22 | 1:A:474:VAL:O    | 2.19                     | 0.43              |
| 1:A:577:ILE:O    | 1:A:580:VAL:HG23 | 2.18                     | 0.43              |
| 1:A:907:THR:HG22 | 1:A:908:LEU:N    | 2.33                     | 0.43              |
| 1:A:935:GLN:O    | 1:A:938:LYS:N    | 2.50                     | 0.43              |
| 2:B:181:LEU:HD22 | 2:B:189:LEU:CD2  | 2.48                     | 0.43              |
| 2:B:331:LEU:HD12 | 2:B:331:LEU:N    | 2.33                     | 0.43              |
| 2:B:449:ASN:O    | 2:B:451:LYS:N    | 2.51                     | 0.43              |
| 2:B:570:VAL:HA   | 2:B:571:PRO:HD2  | 1.74                     | 0.43              |
| 2:B:642:ASP:HB3  | 2:B:649:LYS:HG3  | 2.00                     | 0.43              |
| 3:C:249:ASP:O    | 3:C:252:GLN:HB3  | 2.18                     | 0.43              |
| 4:D:122:GLU:HA   | 4:D:125:SER:OG   | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:141:LEU:HA    | 4:D:141:LEU:HD12  | 1.80                     | 0.43              |
| 6:F:111:LEU:C     | 6:F:113:GLY:N     | 2.70                     | 0.43              |
| 9:I:7:CYS:HB2     | 9:I:34:TYR:CD1    | 2.53                     | 0.43              |
| 1:A:547:LEU:HB3   | 11:K:58:PHE:CE1   | 2.52                     | 0.43              |
| 12:L:70:ARG:HG2   | 12:L:70:ARG:NH1   | 2.32                     | 0.43              |
| 15:T:24:DG:C2'    | 15:T:25:DT:O5'    | 2.63                     | 0.43              |
| 1:A:1243:VAL:HG12 | 1:A:1244:ARG:N    | 2.32                     | 0.43              |
| 1:A:1290:LYS:O    | 1:A:1291:VAL:HG23 | 2.19                     | 0.43              |
| 1:A:1341:ILE:O    | 1:A:1344:GLY:N    | 2.51                     | 0.43              |
| 1:A:1450:LEU:HD11 | 6:F:108:PHE:HZ    | 1.79                     | 0.43              |
| 1:A:248:PRO:O     | 1:A:260:ASP:HB2   | 2.18                     | 0.43              |
| 1:A:699:ALA:HB2   | 9:I:114:GLN:NE2   | 2.32                     | 0.43              |
| 1:A:780:VAL:O     | 1:A:782:ARG:HG2   | 2.18                     | 0.43              |
| 2:B:234:ILE:HD12  | 2:B:234:ILE:N     | 2.33                     | 0.43              |
| 2:B:616:ILE:CD1   | 2:B:616:ILE:N     | 2.81                     | 0.43              |
| 2:B:707:PRO:O     | 2:B:711:GLU:HG3   | 2.18                     | 0.43              |
| 2:B:34:ILE:HD13   | 2:B:747:MET:HE2   | 1.99                     | 0.43              |
| 2:B:827:ILE:HD12  | 2:B:1086:PHE:HD2  | 1.84                     | 0.43              |
| 3:C:8:VAL:HG12    | 3:C:9:LYS:H       | 1.83                     | 0.43              |
| 4:D:209:ARG:O     | 4:D:212:LYS:HB2   | 2.19                     | 0.43              |
| 7:G:17:PHE:C      | 7:G:19:GLY:H      | 2.20                     | 0.43              |
| 7:G:99:PHE:CD1    | 7:G:99:PHE:C      | 2.91                     | 0.43              |
| 8:H:59:ILE:O      | 8:H:60:ALA:HB3    | 2.18                     | 0.43              |
| 9:I:85:PHE:CD1    | 9:I:99:LEU:HD13   | 2.54                     | 0.43              |
| 1:A:1213:GLY:O    | 1:A:1216:ILE:N    | 2.52                     | 0.43              |
| 1:A:1305:VAL:CG1  | 1:A:1306:LEU:N    | 2.81                     | 0.43              |
| 1:A:1101:LEU:HB2  | 1:A:1355:VAL:HG11 | 1.99                     | 0.43              |
| 1:A:388:LEU:HD22  | 1:A:432:VAL:HB    | 1.99                     | 0.43              |
| 1:A:353:ILE:CG2   | 1:A:487:MET:HG3   | 2.45                     | 0.43              |
| 1:A:347:PHE:CE2   | 1:A:493:GLN:OE1   | 2.72                     | 0.43              |
| 1:A:546:VAL:O     | 1:A:546:VAL:HG12  | 2.18                     | 0.43              |
| 1:A:639:PRO:HG2   | 1:A:640:GLN:N     | 2.33                     | 0.43              |
| 1:A:699:ALA:HB1   | 9:I:114:GLN:HB2   | 2.00                     | 0.43              |
| 1:A:802:ASN:ND2   | 1:A:812:GLU:OE1   | 2.42                     | 0.43              |
| 2:B:114:PRO:HG2   | 2:B:115:GLN:N     | 2.28                     | 0.43              |
| 2:B:1156:ASP:O    | 2:B:1157:ALA:O    | 2.37                     | 0.43              |
| 2:B:1181:GLU:O    | 2:B:1182:CYS:HB2  | 2.17                     | 0.43              |
| 2:B:281:PRO:O     | 2:B:282:ILE:C     | 2.56                     | 0.43              |
| 2:B:291:ILE:HD13  | 2:B:300:HIS:NE2   | 2.34                     | 0.43              |
| 2:B:309:GLN:HG3   | 9:I:52:ILE:CD1    | 2.48                     | 0.43              |
| 2:B:642:ASP:HB3   | 2:B:649:LYS:CG    | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:661:LEU:C     | 2:B:663:ALA:N     | 2.70                     | 0.43              |
| 2:B:681:TRP:O     | 2:B:684:LEU:N     | 2.51                     | 0.43              |
| 2:B:957:ASN:O     | 2:B:960:GLY:N     | 2.47                     | 0.43              |
| 2:B:997:GLU:H     | 2:B:997:GLU:CD    | 2.22                     | 0.43              |
| 4:D:55:ALA:HB3    | 4:D:148:LEU:HD21  | 1.99                     | 0.43              |
| 5:E:88:VAL:HG12   | 5:E:89:GLY:N      | 2.33                     | 0.43              |
| 7:G:26:LEU:HA     | 7:G:26:LEU:HD23   | 1.85                     | 0.43              |
| 8:H:95:TYR:HB3    | 8:H:144:ILE:HB    | 1.99                     | 0.43              |
| 8:H:23:VAL:HG22   | 8:H:43:ASN:HA     | 2.00                     | 0.43              |
| 15:T:10:DA:H1'    | 15:T:11:DG:C8     | 2.54                     | 0.43              |
| 2:B:1123:SER:HB3  | 15:T:24:DG:P      | 2.58                     | 0.43              |
| 1:A:1209:MET:CE   | 1:A:1236:LEU:HB3  | 2.48                     | 0.43              |
| 1:A:1226:VAL:HG22 | 1:A:1240:CYS:HB3  | 2.00                     | 0.43              |
| 1:A:1316:VAL:HG12 | 1:A:1316:VAL:O    | 2.19                     | 0.43              |
| 1:A:1404:GLU:O    | 1:A:1407:GLU:HB2  | 2.18                     | 0.43              |
| 1:A:239:LEU:HA    | 1:A:240:PRO:HD2   | 1.89                     | 0.43              |
| 1:A:608:ILE:HG13  | 1:A:613:ILE:HD12  | 2.01                     | 0.43              |
| 1:A:871:ASP:OD1   | 1:A:1366:ARG:NH2  | 2.52                     | 0.43              |
| 1:A:92:HIS:O      | 1:A:93:VAL:C      | 2.56                     | 0.43              |
| 1:A:958:VAL:HG12  | 1:A:960:ILE:HG13  | 2.01                     | 0.43              |
| 2:B:1074:ASN:HB2  | 2:B:1081:LEU:HD21 | 2.00                     | 0.43              |
| 2:B:496:ARG:NH1   | 2:B:496:ARG:HB3   | 2.33                     | 0.43              |
| 2:B:765:PRO:O     | 2:B:768:THR:N     | 2.51                     | 0.43              |
| 3:C:213:PRO:O     | 3:C:214:ASN:CB    | 2.60                     | 0.43              |
| 3:C:86:CYS:O      | 3:C:88:CYS:N      | 2.52                     | 0.43              |
| 4:D:51:ASN:C      | 4:D:52:LEU:O      | 2.56                     | 0.43              |
| 5:E:153:HIS:O     | 5:E:154:ILE:CG1   | 2.67                     | 0.43              |
| 5:E:46:TYR:CE2    | 5:E:58:MET:HA     | 2.54                     | 0.43              |
| 6:F:118:LEU:HG    | 6:F:118:LEU:O     | 2.18                     | 0.43              |
| 7:G:9:LEU:HD12    | 7:G:10:ASN:N      | 2.34                     | 0.43              |
| 10:J:34:THR:O     | 10:J:35:ALA:C     | 2.56                     | 0.43              |
| 10:J:53:HIS:NE2   | 10:J:55:ASP:HA    | 2.34                     | 0.43              |
| 13:N:0:DT:O4      | 15:T:18:DT:O2     | 2.35                     | 0.43              |
| 1:A:335:ARG:N     | 1:A:339:ASN:HD22  | 2.17                     | 0.43              |
| 1:A:47:ARG:O      | 1:A:48:ALA:HB2    | 2.18                     | 0.43              |
| 1:A:618:GLU:OE2   | 1:A:620:LYS:HB2   | 2.19                     | 0.43              |
| 1:A:723:ASN:C     | 1:A:725:ALA:N     | 2.72                     | 0.43              |
| 1:A:795:GLU:CD    | 1:A:795:GLU:H     | 2.22                     | 0.43              |
| 2:B:1115:THR:HG22 | 2:B:1117:GLN:HG3  | 2.00                     | 0.43              |
| 2:B:247:GLY:O     | 2:B:249:ARG:N     | 2.51                     | 0.43              |
| 2:B:628:THR:CG2   | 2:B:628:THR:O     | 2.66                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:825:VAL:HG12  | 2:B:826:ALA:N    | 2.33                     | 0.43              |
| 2:B:857:ARG:HH21  | 2:B:942:ARG:NH1  | 2.16                     | 0.43              |
| 3:C:189:THR:CG2   | 3:C:190:ASP:N    | 2.81                     | 0.43              |
| 4:D:13:ARG:HB2    | 4:D:17:LYS:NZ    | 2.34                     | 0.43              |
| 4:D:47:LEU:CD1    | 4:D:48:ILE:N     | 2.81                     | 0.43              |
| 5:E:124:VAL:CG1   | 5:E:132:ILE:HB   | 2.46                     | 0.43              |
| 5:E:136:ASN:OD1   | 5:E:138:ALA:N    | 2.52                     | 0.43              |
| 6:F:121:ALA:O     | 6:F:122:MET:C    | 2.57                     | 0.43              |
| 7:G:99:PHE:CZ     | 7:G:143:ILE:HD13 | 2.54                     | 0.43              |
| 9:I:33:SER:O      | 9:I:35:VAL:HG23  | 2.18                     | 0.43              |
| 2:B:193:LYS:NZ    | 12:L:32:ALA:HB1  | 2.32                     | 0.43              |
| 1:A:1313:LEU:HD23 | 1:A:1338:VAL:HB  | 2.01                     | 0.43              |
| 1:A:1362:TYR:HD1  | 1:A:1363:VAL:H   | 1.65                     | 0.43              |
| 1:A:1385:THR:O    | 1:A:1386:ARG:C   | 2.57                     | 0.43              |
| 1:A:265:LYS:HE2   | 1:A:322:VAL:HG13 | 1.98                     | 0.43              |
| 1:A:696:GLU:HG2   | 1:A:696:GLU:O    | 2.18                     | 0.43              |
| 1:A:857:ARG:NH2   | 6:F:139:PRO:HG3  | 2.33                     | 0.43              |
| 1:A:877:HIS:O     | 1:A:878:ILE:HG12 | 2.19                     | 0.43              |
| 2:B:1184:GLY:C    | 2:B:1186:ASP:N   | 2.68                     | 0.43              |
| 2:B:189:LEU:O     | 2:B:190:TYR:C    | 2.55                     | 0.43              |
| 2:B:258:LEU:HG    | 2:B:258:LEU:O    | 2.18                     | 0.43              |
| 2:B:29:ASP:HB3    | 2:B:658:ILE:HD11 | 1.99                     | 0.43              |
| 2:B:410:GLY:O     | 2:B:412:LEU:N    | 2.52                     | 0.43              |
| 2:B:39:ARG:HH21   | 2:B:665:GLU:CG   | 2.31                     | 0.43              |
| 2:B:895:ASP:C     | 2:B:897:GLY:H    | 2.22                     | 0.43              |
| 3:C:262:LEU:HA    | 3:C:262:LEU:HD23 | 1.84                     | 0.43              |
| 3:C:69:LEU:HB3    | 10:J:6:ARG:HD3   | 1.99                     | 0.43              |
| 4:D:71:LYS:HA     | 4:D:74:GLN:CB    | 2.46                     | 0.43              |
| 7:G:112:LYS:NZ    | 7:G:120:THR:HA   | 2.33                     | 0.43              |
| 11:K:44:ASN:N     | 11:K:61:TYR:CE1  | 2.87                     | 0.43              |
| 1:A:1074:GLU:HB3  | 1:A:1075:PRO:HD3 | 2.01                     | 0.43              |
| 1:A:35:ILE:HB     | 1:A:83:HIS:O     | 2.18                     | 0.43              |
| 2:B:515:HIS:O     | 2:B:518:HIS:HB2  | 2.19                     | 0.43              |
| 2:B:583:ASN:OD1   | 2:B:628:THR:N    | 2.50                     | 0.43              |
| 2:B:95:ILE:HG13   | 2:B:130:VAL:HG22 | 1.99                     | 0.43              |
| 7:G:51:TYR:O      | 7:G:51:TYR:CD2   | 2.71                     | 0.43              |
| 12:L:43:THR:O     | 12:L:43:THR:HG22 | 2.19                     | 0.43              |
| 1:A:370:ILE:O     | 1:A:373:THR:N    | 2.43                     | 0.43              |
| 1:A:481:ASP:OD1   | 1:A:483:ASP:OD2  | 2.37                     | 0.43              |
| 1:A:506:ALA:C     | 1:A:508:PRO:HD2  | 2.39                     | 0.43              |
| 1:A:570:PRO:O     | 1:A:571:LEU:HD12 | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:76:GLU:O      | 1:A:78:PRO:HD3    | 2.19                     | 0.43              |
| 2:B:1060:ARG:HA   | 2:B:1060:ARG:HD2  | 1.63                     | 0.43              |
| 2:B:1064:TYR:O    | 2:B:1065:GLN:O    | 2.37                     | 0.43              |
| 2:B:1065:GLN:NE2  | 2:B:1067:ARG:HG2  | 2.33                     | 0.43              |
| 2:B:1147:LEU:CD2  | 2:B:1151:LEU:HD22 | 2.48                     | 0.43              |
| 2:B:47:GLN:O      | 2:B:173:MET:HE1   | 2.19                     | 0.43              |
| 2:B:376:PHE:HE2   | 2:B:569:TYR:HD2   | 1.65                     | 0.43              |
| 2:B:642:ASP:CA    | 2:B:649:LYS:HA    | 2.40                     | 0.43              |
| 2:B:797:TYR:HB2   | 2:B:852:ARG:O     | 2.19                     | 0.43              |
| 3:C:176:ILE:HG22  | 3:C:177:GLU:O     | 2.19                     | 0.43              |
| 5:E:195:VAL:HG22  | 5:E:213:ILE:HG13  | 2.01                     | 0.43              |
| 8:H:39:THR:HB     | 8:H:124:ARG:HB3   | 2.00                     | 0.43              |
| 8:H:30:SER:CB     | 8:H:36:CYS:HB3    | 2.48                     | 0.43              |
| 10:J:2:ILE:HG22   | 10:J:3:VAL:O      | 2.18                     | 0.43              |
| 11:K:5:ASP:O      | 11:K:6:ARG:C      | 2.57                     | 0.43              |
| 11:K:57:LEU:HB2   | 11:K:76:GLN:HG2   | 2.01                     | 0.43              |
| 1:A:1127:ASP:O    | 1:A:1128:GLN:C    | 2.57                     | 0.43              |
| 1:A:1130:GLN:O    | 1:A:1134:ILE:HG13 | 2.19                     | 0.43              |
| 1:A:577:ILE:C     | 1:A:579:SER:N     | 2.69                     | 0.43              |
| 1:A:601:LYS:HB2   | 1:A:603:ASN:HD21  | 1.84                     | 0.43              |
| 1:A:49:LYS:CE     | 1:A:61:ILE:HD12   | 2.42                     | 0.43              |
| 1:A:672:ASP:O     | 1:A:673:GLY:C     | 2.58                     | 0.43              |
| 1:A:877:HIS:C     | 1:A:878:ILE:CG1   | 2.87                     | 0.43              |
| 1:A:341:MET:HE3   | 2:B:1135:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:78:PRO:HB2    | 2:B:1201:LYS:HE3  | 2.01                     | 0.43              |
| 2:B:1202:LEU:HD22 | 2:B:1206:GLU:CD   | 2.39                     | 0.43              |
| 2:B:251:ILE:HG22  | 2:B:251:ILE:O     | 2.19                     | 0.43              |
| 2:B:343:ILE:HB    | 2:B:348:ARG:HE    | 1.84                     | 0.43              |
| 2:B:361:LEU:N     | 2:B:362:PRO:CD    | 2.81                     | 0.43              |
| 2:B:785:TYR:C     | 2:B:785:TYR:CD1   | 2.91                     | 0.43              |
| 2:B:890:TYR:O     | 2:B:892:LYS:N     | 2.51                     | 0.43              |
| 2:B:60:GLN:OE1    | 2:B:95:ILE:HG22   | 2.19                     | 0.43              |
| 3:C:120:ILE:HD11  | 3:C:130:GLY:O     | 2.19                     | 0.43              |
| 3:C:38:ILE:HA     | 3:C:173:ALA:HB2   | 2.00                     | 0.43              |
| 3:C:27:LEU:HD13   | 3:C:228:PHE:CE2   | 2.54                     | 0.43              |
| 3:C:3:GLU:O       | 3:C:4:GLU:CG      | 2.67                     | 0.43              |
| 4:D:51:ASN:ND2    | 4:D:54:GLU:OE2    | 2.52                     | 0.43              |
| 4:D:60:LYS:O      | 4:D:64:VAL:HG23   | 2.19                     | 0.43              |
| 5:E:55:ARG:HD2    | 5:E:83:CYS:O      | 2.19                     | 0.43              |
| 7:G:34:VAL:HG11   | 7:G:74:TYR:HE1    | 1.84                     | 0.43              |
| 11:K:57:LEU:N     | 11:K:76:GLN:O     | 2.52                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1011:GLN:O    | 1:A:1015:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:1025:ARG:O    | 1:A:1026:LEU:HD23 | 2.19                     | 0.42              |
| 1:A:203:SER:OG    | 1:A:206:GLU:HB2   | 2.19                     | 0.42              |
| 1:A:350:ARG:HG3   | 1:A:350:ARG:NH1   | 2.33                     | 0.42              |
| 1:A:40:THR:C      | 1:A:41:MET:HG3    | 2.39                     | 0.42              |
| 1:A:925:LEU:O     | 1:A:927:VAL:N     | 2.52                     | 0.42              |
| 2:B:382:ILE:O     | 2:B:386:LEU:HG    | 2.19                     | 0.42              |
| 2:B:764:SER:HB3   | 2:B:765:PRO:CD    | 2.49                     | 0.42              |
| 3:C:27:LEU:O      | 3:C:28:ALA:C      | 2.57                     | 0.42              |
| 3:C:61:GLU:HA     | 3:C:64:ALA:HB3    | 2.00                     | 0.42              |
| 4:D:145:MET:O     | 4:D:149:THR:HB    | 2.19                     | 0.42              |
| 6:F:101:ILE:HD11  | 6:F:124:GLU:OE1   | 2.18                     | 0.42              |
| 7:G:79:PHE:CE2    | 7:G:105:PRO:HG2   | 2.54                     | 0.42              |
| 8:H:139:ASN:O     | 8:H:140:ALA:HB2   | 2.19                     | 0.42              |
| 9:I:56:ALA:O      | 9:I:57:GLY:C      | 2.57                     | 0.42              |
| 1:A:1057:VAL:CG1  | 1:A:1058:VAL:N    | 2.82                     | 0.42              |
| 1:A:1205:LYS:O    | 1:A:1206:ASP:C    | 2.57                     | 0.42              |
| 1:A:1424:VAL:HG22 | 1:A:1436:ILE:HD11 | 2.01                     | 0.42              |
| 1:A:92:HIS:HD2    | 1:A:304:MET:CE    | 2.32                     | 0.42              |
| 1:A:335:ARG:O     | 1:A:336:ILE:C     | 2.55                     | 0.42              |
| 1:A:674:PRO:C     | 1:A:676:MET:N     | 2.72                     | 0.42              |
| 1:A:412:ARG:NH2   | 2:B:1108:ARG:HH12 | 2.17                     | 0.42              |
| 2:B:1197:PRO:O    | 2:B:1200:ALA:N    | 2.51                     | 0.42              |
| 2:B:654:ARG:C     | 2:B:656:GLY:N     | 2.72                     | 0.42              |
| 2:B:693:ILE:HG22  | 2:B:694:ASP:O     | 2.20                     | 0.42              |
| 3:C:41:ILE:HD11   | 3:C:247:GLY:HA2   | 2.00                     | 0.42              |
| 5:E:160:GLU:O     | 5:E:163:GLU:HB3   | 2.19                     | 0.42              |
| 6:F:85:MET:HE1    | 6:F:93:ILE:HD12   | 2.01                     | 0.42              |
| 7:G:66:GLY:O      | 7:G:67:SER:C      | 2.55                     | 0.42              |
| 8:H:56:THR:HG21   | 8:H:145:ARG:HE    | 1.84                     | 0.42              |
| 9:I:101:PHE:HB2   | 9:I:110:PHE:CE2   | 2.55                     | 0.42              |
| 9:I:59:VAL:C      | 9:I:61:ASP:H      | 2.22                     | 0.42              |
| 1:A:1400:CYS:O    | 1:A:1405:THR:HG23 | 2.20                     | 0.42              |
| 1:A:1430:LEU:HB2  | 1:A:1432:GLN:HG3  | 2.00                     | 0.42              |
| 1:A:1437:GLY:O    | 1:A:1438:THR:C    | 2.58                     | 0.42              |
| 1:A:299:HIS:C     | 1:A:301:ALA:H     | 2.23                     | 0.42              |
| 1:A:372:LYS:HA    | 1:A:435:HIS:HD1   | 1.81                     | 0.42              |
| 1:A:49:LYS:HZ2    | 1:A:60:SER:HA     | 1.84                     | 0.42              |
| 1:A:870:GLU:HG2   | 5:E:208:TYR:CD1   | 2.54                     | 0.42              |
| 1:A:907:THR:HG23  | 1:A:908:LEU:N     | 2.33                     | 0.42              |
| 2:B:1162:ILE:O    | 2:B:1171:VAL:HG21 | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:37:PHE:CE2   | 2:B:542:MET:HA   | 2.55                     | 0.42              |
| 2:B:857:ARG:NH2  | 2:B:942:ARG:NH1  | 2.68                     | 0.42              |
| 4:D:118:THR:HG22 | 4:D:118:THR:O    | 2.19                     | 0.42              |
| 5:E:179:GLN:HB2  | 5:E:182:ASP:HB2  | 2.01                     | 0.42              |
| 5:E:61:GLN:HG2   | 5:E:62:ALA:H     | 1.83                     | 0.42              |
| 6:F:79:ARG:HH22  | 6:F:150:GLU:CD   | 2.22                     | 0.42              |
| 7:G:13:LEU:HD21  | 7:G:17:PHE:CB    | 2.28                     | 0.42              |
| 1:A:1237:ILE:CG2 | 1:A:1238:ILE:N   | 2.83                     | 0.42              |
| 1:A:122:MET:O    | 1:A:123:ARG:C    | 2.58                     | 0.42              |
| 1:A:1386:ARG:HE  | 1:A:1386:ARG:HB3 | 1.68                     | 0.42              |
| 1:A:1387:HIS:CE1 | 13:N:4:DT:C4'    | 3.00                     | 0.42              |
| 1:A:774:ARG:CZ   | 1:A:797:LYS:HG3  | 2.48                     | 0.42              |
| 2:B:221:ASN:OD1  | 2:B:242:SER:HA   | 2.18                     | 0.42              |
| 2:B:364:ILE:HG22 | 2:B:365:THR:N    | 2.33                     | 0.42              |
| 2:B:45:SER:O     | 2:B:46:GLN:C     | 2.57                     | 0.42              |
| 2:B:467:GLY:CA   | 2:B:475:SER:HB3  | 2.49                     | 0.42              |
| 3:C:45:ALA:O     | 3:C:159:ALA:HA   | 2.20                     | 0.42              |
| 8:H:95:TYR:CE2   | 8:H:97:MET:CG    | 3.02                     | 0.42              |
| 9:I:53:GLY:O     | 9:I:89:GLN:HB2   | 2.18                     | 0.42              |
| 11:K:61:TYR:O    | 11:K:61:TYR:CD2  | 2.72                     | 0.42              |
| 1:A:1198:ASP:HB3 | 1:A:1201:ALA:HB3 | 2.01                     | 0.42              |
| 1:A:1315:GLU:C   | 1:A:1317:MET:N   | 2.72                     | 0.42              |
| 1:A:1370:LEU:O   | 1:A:1373:ASP:HB2 | 2.20                     | 0.42              |
| 1:A:1398:MET:HB2 | 1:A:1426:GLU:OE2 | 2.19                     | 0.42              |
| 1:A:208:LEU:HD23 | 1:A:208:LEU:O    | 2.20                     | 0.42              |
| 1:A:817:ALA:O    | 1:A:818:MET:C    | 2.56                     | 0.42              |
| 1:A:890:ASP:H    | 1:A:1296:GLY:HA3 | 1.83                     | 0.42              |
| 1:A:907:THR:HG23 | 1:A:908:LEU:H    | 1.85                     | 0.42              |
| 1:A:964:ILE:O    | 1:A:965:GLN:C    | 2.57                     | 0.42              |
| 2:B:1222:ARG:HG2 | 2:B:1222:ARG:O   | 2.19                     | 0.42              |
| 2:B:129:PHE:HE2  | 2:B:166:PHE:CD1  | 2.37                     | 0.42              |
| 2:B:129:PHE:CE2  | 2:B:166:PHE:HD1  | 2.35                     | 0.42              |
| 2:B:405:ARG:NE   | 2:B:632:ARG:HG2  | 2.34                     | 0.42              |
| 2:B:45:SER:OG    | 2:B:46:GLN:N     | 2.49                     | 0.42              |
| 2:B:758:PHE:N    | 2:B:759:PRO:HD2  | 2.34                     | 0.42              |
| 2:B:806:THR:HG22 | 2:B:808:ALA:CB   | 2.49                     | 0.42              |
| 3:C:239:PRO:O    | 3:C:241:ASP:N    | 2.53                     | 0.42              |
| 3:C:94:LYS:HB2   | 3:C:94:LYS:HE3   | 1.87                     | 0.42              |
| 1:A:852:TYR:CE1  | 6:F:136:ARG:HG2  | 2.54                     | 0.42              |
| 6:F:86:THR:HG23  | 6:F:89:GLU:CD    | 2.39                     | 0.42              |
| 7:G:115:MET:CB   | 7:G:116:PRO:CD   | 2.98                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:10:PHE:HA     | 8:H:29:ALA:O      | 2.18                     | 0.42              |
| 1:A:477:PRO:HG3   | 1:A:521:MET:HG2   | 2.02                     | 0.42              |
| 1:A:543:LEU:HD12  | 1:A:547:LEU:HG    | 2.01                     | 0.42              |
| 1:A:53:LEU:O      | 1:A:54:ASN:C      | 2.57                     | 0.42              |
| 1:A:568:PRO:HB2   | 3:C:221:TYR:CZ    | 2.54                     | 0.42              |
| 1:A:842:VAL:O     | 1:A:844:ALA:N     | 2.52                     | 0.42              |
| 2:B:1208:MET:O    | 2:B:1211:ASN:N    | 2.51                     | 0.42              |
| 2:B:597:MET:C     | 2:B:599:THR:N     | 2.73                     | 0.42              |
| 2:B:641:GLU:HA    | 2:B:641:GLU:OE1   | 2.20                     | 0.42              |
| 4:D:7:THR:HB      | 7:G:42:PHE:CZ     | 2.55                     | 0.42              |
| 5:E:180:ARG:NH2   | 5:E:192:ARG:HD2   | 2.34                     | 0.42              |
| 8:H:95:TYR:HE2    | 8:H:97:MET:CG     | 2.32                     | 0.42              |
| 9:I:100:PHE:CD1   | 9:I:100:PHE:N     | 2.88                     | 0.42              |
| 10:J:32:GLU:O     | 10:J:33:GLY:C     | 2.57                     | 0.42              |
| 12:L:29:TYR:CD2   | 12:L:29:TYR:N     | 2.84                     | 0.42              |
| 12:L:60:ARG:HG2   | 12:L:61:THR:N     | 2.35                     | 0.42              |
| 3:C:47:ASP:CA     | 12:L:69:ALA:CB    | 2.94                     | 0.42              |
| 1:A:1074:GLU:N    | 1:A:1075:PRO:HD2  | 2.35                     | 0.42              |
| 1:A:1226:VAL:HG22 | 1:A:1240:CYS:CB   | 2.50                     | 0.42              |
| 1:A:1118:VAL:O    | 1:A:1305:VAL:HG13 | 2.20                     | 0.42              |
| 1:A:1315:GLU:C    | 1:A:1317:MET:H    | 2.22                     | 0.42              |
| 1:A:1389:PHE:C    | 1:A:1391:ARG:H    | 2.22                     | 0.42              |
| 1:A:507:VAL:N     | 1:A:508:PRO:CD    | 2.82                     | 0.42              |
| 1:A:746:MET:CE    | 2:B:1018:PRO:HG2  | 2.50                     | 0.42              |
| 1:A:846:GLU:HB2   | 1:A:847:ASP:H     | 1.68                     | 0.42              |
| 2:B:559:SER:HA    | 2:B:563:MET:HB3   | 2.02                     | 0.42              |
| 2:B:519:TRP:HE1   | 2:B:635:ARG:NH2   | 2.18                     | 0.42              |
| 2:B:693:ILE:HD11  | 2:B:740:HIS:CD2   | 2.54                     | 0.42              |
| 2:B:781:PHE:O     | 2:B:782:LEU:HD23  | 2.19                     | 0.42              |
| 3:C:98:VAL:C      | 3:C:99:LEU:CD2    | 2.88                     | 0.42              |
| 6:F:87:LYS:HG3    | 6:F:88:TYR:CE1    | 2.54                     | 0.42              |
| 12:L:28:LYS:HB2   | 12:L:39:SER:HA    | 2.02                     | 0.42              |
| 1:A:1447:GLU:OE2  | 7:G:23:LYS:HB2    | 2.19                     | 0.42              |
| 1:A:274:ILE:O     | 1:A:275:SER:C     | 2.57                     | 0.42              |
| 1:A:381:THR:O     | 1:A:384:ASN:N     | 2.50                     | 0.42              |
| 1:A:665:GLY:O     | 1:A:666:ILE:C     | 2.58                     | 0.42              |
| 1:A:841:LEU:O     | 1:A:845:LEU:HG    | 2.20                     | 0.42              |
| 2:B:102:VAL:HG23  | 2:B:112:LEU:HB2   | 2.02                     | 0.42              |
| 2:B:458:LYS:O     | 2:B:459:TYR:C     | 2.58                     | 0.42              |
| 3:C:124:LEU:HD22  | 3:C:129:ILE:HG22  | 2.01                     | 0.42              |
| 4:D:170:THR:CG2   | 4:D:172:LEU:HG    | 2.50                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:F:81:THR:HB     | 6:F:136:ARG:HH11 | 1.85                     | 0.42              |
| 7:G:56:ILE:O      | 7:G:57:GLN:HB2   | 2.20                     | 0.42              |
| 10:J:1:MET:H3     | 10:J:56:LEU:H    | 1.68                     | 0.42              |
| 15:T:12:DT:H2"    | 15:T:13:DA:OP2   | 2.18                     | 0.42              |
| 1:A:1437:GLY:HA3  | 6:F:88:TYR:CD2   | 2.55                     | 0.42              |
| 1:A:1438:THR:HB   | 2:B:1144:ALA:CB  | 2.46                     | 0.42              |
| 1:A:162:VAL:HG12  | 1:A:163:SER:N    | 2.34                     | 0.42              |
| 1:A:270:LEU:O     | 1:A:271:LYS:C    | 2.57                     | 0.42              |
| 1:A:598:LEU:O     | 1:A:599:SER:C    | 2.58                     | 0.42              |
| 1:A:608:ILE:C     | 1:A:610:GLY:H    | 2.22                     | 0.42              |
| 1:A:785:PRO:HG2   | 1:A:786:HIS:CD2  | 2.52                     | 0.42              |
| 2:B:1085:ILE:CD1  | 2:B:1085:ILE:N   | 2.79                     | 0.42              |
| 2:B:235:SER:HA    | 2:B:261:ARG:NH1  | 2.34                     | 0.42              |
| 2:B:597:MET:O     | 2:B:599:THR:N    | 2.53                     | 0.42              |
| 2:B:616:ILE:HG12  | 2:B:697:GLU:HA   | 2.01                     | 0.42              |
| 2:B:914:LYS:HD3   | 2:B:937:ALA:CB   | 2.50                     | 0.42              |
| 3:C:166:GLU:O     | 3:C:167:HIS:HB2  | 2.20                     | 0.42              |
| 3:C:208:GLU:C     | 3:C:210:GLU:N    | 2.71                     | 0.42              |
| 3:C:213:PRO:HG2   | 3:C:214:ASN:H    | 1.84                     | 0.42              |
| 3:C:23:SER:O      | 3:C:24:ASN:HB3   | 2.19                     | 0.42              |
| 2:B:798:TYR:HE2   | 3:C:62:PHE:CE2   | 2.36                     | 0.42              |
| 4:D:64:VAL:C      | 4:D:66:ARG:N     | 2.73                     | 0.42              |
| 5:E:73:PRO:O      | 5:E:75:MET:N     | 2.48                     | 0.42              |
| 1:A:1441:PHE:CE2  | 6:F:89:GLU:HG2   | 2.55                     | 0.42              |
| 9:I:4:PHE:HE1     | 9:I:6:PHE:CE2    | 2.38                     | 0.42              |
| 1:A:975:HIS:HA    | 1:A:1036:ARG:HG3 | 2.02                     | 0.42              |
| 1:A:1215:ARG:HA   | 1:A:1215:ARG:HD2 | 1.72                     | 0.42              |
| 1:A:1279:ILE:HG23 | 1:A:1308:THR:OG1 | 2.20                     | 0.42              |
| 1:A:353:ILE:HD13  | 1:A:487:MET:CE   | 2.49                     | 0.42              |
| 1:A:382:PRO:CB    | 1:A:428:TYR:CE2  | 2.97                     | 0.42              |
| 1:A:472:LEU:O     | 1:A:475:THR:CB   | 2.60                     | 0.42              |
| 1:A:7:SER:OG      | 2:B:1193:GLN:NE2 | 2.53                     | 0.42              |
| 1:A:856:THR:CB    | 1:A:865:GLN:HB2  | 2.47                     | 0.42              |
| 1:A:925:LEU:C     | 1:A:927:VAL:H    | 2.23                     | 0.42              |
| 2:B:1006:ILE:HD13 | 10:J:44:TYR:HE2  | 1.81                     | 0.42              |
| 2:B:977:GLY:HA3   | 2:B:1099:VAL:CG2 | 2.49                     | 0.42              |
| 2:B:28:GLU:HG3    | 2:B:28:GLU:O     | 2.20                     | 0.42              |
| 2:B:763:GLN:O     | 2:B:765:PRO:N    | 2.53                     | 0.42              |
| 2:B:882:THR:HG21  | 2:B:884:ARG:HB2  | 2.02                     | 0.42              |
| 5:E:144:ILE:HD13  | 5:E:183:PRO:HB3  | 2.01                     | 0.42              |
| 7:G:144:ARG:O     | 7:G:168:LEU:HD22 | 2.20                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:G:38:CYS:HB3    | 7:G:155:SER:HA   | 2.02                     | 0.42              |
| 8:H:10:PHE:HE1    | 8:H:57:VAL:HB    | 1.85                     | 0.42              |
| 8:H:98:TYR:C      | 8:H:118:PHE:HD2  | 2.23                     | 0.42              |
| 11:K:50:LEU:HD11  | 11:K:75:ILE:CD1  | 2.50                     | 0.42              |
| 14:P:1:U:O2'      | 14:P:2:C:C5'     | 2.67                     | 0.42              |
| 1:A:130:ASP:HB3   | 1:A:133:LYS:HB2  | 2.02                     | 0.41              |
| 1:A:146:MET:HA    | 1:A:171:GLN:HB2  | 2.01                     | 0.41              |
| 1:A:61:ILE:HG22   | 1:A:62:ASP:N     | 2.32                     | 0.41              |
| 1:A:786:HIS:O     | 1:A:787:PHE:HD2  | 2.03                     | 0.41              |
| 2:B:753:ALA:O     | 2:B:755:ILE:N    | 2.53                     | 0.41              |
| 2:B:769:TYR:O     | 2:B:772:ALA:N    | 2.53                     | 0.41              |
| 2:B:957:ASN:O     | 2:B:958:GLN:C    | 2.58                     | 0.41              |
| 2:B:953:LEU:HD23  | 2:B:965:LYS:H    | 1.85                     | 0.41              |
| 6:F:97:ARG:HA     | 6:F:97:ARG:HD2   | 1.83                     | 0.41              |
| 7:G:91:VAL:HA     | 7:G:101:VAL:HA   | 2.02                     | 0.41              |
| 7:G:22:MET:O      | 7:G:25:TYR:N     | 2.53                     | 0.41              |
| 11:K:42:LEU:HD21  | 11:K:46:ILE:CD1  | 2.50                     | 0.41              |
| 1:A:108:MET:O     | 1:A:109:HIS:HB2  | 2.19                     | 0.41              |
| 1:A:1394:THR:HG22 | 1:A:1395:GLY:N   | 2.35                     | 0.41              |
| 1:A:469:ARG:HB3   | 1:A:469:ARG:HH11 | 1.85                     | 0.41              |
| 1:A:719:VAL:C     | 1:A:721:PHE:N    | 2.73                     | 0.41              |
| 1:A:842:VAL:O     | 1:A:843:LYS:C    | 2.57                     | 0.41              |
| 1:A:98:LYS:O      | 1:A:101:LYS:N    | 2.54                     | 0.41              |
| 2:B:263:GLY:O     | 2:B:264:SER:C    | 2.58                     | 0.41              |
| 2:B:523:CYS:SG    | 2:B:524:PRO:HD2  | 2.60                     | 0.41              |
| 2:B:53:GLN:NE2    | 2:B:57:TYR:HB2   | 2.35                     | 0.41              |
| 2:B:620:ARG:NH2   | 9:I:89:GLN:NE2   | 2.68                     | 0.41              |
| 2:B:862:GLN:CG    | 2:B:963:PHE:HD1  | 2.33                     | 0.41              |
| 3:C:51:VAL:HG22   | 3:C:155:LEU:HD22 | 2.01                     | 0.41              |
| 3:C:53:THR:O      | 3:C:153:LEU:HA   | 2.20                     | 0.41              |
| 4:D:180:LEU:HD23  | 4:D:180:LEU:HA   | 1.88                     | 0.41              |
| 5:E:157:SER:OG    | 5:E:159:ASP:HB2  | 2.21                     | 0.41              |
| 5:E:177:ARG:HD3   | 5:E:215:MET:HG2  | 2.02                     | 0.41              |
| 5:E:92:THR:HG22   | 5:E:92:THR:O     | 2.20                     | 0.41              |
| 8:H:20:TYR:O      | 8:H:22:LYS:N     | 2.52                     | 0.41              |
| 8:H:76:THR:HG22   | 8:H:76:THR:O     | 2.19                     | 0.41              |
| 9:I:54:GLU:HB3    | 9:I:100:PHE:CE2  | 2.55                     | 0.41              |
| 1:A:117:GLU:H     | 1:A:117:GLU:CD   | 2.23                     | 0.41              |
| 1:A:1329:THR:CG2  | 1:A:1331:SER:HB3 | 2.51                     | 0.41              |
| 1:A:697:ALA:C     | 1:A:699:ALA:H    | 2.23                     | 0.41              |
| 1:A:722:LEU:HD21  | 1:A:794:PRO:HB3  | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:845:LEU:O    | 1:A:846:GLU:C    | 2.58                     | 0.41              |
| 1:A:90:VAL:HG12  | 1:A:91:PHE:N     | 2.34                     | 0.41              |
| 2:B:169:ARG:N    | 2:B:454:THR:OG1  | 2.54                     | 0.41              |
| 2:B:224:GLN:HA   | 2:B:396:ASP:OD2  | 2.19                     | 0.41              |
| 2:B:429:PHE:HA   | 2:B:432:MET:CE   | 2.50                     | 0.41              |
| 2:B:95:ILE:HB    | 2:B:130:VAL:HG22 | 2.01                     | 0.41              |
| 3:C:236:GLY:O    | 3:C:237:SER:C    | 2.59                     | 0.41              |
| 3:C:29:MET:HE1   | 11:K:98:LEU:CD2  | 2.50                     | 0.41              |
| 6:F:143:PHE:C    | 6:F:143:PHE:HD1  | 2.23                     | 0.41              |
| 8:H:83:GLN:O     | 8:H:85:GLY:N     | 2.53                     | 0.41              |
| 10:J:28:ASP:O    | 10:J:29:GLU:C    | 2.59                     | 0.41              |
| 11:K:91:CYS:O    | 11:K:94:ILE:HB   | 2.21                     | 0.41              |
| 1:A:1157:ASP:C   | 1:A:1159:ARG:H   | 2.24                     | 0.41              |
| 1:A:11:LEU:HG    | 1:A:11:LEU:O     | 2.16                     | 0.41              |
| 1:A:1444:MET:HG2 | 7:G:59:GLY:O     | 2.20                     | 0.41              |
| 1:A:596:THR:O    | 1:A:597:LEU:C    | 2.59                     | 0.41              |
| 1:A:825:ILE:O    | 1:A:828:ALA:N    | 2.48                     | 0.41              |
| 2:B:1085:ILE:CG2 | 2:B:1086:PHE:N   | 2.82                     | 0.41              |
| 2:B:1115:THR:CG2 | 2:B:1117:GLN:CG  | 2.98                     | 0.41              |
| 2:B:51:PHE:CD2   | 2:B:173:MET:HB3  | 2.56                     | 0.41              |
| 2:B:97:VAL:HG12  | 2:B:178:ASN:HD21 | 1.85                     | 0.41              |
| 2:B:273:LEU:HD12 | 2:B:280:ILE:HD12 | 2.01                     | 0.41              |
| 2:B:336:ARG:NH2  | 2:B:345:LYS:CE   | 2.77                     | 0.41              |
| 2:B:48:LEU:O     | 2:B:51:PHE:N     | 2.51                     | 0.41              |
| 2:B:581:PHE:HA   | 2:B:585:VAL:O    | 2.20                     | 0.41              |
| 4:D:153:ARG:C    | 4:D:154:PHE:CD1  | 2.93                     | 0.41              |
| 4:D:33:PHE:CE2   | 7:G:80:LYS:NZ    | 2.82                     | 0.41              |
| 10:J:22:LEU:O    | 10:J:25:LEU:HB2  | 2.20                     | 0.41              |
| 10:J:2:ILE:HG12  | 10:J:57:ILE:HD12 | 2.02                     | 0.41              |
| 1:A:1010:ALA:O   | 1:A:1011:GLN:C   | 2.59                     | 0.41              |
| 1:A:1018:PHE:O   | 1:A:1021:LEU:HB3 | 2.20                     | 0.41              |
| 1:A:1445:ILE:H   | 1:A:1445:ILE:CD1 | 1.98                     | 0.41              |
| 1:A:265:LYS:NZ   | 1:A:322:VAL:HG13 | 2.36                     | 0.41              |
| 1:A:305:ASP:CG   | 1:A:326:ARG:HD2  | 2.41                     | 0.41              |
| 1:A:335:ARG:HB3  | 1:A:336:ILE:H    | 1.68                     | 0.41              |
| 1:A:353:ILE:HG21 | 1:A:487:MET:CE   | 2.49                     | 0.41              |
| 1:A:562:THR:HA   | 1:A:563:PRO:HD3  | 1.87                     | 0.41              |
| 1:A:818:MET:HG2  | 2:B:514:LEU:HG   | 2.03                     | 0.41              |
| 1:A:886:ILE:HG22 | 1:A:887:GLY:H    | 1.78                     | 0.41              |
| 2:B:980:PHE:HE2  | 2:B:1094:ARG:CB  | 2.33                     | 0.41              |
| 2:B:1142:GLY:O   | 2:B:1144:ALA:N   | 2.53                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:446:LEU:HD23 | 2:B:446:LEU:N     | 2.36                     | 0.41              |
| 2:B:705:MET:CE   | 2:B:745:PRO:HB3   | 2.51                     | 0.41              |
| 2:B:750:GLY:O    | 2:B:751:VAL:C     | 2.59                     | 0.41              |
| 2:B:806:THR:C    | 2:B:808:ALA:N     | 2.71                     | 0.41              |
| 2:B:807:ARG:O    | 2:B:811:TYR:HE1   | 2.03                     | 0.41              |
| 3:C:116:LYS:HD3  | 3:C:140:ASN:HA    | 2.02                     | 0.41              |
| 3:C:70:ILE:HA    | 3:C:71:PRO:HD2    | 1.89                     | 0.41              |
| 4:D:40:HIS:C     | 4:D:42:GLY:N      | 2.72                     | 0.41              |
| 10:J:32:GLU:O    | 10:J:35:ALA:N     | 2.53                     | 0.41              |
| 10:J:53:HIS:CD2  | 10:J:54:VAL:N     | 2.88                     | 0.41              |
| 1:A:1074:GLU:HB3 | 1:A:1075:PRO:CD   | 2.50                     | 0.41              |
| 1:A:116:ASP:C    | 1:A:118:HIS:H     | 2.24                     | 0.41              |
| 1:A:860:LEU:HD11 | 1:A:1393:ASN:HB2  | 2.02                     | 0.41              |
| 1:A:47:ARG:HH12  | 1:A:254:GLU:CG    | 2.33                     | 0.41              |
| 1:A:62:ASP:HB3   | 1:A:64:ASN:HD21   | 1.83                     | 0.41              |
| 1:A:920:LEU:HD23 | 1:A:920:LEU:C     | 2.40                     | 0.41              |
| 2:B:1002:THR:CG2 | 2:B:1006:ILE:HG13 | 2.49                     | 0.41              |
| 2:B:1074:ASN:O   | 2:B:1078:GLY:N    | 2.51                     | 0.41              |
| 2:B:1110:PRO:HB2 | 2:B:1119:VAL:CG2  | 2.51                     | 0.41              |
| 2:B:400:HIS:O    | 2:B:402:GLY:N     | 2.53                     | 0.41              |
| 2:B:458:LYS:O    | 2:B:462:ALA:N     | 2.54                     | 0.41              |
| 2:B:651:LEU:HD11 | 2:B:707:PRO:CB    | 2.51                     | 0.41              |
| 2:B:863:GLU:OE1  | 2:B:962:LYS:HB2   | 2.20                     | 0.41              |
| 3:C:76:ASP:O     | 3:C:79:GLN:HG2    | 2.21                     | 0.41              |
| 5:E:42:PHE:O     | 5:E:43:LYS:C      | 2.59                     | 0.41              |
| 6:F:147:SER:OG   | 6:F:150:GLU:HG3   | 2.20                     | 0.41              |
| 7:G:165:GLU:HB2  | 7:G:168:LEU:HD12  | 2.02                     | 0.41              |
| 7:G:62:LEU:HD23  | 7:G:62:LEU:HA     | 1.89                     | 0.41              |
| 10:J:21:TYR:C    | 10:J:21:TYR:CD2   | 2.94                     | 0.41              |
| 12:L:40:LEU:HD22 | 12:L:44:ASP:CB    | 2.51                     | 0.41              |
| 14:P:6:C:H2'     | 14:P:7:A:O4'      | 2.20                     | 0.41              |
| 1:A:252:PHE:HB2  | 1:A:256:GLN:CD    | 2.41                     | 0.41              |
| 1:A:42:ASP:OD1   | 1:A:45:GLN:O      | 2.39                     | 0.41              |
| 1:A:526:ASP:O    | 1:A:527:THR:C     | 2.59                     | 0.41              |
| 1:A:629:LEU:O    | 1:A:633:VAL:HG23  | 2.21                     | 0.41              |
| 1:A:65:LEU:O     | 1:A:66:LYS:C      | 2.59                     | 0.41              |
| 1:A:699:ALA:HB2  | 9:I:114:GLN:CD    | 2.41                     | 0.41              |
| 1:A:89:PRO:HB3   | 1:A:208:LEU:HD12  | 2.03                     | 0.41              |
| 2:B:1023:VAL:O   | 2:B:1024:ALA:C    | 2.59                     | 0.41              |
| 2:B:324:ILE:CG2  | 2:B:325:GLN:N     | 2.83                     | 0.41              |
| 2:B:469:GLN:HB2  | 2:B:470:LYS:H     | 1.52                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:642:ASP:CA    | 2:B:649:LYS:HG3   | 2.50                     | 0.41              |
| 3:C:59:ALA:O      | 3:C:60:ASP:C      | 2.58                     | 0.41              |
| 5:E:114:ASN:O     | 5:E:115:ASN:CB    | 2.63                     | 0.41              |
| 6:F:97:ARG:NH2    | 6:F:106:PRO:O     | 2.54                     | 0.41              |
| 10:J:57:ILE:HG23  | 10:J:58:GLU:N     | 2.35                     | 0.41              |
| 15:T:16:DT:C4     | 15:T:17:DT:C4     | 3.09                     | 0.41              |
| 1:A:1076:ALA:HA   | 1:A:1079:MET:HE3  | 2.01                     | 0.41              |
| 1:A:1170:ILE:HG13 | 1:A:1170:ILE:H    | 1.55                     | 0.41              |
| 1:A:1214:GLU:OE1  | 1:A:1214:GLU:HA   | 2.21                     | 0.41              |
| 1:A:135:PHE:HB2   | 1:A:223:GLY:H     | 1.85                     | 0.41              |
| 1:A:268:ASP:O     | 1:A:269:ILE:C     | 2.59                     | 0.41              |
| 1:A:322:VAL:HG12  | 1:A:322:VAL:O     | 2.19                     | 0.41              |
| 1:A:56:PRO:O      | 1:A:57:ARG:NE     | 2.47                     | 0.41              |
| 1:A:715:GLU:O     | 1:A:716:ASP:C     | 2.59                     | 0.41              |
| 1:A:77:CYS:C      | 1:A:78:PRO:O      | 2.55                     | 0.41              |
| 1:A:98:LYS:O      | 1:A:100:LYS:N     | 2.53                     | 0.41              |
| 2:B:1034:VAL:O    | 2:B:1036:ALA:N    | 2.54                     | 0.41              |
| 2:B:762:ASN:OD1   | 2:B:1024:ALA:HB3  | 2.21                     | 0.41              |
| 3:C:143:LEU:HD21  | 3:C:146:LYS:HE2   | 2.03                     | 0.41              |
| 3:C:256:ALA:O     | 3:C:258:ILE:N     | 2.54                     | 0.41              |
| 3:C:66:ARG:CZ     | 10:J:2:ILE:CG2    | 2.98                     | 0.41              |
| 4:D:187:THR:HG22  | 4:D:188:ALA:H     | 1.84                     | 0.41              |
| 6:F:147:SER:O     | 6:F:148:VAL:C     | 2.58                     | 0.41              |
| 6:F:89:GLU:O      | 6:F:93:ILE:HG13   | 2.20                     | 0.41              |
| 7:G:87:VAL:CG2    | 7:G:103:VAL:HG21  | 2.51                     | 0.41              |
| 9:I:101:PHE:CE1   | 9:I:112:SER:HB2   | 2.56                     | 0.41              |
| 10:J:31:ASP:O     | 10:J:32:GLU:C     | 2.59                     | 0.41              |
| 12:L:60:ARG:HH21  | 12:L:65:VAL:HG21  | 1.86                     | 0.41              |
| 1:A:24:PRO:HD2    | 1:A:233:TRP:CD1   | 2.55                     | 0.41              |
| 1:A:269:ILE:HG12  | 1:A:299:HIS:HB3   | 2.03                     | 0.41              |
| 1:A:338:GLY:HA2   | 2:B:1129:ARG:HH22 | 1.86                     | 0.41              |
| 1:A:335:ARG:CA    | 1:A:339:ASN:HD22  | 2.28                     | 0.41              |
| 1:A:573:SER:OG    | 1:A:576:GLN:HB2   | 2.21                     | 0.41              |
| 1:A:68:GLN:HE22   | 1:A:80:HIS:CG     | 2.39                     | 0.41              |
| 1:A:722:LEU:HD22  | 1:A:799:PHE:CG    | 2.56                     | 0.41              |
| 1:A:976:THR:HG23  | 8:H:136:LYS:NZ    | 2.36                     | 0.41              |
| 2:B:1010:LEU:HA   | 2:B:1010:LEU:HD12 | 1.81                     | 0.41              |
| 2:B:1107:ALA:O    | 2:B:1108:ARG:O    | 2.39                     | 0.41              |
| 2:B:181:LEU:O     | 2:B:182:SER:C     | 2.59                     | 0.41              |
| 2:B:583:ASN:HD21  | 2:B:628:THR:HB    | 1.86                     | 0.41              |
| 2:B:603:LEU:HA    | 2:B:603:LEU:HD22  | 1.95                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:751:VAL:HG13  | 2:B:812:LEU:CD2   | 2.47                     | 0.41              |
| 2:B:812:LEU:O     | 2:B:813:LYS:C     | 2.59                     | 0.41              |
| 3:C:236:GLY:C     | 3:C:238:ILE:N     | 2.73                     | 0.41              |
| 4:D:176:GLU:HG2   | 4:D:197:SER:OG    | 2.21                     | 0.41              |
| 4:D:56:ARG:NH2    | 4:D:57:LEU:HD21   | 2.35                     | 0.41              |
| 5:E:153:HIS:O     | 5:E:154:ILE:HG13  | 2.20                     | 0.41              |
| 5:E:56:LYS:HE3    | 5:E:84:ASP:HB2    | 2.02                     | 0.41              |
| 5:E:58:MET:O      | 5:E:59:SER:O      | 2.38                     | 0.41              |
| 7:G:27:LYS:O      | 7:G:30:LEU:N      | 2.54                     | 0.41              |
| 8:H:83:GLN:C      | 8:H:85:GLY:N      | 2.74                     | 0.41              |
| 8:H:95:TYR:CE2    | 8:H:97:MET:HG3    | 2.56                     | 0.41              |
| 12:L:61:THR:CG2   | 12:L:63:ARG:HG2   | 2.50                     | 0.41              |
| 15:T:18:DT:O3'    | 15:T:19:TT:C4'    | 2.63                     | 0.41              |
| 1:A:1161:THR:HG22 | 1:A:1162:VAL:N    | 2.35                     | 0.41              |
| 1:A:1362:TYR:CD1  | 1:A:1362:TYR:C    | 2.92                     | 0.41              |
| 1:A:23:SER:HB3    | 1:A:233:TRP:CE2   | 2.56                     | 0.41              |
| 1:A:265:LYS:O     | 1:A:269:ILE:HG13  | 2.21                     | 0.41              |
| 1:A:337:ARG:CZ    | 1:A:839:ARG:NH1   | 2.84                     | 0.41              |
| 1:A:41:MET:O      | 1:A:50:ILE:HG13   | 2.21                     | 0.41              |
| 1:A:608:ILE:O     | 1:A:610:GLY:N     | 2.54                     | 0.41              |
| 2:B:189:LEU:O     | 2:B:192:LEU:HB2   | 2.21                     | 0.41              |
| 2:B:205:ILE:N     | 2:B:205:ILE:CD1   | 2.83                     | 0.41              |
| 2:B:24:PRO:O      | 2:B:655:LYS:HB2   | 2.21                     | 0.41              |
| 2:B:593:PRO:HG2   | 2:B:617:ARG:CZ    | 2.51                     | 0.41              |
| 2:B:597:MET:C     | 2:B:599:THR:H     | 2.22                     | 0.41              |
| 2:B:909:ASP:N     | 2:B:909:ASP:OD1   | 2.51                     | 0.41              |
| 1:A:106:VAL:HA    | 1:A:114:LEU:HD21  | 2.04                     | 0.41              |
| 1:A:1074:GLU:C    | 1:A:1076:ALA:H    | 2.25                     | 0.41              |
| 1:A:1332:PHE:HE1  | 1:A:1348:LEU:HD13 | 1.85                     | 0.41              |
| 1:A:188:ASP:OD1   | 1:A:189:ARG:N     | 2.53                     | 0.41              |
| 1:A:354:SER:HA    | 1:A:482:PHE:CD2   | 2.56                     | 0.41              |
| 1:A:532:ARG:O     | 1:A:535:THR:HB    | 2.21                     | 0.41              |
| 1:A:604:GLY:O     | 1:A:605:MET:HB2   | 2.21                     | 0.41              |
| 2:B:245:GLU:C     | 2:B:246:LYS:HG3   | 2.41                     | 0.41              |
| 2:B:743:ILE:H     | 2:B:743:ILE:HG12  | 1.64                     | 0.41              |
| 2:B:895:ASP:C     | 2:B:897:GLY:N     | 2.74                     | 0.41              |
| 2:B:953:LEU:HD22  | 2:B:965:LYS:HB2   | 1.98                     | 0.41              |
| 3:C:174:ALA:O     | 3:C:175:ALA:CB    | 2.67                     | 0.41              |
| 3:C:97:VAL:HG12   | 3:C:99:LEU:HD21   | 2.03                     | 0.41              |
| 5:E:191:LYS:O     | 5:E:192:ARG:C     | 2.58                     | 0.41              |
| 7:G:21:ARG:HD3    | 7:G:21:ARG:HA     | 1.81                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:34:VAL:HG11  | 7:G:74:TYR:CE1    | 2.56                     | 0.41              |
| 8:H:145:ARG:O    | 8:H:146:ARG:HB2   | 2.21                     | 0.41              |
| 2:B:309:GLN:CD   | 9:I:52:ILE:HD11   | 2.41                     | 0.41              |
| 9:I:77:LYS:O     | 9:I:79:HIS:N      | 2.54                     | 0.41              |
| 10:J:57:ILE:O    | 10:J:60:PHE:HB2   | 2.21                     | 0.41              |
| 11:K:42:LEU:O    | 11:K:42:LEU:HG    | 2.22                     | 0.41              |
| 11:K:65:HIS:CD2  | 11:K:67:PHE:HB2   | 2.56                     | 0.41              |
| 1:A:219:PHE:O    | 1:A:222:LEU:O     | 2.38                     | 0.40              |
| 1:A:26:GLU:O     | 1:A:27:VAL:C      | 2.59                     | 0.40              |
| 1:A:31:SER:HA    | 1:A:81:PHE:O      | 2.22                     | 0.40              |
| 1:A:391:LEU:O    | 1:A:394:ASN:HB2   | 2.21                     | 0.40              |
| 1:A:606:LEU:CB   | 1:A:614:PHE:CE2   | 3.03                     | 0.40              |
| 2:B:999:MET:HG2  | 2:B:1007:VAL:HG22 | 2.02                     | 0.40              |
| 2:B:95:ILE:CB    | 2:B:130:VAL:HG22  | 2.51                     | 0.40              |
| 2:B:29:ASP:O     | 2:B:30:SER:C      | 2.60                     | 0.40              |
| 2:B:313:MET:CE   | 2:B:386:LEU:HD22  | 2.51                     | 0.40              |
| 2:B:337:ARG:C    | 2:B:338:GLY:CA    | 2.90                     | 0.40              |
| 2:B:638:PHE:HB3  | 2:B:651:LEU:HD22  | 2.03                     | 0.40              |
| 2:B:710:LEU:O    | 2:B:711:GLU:OE2   | 2.38                     | 0.40              |
| 2:B:744:HIS:CD2  | 2:B:746:SER:HB3   | 2.56                     | 0.40              |
| 2:B:834:ASN:CA   | 2:B:838:SER:O     | 2.69                     | 0.40              |
| 3:C:172:PRO:O    | 3:C:235:VAL:HG23  | 2.20                     | 0.40              |
| 4:D:192:LYS:HB3  | 4:D:192:LYS:NZ    | 2.34                     | 0.40              |
| 4:D:195:ILE:N    | 4:D:196:PRO:CD    | 2.85                     | 0.40              |
| 8:H:39:THR:O     | 8:H:124:ARG:N     | 2.52                     | 0.40              |
| 8:H:82:PRO:C     | 8:H:84:ALA:N      | 2.73                     | 0.40              |
| 9:I:34:TYR:O     | 9:I:35:VAL:CG2    | 2.69                     | 0.40              |
| 10:J:13:VAL:C    | 10:J:14:VAL:HG23  | 2.40                     | 0.40              |
| 1:A:547:LEU:HD13 | 11:K:58:PHE:CD1   | 2.56                     | 0.40              |
| 1:A:1364:ASN:C   | 1:A:1364:ASN:HD22 | 2.24                     | 0.40              |
| 1:A:1405:THR:HB  | 1:A:1406:VAL:H    | 1.55                     | 0.40              |
| 1:A:1409:LEU:O   | 1:A:1412:ALA:HB3  | 2.21                     | 0.40              |
| 1:A:308:ILE:HG22 | 1:A:309:ALA:N     | 2.25                     | 0.40              |
| 1:A:376:TYR:HA   | 1:A:377:PRO:HD2   | 1.93                     | 0.40              |
| 1:A:525:GLN:HG3  | 2:B:836:GLU:HG2   | 2.02                     | 0.40              |
| 1:A:567:LYS:NZ   | 8:H:47:PHE:HB3    | 2.36                     | 0.40              |
| 1:A:824:LEU:HD23 | 1:A:824:LEU:HA    | 1.85                     | 0.40              |
| 1:A:879:GLU:OE1  | 1:A:962:ARG:NH2   | 2.53                     | 0.40              |
| 1:A:964:ILE:O    | 1:A:966:ASN:N     | 2.54                     | 0.40              |
| 2:B:175:ARG:NH1  | 2:B:175:ARG:CG    | 2.84                     | 0.40              |
| 2:B:298:LEU:N    | 2:B:298:LEU:HD22  | 2.36                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:448:ILE:O     | 2:B:450:ALA:N     | 2.55                     | 0.40              |
| 2:B:773:MET:HB3   | 2:B:1095:LEU:HD23 | 2.02                     | 0.40              |
| 3:C:181:ASP:N     | 3:C:182:PRO:CD    | 2.84                     | 0.40              |
| 4:D:192:LYS:HG2   | 4:D:207:LEU:CD2   | 2.51                     | 0.40              |
| 5:E:72:PHE:CE2    | 5:E:155:ARG:NH2   | 2.89                     | 0.40              |
| 8:H:59:ILE:CG2    | 8:H:60:ALA:N      | 2.65                     | 0.40              |
| 9:I:103:CYS:CB    | 9:I:106:CYS:SG    | 3.09                     | 0.40              |
| 11:K:46:ILE:O     | 11:K:50:LEU:HB2   | 2.21                     | 0.40              |
| 11:K:50:LEU:HD11  | 11:K:75:ILE:HD13  | 2.04                     | 0.40              |
| 12:L:46:VAL:O     | 12:L:46:VAL:HG12  | 2.22                     | 0.40              |
| 12:L:49:LYS:O     | 12:L:50:ASP:HB3   | 2.22                     | 0.40              |
| 1:A:1031:VAL:HG12 | 1:A:1031:VAL:O    | 2.22                     | 0.40              |
| 1:A:1053:PHE:O    | 1:A:1056:SER:N    | 2.51                     | 0.40              |
| 1:A:1450:LEU:CD1  | 6:F:108:PHE:CZ    | 3.04                     | 0.40              |
| 1:A:225:ASN:HD22  | 1:A:228:PHE:N     | 1.88                     | 0.40              |
| 1:A:230:ARG:N     | 1:A:233:TRP:HE3   | 2.11                     | 0.40              |
| 1:A:34:LYS:H      | 1:A:57:ARG:HH22   | 1.68                     | 0.40              |
| 1:A:356:ASP:HB2   | 1:A:469:ARG:HH12  | 1.81                     | 0.40              |
| 1:A:408:ASP:C     | 1:A:410:GLY:H     | 2.24                     | 0.40              |
| 1:A:481:ASP:OD1   | 1:A:483:ASP:CG    | 2.60                     | 0.40              |
| 1:A:482:PHE:C     | 1:A:484:GLY:N     | 2.71                     | 0.40              |
| 1:A:58:LEU:HG     | 1:A:59:GLY:H      | 1.82                     | 0.40              |
| 1:A:834:THR:HG22  | 1:A:835:GLY:N     | 2.35                     | 0.40              |
| 1:A:869:GLY:O     | 1:A:870:GLU:HB2   | 2.21                     | 0.40              |
| 1:A:925:LEU:C     | 1:A:927:VAL:N     | 2.73                     | 0.40              |
| 2:B:774:GLY:HA2   | 2:B:1093:GLN:HE22 | 1.85                     | 0.40              |
| 2:B:315:LYS:N     | 2:B:316:PRO:CD    | 2.83                     | 0.40              |
| 2:B:658:ILE:O     | 2:B:661:LEU:N     | 2.42                     | 0.40              |
| 2:B:824:ILE:CG2   | 2:B:1087:PHE:CE2  | 2.95                     | 0.40              |
| 3:C:16:ASP:O      | 3:C:17:ASN:CG     | 2.59                     | 0.40              |
| 7:G:109:PHE:O     | 7:G:160:ILE:HA    | 2.22                     | 0.40              |
| 7:G:17:PHE:N      | 7:G:17:PHE:HD2    | 2.17                     | 0.40              |
| 7:G:27:LYS:O      | 7:G:30:LEU:HB3    | 2.20                     | 0.40              |
| 9:I:8:ARG:O       | 9:I:10:CYS:N      | 2.54                     | 0.40              |
| 2:B:309:GLN:CG    | 9:I:52:ILE:HD11   | 2.51                     | 0.40              |
| 9:I:56:ALA:O      | 9:I:57:GLY:O      | 2.39                     | 0.40              |
| 1:A:1134:ILE:O    | 1:A:1135:ARG:C    | 2.59                     | 0.40              |
| 1:A:263:THR:HG22  | 1:A:263:THR:O     | 2.22                     | 0.40              |
| 1:A:332:LYS:O     | 1:A:334:GLY:N     | 2.55                     | 0.40              |
| 1:A:388:LEU:HD22  | 1:A:432:VAL:CB    | 2.51                     | 0.40              |
| 1:A:466:SER:HB3   | 2:B:1103:ILE:HG12 | 2.02                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:711:ARG:O    | 1:A:714:PHE:HB3   | 2.21                     | 0.40              |
| 1:A:823:GLY:O    | 1:A:825:ILE:N     | 2.55                     | 0.40              |
| 2:B:1030:LEU:HA  | 2:B:1030:LEU:HD12 | 1.96                     | 0.40              |
| 2:B:288:ALA:HA   | 2:B:331:LEU:CD1   | 2.49                     | 0.40              |
| 2:B:294:ASP:C    | 2:B:296:GLU:H     | 2.24                     | 0.40              |
| 2:B:460:ALA:HB1  | 2:B:466:TRP:CZ3   | 2.57                     | 0.40              |
| 2:B:498:THR:CG2  | 2:B:499:ASN:N     | 2.84                     | 0.40              |
| 2:B:22:SER:HA    | 2:B:654:ARG:HG3   | 2.03                     | 0.40              |
| 2:B:732:SER:HB2  | 2:B:734:HIS:CD2   | 2.57                     | 0.40              |
| 2:B:782:LEU:HB3  | 2:B:784:ASN:OD1   | 2.21                     | 0.40              |
| 3:C:10:ILE:HG22  | 3:C:11:ARG:O      | 2.21                     | 0.40              |
| 3:C:187:LYS:HG3  | 3:C:219:PHE:CE1   | 2.56                     | 0.40              |
| 3:C:58:LEU:N     | 3:C:58:LEU:CD2    | 2.84                     | 0.40              |
| 3:C:58:LEU:N     | 3:C:58:LEU:HD22   | 2.37                     | 0.40              |
| 1:A:852:TYR:CD1  | 6:F:136:ARG:HB3   | 2.56                     | 0.40              |
| 7:G:14:HIS:ND1   | 7:G:15:PRO:CD     | 2.78                     | 0.40              |
| 8:H:38:LEU:HD13  | 8:H:125:LEU:CD1   | 2.51                     | 0.40              |
| 1:A:1019:CYS:O   | 1:A:1022:LEU:N    | 2.54                     | 0.40              |
| 1:A:1036:ARG:NH1 | 1:A:1036:ARG:CG   | 2.80                     | 0.40              |
| 1:A:1168:GLU:O   | 1:A:1172:LEU:HG   | 2.21                     | 0.40              |
| 1:A:1260:LEU:CG  | 1:A:1260:LEU:O    | 2.70                     | 0.40              |
| 1:A:299:HIS:C    | 1:A:301:ALA:N     | 2.74                     | 0.40              |
| 1:A:414:ASP:OD1  | 1:A:414:ASP:C     | 2.60                     | 0.40              |
| 1:A:545:GLN:C    | 1:A:547:LEU:N     | 2.73                     | 0.40              |
| 1:A:56:PRO:O     | 1:A:57:ARG:CG     | 2.70                     | 0.40              |
| 1:A:34:LYS:N     | 1:A:57:ARG:NH2    | 2.65                     | 0.40              |
| 1:A:682:THR:HG22 | 1:A:682:THR:O     | 2.22                     | 0.40              |
| 1:A:685:GLU:HG3  | 1:A:686:ALA:N     | 2.36                     | 0.40              |
| 1:A:939:ASP:O    | 1:A:940:ARG:C     | 2.59                     | 0.40              |
| 1:A:351:THR:CG2  | 2:B:1103:ILE:HG13 | 2.51                     | 0.40              |
| 2:B:225:VAL:O    | 2:B:226:PHE:CD2   | 2.74                     | 0.40              |
| 2:B:223:VAL:HG11 | 2:B:381:MET:HG2   | 2.03                     | 0.40              |
| 2:B:765:PRO:O    | 2:B:766:ARG:C     | 2.59                     | 0.40              |
| 2:B:766:ARG:HD3  | 2:B:766:ARG:HA    | 1.73                     | 0.40              |
| 2:B:785:TYR:CD1  | 2:B:786:ASN:N     | 2.89                     | 0.40              |
| 3:C:137:LYS:HB3  | 3:C:138:GLU:OE1   | 2.21                     | 0.40              |
| 4:D:207:LEU:O    | 4:D:211:LEU:HG    | 2.22                     | 0.40              |
| 5:E:114:ASN:HD22 | 5:E:114:ASN:HA    | 1.68                     | 0.40              |
| 5:E:11:ARG:HH21  | 5:E:141:VAL:HG21  | 1.87                     | 0.40              |
| 5:E:35:VAL:C     | 5:E:37:LEU:N      | 2.75                     | 0.40              |
| 6:F:111:LEU:O    | 6:F:113:GLY:N     | 2.52                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 11:K:110:ASN:C  | 11:K:111:LEU:CG | 2.89                     | 0.40              |
| 11:K:62:LYS:O   | 11:K:71:PHE:HB2 | 2.21                     | 0.40              |
| 11:K:58:PHE:HB3 | 11:K:76:GLN:HB3 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-----------|-------------|----|
| 1   | A     | 1410/1733 (81%) | 962 (68%)  | 299 (21%) | 149 (11%) | 0           | 8  |
| 2   | B     | 1096/1224 (90%) | 767 (70%)  | 219 (20%) | 110 (10%) | 0           | 9  |
| 3   | C     | 264/318 (83%)   | 171 (65%)  | 62 (24%)  | 31 (12%)  | 0           | 6  |
| 4   | D     | 173/221 (78%)   | 125 (72%)  | 29 (17%)  | 19 (11%)  | 0           | 8  |
| 5   | E     | 212/215 (99%)   | 157 (74%)  | 44 (21%)  | 11 (5%)   | 2           | 23 |
| 6   | F     | 84/155 (54%)    | 67 (80%)   | 15 (18%)  | 2 (2%)    | 6           | 37 |
| 7   | G     | 169/171 (99%)   | 125 (74%)  | 34 (20%)  | 10 (6%)   | 1           | 21 |
| 8   | H     | 131/146 (90%)   | 84 (64%)   | 30 (23%)  | 17 (13%)  | 0           | 5  |
| 9   | I     | 114/122 (93%)   | 80 (70%)   | 21 (18%)  | 13 (11%)  | 0           | 7  |
| 10  | J     | 63/70 (90%)     | 35 (56%)   | 13 (21%)  | 15 (24%)  | 0           | 1  |
| 11  | K     | 112/120 (93%)   | 86 (77%)   | 16 (14%)  | 10 (9%)   | 1           | 12 |
| 12  | L     | 44/70 (63%)     | 17 (39%)   | 17 (39%)  | 10 (23%)  | 0           | 1  |
| All | All   | 3872/4565 (85%) | 2676 (69%) | 799 (21%) | 397 (10%) | 0           | 9  |

All (397) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 44  | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 48   | ALA  |
| 1   | A     | 57   | ARG  |
| 1   | A     | 62   | ASP  |
| 1   | A     | 65   | LEU  |
| 1   | A     | 74   | MET  |
| 1   | A     | 93   | VAL  |
| 1   | A     | 167  | CYS  |
| 1   | A     | 219  | PHE  |
| 1   | A     | 223  | GLY  |
| 1   | A     | 255  | SER  |
| 1   | A     | 286  | HIS  |
| 1   | A     | 311  | GLN  |
| 1   | A     | 312  | PRO  |
| 1   | A     | 318  | SER  |
| 1   | A     | 322  | VAL  |
| 1   | A     | 335  | ARG  |
| 1   | A     | 385  | ILE  |
| 1   | A     | 423  | ASP  |
| 1   | A     | 465  | TYR  |
| 1   | A     | 536  | LEU  |
| 1   | A     | 543  | LEU  |
| 1   | A     | 567  | LYS  |
| 1   | A     | 597  | LEU  |
| 1   | A     | 626  | ASN  |
| 1   | A     | 666  | ILE  |
| 1   | A     | 753  | GLY  |
| 1   | A     | 789  | LYS  |
| 1   | A     | 847  | ASP  |
| 1   | A     | 875  | ALA  |
| 1   | A     | 968  | GLN  |
| 1   | A     | 969  | GLN  |
| 1   | A     | 986  | ILE  |
| 1   | A     | 1002 | GLY  |
| 1   | A     | 1036 | ARG  |
| 1   | A     | 1096 | SER  |
| 1   | A     | 1114 | PRO  |
| 1   | A     | 1115 | SER  |
| 1   | A     | 1122 | PRO  |
| 1   | A     | 1212 | VAL  |
| 1   | A     | 1223 | ASP  |
| 1   | A     | 1281 | ARG  |
| 1   | A     | 1314 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1341 | ILE  |
| 1   | A     | 1365 | TYR  |
| 1   | A     | 1378 | GLN  |
| 1   | A     | 1405 | THR  |
| 1   | A     | 1438 | THR  |
| 2   | B     | 45   | SER  |
| 2   | B     | 46   | GLN  |
| 2   | B     | 108  | VAL  |
| 2   | B     | 115  | GLN  |
| 2   | B     | 186  | GLU  |
| 2   | B     | 258  | LEU  |
| 2   | B     | 345  | LYS  |
| 2   | B     | 367  | LEU  |
| 2   | B     | 467  | GLY  |
| 2   | B     | 474  | SER  |
| 2   | B     | 643  | ASP  |
| 2   | B     | 709  | ASP  |
| 2   | B     | 727  | LYS  |
| 2   | B     | 731  | VAL  |
| 2   | B     | 764  | SER  |
| 2   | B     | 831  | SER  |
| 2   | B     | 943  | SER  |
| 2   | B     | 958  | GLN  |
| 2   | B     | 1046 | PRO  |
| 2   | B     | 1069 | PHE  |
| 2   | B     | 1097 | HIS  |
| 2   | B     | 1108 | ARG  |
| 2   | B     | 1156 | ASP  |
| 2   | B     | 1157 | ALA  |
| 2   | B     | 1167 | GLY  |
| 2   | B     | 1175 | LEU  |
| 2   | B     | 1178 | ASN  |
| 2   | B     | 1181 | GLU  |
| 2   | B     | 1182 | CYS  |
| 2   | B     | 1188 | LYS  |
| 3   | C     | 4    | GLU  |
| 3   | C     | 6    | PRO  |
| 3   | C     | 78   | GLU  |
| 3   | C     | 87   | PHE  |
| 3   | C     | 141  | GLY  |
| 3   | C     | 149  | LYS  |
| 3   | C     | 156  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 161 | LYS  |
| 3   | C     | 184 | ASN  |
| 3   | C     | 209 | TYR  |
| 3   | C     | 214 | ASN  |
| 3   | C     | 215 | GLU  |
| 4   | D     | 5   | THR  |
| 4   | D     | 8   | PHE  |
| 4   | D     | 19  | GLU  |
| 4   | D     | 20  | GLU  |
| 4   | D     | 52  | LEU  |
| 4   | D     | 131 | GLU  |
| 4   | D     | 177 | VAL  |
| 4   | D     | 199 | ASN  |
| 5   | E     | 3   | GLN  |
| 5   | E     | 36  | GLU  |
| 5   | E     | 59  | SER  |
| 5   | E     | 73  | PRO  |
| 5   | E     | 74  | ASP  |
| 5   | E     | 106 | GLN  |
| 5   | E     | 130 | ALA  |
| 5   | E     | 206 | GLY  |
| 7   | G     | 63  | PRO  |
| 7   | G     | 139 | ILE  |
| 8   | H     | 17  | PRO  |
| 8   | H     | 62  | SER  |
| 8   | H     | 81  | PRO  |
| 8   | H     | 82  | PRO  |
| 8   | H     | 108 | SER  |
| 8   | H     | 128 | ASN  |
| 9   | I     | 3   | THR  |
| 9   | I     | 9   | ASP  |
| 9   | I     | 79  | HIS  |
| 10  | J     | 2   | ILE  |
| 10  | J     | 6   | ARG  |
| 10  | J     | 32  | GLU  |
| 10  | J     | 64  | ASN  |
| 11  | K     | 110 | ASN  |
| 12  | L     | 35  | SER  |
| 12  | L     | 50  | ASP  |
| 12  | L     | 59  | ALA  |
| 12  | L     | 60  | ARG  |
| 1   | A     | 42  | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 54   | ASN  |
| 1   | A     | 59   | GLY  |
| 1   | A     | 61   | ILE  |
| 1   | A     | 66   | LYS  |
| 1   | A     | 70   | CYS  |
| 1   | A     | 76   | GLU  |
| 1   | A     | 84   | ILE  |
| 1   | A     | 148  | CYS  |
| 1   | A     | 154  | SER  |
| 1   | A     | 250  | ILE  |
| 1   | A     | 253  | ASN  |
| 1   | A     | 283  | GLY  |
| 1   | A     | 386  | ASP  |
| 1   | A     | 394  | ASN  |
| 1   | A     | 399  | HIS  |
| 1   | A     | 439  | ASN  |
| 1   | A     | 517  | ASN  |
| 1   | A     | 619  | LYS  |
| 1   | A     | 661  | GLY  |
| 1   | A     | 731  | ARG  |
| 1   | A     | 780  | VAL  |
| 1   | A     | 979  | SER  |
| 1   | A     | 1054 | LEU  |
| 1   | A     | 1116 | LEU  |
| 1   | A     | 1120 | LEU  |
| 1   | A     | 1124 | HIS  |
| 1   | A     | 1127 | ASP  |
| 1   | A     | 1233 | ASP  |
| 1   | A     | 1280 | GLU  |
| 1   | A     | 1377 | THR  |
| 1   | A     | 1386 | ARG  |
| 1   | A     | 1395 | GLY  |
| 1   | A     | 1402 | PHE  |
| 2   | B     | 28   | GLU  |
| 2   | B     | 48   | LEU  |
| 2   | B     | 65   | GLU  |
| 2   | B     | 260  | GLY  |
| 2   | B     | 264  | SER  |
| 2   | B     | 266  | ALA  |
| 2   | B     | 282  | ILE  |
| 2   | B     | 387  | LEU  |
| 2   | B     | 401  | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 450  | ALA  |
| 2   | B     | 466  | TRP  |
| 2   | B     | 605  | ARG  |
| 2   | B     | 613  | VAL  |
| 2   | B     | 619  | ILE  |
| 2   | B     | 641  | GLU  |
| 2   | B     | 655  | LYS  |
| 2   | B     | 708  | GLU  |
| 2   | B     | 746  | SER  |
| 2   | B     | 751  | VAL  |
| 2   | B     | 792  | MET  |
| 2   | B     | 869  | SER  |
| 2   | B     | 881  | ASN  |
| 2   | B     | 891  | ASP  |
| 2   | B     | 907  | GLY  |
| 2   | B     | 945  | GLU  |
| 2   | B     | 1065 | GLN  |
| 2   | B     | 1100 | ASP  |
| 2   | B     | 1155 | SER  |
| 2   | B     | 1171 | VAL  |
| 2   | B     | 1183 | LYS  |
| 2   | B     | 1186 | ASP  |
| 3   | C     | 81   | GLU  |
| 3   | C     | 110  | THR  |
| 3   | C     | 175  | ALA  |
| 3   | C     | 213  | PRO  |
| 3   | C     | 216  | GLY  |
| 3   | C     | 240  | VAL  |
| 4   | D     | 12   | ARG  |
| 4   | D     | 21   | GLU  |
| 4   | D     | 65   | GLU  |
| 4   | D     | 192  | LYS  |
| 5   | E     | 45   | LYS  |
| 7   | G     | 19   | GLY  |
| 8   | H     | 21   | ASN  |
| 8   | H     | 32   | THR  |
| 8   | H     | 59   | ILE  |
| 8   | H     | 77   | ARG  |
| 8   | H     | 84   | ALA  |
| 8   | H     | 140  | ALA  |
| 9   | I     | 11   | ASN  |
| 9   | I     | 34   | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | I     | 57   | GLY  |
| 9   | I     | 78   | CYS  |
| 9   | I     | 106  | CYS  |
| 10  | J     | 14   | VAL  |
| 10  | J     | 17   | LYS  |
| 10  | J     | 27   | GLU  |
| 10  | J     | 28   | ASP  |
| 10  | J     | 29   | GLU  |
| 11  | K     | 7    | PHE  |
| 11  | K     | 15   | GLY  |
| 12  | L     | 26   | THR  |
| 12  | L     | 53   | HIS  |
| 12  | L     | 55   | ILE  |
| 1   | A     | 263  | THR  |
| 1   | A     | 336  | ILE  |
| 1   | A     | 409  | SER  |
| 1   | A     | 418  | SER  |
| 1   | A     | 424  | ILE  |
| 1   | A     | 525  | GLN  |
| 1   | A     | 526  | ASP  |
| 1   | A     | 544  | ASP  |
| 1   | A     | 592  | ASP  |
| 1   | A     | 648  | ASN  |
| 1   | A     | 649  | ILE  |
| 1   | A     | 673  | GLY  |
| 1   | A     | 759  | ALA  |
| 1   | A     | 846  | GLU  |
| 1   | A     | 871  | ASP  |
| 1   | A     | 1014 | ALA  |
| 1   | A     | 1165 | GLU  |
| 1   | A     | 1221 | LYS  |
| 1   | A     | 1335 | ILE  |
| 1   | A     | 1392 | SER  |
| 2   | B     | 94   | LYS  |
| 2   | B     | 114  | PRO  |
| 2   | B     | 124  | TYR  |
| 2   | B     | 259  | TYR  |
| 2   | B     | 591  | ARG  |
| 2   | B     | 629  | ASP  |
| 2   | B     | 711  | GLU  |
| 2   | B     | 754  | SER  |
| 2   | B     | 772  | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 818  | PRO  |
| 2   | B     | 951  | GLN  |
| 2   | B     | 1041 | GLU  |
| 3   | C     | 51   | VAL  |
| 3   | C     | 56   | THR  |
| 3   | C     | 60   | ASP  |
| 3   | C     | 148  | ARG  |
| 3   | C     | 264  | GLN  |
| 4   | D     | 6    | SER  |
| 4   | D     | 9    | GLN  |
| 4   | D     | 30   | GLY  |
| 4   | D     | 53   | SER  |
| 5   | E     | 115  | ASN  |
| 5   | E     | 192  | ARG  |
| 6   | F     | 81   | THR  |
| 7   | G     | 140  | LYS  |
| 8   | H     | 92   | ASP  |
| 9   | I     | 47   | GLU  |
| 9   | I     | 62   | ILE  |
| 10  | J     | 24   | LEU  |
| 10  | J     | 33   | GLY  |
| 10  | J     | 55   | ASP  |
| 11  | K     | 29   | ASN  |
| 11  | K     | 53   | ASP  |
| 11  | K     | 88   | LYS  |
| 11  | K     | 104  | ASN  |
| 1   | A     | 113  | LEU  |
| 1   | A     | 169  | ASN  |
| 1   | A     | 245  | PRO  |
| 1   | A     | 317  | LYS  |
| 1   | A     | 332  | LYS  |
| 1   | A     | 483  | ASP  |
| 1   | A     | 516  | SER  |
| 1   | A     | 591  | PHE  |
| 1   | A     | 605  | MET  |
| 1   | A     | 636  | GLU  |
| 1   | A     | 975  | HIS  |
| 1   | A     | 1277 | GLU  |
| 1   | A     | 1366 | ARG  |
| 1   | A     | 1454 | MET  |
| 2   | B     | 56   | ASP  |
| 2   | B     | 58   | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 229  | ALA  |
| 2   | B     | 257  | LYS  |
| 2   | B     | 283  | VAL  |
| 2   | B     | 322  | PHE  |
| 2   | B     | 389  | ALA  |
| 2   | B     | 894  | ASP  |
| 2   | B     | 1003 | ALA  |
| 2   | B     | 1017 | ILE  |
| 2   | B     | 1035 | ALA  |
| 3   | C     | 117  | ASP  |
| 3   | C     | 167  | HIS  |
| 6   | F     | 154  | ASP  |
| 7   | G     | 17   | PHE  |
| 7   | G     | 20   | PRO  |
| 7   | G     | 62   | LEU  |
| 7   | G     | 154  | VAL  |
| 8   | H     | 52   | GLN  |
| 8   | H     | 90   | ALA  |
| 9   | I     | 107  | SER  |
| 9   | I     | 113  | ASP  |
| 10  | J     | 8    | PHE  |
| 10  | J     | 63   | TYR  |
| 11  | K     | 90   | ALA  |
| 1   | A     | 69   | THR  |
| 1   | A     | 86   | LEU  |
| 1   | A     | 226  | GLU  |
| 1   | A     | 244  | PRO  |
| 1   | A     | 290  | GLU  |
| 1   | A     | 400  | PRO  |
| 1   | A     | 604  | GLY  |
| 1   | A     | 720  | ARG  |
| 1   | A     | 824  | LEU  |
| 1   | A     | 895  | LYS  |
| 1   | A     | 926  | GLN  |
| 1   | A     | 958  | VAL  |
| 1   | A     | 1389 | PHE  |
| 2   | B     | 61   | ASP  |
| 2   | B     | 231  | PRO  |
| 2   | B     | 245  | GLU  |
| 2   | B     | 248  | SER  |
| 2   | B     | 365  | THR  |
| 2   | B     | 369  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 571  | PRO  |
| 2   | B     | 728  | ARG  |
| 2   | B     | 770  | GLN  |
| 2   | B     | 848  | ARG  |
| 2   | B     | 880  | THR  |
| 2   | B     | 1103 | ILE  |
| 3   | C     | 142  | VAL  |
| 3   | C     | 208  | GLU  |
| 4   | D     | 119  | ARG  |
| 4   | D     | 218  | GLU  |
| 7   | G     | 115  | MET  |
| 8   | H     | 43   | ASN  |
| 8   | H     | 44   | VAL  |
| 9   | I     | 59   | VAL  |
| 10  | J     | 18   | TRP  |
| 11  | K     | 112  | GLN  |
| 12  | L     | 39   | SER  |
| 12  | L     | 57   | LEU  |
| 1   | A     | 43   | GLU  |
| 1   | A     | 71   | GLN  |
| 1   | A     | 96   | ILE  |
| 1   | A     | 111  | GLY  |
| 1   | A     | 135  | PHE  |
| 1   | A     | 825  | ILE  |
| 2   | B     | 100  | PRO  |
| 2   | B     | 341  | LEU  |
| 2   | B     | 530  | GLY  |
| 2   | B     | 752  | ALA  |
| 2   | B     | 824  | ILE  |
| 3   | C     | 126  | GLY  |
| 4   | D     | 196  | PRO  |
| 11  | K     | 41   | THR  |
| 12  | L     | 54   | ARG  |
| 1   | A     | 196  | GLU  |
| 2   | B     | 1018 | PRO  |
| 2   | B     | 1214 | PRO  |
| 1   | A     | 55   | ASP  |
| 1   | A     | 1158 | PRO  |
| 1   | A     | 1164 | PRO  |
| 2   | B     | 364  | ILE  |
| 2   | B     | 611  | PRO  |
| 2   | B     | 729  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 901 | PRO  |
| 7   | G     | 34  | VAL  |
| 1   | A     | 357 | PRO  |
| 1   | A     | 364 | VAL  |
| 1   | A     | 410 | GLY  |
| 1   | A     | 492 | PRO  |
| 1   | A     | 718 | VAL  |
| 3   | C     | 212 | PRO  |
| 3   | C     | 255 | VAL  |
| 1   | A     | 35  | ILE  |
| 1   | A     | 99  | ILE  |
| 1   | A     | 842 | VAL  |
| 2   | B     | 758 | PHE  |
| 2   | B     | 867 | GLY  |
| 3   | C     | 139 | GLY  |
| 1   | A     | 652 | VAL  |
| 1   | A     | 653 | VAL  |
| 2   | B     | 636 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 1244/1520 (82%) | 1138 (92%) | 106 (8%) | 10          | 40 |
| 2   | B     | 967/1061 (91%)  | 890 (92%)  | 77 (8%)  | 12          | 42 |
| 3   | C     | 235/274 (86%)   | 215 (92%)  | 20 (8%)  | 10          | 40 |
| 4   | D     | 159/200 (80%)   | 136 (86%)  | 23 (14%) | 3           | 19 |
| 5   | E     | 196/197 (100%)  | 191 (97%)  | 5 (3%)   | 46          | 69 |
| 6   | F     | 77/137 (56%)    | 68 (88%)   | 9 (12%)  | 5           | 27 |
| 7   | G     | 152/152 (100%)  | 140 (92%)  | 12 (8%)  | 12          | 42 |
| 8   | H     | 119/128 (93%)   | 112 (94%)  | 7 (6%)   | 19          | 51 |
| 9   | I     | 110/116 (95%)   | 97 (88%)   | 13 (12%) | 5           | 26 |
| 10  | J     | 60/65 (92%)     | 53 (88%)   | 7 (12%)  | 5           | 27 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 11  | K     | 99/102 (97%)    | 86 (87%)   | 13 (13%) | 4           | 23 |
| 12  | L     | 40/57 (70%)     | 36 (90%)   | 4 (10%)  | 7           | 32 |
| All | All   | 3458/4009 (86%) | 3162 (91%) | 296 (9%) | 10          | 40 |

All (296) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | VAL  |
| 1   | A     | 5   | GLN  |
| 1   | A     | 11  | LEU  |
| 1   | A     | 34  | LYS  |
| 1   | A     | 37  | PHE  |
| 1   | A     | 38  | PRO  |
| 1   | A     | 62  | ASP  |
| 1   | A     | 67  | CYS  |
| 1   | A     | 83  | HIS  |
| 1   | A     | 93  | VAL  |
| 1   | A     | 108 | MET  |
| 1   | A     | 122 | MET  |
| 1   | A     | 130 | ASP  |
| 1   | A     | 142 | CYS  |
| 1   | A     | 198 | GLU  |
| 1   | A     | 200 | ARG  |
| 1   | A     | 215 | SER  |
| 1   | A     | 245 | PRO  |
| 1   | A     | 270 | LEU  |
| 1   | A     | 302 | THR  |
| 1   | A     | 312 | PRO  |
| 1   | A     | 320 | ARG  |
| 1   | A     | 326 | ARG  |
| 1   | A     | 335 | ARG  |
| 1   | A     | 344 | ARG  |
| 1   | A     | 350 | ARG  |
| 1   | A     | 381 | THR  |
| 1   | A     | 385 | ILE  |
| 1   | A     | 404 | TYR  |
| 1   | A     | 406 | ILE  |
| 1   | A     | 407 | ARG  |
| 1   | A     | 408 | ASP  |
| 1   | A     | 412 | ARG  |
| 1   | A     | 418 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 425  | GLN  |
| 1   | A     | 443  | LEU  |
| 1   | A     | 445  | ASN  |
| 1   | A     | 450  | LEU  |
| 1   | A     | 451  | HIS  |
| 1   | A     | 462  | VAL  |
| 1   | A     | 466  | SER  |
| 1   | A     | 470  | LEU  |
| 1   | A     | 475  | THR  |
| 1   | A     | 481  | ASP  |
| 1   | A     | 493  | GLN  |
| 1   | A     | 515  | GLN  |
| 1   | A     | 527  | THR  |
| 1   | A     | 560  | ILE  |
| 1   | A     | 562  | THR  |
| 1   | A     | 577  | ILE  |
| 1   | A     | 618  | GLU  |
| 1   | A     | 626  | ASN  |
| 1   | A     | 629  | LEU  |
| 1   | A     | 666  | ILE  |
| 1   | A     | 670  | ILE  |
| 1   | A     | 711  | ARG  |
| 1   | A     | 768  | GLN  |
| 1   | A     | 774  | ARG  |
| 1   | A     | 779  | PHE  |
| 1   | A     | 821  | ARG  |
| 1   | A     | 831  | THR  |
| 1   | A     | 845  | LEU  |
| 1   | A     | 858  | ASN  |
| 1   | A     | 859  | SER  |
| 1   | A     | 886  | ILE  |
| 1   | A     | 890  | ASP  |
| 1   | A     | 903  | ASN  |
| 1   | A     | 906  | HIS  |
| 1   | A     | 907  | THR  |
| 1   | A     | 929  | LEU  |
| 1   | A     | 940  | ARG  |
| 1   | A     | 969  | GLN  |
| 1   | A     | 992  | ASP  |
| 1   | A     | 1029 | ARG  |
| 1   | A     | 1030 | ARG  |
| 1   | A     | 1035 | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1052 | GLN  |
| 1   | A     | 1067 | LEU  |
| 1   | A     | 1110 | ASN  |
| 1   | A     | 1116 | LEU  |
| 1   | A     | 1122 | PRO  |
| 1   | A     | 1127 | ASP  |
| 1   | A     | 1170 | ILE  |
| 1   | A     | 1187 | GLN  |
| 1   | A     | 1206 | ASP  |
| 1   | A     | 1264 | GLU  |
| 1   | A     | 1271 | ILE  |
| 1   | A     | 1291 | VAL  |
| 1   | A     | 1295 | THR  |
| 1   | A     | 1309 | ASP  |
| 1   | A     | 1332 | PHE  |
| 1   | A     | 1333 | ILE  |
| 1   | A     | 1359 | ASP  |
| 1   | A     | 1364 | ASN  |
| 1   | A     | 1366 | ARG  |
| 1   | A     | 1372 | VAL  |
| 1   | A     | 1376 | THR  |
| 1   | A     | 1385 | THR  |
| 1   | A     | 1386 | ARG  |
| 1   | A     | 1389 | PHE  |
| 1   | A     | 1405 | THR  |
| 1   | A     | 1432 | GLN  |
| 1   | A     | 1442 | ASP  |
| 1   | A     | 1443 | VAL  |
| 1   | A     | 1444 | MET  |
| 1   | A     | 1445 | ILE  |
| 2   | B     | 30   | SER  |
| 2   | B     | 35   | SER  |
| 2   | B     | 37   | PHE  |
| 2   | B     | 57   | TYR  |
| 2   | B     | 106  | ASP  |
| 2   | B     | 128  | LEU  |
| 2   | B     | 175  | ARG  |
| 2   | B     | 180  | TYR  |
| 2   | B     | 188  | ASP  |
| 2   | B     | 194  | GLU  |
| 2   | B     | 199  | MET  |
| 2   | B     | 217  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 218 | SER  |
| 2   | B     | 223 | VAL  |
| 2   | B     | 268 | THR  |
| 2   | B     | 298 | LEU  |
| 2   | B     | 365 | THR  |
| 2   | B     | 371 | GLU  |
| 2   | B     | 393 | LYS  |
| 2   | B     | 396 | ASP  |
| 2   | B     | 399 | ASP  |
| 2   | B     | 427 | ASP  |
| 2   | B     | 429 | PHE  |
| 2   | B     | 463 | THR  |
| 2   | B     | 465 | ASN  |
| 2   | B     | 466 | TRP  |
| 2   | B     | 485 | ARG  |
| 2   | B     | 496 | ARG  |
| 2   | B     | 498 | THR  |
| 2   | B     | 502 | ILE  |
| 2   | B     | 513 | GLN  |
| 2   | B     | 516 | ASN  |
| 2   | B     | 557 | PHE  |
| 2   | B     | 582 | VAL  |
| 2   | B     | 593 | PRO  |
| 2   | B     | 603 | LEU  |
| 2   | B     | 615 | MET  |
| 2   | B     | 635 | ARG  |
| 2   | B     | 644 | GLU  |
| 2   | B     | 682 | SER  |
| 2   | B     | 684 | LEU  |
| 2   | B     | 724 | ASP  |
| 2   | B     | 737 | THR  |
| 2   | B     | 742 | GLU  |
| 2   | B     | 790 | ASP  |
| 2   | B     | 811 | TYR  |
| 2   | B     | 830 | TYR  |
| 2   | B     | 835 | GLN  |
| 2   | B     | 837 | ASP  |
| 2   | B     | 839 | MET  |
| 2   | B     | 857 | ARG  |
| 2   | B     | 878 | GLN  |
| 2   | B     | 901 | PRO  |
| 2   | B     | 909 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 935  | ARG  |
| 2   | B     | 939  | THR  |
| 2   | B     | 953  | LEU  |
| 2   | B     | 999  | MET  |
| 2   | B     | 1002 | THR  |
| 2   | B     | 1006 | ILE  |
| 2   | B     | 1022 | THR  |
| 2   | B     | 1047 | PHE  |
| 2   | B     | 1069 | PHE  |
| 2   | B     | 1084 | GLN  |
| 2   | B     | 1087 | PHE  |
| 2   | B     | 1092 | TYR  |
| 2   | B     | 1095 | LEU  |
| 2   | B     | 1099 | VAL  |
| 2   | B     | 1106 | ARG  |
| 2   | B     | 1108 | ARG  |
| 2   | B     | 1159 | ARG  |
| 2   | B     | 1160 | VAL  |
| 2   | B     | 1170 | THR  |
| 2   | B     | 1176 | ASN  |
| 2   | B     | 1183 | LYS  |
| 2   | B     | 1202 | LEU  |
| 2   | B     | 1216 | LEU  |
| 3   | C     | 22   | LEU  |
| 3   | C     | 48   | SER  |
| 3   | C     | 56   | THR  |
| 3   | C     | 58   | LEU  |
| 3   | C     | 62   | PHE  |
| 3   | C     | 77   | ILE  |
| 3   | C     | 99   | LEU  |
| 3   | C     | 104  | PHE  |
| 3   | C     | 108  | GLU  |
| 3   | C     | 129  | ILE  |
| 3   | C     | 140  | ASN  |
| 3   | C     | 145  | CYS  |
| 3   | C     | 147  | LEU  |
| 3   | C     | 151  | GLN  |
| 3   | C     | 163  | ILE  |
| 3   | C     | 193  | TYR  |
| 3   | C     | 214  | ASN  |
| 3   | C     | 240  | VAL  |
| 3   | C     | 259  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 266 | ASP  |
| 4   | D     | 8   | PHE  |
| 4   | D     | 13  | ARG  |
| 4   | D     | 16  | LYS  |
| 4   | D     | 17  | LYS  |
| 4   | D     | 19  | GLU  |
| 4   | D     | 22  | GLU  |
| 4   | D     | 47  | LEU  |
| 4   | D     | 63  | LEU  |
| 4   | D     | 70  | PHE  |
| 4   | D     | 137 | ASN  |
| 4   | D     | 139 | LYS  |
| 4   | D     | 148 | LEU  |
| 4   | D     | 149 | THR  |
| 4   | D     | 156 | ASP  |
| 4   | D     | 159 | THR  |
| 4   | D     | 170 | THR  |
| 4   | D     | 174 | PRO  |
| 4   | D     | 182 | SER  |
| 4   | D     | 187 | THR  |
| 4   | D     | 192 | LYS  |
| 4   | D     | 193 | THR  |
| 4   | D     | 208 | GLU  |
| 4   | D     | 221 | TYR  |
| 5   | E     | 60  | PHE  |
| 5   | E     | 74  | ASP  |
| 5   | E     | 104 | ASN  |
| 5   | E     | 114 | ASN  |
| 5   | E     | 183 | PRO  |
| 6   | F     | 79  | ARG  |
| 6   | F     | 90  | ARG  |
| 6   | F     | 99  | LEU  |
| 6   | F     | 111 | LEU  |
| 6   | F     | 119 | ARG  |
| 6   | F     | 123 | LYS  |
| 6   | F     | 143 | PHE  |
| 6   | F     | 148 | VAL  |
| 6   | F     | 153 | VAL  |
| 7   | G     | 1   | MET  |
| 7   | G     | 13  | LEU  |
| 7   | G     | 17  | PHE  |
| 7   | G     | 74  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 78  | VAL  |
| 7   | G     | 80  | LYS  |
| 7   | G     | 88  | ASP  |
| 7   | G     | 96  | GLN  |
| 7   | G     | 115 | MET  |
| 7   | G     | 118 | ASP  |
| 7   | G     | 126 | ASN  |
| 7   | G     | 171 | ILE  |
| 8   | H     | 86  | ASP  |
| 8   | H     | 93  | TYR  |
| 8   | H     | 95  | TYR  |
| 8   | H     | 102 | TYR  |
| 8   | H     | 130 | ARG  |
| 8   | H     | 134 | ASN  |
| 8   | H     | 143 | LEU  |
| 9   | I     | 8   | ARG  |
| 9   | I     | 9   | ASP  |
| 9   | I     | 15  | TYR  |
| 9   | I     | 34  | TYR  |
| 9   | I     | 40  | SER  |
| 9   | I     | 75  | CYS  |
| 9   | I     | 78  | CYS  |
| 9   | I     | 85  | PHE  |
| 9   | I     | 86  | PHE  |
| 9   | I     | 94  | ASP  |
| 9   | I     | 99  | LEU  |
| 9   | I     | 101 | PHE  |
| 9   | I     | 106 | CYS  |
| 10  | J     | 7   | CYS  |
| 10  | J     | 9   | SER  |
| 10  | J     | 10  | CYS  |
| 10  | J     | 28  | ASP  |
| 10  | J     | 44  | TYR  |
| 10  | J     | 46  | CYS  |
| 10  | J     | 48  | ARG  |
| 11  | K     | 5   | ASP  |
| 11  | K     | 10  | PHE  |
| 11  | K     | 25  | THR  |
| 11  | K     | 42  | LEU  |
| 11  | K     | 47  | ARG  |
| 11  | K     | 50  | LEU  |
| 11  | K     | 61  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | K     | 68  | PHE  |
| 11  | K     | 78  | THR  |
| 11  | K     | 81  | TYR  |
| 11  | K     | 111 | LEU  |
| 11  | K     | 112 | GLN  |
| 11  | K     | 113 | THR  |
| 12  | L     | 51  | CYS  |
| 12  | L     | 55  | ILE  |
| 12  | L     | 65  | VAL  |
| 12  | L     | 70  | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 54   | ASN  |
| 1   | A     | 64   | ASN  |
| 1   | A     | 68   | GLN  |
| 1   | A     | 71   | GLN  |
| 1   | A     | 83   | HIS  |
| 1   | A     | 92   | HIS  |
| 1   | A     | 225  | ASN  |
| 1   | A     | 339  | ASN  |
| 1   | A     | 358  | ASN  |
| 1   | A     | 435  | HIS  |
| 1   | A     | 479  | ASN  |
| 1   | A     | 517  | ASN  |
| 1   | A     | 631  | HIS  |
| 1   | A     | 654  | ASN  |
| 1   | A     | 698  | GLN  |
| 1   | A     | 736  | ASN  |
| 1   | A     | 741  | ASN  |
| 1   | A     | 757  | ASN  |
| 1   | A     | 767  | GLN  |
| 1   | A     | 768  | GLN  |
| 1   | A     | 786  | HIS  |
| 1   | A     | 858  | ASN  |
| 1   | A     | 903  | ASN  |
| 1   | A     | 926  | GLN  |
| 1   | A     | 965  | GLN  |
| 1   | A     | 1140 | HIS  |
| 1   | A     | 1218 | GLN  |
| 1   | A     | 1364 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1432 | GLN  |
| 2   | B     | 121  | ASN  |
| 2   | B     | 178  | ASN  |
| 2   | B     | 215  | GLN  |
| 2   | B     | 236  | HIS  |
| 2   | B     | 363  | HIS  |
| 2   | B     | 366  | GLN  |
| 2   | B     | 449  | ASN  |
| 2   | B     | 465  | ASN  |
| 2   | B     | 513  | GLN  |
| 2   | B     | 515  | HIS  |
| 2   | B     | 516  | ASN  |
| 2   | B     | 518  | HIS  |
| 2   | B     | 538  | ASN  |
| 2   | B     | 734  | HIS  |
| 2   | B     | 744  | HIS  |
| 2   | B     | 776  | GLN  |
| 2   | B     | 794  | ASN  |
| 2   | B     | 821  | GLN  |
| 2   | B     | 842  | ASN  |
| 2   | B     | 975  | GLN  |
| 2   | B     | 1015 | HIS  |
| 2   | B     | 1025 | HIS  |
| 2   | B     | 1065 | GLN  |
| 2   | B     | 1076 | HIS  |
| 2   | B     | 1084 | GLN  |
| 2   | B     | 1117 | GLN  |
| 2   | B     | 1141 | HIS  |
| 2   | B     | 1179 | GLN  |
| 2   | B     | 1193 | GLN  |
| 3   | C     | 73   | GLN  |
| 3   | C     | 112  | ASN  |
| 3   | C     | 123  | ASN  |
| 3   | C     | 167  | HIS  |
| 3   | C     | 231  | ASN  |
| 3   | C     | 252  | GLN  |
| 4   | D     | 39   | ASN  |
| 4   | D     | 40   | HIS  |
| 4   | D     | 137  | ASN  |
| 5   | E     | 8    | ASN  |
| 5   | E     | 101  | GLN  |
| 5   | E     | 104  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 114 | ASN  |
| 5   | E     | 147 | HIS  |
| 7   | G     | 53  | ASN  |
| 7   | G     | 97  | HIS  |
| 7   | G     | 122 | ASN  |
| 7   | G     | 126 | ASN  |
| 9   | I     | 12  | ASN  |
| 9   | I     | 90  | GLN  |
| 10  | J     | 53  | HIS  |
| 10  | J     | 64  | ASN  |
| 11  | K     | 44  | ASN  |
| 11  | K     | 65  | HIS  |
| 11  | K     | 76  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed   | Backbone Outliers | Pucker Outliers |
|-----|-------|------------|-------------------|-----------------|
| 14  | P     | 9/11 (81%) | 3 (33%)           | 1 (11%)         |

All (3) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | P     | 7   | A    |
| 14  | P     | 8   | G    |
| 14  | P     | 9   | A    |

All (1) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | P     | 7   | A    |

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | BRU  | T     | 22  | 15,14 | 15,21,22     | 1.58 | 3 (20%)  | 17,30,33    | 4.18 | 4 (23%)  |
| 15  | TT   | T     | 19  | 15    | 40,43,44     | 4.90 | 12 (30%) | 59,69,72    | 2.36 | 17 (28%) |

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

| Mol | Type | Chain | Res | Link  | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|-------|---------|---------------|---------|
| 15  | BRU  | T     | 22  | 15,14 | -       | 0/4/21/22     | 0/2/2/2 |
| 15  | TT   | T     | 19  | 15    | -       | 11/18/105/106 | 0/5/6/6 |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 15  | T     | 19  | TT   | C5-C6   | -21.02 | 1.31        | 1.55     |
| 15  | T     | 19  | TT   | C5T-C6T | -20.02 | 1.32        | 1.55     |
| 15  | T     | 19  | TT   | C6-N1   | -5.36  | 1.38        | 1.46     |
| 15  | T     | 22  | BRU  | C4-C5   | 4.86   | 1.44        | 1.38     |
| 15  | T     | 19  | TT   | C1'-N1  | 4.04   | 1.50        | 1.45     |
| 15  | T     | 19  | TT   | C6T-N1T | -3.72  | 1.40        | 1.46     |
| 15  | T     | 22  | BRU  | C4-N3   | 2.76   | 1.37        | 1.33     |
| 15  | T     | 19  | TT   | O3'-C3' | 2.66   | 1.48        | 1.43     |
| 15  | T     | 19  | TT   | C2-N1   | 2.58   | 1.41        | 1.36     |
| 15  | T     | 19  | TT   | C6T-C6  | 2.54   | 1.64        | 1.56     |
| 15  | T     | 19  | TT   | C1R-N1T | 2.53   | 1.49        | 1.45     |
| 15  | T     | 19  | TT   | O4-C4   | 2.24   | 1.26        | 1.22     |
| 15  | T     | 22  | BRU  | C6-C5   | -2.09  | 1.34        | 1.39     |
| 15  | T     | 19  | TT   | C4-N3   | 2.07   | 1.40        | 1.37     |
| 15  | T     | 19  | TT   | O5'-C5' | 2.01   | 1.49        | 1.44     |

All (21) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | T     | 22  | BRU  | C4-N3-C2    | 14.88 | 127.70      | 115.14   |
| 15  | T     | 19  | TT   | C5-C6-N1    | 8.44  | 127.43      | 115.61   |
| 15  | T     | 22  | BRU  | C5-C4-N3    | -7.01 | 115.24      | 123.64   |
| 15  | T     | 19  | TT   | C5T-C6T-N1T | 6.14  | 124.22      | 115.61   |
| 15  | T     | 19  | TT   | C5T-C5-C6   | 6.02  | 95.86       | 88.38    |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | T     | 19  | TT   | C5-C6-C6T   | -5.71 | 79.91       | 89.28    |
| 15  | T     | 19  | TT   | C5-C5T-C6T  | -5.45 | 81.59       | 88.38    |
| 15  | T     | 19  | TT   | O4-C4-C5    | 3.62  | 125.77      | 122.88   |
| 15  | T     | 19  | TT   | C5'-C4'-C3' | 3.08  | 121.57      | 114.53   |
| 15  | T     | 19  | TT   | N3T-C2T-N1T | -2.94 | 113.64      | 116.69   |
| 15  | T     | 22  | BRU  | C5-C6-N1    | 2.89  | 123.71      | 119.97   |
| 15  | T     | 19  | TT   | O4R-C4R-C5R | 2.82  | 118.67      | 109.37   |
| 15  | T     | 19  | TT   | N3-C2-N1    | -2.55 | 114.04      | 116.69   |
| 15  | T     | 22  | BRU  | BR-C5-C6    | 2.47  | 122.94      | 117.31   |
| 15  | T     | 19  | TT   | C6-C6T-N1T  | 2.46  | 128.06      | 118.20   |
| 15  | T     | 19  | TT   | C2R-C1R-N1T | -2.31 | 112.47      | 115.59   |
| 15  | T     | 19  | TT   | C5A-C5-C6   | -2.30 | 107.08      | 114.16   |
| 15  | T     | 19  | TT   | C5T-C6T-C6  | 2.26  | 92.99       | 89.28    |
| 15  | T     | 19  | TT   | O4T-C4T-C5T | 2.14  | 124.58      | 122.88   |
| 15  | T     | 19  | TT   | C5-C4-N3    | -2.13 | 114.20      | 116.06   |
| 15  | T     | 19  | TT   | O3R-C3R-C4R | -2.06 | 102.21      | 110.10   |

There are no chirality outliers.

All (11) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | T     | 19  | TT   | C4'-C5'-O5'-P   |
| 15  | T     | 19  | TT   | O3'-C7-O5R-C5R  |
| 15  | T     | 19  | TT   | C2R-C1R-N1T-C6T |
| 15  | T     | 19  | TT   | C2'-C1'-N1-C6   |
| 15  | T     | 19  | TT   | C2'-C1'-N1-C2   |
| 15  | T     | 19  | TT   | O4'-C1'-N1-C2   |
| 15  | T     | 19  | TT   | O4'-C1'-N1-C6   |
| 15  | T     | 19  | TT   | O4R-C1R-N1T-C6T |
| 15  | T     | 19  | TT   | O5R-C7-O3'-C3'  |
| 15  | T     | 19  | TT   | C4R-C5R-O5R-C7  |
| 15  | T     | 19  | TT   | O4R-C1R-N1T-C2T |

There are no ring outliers.

2 monomers are involved in 31 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 15  | T     | 22  | BRU  | 5       | 0            |
| 15  | T     | 19  | TT   | 26      | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | B     | 2                |
| 1   | A     | 1                |
| 15  | T     | 1                |
| 3   | C     | 1                |
| 6   | F     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | T     | 19:TT     | O3'    | 21:DC     | P      | 6.48         |
| 1     | C     | 2:SER     | C      | 3:GLU     | N      | 4.15         |
| 1     | B     | 18:PHE    | C      | 19:GLU    | N      | 3.85         |
| 1     | F     | 69:LEU    | C      | 70:LYS    | N      | 3.50         |
| 1     | A     | 1175:SER  | C      | 1176:LEU  | N      | 3.39         |
| 1     | B     | 337:ARG   | C      | 338:GLY   | N      | 2.64         |

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 1421/1733 (81%) | -0.37  | 9 (0%) 89 85  | 17, 78, 152, 199      | 0     |
| 2   | B     | 1115/1224 (91%) | -0.28  | 12 (1%) 80 74 | 20, 91, 167, 200      | 0     |
| 3   | C     | 267/318 (83%)   | -0.41  | 0 100 100     | 39, 77, 139, 165      | 0     |
| 4   | D     | 177/221 (80%)   | -0.17  | 2 (1%) 80 74  | 61, 111, 160, 175     | 0     |
| 5   | E     | 214/215 (99%)   | -0.28  | 2 (0%) 84 79  | 50, 133, 184, 188     | 0     |
| 6   | F     | 87/155 (56%)    | -0.52  | 0 100 100     | 27, 56, 100, 138      | 0     |
| 7   | G     | 171/171 (100%)  | -0.28  | 0 100 100     | 57, 80, 126, 137      | 0     |
| 8   | H     | 135/146 (92%)   | 0.24   | 3 (2%) 62 54  | 95, 138, 173, 183     | 0     |
| 9   | I     | 116/122 (95%)   | -0.12  | 1 (0%) 84 79  | 75, 134, 166, 186     | 0     |
| 10  | J     | 65/70 (92%)     | -0.61  | 0 100 100     | 42, 73, 117, 125      | 0     |
| 11  | K     | 114/120 (95%)   | -0.33  | 2 (1%) 68 61  | 38, 83, 112, 167      | 0     |
| 12  | L     | 46/70 (65%)     | 0.16   | 2 (4%) 35 30  | 78, 156, 175, 181     | 0     |
| 13  | N     | 8/14 (57%)      | 0.51   | 0 100 100     | 129, 140, 153, 155    | 0     |
| 14  | P     | 10/11 (90%)     | 0.12   | 1 (10%) 7 6   | 115, 126, 152, 158    | 0     |
| 15  | T     | 17/25 (68%)     | 0.37   | 0 100 100     | 125, 138, 151, 153    | 0     |
| All | All   | 3963/4615 (85%) | -0.29  | 34 (0%) 84 79 | 17, 89, 165, 200      | 0     |

All (34) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 11  | K     | 114  | LEU  | 7.5  |
| 2   | B     | 471  | LYS  | 6.3  |
| 11  | K     | 113  | THR  | 5.0  |
| 2   | B     | 882  | THR  | 4.0  |
| 2   | B     | 883  | LEU  | 3.4  |
| 1   | A     | 1257 | ASP  | 3.2  |
| 2   | B     | 334  | ILE  | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 472  | ALA  | 3.0  |
| 5   | E     | 110  | PHE  | 2.8  |
| 8   | H     | 139  | ASN  | 2.6  |
| 2   | B     | 734  | HIS  | 2.6  |
| 1   | A     | 257  | ARG  | 2.5  |
| 2   | B     | 341  | LEU  | 2.5  |
| 2   | B     | 709  | ASP  | 2.5  |
| 1   | A     | 253  | ASN  | 2.4  |
| 2   | B     | 340  | ALA  | 2.4  |
| 1   | A     | 159  | THR  | 2.4  |
| 1   | A     | 1455 | PRO  | 2.3  |
| 5   | E     | 82   | PHE  | 2.3  |
| 1   | A     | 171  | GLN  | 2.3  |
| 12  | L     | 50   | ASP  | 2.2  |
| 9   | I     | 55   | THR  | 2.2  |
| 12  | L     | 43   | THR  | 2.2  |
| 14  | P     | 8    | G    | 2.2  |
| 1   | A     | 251  | SER  | 2.2  |
| 2   | B     | 113  | TYR  | 2.2  |
| 8   | H     | 112  | ILE  | 2.1  |
| 4   | D     | 9    | GLN  | 2.1  |
| 8   | H     | 140  | ALA  | 2.1  |
| 1   | A     | 158  | PRO  | 2.1  |
| 2   | B     | 133  | LYS  | 2.1  |
| 2   | B     | 884  | ARG  | 2.1  |
| 1   | A     | 145  | LYS  | 2.0  |
| 4   | D     | 8    | PHE  | 2.1  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 15  | BRU  | T     | 22  | 20/21 | 0.78 | 0.24 | 112,118,124,128             | 0     |
| 15  | TT   | T     | 19  | 38/39 | 0.84 | 0.27 | 130,144,163,166             | 0     |

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 17  | ZN   | A     | 2461 | 1/1   | 0.95 | 0.12 | 200,200,200,200             | 0     |
| 17  | ZN   | A     | 2464 | 1/1   | 0.98 | 0.07 | 87,87,87,87                 | 0     |
| 17  | ZN   | A     | 2459 | 1/1   | 0.98 | 0.03 | 125,125,125,125             | 0     |
| 17  | ZN   | A     | 2460 | 1/1   | 0.99 | 0.14 | 88,88,88,88                 | 0     |
| 17  | ZN   | A     | 2465 | 1/1   | 0.99 | 0.06 | 39,39,39,39                 | 0     |
| 17  | ZN   | A     | 2458 | 1/1   | 0.99 | 0.16 | 57,57,57,57                 | 0     |
| 17  | ZN   | A     | 2463 | 1/1   | 0.99 | 0.14 | 47,47,47,47                 | 0     |
| 17  | ZN   | A     | 2462 | 1/1   | 0.99 | 0.07 | 39,39,39,39                 | 0     |
| 16  | MG   | A     | 2457 | 1/1   | 0.99 | 0.16 | 35,35,35,35                 | 0     |

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

There are no such residues in this entry.