



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:28 AM GMT

PDB ID : 3ER8  
Title : Crystal structure of the heterodimeric vaccinia virus mRNA polyadenylate polymerase complex with two fragments of RNA  
Authors : Li, C.; Li, H; Zhou, S.; Poulos, T.L.; Gershon, P.D.  
Deposited on : 2008-10-01  
Resolution : 3.18 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

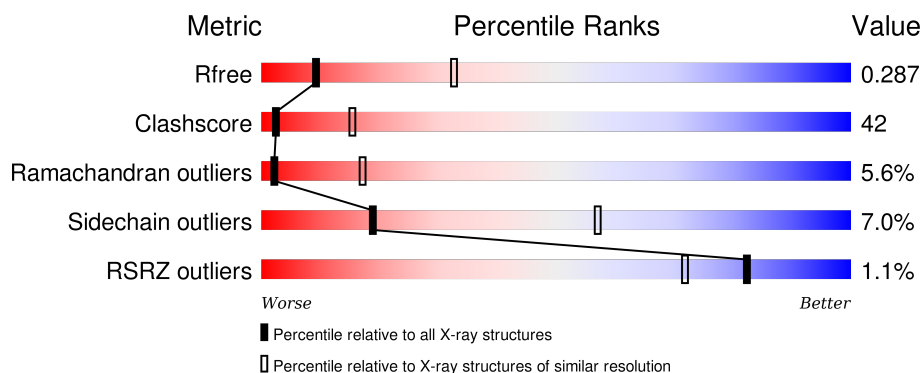
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.18 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.



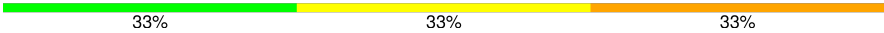
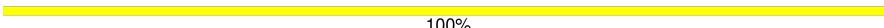
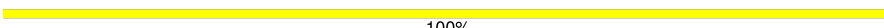
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1115 (3.22-3.14)                                      |
| Clashscore            | 102246                      | 1125 (3.20-3.16)                                      |
| Ramachandran outliers | 100387                      | 1105 (3.20-3.16)                                      |
| Sidechain outliers    | 100360                      | 1104 (3.20-3.16)                                      |
| RSRZ outliers         | 91569                       | 1120 (3.22-3.14)                                      |

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. 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     | 297    | <div> <div>48%</div> <div>43%</div> <div>5%</div> <div>.</div> </div>                |
| 1   | B     | 297    | <div> <div>48%</div> <div>45%</div> <div>.</div> <div>.</div> </div>                 |
| 2   | C     | 479    | <div> <div>2%</div> <div>29%</div> <div>55%</div> <div>8%</div> <div>7%</div> </div> |
| 2   | D     | 479    | <div> <div>30%</div> <div>54%</div> <div>8%</div> <div>7%</div> </div>               |
| 3   | E     | 5      | <div> <div>40%</div> <div>60%</div> </div>   |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 4   | F     | 3      | <br>33% 33% 33% |
| 5   | G     | 3      | <br>100%        |
| 5   | H     | 3      | <br>100%        |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12289 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 Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 288      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2382  | 1552 | 394 | 424 | 12 |         |         |       |
| 1   | B     | 288      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2382  | 1552 | 394 | 424 | 12 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment    | Reference  |
|-------|---------|----------|--------|------------|------------|
| A     | 140     | ALA      | ARG    | ENGINEERED | UNP P07617 |
| A     | 142     | ALA      | LYS    | ENGINEERED | UNP P07617 |
| A     | 143     | ALA      | ARG    | ENGINEERED | UNP P07617 |
| B     | 140     | ALA      | ARG    | ENGINEERED | UNP P07617 |
| B     | 142     | ALA      | LYS    | ENGINEERED | UNP P07617 |
| B     | 143     | ALA      | ARG    | ENGINEERED | UNP P07617 |

- Molecule 2 is a protein called Poly(A) polymerase catalytic subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | C     | 445      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3627  | 2318 | 605 | 680 | 24 |         |         |       |
| 2   | D     | 445      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3627  | 2318 | 605 | 680 | 24 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment    | Reference  |
|-------|---------|----------|--------|------------|------------|
| C     | 36      | SER      | LEU    | ENGINEERED | UNP P23371 |
| D     | 36      | SER      | LEU    | ENGINEERED | UNP P23371 |

- Molecule 3 is DNA/RNA hybrid called RNA/DNA chimera 5'-D(CP\*CP\*)R(UP\*UP\*)D(C)-3'.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 3   | E     | 5        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 94    | 45 | 13 | 32 | 4 |         |         |       |

- Molecule 4 is DNA/RNA hybrid called RNA/DNA chimera 5'-R(P\*UP\*UP\*)D(C)-3'.

| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|---------|-------|
| 4   | F     | 3        | Total | C  | N | O  | P | 0       | 0       | 0     |
|     |       |          | 59    | 27 | 7 | 22 | 3 |         |         |       |

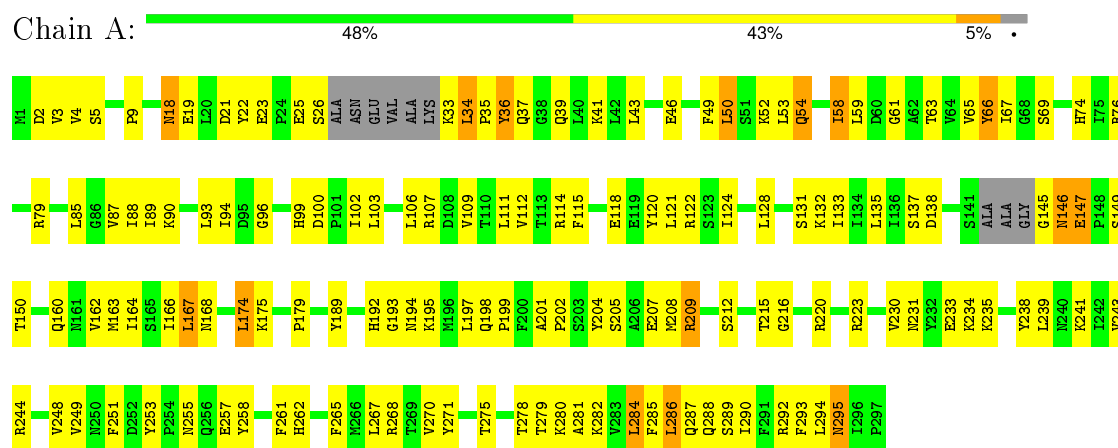
- Molecule 5 is DNA/RNA hybrid called RNA/DNA chimera 5'-D(P\*CP\*)R(UP\*U)-3'.

| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|---------|-------|
| 5   | G     | 3        | Total | C  | N | O  | P | 0       | 0       | 0     |
|     |       |          | 59    | 27 | 7 | 22 | 3 |         |         |       |
| 5   | H     | 3        | Total | C  | N | O  | P | 0       | 0       | 0     |
|     |       |          | 59    | 27 | 7 | 22 | 3 |         |         |       |

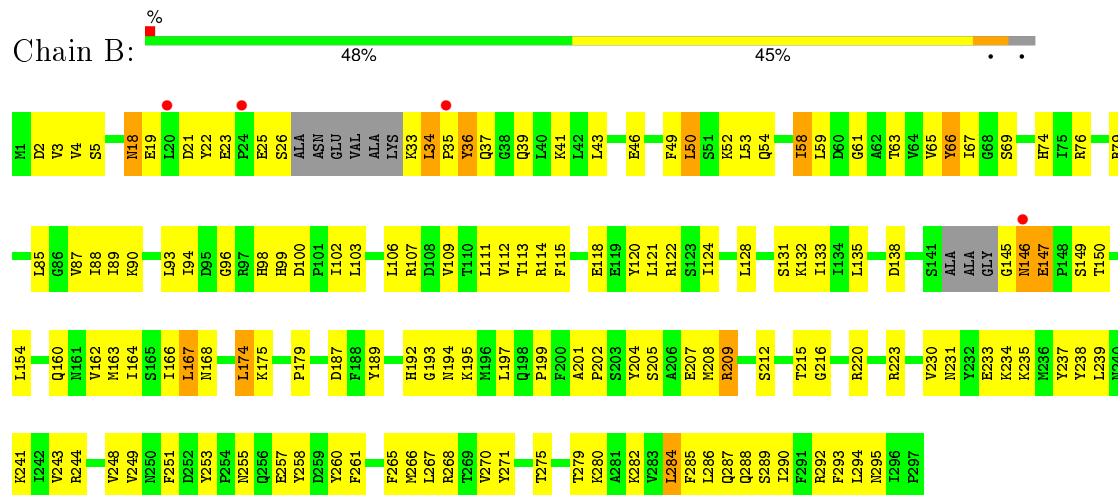
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

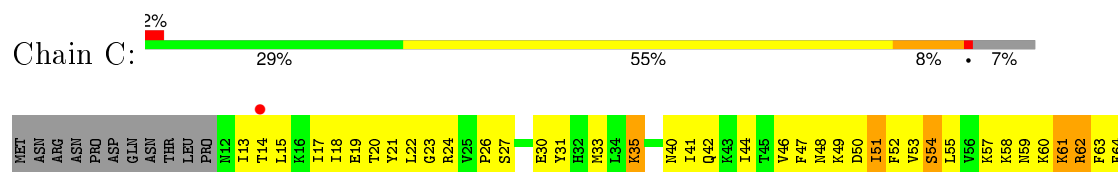
- Molecule 1: Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase

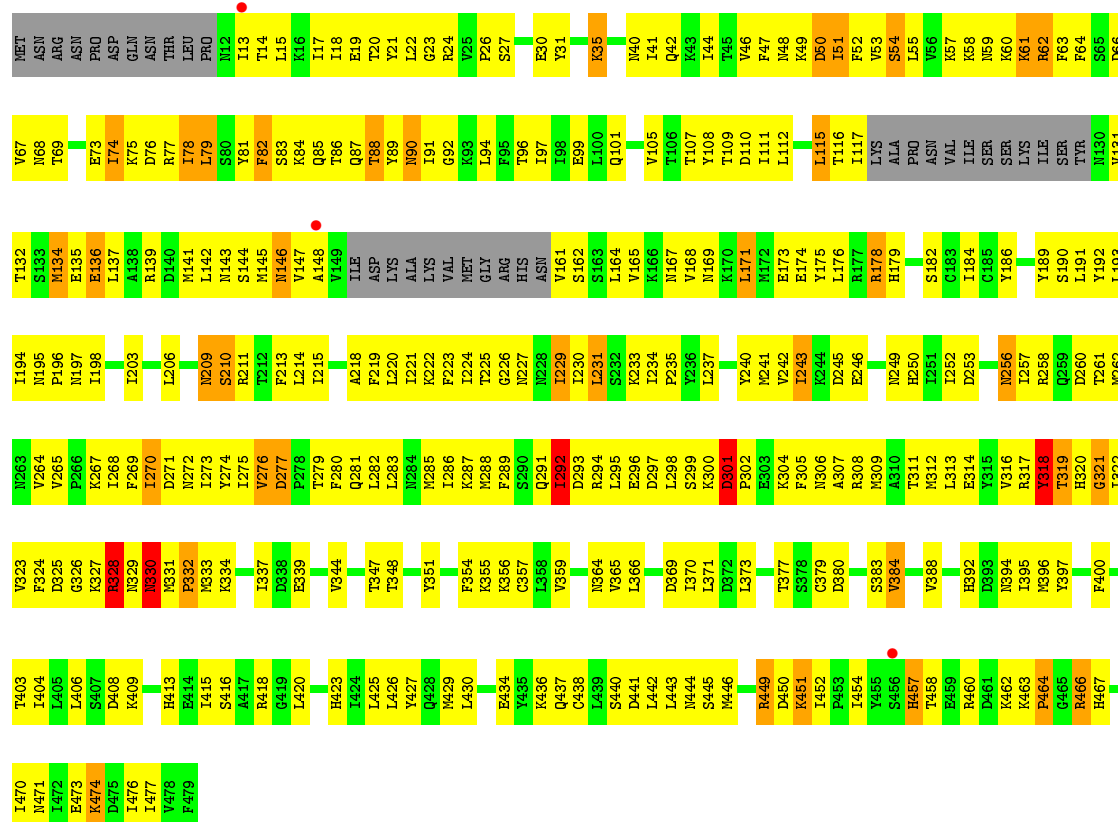
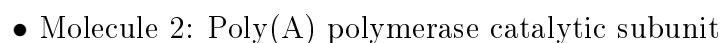


- Molecule 1: Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase



- Molecule 2: Poly(A) polymerase catalytic subunit





- Molecule 3: RNA/DNA chimera 5'-D(CP\*CP\*)R(UP\*UP\*)D(C)-3'

Chain E:  40% 60%

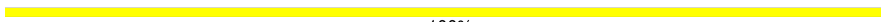
  
C600  
C601  
U602  
U603  
C604

- Molecule 4: RNA/DNA chimera 5'-R(P\*UP\*UP\*)D(C)-3'

Chain F:  33% 33% 33%

  
U702  
U703  
C704

- Molecule 5: RNA/DNA chimera 5'-D(P\*CP\*)R(UP\*U)-3'

Chain G:  100%

  
C800  
U801  
U802

- Molecule 5: RNA/DNA chimera 5'-D(P\*CP\*)R(UP\*U)-3'

Chain H:  100%

  
C900  
U901  
U902



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 70.61Å 77.24Å 106.85Å<br>74.88° 74.00° 63.69°               | Depositor        |
| Resolution (Å)  | 38.90 – 3.18<br>38.90 – 3.15                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.3 (38.90-3.18)<br>87.5 (38.90-3.15)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.08  | Depositor        |
| $R_{sym}$   | 0.08  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.18 (at 3.12Å)   | Xtriage          |
| Refinement program  | CNS 1.2   | Depositor        |
| R, $R_{free}$   | 0.243 , 0.285<br>0.244 , 0.287                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1492 reflections (4.95%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 69.3  | Xtriage          |
| Anisotropy  | 0.359   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 74.5   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Outliers  | 0 of 30648 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 12289   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 81.0  | wwPDB-VP         |

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

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

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

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$    |
| 1   | A     | 0.50         | 0/2444         | 0.69        | 0/3308         |
| 1   | B     | 0.49         | 0/2444         | 0.69        | 0/3308         |
| 2   | C     | 0.59         | 0/3686         | 0.69        | 0/4972         |
| 2   | D     | 0.57         | 0/3686         | 0.69        | 0/4972         |
| 3   | E     | 0.92         | 0/103          | 1.02        | 0/156          |
| 4   | F     | 1.09         | 1/64 (1.6%)    | 0.84        | 1/96 (1.0%)    |
| 5   | G     | 1.29         | 0/64           | 1.27        | 0/96           |
| 5   | H     | 1.34         | 0/64           | 1.32        | 1/96 (1.0%)    |
| All | All   | 0.57         | 1/12555 (0.0%) | 0.70        | 2/17004 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4   | F     | 702 | U    | P-O5' | 5.03 | 1.64        | 1.59     |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | H     | 902 | U    | C3'-C2'-C1' | 5.41  | 105.83      | 101.50   |
| 4   | F     | 702 | U    | OP1-P-OP2   | -5.21 | 111.78      | 119.60   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2382  | 0        | 2389     | 141     | 0            |
| 1   | B     | 2382  | 0        | 2389     | 139     | 0            |
| 2   | C     | 3627  | 0        | 3689     | 392     | 0            |
| 2   | D     | 3627  | 0        | 3689     | 376     | 0            |
| 3   | E     | 94    | 0        | 55       | 14      | 0            |
| 4   | F     | 59    | 0        | 32       | 8       | 0            |
| 5   | G     | 59    | 0        | 32       | 4       | 0            |
| 5   | H     | 59    | 0        | 32       | 3       | 0            |
| All | All   | 12289 | 0        | 12307    | 1038    | 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 42.

All (1038) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:603:U:H5'    | 3:E:603:U:H6     | 1.12                     | 1.12              |
| 1:B:106:LEU:HB2  | 1:B:109:VAL:HG22 | 1.31                     | 1.08              |
| 1:A:106:LEU:HB2  | 1:A:109:VAL:HG22 | 1.34                     | 1.05              |
| 2:D:256:ASN:HD22 | 2:D:257:ILE:N    | 1.59                     | 1.01              |
| 2:D:474:LYS:HA   | 2:D:474:LYS:HE3  | 1.42                     | 1.00              |
| 2:C:256:ASN:HD22 | 2:C:257:ILE:N    | 1.60                     | 0.99              |
| 2:C:291:GLN:HE21 | 2:C:293:ASP:H    | 1.07                     | 0.97              |
| 2:C:474:LYS:HA   | 2:C:474:LYS:HE3  | 1.43                     | 0.97              |
| 1:B:131:SER:HB3  | 2:C:466:ARG:HG2  | 1.47                     | 0.96              |
| 1:A:131:SER:HB3  | 2:D:466:ARG:HG2  | 1.47                     | 0.95              |
| 2:D:291:GLN:HE21 | 2:D:293:ASP:H    | 1.11                     | 0.94              |
| 2:D:148:ALA:HB2  | 2:D:295:LEU:HB3  | 1.49                     | 0.94              |
| 2:C:288:MET:HG2  | 2:C:294:ARG:HG3  | 1.48                     | 0.94              |
| 3:E:603:U:C6     | 3:E:603:U:H5'    | 2.03                     | 0.93              |
| 2:D:270:ILE:HG22 | 2:D:271:ASP:N    | 1.84                     | 0.93              |
| 2:C:148:ALA:HB2  | 2:C:295:LEU:HB3  | 1.51                     | 0.93              |
| 2:C:270:ILE:HG22 | 2:C:271:ASP:N    | 1.84                     | 0.92              |
| 2:D:288:MET:HG2  | 2:D:294:ARG:HG3  | 1.50                     | 0.91              |
| 2:C:443:LEU:HA   | 2:C:446:MET:HE2  | 1.52                     | 0.91              |
| 2:C:178:ARG:HA   | 2:C:178:ARG:HH11 | 1.35                     | 0.91              |
| 2:D:443:LEU:HA   | 2:D:446:MET:HE2  | 1.51                     | 0.91              |
| 2:C:316:VAL:HG22 | 2:C:322:ILE:HG13 | 1.51                     | 0.90              |
| 2:D:229:ILE:HD13 | 2:D:229:ILE:H    | 1.36                     | 0.90              |
| 2:D:178:ARG:HA   | 2:D:178:ARG:HH11 | 1.37                     | 0.89              |
| 2:D:283:LEU:HD23 | 2:D:426:LEU:HD23 | 1.55                     | 0.89              |
| 2:D:73:GLU:HB3   | 2:D:77:ARG:NH1   | 1.87                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:418:ARG:NE   | 2:C:446:MET:HG2  | 1.88                     | 0.88              |
| 2:C:73:GLU:HB3   | 2:C:77:ARG:NH1   | 1.86                     | 0.88              |
| 5:G:801:U:O2'    | 5:G:802:U:H5''   | 1.71                     | 0.88              |
| 2:C:229:ILE:H    | 2:C:229:ILE:HD13 | 1.39                     | 0.87              |
| 2:C:13:ILE:O     | 2:C:17:ILE:HG12  | 1.75                     | 0.87              |
| 1:B:106:LEU:HB2  | 1:B:109:VAL:CG2  | 2.05                     | 0.86              |
| 2:C:283:LEU:HD23 | 2:C:426:LEU:HD23 | 1.58                     | 0.86              |
| 2:C:270:ILE:HG22 | 2:C:271:ASP:H    | 1.38                     | 0.86              |
| 2:C:195:ASN:HD22 | 2:C:198:ILE:HG12 | 1.39                     | 0.85              |
| 2:D:21:TYR:CE2   | 2:D:85:GLN:HG2   | 2.10                     | 0.85              |
| 2:D:316:VAL:HG22 | 2:D:322:ILE:HG13 | 1.55                     | 0.85              |
| 2:D:270:ILE:HG22 | 2:D:271:ASP:H    | 1.39                     | 0.85              |
| 2:C:60:LYS:HE2   | 2:C:67:VAL:HB    | 1.56                     | 0.85              |
| 2:C:256:ASN:HD22 | 2:C:257:ILE:H    | 1.22                     | 0.84              |
| 2:C:21:TYR:CE2   | 2:C:85:GLN:HG2   | 2.11                     | 0.84              |
| 2:D:60:LYS:HE2   | 2:D:67:VAL:HB    | 1.56                     | 0.84              |
| 2:D:256:ASN:HD22 | 2:D:257:ILE:H    | 1.21                     | 0.84              |
| 2:C:53:VAL:HG11  | 2:C:75:LYS:HG2   | 1.60                     | 0.84              |
| 2:D:146:ASN:HD21 | 2:D:302:PRO:HB3  | 1.41                     | 0.84              |
| 1:A:106:LEU:HB2  | 1:A:109:VAL:CG2  | 2.08                     | 0.83              |
| 2:D:418:ARG:NE   | 2:D:446:MET:HG2  | 1.92                     | 0.83              |
| 1:A:168:ASN:HD22 | 1:B:223:ARG:CZ   | 1.91                     | 0.83              |
| 2:D:195:ASN:HD22 | 2:D:198:ILE:HG12 | 1.41                     | 0.83              |
| 2:D:53:VAL:HG11  | 2:D:75:LYS:HG2   | 1.61                     | 0.82              |
| 2:D:13:ILE:O     | 2:D:17:ILE:HG12  | 1.79                     | 0.82              |
| 2:C:146:ASN:HD21 | 2:C:302:PRO:HB3  | 1.45                     | 0.81              |
| 5:G:800:DC:H2''  | 5:G:801:U:OP2    | 1.81                     | 0.81              |
| 2:D:60:LYS:HA    | 2:D:64:PHE:HB2   | 1.63                     | 0.80              |
| 2:C:473:GLU:HG3  | 2:C:474:LYS:N    | 1.97                     | 0.80              |
| 2:D:84:LYS:HG3   | 2:D:97:ILE:HD13  | 1.63                     | 0.79              |
| 2:C:90:ASN:HD22  | 2:C:91:ILE:N     | 1.82                     | 0.78              |
| 2:C:60:LYS:HA    | 2:C:64:PHE:HB2   | 1.65                     | 0.78              |
| 2:C:84:LYS:HG3   | 2:C:97:ILE:HD13  | 1.63                     | 0.78              |
| 2:D:74:ILE:HG13  | 2:D:224:ILE:HA   | 1.66                     | 0.78              |
| 2:D:225:THR:HG21 | 2:D:227:ASN:HB2  | 1.65                     | 0.78              |
| 2:C:148:ALA:HA   | 2:C:454:ILE:CD1  | 2.14                     | 0.77              |
| 2:C:184:ILE:CG2  | 2:C:206:LEU:HB2  | 2.15                     | 0.77              |
| 2:C:344:VAL:HG11 | 2:C:420:LEU:HD11 | 1.66                     | 0.77              |
| 2:C:74:ILE:HG13  | 2:C:224:ILE:HA   | 1.67                     | 0.77              |
| 2:D:473:GLU:HG3  | 2:D:474:LYS:N    | 1.99                     | 0.77              |
| 2:D:30:GLU:HG2   | 2:D:91:ILE:HD11  | 1.66                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:53:LEU:HD22  | 1:B:58:ILE:HG12  | 1.66                     | 0.77              |
| 2:D:90:ASN:HD22  | 2:D:91:ILE:N     | 1.83                     | 0.77              |
| 2:D:473:GLU:HG3  | 2:D:474:LYS:H    | 1.51                     | 0.76              |
| 2:C:473:GLU:HG3  | 2:C:474:LYS:H    | 1.51                     | 0.76              |
| 2:C:344:VAL:HG11 | 2:C:420:LEU:CD1  | 2.15                     | 0.76              |
| 2:C:59:ASN:HD21  | 2:C:220:LEU:HD21 | 1.51                     | 0.76              |
| 2:D:148:ALA:HA   | 2:D:454:ILE:CD1  | 2.16                     | 0.76              |
| 2:D:184:ILE:CG2  | 2:D:206:LEU:HB2  | 2.16                     | 0.76              |
| 1:B:23:GLU:HB3   | 1:B:25:GLU:OE1   | 1.86                     | 0.75              |
| 2:C:323:VAL:HG22 | 2:C:325:ASP:OD1  | 1.86                     | 0.75              |
| 1:A:23:GLU:HB3   | 1:A:25:GLU:OE1   | 1.86                     | 0.75              |
| 2:C:30:GLU:HG2   | 2:C:91:ILE:HD11  | 1.68                     | 0.75              |
| 2:C:269:PHE:CZ   | 2:C:272:ASN:HA   | 2.22                     | 0.74              |
| 2:D:323:VAL:HG22 | 2:D:325:ASP:OD1  | 1.87                     | 0.74              |
| 1:A:53:LEU:HD22  | 1:A:58:ILE:HG12  | 1.68                     | 0.74              |
| 2:C:333:MET:HE2  | 2:C:348:THR:HA   | 1.68                     | 0.74              |
| 2:C:225:THR:HG21 | 2:C:227:ASN:HB2  | 1.69                     | 0.74              |
| 2:C:470:ILE:HG23 | 2:C:477:ILE:HG12 | 1.67                     | 0.74              |
| 2:C:288:MET:HE3  | 2:C:294:ARG:HD2  | 1.69                     | 0.74              |
| 2:C:73:GLU:HB3   | 2:C:77:ARG:HH12  | 1.50                     | 0.74              |
| 2:D:19:GLU:HG3   | 2:D:24:ARG:O     | 1.88                     | 0.74              |
| 2:D:73:GLU:HB3   | 2:D:77:ARG:HH12  | 1.50                     | 0.74              |
| 2:D:331:MET:HG2  | 2:D:442:LEU:HA   | 1.70                     | 0.74              |
| 2:D:344:VAL:HG11 | 2:D:420:LEU:HD11 | 1.69                     | 0.74              |
| 1:A:66:TYR:CD1   | 1:A:69:SER:HB3   | 2.23                     | 0.74              |
| 2:C:19:GLU:HG3   | 2:C:24:ARG:O     | 1.88                     | 0.74              |
| 1:A:121:LEU:HD13 | 1:A:163:MET:HA   | 1.70                     | 0.73              |
| 2:D:470:ILE:HG23 | 2:D:477:ILE:HG12 | 1.69                     | 0.73              |
| 2:D:59:ASN:HD21  | 2:D:220:LEU:HD21 | 1.53                     | 0.73              |
| 2:D:344:VAL:HG11 | 2:D:420:LEU:CD1  | 2.18                     | 0.73              |
| 2:C:195:ASN:ND2  | 2:C:198:ILE:HG12 | 2.03                     | 0.73              |
| 2:C:31:TYR:O     | 2:C:35:LYS:HB2   | 1.88                     | 0.72              |
| 1:B:66:TYR:CD1   | 1:B:69:SER:HB3   | 2.24                     | 0.72              |
| 1:B:121:LEU:HD13 | 1:B:163:MET:HA   | 1.71                     | 0.72              |
| 2:D:261:THR:O    | 2:D:265:VAL:HG23 | 1.88                     | 0.72              |
| 2:C:300:LYS:O    | 2:C:301:ASP:HB2  | 1.88                     | 0.72              |
| 2:C:229:ILE:O    | 2:C:230:ILE:HD13 | 1.90                     | 0.72              |
| 2:C:162:SER:HB3  | 2:C:245:ASP:OD1  | 1.89                     | 0.72              |
| 2:D:162:SER:HB3  | 2:D:245:ASP:OD1  | 1.89                     | 0.72              |
| 2:D:195:ASN:ND2  | 2:D:198:ILE:HG12 | 2.05                     | 0.71              |
| 2:C:331:MET:HB3  | 2:C:332:PRO:HD3  | 1.71                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:331:MET:HB3  | 2:D:332:PRO:HD3  | 1.72                     | 0.71              |
| 2:D:90:ASN:ND2   | 2:D:92:GLY:H     | 1.89                     | 0.71              |
| 2:D:69:THR:OG1   | 2:D:74:ILE:HD11  | 1.90                     | 0.71              |
| 2:C:69:THR:OG1   | 2:C:74:ILE:HD11  | 1.90                     | 0.71              |
| 2:C:261:THR:O    | 2:C:265:VAL:HG23 | 1.89                     | 0.71              |
| 2:D:328:ARG:HA   | 2:D:328:ARG:NE   | 2.05                     | 0.71              |
| 1:B:267:LEU:HB3  | 1:B:286:LEU:HD12 | 1.71                     | 0.71              |
| 2:C:331:MET:HG2  | 2:C:442:LEU:HA   | 1.74                     | 0.70              |
| 2:D:229:ILE:H    | 2:D:229:ILE:CD1  | 2.02                     | 0.70              |
| 2:D:229:ILE:HD13 | 2:D:229:ILE:N    | 2.06                     | 0.70              |
| 2:D:31:TYR:O     | 2:D:35:LYS:HB2   | 1.90                     | 0.70              |
| 2:C:58:LYS:NZ    | 2:C:116:THR:HB   | 2.07                     | 0.70              |
| 1:A:174:LEU:H    | 1:A:174:LEU:HD12 | 1.57                     | 0.70              |
| 2:D:288:MET:HE3  | 2:D:294:ARG:HD2  | 1.73                     | 0.70              |
| 1:A:33:LYS:HG2   | 1:A:34:LEU:H     | 1.55                     | 0.70              |
| 2:D:58:LYS:NZ    | 2:D:116:THR:HB   | 2.06                     | 0.70              |
| 2:C:291:GLN:HE21 | 2:C:293:ASP:N    | 1.88                     | 0.70              |
| 2:C:90:ASN:ND2   | 2:C:92:GLY:H     | 1.90                     | 0.70              |
| 2:C:301:ASP:H    | 2:C:302:PRO:HD3  | 1.57                     | 0.70              |
| 1:A:267:LEU:HB3  | 1:A:286:LEU:HD12 | 1.71                     | 0.70              |
| 2:C:328:ARG:HA   | 2:C:328:ARG:NE   | 2.07                     | 0.70              |
| 1:B:150:THR:HG23 | 1:B:179:PRO:HB3  | 1.74                     | 0.70              |
| 2:C:148:ALA:HB3  | 2:C:299:SER:OG   | 1.91                     | 0.69              |
| 2:C:17:ILE:HD12  | 2:C:42:GLN:HB2   | 1.74                     | 0.69              |
| 2:D:240:TYR:HE1  | 2:D:253:ASP:HB2  | 1.56                     | 0.69              |
| 2:D:269:PHE:CZ   | 2:D:272:ASN:HA   | 2.28                     | 0.69              |
| 1:A:100:ASP:OD1  | 1:A:102:ILE:HG12 | 1.91                     | 0.69              |
| 2:D:229:ILE:O    | 2:D:230:ILE:HD13 | 1.93                     | 0.69              |
| 1:B:53:LEU:HB3   | 1:B:58:ILE:HG13  | 1.74                     | 0.69              |
| 2:D:301:ASP:H    | 2:D:302:PRO:HD3  | 1.58                     | 0.69              |
| 1:B:50:LEU:HD12  | 1:B:53:LEU:HD12  | 1.75                     | 0.69              |
| 2:D:111:ILE:HG23 | 2:D:175:TYR:OH   | 1.93                     | 0.69              |
| 2:C:111:ILE:HG23 | 2:C:175:TYR:OH   | 1.93                     | 0.68              |
| 1:A:150:THR:HG23 | 1:A:179:PRO:HB3  | 1.75                     | 0.68              |
| 2:C:92:GLY:HA3   | 5:H:901:U:H5"    | 1.75                     | 0.68              |
| 1:A:53:LEU:HB3   | 1:A:58:ILE:HG13  | 1.75                     | 0.68              |
| 2:C:413:HIS:CD2  | 2:C:415:ILE:H    | 2.12                     | 0.68              |
| 2:C:229:ILE:N    | 2:C:229:ILE:HD13 | 2.09                     | 0.68              |
| 2:D:300:LYS:O    | 2:D:301:ASP:HB2  | 1.92                     | 0.68              |
| 2:C:316:VAL:HG22 | 2:C:322:ILE:CG1  | 2.23                     | 0.68              |
| 2:C:21:TYR:CG    | 2:C:41:ILE:HG23  | 2.29                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:229:ILE:H    | 2:C:229:ILE:CD1  | 2.05                     | 0.68              |
| 2:D:413:HIS:CD2  | 2:D:415:ILE:H    | 2.12                     | 0.68              |
| 2:C:240:TYR:HE1  | 2:C:253:ASP:HB2  | 1.57                     | 0.68              |
| 1:B:160:GLN:O    | 1:B:164:ILE:HG12 | 1.94                     | 0.67              |
| 2:C:131:VAL:CG1  | 2:C:311:THR:HA   | 2.24                     | 0.67              |
| 1:A:50:LEU:HD12  | 1:A:53:LEU:HD12  | 1.77                     | 0.67              |
| 2:C:184:ILE:HG22 | 2:C:206:LEU:HB2  | 1.76                     | 0.67              |
| 1:B:174:LEU:HD12 | 1:B:174:LEU:H    | 1.60                     | 0.67              |
| 1:B:33:LYS:HG2   | 1:B:34:LEU:H     | 1.58                     | 0.67              |
| 2:D:474:LYS:HE3  | 2:D:474:LYS:CA   | 2.21                     | 0.67              |
| 2:C:327:LYS:O    | 2:C:327:LYS:HE2  | 1.93                     | 0.67              |
| 2:C:21:TYR:CD1   | 2:C:41:ILE:HG23  | 2.29                     | 0.67              |
| 2:D:327:LYS:HE2  | 2:D:327:LYS:O    | 1.93                     | 0.67              |
| 1:A:195:LYS:N    | 1:A:195:LYS:HD2  | 2.09                     | 0.66              |
| 2:D:21:TYR:CG    | 2:D:41:ILE:HG23  | 2.31                     | 0.66              |
| 2:C:176:LEU:HD13 | 2:C:273:ILE:HD12 | 1.78                     | 0.66              |
| 2:D:286:ILE:N    | 2:D:286:ILE:HD12 | 2.11                     | 0.66              |
| 2:C:291:GLN:NE2  | 2:C:293:ASP:H    | 1.89                     | 0.66              |
| 2:D:17:ILE:HD12  | 2:D:42:GLN:HB2   | 1.78                     | 0.66              |
| 1:A:53:LEU:HD13  | 1:A:58:ILE:HD11  | 1.78                     | 0.66              |
| 1:B:53:LEU:HD13  | 1:B:58:ILE:HD11  | 1.78                     | 0.66              |
| 2:C:164:LEU:HA   | 2:C:167:ASN:HB3  | 1.78                     | 0.66              |
| 2:C:148:ALA:HA   | 2:C:454:ILE:HD11 | 1.78                     | 0.65              |
| 2:D:148:ALA:HB3  | 2:D:299:SER:OG   | 1.96                     | 0.65              |
| 2:D:146:ASN:ND2  | 2:D:302:PRO:HB3  | 2.11                     | 0.65              |
| 1:A:231:ASN:HD21 | 1:A:235:LYS:HE3  | 1.60                     | 0.65              |
| 2:D:148:ALA:HA   | 2:D:454:ILE:HD11 | 1.79                     | 0.65              |
| 2:D:30:GLU:HG2   | 2:D:91:ILE:CD1   | 2.26                     | 0.65              |
| 1:A:118:GLU:HG2  | 1:A:122:ARG:NH1  | 2.10                     | 0.65              |
| 1:A:174:LEU:HD12 | 1:A:174:LEU:N    | 2.11                     | 0.65              |
| 1:B:100:ASP:OD1  | 1:B:102:ILE:HG12 | 1.95                     | 0.65              |
| 2:C:474:LYS:HE3  | 2:C:474:LYS:CA   | 2.24                     | 0.65              |
| 1:A:160:GLN:O    | 1:A:164:ILE:HG12 | 1.97                     | 0.65              |
| 2:D:21:TYR:CD1   | 2:D:41:ILE:HG23  | 2.31                     | 0.65              |
| 2:D:184:ILE:HG22 | 2:D:206:LEU:HB2  | 1.78                     | 0.65              |
| 2:D:331:MET:HG2  | 2:D:442:LEU:CA   | 2.27                     | 0.65              |
| 2:D:27:SER:OG    | 2:D:30:GLU:HG3   | 1.97                     | 0.64              |
| 1:B:174:LEU:HD12 | 1:B:174:LEU:N    | 2.12                     | 0.64              |
| 1:A:204:TYR:OH   | 1:A:241:LYS:HD2  | 1.98                     | 0.64              |
| 2:D:139:ARG:HG2  | 2:D:139:ARG:HH11 | 1.63                     | 0.64              |
| 2:C:331:MET:CE   | 2:C:441:ASP:HB2  | 2.28                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:195:LYS:N    | 1:B:195:LYS:HD2  | 2.12                     | 0.64              |
| 2:D:58:LYS:HD2   | 3:E:601:DC:C2    | 2.33                     | 0.64              |
| 2:C:146:ASN:ND2  | 2:C:302:PRO:HB3  | 2.13                     | 0.64              |
| 1:B:26:SER:HB3   | 1:B:204:TYR:CE2  | 2.33                     | 0.64              |
| 2:C:74:ILE:N     | 2:C:74:ILE:HD12  | 2.12                     | 0.63              |
| 1:A:118:GLU:HG2  | 1:A:122:ARG:HH12 | 1.62                     | 0.63              |
| 2:D:225:THR:CG2  | 2:D:227:ASN:HB2  | 2.28                     | 0.63              |
| 2:C:141:MET:HE1  | 2:C:443:LEU:O    | 1.99                     | 0.63              |
| 2:C:331:MET:HE3  | 2:C:441:ASP:HB2  | 1.80                     | 0.63              |
| 2:C:161:VAL:HA   | 2:C:165:VAL:HG21 | 1.79                     | 0.63              |
| 2:D:210:SER:HA   | 2:D:213:PHE:HB3  | 1.81                     | 0.63              |
| 1:B:231:ASN:HD21 | 1:B:235:LYS:HE3  | 1.63                     | 0.63              |
| 2:C:331:MET:HG2  | 2:C:442:LEU:CA   | 2.29                     | 0.63              |
| 2:D:331:MET:HE3  | 2:D:441:ASP:HB2  | 1.80                     | 0.63              |
| 2:C:285:MET:O    | 2:C:288:MET:HB3  | 1.98                     | 0.63              |
| 2:D:131:VAL:CG1  | 2:D:311:THR:HA   | 2.29                     | 0.63              |
| 2:D:331:MET:CE   | 2:D:441:ASP:HB2  | 2.29                     | 0.63              |
| 2:D:198:ILE:HD12 | 2:D:308:ARG:HD3  | 1.80                     | 0.63              |
| 2:D:443:LEU:HA   | 2:D:446:MET:CE   | 2.28                     | 0.63              |
| 1:B:204:TYR:OH   | 1:B:241:LYS:HD2  | 1.99                     | 0.63              |
| 2:C:245:ASP:OD1  | 2:C:249:ASN:HB2  | 1.99                     | 0.62              |
| 2:D:161:VAL:HA   | 2:D:165:VAL:HG21 | 1.79                     | 0.62              |
| 2:D:164:LEU:HA   | 2:D:167:ASN:HB3  | 1.81                     | 0.62              |
| 2:C:210:SER:HA   | 2:C:213:PHE:HB3  | 1.82                     | 0.62              |
| 2:C:27:SER:OG    | 2:C:30:GLU:HG3   | 2.00                     | 0.62              |
| 2:C:234:ILE:HD12 | 2:C:240:TYR:HE2  | 1.65                     | 0.62              |
| 2:C:30:GLU:HG2   | 2:C:91:ILE:CD1   | 2.29                     | 0.62              |
| 2:C:286:ILE:N    | 2:C:286:ILE:HD12 | 2.15                     | 0.62              |
| 1:B:118:GLU:HG2  | 1:B:122:ARG:NH1  | 2.14                     | 0.62              |
| 1:A:138:ASP:OD1  | 1:A:209:ARG:NH2  | 2.25                     | 0.62              |
| 1:B:4:VAL:HG22   | 1:B:5:SER:N      | 2.14                     | 0.61              |
| 2:D:316:VAL:HG22 | 2:D:322:ILE:CG1  | 2.27                     | 0.61              |
| 2:D:74:ILE:N     | 2:D:74:ILE:HD12  | 2.15                     | 0.61              |
| 2:C:288:MET:CG   | 2:C:294:ARG:HG3  | 2.27                     | 0.61              |
| 2:D:60:LYS:O     | 2:D:64:PHE:C     | 2.39                     | 0.61              |
| 1:A:163:MET:O    | 1:A:167:LEU:HB2  | 2.01                     | 0.61              |
| 1:B:118:GLU:HG2  | 1:B:122:ARG:HH12 | 1.65                     | 0.61              |
| 1:A:175:LYS:NZ   | 1:A:207:GLU:OE2  | 2.23                     | 0.61              |
| 2:D:47:PHE:CD1   | 2:D:105:VAL:HG13 | 2.35                     | 0.61              |
| 2:C:61:LYS:HZ3   | 2:C:62:ARG:HB2   | 1.65                     | 0.61              |
| 2:D:53:VAL:HG12  | 2:D:57:LYS:HE3   | 1.81                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:40:ASN:O     | 2:D:44:ILE:HG13  | 2.00                     | 0.61              |
| 2:D:195:ASN:C    | 2:D:197:ASN:H    | 2.04                     | 0.61              |
| 2:D:331:MET:HB2  | 2:D:441:ASP:HB3  | 1.83                     | 0.61              |
| 2:C:198:ILE:HD12 | 2:C:308:ARG:HD3  | 1.82                     | 0.61              |
| 2:D:134:MET:HG3  | 2:D:137:LEU:HD23 | 1.83                     | 0.61              |
| 2:C:142:LEU:HD11 | 2:C:306:ASN:N    | 2.15                     | 0.61              |
| 2:D:333:MET:CE   | 2:D:348:THR:HA   | 2.30                     | 0.61              |
| 2:D:333:MET:HE2  | 2:D:348:THR:HA   | 1.82                     | 0.61              |
| 1:A:26:SER:HB3   | 1:A:204:TYR:CE2  | 2.36                     | 0.61              |
| 1:B:88:ILE:HD11  | 2:C:211:ARG:HD3  | 1.83                     | 0.61              |
| 1:A:106:LEU:O    | 5:G:800:DC:N4    | 2.34                     | 0.61              |
| 2:C:148:ALA:HA   | 2:C:454:ILE:HD12 | 1.81                     | 0.61              |
| 1:A:25:GLU:CD    | 1:A:25:GLU:H     | 2.03                     | 0.61              |
| 2:C:331:MET:HG2  | 2:C:442:LEU:N    | 2.16                     | 0.61              |
| 2:D:74:ILE:HG22  | 2:D:74:ILE:O     | 2.01                     | 0.60              |
| 2:D:328:ARG:HB3  | 2:D:444:ASN:HB2  | 1.82                     | 0.60              |
| 1:A:294:LEU:O    | 1:A:295:ASN:HB2  | 1.99                     | 0.60              |
| 2:D:291:GLN:NE2  | 2:D:293:ASP:H    | 1.93                     | 0.60              |
| 2:C:53:VAL:HG12  | 2:C:57:LYS:HE3   | 1.82                     | 0.60              |
| 2:D:148:ALA:HA   | 2:D:454:ILE:HD12 | 1.82                     | 0.60              |
| 2:C:134:MET:HA   | 2:C:134:MET:HE2  | 1.83                     | 0.60              |
| 2:C:134:MET:HG3  | 2:C:137:LEU:HD23 | 1.83                     | 0.60              |
| 2:C:22:LEU:O     | 2:C:86:THR:HA    | 2.01                     | 0.60              |
| 2:D:22:LEU:O     | 2:D:86:THR:HA    | 2.01                     | 0.60              |
| 2:D:143:ASN:O    | 2:D:451:LYS:HE2  | 2.02                     | 0.60              |
| 2:D:134:MET:HE2  | 2:D:134:MET:HA   | 1.84                     | 0.60              |
| 2:D:145:MET:HB3  | 2:D:415:ILE:HD11 | 1.83                     | 0.60              |
| 2:C:331:MET:HB2  | 2:C:441:ASP:HB3  | 1.84                     | 0.60              |
| 2:C:233:LYS:HG3  | 2:C:240:TYR:O    | 2.02                     | 0.60              |
| 1:B:160:GLN:HB3  | 1:B:174:LEU:HD23 | 1.82                     | 0.60              |
| 2:D:285:MET:O    | 2:D:288:MET:HB3  | 2.02                     | 0.60              |
| 2:C:23:GLY:HA3   | 2:C:86:THR:HG22  | 1.82                     | 0.60              |
| 2:D:331:MET:O    | 2:D:333:MET:N    | 2.35                     | 0.60              |
| 1:B:26:SER:HB3   | 1:B:204:TYR:CD2  | 2.36                     | 0.60              |
| 2:D:147:VAL:HG12 | 2:D:451:LYS:HB3  | 1.84                     | 0.59              |
| 2:D:234:ILE:HD12 | 2:D:240:TYR:HE2  | 1.67                     | 0.59              |
| 2:D:44:ILE:O     | 2:D:49:LYS:HE3   | 2.02                     | 0.59              |
| 2:C:44:ILE:O     | 2:C:49:LYS:HE3   | 2.02                     | 0.59              |
| 2:C:109:THR:HG23 | 4:F:702:U:O2'    | 2.03                     | 0.59              |
| 2:C:331:MET:O    | 2:C:333:MET:N    | 2.35                     | 0.59              |
| 1:B:59:LEU:HD11  | 1:B:89:ILE:HD13  | 1.84                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:142:LEU:HD11 | 2:D:306:ASN:N    | 2.17                     | 0.59              |
| 2:D:474:LYS:CE   | 2:D:474:LYS:HA   | 2.24                     | 0.59              |
| 2:C:301:ASP:N    | 2:C:302:PRO:HD3  | 2.17                     | 0.59              |
| 2:C:74:ILE:HG22  | 2:C:74:ILE:O     | 2.02                     | 0.59              |
| 1:B:46:GLU:OE2   | 1:B:66:TYR:OH    | 2.21                     | 0.59              |
| 2:C:139:ARG:HH11 | 2:C:139:ARG:HG2  | 1.68                     | 0.59              |
| 2:D:191:LEU:HB2  | 2:D:198:ILE:HG21 | 1.84                     | 0.59              |
| 2:D:198:ILE:HD11 | 2:D:311:THR:OG1  | 2.02                     | 0.59              |
| 2:D:331:MET:HG2  | 2:D:442:LEU:N    | 2.17                     | 0.59              |
| 1:A:160:GLN:HB3  | 1:A:174:LEU:HD23 | 1.82                     | 0.59              |
| 2:C:195:ASN:C    | 2:C:197:ASN:H    | 2.06                     | 0.59              |
| 2:D:84:LYS:CG    | 2:D:97:ILE:HD13  | 2.33                     | 0.59              |
| 2:D:333:MET:HB3  | 2:D:347:THR:O    | 2.03                     | 0.59              |
| 1:A:26:SER:HB3   | 1:A:204:TYR:CD2  | 2.37                     | 0.59              |
| 1:B:147:GLU:OE1  | 1:B:147:GLU:HA   | 2.01                     | 0.59              |
| 3:E:602:U:H4'    | 3:E:603:U:H5''   | 1.84                     | 0.59              |
| 2:C:131:VAL:HA   | 2:C:314:GLU:HG2  | 1.84                     | 0.59              |
| 1:A:59:LEU:HD11  | 1:A:89:ILE:HD13  | 1.85                     | 0.59              |
| 1:B:163:MET:O    | 1:B:167:LEU:HB2  | 2.03                     | 0.59              |
| 2:D:291:GLN:HE21 | 2:D:293:ASP:N    | 1.92                     | 0.59              |
| 2:D:288:MET:CG   | 2:D:294:ARG:HG3  | 2.30                     | 0.59              |
| 2:C:134:MET:CG   | 2:C:137:LEU:HD23 | 2.32                     | 0.59              |
| 2:C:333:MET:CE   | 2:C:348:THR:HA   | 2.32                     | 0.59              |
| 2:C:225:THR:CG2  | 2:C:227:ASN:HB2  | 2.33                     | 0.59              |
| 2:D:61:LYS:HZ3   | 2:D:62:ARG:HB2   | 1.67                     | 0.59              |
| 2:C:198:ILE:CD1  | 2:C:308:ARG:HH11 | 2.15                     | 0.58              |
| 2:C:333:MET:HB3  | 2:C:347:THR:O    | 2.03                     | 0.58              |
| 2:C:109:THR:HG22 | 2:C:110:ASP:N    | 2.18                     | 0.58              |
| 1:A:88:ILE:HD11  | 2:D:211:ARG:HD3  | 1.85                     | 0.58              |
| 2:D:179:HIS:HB3  | 2:D:182:SER:OG   | 2.03                     | 0.58              |
| 2:C:147:VAL:HG12 | 2:C:451:LYS:HB3  | 1.85                     | 0.58              |
| 2:D:283:LEU:HD21 | 2:D:425:LEU:HB2  | 1.85                     | 0.58              |
| 2:D:406:LEU:HA   | 2:D:413:HIS:H    | 1.68                     | 0.58              |
| 2:D:245:ASP:OD1  | 2:D:249:ASN:HB2  | 2.04                     | 0.58              |
| 2:C:258:ARG:NH2  | 2:C:380:ASP:O    | 2.36                     | 0.58              |
| 2:D:258:ARG:NH2  | 2:D:380:ASP:O    | 2.36                     | 0.58              |
| 2:D:176:LEU:HD13 | 2:D:273:ILE:HD12 | 1.86                     | 0.58              |
| 2:D:186:TYR:HA   | 2:D:190:SER:HB2  | 1.86                     | 0.58              |
| 1:A:4:VAL:HG22   | 1:A:5:SER:N      | 2.18                     | 0.58              |
| 2:D:301:ASP:N    | 2:D:302:PRO:HD3  | 2.18                     | 0.58              |
| 2:C:328:ARG:HB3  | 2:C:444:ASN:HB2  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:135:GLU:O    | 2:D:139:ARG:HB2  | 2.04                     | 0.58              |
| 2:C:47:PHE:CD1   | 2:C:105:VAL:HG13 | 2.37                     | 0.58              |
| 1:A:33:LYS:O     | 1:A:34:LEU:O     | 2.21                     | 0.58              |
| 2:C:406:LEU:HA   | 2:C:413:HIS:H    | 1.68                     | 0.58              |
| 2:C:176:LEU:HB3  | 2:C:273:ILE:HB   | 1.85                     | 0.58              |
| 2:D:145:MET:CB   | 2:D:415:ILE:HD11 | 2.32                     | 0.58              |
| 1:A:61:GLY:HA2   | 1:A:88:ILE:O     | 2.04                     | 0.58              |
| 1:A:192:HIS:O    | 1:A:212:SER:HB3  | 2.04                     | 0.58              |
| 2:D:231:LEU:HD13 | 2:D:241:MET:HE2  | 1.86                     | 0.58              |
| 2:D:233:LYS:HG3  | 2:D:240:TYR:O    | 2.04                     | 0.58              |
| 2:D:90:ASN:C     | 2:D:90:ASN:HD22  | 2.06                     | 0.58              |
| 2:C:198:ILE:HD11 | 2:C:311:THR:OG1  | 2.04                     | 0.58              |
| 1:A:162:VAL:O    | 1:A:166:ILE:HG12 | 2.04                     | 0.58              |
| 2:D:404:ILE:O    | 2:D:457:HIS:HA   | 2.04                     | 0.57              |
| 2:C:164:LEU:HD23 | 2:C:167:ASN:HD22 | 1.68                     | 0.57              |
| 1:B:294:LEU:O    | 1:B:295:ASN:HB2  | 2.03                     | 0.57              |
| 2:C:189:TYR:CE2  | 2:C:193:LEU:HD21 | 2.39                     | 0.57              |
| 2:C:270:ILE:CG2  | 2:C:271:ASP:N    | 2.54                     | 0.57              |
| 1:A:107:ARG:CZ   | 2:D:477:ILE:HG21 | 2.34                     | 0.57              |
| 2:C:73:GLU:C     | 2:C:75:LYS:H     | 2.06                     | 0.57              |
| 2:C:164:LEU:CD2  | 2:C:167:ASN:HD22 | 2.16                     | 0.57              |
| 2:C:186:TYR:HA   | 2:C:190:SER:HB2  | 1.87                     | 0.57              |
| 2:D:283:LEU:HD22 | 2:D:429:MET:CE   | 2.34                     | 0.57              |
| 2:C:59:ASN:ND2   | 2:C:220:LEU:HD21 | 2.17                     | 0.57              |
| 2:C:234:ILE:HD12 | 2:C:240:TYR:CE2  | 2.39                     | 0.57              |
| 1:A:39:GLN:HB3   | 1:A:294:LEU:HD22 | 1.87                     | 0.57              |
| 2:D:131:VAL:HA   | 2:D:314:GLU:HG2  | 1.86                     | 0.57              |
| 2:D:109:THR:HG22 | 2:D:110:ASP:N    | 2.19                     | 0.57              |
| 2:C:143:ASN:O    | 2:C:451:LYS:HE2  | 2.05                     | 0.57              |
| 2:C:40:ASN:O     | 2:C:44:ILE:HG13  | 2.04                     | 0.57              |
| 1:A:43:LEU:O     | 1:A:43:LEU:HD12  | 2.05                     | 0.57              |
| 2:C:90:ASN:HD22  | 2:C:90:ASN:C     | 2.07                     | 0.57              |
| 1:B:25:GLU:CD    | 1:B:25:GLU:H     | 2.07                     | 0.57              |
| 2:C:179:HIS:HB3  | 2:C:182:SER:OG   | 2.05                     | 0.57              |
| 2:C:134:MET:HG3  | 2:C:137:LEU:HB3  | 1.87                     | 0.57              |
| 2:D:73:GLU:C     | 2:D:75:LYS:H     | 2.06                     | 0.57              |
| 2:D:22:LEU:HD23  | 2:D:85:GLN:HB3   | 1.85                     | 0.57              |
| 1:A:46:GLU:OE2   | 1:A:66:TYR:OH    | 2.23                     | 0.57              |
| 2:C:24:ARG:HD3   | 2:C:89:TYR:CE2   | 2.40                     | 0.57              |
| 2:D:58:LYS:HZ3   | 2:D:116:THR:HB   | 1.68                     | 0.57              |
| 2:C:135:GLU:O    | 2:C:139:ARG:HB2  | 2.05                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:79:ARG:HD3   | 1:B:79:ARG:C     | 2.26                     | 0.57              |
| 2:D:23:GLY:HA3   | 2:D:86:THR:HG22  | 1.86                     | 0.56              |
| 2:C:325:ASP:OD2  | 2:C:327:LYS:HE2  | 2.03                     | 0.56              |
| 2:C:132:THR:HA   | 2:C:135:GLU:HG3  | 1.86                     | 0.56              |
| 2:C:474:LYS:HA   | 2:C:474:LYS:CE   | 2.27                     | 0.56              |
| 2:C:191:LEU:HB2  | 2:C:198:ILE:HG21 | 1.86                     | 0.56              |
| 2:C:198:ILE:HD13 | 2:C:308:ARG:NH1  | 2.20                     | 0.56              |
| 2:C:44:ILE:HG12  | 2:C:105:VAL:HG21 | 1.87                     | 0.56              |
| 2:C:283:LEU:HD21 | 2:C:425:LEU:HB2  | 1.87                     | 0.56              |
| 2:D:234:ILE:HD12 | 2:D:240:TYR:CE2  | 2.41                     | 0.56              |
| 1:A:265:PHE:HA   | 1:A:268:ARG:HD3  | 1.86                     | 0.56              |
| 1:A:147:GLU:HA   | 1:A:147:GLU:OE1  | 2.05                     | 0.56              |
| 1:B:3:VAL:HB     | 1:B:249:VAL:HG13 | 1.86                     | 0.56              |
| 1:B:192:HIS:O    | 1:B:212:SER:HB3  | 2.06                     | 0.56              |
| 1:B:43:LEU:O     | 1:B:43:LEU:HD12  | 2.06                     | 0.56              |
| 2:D:44:ILE:HG12  | 2:D:105:VAL:HG21 | 1.86                     | 0.56              |
| 1:B:39:GLN:HB3   | 1:B:294:LEU:HD22 | 1.88                     | 0.56              |
| 2:D:198:ILE:CD1  | 2:D:308:ARG:HH11 | 2.18                     | 0.56              |
| 2:C:443:LEU:HA   | 2:C:446:MET:CE   | 2.29                     | 0.56              |
| 1:A:4:VAL:O      | 1:A:249:VAL:HG22 | 2.04                     | 0.56              |
| 1:B:33:LYS:O     | 1:B:34:LEU:O     | 2.24                     | 0.55              |
| 2:D:19:GLU:HB2   | 2:D:26:PRO:HD3   | 1.89                     | 0.55              |
| 2:D:198:ILE:HD13 | 2:D:308:ARG:NH1  | 2.21                     | 0.55              |
| 2:D:141:MET:HE1  | 2:D:443:LEU:O    | 2.06                     | 0.55              |
| 1:B:107:ARG:CZ   | 2:C:477:ILE:HG21 | 2.36                     | 0.55              |
| 2:D:176:LEU:HB3  | 2:D:273:ILE:HB   | 1.88                     | 0.55              |
| 2:C:143:ASN:HA   | 2:C:146:ASN:HB2  | 1.88                     | 0.55              |
| 2:D:51:ILE:HD12  | 3:E:603:U:C4     | 2.41                     | 0.55              |
| 2:D:134:MET:CG   | 2:D:137:LEU:HD23 | 2.36                     | 0.55              |
| 1:A:112:VAL:CG1  | 1:A:114:ARG:HG2  | 2.37                     | 0.55              |
| 2:D:132:THR:HA   | 2:D:135:GLU:HG3  | 1.88                     | 0.55              |
| 1:B:61:GLY:HA2   | 1:B:88:ILE:O     | 2.07                     | 0.55              |
| 2:D:298:LEU:HD13 | 2:D:305:PHE:CD1  | 2.42                     | 0.55              |
| 2:C:325:ASP:O    | 2:C:327:LYS:N    | 2.40                     | 0.55              |
| 1:B:87:VAL:HG12  | 1:B:89:ILE:HG13  | 1.88                     | 0.55              |
| 2:C:51:ILE:HG23  | 4:F:703:U:N3     | 2.21                     | 0.55              |
| 2:D:134:MET:O    | 2:D:137:LEU:HB3  | 2.06                     | 0.55              |
| 2:C:227:ASN:OD1  | 2:C:246:GLU:HG3  | 2.05                     | 0.55              |
| 2:C:449:ARG:NH1  | 2:C:449:ARG:HB3  | 2.22                     | 0.55              |
| 2:D:51:ILE:HG23  | 3:E:603:U:C4     | 2.42                     | 0.55              |
| 2:C:60:LYS:O     | 2:C:64:PHE:C     | 2.46                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:109:VAL:O    | 1:A:109:VAL:HG23 | 2.06                     | 0.54              |
| 2:D:44:ILE:O     | 2:D:47:PHE:HB3   | 2.06                     | 0.54              |
| 1:A:114:ARG:HD3  | 1:A:120:TYR:CE1  | 2.42                     | 0.54              |
| 2:D:63:PHE:CD2   | 2:D:171:LEU:HA   | 2.42                     | 0.54              |
| 2:C:108:TYR:CE1  | 2:C:112:LEU:HB2  | 2.42                     | 0.54              |
| 2:D:331:MET:CG   | 2:D:442:LEU:HA   | 2.36                     | 0.54              |
| 1:B:138:ASP:OD1  | 1:B:209:ARG:NH2  | 2.26                     | 0.54              |
| 1:B:162:VAL:O    | 1:B:166:ILE:HG12 | 2.07                     | 0.54              |
| 2:C:145:MET:CB   | 2:C:415:ILE:HD11 | 2.36                     | 0.54              |
| 2:C:276:VAL:O    | 2:C:281:GLN:HG3  | 2.06                     | 0.54              |
| 2:C:404:ILE:O    | 2:C:457:HIS:HA   | 2.08                     | 0.54              |
| 2:C:44:ILE:O     | 2:C:47:PHE:HB3   | 2.07                     | 0.54              |
| 1:B:265:PHE:HA   | 1:B:268:ARG:HD3  | 1.88                     | 0.54              |
| 1:B:106:LEU:HD12 | 1:B:109:VAL:HG11 | 1.90                     | 0.54              |
| 2:D:351:TYR:HD2  | 2:D:438:CYS:HG   | 1.55                     | 0.54              |
| 1:A:121:LEU:C    | 1:A:166:ILE:HG21 | 2.27                     | 0.54              |
| 1:A:3:VAL:HB     | 1:A:249:VAL:HG13 | 1.88                     | 0.54              |
| 2:D:240:TYR:CE1  | 2:D:253:ASP:HB2  | 2.41                     | 0.54              |
| 2:D:134:MET:HG3  | 2:D:137:LEU:HB3  | 1.90                     | 0.54              |
| 1:B:121:LEU:C    | 1:B:166:ILE:HG21 | 2.28                     | 0.54              |
| 2:C:63:PHE:CD2   | 2:C:171:LEU:HA   | 2.43                     | 0.54              |
| 2:C:283:LEU:HD22 | 2:C:429:MET:CE   | 2.37                     | 0.54              |
| 5:H:900:DC:H4'   | 5:H:901:U:H5''   | 1.90                     | 0.54              |
| 2:C:145:MET:HB3  | 2:C:415:ILE:HD11 | 1.89                     | 0.54              |
| 2:C:174:GLU:O    | 2:C:178:ARG:HG2  | 2.08                     | 0.54              |
| 2:D:59:ASN:ND2   | 2:D:220:LEU:HD21 | 2.21                     | 0.54              |
| 2:D:24:ARG:HD3   | 2:D:89:TYR:CE2   | 2.43                     | 0.54              |
| 1:A:87:VAL:HG12  | 1:A:89:ILE:HG13  | 1.90                     | 0.54              |
| 1:A:79:ARG:C     | 1:A:79:ARG:HD3   | 2.29                     | 0.54              |
| 1:A:223:ARG:HD2  | 1:B:168:ASN:ND2  | 2.23                     | 0.54              |
| 2:C:116:THR:O    | 2:C:117:ILE:HG13 | 2.08                     | 0.54              |
| 2:D:116:THR:O    | 2:D:117:ILE:HG13 | 2.08                     | 0.54              |
| 1:B:4:VAL:O      | 1:B:249:VAL:HG22 | 2.06                     | 0.54              |
| 2:C:331:MET:CG   | 2:C:442:LEU:HA   | 2.37                     | 0.53              |
| 1:B:286:LEU:O    | 1:B:289:SER:N    | 2.37                     | 0.53              |
| 2:C:51:ILE:HD13  | 2:C:51:ILE:O     | 2.08                     | 0.53              |
| 2:D:141:MET:O    | 2:D:144:SER:HB2  | 2.08                     | 0.53              |
| 1:A:286:LEU:O    | 1:A:289:SER:N    | 2.38                     | 0.53              |
| 2:D:164:LEU:CD2  | 2:D:167:ASN:HD22 | 2.21                     | 0.53              |
| 2:C:20:THR:O     | 2:C:20:THR:HG22  | 2.08                     | 0.53              |
| 1:B:114:ARG:HD3  | 1:B:120:TYR:CE1  | 2.43                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:109:VAL:HG23 | 1:B:109:VAL:O    | 2.07                     | 0.53              |
| 2:D:147:VAL:CG1  | 2:D:451:LYS:HB3  | 2.39                     | 0.53              |
| 2:D:280:PHE:HD1  | 2:D:429:MET:SD   | 2.31                     | 0.53              |
| 2:C:84:LYS:CG    | 2:C:97:ILE:HD13  | 2.34                     | 0.53              |
| 2:C:51:ILE:HG23  | 4:F:703:U:H3     | 1.73                     | 0.53              |
| 2:C:356:LYS:HE3  | 2:C:395:ILE:HD12 | 1.90                     | 0.53              |
| 1:A:106:LEU:HD12 | 1:A:109:VAL:HG11 | 1.91                     | 0.53              |
| 2:C:189:TYR:CZ   | 2:C:193:LEU:HD21 | 2.44                     | 0.53              |
| 2:C:22:LEU:HD23  | 2:C:85:GLN:HB3   | 1.89                     | 0.53              |
| 2:D:449:ARG:NH1  | 2:D:449:ARG:HB3  | 2.23                     | 0.53              |
| 2:C:141:MET:CE   | 2:C:446:MET:HB2  | 2.38                     | 0.53              |
| 2:D:112:LEU:HD13 | 2:D:220:LEU:HD22 | 1.89                     | 0.53              |
| 2:C:240:TYR:CE1  | 2:C:253:ASP:HB2  | 2.42                     | 0.53              |
| 2:C:90:ASN:ND2   | 2:C:90:ASN:C     | 2.60                     | 0.53              |
| 1:B:35:PRO:O     | 1:B:36:TYR:HB2   | 2.09                     | 0.53              |
| 2:C:366:LEU:O    | 2:C:370:ILE:HG13 | 2.08                     | 0.53              |
| 2:C:434:GLU:HA   | 2:C:434:GLU:OE1  | 2.08                     | 0.53              |
| 2:C:267:LYS:HD3  | 2:C:274:TYR:CD2  | 2.43                     | 0.53              |
| 2:D:20:THR:O     | 2:D:20:THR:HG22  | 2.09                     | 0.53              |
| 2:C:283:LEU:HD21 | 2:C:425:LEU:CB   | 2.38                     | 0.53              |
| 2:C:286:ILE:HG12 | 2:C:442:LEU:HD21 | 1.91                     | 0.53              |
| 2:D:164:LEU:HD23 | 2:D:167:ASN:HD22 | 1.74                     | 0.53              |
| 2:C:357:CYS:HA   | 2:C:396:MET:O    | 2.09                     | 0.53              |
| 2:D:397:TYR:CD1  | 2:D:397:TYR:N    | 2.77                     | 0.53              |
| 2:D:283:LEU:HD21 | 2:D:425:LEU:CB   | 2.38                     | 0.53              |
| 2:D:286:ILE:HG12 | 2:D:442:LEU:HD21 | 1.91                     | 0.53              |
| 2:C:58:LYS:HZ3   | 2:C:116:THR:HB   | 1.74                     | 0.53              |
| 2:C:168:VAL:O    | 2:C:171:LEU:N    | 2.42                     | 0.52              |
| 1:A:168:ASN:HD22 | 1:B:223:ARG:NE   | 2.07                     | 0.52              |
| 2:C:198:ILE:HD12 | 2:C:308:ARG:HH11 | 1.74                     | 0.52              |
| 2:C:134:MET:O    | 2:C:137:LEU:HB3  | 2.09                     | 0.52              |
| 2:D:143:ASN:HA   | 2:D:146:ASN:HB2  | 1.90                     | 0.52              |
| 1:B:112:VAL:CG1  | 1:B:114:ARG:HG2  | 2.39                     | 0.52              |
| 2:D:168:VAL:O    | 2:D:171:LEU:N    | 2.43                     | 0.52              |
| 2:C:231:LEU:HD13 | 2:C:241:MET:HE2  | 1.91                     | 0.52              |
| 1:A:124:ILE:O    | 1:A:128:LEU:HD13 | 2.09                     | 0.52              |
| 2:C:57:LYS:C     | 2:C:59:ASN:H     | 2.13                     | 0.52              |
| 2:C:317:ARG:HH11 | 2:C:317:ARG:HG2  | 1.73                     | 0.52              |
| 2:C:19:GLU:HB2   | 2:C:26:PRO:HD3   | 1.92                     | 0.52              |
| 1:B:286:LEU:O    | 1:B:287:GLN:C    | 2.48                     | 0.52              |
| 2:D:276:VAL:O    | 2:D:281:GLN:HG3  | 2.08                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:189:TYR:CE2  | 2:D:193:LEU:HD21 | 2.45                     | 0.52              |
| 2:C:198:ILE:CD1  | 2:C:308:ARG:NH1  | 2.73                     | 0.52              |
| 2:C:112:LEU:HD13 | 2:C:220:LEU:HD22 | 1.91                     | 0.52              |
| 1:A:168:ASN:ND2  | 1:B:223:ARG:CZ   | 2.69                     | 0.52              |
| 2:D:331:MET:HE3  | 2:D:438:CYS:O    | 2.10                     | 0.52              |
| 1:A:22:TYR:HB2   | 1:A:233:GLU:HG2  | 1.92                     | 0.52              |
| 1:A:35:PRO:O     | 1:A:36:TYR:HB2   | 2.10                     | 0.52              |
| 2:D:267:LYS:HD3  | 2:D:274:TYR:CD2  | 2.44                     | 0.52              |
| 2:C:298:LEU:HD13 | 2:C:305:PHE:CD1  | 2.45                     | 0.52              |
| 2:C:141:MET:O    | 2:C:144:SER:HB2  | 2.10                     | 0.52              |
| 2:C:178:ARG:HH11 | 2:C:178:ARG:CA   | 2.17                     | 0.52              |
| 1:B:280:LYS:O    | 1:B:284:LEU:HB2  | 2.10                     | 0.52              |
| 2:C:110:ASP:O    | 2:C:179:HIS:HE1  | 1.92                     | 0.52              |
| 2:D:108:TYR:CE1  | 2:D:112:LEU:HB2  | 2.45                     | 0.52              |
| 2:D:221:ILE:O    | 2:D:225:THR:HB   | 2.10                     | 0.52              |
| 1:B:43:LEU:HD23  | 1:B:290:ILE:HG23 | 1.92                     | 0.52              |
| 2:D:434:GLU:OE1  | 2:D:434:GLU:HA   | 2.09                     | 0.52              |
| 2:D:270:ILE:CG2  | 2:D:271:ASP:N    | 2.55                     | 0.51              |
| 2:C:178:ARG:HA   | 2:C:178:ARG:NH1  | 2.15                     | 0.51              |
| 2:C:58:LYS:C     | 2:C:61:LYS:HZ2   | 2.13                     | 0.51              |
| 2:C:49:LYS:HZ3   | 2:C:82:PHE:HD2   | 1.58                     | 0.51              |
| 2:D:289:PHE:CE2  | 2:D:298:LEU:HD22 | 2.45                     | 0.51              |
| 2:C:397:TYR:N    | 2:C:397:TYR:CD1  | 2.78                     | 0.51              |
| 2:C:289:PHE:CE2  | 2:C:298:LEU:HD22 | 2.45                     | 0.51              |
| 2:D:57:LYS:C     | 2:D:59:ASN:H     | 2.14                     | 0.51              |
| 2:D:325:ASP:OD2  | 2:D:327:LYS:HE2  | 2.09                     | 0.51              |
| 2:C:351:TYR:HD2  | 2:C:438:CYS:HG   | 1.58                     | 0.51              |
| 1:A:33:LYS:O     | 1:A:34:LEU:C     | 2.48                     | 0.51              |
| 2:D:61:LYS:HZ3   | 2:D:62:ARG:CB    | 2.24                     | 0.51              |
| 2:D:227:ASN:OD1  | 2:D:246:GLU:HG3  | 2.09                     | 0.51              |
| 1:A:292:ARG:HG3  | 1:A:292:ARG:HH11 | 1.76                     | 0.51              |
| 1:B:18:ASN:HB2   | 1:B:238:TYR:CZ   | 2.46                     | 0.51              |
| 2:C:288:MET:CE   | 2:C:294:ARG:HD2  | 2.40                     | 0.51              |
| 2:D:195:ASN:O    | 2:D:197:ASN:N    | 2.44                     | 0.51              |
| 2:D:198:ILE:CD1  | 2:D:308:ARG:NH1  | 2.74                     | 0.51              |
| 1:B:76:ARG:HD2   | 1:B:76:ARG:O     | 2.11                     | 0.51              |
| 2:C:344:VAL:HG11 | 2:C:420:LEU:HD13 | 1.91                     | 0.51              |
| 2:C:74:ILE:N     | 2:C:74:ILE:CD1   | 2.73                     | 0.51              |
| 1:A:18:ASN:HB2   | 1:A:238:TYR:CZ   | 2.46                     | 0.51              |
| 1:A:112:VAL:HG12 | 1:A:114:ARG:HG2  | 1.91                     | 0.51              |
| 2:C:318:TYR:O    | 2:C:321:GLY:N    | 2.44                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:317:ARG:HH11 | 2:D:317:ARG:HG2  | 1.75                     | 0.51              |
| 1:A:289:SER:O    | 1:A:292:ARG:HB3  | 2.10                     | 0.51              |
| 2:D:318:TYR:O    | 2:D:321:GLY:N    | 2.43                     | 0.51              |
| 2:C:147:VAL:CG1  | 2:C:451:LYS:HB3  | 2.41                     | 0.50              |
| 2:C:76:ASP:O     | 2:C:77:ARG:C     | 2.48                     | 0.50              |
| 2:D:90:ASN:C     | 2:D:90:ASN:ND2   | 2.62                     | 0.50              |
| 2:C:450:ASP:O    | 2:C:452:ILE:N    | 2.45                     | 0.50              |
| 2:C:218:ALA:O    | 2:C:229:ILE:HD11 | 2.11                     | 0.50              |
| 2:C:61:LYS:HZ3   | 2:C:62:ARG:CB    | 2.24                     | 0.50              |
| 1:A:99:HIS:HB3   | 1:A:103:LEU:HD12 | 1.94                     | 0.50              |
| 1:B:124:ILE:O    | 1:B:128:LEU:HD13 | 2.10                     | 0.50              |
| 3:E:602:U:H4'    | 3:E:603:U:C5'    | 2.40                     | 0.50              |
| 2:C:90:ASN:HD21  | 2:C:92:GLY:H     | 1.58                     | 0.50              |
| 2:C:462:LYS:HB2  | 2:C:462:LYS:NZ   | 2.25                     | 0.50              |
| 2:D:462:LYS:HB2  | 2:D:462:LYS:NZ   | 2.26                     | 0.50              |
| 1:B:93:LEU:HD12  | 1:B:111:LEU:HD21 | 1.92                     | 0.50              |
| 2:D:112:LEU:O    | 2:D:115:LEU:HB2  | 2.12                     | 0.50              |
| 2:C:221:ILE:O    | 2:C:225:THR:HB   | 2.11                     | 0.50              |
| 2:C:58:LYS:HZ2   | 2:C:116:THR:HB   | 1.76                     | 0.50              |
| 1:B:22:TYR:HB2   | 1:B:233:GLU:HG2  | 1.93                     | 0.50              |
| 2:D:366:LEU:O    | 2:D:370:ILE:HG13 | 2.11                     | 0.50              |
| 2:D:450:ASP:O    | 2:D:452:ILE:N    | 2.45                     | 0.50              |
| 2:C:331:MET:HE3  | 2:C:438:CYS:O    | 2.12                     | 0.50              |
| 1:B:292:ARG:HG3  | 1:B:292:ARG:HH11 | 1.77                     | 0.50              |
| 2:C:195:ASN:HD22 | 2:C:198:ILE:CG1  | 2.17                     | 0.50              |
| 2:C:75:LYS:CE    | 2:C:79:LEU:HD11  | 2.42                     | 0.50              |
| 2:C:322:ILE:HG21 | 2:C:443:LEU:CD1  | 2.42                     | 0.50              |
| 2:D:178:ARG:HA   | 2:D:178:ARG:NH1  | 2.16                     | 0.50              |
| 2:D:76:ASP:O     | 2:D:77:ARG:C     | 2.49                     | 0.50              |
| 2:D:51:ILE:O     | 2:D:51:ILE:HD13  | 2.11                     | 0.50              |
| 2:D:50:ASP:C     | 2:D:52:PHE:N     | 2.64                     | 0.50              |
| 2:D:325:ASP:O    | 2:D:327:LYS:N    | 2.45                     | 0.50              |
| 2:D:471:ASN:OD1  | 2:D:473:GLU:HG2  | 2.12                     | 0.50              |
| 2:C:292:ILE:HG13 | 2:C:457:HIS:ND1  | 2.26                     | 0.50              |
| 2:C:280:PHE:HD1  | 2:C:429:MET:SD   | 2.35                     | 0.50              |
| 2:C:320:HIS:O    | 2:C:321:GLY:C    | 2.50                     | 0.50              |
| 2:C:112:LEU:O    | 2:C:115:LEU:HB2  | 2.12                     | 0.49              |
| 5:H:900:DC:H4'   | 5:H:901:U:C5'    | 2.41                     | 0.49              |
| 2:C:44:ILE:HD13  | 2:C:101:GLN:HE21 | 1.76                     | 0.49              |
| 2:C:50:ASP:C     | 2:C:52:PHE:N     | 2.65                     | 0.49              |
| 2:D:58:LYS:C     | 2:D:61:LYS:HZ2   | 2.16                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:280:LYS:O    | 1:A:284:LEU:HB2  | 2.12                     | 0.49              |
| 1:A:286:LEU:O    | 1:A:287:GLN:C    | 2.51                     | 0.49              |
| 2:C:207:GLN:NE2  | 2:C:213:PHE:CD2  | 2.71                     | 0.49              |
| 2:D:110:ASP:O    | 2:D:179:HIS:HE1  | 1.95                     | 0.49              |
| 2:C:148:ALA:HB1  | 2:C:296:GLU:HG2  | 1.94                     | 0.49              |
| 2:D:47:PHE:CD2   | 2:D:105:VAL:HG22 | 2.48                     | 0.49              |
| 3:E:603:U:H6     | 3:E:603:U:C5'    | 2.03                     | 0.49              |
| 2:C:420:LEU:O    | 2:C:423:HIS:HB3  | 2.13                     | 0.49              |
| 1:B:289:SER:O    | 1:B:292:ARG:HB3  | 2.11                     | 0.49              |
| 2:D:252:ILE:HD12 | 2:D:253:ASP:H    | 1.77                     | 0.49              |
| 2:D:337:ILE:HD12 | 2:D:404:ILE:HG21 | 1.93                     | 0.49              |
| 2:D:90:ASN:HD21  | 2:D:92:GLY:H     | 1.59                     | 0.49              |
| 2:D:231:LEU:HD22 | 2:D:241:MET:HE2  | 1.94                     | 0.49              |
| 1:B:99:HIS:HB3   | 1:B:103:LEU:HD12 | 1.95                     | 0.49              |
| 1:A:253:TYR:OH   | 1:A:287:GLN:NE2  | 2.45                     | 0.49              |
| 2:D:47:PHE:CG    | 2:D:105:VAL:HG13 | 2.47                     | 0.49              |
| 1:A:223:ARG:CD   | 1:B:168:ASN:ND2  | 2.75                     | 0.49              |
| 1:A:215:THR:HG23 | 2:D:364:ASN:ND2  | 2.27                     | 0.49              |
| 2:D:141:MET:CE   | 2:D:446:MET:HB2  | 2.42                     | 0.49              |
| 2:C:231:LEU:HD22 | 2:C:241:MET:HE2  | 1.95                     | 0.49              |
| 1:B:18:ASN:O     | 1:B:235:LYS:HG2  | 2.13                     | 0.49              |
| 2:C:47:PHE:CG    | 2:C:105:VAL:HG13 | 2.47                     | 0.49              |
| 1:B:220:ARG:HG3  | 1:B:220:ARG:HH11 | 1.77                     | 0.49              |
| 2:D:148:ALA:HB1  | 2:D:296:GLU:HG2  | 1.94                     | 0.49              |
| 2:C:331:MET:HG2  | 2:C:441:ASP:C    | 2.32                     | 0.49              |
| 2:D:344:VAL:HG11 | 2:D:420:LEU:HD13 | 1.93                     | 0.49              |
| 1:A:202:PRO:HB2  | 1:A:205:SER:HB2  | 1.94                     | 0.49              |
| 1:A:109:VAL:CG2  | 1:A:109:VAL:O    | 2.60                     | 0.48              |
| 2:D:292:ILE:HG13 | 2:D:457:HIS:ND1  | 2.27                     | 0.48              |
| 2:D:292:ILE:O    | 2:D:295:LEU:HB2  | 2.12                     | 0.48              |
| 2:C:194:ILE:HD11 | 2:C:270:ILE:HD11 | 1.95                     | 0.48              |
| 2:D:145:MET:HB3  | 2:D:415:ILE:CD1  | 2.42                     | 0.48              |
| 2:C:51:ILE:HD12  | 4:F:703:U:C4     | 2.48                     | 0.48              |
| 2:D:189:TYR:CZ   | 2:D:193:LEU:HD21 | 2.48                     | 0.48              |
| 2:D:51:ILE:HD13  | 2:D:55:LEU:HG    | 1.95                     | 0.48              |
| 2:C:471:ASN:OD1  | 2:C:473:GLU:HG2  | 2.13                     | 0.48              |
| 2:D:194:ILE:HD11 | 2:D:270:ILE:HD11 | 1.95                     | 0.48              |
| 2:C:195:ASN:O    | 2:C:197:ASN:N    | 2.46                     | 0.48              |
| 2:C:137:LEU:HG   | 2:C:313:LEU:HD13 | 1.96                     | 0.48              |
| 2:C:51:ILE:CG2   | 4:F:703:U:N3     | 2.76                     | 0.48              |
| 2:D:198:ILE:HD12 | 2:D:308:ARG:HH11 | 1.78                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:251:PHE:CE2  | 1:B:253:TYR:HB3  | 2.48                     | 0.48              |
| 2:C:252:ILE:HD12 | 2:C:253:ASP:H    | 1.78                     | 0.48              |
| 2:D:273:ILE:O    | 2:D:273:ILE:HG13 | 2.13                     | 0.48              |
| 2:C:136:GLU:H    | 2:C:136:GLU:CD   | 2.15                     | 0.48              |
| 2:D:357:CYS:HA   | 2:D:396:MET:O    | 2.13                     | 0.48              |
| 2:D:270:ILE:O    | 2:D:272:ASN:N    | 2.44                     | 0.48              |
| 2:D:420:LEU:O    | 2:D:423:HIS:HB3  | 2.14                     | 0.48              |
| 1:B:67:ILE:HD12  | 1:B:135:LEU:HD11 | 1.95                     | 0.48              |
| 2:D:75:LYS:CE    | 2:D:79:LEU:HD11  | 2.43                     | 0.48              |
| 1:B:33:LYS:O     | 1:B:34:LEU:C     | 2.51                     | 0.48              |
| 2:C:418:ARG:CD   | 2:C:446:MET:HG2  | 2.43                     | 0.48              |
| 2:D:174:GLU:O    | 2:D:178:ARG:HG2  | 2.14                     | 0.48              |
| 2:C:90:ASN:ND2   | 2:C:91:ILE:N     | 2.57                     | 0.48              |
| 1:B:255:ASN:OD1  | 1:B:260:TYR:CD1  | 2.67                     | 0.48              |
| 2:C:75:LYS:HE3   | 2:C:79:LEU:HD11  | 1.95                     | 0.48              |
| 1:A:33:LYS:HG2   | 1:A:34:LEU:N     | 2.26                     | 0.48              |
| 1:A:253:TYR:HE2  | 1:A:287:GLN:HE22 | 1.62                     | 0.48              |
| 1:B:112:VAL:HG12 | 1:B:114:ARG:HG2  | 1.94                     | 0.48              |
| 1:B:109:VAL:O    | 1:B:109:VAL:CG2  | 2.61                     | 0.48              |
| 2:C:293:ASP:O    | 2:C:296:GLU:N    | 2.47                     | 0.48              |
| 2:D:195:ASN:HD22 | 2:D:198:ILE:CG1  | 2.20                     | 0.48              |
| 2:D:418:ARG:CD   | 2:D:446:MET:HG2  | 2.44                     | 0.48              |
| 2:D:50:ASP:O     | 2:D:53:VAL:N     | 2.46                     | 0.48              |
| 2:C:413:HIS:HE1  | 2:C:452:ILE:O    | 1.97                     | 0.48              |
| 2:D:74:ILE:N     | 2:D:74:ILE:CD1   | 2.76                     | 0.47              |
| 2:D:286:ILE:N    | 2:D:286:ILE:CD1  | 2.76                     | 0.47              |
| 2:C:184:ILE:HB   | 2:C:262:MET:HE1  | 1.95                     | 0.47              |
| 2:D:331:MET:HG2  | 2:D:441:ASP:C    | 2.34                     | 0.47              |
| 2:D:14:THR:O     | 2:D:18:ILE:HG13  | 2.13                     | 0.47              |
| 2:D:136:GLU:H    | 2:D:136:GLU:CD   | 2.16                     | 0.47              |
| 1:B:202:PRO:HB2  | 1:B:205:SER:HB2  | 1.94                     | 0.47              |
| 2:D:289:PHE:CE1  | 2:D:309:MET:CE   | 2.97                     | 0.47              |
| 1:B:265:PHE:HA   | 1:B:268:ARG:CD   | 2.44                     | 0.47              |
| 1:B:85:LEU:HD11  | 1:B:271:TYR:O    | 2.14                     | 0.47              |
| 2:D:137:LEU:HG   | 2:D:313:LEU:HD13 | 1.97                     | 0.47              |
| 2:D:322:ILE:HG21 | 2:D:443:LEU:CD1  | 2.45                     | 0.47              |
| 1:A:265:PHE:HA   | 1:A:268:ARG:CD   | 2.44                     | 0.47              |
| 1:A:244:ARG:HA   | 1:A:258:TYR:CD2  | 2.49                     | 0.47              |
| 1:A:168:ASN:ND2  | 1:B:223:ARG:HD2  | 2.29                     | 0.47              |
| 1:A:195:LYS:N    | 1:A:195:LYS:CD   | 2.77                     | 0.47              |
| 2:C:298:LEU:HD13 | 2:C:305:PHE:HD1  | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:356:LYS:HE3  | 2:D:395:ILE:HD12 | 1.96                     | 0.47              |
| 2:C:373:LEU:HB3  | 2:C:392:HIS:CD2  | 2.49                     | 0.47              |
| 1:A:93:LEU:HD12  | 1:A:111:LEU:HD21 | 1.95                     | 0.47              |
| 2:C:292:ILE:O    | 2:C:295:LEU:HB2  | 2.13                     | 0.47              |
| 2:C:337:ILE:HD12 | 2:C:404:ILE:HG21 | 1.95                     | 0.47              |
| 2:D:307:ALA:HB1  | 2:D:308:ARG:NH1  | 2.30                     | 0.47              |
| 2:C:194:ILE:CD1  | 2:C:270:ILE:HD11 | 2.44                     | 0.47              |
| 2:C:60:LYS:C     | 2:C:60:LYS:HD3   | 2.35                     | 0.47              |
| 2:D:84:LYS:O     | 2:D:88:THR:HB    | 2.15                     | 0.47              |
| 2:C:58:LYS:O     | 2:C:116:THR:HG21 | 2.15                     | 0.47              |
| 2:D:49:LYS:HZ3   | 2:D:82:PHE:HD2   | 1.62                     | 0.47              |
| 2:D:49:LYS:HE2   | 2:D:82:PHE:HD2   | 1.80                     | 0.47              |
| 2:D:298:LEU:HD13 | 2:D:305:PHE:HD1  | 1.79                     | 0.47              |
| 2:D:304:LYS:HD3  | 2:D:305:PHE:CE1  | 2.50                     | 0.47              |
| 2:C:46:VAL:O     | 2:C:46:VAL:HG12  | 2.14                     | 0.47              |
| 1:A:168:ASN:ND2  | 1:B:223:ARG:CD   | 2.77                     | 0.47              |
| 2:D:19:GLU:HB2   | 2:D:26:PRO:CD    | 2.44                     | 0.47              |
| 2:C:162:SER:N    | 2:C:165:VAL:HG23 | 2.30                     | 0.47              |
| 1:A:43:LEU:HD23  | 1:A:290:ILE:HG23 | 1.96                     | 0.47              |
| 2:D:194:ILE:CD1  | 2:D:270:ILE:HD11 | 2.44                     | 0.47              |
| 2:D:413:HIS:HE1  | 2:D:452:ILE:O    | 1.98                     | 0.47              |
| 1:B:189:TYR:CE2  | 1:B:223:ARG:HB2  | 2.50                     | 0.47              |
| 2:D:277:ASP:OD1  | 2:D:279:THR:N    | 2.43                     | 0.47              |
| 3:E:602:U:C4'    | 3:E:603:U:OP2    | 2.63                     | 0.47              |
| 2:D:293:ASP:O    | 2:D:296:GLU:N    | 2.48                     | 0.47              |
| 2:D:75:LYS:HE3   | 2:D:79:LEU:HD11  | 1.96                     | 0.47              |
| 2:C:276:VAL:O    | 2:C:277:ASP:C    | 2.53                     | 0.47              |
| 2:D:288:MET:CE   | 2:D:294:ARG:HD2  | 2.45                     | 0.46              |
| 2:D:58:LYS:HD2   | 3:E:601:DC:N3    | 2.30                     | 0.46              |
| 2:D:289:PHE:HE1  | 2:D:309:MET:CE   | 2.28                     | 0.46              |
| 2:C:51:ILE:C     | 2:C:51:ILE:HD13  | 2.36                     | 0.46              |
| 1:B:285:PHE:O    | 1:B:288:GLN:HB3  | 2.15                     | 0.46              |
| 2:C:145:MET:HG2  | 2:C:415:ILE:HG12 | 1.98                     | 0.46              |
| 1:B:43:LEU:HB2   | 1:B:74:HIS:HB2   | 1.97                     | 0.46              |
| 1:B:230:VAL:O    | 1:B:234:LYS:HG2  | 2.16                     | 0.46              |
| 2:C:270:ILE:O    | 2:C:272:ASN:N    | 2.45                     | 0.46              |
| 2:C:47:PHE:CD2   | 2:C:105:VAL:HG22 | 2.51                     | 0.46              |
| 2:D:218:ALA:O    | 2:D:229:ILE:HD11 | 2.15                     | 0.46              |
| 2:C:141:MET:CE   | 2:C:443:LEU:O    | 2.63                     | 0.46              |
| 1:A:168:ASN:ND2  | 1:B:223:ARG:NE   | 2.64                     | 0.46              |
| 2:C:396:MET:HE2  | 2:C:427:TYR:CD2  | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:192:TYR:CD2  | 2:D:193:LEU:HD22 | 2.50                     | 0.46              |
| 1:B:239:LEU:HA   | 1:B:243:VAL:CG2  | 2.46                     | 0.46              |
| 1:A:96:GLY:HA3   | 1:A:115:PHE:CE1  | 2.51                     | 0.46              |
| 1:B:49:PHE:CD2   | 1:B:50:LEU:HD13  | 2.51                     | 0.46              |
| 1:B:267:LEU:HA   | 1:B:270:VAL:HG23 | 1.98                     | 0.46              |
| 2:C:289:PHE:CE1  | 2:C:309:MET:CE   | 2.98                     | 0.46              |
| 2:C:50:ASP:O     | 2:C:53:VAL:N     | 2.48                     | 0.46              |
| 2:C:17:ILE:HD12  | 2:C:42:GLN:CB    | 2.44                     | 0.46              |
| 2:C:49:LYS:HE2   | 2:C:82:PHE:HD2   | 1.81                     | 0.46              |
| 2:D:78:ILE:HG12  | 2:D:223:PHE:CD1  | 2.51                     | 0.46              |
| 2:D:60:LYS:C     | 2:D:60:LYS:HD3   | 2.36                     | 0.46              |
| 2:D:289:PHE:HE1  | 2:D:309:MET:HE1  | 1.81                     | 0.46              |
| 2:C:275:ILE:HG13 | 2:C:275:ILE:O    | 2.15                     | 0.46              |
| 1:A:251:PHE:CE2  | 1:A:253:TYR:HB3  | 2.50                     | 0.46              |
| 2:D:169:ASN:O    | 2:D:173:GLU:HG3  | 2.16                     | 0.46              |
| 1:B:59:LEU:HG    | 1:B:59:LEU:O     | 2.16                     | 0.46              |
| 2:C:277:ASP:OD1  | 2:C:279:THR:N    | 2.44                     | 0.46              |
| 1:B:94:ILE:HG23  | 1:B:112:VAL:HB   | 1.97                     | 0.46              |
| 2:D:320:HIS:O    | 2:D:321:GLY:C    | 2.54                     | 0.46              |
| 2:D:134:MET:HA   | 2:D:134:MET:CE   | 2.46                     | 0.46              |
| 2:D:322:ILE:HB   | 2:D:324:PHE:HE1  | 1.81                     | 0.46              |
| 2:D:44:ILE:HD13  | 2:D:101:GLN:HE21 | 1.80                     | 0.46              |
| 2:D:289:PHE:CE1  | 2:D:309:MET:HE1  | 2.50                     | 0.46              |
| 1:A:94:ILE:HG23  | 1:A:112:VAL:HB   | 1.97                     | 0.46              |
| 2:C:51:ILE:HD13  | 2:C:55:LEU:HG    | 1.98                     | 0.46              |
| 1:A:189:TYR:CE2  | 1:A:223:ARG:HB2  | 2.51                     | 0.46              |
| 1:B:215:THR:HG23 | 2:C:364:ASN:ND2  | 2.31                     | 0.46              |
| 1:A:220:ARG:HG3  | 1:A:220:ARG:HH11 | 1.80                     | 0.46              |
| 1:A:63:THR:HG23  | 1:A:90:LYS:HG3   | 1.97                     | 0.46              |
| 1:B:52:LYS:HD3   | 2:C:371:LEU:HD13 | 1.98                     | 0.46              |
| 2:D:426:LEU:O    | 2:D:430:LEU:HG   | 2.16                     | 0.45              |
| 1:A:43:LEU:HB2   | 1:A:74:HIS:HB2   | 1.98                     | 0.45              |
| 2:D:366:LEU:HD11 | 2:D:370:ILE:HD11 | 1.98                     | 0.45              |
| 2:D:51:ILE:HD12  | 3:E:603:U:C5     | 2.52                     | 0.45              |
| 2:D:53:VAL:CG1   | 2:D:57:LYS:HE3   | 2.47                     | 0.45              |
| 1:A:18:ASN:O     | 1:A:235:LYS:HG2  | 2.16                     | 0.45              |
| 1:B:3:VAL:HB     | 1:B:249:VAL:CG1  | 2.46                     | 0.45              |
| 2:D:214:LEU:HD22 | 2:D:243:ILE:HD11 | 1.96                     | 0.45              |
| 1:A:285:PHE:O    | 1:A:288:GLN:HB3  | 2.15                     | 0.45              |
| 2:C:379:CYS:C    | 2:C:388:VAL:HG23 | 2.36                     | 0.45              |
| 1:A:67:ILE:HD12  | 1:A:135:LEU:HD11 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:192:TYR:CD2  | 2:C:193:LEU:HD22 | 2.51                     | 0.45              |
| 1:B:253:TYR:OH   | 1:B:287:GLN:NE2  | 2.49                     | 0.45              |
| 2:C:169:ASN:O    | 2:C:173:GLU:HG3  | 2.17                     | 0.45              |
| 2:C:289:PHE:CE1  | 2:C:309:MET:HE1  | 2.51                     | 0.45              |
| 2:C:319:THR:HG22 | 2:C:320:HIS:CD2  | 2.52                     | 0.45              |
| 2:C:328:ARG:HB3  | 2:C:444:ASN:CB   | 2.45                     | 0.45              |
| 2:D:19:GLU:CB    | 2:D:26:PRO:HD3   | 2.46                     | 0.45              |
| 2:D:58:LYS:O     | 2:D:116:THR:HG21 | 2.17                     | 0.45              |
| 1:A:100:ASP:CG   | 1:A:102:ILE:HG12 | 2.36                     | 0.45              |
| 2:D:59:ASN:HD22  | 2:D:220:LEU:HD11 | 1.82                     | 0.45              |
| 2:C:273:ILE:HG13 | 2:C:273:ILE:O    | 2.16                     | 0.45              |
| 2:D:145:MET:HG2  | 2:D:415:ILE:HG12 | 1.99                     | 0.45              |
| 2:D:406:LEU:C    | 2:D:413:HIS:HB2  | 2.37                     | 0.45              |
| 1:A:122:ARG:HG2  | 1:A:166:ILE:HG23 | 1.98                     | 0.45              |
| 2:D:276:VAL:O    | 2:D:277:ASP:C    | 2.54                     | 0.45              |
| 2:C:289:PHE:HE1  | 2:C:309:MET:HE1  | 1.82                     | 0.45              |
| 1:B:244:ARG:HA   | 1:B:258:TYR:CD2  | 2.51                     | 0.45              |
| 1:B:258:TYR:O    | 1:B:261:PHE:HB3  | 2.16                     | 0.45              |
| 1:B:63:THR:HG23  | 1:B:90:LYS:HG3   | 1.97                     | 0.45              |
| 1:A:49:PHE:CD2   | 1:A:50:LEU:HD13  | 2.52                     | 0.45              |
| 2:C:96:THR:HG23  | 2:C:477:ILE:HG13 | 1.98                     | 0.45              |
| 1:A:37:GLN:C     | 1:A:39:GLN:H     | 2.20                     | 0.45              |
| 2:D:191:LEU:O    | 2:D:194:ILE:HB   | 2.17                     | 0.45              |
| 2:C:78:ILE:HG12  | 2:C:223:PHE:CD1  | 2.51                     | 0.45              |
| 2:C:331:MET:HB3  | 2:C:445:SER:OG   | 2.17                     | 0.45              |
| 1:B:195:LYS:CD   | 1:B:195:LYS:N    | 2.79                     | 0.45              |
| 1:A:76:ARG:O     | 1:A:76:ARG:HD2   | 2.17                     | 0.45              |
| 2:D:373:LEU:HB3  | 2:D:392:HIS:CD2  | 2.51                     | 0.45              |
| 2:D:256:ASN:C    | 2:D:256:ASN:HD22 | 2.16                     | 0.45              |
| 2:C:75:LYS:HD3   | 2:C:75:LYS:O     | 2.16                     | 0.45              |
| 2:D:184:ILE:HB   | 2:D:262:MET:HE1  | 1.98                     | 0.45              |
| 2:D:24:ARG:HD3   | 2:D:89:TYR:HE2   | 1.82                     | 0.45              |
| 1:B:175:LYS:NZ   | 1:B:207:GLU:OE2  | 2.25                     | 0.45              |
| 1:B:33:LYS:HG2   | 1:B:34:LEU:N     | 2.28                     | 0.45              |
| 2:C:304:LYS:HD3  | 2:C:305:PHE:CE1  | 2.52                     | 0.45              |
| 2:D:51:ILE:HD13  | 2:D:51:ILE:C     | 2.38                     | 0.44              |
| 2:C:44:ILE:HG21  | 2:C:101:GLN:NE2  | 2.32                     | 0.44              |
| 1:A:3:VAL:HB     | 1:A:249:VAL:CG1  | 2.47                     | 0.44              |
| 1:A:258:TYR:O    | 1:A:261:PHE:HB3  | 2.17                     | 0.44              |
| 2:C:14:THR:O     | 2:C:18:ILE:HG13  | 2.16                     | 0.44              |
| 1:B:96:GLY:HA3   | 1:B:115:PHE:CE1  | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:316:VAL:CG2  | 2:C:322:ILE:HG13 | 2.36                     | 0.44              |
| 2:C:325:ASP:C    | 2:C:327:LYS:N    | 2.70                     | 0.44              |
| 1:A:121:LEU:CD1  | 1:A:163:MET:HA   | 2.45                     | 0.44              |
| 1:B:253:TYR:HE2  | 1:B:287:GLN:HE22 | 1.65                     | 0.44              |
| 1:B:150:THR:O    | 1:B:154:LEU:HG   | 2.16                     | 0.44              |
| 1:A:52:LYS:HD3   | 2:D:371:LEU:HD13 | 1.99                     | 0.44              |
| 2:D:476:ILE:HD13 | 5:G:802:U:H4'    | 1.99                     | 0.44              |
| 2:C:53:VAL:HG13  | 2:C:75:LYS:HA    | 1.99                     | 0.44              |
| 1:A:66:TYR:CG    | 1:A:69:SER:HB3   | 2.52                     | 0.44              |
| 1:B:93:LEU:HB2   | 1:B:111:LEU:CD2  | 2.47                     | 0.44              |
| 2:C:59:ASN:HD22  | 2:C:220:LEU:HD11 | 1.82                     | 0.44              |
| 2:C:24:ARG:HD3   | 2:C:89:TYR:HE2   | 1.79                     | 0.44              |
| 2:D:44:ILE:HG21  | 2:D:101:GLN:NE2  | 2.33                     | 0.44              |
| 1:A:293:PHE:C    | 1:A:293:PHE:CD2  | 2.91                     | 0.44              |
| 1:A:239:LEU:HA   | 1:A:243:VAL:CG2  | 2.48                     | 0.44              |
| 2:C:53:VAL:O     | 2:C:57:LYS:HG3   | 2.18                     | 0.44              |
| 2:C:437:GLN:O    | 2:C:440:SER:HB3  | 2.18                     | 0.44              |
| 2:D:437:GLN:O    | 2:D:440:SER:HB3  | 2.18                     | 0.44              |
| 2:D:53:VAL:HG13  | 2:D:75:LYS:HA    | 2.00                     | 0.44              |
| 2:D:75:LYS:O     | 2:D:75:LYS:HD3   | 2.17                     | 0.44              |
| 2:D:94:LEU:O     | 2:D:97:ILE:N     | 2.48                     | 0.44              |
| 2:D:169:ASN:OD1  | 2:D:203:ILE:HG13 | 2.17                     | 0.44              |
| 2:C:49:LYS:CE    | 2:C:82:PHE:HD2   | 2.30                     | 0.44              |
| 2:D:230:ILE:HD12 | 2:D:471:ASN:ND2  | 2.31                     | 0.44              |
| 2:C:134:MET:HA   | 2:C:134:MET:CE   | 2.48                     | 0.44              |
| 2:C:174:GLU:OE1  | 2:C:178:ARG:HD3  | 2.18                     | 0.44              |
| 2:C:21:TYR:CG    | 2:C:41:ILE:CG2   | 2.99                     | 0.44              |
| 1:B:122:ARG:HG2  | 1:B:166:ILE:HG23 | 1.99                     | 0.44              |
| 2:D:328:ARG:HB3  | 2:D:444:ASN:CB   | 2.45                     | 0.44              |
| 2:C:406:LEU:C    | 2:C:413:HIS:HB2  | 2.38                     | 0.44              |
| 2:C:203:ILE:O    | 2:C:252:ILE:HD11 | 2.17                     | 0.44              |
| 1:B:59:LEU:HG    | 1:B:89:ILE:HD11  | 2.00                     | 0.44              |
| 1:A:58:ILE:HD12  | 1:A:58:ILE:O     | 2.18                     | 0.44              |
| 2:C:286:ILE:N    | 2:C:286:ILE:CD1  | 2.79                     | 0.44              |
| 1:A:278:THR:O    | 1:A:281:ALA:HB3  | 2.18                     | 0.44              |
| 2:C:354:PHE:HB2  | 2:C:394:ASN:O    | 2.18                     | 0.44              |
| 2:C:322:ILE:HB   | 2:C:324:PHE:HE1  | 1.83                     | 0.44              |
| 2:C:115:LEU:CD1  | 2:C:171:LEU:CD2  | 2.96                     | 0.44              |
| 2:C:48:ASN:HB3   | 4:F:703:U:O2     | 2.18                     | 0.44              |
| 1:B:248:VAL:HG21 | 1:B:261:PHE:CD2  | 2.53                     | 0.44              |
| 2:D:235:PRO:HD2  | 2:D:467:HIS:ND1  | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:59:ASN:ND2   | 2:D:220:LEU:HD11 | 2.33                     | 0.43              |
| 2:D:73:GLU:CB    | 2:D:77:ARG:HH12  | 2.24                     | 0.43              |
| 2:C:53:VAL:CG1   | 2:C:57:LYS:HE3   | 2.48                     | 0.43              |
| 2:D:74:ILE:CG1   | 2:D:224:ILE:HA   | 2.42                     | 0.43              |
| 2:C:366:LEU:HD11 | 2:C:370:ILE:HD11 | 2.00                     | 0.43              |
| 1:B:279:THR:O    | 1:B:282:LYS:N    | 2.50                     | 0.43              |
| 2:C:317:ARG:NH1  | 2:C:317:ARG:HG2  | 2.32                     | 0.43              |
| 2:D:319:THR:HG22 | 2:D:320:HIS:CD2  | 2.54                     | 0.43              |
| 1:B:293:PHE:C    | 1:B:293:PHE:CD2  | 2.92                     | 0.43              |
| 2:D:51:ILE:O     | 2:D:54:SER:HB2   | 2.17                     | 0.43              |
| 2:C:256:ASN:C    | 2:C:256:ASN:HD22 | 2.18                     | 0.43              |
| 2:D:291:GLN:O    | 2:D:292:ILE:C    | 2.56                     | 0.43              |
| 2:C:307:ALA:HB1  | 2:C:308:ARG:NH1  | 2.33                     | 0.43              |
| 2:D:53:VAL:O     | 2:D:57:LYS:HG3   | 2.19                     | 0.43              |
| 2:C:77:ARG:NE    | 2:C:226:GLY:HA2  | 2.33                     | 0.43              |
| 1:B:58:ILE:HD12  | 1:B:58:ILE:O     | 2.18                     | 0.43              |
| 2:C:145:MET:HB3  | 2:C:415:ILE:CD1  | 2.47                     | 0.43              |
| 1:B:37:GLN:C     | 1:B:39:GLN:H     | 2.22                     | 0.43              |
| 1:A:248:VAL:HG21 | 1:A:261:PHE:CD2  | 2.53                     | 0.43              |
| 2:C:468:GLY:O    | 2:C:469:PHE:HB3  | 2.18                     | 0.43              |
| 2:D:379:CYS:C    | 2:D:388:VAL:HG23 | 2.38                     | 0.43              |
| 2:D:96:THR:HG23  | 2:D:477:ILE:HG13 | 1.99                     | 0.43              |
| 1:A:253:TYR:OH   | 1:A:284:LEU:HA   | 2.17                     | 0.43              |
| 1:A:192:HIS:O    | 1:A:212:SER:CB   | 2.66                     | 0.43              |
| 2:C:276:VAL:O    | 2:C:281:GLN:NE2  | 2.39                     | 0.43              |
| 2:D:473:GLU:CG   | 2:D:474:LYS:H    | 2.25                     | 0.43              |
| 2:D:174:GLU:OE1  | 2:D:178:ARG:HD3  | 2.19                     | 0.43              |
| 2:C:84:LYS:O     | 2:C:88:THR:HB    | 2.19                     | 0.43              |
| 1:B:34:LEU:HD11  | 1:B:260:TYR:OH   | 2.18                     | 0.43              |
| 2:C:473:GLU:CG   | 2:C:474:LYS:H    | 2.26                     | 0.43              |
| 2:C:288:MET:SD   | 2:C:294:ARG:NE   | 2.91                     | 0.43              |
| 1:B:121:LEU:CD1  | 1:B:163:MET:HA   | 2.46                     | 0.43              |
| 1:B:4:VAL:CG2    | 1:B:5:SER:N      | 2.81                     | 0.43              |
| 2:D:49:LYS:CE    | 2:D:82:PHE:HD2   | 2.31                     | 0.43              |
| 2:C:289:PHE:HE1  | 2:C:309:MET:CE   | 2.31                     | 0.43              |
| 2:D:46:VAL:HG12  | 2:D:46:VAL:O     | 2.18                     | 0.43              |
| 3:E:603:U:C6     | 3:E:603:U:C5'    | 2.90                     | 0.43              |
| 2:D:77:ARG:NE    | 2:D:226:GLY:HA2  | 2.34                     | 0.43              |
| 2:C:19:GLU:HB2   | 2:C:26:PRO:CD    | 2.48                     | 0.43              |
| 1:A:267:LEU:HA   | 1:A:270:VAL:HG23 | 2.01                     | 0.43              |
| 2:C:395:ILE:HB   | 2:C:397:TYR:CE1  | 2.54                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:229:ILE:C    | 2:C:230:ILE:HD13 | 2.39                     | 0.43              |
| 2:C:137:LEU:HD21 | 2:C:324:PHE:CD2  | 2.54                     | 0.43              |
| 2:C:141:MET:HE1  | 2:C:446:MET:HB2  | 2.00                     | 0.43              |
| 2:D:316:VAL:HG13 | 2:D:317:ARG:N    | 2.34                     | 0.43              |
| 2:C:264:VAL:HB   | 2:C:430:LEU:O    | 2.18                     | 0.43              |
| 1:B:257:GLU:N    | 1:B:257:GLU:OE2  | 2.51                     | 0.43              |
| 2:C:331:MET:HE2  | 2:C:441:ASP:HB2  | 1.99                     | 0.43              |
| 2:D:203:ILE:O    | 2:D:252:ILE:HD11 | 2.18                     | 0.43              |
| 1:B:100:ASP:CG   | 1:B:102:ILE:HG12 | 2.38                     | 0.43              |
| 1:A:39:GLN:NE2   | 1:A:39:GLN:HA    | 2.33                     | 0.43              |
| 1:A:54:GLN:HB2   | 1:A:59:LEU:HD23  | 2.01                     | 0.43              |
| 1:A:93:LEU:HB2   | 1:A:111:LEU:CD2  | 2.48                     | 0.43              |
| 1:B:41:LYS:HE2   | 1:B:41:LYS:HB3   | 1.78                     | 0.43              |
| 1:A:257:GLU:OE2  | 1:A:257:GLU:N    | 2.51                     | 0.43              |
| 2:D:396:MET:HE2  | 2:D:427:TYR:CD2  | 2.54                     | 0.43              |
| 1:B:132:LYS:HD3  | 2:C:464:PRO:HB2  | 2.00                     | 0.43              |
| 1:B:145:GLY:O    | 1:B:146:ASN:HB2  | 2.19                     | 0.43              |
| 2:C:292:ILE:CG2  | 2:C:293:ASP:N    | 2.81                     | 0.42              |
| 2:C:296:GLU:O    | 2:C:299:SER:HB2  | 2.18                     | 0.42              |
| 1:A:253:TYR:CE1  | 1:A:284:LEU:HG   | 2.54                     | 0.42              |
| 2:C:268:ILE:CG1  | 2:C:277:ASP:HA   | 2.49                     | 0.42              |
| 2:D:287:LYS:HG2  | 2:D:287:LYS:O    | 2.17                     | 0.42              |
| 2:D:471:ASN:OD1  | 2:D:473:GLU:CG   | 2.68                     | 0.42              |
| 2:C:322:ILE:HG21 | 2:C:443:LEU:HD12 | 1.99                     | 0.42              |
| 2:C:19:GLU:CB    | 2:C:26:PRO:HD3   | 2.49                     | 0.42              |
| 2:D:105:VAL:O    | 2:D:105:VAL:HG12 | 2.17                     | 0.42              |
| 1:A:59:LEU:HG    | 1:A:89:ILE:HD11  | 2.02                     | 0.42              |
| 1:A:255:ASN:OD1  | 1:A:257:GLU:OE2  | 2.36                     | 0.42              |
| 1:B:65:VAL:HG23  | 1:B:133:ILE:HG23 | 2.00                     | 0.42              |
| 2:C:191:LEU:O    | 2:C:194:ILE:HB   | 2.19                     | 0.42              |
| 2:D:242:VAL:HG23 | 2:D:252:ILE:O    | 2.19                     | 0.42              |
| 2:D:268:ILE:CG1  | 2:D:277:ASP:HA   | 2.49                     | 0.42              |
| 1:A:239:LEU:O    | 1:A:243:VAL:HB   | 2.19                     | 0.42              |
| 2:D:282:LEU:HD13 | 2:D:312:MET:HE3  | 2.00                     | 0.42              |
| 1:A:137:SER:OG   | 1:A:160:GLN:HG2  | 2.19                     | 0.42              |
| 1:B:18:ASN:HB2   | 1:B:238:TYR:CE2  | 2.54                     | 0.42              |
| 2:C:109:THR:CG2  | 4:F:702:U:O2'    | 2.66                     | 0.42              |
| 2:D:462:LYS:HZ3  | 2:D:462:LYS:HB2  | 1.84                     | 0.42              |
| 2:D:366:LEU:HD12 | 2:D:370:ILE:HG13 | 2.02                     | 0.42              |
| 2:D:275:ILE:HG13 | 2:D:275:ILE:O    | 2.19                     | 0.42              |
| 2:C:383:SER:O    | 2:C:384:VAL:C    | 2.58                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:55:LEU:HD22  | 3:E:602:U:C5     | 2.54                     | 0.42              |
| 2:C:94:LEU:O     | 2:C:97:ILE:N     | 2.50                     | 0.42              |
| 2:D:325:ASP:C    | 2:D:327:LYS:N    | 2.73                     | 0.42              |
| 2:D:162:SER:O    | 2:D:165:VAL:HB   | 2.20                     | 0.42              |
| 2:C:235:PRO:HD2  | 2:C:467:HIS:ND1  | 2.34                     | 0.42              |
| 1:A:65:VAL:HG23  | 1:A:133:ILE:HG23 | 2.00                     | 0.42              |
| 2:D:354:PHE:HB2  | 2:D:394:ASN:O    | 2.20                     | 0.42              |
| 2:C:291:GLN:O    | 2:C:292:ILE:C    | 2.57                     | 0.42              |
| 2:D:137:LEU:HD21 | 2:D:324:PHE:CD2  | 2.55                     | 0.42              |
| 2:C:78:ILE:O     | 2:C:80:SER:N     | 2.53                     | 0.42              |
| 2:D:21:TYR:CG    | 2:D:41:ILE:CG2   | 3.01                     | 0.42              |
| 2:C:327:LYS:O    | 2:C:328:ARG:HB2  | 2.18                     | 0.42              |
| 2:C:96:THR:HG23  | 2:C:477:ILE:HD12 | 2.02                     | 0.42              |
| 2:D:209:ASN:O    | 2:D:211:ARG:N    | 2.52                     | 0.42              |
| 2:C:366:LEU:HD12 | 2:C:370:ILE:HG13 | 2.02                     | 0.42              |
| 1:A:198:GLN:HA   | 1:A:199:PRO:HD3  | 1.73                     | 0.42              |
| 1:B:122:ARG:N    | 1:B:166:ILE:HG21 | 2.34                     | 0.42              |
| 2:C:211:ARG:O    | 2:C:215:ILE:HG13 | 2.19                     | 0.42              |
| 2:D:189:TYR:O    | 2:D:193:LEU:HD23 | 2.19                     | 0.42              |
| 2:D:365:VAL:HG12 | 2:D:369:ASP:OD2  | 2.20                     | 0.42              |
| 2:D:264:VAL:HB   | 2:D:430:LEU:O    | 2.19                     | 0.42              |
| 2:C:78:ILE:O     | 2:C:81:TYR:N     | 2.53                     | 0.42              |
| 2:C:74:ILE:CD1   | 2:C:74:ILE:H     | 2.33                     | 0.42              |
| 2:D:331:MET:HB3  | 2:D:445:SER:OG   | 2.20                     | 0.42              |
| 2:C:209:ASN:O    | 2:C:211:ARG:N    | 2.53                     | 0.42              |
| 1:B:201:ALA:O    | 1:B:202:PRO:C    | 2.58                     | 0.42              |
| 2:D:463:LYS:HA   | 2:D:464:PRO:HD3  | 1.89                     | 0.42              |
| 1:A:19:GLU:HB2   | 1:A:234:LYS:HB3  | 2.02                     | 0.42              |
| 2:C:473:GLU:CG   | 2:C:474:LYS:N    | 2.74                     | 0.42              |
| 2:D:317:ARG:NH1  | 2:D:317:ARG:HG2  | 2.34                     | 0.42              |
| 2:D:53:VAL:HG11  | 2:D:75:LYS:CG    | 2.43                     | 0.42              |
| 1:B:121:LEU:CB   | 1:B:166:ILE:HG21 | 2.50                     | 0.42              |
| 2:D:268:ILE:HG12 | 2:D:277:ASP:HA   | 2.02                     | 0.42              |
| 2:C:250:HIS:C    | 2:C:250:HIS:CD2  | 2.93                     | 0.42              |
| 2:C:270:ILE:CG2  | 2:C:271:ASP:H    | 2.05                     | 0.42              |
| 1:B:66:TYR:CG    | 1:B:69:SER:HB3   | 2.55                     | 0.42              |
| 2:C:49:LYS:NZ    | 2:C:82:PHE:HD2   | 2.18                     | 0.42              |
| 2:C:268:ILE:HG12 | 2:C:277:ASP:HA   | 2.02                     | 0.42              |
| 2:C:395:ILE:HB   | 2:C:397:TYR:HE1  | 1.85                     | 0.42              |
| 2:C:403:THR:HG22 | 2:C:458:THR:O    | 2.20                     | 0.42              |
| 2:D:250:HIS:CD2  | 2:D:250:HIS:C    | 2.94                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:145:GLY:O    | 1:A:146:ASN:HB2  | 2.20                     | 0.42              |
| 2:C:147:VAL:HG23 | 2:C:454:ILE:HG13 | 2.02                     | 0.41              |
| 2:C:230:ILE:HD12 | 2:C:471:ASN:ND2  | 2.34                     | 0.41              |
| 1:A:121:LEU:CB   | 1:A:166:ILE:HG21 | 2.50                     | 0.41              |
| 2:D:135:GLU:HB3  | 2:D:139:ARG:NH2  | 2.35                     | 0.41              |
| 2:C:135:GLU:HB3  | 2:C:139:ARG:NH2  | 2.35                     | 0.41              |
| 1:A:9:PRO:HD2    | 1:A:265:PHE:CD2  | 2.54                     | 0.41              |
| 2:C:449:ARG:HH11 | 2:C:449:ARG:HB3  | 1.83                     | 0.41              |
| 2:C:427:TYR:CE1  | 2:C:431:THR:HG21 | 2.55                     | 0.41              |
| 2:C:318:TYR:O    | 2:C:320:HIS:N    | 2.53                     | 0.41              |
| 1:A:230:VAL:O    | 1:A:234:LYS:HG2  | 2.20                     | 0.41              |
| 1:B:199:PRO:HG2  | 1:B:266:MET:SD   | 2.60                     | 0.41              |
| 1:A:41:LYS:HB3   | 1:A:41:LYS:HE2   | 1.79                     | 0.41              |
| 2:D:256:ASN:ND2  | 2:D:257:ILE:H    | 2.02                     | 0.41              |
| 2:C:316:VAL:HG13 | 2:C:317:ARG:N    | 2.36                     | 0.41              |
| 2:D:115:LEU:CD1  | 2:D:171:LEU:CD2  | 2.98                     | 0.41              |
| 2:D:61:LYS:NZ    | 2:D:62:ARG:HG3   | 2.36                     | 0.41              |
| 1:A:59:LEU:O     | 1:A:59:LEU:HG    | 2.21                     | 0.41              |
| 2:D:395:ILE:HB   | 2:D:397:TYR:CE1  | 2.55                     | 0.41              |
| 1:A:201:ALA:O    | 1:A:202:PRO:C    | 2.59                     | 0.41              |
| 1:B:248:VAL:HG21 | 1:B:261:PHE:CG   | 2.55                     | 0.41              |
| 2:D:473:GLU:CG   | 2:D:474:LYS:N    | 2.75                     | 0.41              |
| 2:C:143:ASN:HA   | 2:C:146:ASN:HD22 | 1.85                     | 0.41              |
| 2:C:301:ASP:O    | 2:C:303:GLU:N    | 2.53                     | 0.41              |
| 2:D:292:ILE:CG2  | 2:D:293:ASP:N    | 2.82                     | 0.41              |
| 2:D:143:ASN:HA   | 2:D:146:ASN:HD22 | 1.85                     | 0.41              |
| 1:A:292:ARG:NH1  | 1:A:292:ARG:HG3  | 2.34                     | 0.41              |
| 2:D:211:ARG:O    | 2:D:215:ILE:HG13 | 2.20                     | 0.41              |
| 1:A:193:GLY:HA3  | 1:A:212:SER:HB3  | 2.02                     | 0.41              |
| 2:D:322:ILE:HB   | 2:D:324:PHE:CE1  | 2.55                     | 0.41              |
| 2:D:283:LEU:HD22 | 2:D:429:MET:HE2  | 2.01                     | 0.41              |
| 2:D:318:TYR:O    | 2:D:320:HIS:N    | 2.53                     | 0.41              |
| 2:D:329:ASN:HB2  | 2:D:330:ASN:H    | 1.71                     | 0.41              |
| 2:D:48:ASN:N     | 3:E:603:U:O2     | 2.54                     | 0.41              |
| 2:D:77:ARG:HE    | 2:D:226:GLY:HA2  | 1.85                     | 0.41              |
| 2:C:347:THR:CG2  | 2:C:349:LYS:HG2  | 2.50                     | 0.41              |
| 2:C:162:SER:N    | 2:C:165:VAL:CG2  | 2.83                     | 0.41              |
| 2:D:49:LYS:HG3   | 2:D:82:PHE:CD2   | 2.55                     | 0.41              |
| 1:B:192:HIS:O    | 1:B:212:SER:CB   | 2.68                     | 0.41              |
| 2:C:462:LYS:HZ3  | 2:C:462:LYS:HB2  | 1.85                     | 0.41              |
| 1:A:248:VAL:HG21 | 1:A:261:PHE:CG   | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:98:HIS:CE1   | 1:B:113:THR:HG21 | 2.55                     | 0.41              |
| 2:C:256:ASN:ND2  | 2:C:257:ILE:H    | 2.03                     | 0.41              |
| 2:D:17:ILE:HD12  | 2:D:42:GLN:CB    | 2.47                     | 0.41              |
| 2:C:90:ASN:OD1   | 2:C:93:LYS:HG3   | 2.21                     | 0.41              |
| 2:D:286:ILE:H    | 2:D:286:ILE:CD1  | 2.33                     | 0.41              |
| 2:C:58:LYS:C     | 2:C:61:LYS:NZ    | 2.73                     | 0.41              |
| 2:C:233:LYS:HB2  | 2:C:241:MET:HG2  | 2.02                     | 0.41              |
| 1:A:18:ASN:HB2   | 1:A:238:TYR:CE2  | 2.55                     | 0.41              |
| 1:B:193:GLY:HA3  | 1:B:212:SER:HB3  | 2.02                     | 0.41              |
| 2:C:352:PHE:HE2  | 2:C:434:GLU:O    | 2.04                     | 0.41              |
| 2:C:301:ASP:N    | 2:C:302:PRO:CD   | 2.84                     | 0.41              |
| 2:C:81:TYR:O     | 2:C:83:SER:N     | 2.54                     | 0.41              |
| 2:C:74:ILE:CG1   | 2:C:224:ILE:HA   | 2.46                     | 0.41              |
| 2:C:183:CYS:SG   | 2:C:205:ILE:HD12 | 2.60                     | 0.41              |
| 2:D:90:ASN:ND2   | 2:D:91:ILE:N     | 2.60                     | 0.41              |
| 2:C:356:LYS:HG3  | 2:C:395:ILE:HD12 | 2.02                     | 0.41              |
| 2:D:78:ILE:HG22  | 2:D:79:LEU:N     | 2.36                     | 0.41              |
| 2:C:115:LEU:HD13 | 2:C:171:LEU:CD2  | 2.50                     | 0.41              |
| 2:D:331:MET:HE2  | 2:D:441:ASP:HB2  | 2.01                     | 0.41              |
| 2:C:169:ASN:OD1  | 2:C:203:ILE:HG13 | 2.20                     | 0.41              |
| 1:A:4:VAL:CG2    | 1:A:5:SER:N      | 2.83                     | 0.41              |
| 2:C:51:ILE:O     | 2:C:54:SER:HB2   | 2.20                     | 0.41              |
| 1:B:93:LEU:HB2   | 1:B:111:LEU:HD23 | 2.02                     | 0.41              |
| 2:D:81:TYR:O     | 2:D:83:SER:N     | 2.54                     | 0.41              |
| 2:C:359:VAL:CG1  | 2:C:400:PHE:HB2  | 2.51                     | 0.41              |
| 2:D:333:MET:HE1  | 2:D:348:THR:HG22 | 2.02                     | 0.41              |
| 2:C:164:LEU:HD23 | 2:C:167:ASN:ND2  | 2.34                     | 0.41              |
| 1:B:54:GLN:HB2   | 1:B:59:LEU:HD23  | 2.03                     | 0.41              |
| 1:B:19:GLU:HB2   | 1:B:234:LYS:HB3  | 2.03                     | 0.41              |
| 1:A:132:LYS:HD3  | 2:D:464:PRO:HB2  | 2.02                     | 0.41              |
| 2:C:329:ASN:HB2  | 2:C:330:ASN:H    | 1.72                     | 0.41              |
| 2:D:359:VAL:CG1  | 2:D:400:PHE:HB2  | 2.51                     | 0.41              |
| 2:D:229:ILE:C    | 2:D:230:ILE:HD13 | 2.42                     | 0.40              |
| 1:B:237:TYR:OH   | 1:B:241:LYS:HD3  | 2.21                     | 0.40              |
| 2:C:51:ILE:CG2   | 4:F:703:U:H3     | 2.32                     | 0.40              |
| 2:C:287:LYS:O    | 2:C:287:LYS:HG2  | 2.20                     | 0.40              |
| 1:A:85:LEU:HD11  | 1:A:271:TYR:O    | 2.21                     | 0.40              |
| 2:C:294:ARG:HA   | 2:C:297:ASP:OD2  | 2.21                     | 0.40              |
| 2:D:308:ARG:O    | 2:D:312:MET:HG3  | 2.21                     | 0.40              |
| 2:C:193:LEU:HB3  | 2:C:270:ILE:HG21 | 2.03                     | 0.40              |
| 2:C:426:LEU:O    | 2:C:430:LEU:HG   | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:96:THR:HG23  | 2:D:477:ILE:HD12 | 2.03                     | 0.40              |
| 2:D:234:ILE:HG21 | 2:D:237:LEU:HD23 | 2.03                     | 0.40              |
| 2:D:214:LEU:HD11 | 2:D:241:MET:O    | 2.21                     | 0.40              |
| 2:C:364:ASN:OD1  | 2:C:365:VAL:N    | 2.54                     | 0.40              |
| 2:C:365:VAL:HG12 | 2:C:369:ASP:OD2  | 2.21                     | 0.40              |
| 2:D:383:SER:O    | 2:D:384:VAL:C    | 2.60                     | 0.40              |
| 2:C:301:ASP:H    | 2:C:302:PRO:CD   | 2.31                     | 0.40              |
| 2:D:107:THR:O    | 2:D:108:TYR:C    | 2.60                     | 0.40              |
| 2:D:145:MET:O    | 2:D:147:VAL:HG22 | 2.21                     | 0.40              |
| 2:D:301:ASP:N    | 2:D:302:PRO:CD   | 2.84                     | 0.40              |
| 2:C:96:THR:HG23  | 2:C:477:ILE:CD1  | 2.51                     | 0.40              |
| 2:D:142:LEU:HD22 | 2:D:298:LEU:HD21 | 2.03                     | 0.40              |
| 1:A:199:PRO:HG3  | 1:A:262:HIS:CE1  | 2.56                     | 0.40              |
| 2:D:322:ILE:HG21 | 2:D:443:LEU:HD12 | 2.02                     | 0.40              |
| 2:D:222:LYS:O    | 2:D:226:GLY:N    | 2.55                     | 0.40              |
| 2:C:162:SER:O    | 2:C:165:VAL:HB   | 2.22                     | 0.40              |
| 1:B:253:TYR:OH   | 1:B:284:LEU:HA   | 2.20                     | 0.40              |
| 1:B:239:LEU:O    | 1:B:243:VAL:HB   | 2.21                     | 0.40              |
| 2:C:33:MET:HB3   | 2:C:95:PHE:CZ    | 2.56                     | 0.40              |
| 2:C:33:MET:HB3   | 2:C:95:PHE:HZ    | 1.87                     | 0.40              |
| 2:D:403:THR:HG22 | 2:D:458:THR:O    | 2.22                     | 0.40              |
| 1:A:279:THR:O    | 1:A:282:LYS:N    | 2.55                     | 0.40              |
| 2:D:294:ARG:HA   | 2:D:297:ASP:OD2  | 2.21                     | 0.40              |
| 2:C:78:ILE:O     | 2:C:79:LEU:C     | 2.59                     | 0.40              |
| 1:A:223:ARG:CD   | 1:B:168:ASN:HD22 | 2.35                     | 0.40              |
| 2:D:449:ARG:HH11 | 2:D:449:ARG:HB3  | 1.84                     | 0.40              |
| 2:C:318:TYR:C    | 2:C:318:TYR:CD1  | 2.95                     | 0.40              |
| 2:C:365:VAL:O    | 2:C:368:SER:N    | 2.50                     | 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     | 282/297 (95%)   | 244 (86%)  | 30 (11%)  | 8 (3%)   | 6           | 36 |
| 1   | B     | 282/297 (95%)   | 244 (86%)  | 33 (12%)  | 5 (2%)   | 11          | 50 |
| 2   | C     | 439/479 (92%)   | 330 (75%)  | 74 (17%)  | 35 (8%)  | 1           | 7  |
| 2   | D     | 439/479 (92%)   | 329 (75%)  | 77 (18%)  | 33 (8%)  | 1           | 8  |
| All | All   | 1442/1552 (93%) | 1147 (80%) | 214 (15%) | 81 (6%)  | 2           | 17 |

All (81) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | ASP  |
| 1   | A     | 146 | ASN  |
| 1   | B     | 2   | ASP  |
| 2   | C     | 78  | ILE  |
| 2   | C     | 146 | ASN  |
| 2   | C     | 301 | ASP  |
| 2   | C     | 319 | THR  |
| 2   | C     | 328 | ARG  |
| 2   | C     | 334 | LYS  |
| 2   | C     | 451 | LYS  |
| 2   | D     | 78  | ILE  |
| 2   | D     | 146 | ASN  |
| 2   | D     | 301 | ASP  |
| 2   | D     | 319 | THR  |
| 2   | D     | 334 | LYS  |
| 2   | D     | 451 | LYS  |
| 1   | A     | 34  | LEU  |
| 1   | B     | 34  | LEU  |
| 1   | B     | 146 | ASN  |
| 2   | C     | 66  | ASP  |
| 2   | C     | 82  | PHE  |
| 2   | C     | 115 | LEU  |
| 2   | C     | 209 | ASN  |
| 2   | C     | 210 | SER  |
| 2   | C     | 321 | GLY  |
| 2   | C     | 326 | GLY  |
| 2   | C     | 355 | LYS  |
| 2   | C     | 409 | LYS  |
| 2   | C     | 436 | LYS  |
| 2   | D     | 66  | ASP  |
| 2   | D     | 82  | PHE  |
| 2   | D     | 115 | LEU  |
| 2   | D     | 209 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 210 | SER  |
| 2   | D     | 321 | GLY  |
| 2   | D     | 326 | GLY  |
| 2   | D     | 328 | ARG  |
| 2   | D     | 330 | ASN  |
| 2   | D     | 355 | LYS  |
| 2   | D     | 436 | LYS  |
| 2   | C     | 74  | ILE  |
| 2   | C     | 79  | LEU  |
| 2   | C     | 196 | PRO  |
| 2   | C     | 270 | ILE  |
| 2   | C     | 330 | ASN  |
| 2   | C     | 339 | GLU  |
| 2   | C     | 460 | ARG  |
| 2   | D     | 74  | ILE  |
| 2   | D     | 79  | LEU  |
| 2   | D     | 196 | PRO  |
| 2   | D     | 270 | ILE  |
| 2   | D     | 339 | GLU  |
| 2   | D     | 409 | LYS  |
| 2   | C     | 276 | VAL  |
| 2   | C     | 318 | TYR  |
| 2   | C     | 384 | VAL  |
| 2   | C     | 464 | PRO  |
| 2   | D     | 318 | TYR  |
| 2   | D     | 460 | ARG  |
| 2   | D     | 464 | PRO  |
| 1   | A     | 36  | TYR  |
| 1   | A     | 54  | GLN  |
| 1   | A     | 295 | ASN  |
| 1   | B     | 36  | TYR  |
| 1   | B     | 216 | GLY  |
| 2   | C     | 68  | ASN  |
| 2   | C     | 183 | CYS  |
| 2   | C     | 332 | PRO  |
| 2   | D     | 276 | VAL  |
| 2   | D     | 292 | ILE  |
| 2   | D     | 332 | PRO  |
| 2   | D     | 384 | VAL  |
| 1   | A     | 286 | LEU  |
| 2   | C     | 35  | LYS  |
| 2   | C     | 292 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 35  | LYS  |
| 2   | D     | 68  | ASN  |
| 1   | A     | 216 | GLY  |
| 2   | C     | 277 | ASP  |
| 2   | D     | 277 | ASP  |
| 2   | C     | 412 | VAL  |

### 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     | 266/270 (98%)   | 251 (94%)  | 15 (6%)  | 26          | 66 |
| 1   | B     | 266/270 (98%)   | 250 (94%)  | 16 (6%)  | 24          | 63 |
| 2   | C     | 422/453 (93%)   | 389 (92%)  | 33 (8%)  | 16          | 52 |
| 2   | D     | 422/453 (93%)   | 390 (92%)  | 32 (8%)  | 16          | 53 |
| All | All   | 1376/1446 (95%) | 1280 (93%) | 96 (7%)  | 19          | 57 |

All (96) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | ASN  |
| 1   | A     | 21  | ASP  |
| 1   | A     | 50  | LEU  |
| 1   | A     | 58  | ILE  |
| 1   | A     | 66  | TYR  |
| 1   | A     | 147 | GLU  |
| 1   | A     | 149 | SER  |
| 1   | A     | 167 | LEU  |
| 1   | A     | 174 | LEU  |
| 1   | A     | 194 | ASN  |
| 1   | A     | 197 | LEU  |
| 1   | A     | 208 | MET  |
| 1   | A     | 209 | ARG  |
| 1   | A     | 275 | THR  |
| 1   | A     | 284 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 18  | ASN  |
| 1   | B     | 21  | ASP  |
| 1   | B     | 50  | LEU  |
| 1   | B     | 58  | ILE  |
| 1   | B     | 66  | TYR  |
| 1   | B     | 147 | GLU  |
| 1   | B     | 149 | SER  |
| 1   | B     | 167 | LEU  |
| 1   | B     | 174 | LEU  |
| 1   | B     | 187 | ASP  |
| 1   | B     | 194 | ASN  |
| 1   | B     | 197 | LEU  |
| 1   | B     | 208 | MET  |
| 1   | B     | 209 | ARG  |
| 1   | B     | 275 | THR  |
| 1   | B     | 284 | LEU  |
| 2   | C     | 15  | LEU  |
| 2   | C     | 51  | ILE  |
| 2   | C     | 54  | SER  |
| 2   | C     | 61  | LYS  |
| 2   | C     | 62  | ARG  |
| 2   | C     | 75  | LYS  |
| 2   | C     | 87  | GLN  |
| 2   | C     | 88  | THR  |
| 2   | C     | 90  | ASN  |
| 2   | C     | 99  | GLU  |
| 2   | C     | 134 | MET  |
| 2   | C     | 136 | GLU  |
| 2   | C     | 171 | LEU  |
| 2   | C     | 178 | ARG  |
| 2   | C     | 183 | CYS  |
| 2   | C     | 219 | PHE  |
| 2   | C     | 229 | ILE  |
| 2   | C     | 231 | LEU  |
| 2   | C     | 243 | ILE  |
| 2   | C     | 256 | ASN  |
| 2   | C     | 260 | ASP  |
| 2   | C     | 292 | ILE  |
| 2   | C     | 301 | ASP  |
| 2   | C     | 318 | TYR  |
| 2   | C     | 328 | ARG  |
| 2   | C     | 330 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 377 | THR  |
| 2   | C     | 408 | ASP  |
| 2   | C     | 416 | SER  |
| 2   | C     | 449 | ARG  |
| 2   | C     | 457 | HIS  |
| 2   | C     | 466 | ARG  |
| 2   | C     | 474 | LYS  |
| 2   | D     | 15  | LEU  |
| 2   | D     | 50  | ASP  |
| 2   | D     | 51  | ILE  |
| 2   | D     | 54  | SER  |
| 2   | D     | 61  | LYS  |
| 2   | D     | 62  | ARG  |
| 2   | D     | 87  | GLN  |
| 2   | D     | 88  | THR  |
| 2   | D     | 90  | ASN  |
| 2   | D     | 99  | GLU  |
| 2   | D     | 134 | MET  |
| 2   | D     | 136 | GLU  |
| 2   | D     | 171 | LEU  |
| 2   | D     | 178 | ARG  |
| 2   | D     | 219 | PHE  |
| 2   | D     | 229 | ILE  |
| 2   | D     | 231 | LEU  |
| 2   | D     | 243 | ILE  |
| 2   | D     | 256 | ASN  |
| 2   | D     | 260 | ASP  |
| 2   | D     | 292 | ILE  |
| 2   | D     | 301 | ASP  |
| 2   | D     | 318 | TYR  |
| 2   | D     | 328 | ARG  |
| 2   | D     | 330 | ASN  |
| 2   | D     | 377 | THR  |
| 2   | D     | 408 | ASP  |
| 2   | D     | 416 | SER  |
| 2   | D     | 449 | ARG  |
| 2   | D     | 457 | HIS  |
| 2   | D     | 466 | ARG  |
| 2   | D     | 474 | LYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 37  | GLN  |
| 1   | A     | 84  | ASN  |
| 1   | A     | 98  | HIS  |
| 1   | A     | 146 | ASN  |
| 1   | A     | 160 | GLN  |
| 1   | A     | 168 | ASN  |
| 1   | A     | 183 | GLN  |
| 1   | A     | 194 | ASN  |
| 1   | A     | 231 | ASN  |
| 1   | A     | 287 | GLN  |
| 1   | A     | 288 | GLN  |
| 1   | B     | 37  | GLN  |
| 1   | B     | 54  | GLN  |
| 1   | B     | 84  | ASN  |
| 1   | B     | 98  | HIS  |
| 1   | B     | 146 | ASN  |
| 1   | B     | 160 | GLN  |
| 1   | B     | 168 | ASN  |
| 1   | B     | 183 | GLN  |
| 1   | B     | 194 | ASN  |
| 1   | B     | 287 | GLN  |
| 1   | B     | 288 | GLN  |
| 2   | C     | 29  | ASN  |
| 2   | C     | 42  | GLN  |
| 2   | C     | 59  | ASN  |
| 2   | C     | 85  | GLN  |
| 2   | C     | 90  | ASN  |
| 2   | C     | 101 | GLN  |
| 2   | C     | 146 | ASN  |
| 2   | C     | 167 | ASN  |
| 2   | C     | 179 | HIS  |
| 2   | C     | 180 | ASN  |
| 2   | C     | 247 | ASN  |
| 2   | C     | 250 | HIS  |
| 2   | C     | 256 | ASN  |
| 2   | C     | 291 | GLN  |
| 2   | C     | 320 | HIS  |
| 2   | C     | 394 | ASN  |
| 2   | C     | 413 | HIS  |
| 2   | D     | 29  | ASN  |
| 2   | D     | 42  | GLN  |
| 2   | D     | 59  | ASN  |
| 2   | D     | 85  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 90  | ASN  |
| 2   | D     | 101 | GLN  |
| 2   | D     | 146 | ASN  |
| 2   | D     | 167 | ASN  |
| 2   | D     | 179 | HIS  |
| 2   | D     | 180 | ASN  |
| 2   | D     | 247 | ASN  |
| 2   | D     | 250 | HIS  |
| 2   | D     | 256 | ASN  |
| 2   | D     | 291 | GLN  |
| 2   | D     | 320 | HIS  |
| 2   | D     | 394 | ASN  |
| 2   | D     | 413 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 288/297 (96%)   | -0.29  | 0 100 100     | 36, 61, 94, 135       | 0     |
| 1   | B     | 288/297 (96%)   | -0.31  | 4 (1%) 78 65  | 38, 62, 95, 147       | 0     |
| 2   | C     | 445/479 (92%)   | 0.08   | 9 (2%) 68 54  | 46, 93, 130, 149      | 0     |
| 2   | D     | 445/479 (92%)   | 0.01   | 3 (0%) 89 82  | 43, 88, 122, 156      | 0     |
| 3   | E     | 5/5 (100%)      | 0.28   | 0 100 100     | 74, 92, 107, 119      | 0     |
| 4   | F     | 3/3 (100%)      | -0.18  | 0 100 100     | 87, 87, 110, 112      | 0     |
| 5   | G     | 3/3 (100%)      | 0.51   | 0 100 100     | 115, 115, 118, 123    | 0     |
| 5   | H     | 3/3 (100%)      | 0.45   | 0 100 100     | 106, 106, 112, 124    | 0     |
| All | All   | 1480/1566 (94%) | -0.09  | 16 (1%) 82 72 | 36, 79, 123, 156      | 0     |

All (16) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | C     | 434 | GLU  | 4.1  |
| 2   | D     | 148 | ALA  | 3.7  |
| 1   | B     | 146 | ASN  | 2.9  |
| 1   | B     | 20  | LEU  | 2.8  |
| 2   | C     | 323 | VAL  | 2.6  |
| 2   | C     | 68  | ASN  | 2.5  |
| 2   | D     | 456 | SER  | 2.5  |
| 2   | D     | 13  | ILE  | 2.5  |
| 1   | B     | 24  | PRO  | 2.5  |
| 2   | C     | 227 | ASN  | 2.4  |
| 2   | C     | 456 | SER  | 2.4  |
| 2   | C     | 149 | VAL  | 2.3  |
| 1   | B     | 35  | PRO  | 2.2  |
| 2   | C     | 330 | ASN  | 2.1  |
| 2   | C     | 14  | THR  | 2.1  |
| 2   | C     | 324 | PHE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.