



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:04 pm GMT

PDB ID : 3LC6  
Title : The alternative conformation structure of isocitrate dehydrogenase kinase/phosphatase from E. Coli  
Authors : Zheng, J.; Jia, Z.  
Deposited on : 2010-01-09  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<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

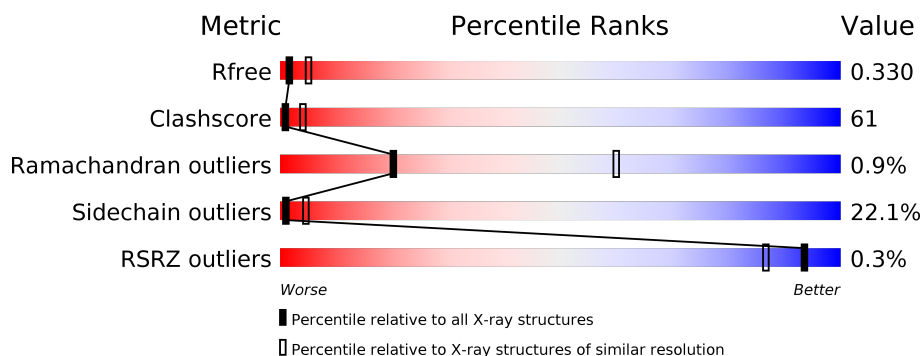
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1001 (3.12-3.08)                                      |
| Clashscore            | 112137                      | 1099 (3.12-3.08)                                      |
| Ramachandran outliers | 110173                      | 1057 (3.12-3.08)                                      |
| Sidechain outliers    | 110143                      | 1057 (3.12-3.08)                                      |
| RSRZ outliers         | 101464                      | 1006 (3.12-3.08)                                      |

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     | 578    | <div> <div></div> <div>24% 56% 14% 5%</div> </div> |
| 1   | B     | 578    | <div> <div></div> <div>27% 52% 14% 7%</div> </div> |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9107 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 Isocitrate dehydrogenase kinase/phosphatase.

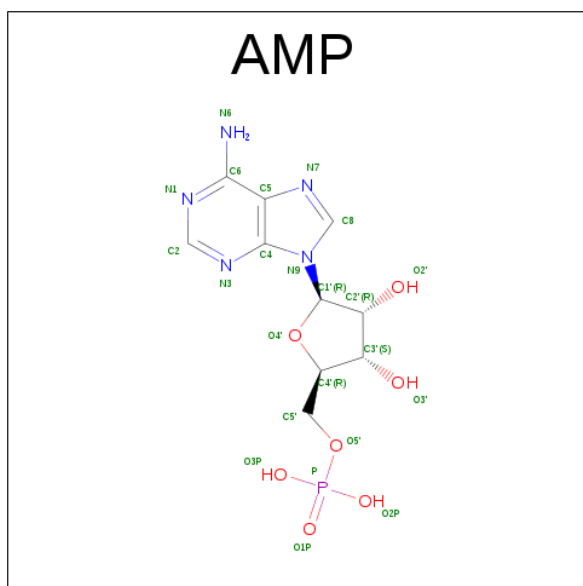
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 547      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4526  | 2906 | 800 | 799 | 21 |         |         |       |
| 1   | B     | 539      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4454  | 2861 | 785 | 788 | 20 |         |         |       |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 4   | B     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 23    | 10 | 5 | 7 | 1 |         |         |

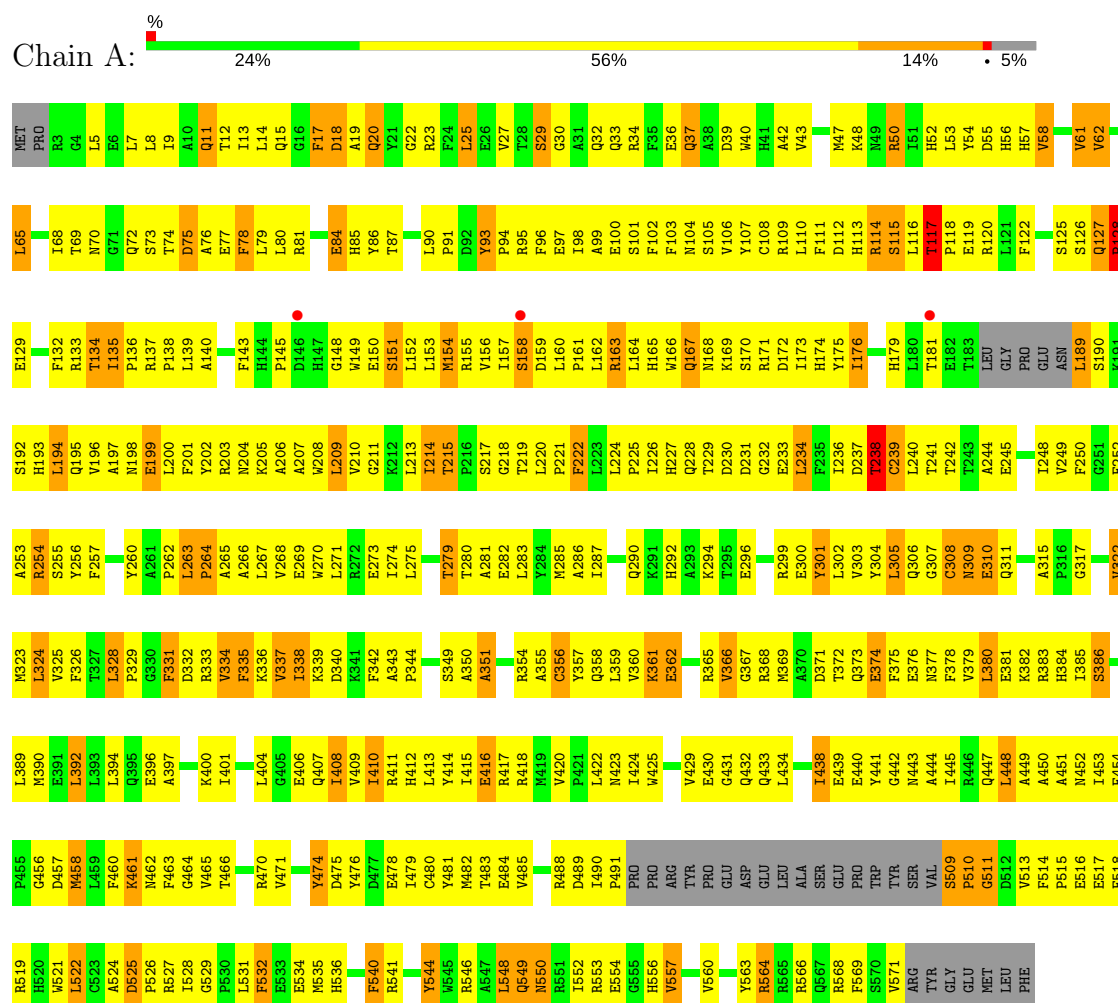
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 31       | Total | O  | 0       | 0       |
|     |       |          | 31    | 31 |         |         |
| 5   | B     | 45       | Total | O  | 0       | 0       |
|     |       |          | 45    | 45 |         |         |

### 3 Residue-property plots

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

- Molecule 1: Isocitrate dehydrogenase kinase/phosphatase



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| F518 | F519 | F520 | H521 | L522 |      | D525 |      | I528 | G529 | F530 | G531 | L531 | F532 |      | M535 | H536 | A537 | D538 | L539 | F540 | R541 | D542 | D543 | Y544 | W545 | R546 | A547 | L548 | Q549 | N550 | R551 | I552 | R553 | E554 |      | D558 | G559 | P560 | Y561 | A562 | Y563 | R564 | R565 | R566 | Q567 | R568 | F569 | S570 | V571 | Y572 | Y573 | G574 | GLU  | MET  | LEU  | PHE  |      |      |      |      |
| L453 | F454 | P455 |      |      |      | M458 | L459 | F460 | K461 | M462 | F463 | G464 | V465 | T466 | R467 |      | R470 | V471 | V472 | F473 | Y474 | D475 | Y476 | D477 | E478 | I479 | G480 | Y481 | M482 | T483 | N484 | V485 |      | D489 | I490 | PRO  | PRO  | PRO  | ASP  | GLU  | LEU  | ALA  | SER  | GLU  | PRO  | TRP  | SER  | VAL  | SER  | PRO  | G511 |      | F514 | P515 | E516 | E517 |      |      |      |      |
| L392 | L393 | L394 | Q395 | E396 | F397 | A398 | E399 | K400 | I401 | D402 | D403 | L404 |      |      | Q407 | I408 | V409 | I410 | R411 | H412 | L413 | Y414 | I415 | E416 | R417 | R418 | M419 | V420 | F421 | L422 | N423 | I424 | W425 | L426 | E427 | Q428 | V429 | E430 | G431 | Q432 | Q433 | L434 | R435 | D436 | A437 | I438 | E439 | E440 | Y441 | G442 | M443 | A444 | I445 | R446 | Q447 | L448 | A449 | A450 | A451 | N452 |
| F331 | D332 | R333 | V334 | F335 | K336 | V337 | I338 | I339 | T340 | K341 | F342 | ALA  | PRO  | GLN  | LYS  | GLU  | MET  | SER  | ALA  | A351 | H352 | V353 | R354 | A355 | C356 | Y357 | Q358 | L359 | V360 | K361 | E362 | H363 | R364 | V366 | G367 | R368 | K369 | A370 | D371 | T372 | Q373 | E374 | F375 | E376 | F378 | V379 | L380 | E381 | K382 | R383 | H384 |      | P387 | A388 | L389 | K390 | E391 |      |      |      |
| V268 | E269 | W270 | L271 |      | I274 | L275 | P276 | G277 | T278 | T279 | T280 | A281 | E282 | L283 | Y284 | M285 | A286 | I287 | G288 | C289 | Q290 | D291 | H292 | A293 | K294 | T295 | E296 | S297 | Y298 | R299 | E300 | Y301 | Y304 | L305 | T306 | A244 | E245 | A246 | S247 | I248 | V249 | F250 | G251 | F252 | A253 | R254 | S255 | Y256 | F257 | M258 | V259 | M260 | L261 | P262 | L263 | F264 | A265 | A266 | L267 |      |
| T134 | I135 | P136 | R137 | L138 | L139 | A140 | K141 | D142 | F143 | H144 | P145 |      | W149 |      | L152 | L153 | M154 | R155 | V156 | I157 | S158 | D159 | L160 | P161 | L162 | R163 | S101 | F102 | M168 | K169 | S170 | R171 | D172 | H173 | H174 | Y175 | I176 | I177 | R178 | H179 | L180 | T181 |      | P186 |      | L189 |      | S192 | H193 | L194 | Q195 | S125 | V196 | A197 | N198 | E199 | L200 | F201 | Y202 | R203 |
| Q72  |      | D75  |      | F78  | L79  | L80  | R81  | V82  |      | H85  | Y86  |      | T87  | R88  | L89  | L90  | P91  | D92  | Y93  | P94  | R95  | F96  | E97  |      | A99  | E100 | S101 | F102 | N104 | S105 | V106 | Y107 | C108 | R109 | L110 | PHE  |      | D112 | H113 | R114 | S115 | L116 | T117 | P118 | E119 | L121 | F122 | I123 | F124 | S125 | V126 | Q127 | P128 | GLU  | ARG  | ARG  | PHE  | ARG  |      |      |

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 64.14Å 133.76Å 187.34Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)  | 10.00 – 3.10<br>10.00 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 83.1 (10.00-3.10)<br>83.7 (10.00-3.10)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.10  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 16.46 (at 3.10Å)  | Xtriage          |
| Refinement program  | REFMAC 5.5.0102   | Depositor        |
| R, $R_{free}$   | 0.287 , 0.332<br>0.292 , 0.330                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1191 reflections (5.15%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 51.5  | Xtriage          |
| Anisotropy  | 0.051   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 82.0   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.72  | EDS              |
| Total number of atoms   | 9107  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 17.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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: AMP, MG, ADP

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     | 0.62         | 2/4643 (0.0%) | 0.80        | 7/6283 (0.1%)  |
| 1   | B     | 0.57         | 1/4567 (0.0%) | 0.77        | 1/6179 (0.0%)  |
| All | All   | 0.60         | 3/9210 (0.0%) | 0.79        | 8/12462 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 1                   | 5                   |
| 1   | B     | 0                   | 2                   |
| All | All   | 1                   | 7                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 239 | CYS  | CB-SG | -6.93 | 1.70        | 1.82     |
| 1   | A     | 511 | GLY  | N-CA  | 6.30  | 1.55        | 1.46     |
| 1   | A     | 356 | CYS  | CB-SG | -5.39 | 1.73        | 1.81     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 128 | PRO  | N-CA-C   | -8.62 | 89.69       | 112.10   |
| 1   | A     | 239 | CYS  | N-CA-C   | 7.35  | 130.85      | 111.00   |
| 1   | A     | 509 | SER  | N-CA-CB  | -6.98 | 100.02      | 110.50   |
| 1   | A     | 238 | THR  | N-CA-C   | 6.78  | 129.31      | 111.00   |
| 1   | B     | 240 | LEU  | CA-CB-CG | 6.74  | 130.80      | 115.30   |
| 1   | A     | 75  | ASP  | N-CA-C   | -6.36 | 93.83       | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 118 | PRO  | N-CA-C | 5.33  | 125.96      | 112.10   |
| 1   | A     | 117 | THR  | C-N-CD | -5.26 | 109.03      | 120.60   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 239 | CYS  | CA   |

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 117 | THR  | Peptide |
| 1   | A     | 128 | PRO  | Peptide |
| 1   | A     | 230 | ASP  | Peptide |
| 1   | A     | 350 | ALA  | Peptide |
| 1   | A     | 510 | PRO  | Peptide |
| 1   | B     | 117 | THR  | Peptide |
| 1   | B     | 278 | LYS  | Peptide |

## 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     | 4526  | 0        | 4449     | 592     | 7            |
| 1   | B     | 4454  | 0        | 4376     | 518     | 7            |
| 2   | A     | 27    | 0        | 12       | 5       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 23    | 0        | 12       | 2       | 0            |
| 5   | A     | 31    | 0        | 0        | 12      | 0            |
| 5   | B     | 45    | 0        | 0        | 11      | 0            |
| All | All   | 9107  | 0        | 8849     | 1095    | 7            |

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 61.

All (1095) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:279:THR:OG1  | 1:A:282:GLU:HG3  | 1.16                     | 1.29              |
| 1:A:128:PRO:HB2  | 1:A:129:GLU:CA   | 1.56                     | 1.29              |
| 1:A:200:LEU:HD23 | 1:A:201:PHE:N    | 1.48                     | 1.29              |
| 1:B:550:ASN:O    | 1:B:554:GLU:HG3  | 1.31                     | 1.29              |
| 1:A:23:ARG:O     | 1:A:27:VAL:HG23  | 1.37                     | 1.25              |
| 1:A:128:PRO:CB   | 1:A:129:GLU:HA   | 1.57                     | 1.24              |
| 1:B:434:LEU:O    | 1:B:438:ILE:HG23 | 1.38                     | 1.24              |
| 1:B:376:GLU:O    | 1:B:411:ARG:HA   | 1.38                     | 1.23              |
| 1:A:200:LEU:HD23 | 1:A:200:LEU:C    | 1.56                     | 1.23              |
| 1:A:8:LEU:HD12   | 5:A:596:HOH:O    | 1.33                     | 1.21              |
| 1:A:416:GLU:OE2  | 2:A:1762:ADP:N6  | 1.71                     | 1.21              |
| 1:B:228:GLN:HB2  | 1:B:233:GLU:O    | 1.37                     | 1.20              |
| 1:B:5:LEU:O      | 1:B:9:ILE:CG2    | 1.89                     | 1.20              |
| 1:A:279:THR:OG1  | 1:A:282:GLU:CG   | 1.90                     | 1.17              |
| 1:A:311:GLN:NE2  | 5:A:590:HOH:O    | 1.74                     | 1.17              |
| 1:B:237:ASP:O    | 1:B:238:THR:HG22 | 1.41                     | 1.16              |
| 1:B:124:PHE:HB2  | 1:B:299:ARG:CG   | 1.75                     | 1.16              |
| 1:B:382:LYS:NZ   | 1:B:403:ASP:OD1  | 1.79                     | 1.16              |
| 1:A:240:LEU:CD2  | 1:A:245:GLU:HG3  | 1.75                     | 1.15              |
| 1:B:124:PHE:HB2  | 1:B:299:ARG:HG2  | 1.28                     | 1.14              |
| 1:B:117:THR:OG1  | 1:B:118:PRO:HA   | 1.45                     | 1.12              |
| 1:B:5:LEU:O      | 1:B:9:ILE:HG22   | 0.95                     | 1.11              |
| 1:A:107:TYR:HE2  | 1:A:115:SER:HB3  | 1.16                     | 1.10              |
| 1:B:304:TYR:CD2  | 1:B:305:LEU:HD12 | 1.88                     | 1.08              |
| 1:B:413:LEU:HD23 | 1:B:413:LEU:O    | 1.54                     | 1.07              |
| 1:B:203:ARG:NH2  | 1:B:254:ARG:HD2  | 1.70                     | 1.07              |
| 1:A:308:CYS:C    | 1:A:309:ASN:HD22 | 1.56                     | 1.07              |
| 1:A:168:ASN:HD22 | 1:A:171:ARG:HB2  | 1.18                     | 1.07              |
| 1:B:124:PHE:CB   | 1:B:299:ARG:HG2  | 1.84                     | 1.06              |
| 1:A:30:GLY:O     | 1:A:34:ARG:HG3   | 1.55                     | 1.06              |
| 1:B:253:ALA:CB   | 1:B:367:GLY:HA2  | 1.87                     | 1.05              |
| 1:B:178:ARG:HA   | 1:B:181:THR:HG22 | 1.07                     | 1.04              |
| 1:B:304:TYR:HD2  | 1:B:305:LEU:CD1  | 1.69                     | 1.04              |
| 1:A:155:ARG:O    | 1:A:159:ASP:OD2  | 1.74                     | 1.04              |
| 1:A:189:LEU:C    | 1:A:189:LEU:HD23 | 1.79                     | 1.03              |
| 1:B:127:GLN:HB3  | 1:B:128:PRO:HD3  | 1.38                     | 1.03              |
| 1:B:253:ALA:HB3  | 1:B:367:GLY:HA2  | 1.35                     | 1.03              |
| 1:B:304:TYR:CD2  | 1:B:305:LEU:CD1  | 2.42                     | 1.03              |
| 1:A:126:SER:O    | 1:A:128:PRO:HD3  | 1.57                     | 1.02              |
| 1:A:167:GLN:HG2  | 1:A:233:GLU:HB2  | 1.39                     | 1.01              |
| 1:B:257:PHE:HB2  | 1:B:286:ALA:O    | 1.58                     | 1.01              |
| 1:A:168:ASN:ND2  | 1:A:171:ARG:HB2  | 1.77                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:189:LEU:O    | 1:A:189:LEU:HD23 | 1.60                     | 0.99              |
| 1:A:200:LEU:CD2  | 1:A:200:LEU:C    | 2.29                     | 0.99              |
| 1:A:240:LEU:HD22 | 1:A:245:GLU:HG3  | 1.39                     | 0.99              |
| 1:B:404:LEU:HB2  | 1:B:407:GLN:HE21 | 1.28                     | 0.99              |
| 1:A:238:THR:HG23 | 1:A:238:THR:O    | 1.63                     | 0.99              |
| 1:A:328:LEU:HD12 | 1:A:329:PRO:HD2  | 1.44                     | 0.99              |
| 1:B:538:ASP:OD1  | 5:B:580:HOH:O    | 1.82                     | 0.97              |
| 1:A:101:SER:HA   | 1:A:104:ASN:ND2  | 1.79                     | 0.97              |
| 1:B:178:ARG:HA   | 1:B:181:THR:CG2  | 1.95                     | 0.97              |
| 1:A:8:LEU:CD1    | 5:A:596:HOH:O    | 1.99                     | 0.97              |
| 1:A:429:VAL:HG12 | 1:A:433:GLN:OE1  | 1.64                     | 0.97              |
| 1:A:430:GLU:OE2  | 1:A:527:ARG:NH1  | 1.97                     | 0.96              |
| 1:A:107:TYR:CE2  | 1:A:115:SER:HB3  | 2.00                     | 0.96              |
| 1:B:61:VAL:O     | 1:B:65:LEU:N     | 1.96                     | 0.96              |
| 1:A:546:ARG:O    | 1:A:550:ASN:HB2  | 1.66                     | 0.95              |
| 1:B:516:GLU:O    | 1:B:519:ARG:HG2  | 1.64                     | 0.95              |
| 1:B:296:GLU:O    | 1:B:300:GLU:HG3  | 1.66                     | 0.95              |
| 1:B:338:ILE:HG12 | 1:B:353:VAL:HG21 | 1.49                     | 0.95              |
| 1:A:96:PHE:CE1   | 1:A:128:PRO:CG   | 2.51                     | 0.94              |
| 1:B:24:PHE:O     | 1:B:28:THR:OG1   | 1.86                     | 0.94              |
| 1:B:366:VAL:HG11 | 1:B:447:GLN:HG2  | 1.47                     | 0.94              |
| 1:B:108:CYS:HB3  | 1:B:113:HIS:CE1  | 2.03                     | 0.93              |
| 1:B:404:LEU:O    | 1:B:407:GLN:NE2  | 2.01                     | 0.93              |
| 1:B:327:THR:CG2  | 1:B:328:LEU:H    | 1.82                     | 0.92              |
| 1:B:541:ARG:NH2  | 1:B:544:TYR:HB2  | 1.84                     | 0.92              |
| 1:A:305:LEU:H    | 1:A:305:LEU:HD13 | 1.30                     | 0.92              |
| 1:B:201:PHE:HB3  | 1:B:257:PHE:CE1  | 2.04                     | 0.92              |
| 1:B:117:THR:OG1  | 1:B:118:PRO:CA   | 2.18                     | 0.92              |
| 1:B:442:GLY:HA3  | 1:B:536:HIS:CD2  | 2.04                     | 0.92              |
| 1:B:361:LYS:HE2  | 1:B:372:THR:O    | 1.69                     | 0.91              |
| 1:A:105:SER:O    | 1:A:109:ARG:HG2  | 1.69                     | 0.91              |
| 1:A:86:TYR:OH    | 1:A:99:ALA:O     | 1.88                     | 0.91              |
| 1:B:455:PRO:HB2  | 1:B:458:MET:HB3  | 1.53                     | 0.91              |
| 1:B:267:LEU:O    | 1:B:271:LEU:HD12 | 1.70                     | 0.91              |
| 1:B:253:ALA:HB1  | 1:B:367:GLY:C    | 1.91                     | 0.91              |
| 1:A:135:ILE:HG12 | 1:A:266:ALA:HB1  | 1.52                     | 0.90              |
| 1:A:192:SER:HB2  | 1:A:214:ILE:O    | 1.71                     | 0.90              |
| 1:B:327:THR:HG22 | 1:B:328:LEU:H    | 1.35                     | 0.90              |
| 1:A:356:CYS:HB2  | 1:A:476:TYR:O    | 1.71                     | 0.90              |
| 1:A:125:SER:CB   | 1:A:129:GLU:HG3  | 2.02                     | 0.90              |
| 1:A:189:LEU:HD23 | 1:A:190:SER:OG   | 1.71                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:173:ILE:HG23 | 5:B:601:HOH:O    | 1.69                     | 0.89              |
| 1:A:454:PHE:HB2  | 1:A:482:MET:SD   | 2.13                     | 0.89              |
| 1:B:178:ARG:CA   | 1:B:181:THR:HG22 | 1.98                     | 0.89              |
| 1:A:96:PHE:CE1   | 1:A:128:PRO:HG2  | 2.08                     | 0.89              |
| 1:B:81:ARG:HH21  | 1:B:81:ARG:HG2   | 1.37                     | 0.89              |
| 1:B:310:GLU:HG3  | 1:B:328:LEU:HD23 | 1.54                     | 0.88              |
| 1:B:450:ALA:HB1  | 1:B:558:GLU:CG   | 2.03                     | 0.88              |
| 1:A:193:HIS:NE2  | 1:A:214:ILE:HG21 | 1.88                     | 0.88              |
| 1:B:228:GLN:CB   | 1:B:233:GLU:O    | 2.21                     | 0.88              |
| 1:B:304:TYR:HD2  | 1:B:305:LEU:HD12 | 1.28                     | 0.88              |
| 1:B:551:ARG:O    | 1:B:556:HIS:HB3  | 1.72                     | 0.88              |
| 1:A:309:ASN:HD22 | 1:A:309:ASN:N    | 1.68                     | 0.88              |
| 1:B:535:MET:O    | 5:B:580:HOH:O    | 1.92                     | 0.88              |
| 1:A:65:LEU:O     | 1:A:69:THR:OG1   | 1.90                     | 0.88              |
| 1:A:356:CYS:CB   | 1:A:476:TYR:O    | 2.22                     | 0.88              |
| 1:B:137:ARG:HB3  | 1:B:138:PRO:HD2  | 1.54                     | 0.87              |
| 1:A:132:PHE:O    | 1:A:134:THR:HG23 | 1.74                     | 0.87              |
| 1:A:193:HIS:CD2  | 1:A:214:ILE:HG21 | 2.09                     | 0.87              |
| 1:B:382:LYS:HZ3  | 1:B:403:ASP:CG   | 1.76                     | 0.87              |
| 1:B:336:LYS:HD2  | 1:B:416:GLU:OE2  | 1.74                     | 0.87              |
| 1:B:327:THR:HG22 | 1:B:328:LEU:N    | 1.87                     | 0.87              |
| 1:A:23:ARG:O     | 1:A:27:VAL:CG2   | 2.23                     | 0.86              |
| 1:A:75:ASP:HB2   | 1:A:77:GLU:HG2   | 1.53                     | 0.86              |
| 1:A:443:ASN:O    | 1:A:447:GLN:HG3  | 1.76                     | 0.86              |
| 1:A:126:SER:C    | 1:A:128:PRO:CD   | 2.43                     | 0.86              |
| 1:A:381:GLU:O    | 1:A:385:ILE:HG12 | 1.74                     | 0.86              |
| 1:B:284:TYR:CE1  | 1:B:292:HIS:HD2  | 1.93                     | 0.86              |
| 1:A:489:ASP:HA   | 1:A:514:PHE:CD1  | 2.11                     | 0.86              |
| 1:A:252:PHE:CE2  | 1:A:417:ARG:HD2  | 2.11                     | 0.85              |
| 1:A:221:PRO:O    | 1:A:241:THR:HG23 | 1.77                     | 0.85              |
| 1:A:96:PHE:CE1   | 1:A:128:PRO:HG3  | 2.11                     | 0.85              |
| 1:A:294:LYS:HG3  | 1:A:373:GLN:HG2  | 1.59                     | 0.85              |
| 1:B:5:LEU:C      | 1:B:9:ILE:HG22   | 1.97                     | 0.84              |
| 1:B:127:GLN:HB3  | 1:B:128:PRO:CD   | 2.07                     | 0.84              |
| 1:A:167:GLN:OE1  | 1:A:167:GLN:HA   | 1.77                     | 0.84              |
| 1:A:240:LEU:HD22 | 1:A:245:GLU:CG   | 2.07                     | 0.83              |
| 1:B:90:LEU:HD22  | 1:B:96:PHE:HB2   | 1.58                     | 0.83              |
| 1:A:444:ALA:O    | 1:A:448:LEU:HD22 | 1.78                     | 0.83              |
| 1:B:253:ALA:CB   | 1:B:367:GLY:CA   | 2.56                     | 0.83              |
| 1:A:113:HIS:HB2  | 1:A:376:GLU:HB3  | 1.61                     | 0.82              |
| 1:A:465:VAL:HA   | 1:A:470:ARG:O    | 1.79                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:192:SER:CB   | 1:A:214:ILE:O    | 2.27                     | 0.82              |
| 1:A:525:ASP:HB3  | 1:A:528:ILE:HG12 | 1.61                     | 0.82              |
| 1:B:7:LEU:O      | 1:B:11:GLN:HG2   | 1.79                     | 0.82              |
| 1:A:335:PHE:HB3  | 1:A:413:LEU:HD11 | 1.60                     | 0.82              |
| 5:A:596:HOH:O    | 1:B:60:LEU:HD11  | 1.78                     | 0.82              |
| 1:A:125:SER:HB3  | 1:A:129:GLU:HG3  | 1.62                     | 0.82              |
| 1:A:489:ASP:OD1  | 1:A:516:GLU:HB3  | 1.80                     | 0.82              |
| 1:B:124:PHE:CB   | 1:B:299:ARG:CG   | 2.52                     | 0.82              |
| 1:A:257:PHE:N    | 1:A:286:ALA:O    | 2.10                     | 0.81              |
| 1:B:108:CYS:HB3  | 1:B:113:HIS:ND1  | 1.95                     | 0.81              |
| 1:B:482:MET:O    | 1:B:549:GLN:NE2  | 2.13                     | 0.81              |
| 1:B:95:ARG:HH22  | 1:B:262:PRO:HB3  | 1.43                     | 0.81              |
| 1:A:332:ASP:OD1  | 1:A:333:ARG:HG3  | 1.80                     | 0.81              |
| 1:A:338:ILE:HD12 | 1:A:338:ILE:N    | 1.96                     | 0.81              |
| 1:A:338:ILE:O    | 1:A:400:LYS:HD2  | 1.80                     | 0.81              |
| 1:A:107:TYR:HE2  | 1:A:115:SER:CB   | 1.94                     | 0.81              |
| 1:A:20:GLN:HA    | 1:A:57:HIS:CD2   | 2.16                     | 0.81              |
| 1:A:325:VAL:HG11 | 2:A:1762:ADP:O4' | 1.80                     | 0.80              |
| 1:A:294:LYS:HG3  | 1:A:373:GLN:CG   | 2.10                     | 0.80              |
| 1:B:538:ASP:HB3  | 1:B:541:ARG:NH2  | 1.95                     | 0.80              |
| 1:A:203:ARG:O    | 5:A:594:HOH:O    | 1.99                     | 0.80              |
| 1:A:382:LYS:HB3  | 1:A:406:GLU:O    | 1.82                     | 0.80              |
| 1:B:450:ALA:HB1  | 1:B:558:GLU:HG2  | 1.64                     | 0.80              |
| 1:A:96:PHE:HE1   | 1:A:128:PRO:HG2  | 1.43                     | 0.80              |
| 1:A:366:VAL:HG13 | 1:A:560:VAL:HB   | 1.64                     | 0.80              |
| 1:A:126:SER:C    | 1:A:128:PRO:HD2  | 2.02                     | 0.80              |
| 1:A:252:PHE:CD2  | 1:A:417:ARG:HD2  | 2.17                     | 0.80              |
| 1:B:153:LEU:O    | 1:B:157:ILE:HD12 | 1.82                     | 0.80              |
| 1:A:238:THR:CG2  | 1:A:238:THR:O    | 2.29                     | 0.80              |
| 1:A:47:MET:SD    | 1:A:362:GLU:O    | 2.40                     | 0.80              |
| 1:B:245:GLU:O    | 1:B:248:ILE:HG22 | 1.82                     | 0.79              |
| 1:A:167:GLN:CG   | 1:A:233:GLU:HB2  | 2.13                     | 0.79              |
| 1:B:438:ILE:HG13 | 1:B:439:GLU:N    | 1.97                     | 0.79              |
| 1:A:189:LEU:O    | 1:A:189:LEU:CD2  | 2.30                     | 0.79              |
| 1:B:201:PHE:HB3  | 1:B:257:PHE:CD1  | 2.17                     | 0.79              |
| 1:B:366:VAL:CG1  | 1:B:447:GLN:HG2  | 2.11                     | 0.79              |
| 1:A:126:SER:O    | 1:A:128:PRO:CD   | 2.30                     | 0.79              |
| 1:A:400:LYS:NZ   | 1:A:412:HIS:NE2  | 2.31                     | 0.79              |
| 1:A:268:VAL:HG13 | 1:A:283:LEU:HB3  | 1.63                     | 0.79              |
| 1:B:100:GLU:O    | 1:B:104:ASN:ND2  | 2.16                     | 0.79              |
| 1:B:208:TRP:CE3  | 1:B:223:LEU:HD22 | 2.18                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:32:GLN:OE1   | 5:B:615:HOH:O    | 2.01                     | 0.78              |
| 1:B:97:GLU:O     | 1:B:100:GLU:HG2  | 1.82                     | 0.78              |
| 1:B:317:GLY:HA2  | 1:B:424:ILE:HD11 | 1.64                     | 0.78              |
| 1:A:108:CYS:O    | 1:A:113:HIS:N    | 2.15                     | 0.78              |
| 1:A:189:LEU:CD2  | 1:A:190:SER:OG   | 2.30                     | 0.78              |
| 1:A:509:SER:N    | 1:A:510:PRO:CD   | 2.47                     | 0.78              |
| 1:A:279:THR:OG1  | 1:A:282:GLU:CD   | 2.21                     | 0.78              |
| 1:A:47:MET:HG3   | 1:A:48:LYS:H     | 1.48                     | 0.78              |
| 1:A:167:GLN:OE1  | 1:A:167:GLN:CA   | 2.30                     | 0.78              |
| 1:A:305:LEU:CD1  | 1:A:305:LEU:H    | 1.96                     | 0.77              |
| 1:B:322:VAL:HG11 | 1:B:475:ASP:OD2  | 1.85                     | 0.77              |
| 1:A:340:ASP:OD1  | 1:A:400:LYS:HG3  | 1.84                     | 0.77              |
| 1:B:208:TRP:CE3  | 1:B:223:LEU:CD2  | 2.68                     | 0.77              |
| 1:B:237:ASP:O    | 1:B:238:THR:CG2  | 2.29                     | 0.77              |
| 1:B:304:TYR:HD2  | 1:B:305:LEU:HD13 | 1.48                     | 0.77              |
| 1:B:387:PRO:HA   | 1:B:390:MET:CB   | 2.14                     | 0.77              |
| 1:B:366:VAL:HG11 | 1:B:447:GLN:CG   | 2.14                     | 0.77              |
| 1:A:128:PRO:HB2  | 1:A:129:GLU:HA   | 0.80                     | 0.77              |
| 1:B:29:SER:HB3   | 1:B:260:TYR:CD1  | 2.20                     | 0.77              |
| 1:B:304:TYR:CD2  | 1:B:305:LEU:HD13 | 2.20                     | 0.77              |
| 1:B:61:VAL:HG23  | 1:B:62:VAL:N     | 2.00                     | 0.77              |
| 1:A:47:MET:HG3   | 1:A:48:LYS:N     | 2.00                     | 0.77              |
| 1:A:488:ARG:O    | 1:A:514:PHE:CE1  | 2.37                     | 0.77              |
| 1:B:117:THR:HG1  | 1:B:118:PRO:HA   | 1.49                     | 0.77              |
| 1:B:550:ASN:O    | 1:B:554:GLU:CG   | 2.24                     | 0.77              |
| 1:A:139:LEU:C    | 1:A:198:ASN:OD1  | 2.24                     | 0.76              |
| 1:B:427:GLU:C    | 1:B:429:VAL:H    | 1.83                     | 0.76              |
| 1:A:125:SER:HB2  | 1:A:129:GLU:HG3  | 1.67                     | 0.76              |
| 1:B:368:ARG:NH1  | 5:B:590:HOH:O    | 2.17                     | 0.76              |
| 1:A:381:GLU:HB2  | 1:A:384:HIS:HB2  | 1.67                     | 0.76              |
| 1:B:89:LEU:C     | 1:B:91:PRO:HD3   | 2.05                     | 0.76              |
| 1:B:203:ARG:HH21 | 1:B:254:ARG:HD2  | 1.49                     | 0.76              |
| 1:B:418:ARG:HG3  | 1:B:418:ARG:O    | 1.84                     | 0.76              |
| 1:A:137:ARG:NH2  | 1:B:199:GLU:OE1  | 2.19                     | 0.75              |
| 1:B:68:ILE:HG13  | 1:B:69:THR:H     | 1.51                     | 0.75              |
| 1:A:423:ASN:OD1  | 1:A:461:LYS:CB   | 2.35                     | 0.75              |
| 1:B:296:GLU:O    | 1:B:300:GLU:CG   | 2.35                     | 0.75              |
| 1:B:90:LEU:N     | 1:B:91:PRO:HD3   | 2.02                     | 0.75              |
| 1:A:268:VAL:HG13 | 1:A:283:LEU:CB   | 2.17                     | 0.74              |
| 1:A:304:TYR:CE2  | 1:A:328:LEU:HD21 | 2.21                     | 0.74              |
| 1:B:564:ARG:HG3  | 1:B:564:ARG:HH21 | 1.52                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:95:ARG:NH2   | 1:B:262:PRO:HB3  | 2.02                     | 0.74              |
| 1:B:253:ALA:HB3  | 1:B:367:GLY:CA   | 2.13                     | 0.74              |
| 1:B:326:PHE:HE2  | 1:B:337:VAL:HG12 | 1.52                     | 0.74              |
| 1:A:292:HIS:CD2  | 1:A:296:GLU:HG2  | 2.23                     | 0.74              |
| 1:B:450:ALA:CB   | 1:B:558:GLU:HG2  | 2.17                     | 0.74              |
| 1:B:81:ARG:HH21  | 1:B:81:ARG:CG    | 2.00                     | 0.74              |
| 1:A:76:ALA:HA    | 1:A:79:LEU:HB2   | 1.68                     | 0.74              |
| 1:B:275:LEU:O    | 1:B:277:GLY:N    | 2.21                     | 0.74              |
| 1:B:376:GLU:HA   | 1:B:412:HIS:H    | 1.52                     | 0.73              |
| 1:A:108:CYS:HB3  | 1:A:113:HIS:CD2  | 2.23                     | 0.73              |
| 1:B:25:LEU:HB3   | 1:B:260:TYR:CE1  | 2.23                     | 0.73              |
| 1:A:128:PRO:CG   | 1:A:129:GLU:HA   | 2.18                     | 0.73              |
| 1:A:304:TYR:HE2  | 1:A:328:LEU:HD21 | 1.53                     | 0.73              |
| 1:A:420:VAL:O    | 1:A:420:VAL:HG23 | 1.86                     | 0.73              |
| 1:B:482:MET:HE2  | 1:B:545:TRP:HZ3  | 1.52                     | 0.73              |
| 1:A:361:LYS:NZ   | 1:A:372:THR:OG1  | 2.22                     | 0.73              |
| 1:A:101:SER:HA   | 1:A:104:ASN:HD22 | 1.52                     | 0.73              |
| 1:A:90:LEU:N     | 1:A:91:PRO:HD3   | 2.03                     | 0.73              |
| 1:B:387:PRO:HA   | 1:B:390:MET:HB2  | 1.69                     | 0.73              |
| 1:B:525:ASP:HB3  | 1:B:528:ILE:HD12 | 1.70                     | 0.73              |
| 1:B:541:ARG:HH22 | 1:B:544:TYR:HB2  | 1.51                     | 0.73              |
| 1:A:338:ILE:HD12 | 1:A:338:ILE:H    | 1.54                     | 0.73              |
| 1:A:107:TYR:CE2  | 1:A:115:SER:CB   | 2.71                     | 0.72              |
| 1:A:192:SER:HB3  | 1:A:215:THR:HA   | 1.71                     | 0.72              |
| 1:A:452:ASN:OD1  | 1:A:552:ILE:HG21 | 1.89                     | 0.72              |
| 1:A:452:ASN:O    | 1:A:453:ILE:HD13 | 1.89                     | 0.72              |
| 1:A:429:VAL:CG1  | 1:A:433:GLN:OE1  | 2.37                     | 0.72              |
| 1:A:440:GLU:HB3  | 1:A:471:VAL:HG23 | 1.71                     | 0.72              |
| 1:B:397:ALA:O    | 1:B:401:ILE:HD12 | 1.89                     | 0.72              |
| 1:B:399:GLU:OE2  | 5:B:617:HOH:O    | 2.06                     | 0.72              |
| 1:B:242:THR:O    | 1:B:245:GLU:HG3  | 1.88                     | 0.72              |
| 1:A:254:ARG:C    | 1:A:365:ARG:NH2  | 2.43                     | 0.72              |
| 1:B:118:PRO:HD2  | 1:B:119:GLU:H    | 1.55                     | 0.72              |
| 1:B:413:LEU:HD23 | 1:B:413:LEU:C    | 2.10                     | 0.72              |
| 1:A:549:GLN:O    | 1:A:553:ARG:HG3  | 1.90                     | 0.72              |
| 1:B:323:MET:SD   | 1:B:338:ILE:HG13 | 2.29                     | 0.72              |
| 1:B:372:THR:HA   | 1:B:415:ILE:O    | 1.90                     | 0.72              |
| 1:A:454:PHE:CZ   | 1:A:513:VAL:HG11 | 2.25                     | 0.71              |
| 1:B:275:LEU:O    | 1:B:275:LEU:HG   | 1.88                     | 0.71              |
| 1:B:253:ALA:HB1  | 1:B:367:GLY:CA   | 2.20                     | 0.71              |
| 1:B:438:ILE:CG1  | 1:B:439:GLU:N    | 2.53                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:488:ARG:HH21 | 1:A:490:ILE:HB   | 1.54                     | 0.71              |
| 1:A:488:ARG:O    | 1:A:514:PHE:CD1  | 2.43                     | 0.71              |
| 1:B:215:THR:O    | 1:B:218:GLY:O    | 2.09                     | 0.71              |
| 1:A:524:ALA:O    | 1:A:526:PRO:HD3  | 1.90                     | 0.71              |
| 1:A:227:HIS:O    | 1:A:234:LEU:HB2  | 1.91                     | 0.71              |
| 1:A:328:LEU:HD12 | 1:A:329:PRO:CD   | 2.18                     | 0.71              |
| 1:B:229:THR:N    | 1:B:233:GLU:OE2  | 2.23                     | 0.71              |
| 1:B:122:PHE:CD2  | 1:B:122:PHE:N    | 2.58                     | 0.70              |
| 1:B:352:HIS:O    | 1:B:356:CYS:HB2  | 1.91                     | 0.70              |
| 1:A:430:GLU:HA   | 1:A:434:LEU:HB2  | 1.72                     | 0.70              |
| 1:A:461:LYS:HD3  | 1:A:461:LYS:H    | 1.56                     | 0.70              |
| 1:A:30:GLY:O     | 1:A:34:ARG:CG    | 2.38                     | 0.70              |
| 1:B:229:THR:HG22 | 1:B:233:GLU:OE2  | 1.90                     | 0.70              |
| 1:A:97:GLU:OE2   | 1:A:265:ALA:HB2  | 1.92                     | 0.70              |
| 1:A:48:LYS:HG2   | 1:A:362:GLU:HB2  | 1.72                     | 0.70              |
| 1:B:354:ARG:NE   | 1:B:374:GLU:OE2  | 2.25                     | 0.70              |
| 1:A:322:VAL:O    | 1:A:339:LYS:HG3  | 1.91                     | 0.70              |
| 1:A:463:PHE:HB3  | 1:A:471:VAL:HG12 | 1.72                     | 0.70              |
| 1:A:77:GLU:HG3   | 1:A:78:PHE:N     | 2.06                     | 0.70              |
| 1:B:208:TRP:HE3  | 1:B:223:LEU:CD2  | 2.03                     | 0.70              |
| 1:B:48:LYS:HE2   | 1:B:362:GLU:CD   | 2.12                     | 0.70              |
| 1:B:122:PHE:H    | 1:B:122:PHE:HD2  | 1.38                     | 0.69              |
| 1:A:166:TRP:C    | 1:A:167:GLN:OE1  | 2.30                     | 0.69              |
| 1:A:228:GLN:HA   | 1:A:234:LEU:HA   | 1.74                     | 0.69              |
| 1:A:281:ALA:O    | 1:A:285:MET:HG3  | 1.92                     | 0.69              |
| 1:B:438:ILE:HD13 | 1:B:531:LEU:HB3  | 1.72                     | 0.69              |
| 1:A:376:GLU:O    | 1:A:411:ARG:HA   | 1.90                     | 0.69              |
| 1:A:357:TYR:CE1  | 1:A:476:TYR:HD2  | 2.09                     | 0.69              |
| 1:A:95:ARG:NH2   | 1:B:26:GLU:HG2   | 2.06                     | 0.69              |
| 1:B:220:LEU:HD12 | 1:B:221:PRO:HD2  | 1.74                     | 0.69              |
| 1:B:412:HIS:CG   | 1:B:412:HIS:O    | 2.46                     | 0.69              |
| 1:B:48:LYS:O     | 1:B:52:HIS:ND1   | 2.25                     | 0.69              |
| 1:B:270:TRP:CE3  | 1:B:271:LEU:HG   | 2.28                     | 0.69              |
| 1:B:274:ILE:HG13 | 1:B:275:LEU:H    | 1.56                     | 0.69              |
| 1:B:87:THR:CG2   | 1:B:122:PHE:HE1  | 2.05                     | 0.69              |
| 1:A:93:TYR:O     | 1:A:96:PHE:HB3   | 1.91                     | 0.69              |
| 1:B:68:ILE:HG13  | 1:B:69:THR:N     | 2.05                     | 0.69              |
| 1:A:153:LEU:CD2  | 1:A:176:ILE:HG21 | 2.23                     | 0.69              |
| 1:A:136:PRO:O    | 1:B:163:ARG:NH1  | 2.25                     | 0.69              |
| 1:B:253:ALA:CB   | 1:B:367:GLY:C    | 2.62                     | 0.69              |
| 1:A:139:LEU:O    | 1:A:198:ASN:OD1  | 2.10                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:200:LEU:HD23 | 1:A:201:PHE:CA   | 2.22                     | 0.68              |
| 1:A:255:SER:HA   | 1:A:365:ARG:HH21 | 1.58                     | 0.68              |
| 1:A:292:HIS:O    | 1:A:292:HIS:HD2  | 1.76                     | 0.68              |
| 1:B:544:TYR:O    | 1:B:548:LEU:HB3  | 1.94                     | 0.68              |
| 1:A:94:PRO:HB2   | 1:A:263:LEU:HD21 | 1.76                     | 0.68              |
| 1:A:454:PHE:HZ   | 1:A:513:VAL:HG11 | 1.59                     | 0.68              |
| 1:B:334:VAL:O    | 1:B:415:ILE:HG23 | 1.94                     | 0.68              |
| 1:B:324:LEU:O    | 1:B:337:VAL:HG13 | 1.94                     | 0.68              |
| 1:B:152:LEU:HD22 | 1:B:152:LEU:N    | 2.08                     | 0.68              |
| 1:B:21:TYR:O     | 1:B:24:PHE:HB3   | 1.94                     | 0.68              |
| 1:A:58:VAL:O     | 1:A:62:VAL:HB    | 1.93                     | 0.67              |
| 1:B:124:PHE:CB   | 1:B:299:ARG:HD3  | 2.25                     | 0.67              |
| 1:B:137:ARG:HB3  | 1:B:138:PRO:CD   | 2.23                     | 0.67              |
| 1:A:371:ASP:CG   | 1:A:372:THR:H    | 1.98                     | 0.67              |
| 1:B:54:TYR:OH    | 1:B:102:PHE:HA   | 1.93                     | 0.67              |
| 1:B:93:TYR:HB3   | 1:B:96:PHE:HB3   | 1.75                     | 0.67              |
| 1:B:118:PRO:CD   | 1:B:119:GLU:H    | 2.08                     | 0.67              |
| 1:B:107:TYR:OH   | 1:B:115:SER:O    | 2.10                     | 0.67              |
| 1:B:203:ARG:NH2  | 1:B:254:ARG:CD   | 2.53                     | 0.67              |
| 1:A:95:ARG:NH2   | 1:B:26:GLU:OE1   | 2.27                     | 0.67              |
| 1:A:343:ALA:HB3  | 1:A:344:PRO:HD3  | 1.76                     | 0.67              |
| 1:A:52:HIS:NE2   | 1:A:362:GLU:OE1  | 2.26                     | 0.67              |
| 1:B:97:GLU:OE1   | 1:B:265:ALA:HB2  | 1.95                     | 0.67              |
| 1:B:376:GLU:O    | 1:B:411:ARG:CA   | 2.31                     | 0.67              |
| 1:A:255:SER:HA   | 1:A:365:ARG:NH2  | 2.11                     | 0.66              |
| 1:A:411:ARG:O    | 1:A:412:HIS:CD2  | 2.48                     | 0.66              |
| 1:B:274:ILE:HG13 | 1:B:275:LEU:N    | 2.09                     | 0.66              |
| 1:B:323:MET:HG3  | 1:B:338:ILE:HA   | 1.77                     | 0.66              |
| 1:A:434:LEU:HD11 | 1:A:528:ILE:HG22 | 1.78                     | 0.66              |
| 1:A:55:ASP:HA    | 1:A:58:VAL:CG1   | 2.25                     | 0.66              |
| 1:B:65:LEU:O     | 1:B:68:ILE:HG12  | 1.96                     | 0.66              |
| 1:A:222:PHE:O    | 1:A:222:PHE:HD2  | 1.79                     | 0.66              |
| 1:B:448:LEU:HD13 | 1:B:453:ILE:CG2  | 2.26                     | 0.66              |
| 1:A:462:ASN:CG   | 1:A:475:ASP:OD2  | 2.34                     | 0.66              |
| 1:A:97:GLU:HB2   | 1:A:292:HIS:HE1  | 1.60                     | 0.66              |
| 1:A:279:THR:CB   | 1:A:282:GLU:HG3  | 2.26                     | 0.66              |
| 1:A:254:ARG:O    | 1:A:365:ARG:NH2  | 2.29                     | 0.66              |
| 1:A:451:ALA:O    | 1:A:453:ILE:N    | 2.29                     | 0.66              |
| 1:A:139:LEU:HD21 | 1:A:267:LEU:HD13 | 1.78                     | 0.65              |
| 1:A:404:LEU:N    | 1:A:407:GLN:O    | 2.28                     | 0.65              |
| 1:A:167:GLN:OE1  | 1:A:167:GLN:N    | 2.29                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:220:LEU:HG   | 1:A:221:PRO:HD3  | 1.78                     | 0.65              |
| 1:B:123:ILE:O    | 1:B:123:ILE:HG12 | 1.95                     | 0.65              |
| 1:B:366:VAL:HG12 | 1:B:366:VAL:O    | 1.96                     | 0.65              |
| 1:A:337:VAL:HG22 | 1:A:413:LEU:HD13 | 1.77                     | 0.65              |
| 1:A:199:GLU:N    | 1:A:199:GLU:OE1  | 2.30                     | 0.65              |
| 1:A:95:ARG:CZ    | 1:B:26:GLU:HG2   | 2.26                     | 0.65              |
| 1:A:157:ILE:CG2  | 1:A:169:LYS:HD2  | 2.26                     | 0.65              |
| 1:A:202:TYR:O    | 1:A:257:PHE:HD1  | 1.80                     | 0.65              |
| 1:A:95:ARG:NE    | 1:A:262:PRO:O    | 2.29                     | 0.65              |
| 1:A:220:LEU:HG   | 1:A:221:PRO:CD   | 2.27                     | 0.65              |
| 1:A:332:ASP:O    | 1:A:418:ARG:N    | 2.26                     | 0.65              |
| 1:A:420:VAL:CG2  | 1:A:465:VAL:HB   | 2.27                     | 0.65              |
| 1:B:427:GLU:C    | 1:B:429:VAL:N    | 2.51                     | 0.65              |
| 1:A:101:SER:CA   | 1:A:104:ASN:ND2  | 2.59                     | 0.65              |
| 1:A:150:GLU:OE1  | 1:A:173:ILE:HD12 | 1.97                     | 0.65              |
| 1:A:377:ASN:ND2  | 1:A:411:ARG:HG2  | 2.12                     | 0.65              |
| 1:A:132:PHE:C    | 1:A:134:THR:HG23 | 2.18                     | 0.64              |
| 1:A:200:LEU:HD11 | 1:A:207:ALA:HB1  | 1.78                     | 0.64              |
| 1:A:516:GLU:OE1  | 1:A:540:PHE:HD1  | 1.80                     | 0.64              |
| 1:A:371:ASP:O    | 1:A:416:GLU:HB2  | 1.97                     | 0.64              |
| 1:B:310:GLU:HG2  | 1:B:311:GLN:N    | 2.12                     | 0.64              |
| 1:A:77:GLU:HG3   | 1:A:78:PHE:H     | 1.63                     | 0.64              |
| 1:A:279:THR:HG1  | 1:A:282:GLU:CD   | 2.00                     | 0.64              |
| 1:A:292:HIS:O    | 1:A:292:HIS:CD2  | 2.50                     | 0.64              |
| 1:A:282:GLU:OE2  | 1:A:417:ARG:NH2  | 2.30                     | 0.64              |
| 1:B:529:GLY:O    | 1:B:532:PHE:HB2  | 1.96                     | 0.64              |
| 1:A:151:SER:O    | 1:A:154:MET:HB2  | 1.97                     | 0.64              |
| 1:A:264:PRO:HB3  | 1:A:287:ILE:HD12 | 1.80                     | 0.64              |
| 1:A:128:PRO:HB2  | 1:A:129:GLU:C    | 2.16                     | 0.63              |
| 1:A:33:GLN:O     | 1:A:37:GLN:HB2   | 1.98                     | 0.63              |
| 1:B:253:ALA:CB   | 1:B:367:GLY:O    | 2.46                     | 0.63              |
| 1:B:284:TYR:CE1  | 1:B:292:HIS:CD2  | 2.83                     | 0.63              |
| 1:A:152:LEU:O    | 1:A:155:ARG:HB2  | 1.98                     | 0.63              |
| 1:A:229:THR:HB   | 1:A:233:GLU:HG2  | 1.78                     | 0.63              |
| 1:A:308:CYS:C    | 1:A:309:ASN:ND2  | 2.41                     | 0.63              |
| 1:B:305:LEU:N    | 1:B:305:LEU:HD13 | 2.12                     | 0.63              |
| 1:B:420:VAL:HG13 | 1:B:465:VAL:HB   | 1.79                     | 0.63              |
| 1:A:104:ASN:OD1  | 1:A:122:PHE:O    | 2.17                     | 0.63              |
| 1:A:519:ARG:HD3  | 1:A:540:PHE:HB2  | 1.79                     | 0.63              |
| 1:A:529:GLY:O    | 1:A:532:PHE:HB2  | 1.99                     | 0.63              |
| 1:B:108:CYS:CB   | 1:B:113:HIS:ND1  | 2.61                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:54:TYR:HH    | 1:B:102:PHE:HA   | 1.63                     | 0.63              |
| 1:A:420:VAL:O    | 1:A:420:VAL:CG2  | 2.45                     | 0.62              |
| 1:A:489:ASP:CA   | 1:A:514:PHE:CD1  | 2.82                     | 0.62              |
| 1:B:370:ALA:N    | 1:B:476:TYR:OH   | 2.28                     | 0.62              |
| 1:A:143:PHE:O    | 1:A:194:LEU:N    | 2.31                     | 0.62              |
| 1:A:145:PRO:HD2  | 1:A:193:HIS:HA   | 1.80                     | 0.62              |
| 1:A:438:ILE:O    | 1:A:536:HIS:HE1  | 1.83                     | 0.62              |
| 1:A:154:MET:O    | 1:A:158:SER:OG   | 2.16                     | 0.62              |
| 1:A:206:ALA:HB3  | 5:A:594:HOH:O    | 1.99                     | 0.62              |
| 1:A:309:ASN:N    | 1:A:309:ASN:ND2  | 2.43                     | 0.62              |
| 1:B:245:GLU:O    | 1:B:248:ILE:CG2  | 2.47                     | 0.62              |
| 1:B:61:VAL:CG2   | 1:B:62:VAL:N     | 2.62                     | 0.62              |
| 1:B:338:ILE:HD11 | 1:B:414:TYR:HD2  | 1.64                     | 0.62              |
| 1:A:292:HIS:HD2  | 1:A:296:GLU:HG2  | 1.63                     | 0.62              |
| 1:A:304:TYR:CE2  | 1:A:328:LEU:CD2  | 2.82                     | 0.62              |
| 1:A:54:TYR:O     | 1:A:58:VAL:HG12  | 1.99                     | 0.62              |
| 1:B:58:VAL:O     | 1:B:61:VAL:HG22  | 2.00                     | 0.62              |
| 1:A:200:LEU:CD2  | 1:A:201:PHE:N    | 2.43                     | 0.61              |
| 1:B:102:PHE:O    | 1:B:106:VAL:HG23 | 2.00                     | 0.61              |
| 1:B:124:PHE:HB2  | 1:B:299:ARG:CD   | 2.29                     | 0.61              |
| 1:A:365:ARG:HB3  | 1:A:369:MET:HB2  | 1.83                     | 0.61              |
| 1:A:422:LEU:HB3  | 1:A:460:PHE:O    | 2.01                     | 0.61              |
| 1:A:516:GLU:OE1  | 1:A:540:PHE:CD1  | 2.53                     | 0.61              |
| 1:A:75:ASP:CB    | 1:A:77:GLU:HG2   | 2.27                     | 0.61              |
| 1:B:220:LEU:HD12 | 1:B:221:PRO:CD   | 2.30                     | 0.61              |
| 1:A:170:SER:O    | 1:A:173:ILE:HG12 | 2.00                     | 0.61              |
| 1:A:414:TYR:C    | 1:A:415:ILE:HD12 | 2.19                     | 0.61              |
| 1:A:509:SER:N    | 1:A:510:PRO:HD2  | 2.13                     | 0.61              |
| 1:A:240:LEU:HD23 | 1:A:245:GLU:HG3  | 1.75                     | 0.61              |
| 1:B:124:PHE:HB2  | 1:B:299:ARG:HG3  | 1.80                     | 0.61              |
| 1:B:215:THR:C    | 1:B:217:SER:H    | 2.04                     | 0.61              |
| 1:B:253:ALA:HB1  | 1:B:367:GLY:O    | 2.00                     | 0.61              |
| 1:A:423:ASN:OD1  | 1:A:461:LYS:HB2  | 2.00                     | 0.61              |
| 1:B:228:GLN:HE21 | 1:B:232:GLY:HA2  | 1.64                     | 0.61              |
| 1:B:413:LEU:O    | 1:B:413:LEU:CD2  | 2.41                     | 0.61              |
| 1:A:127:GLN:N    | 1:A:128:PRO:CD   | 2.61                     | 0.61              |
| 1:A:69:THR:HG22  | 1:A:73:SER:OG    | 2.01                     | 0.61              |
| 1:B:448:LEU:HD13 | 1:B:453:ILE:HG22 | 1.82                     | 0.61              |
| 1:A:119:GLU:OE1  | 1:A:119:GLU:N    | 2.34                     | 0.61              |
| 1:A:133:ARG:O    | 1:A:133:ARG:HG3  | 2.01                     | 0.61              |
| 1:A:108:CYS:SG   | 1:A:113:HIS:HA   | 2.40                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:132:PHE:C    | 1:A:134:THR:H    | 2.02                     | 0.60              |
| 1:A:208:TRP:CZ3  | 1:A:225:PRO:HG3  | 2.36                     | 0.60              |
| 1:B:389:LEU:O    | 1:B:389:LEU:HG   | 2.00                     | 0.60              |
| 1:B:391:GLU:HA   | 1:B:394:LEU:HB3  | 1.83                     | 0.60              |
| 1:B:95:ARG:NH2   | 1:B:262:PRO:O    | 2.25                     | 0.60              |
| 1:B:265:ALA:O    | 1:B:269:GLU:HB2  | 2.01                     | 0.60              |
| 1:A:101:SER:HA   | 1:A:104:ASN:HD21 | 1.63                     | 0.60              |
| 1:A:132:PHE:O    | 1:A:134:THR:N    | 2.28                     | 0.60              |
| 1:A:264:PRO:O    | 1:A:268:VAL:HG23 | 2.01                     | 0.60              |
| 1:A:324:LEU:N    | 1:A:337:VAL:O    | 2.29                     | 0.60              |
| 1:A:86:TYR:O     | 1:A:90:LEU:CD1   | 2.50                     | 0.60              |
| 1:A:420:VAL:HG22 | 1:A:465:VAL:HB   | 1.84                     | 0.60              |
| 1:A:127:GLN:N    | 1:A:128:PRO:HD2  | 2.17                     | 0.60              |
| 1:A:266:ALA:O    | 1:A:269:GLU:HB3  | 2.02                     | 0.60              |
| 1:A:557:VAL:O    | 1:A:557:VAL:CG1  | 2.49                     | 0.60              |
| 1:A:126:SER:O    | 1:A:127:GLN:HB3  | 2.01                     | 0.60              |
| 1:A:229:THR:N    | 1:A:233:GLU:O    | 2.33                     | 0.60              |
| 1:B:315:ALA:HB3  | 1:B:325:VAL:HG11 | 1.84                     | 0.60              |
| 1:B:514:PHE:HD2  | 1:B:517:GLU:HB2  | 1.66                     | 0.60              |
| 1:B:270:TRP:HE3  | 1:B:271:LEU:HG   | 1.66                     | 0.60              |
| 1:A:116:LEU:HD12 | 1:A:117:THR:H    | 1.66                     | 0.59              |
| 1:A:331:PHE:HD1  | 1:A:332:ASP:H    | 1.49                     | 0.59              |
| 1:A:463:PHE:HB3  | 1:A:471:VAL:CG1  | 2.31                     | 0.59              |
| 1:B:525:ASP:CB   | 1:B:528:ILE:HD12 | 2.32                     | 0.59              |
| 1:A:458:MET:HE2  | 5:A:601:HOH:O    | 2.02                     | 0.59              |
| 1:A:488:ARG:O    | 1:A:514:PHE:HE1  | 1.83                     | 0.59              |
| 1:B:108:CYS:CB   | 1:B:113:HIS:HD1  | 2.15                     | 0.59              |
| 1:A:305:LEU:N    | 1:A:305:LEU:HD13 | 2.07                     | 0.59              |
| 1:A:351:ALA:HB3  | 1:A:354:ARG:HG3  | 1.83                     | 0.59              |
| 1:A:357:TYR:CE1  | 1:A:476:TYR:CD2  | 2.89                     | 0.59              |
| 1:A:213:LEU:O    | 1:A:213:LEU:HG   | 2.01                     | 0.59              |
| 1:A:86:TYR:O     | 1:A:90:LEU:HD12  | 2.03                     | 0.59              |
| 1:B:124:PHE:CB   | 1:B:299:ARG:CD   | 2.80                     | 0.59              |
| 1:B:420:VAL:HG21 | 1:B:425:TRP:HD1  | 1.67                     | 0.59              |
| 1:B:482:MET:CE   | 1:B:545:TRP:HZ3  | 2.16                     | 0.59              |
| 1:A:458:MET:CE   | 5:A:601:HOH:O    | 2.50                     | 0.59              |
| 1:B:104:ASN:HB2  | 4:B:1604:AMP:O3' | 2.03                     | 0.59              |
| 1:A:19:ALA:O     | 1:A:22:GLY:N     | 2.36                     | 0.59              |
| 1:B:261:ALA:HB2  | 1:B:267:LEU:HD22 | 1.84                     | 0.59              |
| 1:B:359:LEU:O    | 1:B:363:HIS:HB2  | 2.01                     | 0.59              |
| 1:A:58:VAL:HG23  | 1:A:106:VAL:HG22 | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:489:ASP:HB3  | 1:A:514:PHE:HB3  | 1.85                     | 0.58              |
| 1:A:14:LEU:HD13  | 1:A:86:TYR:OH    | 2.01                     | 0.58              |
| 1:A:61:VAL:O     | 1:A:65:LEU:HB2   | 2.03                     | 0.58              |
| 1:B:116:LEU:C    | 1:B:117:THR:HG22 | 2.23                     | 0.58              |
| 1:A:109:ARG:NH1  | 1:A:374:GLU:OE1  | 2.36                     | 0.58              |
| 1:A:161:PRO:HB3  | 1:B:138:PRO:HB3  | 1.84                     | 0.58              |
| 1:A:252:PHE:O    | 1:A:365:ARG:NH1  | 2.37                     | 0.58              |
| 1:A:301:TYR:HA   | 1:A:331:PHE:HZ   | 1.67                     | 0.58              |
| 1:B:208:TRP:CZ3  | 1:B:223:LEU:HD22 | 2.38                     | 0.58              |
| 1:B:370:ALA:H    | 1:B:476:TYR:HH   | 1.51                     | 0.58              |
| 1:B:433:GLN:HA   | 1:B:433:GLN:OE1  | 2.04                     | 0.58              |
| 1:A:335:PHE:N    | 1:A:335:PHE:CD2  | 2.71                     | 0.58              |
| 1:B:220:LEU:CD1  | 1:B:221:PRO:HD2  | 2.34                     | 0.58              |
| 1:B:310:GLU:CG   | 1:B:328:LEU:HD23 | 2.31                     | 0.58              |
| 1:A:101:SER:CA   | 1:A:104:ASN:HD22 | 2.16                     | 0.58              |
| 1:A:245:GLU:O    | 1:A:249:VAL:HG12 | 2.03                     | 0.58              |
| 1:A:304:TYR:HE2  | 1:A:328:LEU:CD2  | 2.15                     | 0.58              |
| 1:B:442:GLY:O    | 1:B:446:ARG:HG3  | 2.04                     | 0.58              |
| 1:B:95:ARG:NH2   | 1:B:262:PRO:CB   | 2.67                     | 0.58              |
| 1:B:221:PRO:HG3  | 1:B:274:ILE:O    | 2.03                     | 0.58              |
| 1:B:295:THR:HG22 | 1:B:296:GLU:N    | 2.16                     | 0.58              |
| 1:B:541:ARG:O    | 1:B:541:ARG:HG2  | 2.04                     | 0.58              |
| 1:A:39:ASP:O     | 1:A:42:ALA:HB3   | 2.04                     | 0.57              |
| 1:B:32:GLN:HE22  | 1:B:161:PRO:HB3  | 1.69                     | 0.57              |
| 1:B:327:THR:OG1  | 1:B:334:VAL:HA   | 2.04                     | 0.57              |
| 1:B:253:ALA:HA   | 1:B:369:MET:O    | 2.05                     | 0.57              |
| 1:B:450:ALA:HB1  | 1:B:558:GLU:CB   | 2.34                     | 0.57              |
| 1:A:358:GLN:C    | 1:A:360:VAL:H    | 2.06                     | 0.57              |
| 1:A:340:ASP:OD1  | 1:A:400:LYS:CG   | 2.53                     | 0.57              |
| 1:A:325:VAL:HG11 | 2:A:1762:ADP:C1' | 2.34                     | 0.57              |
| 1:A:48:LYS:O     | 1:A:52:HIS:ND1   | 2.37                     | 0.57              |
| 1:B:78:PHE:O     | 1:B:82:VAL:HG23  | 2.04                     | 0.57              |
| 1:B:124:PHE:HB3  | 1:B:299:ARG:HG2  | 1.82                     | 0.57              |
| 1:B:354:ARG:HE   | 1:B:412:HIS:CD2  | 2.23                     | 0.57              |
| 1:A:215:THR:O    | 1:A:218:GLY:O    | 2.23                     | 0.57              |
| 1:A:292:HIS:CD2  | 1:A:296:GLU:CG   | 2.88                     | 0.57              |
| 1:A:145:PRO:CD   | 1:A:193:HIS:HA   | 2.35                     | 0.57              |
| 1:A:449:ALA:CB   | 1:A:548:LEU:HD13 | 2.35                     | 0.57              |
| 1:A:222:PHE:O    | 1:A:222:PHE:CD2  | 2.58                     | 0.56              |
| 1:A:222:PHE:HE2  | 1:A:224:LEU:HD12 | 1.69                     | 0.56              |
| 1:B:356:CYS:SG   | 1:B:479:ILE:HG22 | 2.45                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:294:LYS:HG3  | 1:A:373:GLN:HG3  | 1.87                     | 0.56              |
| 1:A:380:LEU:HD13 | 1:A:410:ILE:HG21 | 1.86                     | 0.56              |
| 1:A:23:ARG:HB3   | 1:A:53:LEU:HD22  | 1.87                     | 0.56              |
| 1:A:315:ALA:HB3  | 1:A:325:VAL:HG13 | 1.87                     | 0.56              |
| 1:B:179:HIS:CD2  | 1:B:241:THR:OG1  | 2.57                     | 0.56              |
| 1:B:334:VAL:HB   | 1:B:418:ARG:HB3  | 1.87                     | 0.56              |
| 1:A:425:TRP:O    | 1:A:429:VAL:HG22 | 2.05                     | 0.56              |
| 1:A:568:ARG:CG   | 1:A:571:VAL:HG12 | 2.35                     | 0.56              |
| 1:A:489:ASP:HA   | 1:A:514:PHE:CE1  | 2.39                     | 0.56              |
| 1:A:68:ILE:HG13  | 1:B:67:CYS:SG    | 2.45                     | 0.56              |
| 1:B:93:TYR:HB3   | 1:B:96:PHE:CB    | 2.35                     | 0.56              |
| 1:B:9:ILE:HG21   | 1:B:82:VAL:HG22  | 1.87                     | 0.56              |
| 1:A:113:HIS:CB   | 1:A:376:GLU:HB3  | 2.35                     | 0.56              |
| 1:B:325:VAL:HG22 | 1:B:334:VAL:HG22 | 1.87                     | 0.56              |
| 1:A:325:VAL:O    | 1:A:325:VAL:HG13 | 2.06                     | 0.56              |
| 1:A:442:GLY:HA3  | 1:A:536:HIS:NE2  | 2.21                     | 0.56              |
| 1:B:326:PHE:CE2  | 1:B:337:VAL:HG12 | 2.36                     | 0.56              |
| 1:A:308:CYS:SG   | 1:A:309:ASN:N    | 2.78                     | 0.55              |
| 1:A:449:ALA:HB1  | 1:A:548:LEU:HD13 | 1.88                     | 0.55              |
| 1:B:327:THR:CG2  | 1:B:328:LEU:N    | 2.46                     | 0.55              |
| 1:A:237:ASP:C    | 1:A:237:ASP:OD1  | 2.43                     | 0.55              |
| 1:A:299:ARG:O    | 1:A:303:VAL:HG23 | 2.06                     | 0.55              |
| 1:A:408:ILE:O    | 1:A:408:ILE:HG12 | 2.05                     | 0.55              |
| 1:B:411:ARG:O    | 1:B:412:HIS:HB3  | 2.06                     | 0.55              |
| 1:B:54:TYR:HH    | 1:B:105:SER:HG   | 1.54                     | 0.55              |
| 1:A:423:ASN:OD1  | 1:A:461:LYS:HB3  | 2.06                     | 0.55              |
| 1:A:488:ARG:NH2  | 1:A:490:ILE:HB   | 2.21                     | 0.55              |
| 1:B:149:TRP:HB3  | 1:B:177:ILE:HD11 | 1.87                     | 0.55              |
| 1:B:318:ILE:HB   | 1:B:461:LYS:CE   | 2.37                     | 0.55              |
| 1:B:95:ARG:NH1   | 5:B:603:HOH:O    | 2.02                     | 0.55              |
| 1:A:108:CYS:CB   | 1:A:113:HIS:HA   | 2.36                     | 0.55              |
| 1:B:394:LEU:HA   | 1:B:401:ILE:HD13 | 1.88                     | 0.55              |
| 1:A:244:ALA:O    | 1:A:248:ILE:HG12 | 2.06                     | 0.55              |
| 1:B:107:TYR:HE2  | 1:B:116:LEU:HA   | 1.72                     | 0.55              |
| 1:B:171:ARG:O    | 1:B:175:TYR:HD2  | 1.90                     | 0.55              |
| 1:B:51:ILE:HD11  | 1:B:256:TYR:HD2  | 1.72                     | 0.55              |
| 1:B:529:GLY:O    | 1:B:532:PHE:N    | 2.27                     | 0.55              |
| 1:A:23:ARG:HB3   | 1:A:53:LEU:CD2   | 2.37                     | 0.55              |
| 1:B:441:TYR:O    | 1:B:444:ALA:HB3  | 2.06                     | 0.55              |
| 1:A:127:GLN:O    | 1:A:128:PRO:C    | 2.42                     | 0.55              |
| 1:A:209:LEU:HB3  | 1:A:224:LEU:HB2  | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:250:PHE:HB2  | 1:A:275:LEU:HD21 | 1.87                     | 0.55              |
| 1:B:372:THR:HG22 | 1:B:415:ILE:O    | 2.07                     | 0.55              |
| 1:A:153:LEU:HD21 | 1:A:176:ILE:HG21 | 1.87                     | 0.55              |
| 1:A:20:GLN:C     | 1:A:20:GLN:NE2   | 2.61                     | 0.55              |
| 1:A:201:PHE:O    | 1:A:208:TRP:HB2  | 2.07                     | 0.54              |
| 1:A:189:LEU:O    | 1:A:190:SER:CB   | 2.55                     | 0.54              |
| 1:A:255:SER:CA   | 1:A:365:ARG:HH21 | 2.18                     | 0.54              |
| 1:A:371:ASP:CG   | 1:A:372:THR:N    | 2.60                     | 0.54              |
| 1:B:134:THR:O    | 1:B:134:THR:HG22 | 2.06                     | 0.54              |
| 1:B:312:PHE:CD2  | 1:B:384:HIS:HB3  | 2.42                     | 0.54              |
| 1:B:338:ILE:HG22 | 1:B:339:LYS:O    | 2.08                     | 0.54              |
| 1:B:237:ASP:OD2  | 1:B:563:TYR:OH   | 2.22                     | 0.54              |
| 1:B:324:LEU:HD13 | 1:B:393:LEU:HD12 | 1.89                     | 0.54              |
| 1:B:61:VAL:CG2   | 1:B:62:VAL:H     | 2.20                     | 0.54              |
| 1:A:25:LEU:O     | 1:A:29:SER:HB3   | 2.06                     | 0.54              |
| 1:B:231:ASP:OD1  | 1:B:231:ASP:N    | 2.29                     | 0.54              |
| 1:A:221:PRO:HB3  | 1:A:274:ILE:HG23 | 1.90                     | 0.54              |
| 1:A:442:GLY:HA3  | 1:A:536:HIS:CE1  | 2.43                     | 0.54              |
| 1:A:128:PRO:CB   | 1:A:129:GLU:CA   | 2.38                     | 0.54              |
| 1:B:195:GLN:O    | 1:B:212:LYS:N    | 2.33                     | 0.54              |
| 1:B:255:SER:OG   | 1:B:364:ASP:OD1  | 2.26                     | 0.54              |
| 1:A:170:SER:O    | 1:A:173:ILE:CG1  | 2.56                     | 0.54              |
| 1:A:97:GLU:HB2   | 1:A:292:HIS:CE1  | 2.42                     | 0.54              |
| 1:A:456:GLY:HA3  | 1:A:478:GLU:O    | 2.08                     | 0.54              |
| 1:A:359:LEU:O    | 1:A:359:LEU:HD23 | 2.08                     | 0.54              |
| 1:A:372:THR:HA   | 1:A:415:ILE:O    | 2.08                     | 0.54              |
| 1:B:290:GLN:HA   | 1:B:293:ALA:HB3  | 1.90                     | 0.54              |
| 1:B:403:ASP:C    | 1:B:404:LEU:HD23 | 2.28                     | 0.54              |
| 1:B:462:ASN:HB3  | 1:B:475:ASP:HB2  | 1.90                     | 0.54              |
| 1:B:118:PRO:CD   | 1:B:119:GLU:N    | 2.71                     | 0.53              |
| 1:B:538:ASP:N    | 1:B:538:ASP:OD1  | 2.41                     | 0.53              |
| 1:B:327:THR:C    | 1:B:328:LEU:HD12 | 2.29                     | 0.53              |
| 1:B:353:VAL:O    | 1:B:357:TYR:HB2  | 2.09                     | 0.53              |
| 1:B:375:PHE:HE2  | 1:B:415:ILE:HD12 | 1.73                     | 0.53              |
| 1:A:366:VAL:O    | 1:A:366:VAL:HG12 | 2.09                     | 0.53              |
| 1:B:280:THR:O    | 1:B:284:TYR:HD2  | 1.90                     | 0.53              |
| 1:B:287:ILE:O    | 1:B:287:ILE:HG22 | 2.08                     | 0.53              |
| 1:B:465:VAL:HA   | 1:B:470:ARG:O    | 2.08                     | 0.53              |
| 1:A:490:ILE:O    | 1:A:491:PRO:O    | 2.25                     | 0.53              |
| 1:A:96:PHE:CZ    | 1:A:128:PRO:CG   | 2.92                     | 0.53              |
| 1:A:194:LEU:CD2  | 1:A:195:GLN:N    | 2.72                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:279:THR:OG1  | 1:A:282:GLU:OE1  | 2.26                     | 0.53              |
| 1:A:292:HIS:HD2  | 1:A:296:GLU:CG   | 2.21                     | 0.53              |
| 1:A:449:ALA:O    | 1:A:451:ALA:O    | 2.25                     | 0.53              |
| 1:A:483:THR:HG23 | 1:A:553:ARG:HD3  | 1.91                     | 0.53              |
| 1:B:561:TYR:HB3  | 1:B:563:TYR:CE1  | 2.43                     | 0.53              |
| 1:A:358:GLN:O    | 1:A:361:LYS:N    | 2.38                     | 0.53              |
| 1:A:489:ASP:HB3  | 1:A:514:PHE:CB   | 2.39                     | 0.53              |
| 1:A:490:ILE:O    | 1:A:491:PRO:C    | 2.46                     | 0.53              |
| 1:A:488:ARG:HB2  | 1:A:546:ARG:HH22 | 1.73                     | 0.53              |
| 1:B:427:GLU:O    | 1:B:429:VAL:N    | 2.39                     | 0.53              |
| 1:B:48:LYS:NZ    | 5:B:610:HOH:O    | 2.30                     | 0.53              |
| 1:B:556:HIS:CE1  | 5:B:579:HOH:O    | 2.60                     | 0.53              |
| 1:A:200:LEU:HD23 | 1:A:200:LEU:O    | 2.05                     | 0.53              |
| 1:B:313:ILE:O    | 1:B:327:THR:N    | 2.40                     | 0.53              |
| 1:B:79:LEU:HD12  | 1:B:120:ARG:HB3  | 1.90                     | 0.53              |
| 1:A:194:LEU:HD23 | 1:A:195:GLN:H    | 1.73                     | 0.53              |
| 1:A:200:LEU:CD2  | 1:A:200:LEU:O    | 2.55                     | 0.53              |
| 1:A:78:PHE:C     | 1:A:80:LEU:H     | 2.11                     | 0.53              |
| 1:B:294:LYS:HG3  | 1:B:373:GLN:OE1  | 2.09                     | 0.53              |
| 1:A:334:VAL:O    | 1:A:415:ILE:HA   | 2.08                     | 0.52              |
| 1:B:127:GLN:CB   | 1:B:128:PRO:HD3  | 2.26                     | 0.52              |
| 1:B:251:GLY:O    | 1:B:254:ARG:HB2  | 2.09                     | 0.52              |
| 1:B:85:HIS:O     | 1:B:88:ARG:HG2   | 2.08                     | 0.52              |
| 1:A:317:GLY:HA2  | 1:A:424:ILE:HD11 | 1.91                     | 0.52              |
| 1:A:359:LEU:HD21 | 1:A:481:TYR:CE1  | 2.44                     | 0.52              |
| 1:B:338:ILE:HG21 | 1:B:353:VAL:HG11 | 1.90                     | 0.52              |
| 1:A:40:TRP:HD1   | 1:A:43:VAL:HB    | 1.74                     | 0.52              |
| 1:B:294:LYS:NZ   | 4:B:1604:AMP:O3P | 2.30                     | 0.52              |
| 1:B:177:ILE:O    | 1:B:181:THR:N    | 2.43                     | 0.52              |
| 1:B:448:LEU:HD12 | 1:B:455:PRO:HG3  | 1.91                     | 0.52              |
| 1:A:264:PRO:CB   | 1:A:287:ILE:HD12 | 2.40                     | 0.52              |
| 1:B:278:LYS:HB2  | 1:B:282:GLU:OE2  | 2.10                     | 0.52              |
| 1:B:286:ALA:O    | 1:B:287:ILE:HD12 | 2.09                     | 0.52              |
| 1:B:63:GLU:O     | 1:B:67:CYS:HB2   | 2.10                     | 0.52              |
| 1:A:200:LEU:CD2  | 1:A:201:PHE:C    | 2.78                     | 0.52              |
| 1:A:445:ILE:HG22 | 1:A:445:ILE:O    | 2.10                     | 0.52              |
| 1:B:186:PRO:HA   | 1:B:189:LEU:HD22 | 1.90                     | 0.52              |
| 1:A:95:ARG:NH2   | 1:B:26:GLU:CG    | 2.72                     | 0.52              |
| 1:B:101:SER:HA   | 1:B:104:ASN:ND2  | 2.25                     | 0.52              |
| 1:B:80:LEU:HD11  | 1:B:119:GLU:O    | 2.08                     | 0.52              |
| 1:B:338:ILE:HG12 | 1:B:353:VAL:CG2  | 2.33                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:552:ILE:C    | 1:B:554:GLU:H    | 2.10                     | 0.52              |
| 1:A:323:MET:HE2  | 1:A:336:LYS:HB3  | 1.92                     | 0.52              |
| 1:A:33:GLN:O     | 1:A:37:GLN:N     | 2.40                     | 0.52              |
| 1:B:176:ILE:HD11 | 1:B:236:ILE:HD12 | 1.92                     | 0.52              |
| 1:B:124:PHE:HB3  | 1:B:299:ARG:HD3  | 1.90                     | 0.52              |
| 1:B:482:MET:CE   | 1:B:545:TRP:CZ3  | 2.92                     | 0.52              |
| 1:A:200:LEU:HD23 | 1:A:201:PHE:C    | 2.29                     | 0.52              |
| 1:B:569:PHE:O    | 1:B:573:TYR:O    | 2.28                     | 0.52              |
| 1:A:336:LYS:HD2  | 1:A:416:GLU:OE1  | 2.09                     | 0.52              |
| 1:A:358:GLN:HA   | 1:A:361:LYS:HB2  | 1.92                     | 0.51              |
| 1:B:54:TYR:OH    | 1:B:105:SER:OG   | 2.25                     | 0.51              |
| 1:B:438:ILE:HB   | 1:B:532:PHE:CE2  | 2.45                     | 0.51              |
| 1:A:127:GLN:O    | 1:A:128:PRO:O    | 2.29                     | 0.51              |
| 1:A:380:LEU:HD13 | 1:A:410:ILE:CG2  | 2.40                     | 0.51              |
| 1:B:222:PHE:O    | 1:B:222:PHE:CD2  | 2.63                     | 0.51              |
| 1:B:514:PHE:CD2  | 1:B:517:GLU:HB2  | 2.45                     | 0.51              |
| 1:A:194:LEU:CD2  | 1:A:195:GLN:H    | 2.23                     | 0.51              |
| 1:A:237:ASP:OD1  | 1:A:238:THR:N    | 2.43                     | 0.51              |
| 1:B:204:ASN:ND2  | 1:B:560:VAL:HG11 | 2.24                     | 0.51              |
| 1:B:564:ARG:HG3  | 1:B:564:ARG:NH2  | 2.24                     | 0.51              |
| 1:A:194:LEU:HD22 | 1:A:195:GLN:N    | 2.25                     | 0.51              |
| 1:B:430:GLU:N    | 1:B:430:GLU:OE2  | 2.44                     | 0.51              |
| 1:B:40:TRP:HD1   | 1:B:43:VAL:HG21  | 1.76                     | 0.51              |
| 1:A:189:LEU:O    | 1:A:190:SER:HB2  | 2.10                     | 0.51              |
| 1:A:57:HIS:O     | 1:A:61:VAL:CG1   | 2.58                     | 0.51              |
| 1:A:74:THR:HA    | 1:A:78:PHE:HE1   | 1.76                     | 0.51              |
| 1:B:374:GLU:HB2  | 1:B:414:TYR:CE1  | 2.46                     | 0.51              |
| 1:A:462:ASN:HB3  | 1:A:475:ASP:HB2  | 1.93                     | 0.51              |
| 1:B:62:VAL:HG21  | 1:B:109:ARG:HB3  | 1.93                     | 0.51              |
| 1:B:154:MET:HG3  | 1:B:173:ILE:HG21 | 1.92                     | 0.51              |
| 1:B:515:PRO:HB3  | 1:B:545:TRP:NE1  | 2.25                     | 0.51              |
| 1:B:569:PHE:O    | 1:B:573:TYR:HB2  | 2.11                     | 0.51              |
| 1:A:138:PRO:HB2  | 1:A:140:ALA:O    | 2.11                     | 0.51              |
| 1:A:81:ARG:O     | 1:A:85:HIS:CD2   | 2.63                     | 0.51              |
| 1:A:33:GLN:HE22  | 1:B:134:THR:HG23 | 1.75                     | 0.51              |
| 1:A:32:GLN:OE1   | 1:B:138:PRO:HD3  | 2.11                     | 0.51              |
| 1:A:449:ALA:HB1  | 1:A:482:MET:CE   | 2.40                     | 0.51              |
| 1:B:116:LEU:O    | 1:B:117:THR:HG22 | 2.11                     | 0.51              |
| 1:B:312:PHE:HD2  | 1:B:384:HIS:HB3  | 1.74                     | 0.51              |
| 1:B:422:LEU:O    | 1:B:425:TRP:N    | 2.44                     | 0.51              |
| 1:B:81:ARG:CG    | 1:B:81:ARG:NH2   | 2.66                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:356:CYS:O    | 1:A:360:VAL:HG23 | 2.11                     | 0.51              |
| 1:B:280:THR:HG22 | 1:B:284:TYR:CE2  | 2.46                     | 0.51              |
| 1:B:327:THR:HG23 | 1:B:328:LEU:H    | 1.73                     | 0.51              |
| 1:A:268:VAL:HG13 | 1:A:283:LEU:HB2  | 1.93                     | 0.51              |
| 1:A:336:LYS:HB2  | 1:A:414:TYR:HB2  | 1.93                     | 0.51              |
| 1:B:382:LYS:HG3  | 1:B:408:ILE:HG12 | 1.92                     | 0.51              |
| 1:B:559:ASP:HB3  | 1:B:561:TYR:CE2  | 2.46                     | 0.51              |
| 1:B:95:ARG:HD3   | 1:B:262:PRO:O    | 2.11                     | 0.51              |
| 1:A:260:TYR:O    | 1:A:260:TYR:CD2  | 2.64                     | 0.50              |
| 1:A:53:LEU:HA    | 1:A:56:HIS:HB3   | 1.93                     | 0.50              |
| 1:B:96:PHE:CD1   | 1:B:96:PHE:C     | 2.84                     | 0.50              |
| 1:B:54:TYR:CG    | 1:B:291:LYS:HD3  | 2.46                     | 0.50              |
| 1:A:439:GLU:HG3  | 1:A:535:MET:HG3  | 1.94                     | 0.50              |
| 1:B:334:VAL:CG1  | 1:B:416:GLU:HG3  | 2.41                     | 0.50              |
| 1:B:518:PHE:O    | 1:B:522:LEU:HB2  | 2.11                     | 0.50              |
| 1:B:525:ASP:HB3  | 1:B:528:ILE:CD1  | 2.40                     | 0.50              |
| 1:B:315:ALA:HB3  | 1:B:325:VAL:CG1  | 2.41                     | 0.50              |
| 1:A:149:TRP:CD1  | 1:A:189:LEU:HG   | 2.47                     | 0.50              |
| 1:A:55:ASP:HA    | 1:A:58:VAL:HG13  | 1.93                     | 0.50              |
| 1:B:29:SER:HB3   | 1:B:260:TYR:HD1  | 1.75                     | 0.50              |
| 1:B:241:THR:N    | 1:B:245:GLU:OE1  | 2.37                     | 0.50              |
| 1:B:353:VAL:O    | 1:B:354:ARG:C    | 2.50                     | 0.50              |
| 1:B:239:CYS:HB2  | 1:B:569:PHE:HZ   | 1.77                     | 0.50              |
| 1:B:318:ILE:HB   | 1:B:461:LYS:HE2  | 1.94                     | 0.50              |
| 1:B:368:ARG:O    | 1:B:473:PHE:HB3  | 2.11                     | 0.50              |
| 1:A:414:TYR:O    | 1:A:415:ILE:HD12 | 2.11                     | 0.50              |
| 1:B:194:LEU:HD12 | 1:B:213:LEU:HA   | 1.94                     | 0.50              |
| 1:A:95:ARG:NH2   | 1:B:26:GLU:CD    | 2.65                     | 0.50              |
| 1:B:61:VAL:HG23  | 1:B:62:VAL:H     | 1.73                     | 0.50              |
| 1:B:21:TYR:O     | 1:B:24:PHE:CB    | 2.59                     | 0.50              |
| 1:A:198:ASN:OD1  | 1:A:198:ASN:O    | 2.30                     | 0.49              |
| 1:A:20:GLN:NE2   | 1:A:20:GLN:O     | 2.45                     | 0.49              |
| 1:A:375:PHE:O    | 1:A:412:HIS:HA   | 2.12                     | 0.49              |
| 1:A:519:ARG:HD3  | 1:A:540:PHE:CB   | 2.42                     | 0.49              |
| 1:B:448:LEU:HD13 | 1:B:453:ILE:HG21 | 1.94                     | 0.49              |
| 1:B:176:ILE:HD11 | 1:B:236:ILE:CD1  | 2.41                     | 0.49              |
| 1:B:275:LEU:C    | 1:B:277:GLY:N    | 2.65                     | 0.49              |
| 1:B:287:ILE:O    | 1:B:287:ILE:CG2  | 2.60                     | 0.49              |
| 1:B:366:VAL:CG1  | 1:B:366:VAL:O    | 2.59                     | 0.49              |
| 1:A:382:LYS:CB   | 1:A:406:GLU:O    | 2.58                     | 0.49              |
| 1:A:76:ALA:O     | 1:A:77:GLU:C     | 2.50                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:196:VAL:HG13 | 1:B:209:LEU:HD21 | 1.93                     | 0.49              |
| 1:B:339:LYS:HD3  | 1:B:342:PHE:HA   | 1.93                     | 0.49              |
| 1:B:376:GLU:HA   | 1:B:412:HIS:N    | 2.25                     | 0.49              |
| 1:A:107:TYR:CZ   | 1:A:120:ARG:HG3  | 2.48                     | 0.49              |
| 1:A:328:LEU:CD1  | 1:A:329:PRO:HD2  | 2.31                     | 0.49              |
| 1:B:310:GLU:OE2  | 1:B:384:HIS:CE1  | 2.66                     | 0.49              |
| 1:B:476:TYR:HB3  | 1:B:479:ILE:HD12 | 1.94                     | 0.49              |
| 1:A:157:ILE:HG22 | 1:A:169:LYS:HD2  | 1.92                     | 0.49              |
| 1:A:197:ALA:HB3  | 1:A:210:VAL:CG1  | 2.43                     | 0.49              |
| 1:A:411:ARG:O    | 1:A:412:HIS:HD2  | 1.93                     | 0.49              |
| 1:A:449:ALA:HB1  | 1:A:482:MET:HE2  | 1.93                     | 0.49              |
| 1:B:223:LEU:HD13 | 1:B:249:VAL:HG11 | 1.94                     | 0.49              |
| 1:A:470:ARG:HB3  | 1:A:470:ARG:CZ   | 2.43                     | 0.49              |
| 1:A:525:ASP:CB   | 1:A:528:ILE:HG12 | 2.39                     | 0.49              |
| 1:A:48:LYS:O     | 1:A:52:HIS:CE1   | 2.65                     | 0.49              |
| 1:A:305:LEU:HD23 | 1:A:381:GLU:OE2  | 2.12                     | 0.49              |
| 1:A:40:TRP:CD1   | 1:A:43:VAL:HB    | 2.48                     | 0.49              |
| 1:B:322:VAL:HG23 | 1:B:323:MET:N    | 2.26                     | 0.49              |
| 1:B:387:PRO:HA   | 1:B:390:MET:HB3  | 1.92                     | 0.49              |
| 1:A:7:LEU:O      | 1:A:11:GLN:HB2   | 2.13                     | 0.49              |
| 1:A:125:SER:HB2  | 1:A:129:GLU:CG   | 2.40                     | 0.49              |
| 1:A:249:VAL:HG13 | 1:A:250:PHE:HD2  | 1.78                     | 0.49              |
| 1:A:339:LYS:HD2  | 1:A:396:GLU:OE1  | 2.12                     | 0.49              |
| 1:A:355:ALA:O    | 1:A:359:LEU:HB2  | 2.13                     | 0.49              |
| 1:B:124:PHE:CD2  | 1:B:299:ARG:HD3  | 2.47                     | 0.49              |
| 1:B:539:LEU:O    | 1:B:545:TRP:NE1  | 2.43                     | 0.49              |
| 1:A:461:LYS:CD   | 1:A:461:LYS:H    | 2.24                     | 0.49              |
| 1:A:453:ILE:HG23 | 1:A:479:ILE:HD12 | 1.95                     | 0.49              |
| 1:A:165:HIS:H    | 1:A:165:HIS:CD2  | 2.30                     | 0.48              |
| 1:B:304:TYR:HB3  | 1:B:305:LEU:HD13 | 1.95                     | 0.48              |
| 1:A:338:ILE:CD1  | 1:A:338:ILE:H    | 2.24                     | 0.48              |
| 1:A:333:ARG:HA   | 1:A:418:ARG:H    | 1.79                     | 0.48              |
| 1:A:441:TYR:O    | 1:A:444:ALA:HB3  | 2.13                     | 0.48              |
| 1:B:328:LEU:HB3  | 1:B:329:PRO:HD2  | 1.96                     | 0.48              |
| 1:B:95:ARG:HH22  | 1:B:262:PRO:CB   | 2.20                     | 0.48              |
| 1:A:132:PHE:C    | 1:A:134:THR:N    | 2.66                     | 0.48              |
| 1:A:240:LEU:HD22 | 1:A:245:GLU:CB   | 2.43                     | 0.48              |
| 1:A:338:ILE:CD1  | 1:A:338:ILE:N    | 2.67                     | 0.48              |
| 1:B:168:ASN:C    | 1:B:170:SER:H    | 2.16                     | 0.48              |
| 1:B:338:ILE:HD11 | 1:B:414:TYR:CD2  | 2.46                     | 0.48              |
| 1:A:222:PHE:HE2  | 1:A:224:LEU:CD1  | 2.26                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:308:CYS:O    | 1:A:309:ASN:ND2  | 2.45                     | 0.48              |
| 1:A:336:LYS:N    | 1:A:414:TYR:O    | 2.31                     | 0.48              |
| 1:A:368:ARG:HH22 | 1:A:440:GLU:HG3  | 1.78                     | 0.48              |
| 1:A:457:ASP:OD1  | 1:A:457:ASP:C    | 2.52                     | 0.48              |
| 1:B:340:ASP:N    | 1:B:340:ASP:OD1  | 2.40                     | 0.48              |
| 1:B:47:MET:O     | 1:B:47:MET:HG3   | 2.14                     | 0.48              |
| 1:A:356:CYS:HB3  | 1:A:476:TYR:O    | 2.10                     | 0.48              |
| 1:A:68:ILE:O     | 1:A:68:ILE:HG22  | 2.14                     | 0.48              |
| 1:B:85:HIS:HA    | 1:B:88:ARG:HD3   | 1.96                     | 0.48              |
| 1:A:116:LEU:CD1  | 1:A:117:THR:H    | 2.27                     | 0.48              |
| 1:A:302:LEU:O    | 1:A:306:GLN:HB2  | 2.14                     | 0.48              |
| 1:B:438:ILE:CD1  | 1:B:531:LEU:HB3  | 2.41                     | 0.48              |
| 1:B:116:LEU:O    | 1:B:117:THR:CB   | 2.56                     | 0.48              |
| 1:B:251:GLY:O    | 1:B:254:ARG:CG   | 2.62                     | 0.48              |
| 1:A:241:THR:O    | 1:A:241:THR:HG22 | 2.13                     | 0.48              |
| 1:B:304:TYR:CE2  | 1:B:305:LEU:HD12 | 2.45                     | 0.48              |
| 1:A:189:LEU:HD21 | 1:A:190:SER:OG   | 2.13                     | 0.48              |
| 1:A:335:PHE:CB   | 1:A:413:LEU:HD11 | 2.37                     | 0.48              |
| 1:B:203:ARG:NH1  | 1:B:255:SER:O    | 2.47                     | 0.48              |
| 1:B:222:PHE:C    | 1:B:222:PHE:CD2  | 2.87                     | 0.48              |
| 1:B:538:ASP:HA   | 1:B:541:ARG:HD3  | 1.95                     | 0.48              |
| 1:A:281:ALA:HB2  | 1:A:296:GLU:HB3  | 1.95                     | 0.47              |
| 1:A:452:ASN:OD1  | 1:A:552:ILE:CG2  | 2.60                     | 0.47              |
| 1:A:450:ALA:O    | 1:A:557:VAL:CG2  | 2.63                     | 0.47              |
| 1:B:108:CYS:HB3  | 1:B:113:HIS:HD1  | 1.74                     | 0.47              |
| 1:B:16:GLY:O     | 1:B:20:GLN:HB2   | 2.14                     | 0.47              |
| 1:B:7:LEU:HD22   | 1:B:8:LEU:N      | 2.28                     | 0.47              |
| 1:A:25:LEU:HB2   | 1:A:260:TYR:CE1  | 2.49                     | 0.47              |
| 1:A:447:GLN:NE2  | 5:A:580:HOH:O    | 2.47                     | 0.47              |
| 1:B:327:THR:HG21 | 1:B:418:ARG:HD3  | 1.96                     | 0.47              |
| 1:A:97:GLU:HG2   | 1:A:98:ILE:N     | 2.30                     | 0.47              |
| 1:B:375:PHE:CE2  | 1:B:415:ILE:HD12 | 2.49                     | 0.47              |
| 1:A:25:LEU:HD13  | 5:B:603:HOH:O    | 2.14                     | 0.47              |
| 1:A:305:LEU:HD22 | 1:A:306:GLN:N    | 2.29                     | 0.47              |
| 1:B:122:PHE:HB3  | 1:B:127:GLN:HB2  | 1.96                     | 0.47              |
| 1:B:145:PRO:HB3  | 1:B:149:TRP:CD1  | 2.49                     | 0.47              |
| 1:B:259:VAL:HG11 | 1:B:267:LEU:HD21 | 1.95                     | 0.47              |
| 1:B:420:VAL:CG2  | 1:B:425:TRP:HD1  | 2.28                     | 0.47              |
| 1:A:100:GLU:O    | 1:A:103:PHE:HB3  | 2.15                     | 0.47              |
| 1:A:156:VAL:O    | 1:A:160:LEU:HG   | 2.13                     | 0.47              |
| 1:A:255:SER:CA   | 1:A:365:ARG:NH2  | 2.76                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:460:PHE:HZ   | 1:A:522:LEU:O    | 1.98                     | 0.47              |
| 1:B:215:THR:C    | 1:B:217:SER:N    | 2.66                     | 0.47              |
| 1:A:65:LEU:HD22  | 1:A:110:LEU:HD11 | 1.97                     | 0.47              |
| 1:A:462:ASN:ND2  | 1:A:475:ASP:OD2  | 2.48                     | 0.47              |
| 1:A:488:ARG:HD2  | 1:A:546:ARG:HH22 | 1.79                     | 0.47              |
| 1:A:544:TYR:CE2  | 1:A:548:LEU:HD11 | 2.49                     | 0.47              |
| 1:B:90:LEU:N     | 1:B:91:PRO:CD    | 2.74                     | 0.47              |
| 1:A:189:LEU:HD23 | 1:A:190:SER:CB   | 2.44                     | 0.47              |
| 1:B:259:VAL:CG1  | 1:B:267:LEU:HD21 | 2.45                     | 0.47              |
| 1:B:290:GLN:O    | 1:B:294:LYS:N    | 2.41                     | 0.47              |
| 1:B:378:PHE:HE2  | 1:B:380:LEU:HD21 | 1.80                     | 0.47              |
| 1:B:539:LEU:HD23 | 1:B:539:LEU:O    | 2.15                     | 0.47              |
| 1:B:90:LEU:HD21  | 1:B:99:ALA:CB    | 2.45                     | 0.47              |
| 1:A:304:TYR:CD2  | 1:A:328:LEU:HD23 | 2.49                     | 0.47              |
| 1:B:58:VAL:HG23  | 1:B:59:GLY:N     | 2.30                     | 0.47              |
| 1:A:557:VAL:O    | 1:A:557:VAL:HG12 | 2.15                     | 0.47              |
| 1:A:32:GLN:NE2   | 1:B:138:PRO:HD3  | 2.30                     | 0.47              |
| 1:A:326:PHE:HE2  | 1:A:337:VAL:HG21 | 1.80                     | 0.46              |
| 1:A:422:LEU:HD13 | 1:A:471:VAL:HG13 | 1.97                     | 0.46              |
| 1:B:137:ARG:CB   | 1:B:138:PRO:CD   | 2.89                     | 0.46              |
| 1:B:203:ARG:HH22 | 1:B:254:ARG:HG3  | 1.80                     | 0.46              |
| 1:B:246:ALA:HA   | 1:B:249:VAL:CG1  | 2.45                     | 0.46              |
| 1:B:380:LEU:CD1  | 1:B:410:ILE:HD11 | 2.45                     | 0.46              |
| 1:B:376:GLU:CA   | 1:B:412:HIS:H    | 2.24                     | 0.46              |
| 1:A:145:PRO:HB3  | 1:A:148:GLY:HA2  | 1.96                     | 0.46              |
| 1:A:430:GLU:HG3  | 1:A:431:GLY:N    | 2.30                     | 0.46              |
| 1:A:84:GLU:HG3   | 1:A:85:HIS:N     | 2.27                     | 0.46              |
| 1:B:189:LEU:C    | 1:B:189:LEU:HD23 | 2.36                     | 0.46              |
| 1:B:257:PHE:CB   | 1:B:286:ALA:O    | 2.46                     | 0.46              |
| 1:A:480:CYS:HB2  | 1:A:484:GLU:OE1  | 2.16                     | 0.46              |
| 1:A:5:LEU:O      | 1:A:9:ILE:HG13   | 2.16                     | 0.46              |
| 1:A:86:TYR:CD2   | 1:A:90:LEU:HD11  | 2.50                     | 0.46              |
| 1:B:173:ILE:N    | 5:B:601:HOH:O    | 2.48                     | 0.46              |
| 1:B:271:LEU:O    | 1:B:274:ILE:HG23 | 2.14                     | 0.46              |
| 1:B:295:THR:O    | 1:B:298:TYR:N    | 2.46                     | 0.46              |
| 1:A:228:GLN:HG2  | 1:A:229:THR:N    | 2.29                     | 0.46              |
| 1:A:448:LEU:O    | 1:A:451:ALA:O    | 2.32                     | 0.46              |
| 1:A:441:TYR:OH   | 1:A:458:MET:O    | 2.30                     | 0.46              |
| 1:B:368:ARG:C    | 1:B:369:MET:HG2  | 2.35                     | 0.46              |
| 1:A:163:ARG:HD2  | 1:A:163:ARG:HA   | 1.66                     | 0.46              |
| 1:A:304:TYR:CD2  | 1:A:328:LEU:CD2  | 2.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:334:VAL:HB   | 1:B:418:ARG:CB   | 2.45                     | 0.46              |
| 1:A:160:LEU:C    | 1:A:162:LEU:H    | 2.19                     | 0.46              |
| 1:A:412:HIS:CG   | 1:A:412:HIS:O    | 2.69                     | 0.46              |
| 1:A:458:MET:HB2  | 5:A:601:HOH:O    | 2.14                     | 0.46              |
| 1:A:516:GLU:C    | 1:A:518:PHE:N    | 2.69                     | 0.46              |
| 1:B:149:TRP:HH2  | 1:B:194:LEU:HD13 | 1.80                     | 0.46              |
| 1:B:304:TYR:C    | 1:B:304:TYR:CD2  | 2.89                     | 0.46              |
| 1:A:101:SER:C    | 1:A:104:ASN:HD22 | 2.18                     | 0.46              |
| 1:A:151:SER:O    | 1:A:154:MET:CB   | 2.62                     | 0.46              |
| 1:A:438:ILE:CD1  | 1:A:531:LEU:HD23 | 2.45                     | 0.46              |
| 1:B:204:ASN:HD22 | 1:B:560:VAL:CG1  | 2.28                     | 0.46              |
| 1:B:290:GLN:O    | 1:B:293:ALA:HB3  | 2.15                     | 0.46              |
| 1:A:365:ARG:O    | 1:A:366:VAL:HB   | 2.15                     | 0.46              |
| 1:A:401:ILE:HA   | 1:A:409:VAL:O    | 2.15                     | 0.46              |
| 1:A:552:ILE:HA   | 1:A:556:HIS:O    | 2.16                     | 0.46              |
| 1:B:402:THR:O    | 1:B:408:ILE:HG22 | 2.16                     | 0.46              |
| 1:B:450:ALA:HB1  | 1:B:558:GLU:CD   | 2.36                     | 0.46              |
| 1:B:78:PHE:HD1   | 1:B:81:ARG:NH2   | 2.13                     | 0.46              |
| 1:A:208:TRP:CE3  | 1:A:225:PRO:HG3  | 2.51                     | 0.46              |
| 1:B:173:ILE:HG13 | 1:B:174:HIS:N    | 2.31                     | 0.46              |
| 1:B:334:VAL:HG12 | 1:B:416:GLU:HG3  | 1.96                     | 0.46              |
| 1:B:72:GLN:H     | 1:B:72:GLN:HG3   | 1.34                     | 0.46              |
| 1:A:114:ARG:C    | 1:A:114:ARG:HD3  | 2.36                     | 0.46              |
| 1:A:86:TYR:O     | 1:A:90:LEU:HD11  | 2.16                     | 0.46              |
| 1:B:299:ARG:HD2  | 1:B:299:ARG:HA   | 1.32                     | 0.46              |
| 1:B:434:LEU:O    | 1:B:438:ILE:CG2  | 2.33                     | 0.46              |
| 1:B:450:ALA:HB1  | 1:B:558:GLU:HB2  | 1.98                     | 0.46              |
| 1:A:228:GLN:OE1  | 1:A:231:ASP:HA   | 2.16                     | 0.45              |
| 1:A:481:TYR:HB2  | 1:A:484:GLU:HG3  | 1.97                     | 0.45              |
| 1:B:458:MET:O    | 1:B:458:MET:HG3  | 2.16                     | 0.45              |
| 1:B:301:TYR:O    | 1:B:305:LEU:HD22 | 2.15                     | 0.45              |
| 1:B:323:MET:CG   | 1:B:338:ILE:HA   | 2.44                     | 0.45              |
| 1:B:33:GLN:O     | 1:B:33:GLN:HG3   | 2.16                     | 0.45              |
| 1:A:488:ARG:HB2  | 1:A:546:ARG:NH2  | 2.30                     | 0.45              |
| 1:B:376:GLU:OE2  | 1:B:411:ARG:NH2  | 2.48                     | 0.45              |
| 1:B:454:PHE:HD1  | 1:B:482:MET:HE2  | 1.81                     | 0.45              |
| 1:A:134:THR:OG1  | 1:A:134:THR:O    | 2.29                     | 0.45              |
| 1:A:153:LEU:O    | 1:A:156:VAL:HG22 | 2.16                     | 0.45              |
| 1:A:227:HIS:O    | 1:A:234:LEU:CB   | 2.62                     | 0.45              |
| 1:A:337:VAL:HG22 | 1:A:413:LEU:CD1  | 2.45                     | 0.45              |
| 1:A:78:PHE:C     | 1:A:80:LEU:N     | 2.68                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:66:ARG:O     | 1:B:69:THR:O     | 2.33                     | 0.45              |
| 1:A:245:GLU:OE1  | 1:A:245:GLU:HA   | 2.17                     | 0.45              |
| 1:A:464:GLY:O    | 1:A:471:VAL:HA   | 2.16                     | 0.45              |
| 1:A:568:ARG:HG3  | 1:A:571:VAL:HG12 | 1.98                     | 0.45              |
| 1:A:90:LEU:N     | 1:A:91:PRO:CD    | 2.78                     | 0.45              |
| 1:A:222:PHE:CD2  | 1:A:222:PHE:C    | 2.90                     | 0.45              |
| 1:B:312:PHE:N    | 1:B:384:HIS:O    | 2.38                     | 0.45              |
| 1:B:75:ASP:O     | 1:B:79:LEU:HB2   | 2.16                     | 0.45              |
| 1:A:366:VAL:O    | 1:A:366:VAL:CG1  | 2.64                     | 0.45              |
| 1:A:57:HIS:O     | 1:A:61:VAL:HG13  | 2.17                     | 0.45              |
| 1:B:125:SER:HA   | 1:B:296:GLU:CG   | 2.47                     | 0.45              |
| 1:B:274:ILE:CG1  | 1:B:275:LEU:H    | 2.25                     | 0.45              |
| 1:B:37:GLN:O     | 1:B:38:ALA:HB3   | 2.17                     | 0.45              |
| 1:A:173:ILE:HG13 | 1:A:174:HIS:N    | 2.32                     | 0.45              |
| 1:B:310:GLU:OE2  | 1:B:384:HIS:ND1  | 2.49                     | 0.45              |
| 1:A:203:ARG:HB2  | 1:A:257:PHE:CE1  | 2.52                     | 0.45              |
| 1:A:430:GLU:HG3  | 1:A:431:GLY:H    | 1.82                     | 0.45              |
| 1:A:357:TYR:CD1  | 1:A:476:TYR:HD2  | 2.35                     | 0.45              |
| 1:A:47:MET:O     | 1:A:50:ARG:N     | 2.48                     | 0.45              |
| 1:A:13:ILE:HA    | 1:A:61:VAL:HG21  | 1.98                     | 0.45              |
| 1:A:126:SER:O    | 1:A:127:GLN:CB   | 2.63                     | 0.45              |
| 1:B:466:THR:CG2  | 1:B:467:ARG:N    | 2.79                     | 0.45              |
| 1:B:420:VAL:O    | 1:B:465:VAL:N    | 2.40                     | 0.44              |
| 1:B:481:TYR:C    | 1:B:483:THR:H    | 2.21                     | 0.44              |
| 1:A:36:GLU:HA    | 1:A:164:LEU:HD11 | 1.98                     | 0.44              |
| 1:A:296:GLU:O    | 1:A:300:GLU:HG3  | 2.17                     | 0.44              |
| 1:B:382:LYS:NZ   | 1:B:403:ASP:CG   | 2.54                     | 0.44              |
| 1:A:234:LEU:O    | 1:A:234:LEU:HD22 | 2.16                     | 0.44              |
| 1:A:371:ASP:OD2  | 1:A:372:THR:N    | 2.51                     | 0.44              |
| 1:A:47:MET:CG    | 1:A:48:LYS:N     | 2.77                     | 0.44              |
| 1:B:162:LEU:H    | 1:B:162:LEU:HD22 | 1.81                     | 0.44              |
| 1:B:226:ILE:CG2  | 1:B:234:LEU:HD22 | 2.47                     | 0.44              |
| 1:B:544:TYR:O    | 1:B:548:LEU:CB   | 2.64                     | 0.44              |
| 1:A:103:PHE:C    | 1:A:103:PHE:CD2  | 2.91                     | 0.44              |
| 1:A:153:LEU:HD11 | 1:A:224:LEU:HD11 | 2.00                     | 0.44              |
| 1:A:301:TYR:HA   | 1:A:331:PHE:CZ   | 2.51                     | 0.44              |
| 1:A:368:ARG:HB2  | 1:A:448:LEU:HD13 | 2.00                     | 0.44              |
| 1:B:196:VAL:CG1  | 1:B:209:LEU:HD21 | 2.48                     | 0.44              |
| 1:B:338:ILE:CG1  | 1:B:353:VAL:HG21 | 2.35                     | 0.44              |
| 1:A:139:LEU:O    | 1:A:139:LEU:HD23 | 2.18                     | 0.44              |
| 1:A:100:GLU:O    | 1:A:104:ASN:ND2  | 2.51                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:116:LEU:HD12 | 1:A:117:THR:N    | 2.32                     | 0.44              |
| 1:A:135:ILE:HG22 | 1:A:137:ARG:O    | 2.16                     | 0.44              |
| 1:A:255:SER:N    | 1:A:365:ARG:NH2  | 2.66                     | 0.44              |
| 1:B:87:THR:HG22  | 1:B:122:PHE:HE1  | 1.80                     | 0.44              |
| 1:B:298:TYR:HA   | 1:B:301:TYR:HB3  | 1.99                     | 0.44              |
| 1:B:565:ARG:O    | 1:B:567:GLN:N    | 2.51                     | 0.44              |
| 1:A:127:GLN:O    | 1:A:127:GLN:HG3  | 2.17                     | 0.44              |
| 1:B:152:LEU:N    | 1:B:152:LEU:CD2  | 2.79                     | 0.44              |
| 1:B:375:PHE:O    | 1:B:413:LEU:N    | 2.50                     | 0.44              |
| 1:B:387:PRO:HA   | 1:B:390:MET:H    | 1.83                     | 0.44              |
| 1:A:153:LEU:HD22 | 1:A:176:ILE:HG21 | 1.99                     | 0.44              |
| 1:A:17:PHE:CG    | 1:A:18:ASP:N     | 2.85                     | 0.44              |
| 1:A:474:TYR:OH   | 2:A:1762:ADP:H2' | 2.18                     | 0.44              |
| 1:B:80:LEU:CD1   | 1:B:119:GLU:O    | 2.66                     | 0.44              |
| 1:B:164:LEU:CD1  | 1:B:228:GLN:HE22 | 2.31                     | 0.44              |
| 1:B:290:GLN:HB3  | 1:B:290:GLN:HE21 | 1.46                     | 0.44              |
| 1:B:323:MET:HE3  | 1:B:323:MET:HB2  | 1.95                     | 0.44              |
| 1:A:155:ARG:C    | 1:A:159:ASP:OD2  | 2.52                     | 0.44              |
| 1:A:394:LEU:HD23 | 1:A:401:ILE:HD11 | 2.00                     | 0.44              |
| 1:B:121:LEU:C    | 1:B:121:LEU:HD12 | 2.38                     | 0.44              |
| 1:B:152:LEU:HD22 | 1:B:152:LEU:H    | 1.82                     | 0.44              |
| 1:B:32:GLN:O     | 1:B:36:GLU:HB2   | 2.18                     | 0.44              |
| 1:B:564:ARG:CG   | 1:B:564:ARG:HH21 | 2.25                     | 0.44              |
| 1:B:565:ARG:C    | 1:B:567:GLN:N    | 2.71                     | 0.44              |
| 1:B:454:PHE:HA   | 1:B:455:PRO:HD3  | 1.87                     | 0.43              |
| 1:B:5:LEU:HB2    | 1:B:78:PHE:CZ    | 2.53                     | 0.43              |
| 1:A:309:ASN:HA   | 1:A:310:GLU:HA   | 1.86                     | 0.43              |
| 1:A:361:LYS:HZ3  | 1:A:372:THR:HG1  | 1.58                     | 0.43              |
| 1:A:255:SER:N    | 1:A:365:ARG:HH21 | 2.17                     | 0.43              |
| 1:A:23:ARG:HE    | 1:A:53:LEU:HD11  | 1.83                     | 0.43              |
| 1:B:297:SER:HA   | 1:B:300:GLU:HG3  | 2.01                     | 0.43              |
| 1:A:458:MET:HE3  | 5:A:601:HOH:O    | 2.17                     | 0.43              |
| 1:A:23:ARG:CD    | 1:A:53:LEU:HD21  | 2.48                     | 0.43              |
| 1:B:246:ALA:HA   | 1:B:249:VAL:HG13 | 2.00                     | 0.43              |
| 1:B:274:ILE:CG1  | 1:B:275:LEU:N    | 2.80                     | 0.43              |
| 1:B:5:LEU:HA     | 1:B:8:LEU:HB3    | 2.00                     | 0.43              |
| 1:B:305:LEU:N    | 1:B:305:LEU:CD1  | 2.80                     | 0.43              |
| 1:B:370:ALA:N    | 1:B:476:TYR:HH   | 2.14                     | 0.43              |
| 1:B:430:GLU:N    | 1:B:430:GLU:CD   | 2.72                     | 0.43              |
| 1:B:288:GLY:O    | 1:B:290:GLN:N    | 2.42                     | 0.43              |
| 1:A:172:ASP:HA   | 1:A:175:TYR:HD2  | 1.84                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:256:TYR:HB3  | 1:A:286:ALA:O    | 2.19                     | 0.43              |
| 1:A:432:GLN:HB3  | 5:A:607:HOH:O    | 2.18                     | 0.43              |
| 1:A:513:VAL:O    | 1:A:515:PRO:HD3  | 2.19                     | 0.43              |
| 1:B:438:ILE:HB   | 1:B:532:PHE:CZ   | 2.53                     | 0.43              |
| 1:A:18:ASP:HB3   | 1:B:19:ALA:HA    | 1.99                     | 0.43              |
| 1:A:371:ASP:OD2  | 1:A:372:THR:O    | 2.36                     | 0.43              |
| 1:A:81:ARG:O     | 1:A:85:HIS:HB2   | 2.19                     | 0.43              |
| 1:B:204:ASN:ND2  | 1:B:560:VAL:CG1  | 2.82                     | 0.43              |
| 1:A:32:GLN:HE22  | 1:B:138:PRO:HD3  | 1.83                     | 0.43              |
| 1:A:113:HIS:CG   | 1:A:376:GLU:HB3  | 2.53                     | 0.43              |
| 1:A:490:ILE:HG23 | 1:A:491:PRO:HD3  | 2.00                     | 0.43              |
| 1:B:448:LEU:HD11 | 1:B:473:PHE:CD2  | 2.53                     | 0.43              |
| 1:B:434:LEU:HD11 | 1:B:528:ILE:HG23 | 2.00                     | 0.43              |
| 1:A:116:LEU:O    | 1:A:120:ARG:HB3  | 2.19                     | 0.43              |
| 1:A:193:HIS:CE1  | 1:A:214:ILE:HG21 | 2.50                     | 0.43              |
| 1:A:253:ALA:O    | 1:A:367:GLY:N    | 2.50                     | 0.43              |
| 1:A:385:ILE:HG22 | 1:A:386:SER:O    | 2.19                     | 0.43              |
| 1:B:123:ILE:O    | 1:B:123:ILE:HG23 | 2.19                     | 0.43              |
| 1:B:441:TYR:C    | 1:B:441:TYR:CD2  | 2.91                     | 0.43              |
| 1:B:49:ASN:O     | 1:B:52:HIS:HB2   | 2.19                     | 0.43              |
| 1:A:170:SER:HA   | 1:A:173:ILE:HG12 | 1.99                     | 0.43              |
| 1:A:202:TYR:O    | 1:A:257:PHE:CD1  | 2.67                     | 0.43              |
| 1:A:301:TYR:HD1  | 1:A:331:PHE:HE2  | 1.67                     | 0.43              |
| 1:B:382:LYS:CE   | 1:B:403:ASP:OD1  | 2.64                     | 0.43              |
| 1:B:564:ARG:CG   | 1:B:564:ARG:NH2  | 2.82                     | 0.43              |
| 1:A:139:LEU:O    | 1:A:139:LEU:CD2  | 2.68                     | 0.42              |
| 1:A:211:GLY:HA2  | 1:A:270:TRP:HH2  | 1.84                     | 0.42              |
| 1:A:23:ARG:HD3   | 1:A:53:LEU:HD21  | 2.01                     | 0.42              |
| 1:A:397:ALA:HB1  | 1:A:400:LYS:HB2  | 2.00                     | 0.42              |
| 1:A:408:ILE:O    | 1:A:408:ILE:CG1  | 2.67                     | 0.42              |
| 1:A:368:ARG:NH2  | 1:A:440:GLU:HG3  | 2.33                     | 0.42              |
| 1:A:535:MET:HE3  | 1:A:535:MET:O    | 2.18                     | 0.42              |
| 1:B:139:LEU:O    | 1:B:198:ASN:OD1  | 2.36                     | 0.42              |
| 1:B:149:TRP:HZ2  | 1:B:192:SER:O    | 2.01                     | 0.42              |
| 1:A:193:HIS:CD2  | 1:A:214:ILE:CG2  | 2.93                     | 0.42              |
| 1:B:101:SER:C    | 1:B:104:ASN:HD22 | 2.22                     | 0.42              |
| 1:A:112:ASP:O    | 1:A:113:HIS:C    | 2.57                     | 0.42              |
| 1:A:175:TYR:HB3  | 1:A:569:PHE:CZ   | 2.53                     | 0.42              |
| 1:A:197:ALA:HB3  | 1:A:210:VAL:HG13 | 2.01                     | 0.42              |
| 1:B:301:TYR:O    | 1:B:305:LEU:CD2  | 2.67                     | 0.42              |
| 1:B:331:PHE:CE2  | 1:B:333:ARG:HG2  | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:363:HIS:CE1  | 1:B:451:ALA:O    | 2.71                     | 0.42              |
| 1:B:9:ILE:HG13   | 1:B:65:LEU:HD21  | 2.02                     | 0.42              |
| 1:A:549:GLN:HG3  | 1:A:553:ARG:HE   | 1.83                     | 0.42              |
| 1:B:422:LEU:O    | 1:B:423:ASN:C    | 2.57                     | 0.42              |
| 1:A:79:LEU:HD11  | 1:A:111:PHE:CZ   | 2.55                     | 0.42              |
| 1:A:311:GLN:HB3  | 1:A:384:HIS:O    | 2.19                     | 0.42              |
| 1:A:440:GLU:O    | 1:A:444:ALA:HB2  | 2.20                     | 0.42              |
| 1:B:543:ASP:O    | 1:B:547:ALA:HB3  | 2.19                     | 0.42              |
| 1:A:116:LEU:HB3  | 1:A:120:ARG:NH1  | 2.34                     | 0.42              |
| 1:A:143:PHE:N    | 1:A:194:LEU:O    | 2.53                     | 0.42              |
| 1:A:221:PRO:O    | 1:A:241:THR:CG2  | 2.60                     | 0.42              |
| 1:A:221:PRO:HD2  | 1:A:241:THR:O    | 2.19                     | 0.42              |
| 1:A:334:VAL:HG22 | 1:A:418:ARG:HA   | 2.01                     | 0.42              |
| 1:A:465:VAL:HG12 | 1:A:466:THR:N    | 2.34                     | 0.42              |
| 1:B:143:PHE:N    | 1:B:143:PHE:CD2  | 2.88                     | 0.42              |
| 1:B:448:LEU:O    | 1:B:453:ILE:N    | 2.51                     | 0.42              |
| 1:B:442:GLY:CA   | 1:B:536:HIS:CD2  | 2.88                     | 0.42              |
| 1:B:450:ALA:HB3  | 1:B:558:GLU:HG2  | 1.98                     | 0.42              |
| 1:A:157:ILE:HG21 | 1:A:169:LYS:HG3  | 2.02                     | 0.42              |
| 1:A:488:ARG:O    | 1:A:514:PHE:HD1  | 1.95                     | 0.42              |
| 1:B:89:LEU:C     | 1:B:91:PRO:CD    | 2.84                     | 0.42              |
| 1:A:489:ASP:CB   | 1:A:514:PHE:CD1  | 3.02                     | 0.42              |
| 1:B:121:LEU:O    | 1:B:121:LEU:HD12 | 2.20                     | 0.42              |
| 1:B:226:ILE:HG22 | 1:B:234:LEU:HD22 | 2.02                     | 0.42              |
| 1:B:459:LEU:O    | 1:B:463:PHE:HD2  | 2.03                     | 0.42              |
| 1:A:200:LEU:HD21 | 1:A:208:TRP:H    | 1.85                     | 0.41              |
| 1:A:32:GLN:HG3   | 1:A:202:TYR:OH   | 2.20                     | 0.41              |
| 1:B:403:ASP:O    | 1:B:404:LEU:HD23 | 2.19                     | 0.41              |
| 1:B:48:LYS:HE2   | 1:B:362:GLU:CG   | 2.49                     | 0.41              |
| 1:A:80:LEU:CD2   | 1:A:119:GLU:O    | 2.68                     | 0.41              |
| 1:A:196:VAL:HG13 | 1:A:209:LEU:HD23 | 2.02                     | 0.41              |
| 1:A:315:ALA:HB3  | 1:A:325:VAL:CG1  | 2.50                     | 0.41              |
| 1:A:379:VAL:O    | 1:A:379:VAL:HG13 | 2.21                     | 0.41              |
| 1:A:325:VAL:CG1  | 2:A:1762:ADP:O4' | 2.61                     | 0.41              |
| 1:A:358:GLN:C    | 1:A:360:VAL:N    | 2.72                     | 0.41              |
| 1:A:390:MET:O    | 1:A:394:LEU:N    | 2.35                     | 0.41              |
| 1:B:168:ASN:C    | 1:B:170:SER:N    | 2.73                     | 0.41              |
| 1:B:285:MET:HB2  | 1:B:285:MET:HE3  | 1.95                     | 0.41              |
| 1:B:32:GLN:O     | 1:B:36:GLU:CB    | 2.68                     | 0.41              |
| 1:B:466:THR:HG23 | 1:B:467:ARG:N    | 2.34                     | 0.41              |
| 1:A:79:LEU:HD11  | 1:A:111:PHE:CE1  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:564:ARG:C    | 1:A:566:ARG:H    | 2.23                     | 0.41              |
| 1:B:318:ILE:O    | 1:B:319:ARG:C    | 2.59                     | 0.41              |
| 1:B:354:ARG:HA   | 1:B:354:ARG:HD3  | 1.79                     | 0.41              |
| 1:B:368:ARG:O    | 1:B:369:MET:HG2  | 2.19                     | 0.41              |
| 1:B:514:PHE:CD2  | 1:B:517:GLU:OE2  | 2.73                     | 0.41              |
| 1:A:157:ILE:CG2  | 1:A:169:LYS:CD   | 2.96                     | 0.41              |
| 1:A:113:HIS:O    | 1:A:377:ASN:HB2  | 2.20                     | 0.41              |
| 1:A:54:TYR:OH    | 1:A:102:PHE:HA   | 2.20                     | 0.41              |
| 1:A:69:THR:O     | 1:A:73:SER:HB2   | 2.21                     | 0.41              |
| 1:B:280:THR:HG22 | 1:B:284:TYR:HE2  | 1.85                     | 0.41              |
| 1:B:432:GLN:O    | 1:B:436:ASP:N    | 2.34                     | 0.41              |
| 1:B:93:TYR:CB    | 1:B:96:PHE:HB3   | 2.48                     | 0.41              |
| 1:A:355:ALA:O    | 1:A:359:LEU:CB   | 2.68                     | 0.41              |
| 1:A:362:GLU:HG2  | 1:A:362:GLU:H    | 1.73                     | 0.41              |
| 1:A:334:VAL:HG23 | 1:A:416:GLU:O    | 2.20                     | 0.41              |
| 1:B:340:ASP:OD1  | 1:B:396:GLU:O    | 2.37                     | 0.41              |
| 1:B:525:ASP:CB   | 1:B:528:ILE:CD1  | 2.99                     | 0.41              |
| 1:B:68:ILE:CG1   | 1:B:69:THR:H     | 2.26                     | 0.41              |
| 1:B:78:PHE:CD1   | 1:B:81:ARG:NH2   | 2.88                     | 0.41              |
| 1:A:222:PHE:CE2  | 1:A:224:LEU:CD1  | 3.03                     | 0.41              |
| 1:A:438:ILE:O    | 1:A:441:TYR:HB3  | 2.21                     | 0.41              |
| 1:B:525:ASP:CG   | 1:B:528:ILE:HD12 | 2.40                     | 0.41              |
| 1:B:549:GLN:C    | 1:B:551:ARG:N    | 2.74                     | 0.41              |
| 1:A:157:ILE:HG21 | 1:A:169:LYS:CD   | 2.51                     | 0.41              |
| 1:A:509:SER:N    | 1:A:510:PRO:HD3  | 2.33                     | 0.41              |
| 1:B:116:LEU:H    | 1:B:116:LEU:HG   | 1.64                     | 0.41              |
| 1:B:253:ALA:O    | 1:B:365:ARG:HB3  | 2.21                     | 0.41              |
| 1:B:541:ARG:HH22 | 1:B:544:TYR:CB   | 2.26                     | 0.41              |
| 1:B:565:ARG:C    | 1:B:567:GLN:H    | 2.24                     | 0.41              |
| 1:A:166:TRP:O    | 1:A:167:GLN:OE1  | 2.38                     | 0.41              |
| 1:A:198:ASN:HA   | 1:A:199:GLU:HA   | 1.71                     | 0.41              |
| 1:A:204:ASN:C    | 1:A:206:ALA:H    | 2.24                     | 0.41              |
| 1:A:204:ASN:HB3  | 1:A:205:LYS:H    | 1.53                     | 0.41              |
| 1:B:58:VAL:HG11  | 1:B:105:SER:HB2  | 2.03                     | 0.41              |
| 1:A:305:LEU:C    | 1:A:307:GLY:H    | 2.24                     | 0.41              |
| 1:A:389:LEU:O    | 1:A:392:LEU:HD23 | 2.21                     | 0.41              |
| 1:B:57:HIS:O     | 1:B:61:VAL:HG13  | 2.21                     | 0.41              |
| 1:B:68:ILE:CG1   | 1:B:69:THR:N     | 2.79                     | 0.41              |
| 1:A:107:TYR:OH   | 1:A:120:ARG:CG   | 2.69                     | 0.40              |
| 1:A:9:ILE:O      | 1:A:12:THR:HB    | 2.22                     | 0.40              |
| 1:A:134:THR:H    | 1:A:134:THR:HG23 | 1.51                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:143:PHE:O    | 1:A:194:LEU:O    | 2.39                     | 0.40              |
| 1:A:234:LEU:H    | 1:A:234:LEU:HD13 | 1.87                     | 0.40              |
| 1:A:240:LEU:HD22 | 1:A:245:GLU:HB3  | 2.03                     | 0.40              |
| 1:A:161:PRO:CB   | 1:B:138:PRO:HB3  | 2.49                     | 0.40              |
| 1:B:529:GLY:O    | 1:B:532:PHE:CB   | 2.66                     | 0.40              |
| 1:B:559:ASP:HB3  | 1:B:561:TYR:HE2  | 1.86                     | 0.40              |
| 1:A:250:PHE:CB   | 1:A:275:LEU:HD21 | 2.51                     | 0.40              |
| 1:A:474:TYR:CD1  | 1:A:474:TYR:C    | 2.95                     | 0.40              |
| 1:B:200:LEU:HB3  | 1:B:208:TRP:O    | 2.21                     | 0.40              |
| 1:B:24:PHE:CE1   | 1:B:50:ARG:HG2   | 2.56                     | 0.40              |
| 1:B:271:LEU:HB2  | 1:B:283:LEU:HD11 | 2.02                     | 0.40              |
| 1:B:34:ARG:HA    | 1:B:34:ARG:HD2   | 1.93                     | 0.40              |
| 1:B:334:VAL:HG12 | 1:B:416:GLU:O    | 2.21                     | 0.40              |
| 1:A:172:ASP:OD1  | 1:A:236:ILE:HB   | 2.21                     | 0.40              |
| 1:B:155:ARG:HA   | 1:B:155:ARG:HD3  | 1.91                     | 0.40              |
| 1:B:203:ARG:NH2  | 1:B:254:ARG:CG   | 2.83                     | 0.40              |
| 1:B:425:TRP:CZ3  | 1:B:429:VAL:HG21 | 2.56                     | 0.40              |
| 1:B:433:GLN:CA   | 1:B:433:GLN:OE1  | 2.68                     | 0.40              |
| 1:A:229:THR:HB   | 1:A:233:GLU:CG   | 2.50                     | 0.40              |
| 1:A:305:LEU:CD1  | 1:A:305:LEU:N    | 2.72                     | 0.40              |
| 1:A:48:LYS:CG    | 1:A:362:GLU:HB2  | 2.45                     | 0.40              |
| 1:A:516:GLU:O    | 1:A:517:GLU:C    | 2.60                     | 0.40              |
| 1:B:101:SER:HA   | 1:B:104:ASN:HD22 | 1.85                     | 0.40              |
| 1:B:126:SER:O    | 1:B:127:GLN:C    | 2.58                     | 0.40              |
| 1:B:195:GLN:HB2  | 1:B:214:ILE:HD11 | 2.04                     | 0.40              |
| 1:A:107:TYR:OH   | 1:A:120:ARG:HG3  | 2.21                     | 0.40              |
| 1:A:220:LEU:HG   | 1:A:221:PRO:HD2  | 1.99                     | 0.40              |
| 1:A:226:ILE:HG23 | 1:A:236:ILE:HG12 | 2.02                     | 0.40              |

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:423:ASN:ND2 | 1:B:427:GLU:CD[2_455]  | 1.48                     | 0.72              |
| 1:A:423:ASN:CG  | 1:B:427:GLU:OE2[2_455] | 1.55                     | 0.65              |
| 1:A:423:ASN:ND2 | 1:B:427:GLU:OE1[2_455] | 1.74                     | 0.46              |
| 1:A:423:ASN:ND2 | 1:B:427:GLU:OE2[2_455] | 1.98                     | 0.22              |
| 1:A:423:ASN:CG  | 1:B:427:GLU:CD[2_455]  | 2.01                     | 0.19              |
| 1:A:423:ASN:OD1 | 1:B:427:GLU:OE2[2_455] | 2.09                     | 0.11              |
| 1:A:423:ASN:CB  | 1:B:427:GLU:OE2[2_455] | 2.13                     | 0.07              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|-----------|-----------|----------|-------------|----|
| 1   | A     | 541/578 (94%)   | 470 (87%) | 65 (12%)  | 6 (1%)   | 17          | 54 |
| 1   | B     | 529/578 (92%)   | 457 (86%) | 68 (13%)  | 4 (1%)   | 22          | 62 |
| All | All   | 1070/1156 (93%) | 927 (87%) | 133 (12%) | 10 (1%)  | 20          | 60 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 127 | GLN  |
| 1   | A     | 232 | GLY  |
| 1   | A     | 366 | VAL  |
| 1   | A     | 511 | GLY  |
| 1   | B     | 118 | PRO  |
| 1   | B     | 566 | ARG  |
| 1   | A     | 264 | PRO  |
| 1   | A     | 351 | ALA  |
| 1   | B     | 90  | LEU  |
| 1   | B     | 216 | 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     | 480/508 (94%)  | 382 (80%) | 98 (20%)  | 1           | 6 |
| 1   | B     | 472/508 (93%)  | 360 (76%) | 112 (24%) | 1           | 3 |
| All | All   | 952/1016 (94%) | 742 (78%) | 210 (22%) | 1           | 4 |

All (210) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | GLN  |
| 1   | A     | 15  | GLN  |
| 1   | A     | 17  | PHE  |
| 1   | A     | 18  | ASP  |
| 1   | A     | 20  | GLN  |
| 1   | A     | 25  | LEU  |
| 1   | A     | 29  | SER  |
| 1   | A     | 37  | GLN  |
| 1   | A     | 50  | ARG  |
| 1   | A     | 58  | VAL  |
| 1   | A     | 61  | VAL  |
| 1   | A     | 62  | VAL  |
| 1   | A     | 65  | LEU  |
| 1   | A     | 70  | ASN  |
| 1   | A     | 72  | GLN  |
| 1   | A     | 78  | PHE  |
| 1   | A     | 84  | GLU  |
| 1   | A     | 87  | THR  |
| 1   | A     | 93  | TYR  |
| 1   | A     | 114 | ARG  |
| 1   | A     | 115 | SER  |
| 1   | A     | 134 | THR  |
| 1   | A     | 135 | ILE  |
| 1   | A     | 151 | SER  |
| 1   | A     | 154 | MET  |
| 1   | A     | 158 | SER  |
| 1   | A     | 163 | ARG  |
| 1   | A     | 167 | GLN  |
| 1   | A     | 176 | ILE  |
| 1   | A     | 179 | HIS  |
| 1   | A     | 181 | THR  |
| 1   | A     | 189 | LEU  |
| 1   | A     | 194 | LEU  |
| 1   | A     | 199 | GLU  |
| 1   | A     | 209 | LEU  |
| 1   | A     | 214 | ILE  |
| 1   | A     | 215 | THR  |
| 1   | A     | 217 | SER  |
| 1   | A     | 219 | THR  |
| 1   | A     | 222 | PHE  |
| 1   | A     | 234 | LEU  |
| 1   | A     | 238 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 239 | CYS  |
| 1   | A     | 242 | THR  |
| 1   | A     | 254 | ARG  |
| 1   | A     | 263 | LEU  |
| 1   | A     | 271 | LEU  |
| 1   | A     | 273 | GLU  |
| 1   | A     | 279 | THR  |
| 1   | A     | 280 | THR  |
| 1   | A     | 290 | GLN  |
| 1   | A     | 301 | TYR  |
| 1   | A     | 305 | LEU  |
| 1   | A     | 308 | CYS  |
| 1   | A     | 309 | ASN  |
| 1   | A     | 310 | GLU  |
| 1   | A     | 322 | VAL  |
| 1   | A     | 324 | LEU  |
| 1   | A     | 328 | LEU  |
| 1   | A     | 331 | PHE  |
| 1   | A     | 334 | VAL  |
| 1   | A     | 335 | PHE  |
| 1   | A     | 337 | VAL  |
| 1   | A     | 338 | ILE  |
| 1   | A     | 342 | PHE  |
| 1   | A     | 349 | SER  |
| 1   | A     | 361 | LYS  |
| 1   | A     | 362 | GLU  |
| 1   | A     | 374 | GLU  |
| 1   | A     | 378 | PHE  |
| 1   | A     | 380 | LEU  |
| 1   | A     | 383 | ARG  |
| 1   | A     | 386 | SER  |
| 1   | A     | 392 | LEU  |
| 1   | A     | 408 | ILE  |
| 1   | A     | 410 | ILE  |
| 1   | A     | 416 | GLU  |
| 1   | A     | 438 | ILE  |
| 1   | A     | 448 | LEU  |
| 1   | A     | 458 | MET  |
| 1   | A     | 461 | LYS  |
| 1   | A     | 474 | TYR  |
| 1   | A     | 485 | VAL  |
| 1   | A     | 521 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 522 | LEU  |
| 1   | A     | 525 | ASP  |
| 1   | A     | 532 | PHE  |
| 1   | A     | 534 | GLU  |
| 1   | A     | 540 | PHE  |
| 1   | A     | 541 | ARG  |
| 1   | A     | 544 | TYR  |
| 1   | A     | 548 | LEU  |
| 1   | A     | 549 | GLN  |
| 1   | A     | 550 | ASN  |
| 1   | A     | 554 | GLU  |
| 1   | A     | 557 | VAL  |
| 1   | A     | 563 | TYR  |
| 1   | A     | 564 | ARG  |
| 1   | B     | 3   | ARG  |
| 1   | B     | 5   | LEU  |
| 1   | B     | 6   | GLU  |
| 1   | B     | 7   | LEU  |
| 1   | B     | 33  | GLN  |
| 1   | B     | 35  | PHE  |
| 1   | B     | 44  | GLN  |
| 1   | B     | 47  | MET  |
| 1   | B     | 53  | LEU  |
| 1   | B     | 67  | CYS  |
| 1   | B     | 72  | GLN  |
| 1   | B     | 79  | LEU  |
| 1   | B     | 80  | LEU  |
| 1   | B     | 81  | ARG  |
| 1   | B     | 89  | LEU  |
| 1   | B     | 93  | TYR  |
| 1   | B     | 95  | ARG  |
| 1   | B     | 96  | PHE  |
| 1   | B     | 109 | ARG  |
| 1   | B     | 112 | ASP  |
| 1   | B     | 113 | HIS  |
| 1   | B     | 116 | LEU  |
| 1   | B     | 117 | THR  |
| 1   | B     | 121 | LEU  |
| 1   | B     | 122 | PHE  |
| 1   | B     | 124 | PHE  |
| 1   | B     | 134 | THR  |
| 1   | B     | 136 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 141 | LYS  |
| 1   | B     | 152 | LEU  |
| 1   | B     | 158 | SER  |
| 1   | B     | 159 | ASP  |
| 1   | B     | 171 | ARG  |
| 1   | B     | 174 | HIS  |
| 1   | B     | 189 | LEU  |
| 1   | B     | 212 | LYS  |
| 1   | B     | 215 | THR  |
| 1   | B     | 219 | THR  |
| 1   | B     | 222 | PHE  |
| 1   | B     | 223 | LEU  |
| 1   | B     | 231 | ASP  |
| 1   | B     | 233 | GLU  |
| 1   | B     | 241 | THR  |
| 1   | B     | 243 | THR  |
| 1   | B     | 245 | GLU  |
| 1   | B     | 247 | SER  |
| 1   | B     | 249 | VAL  |
| 1   | B     | 257 | PHE  |
| 1   | B     | 258 | MET  |
| 1   | B     | 263 | LEU  |
| 1   | B     | 275 | LEU  |
| 1   | B     | 280 | THR  |
| 1   | B     | 287 | ILE  |
| 1   | B     | 290 | GLN  |
| 1   | B     | 291 | LYS  |
| 1   | B     | 294 | LYS  |
| 1   | B     | 295 | THR  |
| 1   | B     | 299 | ARG  |
| 1   | B     | 305 | LEU  |
| 1   | B     | 306 | GLN  |
| 1   | B     | 309 | ASN  |
| 1   | B     | 321 | MET  |
| 1   | B     | 324 | LEU  |
| 1   | B     | 325 | VAL  |
| 1   | B     | 329 | PRO  |
| 1   | B     | 337 | VAL  |
| 1   | B     | 341 | LYS  |
| 1   | B     | 352 | HIS  |
| 1   | B     | 353 | VAL  |
| 1   | B     | 354 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 356 | CYS  |
| 1   | B     | 357 | TYR  |
| 1   | B     | 359 | LEU  |
| 1   | B     | 360 | VAL  |
| 1   | B     | 364 | ASP  |
| 1   | B     | 368 | ARG  |
| 1   | B     | 372 | THR  |
| 1   | B     | 376 | GLU  |
| 1   | B     | 379 | VAL  |
| 1   | B     | 383 | ARG  |
| 1   | B     | 392 | LEU  |
| 1   | B     | 400 | LYS  |
| 1   | B     | 401 | ILE  |
| 1   | B     | 402 | THR  |
| 1   | B     | 404 | LEU  |
| 1   | B     | 408 | ILE  |
| 1   | B     | 411 | ARG  |
| 1   | B     | 413 | LEU  |
| 1   | B     | 417 | ARG  |
| 1   | B     | 418 | ARG  |
| 1   | B     | 420 | VAL  |
| 1   | B     | 425 | TRP  |
| 1   | B     | 426 | LEU  |
| 1   | B     | 427 | GLU  |
| 1   | B     | 428 | GLN  |
| 1   | B     | 430 | GLU  |
| 1   | B     | 433 | GLN  |
| 1   | B     | 459 | LEU  |
| 1   | B     | 466 | THR  |
| 1   | B     | 472 | VAL  |
| 1   | B     | 474 | TYR  |
| 1   | B     | 478 | GLU  |
| 1   | B     | 479 | ILE  |
| 1   | B     | 485 | VAL  |
| 1   | B     | 489 | ASP  |
| 1   | B     | 514 | PHE  |
| 1   | B     | 516 | GLU  |
| 1   | B     | 521 | TRP  |
| 1   | B     | 531 | LEU  |
| 1   | B     | 538 | ASP  |
| 1   | B     | 559 | ASP  |
| 1   | B     | 571 | VAL  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | GLN  |
| 1   | A     | 33  | GLN  |
| 1   | A     | 45  | GLN  |
| 1   | A     | 64  | GLN  |
| 1   | A     | 72  | GLN  |
| 1   | A     | 85  | HIS  |
| 1   | A     | 104 | ASN  |
| 1   | A     | 165 | HIS  |
| 1   | A     | 168 | ASN  |
| 1   | A     | 227 | HIS  |
| 1   | A     | 292 | HIS  |
| 1   | A     | 309 | ASN  |
| 1   | A     | 407 | GLN  |
| 1   | A     | 447 | GLN  |
| 1   | A     | 536 | HIS  |
| 1   | A     | 550 | ASN  |
| 1   | B     | 32  | GLN  |
| 1   | B     | 64  | GLN  |
| 1   | B     | 72  | GLN  |
| 1   | B     | 168 | ASN  |
| 1   | B     | 179 | HIS  |
| 1   | B     | 204 | ASN  |
| 1   | B     | 228 | GLN  |
| 1   | B     | 290 | GLN  |
| 1   | B     | 292 | HIS  |
| 1   | B     | 309 | ASN  |
| 1   | B     | 363 | HIS  |
| 1   | B     | 407 | GLN  |
| 1   | B     | 412 | HIS  |

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | ADP  | A     | 1762 | 3    | 25,29,29     | 0.87 | 1 (4%)      | 24,45,45    | 1.98 | 2 (8%)      |
| 4   | AMP  | B     | 1604 | -    | 22,25,25     | 1.05 | 1 (4%)      | 24,38,38    | 1.90 | 2 (8%)      |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | ADP  | A     | 1762 | 3    | -       | 0/12/32/32 | 0/3/3/3 |
| 4   | AMP  | B     | 1604 | -    | -       | 0/6/26/26  | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2   | A     | 1762 | ADP  | C5-C4 | 2.57 | 1.46        | 1.40     |
| 4   | B     | 1604 | AMP  | C5-C4 | 3.07 | 1.47        | 1.40     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | A     | 1762 | ADP  | N3-C2-N1 | -7.61 | 122.23      | 128.86   |
| 4   | B     | 1604 | AMP  | N3-C2-N1 | -7.09 | 122.69      | 128.86   |
| 4   | B     | 1604 | AMP  | C4-C5-N7 | -3.65 | 105.88      | 109.41   |
| 2   | A     | 1762 | ADP  | C4-C5-N7 | -2.93 | 106.58      | 109.41   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | A     | 1762 | ADP  | 5       | 0            |
| 4   | B     | 1604 | AMP  | 2       | 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 [i](#)

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

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|--------------|-----------------------|-------|
| 1   | A     | 547/578 (94%)   | -0.25  | 3 (0%) 90 80 | 2, 15, 29, 37         | 0     |
| 1   | B     | 539/578 (93%)   | -0.18  | 0 100 100    | 4, 18, 28, 34         | 0     |
| All | All   | 1086/1156 (93%) | -0.21  | 3 (0%) 93 86 | 2, 17, 29, 37         | 0     |

All (3) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 181 | THR  | 3.3  |
| 1   | A     | 158 | SER  | 2.2  |
| 1   | A     | 146 | ASP  | 2.2  |

### 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 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 2   | ADP  | A     | 1762 | 27/27 | 0.95 | 0.15 | -0.90 | 6,10,11,12                  | 0     |
| 4   | AMP  | B     | 1604 | 23/23 | 0.93 | 0.17 | -1.26 | 23,25,31,34                 | 0     |
| 3   | MG   | A     | 579  | 1/1   | 0.98 | 0.20 | -     | 15,15,15,15                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.