



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:16 pm GMT

PDB ID : 3I0S  
Title : crystal structure of HIV reverse transcriptase in complex with inhibitor 7  
Authors : Yan, Y.; Prasad, S.  
Deposited on : 2009-06-25  
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

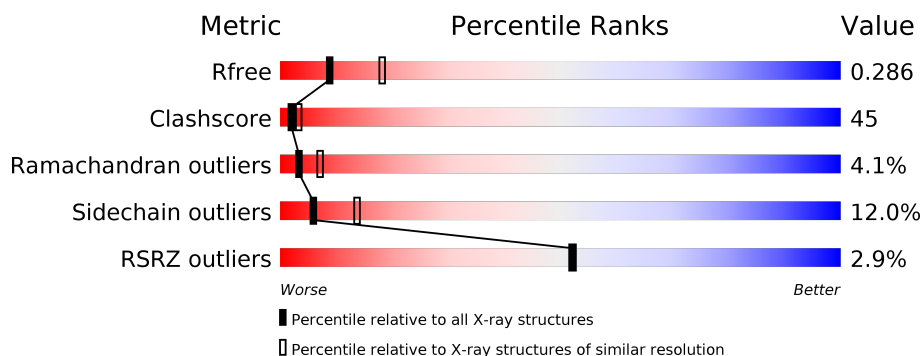
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 2259 (2.70-2.70)                                      |
| Clashscore            | 112137                      | 2590 (2.70-2.70)                                      |
| Ramachandran outliers | 110173                      | 2550 (2.70-2.70)                                      |
| Sidechain outliers    | 110143                      | 2550 (2.70-2.70)                                      |
| RSRZ outliers         | 101464                      | 2275 (2.70-2.70)                                      |

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     | 563    | <div> <div>3%</div> <div> <div></div> <div>48%</div> <div>40%</div> <div>9%</div> <div>..</div> </div> </div> |
| 2   | B     | 443    | <div> <div>2%</div> <div> <div></div> <div>48%</div> <div>35%</div> <div>8%</div> <div>9%</div> </div> </div> |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | RT7  | A     | 601 | -         | -        | X       | -                |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7923 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 Reverse transcriptase/ribonuclease H.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 558      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 4541  | 2934 | 760 | 839 | 8 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -2      | MET      | -      | EXPRESSION TAG | UNP P04585 |
| A     | -1      | ASN      | -      | EXPRESSION TAG | UNP P04585 |
| A     | 0       | SER      | -      | EXPRESSION TAG | UNP P04585 |

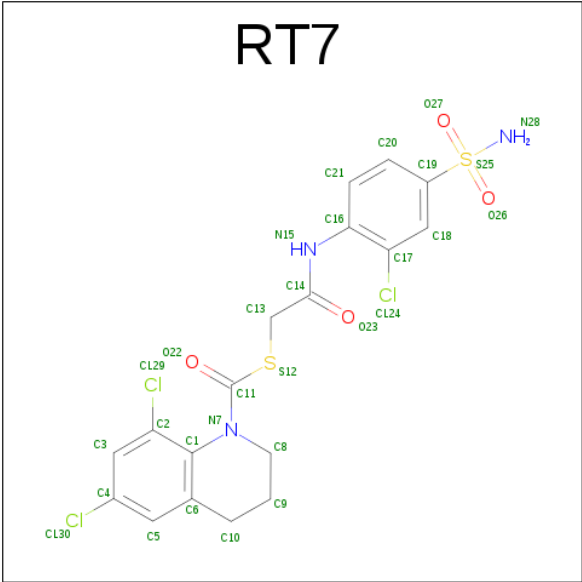
- Molecule 2 is a protein called p51 RT.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 405      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3352  | 2182 | 555 | 609 | 6 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -2      | MET      | -      | EXPRESSION TAG | UNP P04585 |
| B     | -1      | ASN      | -      | EXPRESSION TAG | UNP P04585 |
| B     | 0       | SER      | -      | EXPRESSION TAG | UNP P04585 |

- Molecule 3 is S-{2-[(2-CHLORO-4-SULFAMOYLPHENYL)AMINO]-2-OXOETHYL} 6, 8-DICHLORO-3,4-DIHYDROQUINOLINE-1(2H)-CARBOTHIOATE (three-letter code: RT7) (formula: C<sub>18</sub>H<sub>16</sub>Cl<sub>3</sub>N<sub>3</sub>O<sub>4</sub>S<sub>2</sub>).

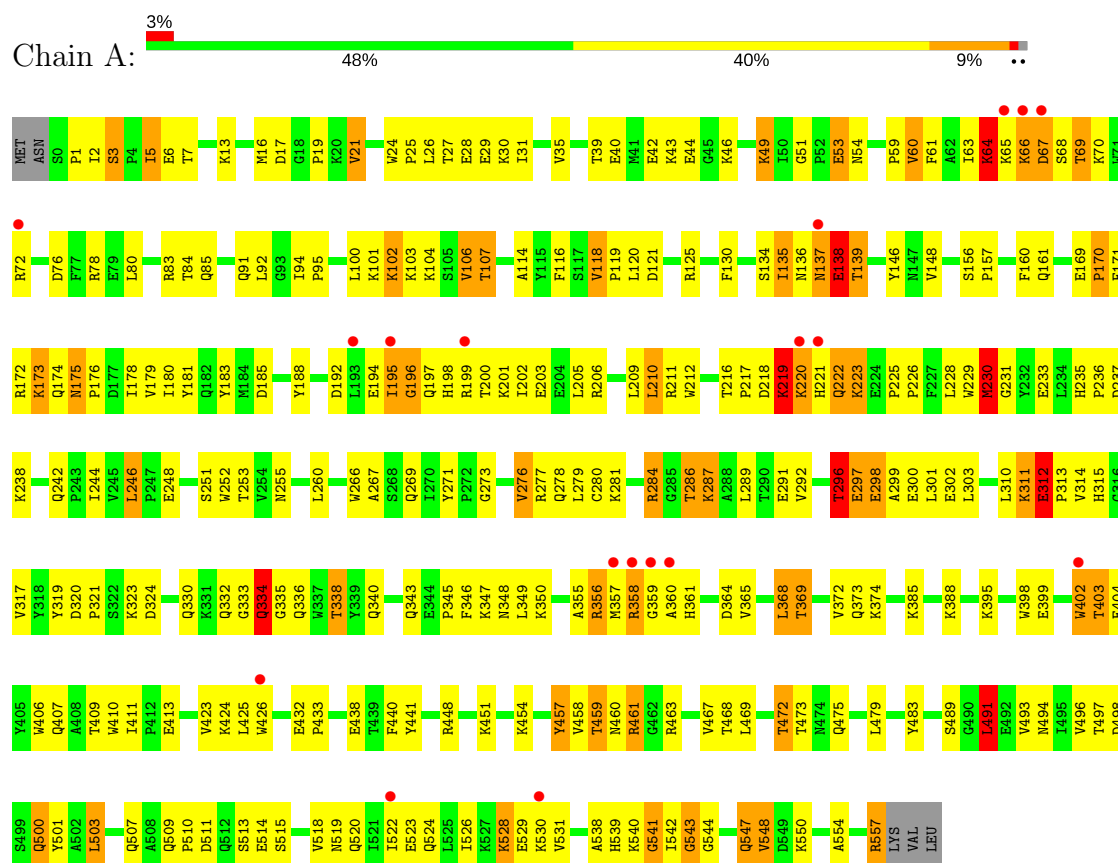


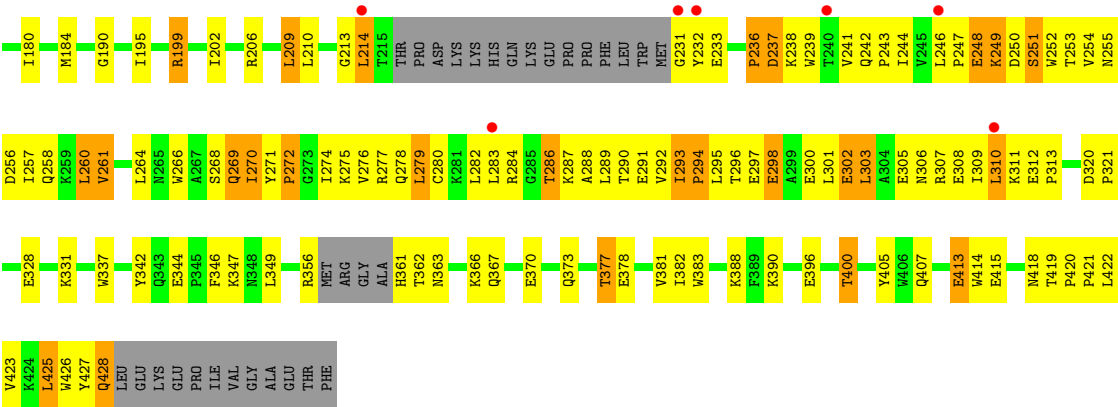
| Mol | Chain | Residues | Atoms |    |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---|---------|---------|
|     |       |          | Total | C  | Cl | N | O | S |         |         |
| 3   | A     | 1        | 30    | 18 | 3  | 3 | 4 | 2 | 0       | 0       |

### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Reverse transcriptase/ribonuclease H





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 2 2 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 119.61Å 154.69Å 155.82Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 50.00 – 2.70<br>47.31 – 2.70                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (50.00-2.70)<br>99.8 (47.31-2.70)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.10  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.27 (at 2.69Å)   | Xtriage          |
| Refinement program  | REFMAC 5.5.0066   | Depositor        |
| R, $R_{free}$   | 0.232 , 0.285<br>0.232 , 0.286                              | Depositor<br>DCC |
| $R_{free}$ test set   | 2003 reflections (5.28%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 60.7  | Xtriage          |
| Anisotropy  | 0.052   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 45.5   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 7923  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 61.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RT7

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     | 0.52         | 0/4658  | 0.64        | 0/6329  |
| 2   | B     | 0.54         | 0/3446  | 0.65        | 0/4682  |
| All | All   | 0.53         | 0/8104  | 0.65        | 0/11011 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4541  | 0        | 4592     | 452     | 0            |
| 2   | B     | 3352  | 0        | 3380     | 276     | 0            |
| 3   | A     | 30    | 0        | 16       | 15      | 0            |
| All | All   | 7923  | 0        | 7988     | 712     | 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 45.

All (712) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:66:LYS:HG3   | 2:B:407:GLN:NE2  | 1.24                     | 1.43              |
| 2:B:66:LYS:CG    | 2:B:407:GLN:HE22 | 1.41                     | 1.32              |
| 2:B:13:LYS:HB2   | 2:B:16:MET:CE    | 1.58                     | 1.32              |
| 1:A:107:THR:HG21 | 1:A:202:ILE:CD1  | 1.59                     | 1.29              |
| 1:A:298:GLU:OE2  | 1:A:298:GLU:N    | 1.65                     | 1.26              |
| 2:B:13:LYS:CB    | 2:B:16:MET:HE3   | 1.66                     | 1.24              |
| 1:A:219:LYS:O    | 1:A:220:LYS:CD   | 1.91                     | 1.19              |
| 1:A:219:LYS:O    | 1:A:220:LYS:HD2  | 1.07                     | 1.19              |
| 2:B:308:GLU:CA   | 2:B:311:LYS:HE2  | 1.75                     | 1.16              |
| 1:A:173:LYS:HE3  | 1:A:173:LYS:HA   | 1.30                     | 1.14              |
| 2:B:396:GLU:O    | 2:B:400:THR:CG2  | 1.96                     | 1.13              |
| 1:A:211:ARG:O    | 1:A:211:ARG:HD3  | 1.47                     | 1.12              |
| 1:A:540:LYS:O    | 1:A:542:ILE:HG13 | 1.46                     | 1.12              |
| 1:A:175:ASN:HD21 | 1:A:201:LYS:NZ   | 1.48                     | 1.11              |
| 1:A:557:ARG:O    | 1:A:557:ARG:HG2  | 1.43                     | 1.11              |
| 1:A:399:GLU:OE1  | 1:A:402:TRP:CZ3  | 2.04                     | 1.11              |
| 1:A:542:ILE:O    | 1:A:543:GLY:O    | 1.67                     | 1.11              |
| 1:A:399:GLU:OE1  | 1:A:402:TRP:HZ3  | 1.32                     | 1.09              |
| 1:A:220:LYS:C    | 1:A:220:LYS:HD3  | 1.70                     | 1.09              |
| 1:A:65:LYS:HE2   | 1:A:72:ARG:HH11  | 0.94                     | 1.09              |
| 2:B:308:GLU:HA   | 2:B:311:LYS:CE   | 1.83                     | 1.08              |
| 1:A:64:LYS:NZ    | 1:A:69:THR:HA    | 1.69                     | 1.08              |
| 2:B:244:ILE:HD13 | 2:B:266:TRP:HZ3  | 1.19                     | 1.08              |
| 1:A:65:LYS:HG2   | 1:A:68:SER:HB3   | 1.37                     | 1.07              |
| 1:A:171:PHE:HA   | 1:A:174:GLN:HE21 | 0.96                     | 1.07              |
| 1:A:357:MET:HE1  | 1:A:360:ALA:O    | 1.52                     | 1.07              |
| 1:A:65:LYS:HE2   | 1:A:72:ARG:NH1   | 1.69                     | 1.07              |
| 2:B:298:GLU:HA   | 2:B:301:LEU:HG   | 1.33                     | 1.07              |
| 1:A:107:THR:HG21 | 1:A:202:ILE:HD11 | 1.22                     | 1.05              |
| 1:A:171:PHE:HA   | 1:A:174:GLN:NE2  | 1.71                     | 1.05              |
| 1:A:220:LYS:HE3  | 1:A:221:HIS:CD2  | 1.92                     | 1.05              |
| 2:B:214:LEU:HD23 | 2:B:214:LEU:H    | 1.19                     | 1.05              |
| 1:A:64:LYS:HZ3   | 1:A:69:THR:HA    | 1.16                     | 1.04              |
| 1:A:220:LYS:CE   | 1:A:221:HIS:CD2  | 2.41                     | 1.03              |
| 1:A:220:LYS:HD3  | 1:A:221:HIS:N    | 1.73                     | 1.03              |
| 2:B:206:ARG:HH22 | 2:B:231:GLY:N    | 1.57                     | 1.02              |
| 2:B:268:SER:O    | 2:B:269:GLN:HB2  | 1.57                     | 1.02              |
| 1:A:21:VAL:HG22  | 1:A:59:PRO:HD3   | 1.40                     | 1.02              |
| 1:A:43:LYS:HE2   | 1:A:43:LYS:HA    | 1.42                     | 1.01              |
| 1:A:107:THR:HG22 | 1:A:198:HIS:HE1  | 1.23                     | 1.01              |
| 2:B:308:GLU:HA   | 2:B:311:LYS:HE2  | 1.04                     | 1.00              |
| 1:A:406:TRP:CZ3  | 1:A:407:GLN:HB2  | 1.95                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:210:LEU:O    | 1:A:210:LEU:HD22 | 1.62                     | 0.99              |
| 1:A:5:ILE:HG22   | 1:A:212:TRP:CE3  | 1.97                     | 0.99              |
| 1:A:107:THR:HG21 | 1:A:202:ILE:HD13 | 1.45                     | 0.98              |
| 1:A:424:LYS:NZ   | 1:A:426:TRP:CZ3  | 2.31                     | 0.98              |
| 1:A:195:ILE:HG23 | 1:A:199:ARG:NE   | 1.79                     | 0.98              |
| 1:A:40:GLU:HG3   | 1:A:44:GLU:OE1   | 1.63                     | 0.97              |
| 1:A:330:GLN:NE2  | 1:A:338:THR:CG2  | 2.26                     | 0.97              |
| 1:A:298:GLU:H    | 1:A:298:GLU:CD   | 1.63                     | 0.97              |
| 1:A:107:THR:CG2  | 1:A:202:ILE:HD11 | 1.92                     | 0.97              |
| 1:A:357:MET:CE   | 1:A:360:ALA:O    | 2.12                     | 0.97              |
| 2:B:13:LYS:CB    | 2:B:16:MET:CE    | 2.32                     | 0.97              |
| 2:B:260:LEU:O    | 2:B:260:LEU:HD22 | 1.65                     | 0.97              |
| 2:B:85:GLN:NE2   | 2:B:89:GLU:OE2   | 1.95                     | 0.97              |
| 1:A:296:THR:HG22 | 1:A:299:ALA:H    | 1.28                     | 0.97              |
| 1:A:395:LYS:O    | 1:A:399:GLU:HG2  | 1.64                     | 0.97              |
| 2:B:253:THR:HG22 | 2:B:256:ASP:CG   | 1.85                     | 0.96              |
| 1:A:330:GLN:HE21 | 1:A:338:THR:CG2  | 1.79                     | 0.95              |
| 2:B:425:LEU:H    | 2:B:425:LEU:HD23 | 1.29                     | 0.95              |
| 1:A:233:GLU:HG2  | 1:A:235:HIS:CE1  | 2.01                     | 0.95              |
| 2:B:274:ILE:HG23 | 2:B:306:ASN:ND2  | 1.82                     | 0.95              |
| 2:B:396:GLU:O    | 2:B:400:THR:HG23 | 1.64                     | 0.94              |
| 2:B:236:PRO:O    | 2:B:238:LYS:N    | 1.99                     | 0.94              |
| 1:A:233:GLU:HG2  | 1:A:235:HIS:HE1  | 1.32                     | 0.94              |
| 1:A:171:PHE:CA   | 1:A:174:GLN:HE21 | 1.80                     | 0.94              |
| 1:A:107:THR:CG2  | 1:A:202:ILE:CD1  | 2.45                     | 0.93              |
| 2:B:271:TYR:HB3  | 2:B:274:ILE:HD11 | 1.49                     | 0.93              |
| 2:B:206:ARG:NH2  | 2:B:231:GLY:N    | 2.16                     | 0.92              |
| 2:B:298:GLU:HA   | 2:B:301:LEU:CG   | 1.99                     | 0.92              |
| 1:A:448:ARG:CG   | 1:A:448:ARG:HH11 | 1.83                     | 0.92              |
| 2:B:396:GLU:O    | 2:B:400:THR:HG22 | 1.67                     | 0.92              |
| 2:B:66:LYS:CG    | 2:B:407:GLN:NE2  | 2.12                     | 0.92              |
| 1:A:65:LYS:CE    | 1:A:72:ARG:HH11  | 1.83                     | 0.92              |
| 1:A:500:GLN:HG3  | 2:B:422:LEU:CD1  | 1.99                     | 0.92              |
| 2:B:300:GLU:HA   | 2:B:303:LEU:HD12 | 1.51                     | 0.91              |
| 1:A:424:LYS:CE   | 1:A:426:TRP:CZ2  | 2.54                     | 0.91              |
| 1:A:424:LYS:HE3  | 1:A:426:TRP:CE2  | 2.06                     | 0.90              |
| 2:B:298:GLU:N    | 2:B:298:GLU:OE2  | 2.05                     | 0.90              |
| 1:A:343:GLN:HG3  | 1:A:349:LEU:HD11 | 1.54                     | 0.90              |
| 1:A:230:MET:HA   | 1:A:230:MET:HE2  | 1.52                     | 0.90              |
| 1:A:1:PRO:C      | 1:A:2:ILE:HD13   | 1.92                     | 0.89              |
| 1:A:373:GLN:OE1  | 2:B:400:THR:HG21 | 1.71                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:199:ARG:HD3  | 2:B:233:GLU:OE1  | 1.72                     | 0.89              |
| 1:A:424:LYS:NZ   | 1:A:426:TRP:CH2  | 2.39                     | 0.89              |
| 2:B:244:ILE:HD13 | 2:B:266:TRP:CZ3  | 2.08                     | 0.89              |
| 2:B:422:LEU:HA   | 2:B:425:LEU:HD21 | 1.53                     | 0.89              |
| 1:A:406:TRP:CH2  | 2:B:418:ASN:HA   | 2.07                     | 0.88              |
| 1:A:424:LYS:HE3  | 1:A:426:TRP:CZ2  | 2.08                     | 0.88              |
| 1:A:458:VAL:HG22 | 1:A:548:VAL:HG22 | 1.54                     | 0.88              |
| 1:A:433:PRO:HG3  | 2:B:255:ASN:ND2  | 1.89                     | 0.88              |
| 1:A:171:PHE:CA   | 1:A:174:GLN:NE2  | 2.35                     | 0.88              |
| 1:A:220:LYS:HE2  | 1:A:221:HIS:CG   | 2.09                     | 0.88              |
| 1:A:539:HIS:O    | 1:A:540:LYS:HD3  | 1.74                     | 0.88              |
| 2:B:266:TRP:NE1  | 2:B:346:PHE:HE2  | 1.72                     | 0.88              |
| 1:A:66:LYS:O     | 1:A:67:ASP:HB3   | 1.74                     | 0.87              |
| 1:A:228:LEU:HB3  | 1:A:242:GLN:NE2  | 1.90                     | 0.87              |
| 2:B:270:ILE:O    | 2:B:272:PRO:HD3  | 1.75                     | 0.87              |
| 2:B:373:GLN:NE2  | 2:B:407:GLN:H    | 1.71                     | 0.87              |
| 1:A:547:GLN:HE21 | 1:A:547:GLN:N    | 1.73                     | 0.87              |
| 2:B:420:PRO:HB2  | 2:B:423:VAL:HG23 | 1.56                     | 0.86              |
| 1:A:433:PRO:HG3  | 2:B:255:ASN:HD22 | 1.40                     | 0.86              |
| 1:A:69:THR:CG2   | 1:A:69:THR:O     | 2.24                     | 0.86              |
| 2:B:373:GLN:HE22 | 2:B:407:GLN:H    | 1.21                     | 0.86              |
| 1:A:3:SER:OG     | 1:A:5:ILE:HD12   | 1.75                     | 0.86              |
| 2:B:199:ARG:NH1  | 2:B:233:GLU:OE2  | 2.09                     | 0.86              |
| 1:A:206:ARG:HH22 | 1:A:218:ASP:HB3  | 1.37                     | 0.85              |
| 2:B:266:TRP:HE1  | 2:B:346:PHE:HE2  | 1.23                     | 0.85              |
| 2:B:337:TRP:HE1  | 2:B:367:GLN:HE21 | 1.25                     | 0.85              |
| 1:A:30:LYS:HE3   | 1:A:61:PHE:CE1   | 2.11                     | 0.85              |
| 1:A:498:ASP:CG   | 1:A:538:ALA:HB2  | 1.96                     | 0.84              |
| 1:A:175:ASN:HD21 | 1:A:201:LYS:CE   | 1.90                     | 0.84              |
| 2:B:253:THR:CG2  | 2:B:256:ASP:H    | 1.90                     | 0.84              |
| 1:A:175:ASN:ND2  | 1:A:201:LYS:HE2  | 1.91                     | 0.84              |
| 2:B:214:LEU:N    | 2:B:214:LEU:HD23 | 1.92                     | 0.84              |
| 1:A:489:SER:OG   | 1:A:493:VAL:HG21 | 1.77                     | 0.84              |
| 1:A:540:LYS:O    | 1:A:542:ILE:CG1  | 2.25                     | 0.84              |
| 1:A:220:LYS:HE2  | 1:A:221:HIS:CE1  | 2.13                     | 0.83              |
| 1:A:175:ASN:HD21 | 1:A:201:LYS:HZ3  | 1.23                     | 0.83              |
| 2:B:13:LYS:HB2   | 2:B:16:MET:HE3   | 0.86                     | 0.83              |
| 1:A:220:LYS:CD   | 1:A:220:LYS:C    | 2.47                     | 0.83              |
| 1:A:540:LYS:O    | 1:A:541:GLY:C    | 2.14                     | 0.82              |
| 2:B:282:LEU:HB3  | 2:B:293:ILE:HD11 | 1.61                     | 0.82              |
| 1:A:220:LYS:HE2  | 1:A:221:HIS:CD2  | 2.14                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:220:LYS:HE3  | 1:A:221:HIS:NE2  | 1.95                     | 0.81              |
| 2:B:388:LYS:HE2  | 2:B:415:GLU:HG3  | 1.60                     | 0.81              |
| 2:B:270:ILE:HB   | 2:B:346:PHE:O    | 1.80                     | 0.81              |
| 1:A:557:ARG:O    | 1:A:557:ARG:CG   | 2.26                     | 0.81              |
| 1:A:27:THR:O     | 1:A:31:ILE:HG13  | 1.81                     | 0.81              |
| 2:B:362:THR:HG22 | 2:B:367:GLN:HG3  | 1.63                     | 0.81              |
| 2:B:428:GLN:HA   | 2:B:428:GLN:NE2  | 1.95                     | 0.81              |
| 1:A:63:ILE:CD1   | 1:A:72:ARG:HB2   | 2.11                     | 0.80              |
| 1:A:65:LYS:CG    | 1:A:68:SER:HB3   | 2.11                     | 0.80              |
| 2:B:366:LYS:HD2  | 2:B:405:TYR:CD1  | 2.16                     | 0.80              |
| 2:B:298:GLU:HA   | 2:B:301:LEU:CD1  | 2.12                     | 0.80              |
| 2:B:244:ILE:CD1  | 2:B:266:TRP:HZ3  | 1.93                     | 0.80              |
| 1:A:500:GLN:HG3  | 2:B:422:LEU:HD11 | 1.61                     | 0.80              |
| 1:A:107:THR:HG22 | 1:A:198:HIS:CE1  | 2.15                     | 0.79              |
| 1:A:175:ASN:ND2  | 1:A:201:LYS:CE   | 2.46                     | 0.79              |
| 1:A:356:ARG:NH2  | 1:A:358:ARG:HD2  | 1.97                     | 0.79              |
| 1:A:220:LYS:CE   | 1:A:221:HIS:NE2  | 2.46                     | 0.79              |
| 1:A:63:ILE:HD12  | 1:A:72:ARG:HB2   | 1.65                     | 0.79              |
| 1:A:198:HIS:O    | 1:A:202:ILE:HG13 | 1.82                     | 0.78              |
| 2:B:244:ILE:CD1  | 2:B:266:TRP:CZ3  | 2.67                     | 0.78              |
| 1:A:409:THR:CG2  | 1:A:410:TRP:N    | 2.47                     | 0.77              |
| 2:B:254:VAL:HG23 | 2:B:291:GLU:O    | 1.83                     | 0.77              |
| 2:B:50:ILE:HD12  | 2:B:54:ASN:HB3   | 1.66                     | 0.77              |
| 1:A:195:ILE:HG23 | 1:A:199:ARG:CD   | 2.15                     | 0.77              |
| 1:A:171:PHE:N    | 1:A:174:GLN:NE2  | 2.32                     | 0.77              |
| 1:A:206:ARG:NH2  | 1:A:218:ASP:HB3  | 1.99                     | 0.77              |
| 1:A:195:ILE:O    | 1:A:196:GLY:O    | 2.03                     | 0.77              |
| 2:B:6:GLU:N      | 2:B:6:GLU:OE1    | 2.19                     | 0.76              |
| 2:B:298:GLU:CA   | 2:B:301:LEU:HG   | 2.12                     | 0.76              |
| 1:A:230:MET:HA   | 1:A:230:MET:CE   | 2.16                     | 0.76              |
| 1:A:197:GLN:O    | 1:A:201:LYS:HB2  | 1.86                     | 0.76              |
| 1:A:1:PRO:O      | 1:A:2:ILE:HD13   | 1.85                     | 0.76              |
| 1:A:333:GLY:O    | 1:A:335:GLY:N    | 2.20                     | 0.75              |
| 2:B:13:LYS:CE    | 2:B:86:ASP:H     | 1.98                     | 0.75              |
| 1:A:330:GLN:HE22 | 1:A:340:GLN:HE22 | 1.32                     | 0.75              |
| 2:B:337:TRP:HE1  | 2:B:367:GLN:NE2  | 1.84                     | 0.75              |
| 1:A:330:GLN:NE2  | 1:A:338:THR:HG23 | 2.01                     | 0.75              |
| 1:A:134:SER:OG   | 1:A:139:THR:HB   | 1.87                     | 0.74              |
| 1:A:279:LEU:HD23 | 1:A:302:GLU:OE1  | 1.86                     | 0.74              |
| 1:A:246:LEU:HD11 | 1:A:310:LEU:HD12 | 1.68                     | 0.74              |
| 2:B:271:TYR:O    | 2:B:274:ILE:HG12 | 1.88                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:308:GLU:C    | 2:B:311:LYS:HE2  | 2.07                     | 0.73              |
| 2:B:5:ILE:HD12   | 2:B:5:ILE:N      | 2.04                     | 0.73              |
| 1:A:175:ASN:ND2  | 1:A:201:LYS:NZ   | 2.32                     | 0.73              |
| 2:B:66:LYS:HG2   | 2:B:407:GLN:HE22 | 1.47                     | 0.73              |
| 1:A:475:GLN:HG2  | 1:A:501:TYR:CD2  | 2.23                     | 0.73              |
| 1:A:21:VAL:HG22  | 1:A:59:PRO:CD    | 2.16                     | 0.73              |
| 1:A:424:LYS:CE   | 1:A:426:TRP:CH2  | 2.72                     | 0.72              |
| 2:B:268:SER:O    | 2:B:269:GLN:CB   | 2.33                     | 0.72              |
| 1:A:266:TRP:O    | 1:A:269:GLN:HG3  | 1.90                     | 0.72              |
| 1:A:106:VAL:HG12 | 3:A:601:RT7:C20  | 2.20                     | 0.72              |
| 2:B:210:LEU:O    | 2:B:210:LEU:HD12 | 1.89                     | 0.72              |
| 2:B:373:GLN:HE22 | 2:B:407:GLN:N    | 1.88                     | 0.72              |
| 1:A:448:ARG:HH11 | 1:A:448:ARG:HG3  | 1.54                     | 0.71              |
| 2:B:13:LYS:HE2   | 2:B:86:ASP:H     | 1.54                     | 0.71              |
| 1:A:228:LEU:HD22 | 1:A:228:LEU:H    | 1.54                     | 0.71              |
| 2:B:428:GLN:HA   | 2:B:428:GLN:HE21 | 1.56                     | 0.71              |
| 1:A:330:GLN:HE21 | 1:A:338:THR:HG21 | 1.54                     | 0.71              |
| 1:A:356:ARG:HH21 | 1:A:358:ARG:HD2  | 1.55                     | 0.71              |
| 3:A:601:RT7:H21  | 3:A:601:RT7:O23  | 1.90                     | 0.71              |
| 2:B:209:LEU:HG   | 2:B:214:LEU:HD12 | 1.71                     | 0.70              |
| 1:A:220:LYS:HE2  | 1:A:221:HIS:ND1  | 2.07                     | 0.70              |
| 1:A:53:GLU:CD    | 1:A:53:GLU:H     | 1.95                     | 0.70              |
| 1:A:69:THR:HG23  | 1:A:69:THR:O     | 1.90                     | 0.70              |
| 1:A:211:ARG:O    | 1:A:211:ARG:CD   | 2.36                     | 0.70              |
| 2:B:257:ILE:O    | 2:B:261:VAL:HG12 | 1.91                     | 0.70              |
| 1:A:406:TRP:CE3  | 1:A:407:GLN:HB2  | 2.26                     | 0.69              |
| 1:A:205:LEU:CD1  | 1:A:209:LEU:HD11 | 2.22                     | 0.69              |
| 1:A:65:LYS:HE2   | 1:A:70:LYS:HE2   | 1.72                     | 0.69              |
| 2:B:253:THR:HG22 | 2:B:256:ASP:H    | 1.56                     | 0.69              |
| 2:B:13:LYS:HE2   | 2:B:86:ASP:N     | 2.08                     | 0.69              |
| 1:A:230:MET:CA   | 1:A:230:MET:HE2  | 2.21                     | 0.69              |
| 1:A:410:TRP:CZ3  | 2:B:363:ASN:HB3  | 2.28                     | 0.69              |
| 2:B:362:THR:HG23 | 2:B:366:LYS:HG2  | 1.73                     | 0.69              |
| 1:A:297:GLU:O    | 1:A:301:LEU:HG   | 1.92                     | 0.69              |
| 1:A:106:VAL:HG12 | 3:A:601:RT7:C21  | 2.23                     | 0.69              |
| 1:A:489:SER:HB2  | 1:A:493:VAL:CG2  | 2.23                     | 0.69              |
| 1:A:5:ILE:HG22   | 1:A:212:TRP:CZ3  | 2.27                     | 0.69              |
| 2:B:253:THR:HG23 | 2:B:256:ASP:H    | 1.58                     | 0.68              |
| 1:A:500:GLN:HG3  | 2:B:422:LEU:HD12 | 1.75                     | 0.68              |
| 2:B:107:THR:CB   | 2:B:202:ILE:HD13 | 2.23                     | 0.68              |
| 2:B:236:PRO:C    | 2:B:238:LYS:H    | 1.96                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:241:VAL:CG2  | 2:B:243:PRO:HG3  | 2.24                     | 0.68              |
| 1:A:66:LYS:O     | 1:A:67:ASP:CB    | 2.41                     | 0.68              |
| 1:A:107:THR:CG2  | 1:A:202:ILE:HD13 | 2.19                     | 0.68              |
| 1:A:228:LEU:HB3  | 1:A:242:GLN:HE22 | 1.57                     | 0.68              |
| 2:B:199:ARG:HH11 | 2:B:233:GLU:CD   | 1.97                     | 0.68              |
| 2:B:362:THR:CG2  | 2:B:367:GLN:HG3  | 2.23                     | 0.68              |
| 2:B:308:GLU:O    | 2:B:311:LYS:CE   | 2.41                     | 0.68              |
| 1:A:402:TRP:CD1  | 1:A:402:TRP:C    | 2.66                     | 0.67              |
| 2:B:241:VAL:HG23 | 2:B:243:PRO:HD3  | 1.76                     | 0.67              |
| 1:A:448:ARG:HH11 | 1:A:448:ARG:HG2  | 1.58                     | 0.67              |
| 1:A:409:THR:HG22 | 1:A:410:TRP:N    | 2.09                     | 0.67              |
| 1:A:438:GLU:HG3  | 1:A:461:ARG:HG3  | 1.77                     | 0.67              |
| 2:B:89:GLU:HG2   | 2:B:90:VAL:HG13  | 1.77                     | 0.67              |
| 2:B:12:LEU:HD23  | 2:B:17:ASP:HA    | 1.75                     | 0.67              |
| 2:B:126:LYS:HA   | 2:B:145:GLN:OE1  | 1.95                     | 0.67              |
| 1:A:365:VAL:O    | 1:A:369:THR:HG23 | 1.95                     | 0.67              |
| 1:A:489:SER:CB   | 1:A:493:VAL:HG21 | 2.26                     | 0.66              |
| 1:A:524:GLN:HE21 | 1:A:524:GLN:HA   | 1.59                     | 0.66              |
| 1:A:64:LYS:HZ1   | 1:A:69:THR:HA    | 1.61                     | 0.66              |
| 2:B:195:ILE:O    | 2:B:199:ARG:HG3  | 1.96                     | 0.66              |
| 2:B:268:SER:HB3  | 2:B:274:ILE:HB   | 1.78                     | 0.66              |
| 2:B:425:LEU:H    | 2:B:425:LEU:CD2  | 2.07                     | 0.66              |
| 2:B:13:LYS:HE3   | 2:B:85:GLN:HB3   | 1.75                     | 0.66              |
| 1:A:475:GLN:HG2  | 1:A:501:TYR:CE2  | 2.30                     | 0.66              |
| 2:B:241:VAL:C    | 2:B:243:PRO:HD3  | 2.16                     | 0.66              |
| 2:B:13:LYS:HE2   | 2:B:86:ASP:HB2   | 1.78                     | 0.66              |
| 1:A:218:ASP:OD2  | 1:A:220:LYS:HE2  | 1.95                     | 0.66              |
| 1:A:399:GLU:OE1  | 1:A:402:TRP:CE3  | 2.48                     | 0.66              |
| 1:A:255:ASN:HB2  | 1:A:289:LEU:HD22 | 1.76                     | 0.66              |
| 1:A:218:ASP:O    | 1:A:219:LYS:O    | 2.13                     | 0.66              |
| 1:A:406:TRP:CH2  | 1:A:407:GLN:HB2  | 2.31                     | 0.66              |
| 1:A:448:ARG:NH1  | 1:A:448:ARG:HG3  | 2.09                     | 0.65              |
| 1:A:489:SER:HB2  | 1:A:493:VAL:HG22 | 1.77                     | 0.65              |
| 1:A:70:LYS:HE3   | 1:A:72:ARG:HG2   | 1.78                     | 0.65              |
| 2:B:13:LYS:CE    | 2:B:86:ASP:N     | 2.59                     | 0.65              |
| 1:A:529:GLU:O    | 1:A:530:LYS:HG2  | 1.96                     | 0.65              |
| 1:A:171:PHE:CE2  | 1:A:205:LEU:HD23 | 2.32                     | 0.65              |
| 1:A:448:ARG:CG   | 1:A:448:ARG:NH1  | 2.52                     | 0.65              |
| 1:A:106:VAL:H    | 3:A:601:RT7:H128 | 1.44                     | 0.65              |
| 1:A:175:ASN:HB3  | 1:A:178:ILE:HD12 | 1.78                     | 0.65              |
| 1:A:220:LYS:CE   | 1:A:221:HIS:CG   | 2.76                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:102:LYS:O    | 2:B:237:ASP:HB3  | 1.97                     | 0.65              |
| 2:B:308:GLU:O    | 2:B:311:LYS:HE2  | 1.97                     | 0.64              |
| 1:A:205:LEU:HD13 | 1:A:209:LEU:HD11 | 1.79                     | 0.64              |
| 1:A:343:GLN:HG3  | 1:A:349:LEU:CD1  | 2.27                     | 0.64              |
| 1:A:195:ILE:CG2  | 1:A:199:ARG:NE   | 2.58                     | 0.64              |
| 1:A:524:GLN:NE2  | 1:A:524:GLN:HA   | 2.12                     | 0.64              |
| 1:A:195:ILE:HG23 | 1:A:199:ARG:HD2  | 1.79                     | 0.64              |
| 1:A:35:VAL:O     | 1:A:39:THR:HG23  | 1.97                     | 0.64              |
| 2:B:241:VAL:HG23 | 2:B:243:PRO:CG   | 2.28                     | 0.64              |
| 1:A:468:THR:C    | 1:A:469:LEU:HG   | 2.17                     | 0.64              |
| 2:B:422:LEU:HB3  | 2:B:426:TRP:CZ2  | 2.33                     | 0.64              |
| 2:B:85:GLN:HA    | 2:B:88:TRP:NE1   | 2.12                     | 0.64              |
| 1:A:457:TYR:HA   | 1:A:548:VAL:HG11 | 1.79                     | 0.64              |
| 2:B:419:THR:HG22 | 2:B:420:PRO:O    | 1.98                     | 0.64              |
| 1:A:311:LYS:O    | 1:A:312:GLU:HB3  | 1.98                     | 0.63              |
| 1:A:542:ILE:O    | 1:A:543:GLY:C    | 2.37                     | 0.63              |
| 1:A:175:ASN:N    | 1:A:176:PRO:HD3  | 2.13                     | 0.63              |
| 2:B:13:LYS:CB    | 2:B:16:MET:HE1   | 2.26                     | 0.63              |
| 2:B:243:PRO:HB3  | 2:B:311:LYS:HA   | 1.78                     | 0.63              |
| 1:A:69:THR:HG22  | 1:A:69:THR:O     | 1.99                     | 0.63              |
| 1:A:522:ILE:O    | 1:A:526:ILE:HG13 | 1.98                     | 0.63              |
| 1:A:220:LYS:CE   | 1:A:221:HIS:CE1  | 2.82                     | 0.62              |
| 1:A:279:LEU:CD2  | 1:A:302:GLU:OE1  | 2.46                     | 0.62              |
| 2:B:246:LEU:HD22 | 2:B:260:LEU:HD21 | 1.80                     | 0.62              |
| 1:A:3:SER:OG     | 1:A:5:ILE:HG23   | 1.99                     | 0.62              |
| 2:B:344:GLU:HB2  | 2:B:347:LYS:HD2  | 1.82                     | 0.62              |
| 1:A:312:GLU:OE2  | 1:A:312:GLU:O    | 2.17                     | 0.62              |
| 1:A:171:PHE:N    | 1:A:174:GLN:HE22 | 1.95                     | 0.62              |
| 1:A:218:ASP:O    | 1:A:221:HIS:HB2  | 1.99                     | 0.62              |
| 1:A:104:LYS:HD3  | 1:A:192:ASP:O    | 1.99                     | 0.62              |
| 1:A:228:LEU:HD22 | 1:A:228:LEU:N    | 2.15                     | 0.62              |
| 1:A:5:ILE:CG2    | 1:A:212:TRP:CE3  | 2.81                     | 0.62              |
| 1:A:173:LYS:CE   | 1:A:173:LYS:HA   | 2.14                     | 0.61              |
| 1:A:491:LEU:N    | 1:A:491:LEU:CD1  | 2.62                     | 0.61              |
| 2:B:278:GLN:HE21 | 2:B:278:GLN:HA   | 1.65                     | 0.61              |
| 1:A:369:THR:HG21 | 1:A:398:TRP:CZ3  | 2.36                     | 0.61              |
| 1:A:205:LEU:HD13 | 1:A:209:LEU:CD1  | 2.30                     | 0.61              |
| 2:B:278:GLN:NE2  | 2:B:278:GLN:HA   | 2.15                     | 0.61              |
| 2:B:66:LYS:HB3   | 2:B:66:LYS:NZ    | 2.15                     | 0.61              |
| 2:B:13:LYS:HB2   | 2:B:16:MET:HE1   | 1.73                     | 0.61              |
| 2:B:107:THR:HB   | 2:B:202:ILE:CD1  | 2.31                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:254:VAL:O    | 2:B:258:GLN:HG3  | 2.00                     | 0.61              |
| 1:A:277:ARG:HB2  | 1:A:336:GLN:NE2  | 2.16                     | 0.60              |
| 2:B:250:ASP:O    | 2:B:251:SER:CB   | 2.48                     | 0.60              |
| 1:A:183:TYR:OH   | 1:A:230:MET:HE1  | 2.02                     | 0.60              |
| 1:A:357:MET:HG2  | 1:A:514:GLU:OE2  | 2.01                     | 0.60              |
| 1:A:503:LEU:HD22 | 1:A:507:GLN:HG3  | 1.84                     | 0.60              |
| 2:B:241:VAL:HG23 | 2:B:243:PRO:HG3  | 1.84                     | 0.60              |
| 2:B:422:LEU:HA   | 2:B:425:LEU:CD2  | 2.29                     | 0.60              |
| 2:B:305:GLU:O    | 2:B:309:ILE:N    | 2.30                     | 0.60              |
| 2:B:274:ILE:CG2  | 2:B:306:ASN:ND2  | 2.62                     | 0.60              |
| 1:A:441:TYR:O    | 1:A:548:VAL:HG21 | 2.02                     | 0.60              |
| 1:A:296:THR:HG22 | 1:A:299:ALA:N    | 2.09                     | 0.59              |
| 1:A:406:TRP:CE3  | 1:A:407:GLN:CA   | 2.85                     | 0.59              |
| 2:B:246:LEU:HD12 | 2:B:307:ARG:HG2  | 1.84                     | 0.59              |
| 2:B:305:GLU:HA   | 2:B:308:GLU:HB3  | 1.84                     | 0.59              |
| 1:A:197:GLN:HA   | 1:A:200:THR:HB   | 1.84                     | 0.59              |
| 1:A:170:PRO:C    | 1:A:174:GLN:NE2  | 2.55                     | 0.59              |
| 1:A:216:THR:HB   | 1:A:217:PRO:HD2  | 1.84                     | 0.59              |
| 1:A:238:LYS:HD2  | 1:A:315:HIS:CD2  | 2.37                     | 0.59              |
| 1:A:13:LYS:O     | 1:A:16:MET:HB2   | 2.02                     | 0.59              |
| 1:A:206:ARG:HH12 | 1:A:218:ASP:CB   | 2.16                     | 0.59              |
| 2:B:65:LYS:HZ1   | 2:B:72:ARG:NE    | 2.00                     | 0.59              |
| 1:A:106:VAL:CG1  | 3:A:601:RT7:C16  | 2.81                     | 0.59              |
| 1:A:233:GLU:CG   | 1:A:235:HIS:HE1  | 2.10                     | 0.59              |
| 2:B:24:TRP:CE3   | 2:B:61:PHE:HZ    | 2.21                     | 0.59              |
| 1:A:106:VAL:CG1  | 3:A:601:RT7:C17  | 2.81                     | 0.58              |
| 1:A:106:VAL:HG11 | 3:A:601:RT7:C16  | 2.33                     | 0.58              |
| 2:B:242:GLN:HG3  | 2:B:242:GLN:O    | 2.01                     | 0.58              |
| 2:B:260:LEU:HD13 | 2:B:264:LEU:HD12 | 1.85                     | 0.58              |
| 1:A:457:TYR:C    | 1:A:457:TYR:CD1  | 2.77                     | 0.58              |
| 1:A:539:HIS:C    | 1:A:540:LYS:HD3  | 2.22                     | 0.58              |
| 2:B:283:LEU:O    | 2:B:284:ARG:HG3  | 2.02                     | 0.58              |
| 1:A:286:THR:HG23 | 1:A:287:LYS:O    | 2.04                     | 0.58              |
| 1:A:355:ALA:O    | 1:A:356:ARG:O    | 2.21                     | 0.58              |
| 1:A:63:ILE:HD11  | 1:A:72:ARG:HB2   | 1.85                     | 0.58              |
| 2:B:241:VAL:HG23 | 2:B:243:PRO:CD   | 2.34                     | 0.58              |
| 1:A:230:MET:CA   | 1:A:230:MET:CE   | 2.79                     | 0.58              |
| 1:A:498:ASP:OD2  | 1:A:538:ALA:HB2  | 2.02                     | 0.58              |
| 1:A:218:ASP:O    | 1:A:219:LYS:C    | 2.41                     | 0.58              |
| 1:A:24:TRP:CD1   | 1:A:25:PRO:HD2   | 2.39                     | 0.58              |
| 2:B:420:PRO:HB2  | 2:B:423:VAL:CG2  | 2.33                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:5:ILE:CD1    | 2:B:5:ILE:N      | 2.67                     | 0.57              |
| 1:A:46:LYS:HE3   | 1:A:116:PHE:HB3  | 1.84                     | 0.57              |
| 2:B:13:LYS:O     | 2:B:16:MET:CE    | 2.53                     | 0.57              |
| 2:B:302:GLU:O    | 2:B:303:LEU:C    | 2.43                     | 0.57              |
| 1:A:195:ILE:HD13 | 1:A:199:ARG:NH2  | 2.19                     | 0.57              |
| 1:A:43:LYS:CE    | 1:A:43:LYS:HA    | 2.23                     | 0.57              |
| 2:B:13:LYS:HB3   | 2:B:16:MET:CE    | 2.30                     | 0.57              |
| 2:B:195:ILE:O    | 2:B:199:ARG:CG   | 2.52                     | 0.57              |
| 1:A:244:ILE:CD1  | 1:A:267:ALA:HB2  | 2.34                     | 0.57              |
| 1:A:529:GLU:O    | 1:A:530:LYS:CG   | 2.51                     | 0.57              |
| 2:B:214:LEU:CD2  | 2:B:214:LEU:H    | 1.97                     | 0.57              |
| 2:B:65:LYS:NZ    | 2:B:72:ARG:HE    | 2.02                     | 0.57              |
| 1:A:330:GLN:NE2  | 1:A:338:THR:HG22 | 2.18                     | 0.57              |
| 2:B:266:TRP:CD1  | 2:B:426:TRP:CE3  | 2.93                     | 0.57              |
| 2:B:266:TRP:NE1  | 2:B:346:PHE:CE2  | 2.64                     | 0.57              |
| 1:A:253:THR:HA   | 1:A:291:GLU:O    | 2.05                     | 0.57              |
| 2:B:28:GLU:HG2   | 2:B:32:LYS:HE2   | 1.87                     | 0.57              |
| 1:A:410:TRP:CZ3  | 2:B:363:ASN:CB   | 2.88                     | 0.57              |
| 1:A:171:PHE:CZ   | 1:A:205:LEU:HD23 | 2.40                     | 0.56              |
| 1:A:355:ALA:O    | 1:A:356:ARG:C    | 2.44                     | 0.56              |
| 1:A:406:TRP:CH2  | 1:A:407:GLN:OE1  | 2.58                     | 0.56              |
| 2:B:75:VAL:HG11  | 2:B:77:PHE:CZ    | 2.40                     | 0.56              |
| 1:A:319:TYR:OH   | 1:A:385:LYS:HE2  | 2.06                     | 0.56              |
| 2:B:253:THR:HG23 | 2:B:255:ASN:N    | 2.20                     | 0.56              |
| 2:B:428:GLN:NE2  | 2:B:428:GLN:CA   | 2.68                     | 0.56              |
| 2:B:107:THR:HB   | 2:B:202:ILE:HD13 | 1.86                     | 0.56              |
| 1:A:106:VAL:HG13 | 3:A:601:RT7:C18  | 2.34                     | 0.56              |
| 1:A:118:VAL:HG23 | 1:A:119:PRO:HD2  | 1.87                     | 0.56              |
| 1:A:440:PHE:CE1  | 1:A:489:SER:HB3  | 2.40                     | 0.56              |
| 2:B:169:GLU:HB3  | 2:B:170:PRO:HD3  | 1.86                     | 0.56              |
| 2:B:244:ILE:HD11 | 2:B:266:TRP:CH2  | 2.41                     | 0.56              |
| 1:A:171:PHE:O    | 1:A:175:ASN:HB2  | 2.06                     | 0.56              |
| 1:A:194:GLU:CD   | 1:A:194:GLU:H    | 2.09                     | 0.56              |
| 1:A:24:TRP:CG    | 1:A:25:PRO:HD2   | 2.41                     | 0.56              |
| 1:A:364:ASP:HB3  | 1:A:423:VAL:HG13 | 1.88                     | 0.56              |
| 2:B:13:LYS:HE3   | 2:B:86:ASP:H     | 1.67                     | 0.56              |
| 1:A:246:LEU:HD23 | 1:A:246:LEU:N    | 2.21                     | 0.56              |
| 1:A:287:LYS:HG2  | 1:A:291:GLU:OE1  | 2.05                     | 0.56              |
| 2:B:246:LEU:HD22 | 2:B:260:LEU:CD2  | 2.36                     | 0.56              |
| 2:B:111:VAL:HG13 | 2:B:111:VAL:O    | 2.05                     | 0.55              |
| 1:A:398:TRP:CZ2  | 1:A:411:ILE:HD12 | 2.40                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:457:TYR:HA   | 1:A:548:VAL:CG1  | 2.36                     | 0.55              |
| 1:A:425:LEU:N    | 1:A:425:LEU:HD22 | 2.22                     | 0.55              |
| 2:B:66:LYS:HB3   | 2:B:66:LYS:HZ3   | 1.71                     | 0.55              |
| 1:A:542:ILE:C    | 1:A:543:GLY:O    | 2.44                     | 0.55              |
| 1:A:3:SER:OG     | 1:A:5:ILE:CD1    | 2.53                     | 0.55              |
| 1:A:424:LYS:HE2  | 1:A:426:TRP:CZ2  | 2.41                     | 0.55              |
| 2:B:46:LYS:HD3   | 2:B:116:PHE:HB2  | 1.88                     | 0.55              |
| 1:A:220:LYS:HE2  | 1:A:221:HIS:NE2  | 2.17                     | 0.55              |
| 1:A:65:LYS:CE    | 1:A:70:LYS:HE2   | 2.36                     | 0.55              |
| 1:A:458:VAL:HG22 | 1:A:548:VAL:CG2  | 2.33                     | 0.55              |
| 1:A:410:TRP:CE3  | 2:B:363:ASN:HB2  | 2.41                     | 0.55              |
| 1:A:278:GLN:HB3  | 1:A:299:ALA:HA   | 1.89                     | 0.55              |
| 1:A:388:LYS:HD2  | 1:A:413:GLU:OE1  | 2.06                     | 0.55              |
| 1:A:171:PHE:CD2  | 1:A:205:LEU:HD23 | 2.42                     | 0.54              |
| 2:B:107:THR:CB   | 2:B:202:ILE:CD1  | 2.85                     | 0.54              |
| 2:B:24:TRP:CE3   | 2:B:61:PHE:CZ    | 2.94                     | 0.54              |
| 1:A:206:ARG:NH1  | 1:A:218:ASP:CB   | 2.70                     | 0.54              |
| 1:A:229:TRP:CD2  | 1:A:230:MET:HB2  | 2.42                     | 0.54              |
| 1:A:229:TRP:O    | 1:A:231:GLY:N    | 2.39                     | 0.54              |
| 1:A:489:SER:CB   | 1:A:493:VAL:CG2  | 2.85                     | 0.54              |
| 1:A:65:LYS:O     | 1:A:67:ASP:N     | 2.40                     | 0.54              |
| 1:A:95:PRO:HA    | 2:B:136:ASN:O    | 2.07                     | 0.54              |
| 1:A:284:ARG:HH11 | 1:A:284:ARG:HB2  | 1.73                     | 0.54              |
| 1:A:273:GLY:HA2  | 1:A:332:GLN:NE2  | 2.21                     | 0.54              |
| 1:A:271:TYR:CE1  | 1:A:314:VAL:HG23 | 2.42                     | 0.54              |
| 2:B:286:THR:O    | 2:B:286:THR:OG1  | 2.25                     | 0.54              |
| 2:B:13:LYS:HZ1   | 2:B:85:GLN:HG2   | 1.72                     | 0.54              |
| 2:B:65:LYS:NZ    | 2:B:72:ARG:NE    | 2.56                     | 0.54              |
| 2:B:96:HIS:HE1   | 2:B:381:VAL:O    | 1.91                     | 0.54              |
| 1:A:287:LYS:HE3  | 1:A:291:GLU:OE2  | 2.07                     | 0.54              |
| 2:B:297:GLU:N    | 2:B:298:GLU:OE2  | 2.41                     | 0.54              |
| 1:A:211:ARG:C    | 1:A:211:ARG:HD3  | 2.24                     | 0.54              |
| 1:A:406:TRP:CE3  | 1:A:407:GLN:N    | 2.76                     | 0.54              |
| 1:A:503:LEU:CD2  | 1:A:507:GLN:HG3  | 2.38                     | 0.54              |
| 1:A:547:GLN:NE2  | 1:A:547:GLN:N    | 2.51                     | 0.54              |
| 2:B:13:LYS:NZ    | 2:B:85:GLN:HG2   | 2.23                     | 0.54              |
| 1:A:330:GLN:HE22 | 1:A:338:THR:HG23 | 1.70                     | 0.53              |
| 1:A:458:VAL:HG23 | 1:A:458:VAL:O    | 2.08                     | 0.53              |
| 1:A:197:GLN:HA   | 1:A:200:THR:CB   | 2.38                     | 0.53              |
| 1:A:218:ASP:OD2  | 1:A:220:LYS:CE   | 2.56                     | 0.53              |
| 1:A:244:ILE:HD13 | 1:A:267:ALA:HB2  | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:275:LYS:H    | 2:B:306:ASN:HD21 | 1.55                     | 0.53              |
| 2:B:13:LYS:CE    | 2:B:85:GLN:HB3   | 2.38                     | 0.53              |
| 2:B:312:GLU:OE2  | 2:B:312:GLU:HA   | 2.08                     | 0.53              |
| 2:B:305:GLU:O    | 2:B:309:ILE:HG13 | 2.09                     | 0.53              |
| 2:B:428:GLN:CA   | 2:B:428:GLN:HE21 | 2.19                     | 0.53              |
| 2:B:91:GLN:O     | 2:B:92:LEU:HD23  | 2.09                     | 0.53              |
| 1:A:311:LYS:O    | 1:A:312:GLU:CB   | 2.56                     | 0.53              |
| 1:A:134:SER:OG   | 1:A:138:GLU:O    | 2.25                     | 0.53              |
| 1:A:357:MET:HE1  | 1:A:360:ALA:C    | 2.28                     | 0.53              |
| 1:A:49:LYS:HB2   | 1:A:49:LYS:NZ    | 2.24                     | 0.53              |
| 1:A:520:GLN:O    | 1:A:523:GLU:HG2  | 2.08                     | 0.53              |
| 2:B:105:SER:O    | 2:B:190:GLY:HA2  | 2.08                     | 0.53              |
| 1:A:406:TRP:CE3  | 1:A:407:GLN:CB   | 2.92                     | 0.52              |
| 1:A:491:LEU:H    | 1:A:491:LEU:HD13 | 1.74                     | 0.52              |
| 2:B:50:ILE:HD12  | 2:B:54:ASN:CB    | 2.38                     | 0.52              |
| 2:B:85:GLN:HA    | 2:B:88:TRP:CE2   | 2.44                     | 0.52              |
| 1:A:287:LYS:CD   | 1:A:291:GLU:OE2  | 2.57                     | 0.52              |
| 1:A:197:GLN:HB2  | 1:A:200:THR:HB   | 1.91                     | 0.52              |
| 1:A:51:GLY:HA3   | 1:A:53:GLU:OE2   | 2.09                     | 0.52              |
| 1:A:2:ILE:N      | 1:A:2:ILE:HD13   | 2.22                     | 0.52              |
| 1:A:458:VAL:CG2  | 1:A:548:VAL:HG22 | 2.33                     | 0.52              |
| 1:A:106:VAL:CG1  | 3:A:601:RT7:C21  | 2.88                     | 0.52              |
| 2:B:241:VAL:O    | 2:B:243:PRO:HD3  | 2.10                     | 0.52              |
| 1:A:170:PRO:O    | 1:A:173:LYS:N    | 2.42                     | 0.52              |
| 1:A:24:TRP:CG    | 1:A:25:PRO:CD    | 2.93                     | 0.52              |
| 1:A:540:LYS:O    | 1:A:541:GLY:O    | 2.27                     | 0.52              |
| 1:A:206:ARG:HH12 | 1:A:218:ASP:HB2  | 1.75                     | 0.51              |
| 2:B:297:GLU:O    | 2:B:301:LEU:HG   | 2.10                     | 0.51              |
| 2:B:309:ILE:O    | 2:B:311:LYS:N    | 2.43                     | 0.51              |
| 1:A:369:THR:HG21 | 1:A:398:TRP:HZ3  | 1.75                     | 0.51              |
| 1:A:42:GLU:OE2   | 1:A:49:LYS:NZ    | 2.42                     | 0.51              |
| 1:A:195:ILE:O    | 1:A:196:GLY:C    | 2.48                     | 0.51              |
| 1:A:547:GLN:O    | 1:A:550:LYS:HG3  | 2.09                     | 0.51              |
| 1:A:65:LYS:CE    | 1:A:72:ARG:NH1   | 2.56                     | 0.51              |
| 2:B:153:TRP:CZ2  | 2:B:155:GLY:HA3  | 2.45                     | 0.51              |
| 1:A:114:ALA:HB1  | 1:A:160:PHE:CE1  | 2.45                     | 0.51              |
| 1:A:399:GLU:O    | 1:A:403:THR:HB   | 2.10                     | 0.51              |
| 1:A:509:GLN:N    | 1:A:510:PRO:CD   | 2.74                     | 0.51              |
| 2:B:261:VAL:HA   | 2:B:264:LEU:HB2  | 1.92                     | 0.51              |
| 2:B:421:PRO:O    | 2:B:425:LEU:CD2  | 2.58                     | 0.51              |
| 2:B:13:LYS:HE3   | 2:B:85:GLN:CB    | 2.40                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:406:TRP:O    | 2:B:331:LYS:HB3  | 2.10                     | 0.51              |
| 1:A:170:PRO:O    | 1:A:171:PHE:C    | 2.48                     | 0.51              |
| 2:B:308:GLU:O    | 2:B:311:LYS:HE3  | 2.09                     | 0.51              |
| 2:B:328:GLU:HG3  | 2:B:390:LYS:HD3  | 1.93                     | 0.51              |
| 1:A:406:TRP:CZ2  | 2:B:418:ASN:OD1  | 2.64                     | 0.51              |
| 2:B:213:GLY:O    | 2:B:214:LEU:C    | 2.49                     | 0.51              |
| 1:A:433:PRO:HB2  | 2:B:290:THR:HG22 | 1.93                     | 0.51              |
| 2:B:292:VAL:HG12 | 2:B:293:ILE:N    | 2.25                     | 0.51              |
| 1:A:228:LEU:HD12 | 1:A:242:GLN:HE21 | 1.76                     | 0.51              |
| 2:B:308:GLU:HA   | 2:B:311:LYS:NZ   | 2.25                     | 0.51              |
| 1:A:296:THR:HG23 | 1:A:297:GLU:N    | 2.26                     | 0.51              |
| 1:A:297:GLU:C    | 1:A:298:GLU:OE2  | 2.42                     | 0.51              |
| 1:A:409:THR:HG23 | 1:A:410:TRP:N    | 2.25                     | 0.51              |
| 2:B:274:ILE:HG23 | 2:B:306:ASN:HD22 | 1.68                     | 0.51              |
| 1:A:542:ILE:CG2  | 1:A:543:GLY:N    | 2.74                     | 0.50              |
| 1:A:409:THR:HG23 | 1:A:410:TRP:H    | 1.76                     | 0.50              |
| 2:B:361:HIS:O    | 2:B:361:HIS:CG   | 2.65                     | 0.50              |
| 1:A:491:LEU:N    | 1:A:491:LEU:HD13 | 2.26                     | 0.50              |
| 1:A:91:GLN:HE21  | 1:A:92:LEU:N     | 2.09                     | 0.50              |
| 2:B:121:ASP:C    | 2:B:121:ASP:OD2  | 2.50                     | 0.50              |
| 1:A:541:GLY:O    | 1:A:542:ILE:HG13 | 2.12                     | 0.50              |
| 1:A:195:ILE:CG2  | 1:A:199:ARG:CZ   | 2.90                     | 0.50              |
| 1:A:197:GLN:CA   | 1:A:200:THR:HB   | 2.42                     | 0.50              |
| 1:A:296:THR:CG2  | 1:A:299:ALA:H    | 2.12                     | 0.50              |
| 2:B:425:LEU:HD23 | 2:B:425:LEU:N    | 2.12                     | 0.50              |
| 1:A:467:VAL:CG1  | 1:A:468:THR:N    | 2.75                     | 0.50              |
| 2:B:13:LYS:O     | 2:B:16:MET:HE3   | 2.11                     | 0.50              |
| 2:B:47:ILE:HD12  | 2:B:144:TYR:CD1  | 2.46                     | 0.49              |
| 2:B:320:ASP:C    | 2:B:320:ASP:OD1  | 2.49                     | 0.49              |
| 2:B:13:LYS:HE3   | 2:B:86:ASP:N     | 2.27                     | 0.49              |
| 1:A:28:GLU:HG2   | 1:A:135:ILE:HG23 | 1.92                     | 0.49              |
| 1:A:235:HIS:HB3  | 1:A:236:PRO:HD2  | 1.94                     | 0.49              |
| 2:B:253:THR:HG22 | 2:B:256:ASP:OD1  | 2.12                     | 0.49              |
| 1:A:70:LYS:HE2   | 1:A:72:ARG:NH1   | 2.27                     | 0.49              |
| 2:B:13:LYS:HE2   | 2:B:86:ASP:CB    | 2.41                     | 0.49              |
| 2:B:13:LYS:CA    | 2:B:16:MET:HE3   | 2.36                     | 0.49              |
| 2:B:305:GLU:O    | 2:B:308:GLU:HB3  | 2.12                     | 0.49              |
| 1:A:438:GLU:OE1  | 1:A:459:THR:HG21 | 2.13                     | 0.49              |
| 2:B:239:TRP:CH2  | 2:B:378:GLU:HG2  | 2.48                     | 0.49              |
| 2:B:248:GLU:O    | 2:B:249:LYS:HB3  | 2.13                     | 0.49              |
| 3:A:601:RT7:CL29 | 3:A:601:RT7:S12  | 3.08                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:241:VAL:HG21 | 2:B:243:PRO:HG3  | 1.92                     | 0.49              |
| 2:B:279:LEU:HD13 | 2:B:282:LEU:HD12 | 1.95                     | 0.49              |
| 1:A:91:GLN:NE2   | 1:A:92:LEU:N     | 2.61                     | 0.48              |
| 2:B:9:PRO:HA     | 2:B:121:ASP:OD1  | 2.13                     | 0.48              |
| 1:A:30:LYS:HE3   | 1:A:61:PHE:HE1   | 1.73                     | 0.48              |
| 1:A:3:SER:CB     | 1:A:5:ILE:HD12   | 2.43                     | 0.48              |
| 2:B:153:TRP:CH2  | 2:B:155:GLY:HA3  | 2.48                     | 0.48              |
| 2:B:247:PRO:HB2  | 2:B:249:LYS:HE3  | 1.95                     | 0.48              |
| 1:A:53:GLU:N     | 1:A:53:GLU:CD    | 2.65                     | 0.48              |
| 1:A:468:THR:HG22 | 1:A:469:LEU:N    | 2.28                     | 0.48              |
| 1:A:544:GLY:HA2  | 2:B:286:THR:HG22 | 1.96                     | 0.48              |
| 1:A:106:VAL:CG1  | 3:A:601:RT7:C18  | 2.91                     | 0.48              |
| 1:A:76:ASP:OD2   | 1:A:78:ARG:HG3   | 2.13                     | 0.48              |
| 2:B:366:LYS:O    | 2:B:370:GLU:HG3  | 2.14                     | 0.48              |
| 2:B:382:ILE:HG22 | 2:B:383:TRP:CD1  | 2.48                     | 0.48              |
| 2:B:260:LEU:HD22 | 2:B:264:LEU:HG   | 1.96                     | 0.48              |
| 2:B:422:LEU:O    | 2:B:425:LEU:HD23 | 2.14                     | 0.48              |
| 1:A:173:LYS:HE3  | 1:A:173:LYS:CA   | 2.22                     | 0.48              |
| 1:A:107:THR:CG2  | 1:A:198:HIS:HE1  | 2.10                     | 0.48              |
| 1:A:457:TYR:HD1  | 1:A:457:TYR:C    | 2.17                     | 0.48              |
| 1:A:64:LYS:HB3   | 1:A:65:LYS:H     | 1.55                     | 0.48              |
| 2:B:260:LEU:HD22 | 2:B:260:LEU:C    | 2.24                     | 0.48              |
| 1:A:406:TRP:CZ3  | 1:A:407:GLN:CB   | 2.85                     | 0.47              |
| 2:B:13:LYS:HZ2   | 2:B:85:GLN:HB3   | 1.78                     | 0.47              |
| 1:A:218:ASP:C    | 1:A:219:LYS:O    | 2.52                     | 0.47              |
| 1:A:372:VAL:HG11 | 1:A:411:ILE:HG23 | 1.96                     | 0.47              |
| 1:A:43:LYS:CA    | 1:A:43:LYS:HE2   | 2.28                     | 0.47              |
| 1:A:458:VAL:O    | 1:A:458:VAL:CG2  | 2.62                     | 0.47              |
| 1:A:21:VAL:CG2   | 1:A:59:PRO:HD3   | 2.29                     | 0.47              |
| 1:A:5:ILE:HG22   | 1:A:212:TRP:HE3  | 1.71                     | 0.47              |
| 1:A:229:TRP:CE2  | 1:A:230:MET:HB2  | 2.49                     | 0.47              |
| 1:A:238:LYS:HD2  | 1:A:315:HIS:CG   | 2.49                     | 0.47              |
| 1:A:280:CYS:O    | 1:A:281:LYS:C    | 2.53                     | 0.47              |
| 1:A:296:THR:HG23 | 1:A:298:GLU:CD   | 2.34                     | 0.47              |
| 1:A:356:ARG:HH21 | 1:A:358:ARG:CD   | 2.23                     | 0.47              |
| 1:A:298:GLU:HA   | 1:A:301:LEU:HD12 | 1.97                     | 0.47              |
| 1:A:114:ALA:HB1  | 1:A:160:PHE:CZ   | 2.50                     | 0.47              |
| 2:B:382:ILE:HG22 | 2:B:383:TRP:CG   | 2.50                     | 0.47              |
| 2:B:382:ILE:HG21 | 2:B:383:TRP:CE2  | 2.49                     | 0.47              |
| 1:A:195:ILE:HG21 | 1:A:199:ARG:CZ   | 2.45                     | 0.47              |
| 1:A:296:THR:O    | 1:A:300:GLU:HG2  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:365:VAL:O    | 1:A:369:THR:CG2  | 2.62                     | 0.47              |
| 2:B:382:ILE:CG2  | 2:B:383:TRP:CE2  | 2.97                     | 0.47              |
| 1:A:181:TYR:CE2  | 1:A:183:TYR:HB2  | 2.49                     | 0.47              |
| 1:A:17:ASP:O     | 1:A:83:ARG:HD3   | 2.14                     | 0.47              |
| 2:B:214:LEU:N    | 2:B:214:LEU:CD2  | 2.64                     | 0.47              |
| 2:B:115:TYR:HB3  | 2:B:149:LEU:HB2  | 1.96                     | 0.47              |
| 2:B:58:THR:HG23  | 2:B:76:ASP:O     | 2.15                     | 0.47              |
| 2:B:12:LEU:HD12  | 2:B:84:THR:HG22  | 1.97                     | 0.47              |
| 1:A:137:ASN:ND2  | 1:A:137:ASN:C    | 2.68                     | 0.46              |
| 1:A:277:ARG:NH1  | 1:A:278:GLN:NE2  | 2.63                     | 0.46              |
| 1:A:296:THR:CG2  | 1:A:297:GLU:N    | 2.74                     | 0.46              |
| 1:A:311:LYS:O    | 1:A:312:GLU:CD   | 2.54                     | 0.46              |
| 1:A:410:TRP:O    | 1:A:411:ILE:HG13 | 2.15                     | 0.46              |
| 2:B:82:LYS:NZ    | 2:B:413:GLU:OE2  | 2.48                     | 0.46              |
| 1:A:369:THR:CG2  | 1:A:398:TRP:CZ3  | 2.99                     | 0.46              |
| 2:B:8:VAL:O      | 2:B:121:ASP:HB2  | 2.16                     | 0.46              |
| 1:A:197:GLN:CB   | 1:A:200:THR:HB   | 2.46                     | 0.46              |
| 2:B:254:VAL:HG21 | 2:B:288:ALA:O    | 2.15                     | 0.46              |
| 2:B:308:GLU:O    | 2:B:311:LYS:HG2  | 2.16                     | 0.46              |
| 1:A:13:LYS:HE3   | 1:A:84:THR:O     | 2.15                     | 0.46              |
| 1:A:273:GLY:HA2  | 1:A:332:GLN:HE22 | 1.81                     | 0.46              |
| 2:B:13:LYS:O     | 2:B:16:MET:HE2   | 2.15                     | 0.46              |
| 2:B:172:ARG:HH21 | 2:B:180:ILE:HB   | 1.79                     | 0.46              |
| 1:A:515:SER:OG   | 1:A:518:VAL:HG23 | 2.16                     | 0.46              |
| 2:B:250:ASP:O    | 2:B:251:SER:HB3  | 2.15                     | 0.46              |
| 1:A:54:ASN:C     | 1:A:54:ASN:OD1   | 2.53                     | 0.46              |
| 1:A:180:ILE:HA   | 1:A:188:TYR:O    | 2.16                     | 0.46              |
| 1:A:104:LYS:HD3  | 1:A:192:ASP:C    | 2.36                     | 0.46              |
| 1:A:102:LYS:HE3  | 1:A:237:ASP:OD1  | 2.16                     | 0.46              |
| 1:A:248:GLU:OE1  | 1:A:248:GLU:HA   | 2.15                     | 0.46              |
| 1:A:496:VAL:HG22 | 1:A:496:VAL:O    | 2.15                     | 0.46              |
| 1:A:2:ILE:HD11   | 1:A:46:LYS:NZ    | 2.30                     | 0.45              |
| 1:A:483:TYR:CE2  | 1:A:520:GLN:NE2  | 2.84                     | 0.45              |
| 1:A:206:ARG:CZ   | 1:A:218:ASP:HB3  | 2.47                     | 0.45              |
| 2:B:111:VAL:HG22 | 2:B:214:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:333:GLY:O    | 1:A:334:GLN:C    | 2.54                     | 0.45              |
| 1:A:433:PRO:HB2  | 2:B:290:THR:CG2  | 2.46                     | 0.45              |
| 2:B:297:GLU:O    | 2:B:301:LEU:CD2  | 2.65                     | 0.45              |
| 2:B:63:ILE:HD13  | 2:B:74:LEU:HD22  | 1.98                     | 0.45              |
| 1:A:169:GLU:N    | 1:A:170:PRO:HD2  | 2.31                     | 0.45              |
| 1:A:438:GLU:OE1  | 1:A:459:THR:OG1  | 2.27                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:312:GLU:OE2  | 2:B:313:PRO:HD2  | 2.15                     | 0.45              |
| 1:A:210:LEU:CD2  | 1:A:210:LEU:O    | 2.50                     | 0.45              |
| 1:A:39:THR:O     | 1:A:43:LYS:HG2   | 2.17                     | 0.45              |
| 1:A:125:ARG:HB3  | 1:A:146:TYR:O    | 2.16                     | 0.45              |
| 1:A:16:MET:CE    | 1:A:83:ARG:HG2   | 2.46                     | 0.45              |
| 2:B:46:LYS:NZ    | 2:B:116:PHE:O    | 2.39                     | 0.45              |
| 2:B:90:VAL:O     | 2:B:90:VAL:HG23  | 2.17                     | 0.45              |
| 1:A:101:LYS:HD3  | 1:A:321:PRO:HG3  | 1.99                     | 0.45              |
| 1:A:498:ASP:CB   | 1:A:538:ALA:HB2  | 2.46                     | 0.45              |
| 2:B:107:THR:HB   | 2:B:202:ILE:HD11 | 1.98                     | 0.45              |
| 2:B:33:ALA:O     | 2:B:37:ILE:HD12  | 2.16                     | 0.45              |
| 1:A:194:GLU:O    | 1:A:195:ILE:C    | 2.56                     | 0.45              |
| 1:A:406:TRP:HZ2  | 2:B:418:ASN:OD1  | 2.00                     | 0.45              |
| 1:A:170:PRO:C    | 1:A:174:GLN:HE22 | 2.19                     | 0.44              |
| 1:A:459:THR:OG1  | 1:A:460:ASN:N    | 2.48                     | 0.44              |
| 1:A:542:ILE:HG22 | 1:A:543:GLY:N    | 2.32                     | 0.44              |
| 1:A:156:SER:HB2  | 1:A:157:PRO:HD3  | 1.98                     | 0.44              |
| 1:A:357:MET:HG3  | 1:A:359:GLY:O    | 2.17                     | 0.44              |
| 1:A:369:THR:CG2  | 1:A:398:TRP:HZ3  | 2.30                     | 0.44              |
| 1:A:46:LYS:HE3   | 1:A:116:PHE:CB   | 2.47                     | 0.44              |
| 1:A:200:THR:O    | 1:A:203:GLU:HB2  | 2.17                     | 0.44              |
| 2:B:266:TRP:CH2  | 2:B:427:TYR:CZ   | 3.05                     | 0.44              |
| 2:B:99:GLY:O     | 2:B:102:LYS:HB2  | 2.17                     | 0.44              |
| 1:A:120:LEU:O    | 1:A:121:ASP:C    | 2.54                     | 0.44              |
| 2:B:158:ALA:O    | 2:B:161:GLN:HB2  | 2.18                     | 0.44              |
| 1:A:403:THR:HG22 | 1:A:404:GLU:HG3  | 2.00                     | 0.44              |
| 2:B:157:PRO:HG3  | 2:B:184:MET:HA   | 1.98                     | 0.44              |
| 2:B:253:THR:CG2  | 2:B:255:ASN:HB3  | 2.48                     | 0.44              |
| 1:A:222:GLN:H    | 1:A:222:GLN:HG2  | 1.58                     | 0.44              |
| 1:A:252:TRP:O    | 1:A:292:VAL:HA   | 2.18                     | 0.44              |
| 1:A:528:LYS:HG2  | 1:A:531:VAL:CG2  | 2.47                     | 0.44              |
| 1:A:64:LYS:NZ    | 1:A:69:THR:CA    | 2.60                     | 0.44              |
| 2:B:266:TRP:CG   | 2:B:426:TRP:CE3  | 3.06                     | 0.44              |
| 2:B:309:ILE:C    | 2:B:311:LYS:H    | 2.21                     | 0.44              |
| 2:B:13:LYS:NZ    | 2:B:85:GLN:HB3   | 2.33                     | 0.44              |
| 2:B:252:TRP:CD1  | 2:B:295:LEU:HD21 | 2.52                     | 0.44              |
| 1:A:513:SER:H    | 1:A:519:ASN:HD21 | 1.65                     | 0.44              |
| 2:B:278:GLN:HE21 | 2:B:278:GLN:CA   | 2.26                     | 0.44              |
| 1:A:101:LYS:CE   | 1:A:321:PRO:HG3  | 2.48                     | 0.44              |
| 1:A:19:PRO:HG3   | 1:A:80:LEU:HB2   | 1.99                     | 0.44              |
| 1:A:287:LYS:CD   | 1:A:287:LYS:N    | 2.81                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:373:GLN:O    | 2:B:377:THR:HG23 | 2.18                     | 0.44              |
| 1:A:369:THR:HG21 | 1:A:398:TRP:CH2  | 2.52                     | 0.43              |
| 1:A:467:VAL:HG12 | 1:A:468:THR:N    | 2.33                     | 0.43              |
| 3:A:601:RT7:O23  | 3:A:601:RT7:C21  | 2.59                     | 0.43              |
| 2:B:282:LEU:HB3  | 2:B:293:ILE:CD1  | 2.39                     | 0.43              |
| 1:A:60:VAL:HG21  | 1:A:130:PHE:HD2  | 1.83                     | 0.43              |
| 1:A:194:GLU:O    | 1:A:196:GLY:N    | 2.51                     | 0.43              |
| 1:A:229:TRP:C    | 1:A:231:GLY:H    | 2.21                     | 0.43              |
| 1:A:229:TRP:C    | 1:A:231:GLY:N    | 2.71                     | 0.43              |
| 1:A:2:ILE:O      | 1:A:3:SER:C      | 2.57                     | 0.43              |
| 1:A:540:LYS:HB2  | 1:A:542:ILE:HD12 | 1.99                     | 0.43              |
| 1:A:27:THR:OG1   | 1:A:30:LYS:HD2   | 2.17                     | 0.43              |
| 2:B:296:THR:C    | 2:B:298:GLU:OE2  | 2.57                     | 0.43              |
| 1:A:225:PRO:HA   | 1:A:226:PRO:C    | 2.38                     | 0.43              |
| 1:A:297:GLU:CA   | 1:A:298:GLU:OE2  | 2.67                     | 0.43              |
| 1:A:440:PHE:CZ   | 1:A:489:SER:HB3  | 2.54                     | 0.43              |
| 2:B:342:TYR:CD2  | 2:B:342:TYR:C    | 2.91                     | 0.43              |
| 2:B:129:ALA:HA   | 2:B:144:TYR:O    | 2.17                     | 0.43              |
| 1:A:175:ASN:N    | 1:A:176:PRO:CD   | 2.81                     | 0.43              |
| 1:A:21:VAL:CG2   | 1:A:59:PRO:CD    | 2.91                     | 0.43              |
| 2:B:36:GLU:O     | 2:B:37:ILE:C     | 2.56                     | 0.43              |
| 2:B:292:VAL:O    | 2:B:293:ILE:HG22 | 2.18                     | 0.43              |
| 1:A:278:GLN:HB2  | 1:A:302:GLU:CD   | 2.40                     | 0.43              |
| 1:A:3:SER:CB     | 1:A:5:ILE:CD1    | 2.97                     | 0.43              |
| 1:A:94:ILE:O     | 1:A:95:PRO:C     | 2.55                     | 0.43              |
| 2:B:422:LEU:HB3  | 2:B:426:TRP:CE2  | 2.54                     | 0.43              |
| 1:A:425:LEU:H    | 1:A:425:LEU:HD22 | 1.83                     | 0.43              |
| 2:B:53:GLU:OE1   | 2:B:53:GLU:N     | 2.44                     | 0.43              |
| 1:A:195:ILE:O    | 1:A:199:ARG:HD2  | 2.19                     | 0.42              |
| 1:A:3:SER:HB3    | 1:A:5:ILE:CD1    | 2.49                     | 0.42              |
| 2:B:421:PRO:HG2  | 2:B:422:LEU:HG   | 2.00                     | 0.42              |
| 1:A:320:ASP:HA   | 1:A:321:PRO:HD2  | 1.94                     | 0.42              |
| 1:A:100:LEU:HD22 | 3:A:601:RT7:H210 | 2.01                     | 0.42              |
| 2:B:236:PRO:O    | 2:B:239:TRP:N    | 2.53                     | 0.42              |
| 2:B:293:ILE:HB   | 2:B:294:PRO:HD2  | 2.01                     | 0.42              |
| 1:A:222:GLN:O    | 1:A:223:LYS:C    | 2.57                     | 0.42              |
| 1:A:402:TRP:CG   | 1:A:403:THR:N    | 2.86                     | 0.42              |
| 2:B:382:ILE:HG22 | 2:B:383:TRP:CD2  | 2.55                     | 0.42              |
| 1:A:106:VAL:HG11 | 3:A:601:RT7:C17  | 2.48                     | 0.42              |
| 1:A:219:LYS:C    | 1:A:221:HIS:H    | 2.22                     | 0.42              |
| 2:B:80:LEU:HD23  | 2:B:80:LEU:HA    | 1.79                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:210:LEU:C    | 1:A:210:LEU:HD22 | 2.25                     | 0.42              |
| 1:A:406:TRP:CE3  | 1:A:407:GLN:HA   | 2.54                     | 0.42              |
| 1:A:454:LYS:NZ   | 1:A:554:ALA:O    | 2.52                     | 0.42              |
| 2:B:103:LYS:HD3  | 2:B:103:LYS:HA   | 1.89                     | 0.42              |
| 1:A:169:GLU:O    | 1:A:172:ARG:HB2  | 2.18                     | 0.42              |
| 1:A:211:ARG:CD   | 1:A:211:ARG:C    | 2.85                     | 0.42              |
| 2:B:13:LYS:HA    | 2:B:14:PRO:HD2   | 1.75                     | 0.42              |
| 1:A:410:TRP:CG   | 1:A:411:ILE:N    | 2.88                     | 0.42              |
| 1:A:103:LYS:HE3  | 1:A:179:VAL:CG1  | 2.50                     | 0.42              |
| 1:A:135:ILE:O    | 1:A:136:ASN:HB2  | 2.20                     | 0.42              |
| 1:A:183:TYR:OH   | 1:A:230:MET:CE   | 2.67                     | 0.42              |
| 1:A:398:TRP:CZ2  | 1:A:411:ILE:CD1  | 3.03                     | 0.42              |
| 1:A:544:GLY:O    | 1:A:548:VAL:HG23 | 2.20                     | 0.42              |
| 2:B:362:THR:CG2  | 2:B:367:GLN:CG   | 2.96                     | 0.42              |
| 1:A:228:LEU:CB   | 1:A:242:GLN:NE2  | 2.75                     | 0.42              |
| 2:B:287:LYS:HE3  | 2:B:291:GLU:OE2  | 2.20                     | 0.42              |
| 1:A:368:LEU:HA   | 1:A:368:LEU:HD23 | 1.80                     | 0.41              |
| 2:B:254:VAL:HG13 | 2:B:283:LEU:HD22 | 2.01                     | 0.41              |
| 2:B:305:GLU:O    | 2:B:306:ASN:C    | 2.59                     | 0.41              |
| 1:A:312:GLU:HA   | 1:A:313:PRO:HD3  | 1.73                     | 0.41              |
| 1:A:16:MET:HE1   | 1:A:83:ARG:HG2   | 2.01                     | 0.41              |
| 1:A:317:VAL:HG22 | 1:A:348:ASN:O    | 2.21                     | 0.41              |
| 2:B:388:LYS:HE2  | 2:B:415:GLU:CG   | 2.41                     | 0.41              |
| 1:A:201:LYS:HD2  | 1:A:201:LYS:HA   | 1.83                     | 0.41              |
| 1:A:491:LEU:HD12 | 1:A:491:LEU:HA   | 1.89                     | 0.41              |
| 2:B:163:SER:O    | 2:B:164:MET:C    | 2.59                     | 0.41              |
| 2:B:153:TRP:CE2  | 2:B:155:GLY:HA3  | 2.55                     | 0.41              |
| 1:A:228:LEU:CD2  | 1:A:228:LEU:H    | 2.28                     | 0.41              |
| 1:A:398:TRP:CH2  | 1:A:411:ILE:HD11 | 2.56                     | 0.41              |
| 1:A:438:GLU:OE1  | 1:A:459:THR:CB   | 2.68                     | 0.41              |
| 1:A:524:GLN:CA   | 1:A:524:GLN:HE21 | 2.20                     | 0.41              |
| 1:A:287:LYS:CE   | 1:A:291:GLU:OE2  | 2.69                     | 0.41              |
| 1:A:410:TRP:CE3  | 2:B:363:ASN:CB   | 3.04                     | 0.41              |
| 2:B:107:THR:OG1  | 2:B:202:ILE:CD1  | 2.69                     | 0.41              |
| 1:A:255:ASN:CB   | 1:A:289:LEU:HD22 | 2.46                     | 0.41              |
| 1:A:116:PHE:HA   | 1:A:148:VAL:HG21 | 2.03                     | 0.41              |
| 1:A:198:HIS:CE1  | 1:A:202:ILE:HD11 | 2.55                     | 0.41              |
| 1:A:511:ASP:OD2  | 1:A:511:ASP:C    | 2.59                     | 0.41              |
| 2:B:298:GLU:HA   | 2:B:301:LEU:HD12 | 2.00                     | 0.41              |
| 2:B:8:VAL:HG23   | 2:B:9:PRO:HD2    | 2.03                     | 0.41              |
| 1:A:137:ASN:O    | 1:A:138:GLU:O    | 2.39                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:170:PRO:O   | 1:A:173:LYS:HB2  | 2.21                     | 0.40              |
| 2:B:5:ILE:O     | 2:B:6:GLU:C      | 2.58                     | 0.40              |
| 1:A:287:LYS:N   | 1:A:287:LYS:HD2  | 2.36                     | 0.40              |
| 2:B:320:ASP:HA  | 2:B:321:PRO:HD3  | 1.74                     | 0.40              |
| 1:A:106:VAL:CG1 | 3:A:601:RT7:C19  | 3.00                     | 0.40              |
| 1:A:323:LYS:HE3 | 1:A:323:LYS:HB2  | 1.61                     | 0.40              |
| 1:A:432:GLU:OE1 | 1:A:432:GLU:HA   | 2.21                     | 0.40              |
| 1:A:64:LYS:HA   | 1:A:64:LYS:HD3   | 1.87                     | 0.40              |
| 2:B:260:LEU:O   | 2:B:264:LEU:HG   | 2.22                     | 0.40              |
| 1:A:101:LYS:HE2 | 1:A:321:PRO:HG3  | 2.03                     | 0.40              |
| 1:A:472:THR:HB  | 1:A:473:THR:H    | 1.66                     | 0.40              |
| 2:B:287:LYS:CE  | 2:B:291:GLU:OE2  | 2.70                     | 0.40              |
| 1:A:494:ASN:HB3 | 2:B:289:LEU:HD12 | 2.03                     | 0.40              |
| 2:B:46:LYS:HA   | 2:B:46:LYS:HE2   | 2.04                     | 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     | 556/563 (99%)  | 486 (87%) | 45 (8%) | 25 (4%)  | 3           | 6 |
| 2   | B     | 399/443 (90%)  | 350 (88%) | 35 (9%) | 14 (4%)  | 4           | 9 |
| All | All   | 955/1006 (95%) | 836 (88%) | 80 (8%) | 39 (4%)  | 3           | 7 |

All (39) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 66  | LYS  |
| 1   | A     | 196 | GLY  |
| 1   | A     | 219 | LYS  |
| 1   | A     | 334 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 543 | GLY  |
| 2   | B     | 237 | ASP  |
| 1   | A     | 67  | ASP  |
| 1   | A     | 223 | LYS  |
| 1   | A     | 356 | ARG  |
| 1   | A     | 541 | GLY  |
| 2   | B     | 14  | PRO  |
| 2   | B     | 91  | GLN  |
| 2   | B     | 251 | SER  |
| 2   | B     | 269 | GLN  |
| 2   | B     | 310 | LEU  |
| 1   | A     | 296 | THR  |
| 1   | A     | 345 | PRO  |
| 1   | A     | 491 | LEU  |
| 1   | A     | 528 | LYS  |
| 2   | B     | 66  | LYS  |
| 2   | B     | 249 | LYS  |
| 2   | B     | 303 | LEU  |
| 1   | A     | 64  | LYS  |
| 1   | A     | 85  | GLN  |
| 1   | A     | 138 | GLU  |
| 1   | A     | 230 | MET  |
| 1   | A     | 139 | THR  |
| 1   | A     | 312 | GLU  |
| 2   | B     | 272 | PRO  |
| 1   | A     | 3   | SER  |
| 1   | A     | 170 | PRO  |
| 1   | A     | 175 | ASN  |
| 1   | A     | 346 | PHE  |
| 2   | B     | 65  | LYS  |
| 2   | B     | 294 | PRO  |
| 2   | B     | 302 | GLU  |
| 1   | A     | 195 | ILE  |
| 1   | A     | 276 | VAL  |
| 2   | B     | 236 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed      | Rotameric | Outliers  | Percentiles |    |
|-----|-------|---------------|-----------|-----------|-------------|----|
| 1   | A     | 497/503 (99%) | 432 (87%) | 65 (13%)  | 5           | 11 |
| 2   | B     | 369/403 (92%) | 330 (89%) | 39 (11%)  | 8           | 18 |
| All | All   | 866/906 (96%) | 762 (88%) | 104 (12%) | 6           | 14 |

All (104) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | ILE  |
| 1   | A     | 6   | GLU  |
| 1   | A     | 7   | THR  |
| 1   | A     | 21  | VAL  |
| 1   | A     | 26  | LEU  |
| 1   | A     | 29  | GLU  |
| 1   | A     | 49  | LYS  |
| 1   | A     | 53  | GLU  |
| 1   | A     | 60  | VAL  |
| 1   | A     | 64  | LYS  |
| 1   | A     | 69  | THR  |
| 1   | A     | 102 | LYS  |
| 1   | A     | 106 | VAL  |
| 1   | A     | 107 | THR  |
| 1   | A     | 118 | VAL  |
| 1   | A     | 135 | ILE  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 138 | GLU  |
| 1   | A     | 161 | GLN  |
| 1   | A     | 173 | LYS  |
| 1   | A     | 185 | ASP  |
| 1   | A     | 210 | LEU  |
| 1   | A     | 219 | LYS  |
| 1   | A     | 220 | LYS  |
| 1   | A     | 222 | GLN  |
| 1   | A     | 230 | MET  |
| 1   | A     | 246 | LEU  |
| 1   | A     | 251 | SER  |
| 1   | A     | 260 | LEU  |
| 1   | A     | 276 | VAL  |
| 1   | A     | 284 | ARG  |
| 1   | A     | 286 | THR  |
| 1   | A     | 287 | LYS  |
| 1   | A     | 296 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 297 | GLU  |
| 1   | A     | 298 | GLU  |
| 1   | A     | 303 | LEU  |
| 1   | A     | 311 | LYS  |
| 1   | A     | 312 | GLU  |
| 1   | A     | 324 | ASP  |
| 1   | A     | 334 | GLN  |
| 1   | A     | 338 | THR  |
| 1   | A     | 347 | LYS  |
| 1   | A     | 350 | LYS  |
| 1   | A     | 358 | ARG  |
| 1   | A     | 361 | HIS  |
| 1   | A     | 368 | LEU  |
| 1   | A     | 369 | THR  |
| 1   | A     | 374 | LYS  |
| 1   | A     | 402 | TRP  |
| 1   | A     | 403 | THR  |
| 1   | A     | 451 | LYS  |
| 1   | A     | 457 | TYR  |
| 1   | A     | 459 | THR  |
| 1   | A     | 461 | ARG  |
| 1   | A     | 463 | ARG  |
| 1   | A     | 472 | THR  |
| 1   | A     | 479 | LEU  |
| 1   | A     | 491 | LEU  |
| 1   | A     | 497 | THR  |
| 1   | A     | 500 | GLN  |
| 1   | A     | 503 | LEU  |
| 1   | A     | 547 | GLN  |
| 1   | A     | 548 | VAL  |
| 1   | A     | 557 | ARG  |
| 2   | B     | 8   | VAL  |
| 2   | B     | 11  | LYS  |
| 2   | B     | 12  | LEU  |
| 2   | B     | 17  | ASP  |
| 2   | B     | 25  | PRO  |
| 2   | B     | 26  | LEU  |
| 2   | B     | 64  | LYS  |
| 2   | B     | 65  | LYS  |
| 2   | B     | 69  | THR  |
| 2   | B     | 72  | ARG  |
| 2   | B     | 80  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 91  | GLN  |
| 2   | B     | 111 | VAL  |
| 2   | B     | 116 | PHE  |
| 2   | B     | 120 | LEU  |
| 2   | B     | 199 | ARG  |
| 2   | B     | 209 | LEU  |
| 2   | B     | 214 | LEU  |
| 2   | B     | 232 | TYR  |
| 2   | B     | 248 | GLU  |
| 2   | B     | 260 | LEU  |
| 2   | B     | 261 | VAL  |
| 2   | B     | 270 | ILE  |
| 2   | B     | 276 | VAL  |
| 2   | B     | 277 | ARG  |
| 2   | B     | 279 | LEU  |
| 2   | B     | 280 | CYS  |
| 2   | B     | 286 | THR  |
| 2   | B     | 293 | ILE  |
| 2   | B     | 298 | GLU  |
| 2   | B     | 310 | LEU  |
| 2   | B     | 349 | LEU  |
| 2   | B     | 356 | ARG  |
| 2   | B     | 377 | THR  |
| 2   | B     | 400 | THR  |
| 2   | B     | 413 | GLU  |
| 2   | B     | 414 | TRP  |
| 2   | B     | 425 | LEU  |
| 2   | B     | 428 | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 57  | ASN  |
| 1   | A     | 91  | GLN  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 147 | ASN  |
| 1   | A     | 161 | GLN  |
| 1   | A     | 174 | GLN  |
| 1   | A     | 175 | ASN  |
| 1   | A     | 198 | HIS  |
| 1   | A     | 235 | HIS  |
| 1   | A     | 242 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 258 | GLN  |
| 1   | A     | 278 | GLN  |
| 1   | A     | 315 | HIS  |
| 1   | A     | 330 | GLN  |
| 1   | A     | 334 | GLN  |
| 1   | A     | 336 | GLN  |
| 1   | A     | 407 | GLN  |
| 1   | A     | 428 | GLN  |
| 1   | A     | 509 | GLN  |
| 1   | A     | 519 | ASN  |
| 1   | A     | 524 | GLN  |
| 1   | A     | 547 | GLN  |
| 2   | B     | 96  | HIS  |
| 2   | B     | 137 | ASN  |
| 2   | B     | 147 | ASN  |
| 2   | B     | 161 | GLN  |
| 2   | B     | 175 | ASN  |
| 2   | B     | 208 | HIS  |
| 2   | B     | 258 | GLN  |
| 2   | B     | 278 | GLN  |
| 2   | B     | 306 | ASN  |
| 2   | B     | 367 | GLN  |
| 2   | B     | 373 | GLN  |
| 2   | B     | 394 | GLN  |
| 2   | B     | 407 | GLN  |
| 2   | B     | 418 | ASN  |
| 2   | B     | 428 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

1 ligand is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | RT7  | A     | 601 | -    | 31,32,32     | 2.45 | 8 (25%)     | 43,47,47    | 2.09 | 16 (37%)    |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | RT7  | A     | 601 | -    | -       | 0/17/29/29 | 0/3/3/3 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | A     | 601 | RT7  | C19-S25  | -8.16 | 1.63        | 1.77     |
| 3   | A     | 601 | RT7  | C11-S12  | -3.89 | 1.69        | 1.78     |
| 3   | A     | 601 | RT7  | C16-N15  | -2.71 | 1.36        | 1.41     |
| 3   | A     | 601 | RT7  | C17-CL24 | 2.46  | 1.79        | 1.73     |
| 3   | A     | 601 | RT7  | C2-CL29  | 2.97  | 1.80        | 1.73     |
| 3   | A     | 601 | RT7  | C16-C17  | 3.41  | 1.48        | 1.39     |
| 3   | A     | 601 | RT7  | C1-C6    | 4.12  | 1.48        | 1.41     |
| 3   | A     | 601 | RT7  | C1-C2    | 6.24  | 1.48        | 1.39     |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 601 | RT7  | O27-S25-O26 | -4.30 | 110.81      | 118.70   |
| 3   | A     | 601 | RT7  | C3-C2-C1    | -2.58 | 117.73      | 120.88   |
| 3   | A     | 601 | RT7  | O23-C14-C13 | -2.45 | 117.30      | 121.63   |
| 3   | A     | 601 | RT7  | C18-C17-C16 | -2.36 | 119.71      | 121.78   |
| 3   | A     | 601 | RT7  | C3-C4-CL30  | -2.32 | 116.25      | 119.14   |
| 3   | A     | 601 | RT7  | C9-C8-N7    | -2.19 | 106.21      | 109.95   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3   | A     | 601 | RT7  | C8-N7-C11   | 2.09 | 124.49      | 118.21   |
| 3   | A     | 601 | RT7  | C10-C6-C1   | 2.09 | 122.76      | 119.35   |
| 3   | A     | 601 | RT7  | C3-C4-C5    | 2.26 | 124.52      | 121.68   |
| 3   | A     | 601 | RT7  | O27-S25-N28 | 2.52 | 111.30      | 107.34   |
| 3   | A     | 601 | RT7  | C21-C20-C19 | 2.79 | 122.48      | 119.46   |
| 3   | A     | 601 | RT7  | O26-S25-C19 | 2.90 | 110.78      | 107.39   |
| 3   | A     | 601 | RT7  | C17-C18-C19 | 2.99 | 120.71      | 118.82   |
| 3   | A     | 601 | RT7  | C13-C14-N15 | 3.32 | 119.36      | 114.39   |
| 3   | A     | 601 | RT7  | C1-C2-CL29  | 3.63 | 125.46      | 120.13   |
| 3   | A     | 601 | RT7  | C13-S12-C11 | 7.16 | 118.50      | 100.80   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 15 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 601 | RT7  | 15      | 0            |

## 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     | 558/563 (99%)  | 0.29   | 18 (3%) | 48 | 48 | 34, 61, 83, 97        | 0     |
| 2   | B     | 405/443 (91%)  | 0.18   | 10 (2%) | 58 | 58 | 36, 54, 95, 105       | 0     |
| All | All   | 963/1006 (95%) | 0.24   | 28 (2%) | 52 | 52 | 34, 59, 91, 105       | 0     |

All (28) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 231 | GLY  | 5.2  |
| 1   | A     | 402 | TRP  | 3.9  |
| 1   | A     | 426 | TRP  | 3.6  |
| 1   | A     | 66  | LYS  | 3.5  |
| 2   | B     | 240 | THR  | 3.5  |
| 2   | B     | 232 | TYR  | 3.3  |
| 1   | A     | 195 | ILE  | 3.0  |
| 1   | A     | 193 | LEU  | 2.9  |
| 2   | B     | 67  | ASP  | 2.8  |
| 1   | A     | 65  | LYS  | 2.8  |
| 1   | A     | 358 | ARG  | 2.7  |
| 1   | A     | 359 | GLY  | 2.6  |
| 2   | B     | 214 | LEU  | 2.5  |
| 1   | A     | 220 | LYS  | 2.4  |
| 1   | A     | 67  | ASP  | 2.4  |
| 2   | B     | 283 | LEU  | 2.3  |
| 1   | A     | 137 | ASN  | 2.3  |
| 1   | A     | 357 | MET  | 2.3  |
| 2   | B     | 14  | PRO  | 2.2  |
| 1   | A     | 522 | ILE  | 2.2  |
| 1   | A     | 530 | LYS  | 2.2  |
| 1   | A     | 199 | ARG  | 2.2  |
| 2   | B     | 246 | LEU  | 2.1  |
| 2   | B     | 13  | LYS  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 310 | LEU  | 2.1  |
| 1   | A     | 360 | ALA  | 2.1  |
| 1   | A     | 72  | ARG  | 2.0  |
| 1   | A     | 221 | HIS  | 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 3   | RT7  | A     | 601 | 30/30 | 0.85 | 0.23 | 0.43 | 61,69,72,73                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.