



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 24, 2017 – 01:00 PM EDT

PDB ID : 5G5L  
EMDB ID: : EMD-3439  
Title : RNA polymerase I-Rrn3 complex at 4.8 Å resolution  
Authors : Engel, C.; Plitzko, J.; Cramer, P.  
Deposited on : unknown  
Resolution : 4.80 Å(reported)  
Based on PDB ID : 4C2M

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

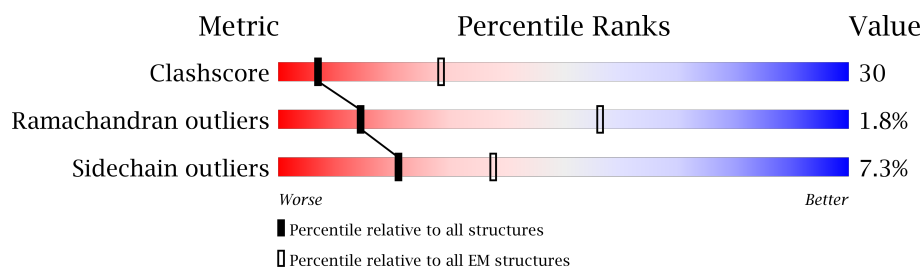
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 125131                      | 1336                        |
| Ramachandran outliers | 121729                      | 1120                        |
| Sidechain outliers    | 121581                      | 1026                        |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1664   | 63% 23% • 11%    |
| 2   | B     | 1203   | 69% 24% • •      |
| 3   | C     | 335    | 61% 26% • • 9%   |
| 4   | D     | 137    | 23% 18% • • 58%  |
| 5   | E     | 215    | 77% 18% • •      |
| 6   | F     | 155    | 53% 10% • 35%    |
| 7   | G     | 326    | 39% 17% • 41%    |
| 8   | H     | 146    | 72% 16% • 10%    |
| 9   | I     | 125    | 54% 30% • 14%    |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 10  | J     | 70     | <div><div></div><div>79%</div><div>17%</div><div>...</div></div>                          |
| 11  | K     | 142    | <div><div></div><div>51%</div><div>19%</div><div>•</div><div>29%</div></div>              |
| 12  | L     | 70     | <div><div></div><div>29%</div><div>27%</div><div>6%</div><div>39%</div></div>             |
| 13  | M     | 415    | <div><div></div><div>17%</div><div>8%</div><div>•</div><div>75%</div></div>               |
| 14  | N     | 233    | <div><div></div><div>47%</div><div>15%</div><div>38%</div></div>                          |
| 15  | O     | 627    | <div><div></div><div>25%</div><div>40%</div><div>8%</div><div>•</div><div>26%</div></div> |

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 37349 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1480     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11686 | 7384 | 2030 | 2211 | 61 |         |       |

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | B     | 1174     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9327  | 5899 | 1635 | 1743 | 50 |         |       |

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | C     | 305      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2423  | 1539 | 416 | 460 | 8 |         |       |

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 4   | D     | 58       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 459   | 289 | 78 | 92 |         |       |

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | E     | 212      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1735  | 1102 | 306 | 316 | 11 |         |       |

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 823   | 522 | 144 | 154 | 3 |         |       |

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 193      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1520  | 982 | 259 | 274 | 5 |         |       |

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1052  | 664 | 176 | 208 | 4 |         |       |

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | I     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 820   | 511 | 138 | 162 | 9 |         |       |

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | J     | 69       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 569   | 362 | 101 | 100 | 6 |         |       |

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 793   | 496 | 130 | 162 | 5 |         |       |

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | L     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 340   | 211 | 66 | 59 | 4 |         |       |

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 13  | M     | 105      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 833   | 528 | 138 | 167 |         |       |

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | N     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1151  | 735 | 188 | 224 | 4 |         |       |

- Molecule 15 is a protein called RNA POLYMERASE I-SPECIFIC TRANSCRIPTION INITIATION FACTOR RRN3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | O     | 463      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3811  | 2473 | 623 | 694 | 21 |         |       |

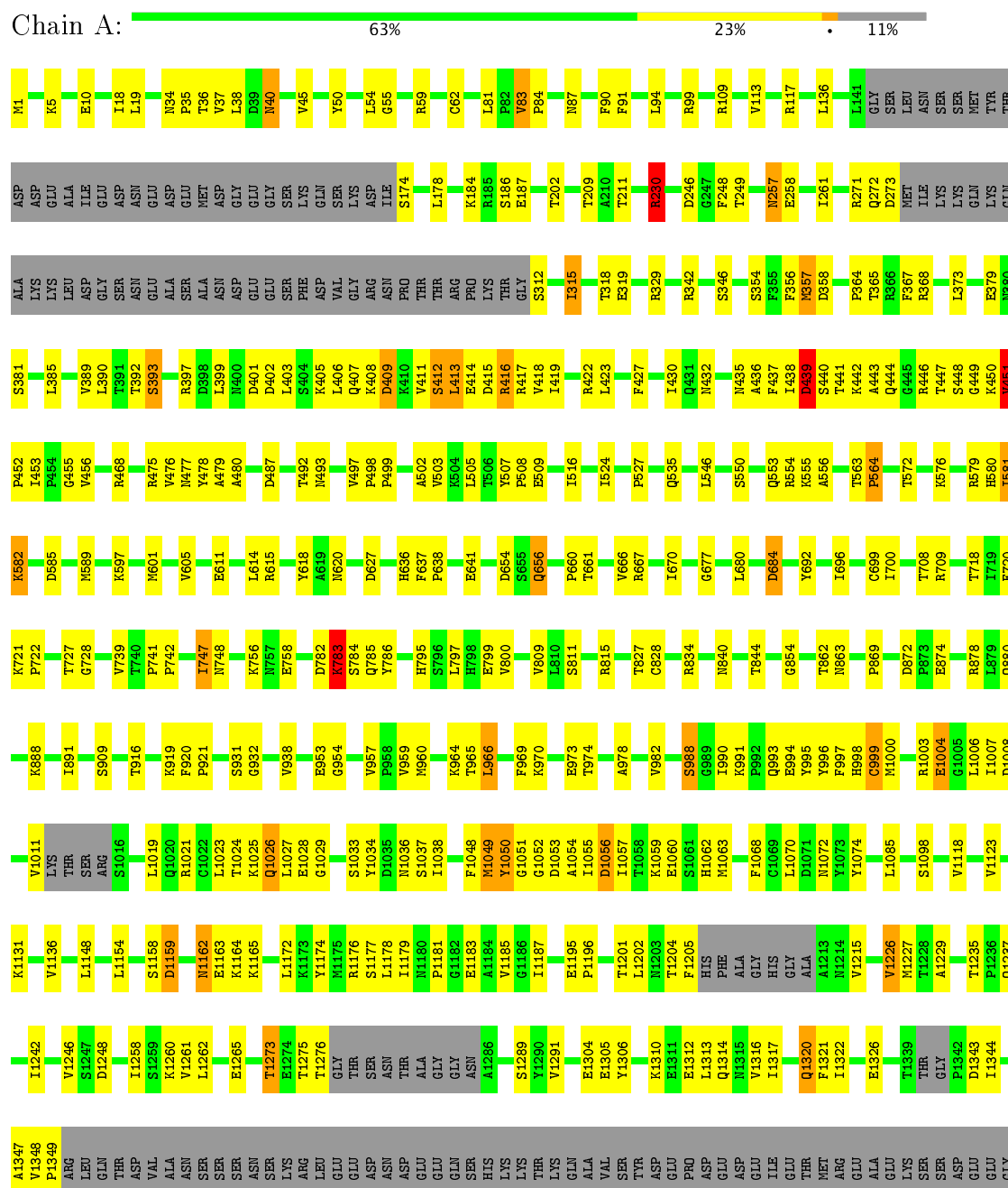
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 16  | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 16  | A     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 16  | L     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 16  | J     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 16  | I     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |

### 3 Residue-property plots

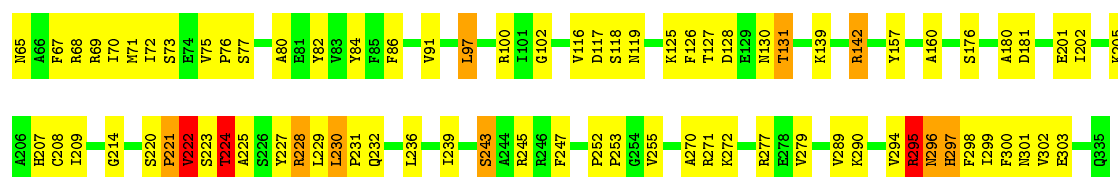
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

- Molecule 1: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190



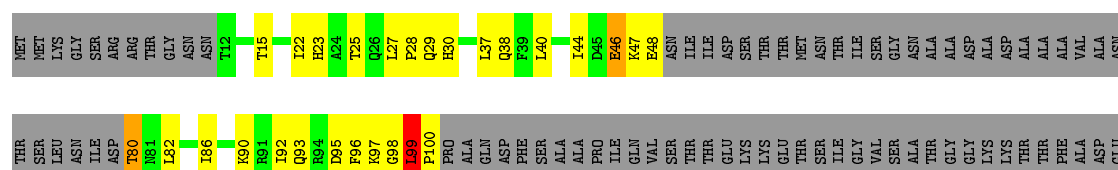






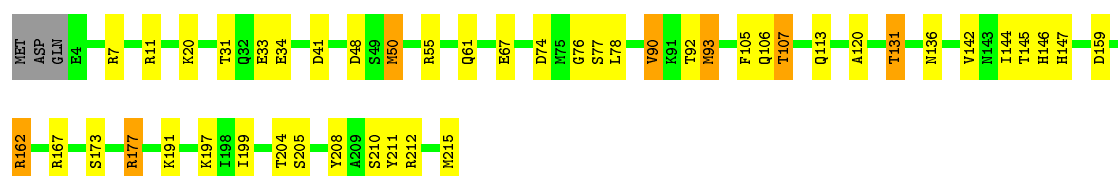
• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14

Chain D: 23% 18% 58%



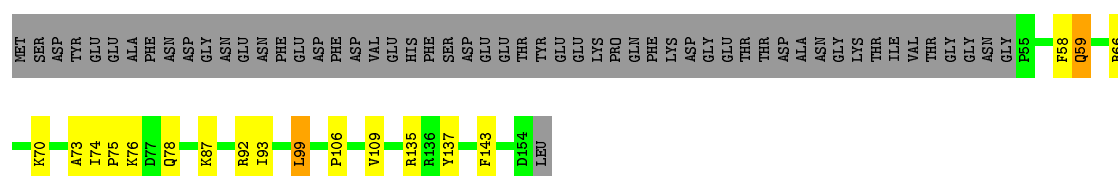
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E: 77% 18%



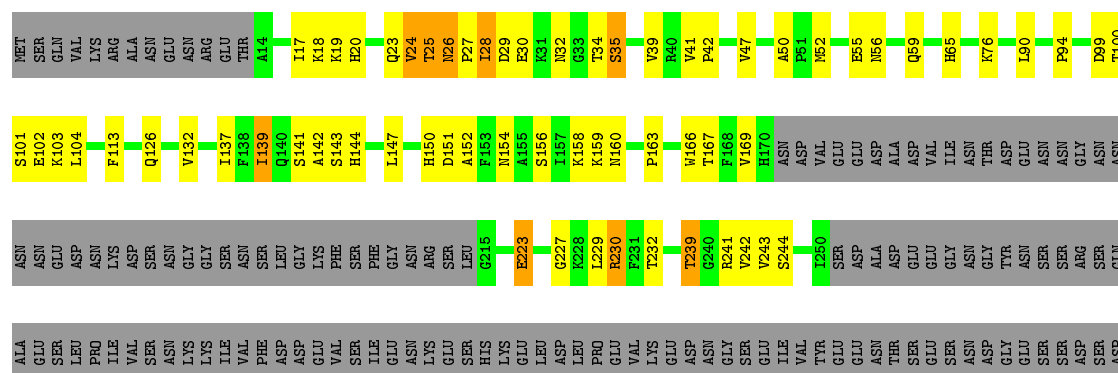
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F: 53% 10% 35%

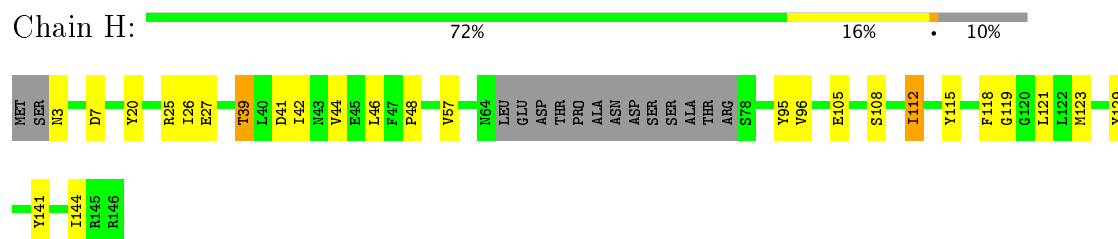


• Molecule 7: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

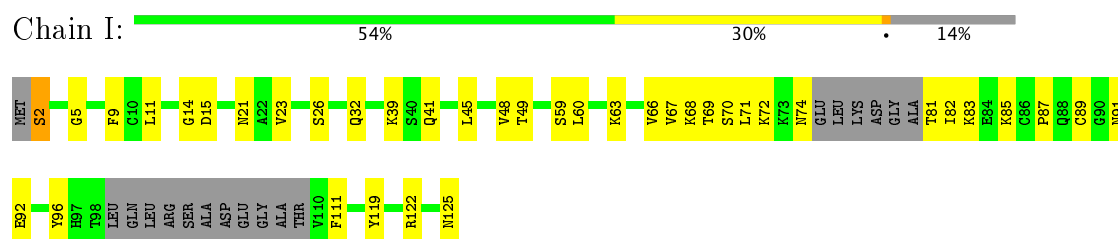
Chain G: 39% 17% 41%



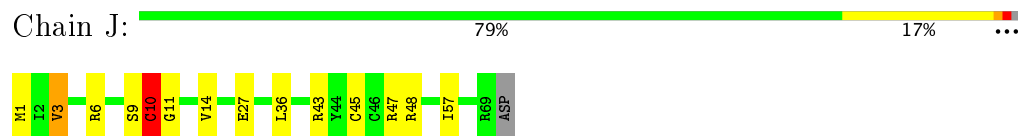
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3



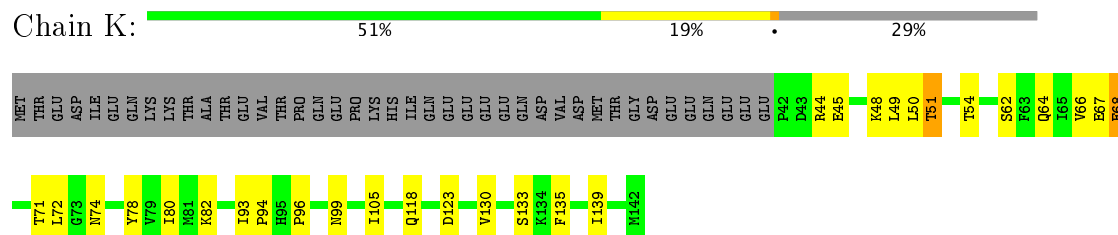
• Molecule 9: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12



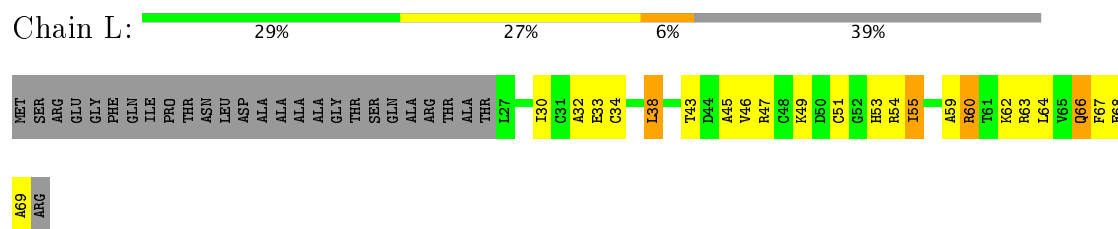
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



• Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2

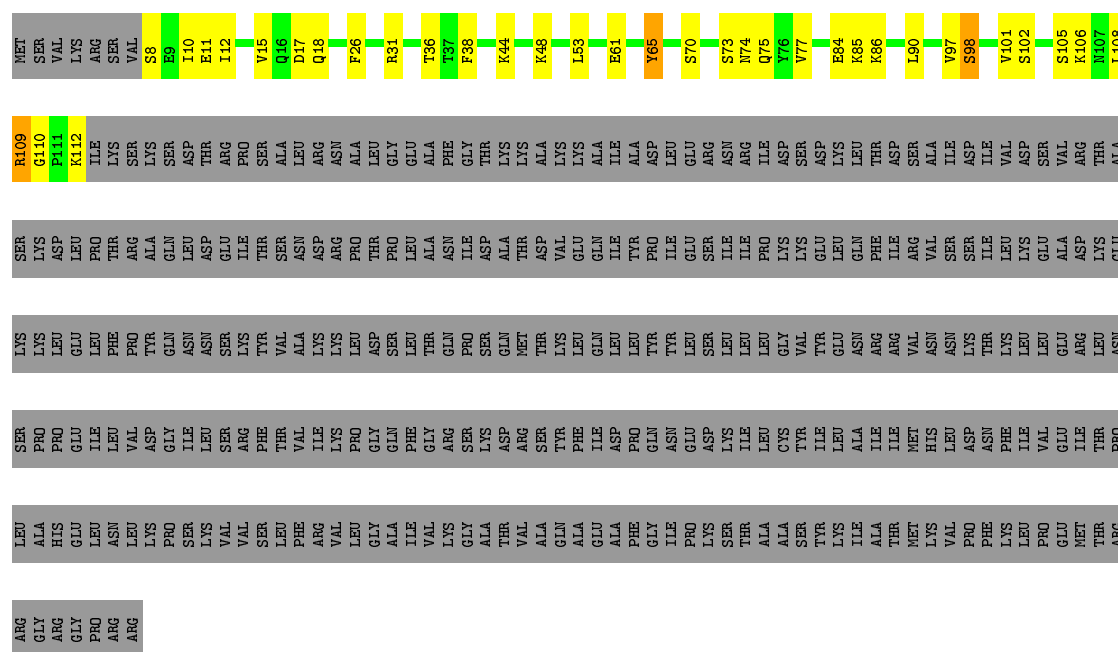


• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

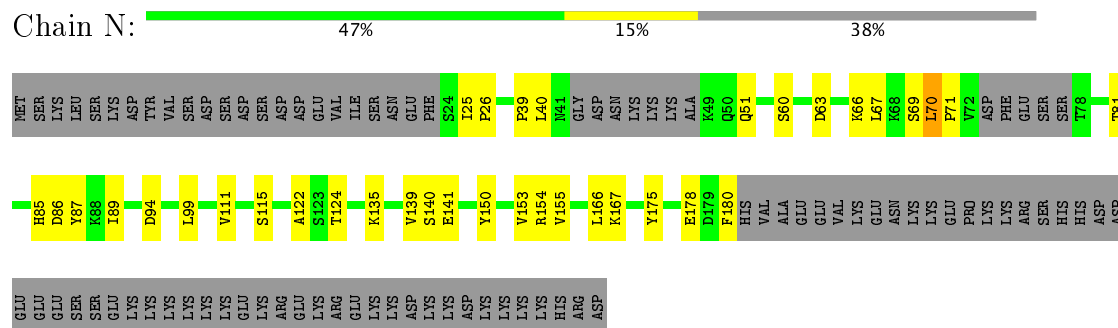


• Molecule 13: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49

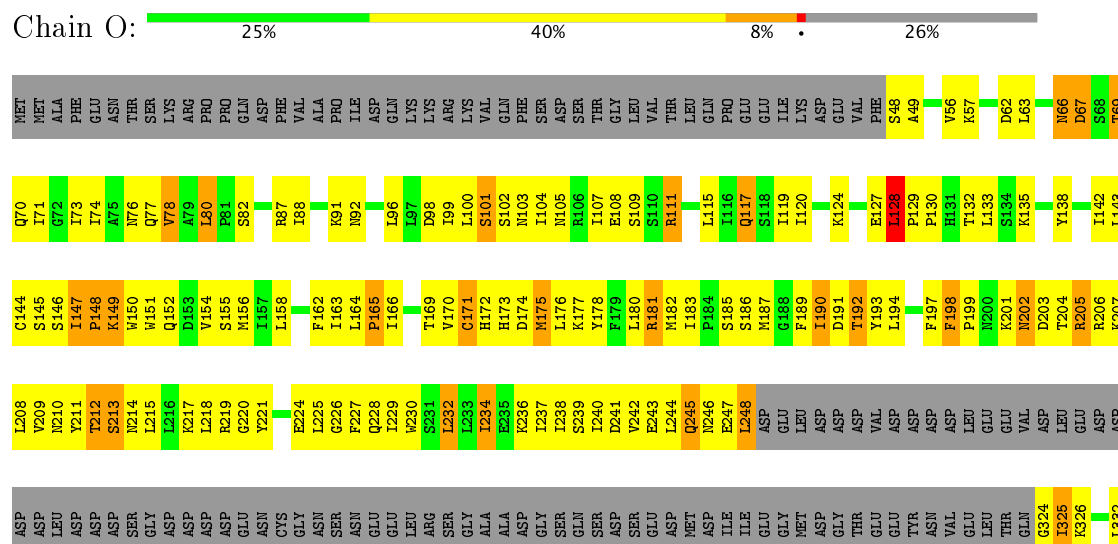




- Molecule 14: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34



● Molecule 15: RNA POLYMERASE I-SPECIFIC TRANSCRIPTION INITIATION FACTOR  
RRN3



|      |      |      |      |      |
|------|------|------|------|------|
| I607 | I531 | D462 | V401 | L336 |
| B608 | V537 | Q463 | T402 | T337 |
| Y609 | Q540 | M467 | I403 |      |
| I611 | I543 | E468 | I404 | T341 |
|      | N547 | R469 | D405 | H342 |
|      | R551 | F470 | I406 | V343 |
|      | LEU  | K471 | S407 |      |
| GLU  | ARG  | F472 | F408 |      |
| ALA  | ILE  | H473 | A409 |      |
| SER  | ILE  | Y474 | V410 | Q346 |
| GLY  | GLY  | A475 | T348 | T347 |
| GLU  | GLY  | F476 | N411 | P349 |
| TYR  | GLY  | Q477 | E412 | E350 |
| GLU  | ASP  | F478 | A413 | S351 |
| ASP  | ASP  | Q479 | A414 | L352 |
| GLY  | GLY  | L480 | E415 | E353 |
| SER  | LYS  | C481 | K416 | S354 |
| ASP  | ALA  | Y482 | K417 | S355 |
| ASP  | ASP  | I483 | I418 | E356 |
|      | SER  | F484 | K419 | G357 |
|      | ASP  | C485 | S420 | V358 |
|      | LYS  | F486 | L421 | G359 |
|      | LYS  | R487 | Q422 | V360 |
|      | GLU  | H488 | Y423 | F361 |
|      | ASN  | R489 | I424 | I362 |
|      | SER  | I490 | G425 | T363 |
|      | ALA  | F491 | S426 | L364 |
|      | ALA  |      | Y427 | T365 |
|      | ALA  | T494 | I428 | T366 |
|      | ASN  | D495 | A429 | L367 |
|      | THR  |      | R430 | F368 |
|      | SER  | E499 | A431 | T369 |
|      | SER  | L502 | K432 | T370 |
|      | SER  |      | K433 | H371 |
|      | SER  |      | L434 | V372 |
|      | SER  |      | S435 | L373 |
|      | TRP  | F505 | R436 | P374 |
|      | SER  | F506 | T437 | T375 |
|      | LEU  | Q507 | Q438 | T376 |
|      | ALA  | R508 | I439 | Y377 |
|      |      |      | I440 | T378 |
|      | T581 | R582 | F441 | R379 |
|      | Q583 | Q584 | V442 | S380 |
|      | F585 | I586 | A443 | T381 |
|      |      |      | S444 | Q382 |
|      | Y591 |      | Y445 | T383 |
|      | F592 |      | I446 | T384 |
|      | P593 |      | T447 | T385 |
|      | Y594 |      | S448 | F386 |
|      | D595 |      | H449 | H387 |
|      | P596 |      | L450 | V388 |
|      | L597 |      |      | S389 |
|      | F598 |      | Y453 | Q390 |
|      | L599 |      | V454 | Q391 |
|      |      |      | R457 | Q392 |
|      | Y602 |      | E458 | L395 |
|      | M606 |      | E459 | H396 |
|      |      |      | E460 | D397 |
|      |      |      | V461 | S398 |

## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, C1                 | Depositor |
| Number of particles used             | 63445                     | Depositor |
| Resolution determination method      | Not provided              | Depositor |
| CTF correction method                | RELION                    | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                        | Depositor |
| Minimum defocus (nm)                 | 800                       | Depositor |
| Maximum defocus (nm)                 | 3600                      | Depositor |
| Magnification                        | 37037                     | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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  > 2$    | RMSZ        | # $ Z  > 2$     |
| 1   | A     | 0.48         | 0/11900        | 0.72        | 22/16073 (0.1%) |
| 10  | J     | 0.57         | 1/578 (0.2%)   | 0.59        | 0/775           |
| 11  | K     | 0.46         | 0/804          | 0.79        | 3/1083 (0.3%)   |
| 12  | L     | 0.38         | 0/342          | 0.55        | 0/454           |
| 13  | M     | 0.42         | 0/849          | 0.56        | 1/1140 (0.1%)   |
| 14  | N     | 0.40         | 0/1172         | 0.54        | 0/1580          |
| 15  | O     | 0.38         | 1/3897 (0.0%)  | 0.58        | 3/5268 (0.1%)   |
| 2   | B     | 0.49         | 1/9533 (0.0%)  | 0.77        | 25/12884 (0.2%) |
| 3   | C     | 0.43         | 0/2475         | 0.68        | 5/3354 (0.1%)   |
| 4   | D     | 0.40         | 0/465          | 0.59        | 0/630           |
| 5   | E     | 0.40         | 0/1771         | 0.66        | 3/2383 (0.1%)   |
| 6   | F     | 0.45         | 0/838          | 0.58        | 0/1129          |
| 7   | G     | 0.39         | 0/1558         | 0.60        | 3/2120 (0.1%)   |
| 8   | H     | 0.42         | 0/1070         | 0.61        | 0/1449          |
| 9   | I     | 0.42         | 0/831          | 0.57        | 0/1117          |
| All | All   | 0.45         | 3/38083 (0.0%) | 0.69        | 65/51439 (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     | 0                   | 1                   |
| 15  | O     | 0                   | 5                   |
| All | All   | 0                   | 6                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 10  | J     | 10  | CYS  | CB-SG | 7.64 | 1.95        | 1.82     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 15  | O     | 198 | PHE  | C-N   | -7.16 | 1.20        | 1.34     |
| 2   | B     | 859 | CYS  | CB-SG | -6.12 | 1.71        | 1.82     |

All (65) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 2   | B     | 1023 | ARG  | NE-CZ-NH2 | -13.90 | 113.35      | 120.30   |
| 2   | B     | 452  | ARG  | NE-CZ-NH2 | -13.35 | 113.63      | 120.30   |
| 1   | A     | 397  | ARG  | NE-CZ-NH1 | 13.22  | 126.91      | 120.30   |
| 1   | A     | 329  | ARG  | NE-CZ-NH2 | -13.12 | 113.74      | 120.30   |
| 2   | B     | 448  | ARG  | NE-CZ-NH2 | -12.97 | 113.81      | 120.30   |
| 1   | A     | 329  | ARG  | NE-CZ-NH1 | 12.94  | 126.77      | 120.30   |
| 2   | B     | 429  | ARG  | NE-CZ-NH2 | -12.81 | 113.89      | 120.30   |
| 1   | A     | 59   | ARG  | NE-CZ-NH1 | 12.81  | 126.70      | 120.30   |
| 1   | A     | 59   | ARG  | NE-CZ-NH2 | -12.78 | 113.91      | 120.30   |
| 5   | E     | 167  | ARG  | NE-CZ-NH1 | 12.52  | 126.56      | 120.30   |
| 5   | E     | 167  | ARG  | NE-CZ-NH2 | -12.50 | 114.05      | 120.30   |
| 1   | A     | 416  | ARG  | NE-CZ-NH2 | -12.41 | 114.09      | 120.30   |
| 11  | K     | 44   | ARG  | NE-CZ-NH2 | -12.29 | 114.15      | 120.30   |
| 2   | B     | 448  | ARG  | NE-CZ-NH1 | 12.28  | 126.44      | 120.30   |
| 2   | B     | 261  | ARG  | NE-CZ-NH1 | 12.22  | 126.41      | 120.30   |
| 2   | B     | 452  | ARG  | NE-CZ-NH1 | 12.22  | 126.41      | 120.30   |
| 2   | B     | 634  | ARG  | NE-CZ-NH2 | -12.21 | 114.19      | 120.30   |
| 2   | B     | 261  | ARG  | NE-CZ-NH2 | -12.11 | 114.25      | 120.30   |
| 2   | B     | 429  | ARG  | NE-CZ-NH1 | 12.07  | 126.33      | 120.30   |
| 11  | K     | 44   | ARG  | NE-CZ-NH1 | 11.97  | 126.29      | 120.30   |
| 1   | A     | 397  | ARG  | NE-CZ-NH2 | -11.89 | 114.35      | 120.30   |
| 3   | C     | 142  | ARG  | NE-CZ-NH2 | -11.52 | 114.54      | 120.30   |
| 1   | A     | 422  | ARG  | NE-CZ-NH2 | -11.46 | 114.57      | 120.30   |
| 3   | C     | 142  | ARG  | NE-CZ-NH1 | 11.44  | 126.02      | 120.30   |
| 1   | A     | 342  | ARG  | NE-CZ-NH2 | -11.35 | 114.62      | 120.30   |
| 1   | A     | 422  | ARG  | NE-CZ-NH1 | 11.12  | 125.86      | 120.30   |
| 2   | B     | 634  | ARG  | NE-CZ-NH1 | 11.02  | 125.81      | 120.30   |
| 1   | A     | 416  | ARG  | NE-CZ-NH1 | 11.00  | 125.80      | 120.30   |
| 1   | A     | 230  | ARG  | NE-CZ-NH1 | 10.85  | 125.72      | 120.30   |
| 1   | A     | 230  | ARG  | NE-CZ-NH2 | -10.79 | 114.91      | 120.30   |
| 2   | B     | 648  | ARG  | NE-CZ-NH2 | -10.72 | 114.94      | 120.30   |
| 2   | B     | 550  | ARG  | NE-CZ-NH2 | -10.51 | 115.04      | 120.30   |
| 2   | B     | 550  | ARG  | NE-CZ-NH1 | 9.88   | 125.24      | 120.30   |
| 2   | B     | 1023 | ARG  | NE-CZ-NH1 | 9.57   | 125.08      | 120.30   |
| 1   | A     | 342  | ARG  | NE-CZ-NH1 | 9.25   | 124.92      | 120.30   |
| 2   | B     | 648  | ARG  | NE-CZ-NH1 | 9.09   | 124.84      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 15  | O     | 460  | GLU  | N-CA-C   | -7.44 | 90.91       | 111.00   |
| 2   | B     | 261  | ARG  | CD-NE-CZ | 6.91  | 133.28      | 123.60   |
| 1   | A     | 397  | ARG  | CD-NE-CZ | 6.90  | 133.25      | 123.60   |
| 15  | O     | 598  | PHE  | N-CA-C   | 6.90  | 129.62      | 111.00   |
| 1   | A     | 59   | ARG  | CD-NE-CZ | 6.61  | 132.86      | 123.60   |
| 2   | B     | 452  | ARG  | CD-NE-CZ | 6.55  | 132.77      | 123.60   |
| 2   | B     | 448  | ARG  | CD-NE-CZ | 6.37  | 132.52      | 123.60   |
| 1   | A     | 329  | ARG  | CD-NE-CZ | 6.33  | 132.46      | 123.60   |
| 11  | K     | 44   | ARG  | CD-NE-CZ | 6.24  | 132.34      | 123.60   |
| 2   | B     | 634  | ARG  | CD-NE-CZ | 6.20  | 132.28      | 123.60   |
| 1   | A     | 416  | ARG  | CD-NE-CZ | 6.18  | 132.25      | 123.60   |
| 1   | A     | 422  | ARG  | CD-NE-CZ | 6.17  | 132.23      | 123.60   |
| 2   | B     | 429  | ARG  | CD-NE-CZ | 6.13  | 132.18      | 123.60   |
| 3   | C     | 142  | ARG  | CD-NE-CZ | 6.00  | 132.00      | 123.60   |
| 5   | E     | 167  | ARG  | CD-NE-CZ | 5.93  | 131.90      | 123.60   |
| 7   | G     | 35   | SER  | O-C-N    | 5.92  | 132.17      | 122.70   |
| 1   | A     | 1622 | LEU  | O-C-N    | 5.78  | 131.94      | 122.70   |
| 1   | A     | 342  | ARG  | CD-NE-CZ | 5.67  | 131.54      | 123.60   |
| 2   | B     | 1103 | VAL  | CB-CA-C  | -5.59 | 100.78      | 111.40   |
| 7   | G     | 35   | SER  | CA-C-N   | -5.54 | 105.02      | 117.20   |
| 2   | B     | 550  | ARG  | CD-NE-CZ | 5.45  | 131.23      | 123.60   |
| 2   | B     | 648  | ARG  | CD-NE-CZ | 5.39  | 131.15      | 123.60   |
| 2   | B     | 1023 | ARG  | CD-NE-CZ | 5.22  | 130.91      | 123.60   |
| 1   | A     | 230  | ARG  | CD-NE-CZ | 5.20  | 130.88      | 123.60   |
| 7   | G     | 26   | ASN  | C-N-CD   | 5.12  | 139.16      | 128.40   |
| 15  | O     | 128  | LEU  | C-N-CD   | 5.08  | 139.06      | 128.40   |
| 13  | M     | 110  | GLY  | C-N-CD   | 5.06  | 139.03      | 128.40   |
| 3   | C     | 220  | SER  | C-N-CD   | 5.05  | 139.00      | 128.40   |
| 3   | C     | 230  | LEU  | C-N-CD   | 5.03  | 138.97      | 128.40   |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1343 | ASP  | Peptide |
| 15  | O     | 374  | PRO  | Peptide |
| 15  | O     | 375  | THR  | Peptide |
| 15  | O     | 411  | ASN  | Peptide |
| 15  | O     | 598  | PHE  | Peptide |
| 15  | O     | 599  | LEU  | 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     | 11686 | 0        | 11770    | 682     | 0            |
| 2   | B     | 9327  | 0        | 9214     | 482     | 0            |
| 3   | C     | 2423  | 0        | 2409     | 283     | 0            |
| 4   | D     | 459   | 0        | 461      | 103     | 0            |
| 5   | E     | 1735  | 0        | 1764     | 40      | 0            |
| 6   | F     | 823   | 0        | 840      | 64      | 0            |
| 7   | G     | 1520  | 0        | 1529     | 162     | 0            |
| 8   | H     | 1052  | 0        | 1021     | 15      | 0            |
| 9   | I     | 820   | 0        | 805      | 71      | 0            |
| 10  | J     | 569   | 0        | 585      | 6       | 0            |
| 11  | K     | 793   | 0        | 790      | 36      | 0            |
| 12  | L     | 340   | 0        | 361      | 47      | 0            |
| 13  | M     | 833   | 0        | 826      | 32      | 0            |
| 14  | N     | 1151  | 0        | 1169     | 44      | 0            |
| 15  | O     | 3811  | 0        | 3800     | 754     | 0            |
| 16  | A     | 2     | 0        | 0        | 0       | 0            |
| 16  | B     | 1     | 0        | 0        | 0       | 0            |
| 16  | I     | 2     | 0        | 0        | 0       | 0            |
| 16  | J     | 1     | 0        | 0        | 0       | 0            |
| 16  | L     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 37349 | 0        | 37344    | 2255    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (2255) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 3:C:75:VAL:HG11 | 3:C:221:PRO:CG    | 1.33                     | 1.52              |
| 1:A:478:TYR:HA  | 2:B:1048:SER:CA   | 1.42                     | 1.50              |
| 1:A:436:ALA:CB  | 1:A:443:ALA:HB2   | 1.43                     | 1.46              |
| 1:A:83:VAL:HG21 | 1:A:427:PHE:CZ    | 1.50                     | 1.46              |
| 15:O:458:GLU:HA | 15:O:461:VAL:CG2  | 1.26                     | 1.44              |
| 15:O:458:GLU:CA | 15:O:461:VAL:HG23 | 1.28                     | 1.41              |
| 15:O:454:VAL:CB | 15:O:514:PHE:HE2  | 1.30                     | 1.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:478:TYR:CA   | 2:B:1048:SER:HA   | 1.53                     | 1.38              |
| 2:B:207:ILE:HG13 | 2:B:503:VAL:CG2   | 1.54                     | 1.37              |
| 15:O:408:PHE:CZ  | 15:O:446:LEU:CD1  | 2.06                     | 1.37              |
| 15:O:408:PHE:CZ  | 15:O:446:LEU:HD11 | 1.59                     | 1.37              |
| 1:A:436:ALA:HB2  | 1:A:443:ALA:CB    | 1.54                     | 1.37              |
| 15:O:471:LYS:HB2 | 15:O:585:PHE:CE1  | 1.58                     | 1.37              |
| 1:A:83:VAL:HG11  | 1:A:427:PHE:CE2   | 1.59                     | 1.36              |
| 15:O:138:TYR:CE2 | 15:O:142:ILE:HD11 | 1.56                     | 1.36              |
| 3:C:31:TRP:CB    | 11:K:82:LYS:HD2   | 1.54                     | 1.35              |
| 15:O:454:VAL:HB  | 15:O:514:PHE:CE2  | 1.61                     | 1.35              |
| 1:A:437:PHE:CZ   | 1:A:456:VAL:HG23  | 1.62                     | 1.35              |
| 7:G:242:VAL:HG11 | 15:O:185:SER:OG   | 1.22                     | 1.35              |
| 1:A:437:PHE:CZ   | 1:A:456:VAL:CG2   | 2.11                     | 1.34              |
| 2:B:42:VAL:CG1   | 2:B:46:ILE:HD11   | 1.57                     | 1.33              |
| 3:C:75:VAL:HG11  | 3:C:221:PRO:CD    | 1.59                     | 1.32              |
| 3:C:75:VAL:CG1   | 3:C:221:PRO:CG    | 2.07                     | 1.31              |
| 3:C:54:PHE:CE2   | 3:C:300:PHE:HB2   | 1.66                     | 1.30              |
| 3:C:55:ASP:CG    | 3:C:299:ILE:HG12  | 1.51                     | 1.29              |
| 1:A:477:ASN:OD1  | 2:B:1059:PRO:HG3  | 1.13                     | 1.29              |
| 3:C:84:TYR:HE2   | 12:L:66:GLN:OE1   | 1.16                     | 1.29              |
| 15:O:198:PHE:CD2 | 15:O:232:LEU:HG   | 1.65                     | 1.29              |
| 4:D:30:HIS:NE2   | 7:G:26:ASN:OD1    | 1.66                     | 1.27              |
| 15:O:432:LYS:HG2 | 15:O:608:GLU:O    | 1.23                     | 1.27              |
| 4:D:25:THR:CG2   | 6:F:59:GLN:HE21   | 1.45                     | 1.27              |
| 3:C:84:TYR:CE2   | 12:L:66:GLN:OE1   | 1.87                     | 1.26              |
| 3:C:75:VAL:CG1   | 3:C:221:PRO:CD    | 2.14                     | 1.26              |
| 1:A:478:TYR:N    | 2:B:1048:SER:O    | 1.66                     | 1.25              |
| 1:A:1008:ASP:OD2 | 1:A:1202:LEU:HD13 | 1.37                     | 1.24              |
| 15:O:431:ALA:CB  | 15:O:434:LEU:HD11 | 1.63                     | 1.24              |
| 3:C:54:PHE:CE2   | 3:C:300:PHE:CB    | 2.20                     | 1.24              |
| 1:A:1348:VAL:HB  | 2:B:268:GLU:O     | 1.35                     | 1.24              |
| 15:O:237:ILE:CB  | 15:O:381:ILE:HD12 | 1.68                     | 1.24              |
| 7:G:158:LYS:CG   | 15:O:105:ASN:OD1  | 1.86                     | 1.23              |
| 15:O:432:LYS:HB3 | 15:O:609:TYR:CA   | 1.69                     | 1.23              |
| 1:A:756:LYS:HD3  | 9:I:85:LYS:NZ     | 1.51                     | 1.23              |
| 15:O:432:LYS:CG  | 15:O:608:GLU:O    | 1.88                     | 1.22              |
| 2:B:769:PHE:CE1  | 2:B:798:PHE:CE1   | 2.26                     | 1.22              |
| 4:D:30:HIS:CE1   | 7:G:26:ASN:OD1    | 1.92                     | 1.22              |
| 2:B:769:PHE:CE1  | 2:B:798:PHE:HE1   | 1.56                     | 1.22              |
| 3:C:230:LEU:CD2  | 3:C:294:VAL:HG21  | 1.67                     | 1.22              |
| 1:A:1605:THR:O   | 1:A:1606:SER:O    | 1.57                     | 1.22              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:454:VAL:CB   | 15:O:514:PHE:CE2  | 2.17                     | 1.22              |
| 3:C:54:PHE:CZ     | 3:C:300:PHE:HB3   | 1.73                     | 1.22              |
| 3:C:131:THR:HG23  | 3:C:209:ILE:CG2   | 1.69                     | 1.21              |
| 15:O:352:LEU:HD23 | 15:O:358:VAL:CG2  | 1.69                     | 1.21              |
| 15:O:373:LEU:HD11 | 15:O:416:LYS:CG   | 1.69                     | 1.21              |
| 15:O:352:LEU:CD2  | 15:O:358:VAL:HG22 | 1.71                     | 1.20              |
| 3:C:31:TRP:CD1    | 11:K:82:LYS:NZ    | 2.10                     | 1.20              |
| 15:O:432:LYS:CB   | 15:O:609:TYR:HA   | 1.71                     | 1.20              |
| 1:A:477:ASN:OD1   | 2:B:1059:PRO:CG   | 1.90                     | 1.20              |
| 3:C:62:SER:HB2    | 11:K:74:ASN:ND2   | 1.51                     | 1.20              |
| 15:O:426:SER:OG   | 15:O:594:TYR:HB2  | 1.42                     | 1.19              |
| 1:A:1050:TYR:CE1  | 1:A:1185:VAL:HG11 | 1.76                     | 1.19              |
| 15:O:247:GLU:OE1  | 15:O:325:ILE:HG12 | 1.42                     | 1.19              |
| 15:O:390:GLN:O    | 15:O:609:TYR:CE1  | 1.94                     | 1.19              |
| 3:C:55:ASP:HA     | 3:C:299:ILE:HA    | 1.20                     | 1.18              |
| 3:C:54:PHE:O      | 3:C:300:PHE:N     | 1.76                     | 1.18              |
| 15:O:237:ILE:CG2  | 15:O:381:ILE:HD12 | 1.73                     | 1.18              |
| 1:A:1008:ASP:OD1  | 1:A:1202:LEU:HD22 | 1.43                     | 1.18              |
| 7:G:141:SER:CB    | 15:O:138:TYR:OH   | 1.92                     | 1.17              |
| 15:O:162:PHE:O    | 15:O:210:ASN:O    | 1.61                     | 1.17              |
| 15:O:237:ILE:HB   | 15:O:381:ILE:HD12 | 1.22                     | 1.17              |
| 1:A:437:PHE:CE1   | 1:A:456:VAL:HG23  | 1.78                     | 1.17              |
| 2:B:207:ILE:CG1   | 2:B:503:VAL:CG2   | 2.22                     | 1.17              |
| 1:A:1006:LEU:CD1  | 2:B:716:MET:SD    | 2.32                     | 1.17              |
| 2:B:207:ILE:CG1   | 2:B:503:VAL:HG21  | 1.73                     | 1.17              |
| 1:A:1006:LEU:HD11 | 2:B:716:MET:SD    | 1.85                     | 1.16              |
| 1:A:83:VAL:HG21   | 1:A:427:PHE:CE2   | 1.78                     | 1.16              |
| 7:G:158:LYS:CD    | 15:O:105:ASN:OD1  | 1.91                     | 1.16              |
| 15:O:430:ARG:NH2  | 15:O:596:PRO:HD3  | 1.60                     | 1.16              |
| 1:A:1048:PHE:CZ   | 5:E:211:TYR:HD1   | 1.64                     | 1.16              |
| 1:A:1011:VAL:HG11 | 1:A:1201:THR:C    | 1.63                     | 1.16              |
| 2:B:207:ILE:HG13  | 2:B:503:VAL:HG22  | 1.26                     | 1.16              |
| 1:A:756:LYS:CD    | 9:I:85:LYS:NZ     | 2.07                     | 1.16              |
| 3:C:59:ILE:HG23   | 3:C:298:PHE:CE1   | 1.79                     | 1.15              |
| 4:D:92:ILE:HG12   | 7:G:152:ALA:HB2   | 1.29                     | 1.15              |
| 7:G:158:LYS:HG2   | 15:O:105:ASN:OD1  | 1.43                     | 1.15              |
| 1:A:1344:ILE:HD12 | 2:B:329:TYR:HE2   | 1.10                     | 1.14              |
| 1:A:556:ALA:HB2   | 15:O:246:ASN:ND2  | 1.63                     | 1.14              |
| 15:O:219:ARG:NH2  | 15:O:360:VAL:HG21 | 1.63                     | 1.14              |
| 15:O:408:PHE:CE2  | 15:O:446:LEU:HD11 | 1.83                     | 1.14              |
| 15:O:408:PHE:CZ   | 15:O:446:LEU:HD13 | 1.81                     | 1.13              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:143:SER:HB2   | 15:O:104:ILE:H    | 1.06                     | 1.13              |
| 15:O:454:VAL:HA   | 15:O:514:PHE:CZ   | 1.83                     | 1.12              |
| 2:B:42:VAL:HB     | 2:B:46:ILE:CD1    | 1.77                     | 1.12              |
| 7:G:28:ILE:HG22   | 7:G:29:ASP:H      | 1.02                     | 1.12              |
| 1:A:1348:VAL:CB   | 2:B:268:GLU:O     | 1.97                     | 1.12              |
| 15:O:247:GLU:OE1  | 15:O:325:ILE:CG1  | 1.97                     | 1.12              |
| 3:C:58:ASN:HA     | 3:C:296:ASN:CB    | 1.79                     | 1.11              |
| 2:B:42:VAL:CG1    | 2:B:46:ILE:CD1    | 2.26                     | 1.11              |
| 3:C:54:PHE:CD2    | 3:C:300:PHE:HB2   | 1.85                     | 1.11              |
| 15:O:370:THR:O    | 15:O:374:PRO:HD3  | 1.51                     | 1.11              |
| 15:O:598:PHE:HB3  | 15:O:599:LEU:HD13 | 1.12                     | 1.11              |
| 6:F:75:PRO:HG2    | 6:F:78:GLN:HB2    | 1.12                     | 1.11              |
| 15:O:156:MET:HG3  | 15:O:197:PHE:CE2  | 1.83                     | 1.11              |
| 15:O:454:VAL:CG2  | 15:O:514:PHE:HE2  | 1.62                     | 1.11              |
| 13:M:101:VAL:CG1  | 13:M:106:LYS:HG3  | 1.81                     | 1.10              |
| 2:B:42:VAL:CB     | 2:B:46:ILE:CD1    | 2.29                     | 1.10              |
| 7:G:158:LYS:HB3   | 15:O:105:ASN:ND2  | 1.65                     | 1.10              |
| 1:A:1226:VAL:O    | 1:A:1598:PHE:HD2  | 1.34                     | 1.10              |
| 15:O:129:PRO:HD2  | 15:O:132:THR:HB   | 1.32                     | 1.10              |
| 15:O:156:MET:SD   | 15:O:197:PHE:CZ   | 2.45                     | 1.10              |
| 15:O:446:LEU:O    | 15:O:449:TRP:HB3  | 1.51                     | 1.10              |
| 1:A:83:VAL:CG1    | 1:A:427:PHE:CE2   | 2.34                     | 1.10              |
| 1:A:480:ALA:HB2   | 2:B:1046:VAL:HG23 | 1.23                     | 1.10              |
| 15:O:240:ILE:HG21 | 15:O:332:LEU:HB2  | 1.24                     | 1.10              |
| 4:D:25:THR:HG22   | 6:F:59:GLN:HE21   | 1.07                     | 1.10              |
| 3:C:31:TRP:CE3    | 11:K:82:LYS:HG3   | 1.86                     | 1.10              |
| 7:G:158:LYS:CB    | 15:O:105:ASN:ND2  | 2.15                     | 1.10              |
| 1:A:1011:VAL:HG11 | 1:A:1201:THR:O    | 1.51                     | 1.10              |
| 3:C:58:ASN:CA     | 3:C:296:ASN:HB2   | 1.81                     | 1.10              |
| 3:C:59:ILE:CG2    | 3:C:298:PHE:CD1   | 2.35                     | 1.09              |
| 1:A:475:ARG:HD2   | 2:B:1059:PRO:O    | 1.51                     | 1.09              |
| 15:O:425:GLY:HA2  | 15:O:483:ILE:HD11 | 1.34                     | 1.09              |
| 3:C:55:ASP:OD1    | 3:C:299:ILE:HG12  | 1.53                     | 1.09              |
| 7:G:158:LYS:HA    | 15:O:105:ASN:HD21 | 1.08                     | 1.09              |
| 15:O:447:THR:O    | 15:O:450:LEU:HB2  | 1.50                     | 1.09              |
| 3:C:56:LEU:HB2    | 3:C:298:PHE:HB2   | 1.35                     | 1.09              |
| 3:C:230:LEU:HD23  | 3:C:294:VAL:CG2   | 1.83                     | 1.09              |
| 3:C:31:TRP:HB3    | 11:K:82:LYS:HD2   | 1.17                     | 1.09              |
| 1:A:436:ALA:CB    | 1:A:443:ALA:CB    | 2.21                     | 1.08              |
| 3:C:230:LEU:HD12  | 3:C:231:PRO:CD    | 1.84                     | 1.08              |
| 1:A:475:ARG:CD    | 2:B:1059:PRO:O    | 2.00                     | 1.08              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:28:PRO:HG2    | 7:G:24:VAL:HG11   | 1.28                     | 1.08              |
| 15:O:138:TYR:CE2  | 15:O:142:ILE:CD1  | 2.35                     | 1.08              |
| 15:O:201:LYS:HD2  | 15:O:239:SER:OG   | 1.54                     | 1.08              |
| 1:A:1011:VAL:CG1  | 1:A:1201:THR:O    | 2.00                     | 1.08              |
| 1:A:478:TYR:CZ    | 2:B:1049:THR:HG23 | 1.88                     | 1.08              |
| 2:B:42:VAL:CB     | 2:B:46:ILE:HD11   | 1.84                     | 1.08              |
| 4:D:25:THR:HA     | 6:F:59:GLN:HG2    | 1.32                     | 1.08              |
| 15:O:129:PRO:CD   | 15:O:132:THR:HB   | 1.83                     | 1.08              |
| 3:C:75:VAL:HB     | 3:C:221:PRO:HD3   | 1.36                     | 1.07              |
| 3:C:57:ILE:HA     | 3:C:297:HIS:HA    | 1.14                     | 1.07              |
| 15:O:156:MET:SD   | 15:O:197:PHE:HZ   | 1.78                     | 1.07              |
| 1:A:478:TYR:CZ    | 2:B:1049:THR:CG2  | 2.38                     | 1.07              |
| 3:C:230:LEU:HD12  | 3:C:231:PRO:HD3   | 1.36                     | 1.07              |
| 15:O:138:TYR:CZ   | 15:O:142:ILE:HD11 | 1.89                     | 1.07              |
| 13:M:101:VAL:HG11 | 13:M:106:LYS:HG3  | 1.27                     | 1.06              |
| 1:A:1008:ASP:O    | 1:A:1011:VAL:HG23 | 1.53                     | 1.06              |
| 1:A:475:ARG:NH2   | 2:B:1061:LYS:HB2  | 1.70                     | 1.06              |
| 15:O:245:GLN:HG3  | 15:O:378:THR:HA   | 1.15                     | 1.06              |
| 4:D:80:THR:OG1    | 15:O:227:PHE:CG   | 2.08                     | 1.06              |
| 15:O:431:ALA:HB3  | 15:O:434:LEU:HD11 | 1.37                     | 1.06              |
| 2:B:42:VAL:HG12   | 2:B:46:ILE:CD1    | 1.84                     | 1.06              |
| 15:O:240:ILE:HG22 | 15:O:332:LEU:HD22 | 1.08                     | 1.06              |
| 3:C:41:GLU:HB3    | 3:C:57:ILE:CG2    | 1.83                     | 1.06              |
| 15:O:198:PHE:CD1  | 15:O:236:LYS:HE3  | 1.90                     | 1.06              |
| 1:A:1053:ASP:OD2  | 1:A:1580:ARG:NH2  | 1.88                     | 1.06              |
| 3:C:75:VAL:HG11   | 3:C:221:PRO:HG2   | 1.06                     | 1.05              |
| 15:O:162:PHE:CA   | 15:O:214:ASN:CB   | 2.33                     | 1.05              |
| 1:A:408:LYS:HA    | 1:A:411:VAL:CG1   | 1.85                     | 1.05              |
| 15:O:152:GLN:HG2  | 15:O:193:TYR:OH   | 1.52                     | 1.05              |
| 15:O:431:ALA:HB1  | 15:O:434:LEU:HD11 | 1.34                     | 1.05              |
| 15:O:240:ILE:CG2  | 15:O:332:LEU:HD22 | 1.87                     | 1.05              |
| 1:A:1179:ILE:HD11 | 1:A:1183:GLU:HG3  | 1.33                     | 1.05              |
| 1:A:1048:PHE:CZ   | 5:E:211:TYR:CD1   | 2.44                     | 1.05              |
| 15:O:198:PHE:CZ   | 15:O:236:LYS:HG3  | 1.92                     | 1.05              |
| 3:C:75:VAL:CB     | 3:C:221:PRO:CD    | 2.35                     | 1.04              |
| 15:O:488:HIS:CG   | 15:O:489:ASN:H    | 1.74                     | 1.04              |
| 15:O:390:GLN:NE2  | 15:O:432:LYS:H    | 1.54                     | 1.04              |
| 3:C:131:THR:HG23  | 3:C:209:ILE:HG22  | 1.08                     | 1.04              |
| 7:G:241:ARG:CB    | 15:O:189:PHE:CE2  | 2.39                     | 1.04              |
| 15:O:152:GLN:CG   | 15:O:193:TYR:OH   | 2.04                     | 1.04              |
| 1:A:83:VAL:HG11   | 1:A:427:PHE:CD2   | 1.90                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:502:ALA:HB1   | 1:A:581:ILE:CG2   | 1.87                     | 1.04              |
| 7:G:141:SER:HB2   | 15:O:138:TYR:OH   | 1.53                     | 1.04              |
| 15:O:174:ASP:HA   | 15:O:177:LYS:HE2  | 1.40                     | 1.03              |
| 15:O:435:SER:HB3  | 15:O:438:GLN:HG3  | 1.37                     | 1.03              |
| 4:D:25:THR:CG2    | 6:F:59:GLN:NE2    | 2.21                     | 1.03              |
| 15:O:237:ILE:HB   | 15:O:381:ILE:CD1  | 1.88                     | 1.03              |
| 12:L:68:GLU:HG2   | 12:L:69:ALA:H     | 1.23                     | 1.03              |
| 1:A:1003:ARG:NE   | 2:B:520:LEU:HB2   | 1.74                     | 1.03              |
| 1:A:1050:TYR:CE1  | 1:A:1185:VAL:CG1  | 2.42                     | 1.02              |
| 1:A:782:ASP:OD2   | 1:A:931:SER:O     | 1.78                     | 1.02              |
| 3:C:59:ILE:CG2    | 3:C:298:PHE:CE1   | 2.43                     | 1.02              |
| 2:B:472:SER:CB    | 2:B:476:LEU:HD12  | 1.88                     | 1.02              |
| 2:B:1155:ASP:OD2  | 7:G:239:THR:OG1   | 1.76                     | 1.02              |
| 1:A:413:LEU:HB3   | 1:A:417:ARG:NH2   | 1.75                     | 1.02              |
| 15:O:241:ASP:OD1  | 15:O:378:THR:HG22 | 1.58                     | 1.02              |
| 1:A:909:SER:OG    | 9:I:83:LYS:CE     | 2.08                     | 1.01              |
| 3:C:51:GLU:HB3    | 3:C:303:GLU:HG2   | 1.42                     | 1.01              |
| 15:O:369:LYS:O    | 15:O:373:LEU:N    | 1.91                     | 1.01              |
| 1:A:392:THR:CG2   | 1:A:430:ILE:HB    | 1.88                     | 1.01              |
| 7:G:158:LYS:HB3   | 15:O:105:ASN:CG   | 1.79                     | 1.01              |
| 1:A:480:ALA:CB    | 2:B:1046:VAL:HG23 | 1.90                     | 1.01              |
| 3:C:56:LEU:CD1    | 3:C:300:PHE:CE1   | 2.44                     | 1.01              |
| 15:O:201:LYS:CD   | 15:O:239:SER:OG   | 2.09                     | 1.01              |
| 2:B:42:VAL:C      | 2:B:46:ILE:HD12   | 1.82                     | 1.00              |
| 15:O:428:ILE:HG23 | 15:O:439:ILE:HG21 | 1.38                     | 1.00              |
| 7:G:158:LYS:CA    | 15:O:105:ASN:HD21 | 1.75                     | 1.00              |
| 3:C:45:SER:HB2    | 3:C:271:ARG:NH2   | 1.76                     | 1.00              |
| 7:G:158:LYS:HZ3   | 15:O:108:GLU:CG   | 1.27                     | 1.00              |
| 15:O:348:THR:HG22 | 15:O:351:SER:HB3  | 1.42                     | 1.00              |
| 1:A:799:GLU:HG3   | 1:A:1062:HIS:CG   | 1.95                     | 1.00              |
| 1:A:408:LYS:HA    | 1:A:411:VAL:HG12  | 1.40                     | 1.00              |
| 15:O:352:LEU:HA   | 15:O:358:VAL:HG23 | 1.44                     | 1.00              |
| 1:A:782:ASP:OD1   | 1:A:783:LYS:N     | 1.93                     | 1.00              |
| 1:A:756:LYS:CD    | 9:I:85:LYS:HZ2    | 1.70                     | 1.00              |
| 15:O:240:ILE:HG21 | 15:O:332:LEU:CB   | 1.92                     | 1.00              |
| 15:O:352:LEU:HD23 | 15:O:358:VAL:HG22 | 1.00                     | 1.00              |
| 15:O:428:ILE:HD12 | 15:O:439:ILE:HG23 | 1.44                     | 1.00              |
| 15:O:471:LYS:CB   | 15:O:585:PHE:CE1  | 2.45                     | 0.99              |
| 2:B:75:ASP:HB3    | 2:B:440:PHE:CE2   | 1.97                     | 0.99              |
| 1:A:1055:ILE:HD12 | 1:A:1063:MET:CE   | 1.91                     | 0.99              |
| 15:O:454:VAL:CG2  | 15:O:514:PHE:CE2  | 2.44                     | 0.99              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:143:SER:CB    | 15:O:104:ILE:H    | 1.75                     | 0.99              |
| 15:O:158:LEU:HD23 | 15:O:172:HIS:HD2  | 1.25                     | 0.99              |
| 1:A:1006:LEU:HD12 | 2:B:716:MET:SD    | 2.01                     | 0.99              |
| 7:G:158:LYS:CA    | 15:O:105:ASN:ND2  | 2.25                     | 0.99              |
| 1:A:1344:ILE:HD12 | 2:B:329:TYR:CE2   | 1.97                     | 0.98              |
| 2:B:70:GLU:CB     | 2:B:98:SER:HB3    | 1.93                     | 0.98              |
| 2:B:1019:GLY:HA3  | 3:C:65:ASN:HB2    | 1.45                     | 0.98              |
| 3:C:54:PHE:CZ     | 3:C:300:PHE:CB    | 2.41                     | 0.98              |
| 3:C:84:TYR:CD2    | 12:L:66:GLN:HB2   | 1.99                     | 0.98              |
| 2:B:70:GLU:HB3    | 2:B:98:SER:HB3    | 0.99                     | 0.98              |
| 15:O:240:ILE:CG2  | 15:O:332:LEU:HD13 | 1.93                     | 0.98              |
| 15:O:373:LEU:HD11 | 15:O:416:LYS:HG3  | 1.43                     | 0.98              |
| 7:G:241:ARG:CB    | 15:O:189:PHE:HE2  | 1.76                     | 0.98              |
| 15:O:598:PHE:CB   | 15:O:599:LEU:HD13 | 1.92                     | 0.98              |
| 1:A:392:THR:HG21  | 1:A:430:ILE:CB    | 1.94                     | 0.98              |
| 6:F:75:PRO:HG2    | 6:F:78:GLN:CB     | 1.92                     | 0.98              |
| 1:A:909:SER:OG    | 9:I:83:LYS:HE2    | 1.62                     | 0.97              |
| 1:A:83:VAL:CG2    | 1:A:427:PHE:CZ    | 2.47                     | 0.97              |
| 4:D:96:PHE:HE1    | 7:G:150:HIS:HB3   | 1.28                     | 0.97              |
| 15:O:423:TYR:HD1  | 15:O:594:TYR:CE2  | 1.82                     | 0.97              |
| 13:M:105:SER:HA   | 13:M:108:LEU:HG   | 1.46                     | 0.97              |
| 1:A:392:THR:HG21  | 1:A:430:ILE:HB    | 0.98                     | 0.97              |
| 1:A:509:GLU:OE2   | 1:A:579:ARG:NE    | 1.97                     | 0.97              |
| 1:A:953:GLU:HG2   | 1:A:1205:PHE:CE2  | 2.00                     | 0.97              |
| 2:B:70:GLU:HB3    | 2:B:98:SER:CB     | 1.93                     | 0.97              |
| 15:O:454:VAL:HB   | 15:O:514:PHE:HE2  | 0.99                     | 0.96              |
| 1:A:480:ALA:HB2   | 2:B:1046:VAL:CG2  | 1.95                     | 0.96              |
| 1:A:476:VAL:HG11  | 2:B:1071:VAL:HG23 | 1.47                     | 0.96              |
| 1:A:1660:VAL:O    | 7:G:102:GLU:HA    | 1.65                     | 0.96              |
| 3:C:59:ILE:HG22   | 3:C:298:PHE:CD1   | 1.98                     | 0.96              |
| 1:A:83:VAL:CG2    | 1:A:427:PHE:CE2   | 2.48                     | 0.96              |
| 1:A:966:LEU:HD22  | 1:A:997:PHE:CZ    | 2.00                     | 0.96              |
| 2:B:769:PHE:CD1   | 2:B:798:PHE:HE1   | 1.83                     | 0.96              |
| 15:O:156:MET:CG   | 15:O:197:PHE:CE2  | 2.48                     | 0.96              |
| 1:A:1055:ILE:HG21 | 1:A:1060:GLU:HG3  | 1.47                     | 0.95              |
| 1:A:502:ALA:HB1   | 1:A:581:ILE:HG21  | 1.46                     | 0.95              |
| 1:A:1:MET:HG2     | 2:B:1098:TYR:CZ   | 2.01                     | 0.95              |
| 7:G:158:LYS:HD3   | 15:O:105:ASN:OD1  | 1.66                     | 0.95              |
| 1:A:516:ILE:HG12  | 15:O:376:TYR:CE2  | 2.01                     | 0.95              |
| 15:O:440:ILE:HG23 | 15:O:491:PHE:HE1  | 1.27                     | 0.95              |
| 15:O:408:PHE:HZ   | 15:O:446:LEU:HD11 | 1.25                     | 0.95              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:502:ALA:CB    | 1:A:581:ILE:HG21  | 1.97                     | 0.95              |
| 2:B:1090:ASP:OD1  | 2:B:1095:SER:OG   | 1.85                     | 0.95              |
| 15:O:454:VAL:HG23 | 15:O:514:PHE:CE2  | 2.01                     | 0.95              |
| 1:A:1344:ILE:CD1  | 2:B:329:TYR:HE2   | 1.78                     | 0.94              |
| 2:B:77:LYS:NZ     | 2:B:438:ILE:O     | 1.99                     | 0.94              |
| 15:O:63:LEU:HD12  | 15:O:71:ILE:HG13  | 1.47                     | 0.94              |
| 15:O:374:PRO:O    | 15:O:419:LYS:NZ   | 2.01                     | 0.94              |
| 1:A:401:ASP:OD2   | 1:A:405:LYS:HE3   | 1.67                     | 0.94              |
| 15:O:234:ILE:CG2  | 15:O:371:HIS:HD2  | 1.81                     | 0.94              |
| 7:G:158:LYS:HD3   | 15:O:105:ASN:CG   | 1.88                     | 0.94              |
| 3:C:75:VAL:HB     | 3:C:221:PRO:CD    | 1.94                     | 0.94              |
| 1:A:799:GLU:HG3   | 1:A:1062:HIS:ND1  | 1.83                     | 0.93              |
| 1:A:990:ILE:HA    | 1:A:994:GLU:OE1   | 1.69                     | 0.93              |
| 2:B:894:LYS:H     | 12:L:54:ARG:NH2   | 1.66                     | 0.93              |
| 15:O:342:HIS:CD2  | 15:O:346:GLN:HE21 | 1.85                     | 0.93              |
| 15:O:417:LYS:HD2  | 15:O:472:HIS:CE1  | 2.02                     | 0.93              |
| 1:A:878:ARG:HG2   | 9:I:67:VAL:HG11   | 1.48                     | 0.93              |
| 15:O:241:ASP:CG   | 15:O:378:THR:HG22 | 1.88                     | 0.93              |
| 2:B:209:GLN:HG2   | 2:B:210:ARG:H     | 1.31                     | 0.93              |
| 2:B:211:ARG:HG2   | 2:B:401:GLU:OE1   | 1.68                     | 0.93              |
| 3:C:57:ILE:HD12   | 3:C:297:HIS:ND1   | 1.82                     | 0.93              |
| 15:O:198:PHE:HD2  | 15:O:232:LEU:HG   | 1.05                     | 0.93              |
| 3:C:62:SER:CB     | 11:K:74:ASN:ND2   | 2.32                     | 0.93              |
| 7:G:242:VAL:HG11  | 15:O:185:SER:HG   | 1.32                     | 0.93              |
| 15:O:342:HIS:O    | 15:O:346:GLN:HG2  | 1.68                     | 0.93              |
| 3:C:75:VAL:CG1    | 3:C:221:PRO:HG2   | 1.89                     | 0.93              |
| 4:D:80:THR:OG1    | 15:O:227:PHE:CD2  | 2.20                     | 0.93              |
| 15:O:358:VAL:O    | 15:O:362:ASN:ND2  | 2.00                     | 0.93              |
| 1:A:413:LEU:HB3   | 1:A:417:ARG:HH21  | 1.29                     | 0.93              |
| 4:D:92:ILE:HG22   | 4:D:96:PHE:CZ     | 2.03                     | 0.93              |
| 7:G:158:LYS:CB    | 15:O:105:ASN:CG   | 2.35                     | 0.93              |
| 7:G:158:LYS:CG    | 15:O:105:ASN:CG   | 2.37                     | 0.93              |
| 3:C:75:VAL:CB     | 3:C:221:PRO:HD2   | 1.97                     | 0.92              |
| 15:O:598:PHE:HB3  | 15:O:599:LEU:CD1  | 1.99                     | 0.92              |
| 3:C:131:THR:CG2   | 3:C:209:ILE:HG22  | 1.98                     | 0.92              |
| 7:G:154:ASN:HD21  | 15:O:182:MET:CE   | 1.82                     | 0.92              |
| 1:A:83:VAL:HG21   | 1:A:427:PHE:HZ    | 1.13                     | 0.92              |
| 15:O:224:GLU:N    | 15:O:224:GLU:OE1  | 2.02                     | 0.92              |
| 1:A:756:LYS:HD3   | 9:I:85:LYS:HZ1    | 1.19                     | 0.92              |
| 3:C:71:MET:SD     | 3:C:225:ALA:HB1   | 2.10                     | 0.92              |
| 15:O:147:ILE:O    | 15:O:149:LYS:N    | 2.03                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:N:85:HIS:HE1   | 14:N:141:GLU:CD   | 1.72                     | 0.92              |
| 15:O:390:GLN:O    | 15:O:609:TYR:HE1  | 1.52                     | 0.92              |
| 15:O:386:PHE:HD2  | 15:O:606:MET:CE   | 1.83                     | 0.92              |
| 15:O:435:SER:CB   | 15:O:438:GLN:HG3  | 1.98                     | 0.92              |
| 1:A:1658:ALA:O    | 7:G:104:LEU:HA    | 1.70                     | 0.91              |
| 15:O:240:ILE:HG22 | 15:O:332:LEU:CD2  | 1.98                     | 0.91              |
| 6:F:74:ILE:HG23   | 6:F:75:PRO:HD2    | 1.51                     | 0.91              |
| 7:G:28:ILE:HG22   | 7:G:29:ASP:N      | 1.81                     | 0.91              |
| 2:B:894:LYS:H     | 12:L:54:ARG:HH21  | 0.92                     | 0.91              |
| 15:O:219:ARG:NH2  | 15:O:360:VAL:CG2  | 2.32                     | 0.91              |
| 15:O:408:PHE:HZ   | 15:O:446:LEU:CD1  | 1.74                     | 0.91              |
| 3:C:253:PRO:HB2   | 14:N:180:PHE:CD1  | 2.06                     | 0.91              |
| 3:C:52:ALA:O      | 3:C:301:ASN:HA    | 1.69                     | 0.91              |
| 15:O:390:GLN:NE2  | 15:O:609:TYR:HB3  | 1.86                     | 0.91              |
| 1:A:478:TYR:C     | 2:B:1047:ARG:O    | 2.08                     | 0.91              |
| 15:O:240:ILE:HG21 | 15:O:332:LEU:HD13 | 1.51                     | 0.91              |
| 1:A:1036:ASN:O    | 1:A:1049:MET:HA   | 1.71                     | 0.91              |
| 15:O:478:GLN:HE21 | 15:O:592:PHE:HZ   | 1.19                     | 0.91              |
| 1:A:412:SER:O     | 1:A:416:ARG:N     | 2.03                     | 0.90              |
| 2:B:42:VAL:HG11   | 2:B:46:ILE:HD11   | 1.52                     | 0.90              |
| 2:B:894:LYS:N     | 12:L:54:ARG:HH21  | 1.69                     | 0.90              |
| 2:B:472:SER:OG    | 2:B:476:LEU:HD12  | 1.71                     | 0.90              |
| 3:C:230:LEU:HD23  | 3:C:294:VAL:HG21  | 0.91                     | 0.90              |
| 15:O:342:HIS:CE1  | 15:O:346:GLN:HG3  | 2.05                     | 0.90              |
| 15:O:426:SER:OG   | 15:O:594:TYR:CB   | 2.18                     | 0.90              |
| 1:A:1055:ILE:HD11 | 1:A:1174:TYR:CE2  | 2.06                     | 0.90              |
| 15:O:240:ILE:CG2  | 15:O:332:LEU:HB2  | 2.01                     | 0.90              |
| 4:D:25:THR:HA     | 6:F:59:GLN:CG     | 1.99                     | 0.90              |
| 15:O:454:VAL:HA   | 15:O:514:PHE:HZ   | 1.34                     | 0.90              |
| 1:A:1048:PHE:HE2  | 5:E:211:TYR:H     | 1.11                     | 0.90              |
| 1:A:756:LYS:CD    | 9:I:85:LYS:HZ1    | 1.76                     | 0.90              |
| 15:O:471:LYS:HB2  | 15:O:585:PHE:HE1  | 1.00                     | 0.90              |
| 1:A:516:ILE:HG21  | 15:O:376:TYR:OH   | 1.72                     | 0.90              |
| 3:C:41:GLU:HB3    | 3:C:57:ILE:HG21   | 1.53                     | 0.90              |
| 4:D:28:PRO:HG2    | 7:G:24:VAL:CG1    | 2.01                     | 0.90              |
| 1:A:413:LEU:O     | 1:A:417:ARG:NE    | 2.05                     | 0.90              |
| 3:C:75:VAL:HG11   | 3:C:221:PRO:HD2   | 1.54                     | 0.90              |
| 15:O:158:LEU:HD23 | 15:O:172:HIS:CD2  | 2.07                     | 0.90              |
| 15:O:426:SER:CB   | 15:O:594:TYR:HB2  | 2.01                     | 0.90              |
| 15:O:432:LYS:HB2  | 15:O:609:TYR:C    | 1.93                     | 0.90              |
| 3:C:31:TRP:CG     | 11:K:82:LYS:HD2   | 2.06                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:86:PHE:CE1    | 12:L:64:LEU:HD13  | 2.07                     | 0.89              |
| 15:O:198:PHE:CG   | 15:O:236:LYS:HE3  | 2.06                     | 0.89              |
| 1:A:1226:VAL:O    | 1:A:1598:PHE:CD2  | 2.24                     | 0.89              |
| 7:G:158:LYS:HA    | 15:O:105:ASN:ND2  | 1.85                     | 0.89              |
| 15:O:194:LEU:O    | 15:O:232:LEU:HD21 | 1.72                     | 0.89              |
| 15:O:421:LEU:HD13 | 15:O:476:ALA:HB2  | 1.54                     | 0.89              |
| 2:B:478:LEU:HD13  | 2:B:484:TYR:CE1   | 2.06                     | 0.89              |
| 4:D:96:PHE:CE1    | 7:G:150:HIS:HB3   | 2.07                     | 0.89              |
| 1:A:1050:TYR:HE1  | 1:A:1185:VAL:CG1  | 1.83                     | 0.89              |
| 1:A:1179:ILE:HD11 | 1:A:1183:GLU:CG   | 2.01                     | 0.89              |
| 15:O:129:PRO:CG   | 15:O:132:THR:HB   | 2.01                     | 0.89              |
| 4:D:80:THR:HG21   | 15:O:227:PHE:HB3  | 1.53                     | 0.89              |
| 3:C:37:LYS:HD2    | 11:K:130:VAL:HG22 | 1.54                     | 0.89              |
| 2:B:42:VAL:CB     | 2:B:46:ILE:HD12   | 2.00                     | 0.89              |
| 15:O:432:LYS:CB   | 15:O:609:TYR:CA   | 2.41                     | 0.89              |
| 15:O:457:ARG:HA   | 15:O:460:GLU:HB2  | 1.54                     | 0.89              |
| 15:O:219:ARG:HH21 | 15:O:360:VAL:CG2  | 1.85                     | 0.89              |
| 1:A:891:ILE:CD1   | 9:I:71:LEU:HB2    | 2.03                     | 0.89              |
| 13:M:102:SER:O    | 13:M:106:LYS:HB2  | 1.73                     | 0.89              |
| 1:A:406:LEU:CD1   | 1:A:411:VAL:HB    | 2.03                     | 0.88              |
| 6:F:66:ARG:CZ     | 7:G:90:LEU:HD13   | 2.02                     | 0.88              |
| 2:B:894:LYS:HG2   | 12:L:47:ARG:CD    | 2.04                     | 0.88              |
| 3:C:58:ASN:H      | 3:C:296:ASN:C     | 1.75                     | 0.88              |
| 1:A:401:ASP:O     | 1:A:405:LYS:HB2   | 1.74                     | 0.88              |
| 3:C:56:LEU:HD11   | 3:C:300:PHE:CE1   | 2.08                     | 0.88              |
| 4:D:28:PRO:CG     | 7:G:24:VAL:HG11   | 2.03                     | 0.88              |
| 1:A:1348:VAL:CG2  | 2:B:268:GLU:O     | 2.21                     | 0.88              |
| 1:A:83:VAL:CG1    | 1:A:427:PHE:HE2   | 1.80                     | 0.88              |
| 1:A:1038:ILE:HG12 | 1:A:1049:MET:O    | 1.74                     | 0.88              |
| 15:O:521:ASN:HD22 | 15:O:524:VAL:H    | 1.22                     | 0.88              |
| 3:C:230:LEU:CD1   | 3:C:231:PRO:CD    | 2.52                     | 0.88              |
| 1:A:556:ALA:HB2   | 15:O:246:ASN:HD22 | 1.38                     | 0.88              |
| 2:B:769:PHE:CE1   | 2:B:798:PHE:CZ    | 2.61                     | 0.88              |
| 15:O:488:HIS:ND1  | 15:O:489:ASN:N    | 2.21                     | 0.88              |
| 15:O:488:HIS:O    | 15:O:490:ILE:N    | 2.06                     | 0.88              |
| 15:O:459:GLU:O    | 15:O:463:GLN:HG3  | 1.73                     | 0.87              |
| 3:C:75:VAL:CB     | 3:C:221:PRO:HD3   | 2.01                     | 0.87              |
| 3:C:230:LEU:CD1   | 3:C:231:PRO:HD2   | 2.04                     | 0.87              |
| 1:A:1662:ASN:HA   | 7:G:101:SER:HB2   | 1.57                     | 0.87              |
| 15:O:417:LYS:CD   | 15:O:472:HIS:CE1  | 2.57                     | 0.87              |
| 1:A:756:LYS:HD2   | 9:I:85:LYS:NZ     | 1.86                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:198:PHE:HD2  | 15:O:232:LEU:CG   | 1.86                     | 0.87              |
| 3:C:131:THR:CG2   | 3:C:209:ILE:CG2   | 2.51                     | 0.87              |
| 1:A:1055:ILE:HD12 | 1:A:1063:MET:SD   | 2.14                     | 0.87              |
| 1:A:475:ARG:HD3   | 2:B:1059:PRO:O    | 1.73                     | 0.87              |
| 7:G:158:LYS:HZ3   | 15:O:108:GLU:HG2  | 1.39                     | 0.87              |
| 1:A:862:THR:O     | 9:I:67:VAL:HG12   | 1.73                     | 0.87              |
| 1:A:1:MET:HA      | 2:B:1098:TYR:CD1  | 2.10                     | 0.87              |
| 3:C:75:VAL:CG1    | 3:C:221:PRO:HG3   | 2.03                     | 0.87              |
| 3:C:70:ILE:HD11   | 11:K:71:THR:CG2   | 2.04                     | 0.87              |
| 1:A:1660:VAL:HG22 | 7:G:103:LYS:O     | 1.75                     | 0.86              |
| 4:D:25:THR:O      | 6:F:59:GLN:HG3    | 1.75                     | 0.86              |
| 4:D:80:THR:CB     | 15:O:227:PHE:CD2  | 2.58                     | 0.86              |
| 1:A:1600:ARG:CD   | 1:A:1616:GLU:OE1  | 2.24                     | 0.86              |
| 1:A:636:HIS:ND1   | 2:B:1091:ARG:NH2  | 2.22                     | 0.86              |
| 11:K:66:VAL:HG12  | 11:K:67:GLU:HG2   | 1.57                     | 0.86              |
| 1:A:1348:VAL:HB   | 2:B:268:GLU:C     | 1.95                     | 0.86              |
| 3:C:56:LEU:HG     | 3:C:300:PHE:CD1   | 2.10                     | 0.86              |
| 1:A:408:LYS:CA    | 1:A:411:VAL:HG12  | 2.04                     | 0.86              |
| 7:G:143:SER:HB2   | 15:O:104:ILE:N    | 1.89                     | 0.86              |
| 3:C:31:TRP:CD2    | 11:K:82:LYS:HG3   | 2.10                     | 0.86              |
| 1:A:475:ARG:HH22  | 2:B:1061:LYS:HB2  | 1.36                     | 0.86              |
| 3:C:59:ILE:HG22   | 3:C:298:PHE:HD1   | 1.38                     | 0.86              |
| 1:A:878:ARG:HE    | 9:I:67:VAL:CG1    | 1.87                     | 0.86              |
| 1:A:1003:ARG:CZ   | 2:B:520:LEU:HB2   | 2.04                     | 0.86              |
| 3:C:31:TRP:HB3    | 11:K:82:LYS:CD    | 2.03                     | 0.86              |
| 15:O:366:THR:O    | 15:O:370:THR:HG23 | 1.75                     | 0.86              |
| 15:O:417:LYS:HB3  | 15:O:472:HIS:NE2  | 1.91                     | 0.86              |
| 1:A:620:ASN:OD1   | 1:A:667:ARG:NH2   | 2.07                     | 0.86              |
| 4:D:80:THR:CG2    | 15:O:227:PHE:HB3  | 2.06                     | 0.86              |
| 1:A:468:ARG:NE    | 1:A:1021:ARG:NH1  | 2.23                     | 0.86              |
| 7:G:141:SER:CA    | 15:O:138:TYR:OH   | 2.24                     | 0.86              |
| 15:O:521:ASN:ND2  | 15:O:523:ASN:H    | 1.74                     | 0.86              |
| 15:O:457:ARG:O    | 15:O:460:GLU:HB2  | 1.76                     | 0.85              |
| 15:O:458:GLU:CA   | 15:O:461:VAL:CG2  | 2.08                     | 0.85              |
| 1:A:1008:ASP:OD1  | 1:A:1202:LEU:CD2  | 2.24                     | 0.85              |
| 15:O:396:MET:HE1  | 15:O:434:LEU:HD12 | 1.57                     | 0.85              |
| 15:O:181:ARG:HH11 | 15:O:181:ARG:CB   | 1.89                     | 0.85              |
| 15:O:163:ILE:HG22 | 15:O:211:TYR:HB2  | 1.58                     | 0.85              |
| 1:A:1661:PRO:C    | 7:G:101:SER:O     | 2.13                     | 0.85              |
| 3:C:64:ALA:C      | 3:C:227:TYR:HE2   | 1.80                     | 0.85              |
| 15:O:408:PHE:CE2  | 15:O:446:LEU:CD1  | 2.50                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1060:GLU:HA   | 1:A:1063:MET:HG3  | 1.55                     | 0.84              |
| 15:O:369:LYS:HZ3  | 15:O:369:LYS:HB3  | 1.37                     | 0.84              |
| 1:A:392:THR:HB    | 1:A:430:ILE:HD13  | 1.59                     | 0.84              |
| 2:B:472:SER:HB3   | 2:B:476:LEU:HD12  | 1.57                     | 0.84              |
| 7:G:25:THR:HG22   | 7:G:26:ASN:H      | 1.40                     | 0.84              |
| 15:O:181:ARG:HB2  | 15:O:181:ARG:HH11 | 1.41                     | 0.84              |
| 15:O:237:ILE:HG22 | 15:O:381:ILE:HD12 | 1.60                     | 0.84              |
| 15:O:361:PHE:O    | 15:O:365:THR:HG23 | 1.78                     | 0.84              |
| 15:O:386:PHE:HD2  | 15:O:606:MET:HE1  | 1.41                     | 0.84              |
| 1:A:1055:ILE:HG23 | 1:A:1063:MET:SD   | 2.17                     | 0.84              |
| 3:C:253:PRO:HB2   | 14:N:180:PHE:HD1  | 1.41                     | 0.84              |
| 15:O:243:GLU:HA   | 15:O:246:ASN:ND2  | 1.90                     | 0.84              |
| 15:O:447:THR:HG22 | 15:O:480:LEU:HD22 | 1.58                     | 0.84              |
| 1:A:1019:LEU:HD12 | 1:A:1227:MET:HG3  | 1.58                     | 0.84              |
| 1:A:1600:ARG:HD2  | 1:A:1616:GLU:OE1  | 1.77                     | 0.84              |
| 1:A:436:ALA:HB2   | 1:A:443:ALA:HB2   | 0.86                     | 0.84              |
| 1:A:413:LEU:C     | 1:A:417:ARG:HH21  | 1.81                     | 0.84              |
| 2:B:472:SER:CB    | 2:B:476:LEU:CD1   | 2.54                     | 0.84              |
| 15:O:240:ILE:CB   | 15:O:332:LEU:HD13 | 2.07                     | 0.84              |
| 2:B:42:VAL:O      | 2:B:46:ILE:HD12   | 1.76                     | 0.84              |
| 2:B:37:LEU:HD13   | 2:B:760:TYR:CZ    | 2.12                     | 0.84              |
| 6:F:74:ILE:CG2    | 6:F:75:PRO:HD2    | 2.08                     | 0.84              |
| 4:D:96:PHE:HE1    | 7:G:150:HIS:CB    | 1.91                     | 0.84              |
| 15:O:422:GLN:NE2  | 15:O:592:PHE:CE2  | 2.45                     | 0.84              |
| 7:G:242:VAL:HG12  | 15:O:185:SER:OG   | 1.77                     | 0.83              |
| 1:A:1008:ASP:CG   | 1:A:1202:LEU:HD13 | 1.98                     | 0.83              |
| 2:B:894:LYS:O     | 2:B:896:GLN:N     | 2.11                     | 0.83              |
| 15:O:398:SER:O    | 15:O:401:VAL:HG12 | 1.79                     | 0.83              |
| 15:O:467:MET:HG3  | 15:O:519:PHE:CZ   | 2.13                     | 0.83              |
| 1:A:436:ALA:CA    | 1:A:443:ALA:HB2   | 2.09                     | 0.83              |
| 3:C:86:PHE:HE1    | 12:L:64:LEU:HD13  | 1.42                     | 0.83              |
| 1:A:863:ASN:ND2   | 9:I:68:LYS:N      | 2.25                     | 0.83              |
| 15:O:359:GLY:HA2  | 15:O:362:ASN:HD22 | 1.43                     | 0.83              |
| 1:A:990:ILE:HB    | 1:A:994:GLU:HB2   | 1.61                     | 0.83              |
| 1:A:990:ILE:CA    | 1:A:994:GLU:OE1   | 2.26                     | 0.83              |
| 3:C:51:GLU:HB3    | 3:C:303:GLU:CG    | 2.08                     | 0.83              |
| 15:O:240:ILE:HG21 | 15:O:332:LEU:CD1  | 2.08                     | 0.83              |
| 15:O:156:MET:CG   | 15:O:197:PHE:CZ   | 2.61                     | 0.83              |
| 15:O:370:THR:O    | 15:O:374:PRO:CD   | 2.25                     | 0.83              |
| 2:B:207:ILE:HG12  | 2:B:503:VAL:HG21  | 1.59                     | 0.83              |
| 15:O:242:VAL:HA   | 15:O:378:THR:HG21 | 1.60                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:390:GLN:NE2  | 15:O:432:LYS:N    | 2.25                     | 0.83              |
| 1:A:1026:GLN:OE1  | 1:A:1603:MET:HB2  | 1.78                     | 0.83              |
| 4:D:25:THR:CA     | 6:F:59:GLN:HG2    | 2.07                     | 0.83              |
| 15:O:428:ILE:CG2  | 15:O:439:ILE:HG21 | 2.09                     | 0.83              |
| 15:O:457:ARG:CA   | 15:O:460:GLU:HB2  | 2.09                     | 0.83              |
| 1:A:1:MET:HA      | 2:B:1098:TYR:CE1  | 2.13                     | 0.83              |
| 1:A:556:ALA:CB    | 15:O:246:ASN:HD22 | 1.90                     | 0.83              |
| 15:O:454:VAL:CA   | 15:O:514:PHE:CE2  | 2.62                     | 0.83              |
| 1:A:1654:PHE:CZ   | 6:F:92:ARG:HD3    | 2.14                     | 0.83              |
| 3:C:253:PRO:HG2   | 14:N:180:PHE:HB3  | 1.61                     | 0.83              |
| 1:A:1179:ILE:CD1  | 1:A:1183:GLU:HG3  | 2.09                     | 0.83              |
| 1:A:1603:MET:HE2  | 1:A:1615:TYR:CD2  | 2.14                     | 0.83              |
| 15:O:352:LEU:O    | 15:O:358:VAL:HG21 | 1.77                     | 0.83              |
| 15:O:488:HIS:CG   | 15:O:489:ASN:N    | 2.40                     | 0.83              |
| 1:A:1575:ILE:CG1  | 9:I:122:ARG:HH12  | 1.92                     | 0.82              |
| 15:O:242:VAL:N    | 15:O:378:THR:HG21 | 1.94                     | 0.82              |
| 15:O:440:ILE:HG23 | 15:O:491:PHE:CE1  | 2.13                     | 0.82              |
| 3:C:31:TRP:CG     | 11:K:82:LYS:NZ    | 2.44                     | 0.82              |
| 1:A:406:LEU:HD13  | 1:A:411:VAL:HB    | 1.60                     | 0.82              |
| 15:O:246:ASN:OD1  | 15:O:247:GLU:N    | 2.11                     | 0.82              |
| 3:C:55:ASP:HA     | 3:C:299:ILE:CA    | 2.07                     | 0.82              |
| 7:G:158:LYS:HD3   | 15:O:105:ASN:CB   | 2.09                     | 0.82              |
| 1:A:437:PHE:CZ    | 1:A:456:VAL:HG21  | 2.14                     | 0.82              |
| 4:D:25:THR:HB     | 6:F:59:GLN:NE2    | 1.94                     | 0.82              |
| 3:C:55:ASP:CA     | 3:C:299:ILE:HA    | 2.08                     | 0.82              |
| 1:A:1:MET:HG2     | 2:B:1098:TYR:CE2  | 2.12                     | 0.82              |
| 1:A:556:ALA:CB    | 15:O:246:ASN:ND2  | 2.41                     | 0.82              |
| 4:D:95:ASP:OD2    | 7:G:150:HIS:HA    | 1.80                     | 0.82              |
| 15:O:245:GLN:HG3  | 15:O:378:THR:CA   | 2.05                     | 0.82              |
| 4:D:25:THR:CA     | 6:F:59:GLN:CG     | 2.57                     | 0.82              |
| 7:G:158:LYS:NZ    | 15:O:108:GLU:HG2  | 1.95                     | 0.82              |
| 4:D:25:THR:HB     | 6:F:59:GLN:CD     | 2.00                     | 0.81              |
| 1:A:863:ASN:HD22  | 9:I:67:VAL:HA     | 1.45                     | 0.81              |
| 15:O:386:PHE:CD2  | 15:O:606:MET:CE   | 2.62                     | 0.81              |
| 15:O:457:ARG:C    | 15:O:460:GLU:HB2  | 2.01                     | 0.81              |
| 2:B:472:SER:HB3   | 2:B:476:LEU:CD1   | 2.11                     | 0.81              |
| 2:B:776:ILE:HB    | 2:B:1026:ILE:HD13 | 1.60                     | 0.81              |
| 15:O:162:PHE:HA   | 15:O:214:ASN:CB   | 2.09                     | 0.81              |
| 15:O:383:TYR:CD2  | 15:O:597:LEU:HD22 | 2.15                     | 0.81              |
| 1:A:50:TYR:HE1    | 1:A:368:ARG:O     | 1.64                     | 0.81              |
| 15:O:237:ILE:CG2  | 15:O:381:ILE:CD1  | 2.57                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:454:VAL:HA   | 15:O:514:PHE:CE2  | 2.15                     | 0.81              |
| 1:A:1011:VAL:HG13 | 1:A:1201:THR:O    | 1.80                     | 0.81              |
| 1:A:782:ASP:CG    | 1:A:931:SER:O     | 2.18                     | 0.81              |
| 1:A:1316:VAL:HG21 | 1:A:1498:ILE:HA   | 1.63                     | 0.81              |
| 4:D:80:THR:HG21   | 15:O:227:PHE:CD2  | 2.16                     | 0.81              |
| 3:C:253:PRO:O     | 14:N:180:PHE:CD1  | 2.34                     | 0.81              |
| 15:O:369:LYS:HE2  | 15:O:370:THR:CG2  | 2.10                     | 0.81              |
| 3:C:75:VAL:HG12   | 3:C:221:PRO:CG    | 2.11                     | 0.81              |
| 15:O:458:GLU:HA   | 15:O:461:VAL:HG21 | 1.59                     | 0.81              |
| 15:O:243:GLU:HA   | 15:O:246:ASN:HD21 | 1.46                     | 0.80              |
| 1:A:564:PRO:HG2   | 15:O:371:HIS:ND1  | 1.97                     | 0.80              |
| 1:A:966:LEU:HD22  | 1:A:997:PHE:HZ    | 1.44                     | 0.80              |
| 12:L:34:CYS:HB3   | 12:L:51:CYS:SG    | 2.21                     | 0.80              |
| 15:O:387:HIS:HB2  | 15:O:606:MET:SD   | 2.21                     | 0.80              |
| 1:A:1004:GLU:HA   | 1:A:1007:ILE:HD12 | 1.64                     | 0.80              |
| 2:B:208:VAL:HG23  | 2:B:401:GLU:HG2   | 1.64                     | 0.80              |
| 3:C:57:ILE:HA     | 3:C:297:HIS:CA    | 2.05                     | 0.80              |
| 4:D:92:ILE:CG2    | 4:D:96:PHE:CZ     | 2.63                     | 0.80              |
| 1:A:1000:MET:HG2  | 2:B:520:LEU:HD23  | 1.62                     | 0.80              |
| 3:C:56:LEU:HD12   | 3:C:300:PHE:HE1   | 1.46                     | 0.80              |
| 4:D:28:PRO:HD2    | 7:G:24:VAL:HG13   | 1.62                     | 0.80              |
| 3:C:37:LYS:HD2    | 11:K:130:VAL:CG2  | 2.11                     | 0.80              |
| 15:O:240:ILE:HG21 | 15:O:332:LEU:CG   | 2.11                     | 0.80              |
| 7:G:141:SER:HA    | 15:O:138:TYR:OH   | 1.82                     | 0.80              |
| 7:G:158:LYS:CD    | 15:O:105:ASN:CG   | 2.48                     | 0.80              |
| 3:C:75:VAL:HG21   | 3:C:221:PRO:HD2   | 1.64                     | 0.80              |
| 15:O:166:ILE:CD1  | 15:O:213:SER:OG   | 2.30                     | 0.80              |
| 6:F:75:PRO:CG     | 6:F:78:GLN:HB2    | 2.05                     | 0.79              |
| 1:A:996:TYR:O     | 1:A:1000:MET:HG3  | 1.83                     | 0.79              |
| 1:A:478:TYR:CE1   | 2:B:1049:THR:HG23 | 2.16                     | 0.79              |
| 3:C:71:MET:HE1    | 3:C:302:VAL:HG22  | 1.64                     | 0.79              |
| 1:A:1655:ASP:HB2  | 6:F:135:ARG:HB3   | 1.65                     | 0.79              |
| 3:C:31:TRP:HB2    | 11:K:82:LYS:HD2   | 1.59                     | 0.79              |
| 1:A:403:LEU:CD1   | 1:A:419:ILE:HG21  | 2.12                     | 0.79              |
| 15:O:234:ILE:HG21 | 15:O:371:HIS:CD2  | 2.18                     | 0.79              |
| 4:D:25:THR:CB     | 6:F:59:GLN:NE2    | 2.46                     | 0.79              |
| 15:O:436:ARG:O    | 15:O:440:ILE:HG13 | 1.82                     | 0.79              |
| 1:A:401:ASP:O     | 1:A:405:LYS:CB    | 2.31                     | 0.79              |
| 1:A:401:ASP:OD2   | 1:A:405:LYS:CE    | 2.31                     | 0.79              |
| 15:O:129:PRO:HG2  | 15:O:132:THR:HB   | 1.63                     | 0.79              |
| 2:B:480:GLN:N     | 2:B:480:GLN:OE1   | 2.14                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:584:GLN:OE1  | 15:O:584:GLN:N    | 2.11                     | 0.78              |
| 1:A:953:GLU:HA    | 1:A:1205:PHE:CD2  | 2.18                     | 0.78              |
| 1:A:638:PRO:HA    | 2:B:1090:ASP:OD2  | 1.82                     | 0.78              |
| 2:B:42:VAL:HG12   | 2:B:46:ILE:CG1    | 2.14                     | 0.78              |
| 3:C:253:PRO:CB    | 14:N:180:PHE:HD1  | 1.95                     | 0.78              |
| 2:B:566:TYR:HD2   | 13:M:73:SER:OG    | 1.66                     | 0.78              |
| 15:O:243:GLU:O    | 15:O:246:ASN:OD1  | 1.99                     | 0.78              |
| 15:O:372:VAL:C    | 15:O:374:PRO:HD2  | 2.04                     | 0.78              |
| 15:O:478:GLN:NE2  | 15:O:592:PHE:HZ   | 1.81                     | 0.78              |
| 1:A:249:THR:OG1   | 1:A:435:ASN:ND2   | 2.16                     | 0.78              |
| 2:B:75:ASP:HB3    | 2:B:440:PHE:CZ    | 2.17                     | 0.78              |
| 1:A:1348:VAL:HG11 | 2:B:268:GLU:HB2   | 1.66                     | 0.78              |
| 15:O:174:ASP:CA   | 15:O:177:LYS:HE2  | 2.12                     | 0.78              |
| 3:C:50:ARG:O      | 3:C:303:GLU:HA    | 1.84                     | 0.78              |
| 1:A:1344:ILE:HG22 | 2:B:333:LYS:HB3   | 1.66                     | 0.78              |
| 3:C:75:VAL:CG2    | 3:C:221:PRO:HD2   | 2.14                     | 0.78              |
| 4:D:23:HIS:CD2    | 6:F:58:PHE:CE2    | 2.71                     | 0.78              |
| 15:O:242:VAL:CA   | 15:O:378:THR:HG21 | 2.14                     | 0.78              |
| 15:O:373:LEU:CD1  | 15:O:416:LYS:HG3  | 2.13                     | 0.78              |
| 1:A:1604:GLU:O    | 1:A:1612:LYS:HE2  | 1.83                     | 0.78              |
| 2:B:934:ILE:HG22  | 3:C:72:ILE:HB     | 1.66                     | 0.78              |
| 15:O:129:PRO:HG2  | 15:O:132:THR:CB   | 2.14                     | 0.78              |
| 15:O:430:ARG:NH2  | 15:O:596:PRO:CD   | 2.44                     | 0.78              |
| 4:D:28:PRO:CG     | 7:G:24:VAL:CG1    | 2.62                     | 0.77              |
| 2:B:68:ILE:HD11   | 2:B:414:LYS:HG3   | 1.66                     | 0.77              |
| 2:B:1043:LYS:HD3  | 2:B:1063:ARG:NH2  | 1.97                     | 0.77              |
| 1:A:1344:ILE:HG22 | 2:B:333:LYS:CB    | 2.15                     | 0.77              |
| 7:G:154:ASN:HD21  | 15:O:182:MET:HE3  | 1.48                     | 0.77              |
| 1:A:1:MET:HB2     | 2:B:1098:TYR:CG   | 2.19                     | 0.77              |
| 1:A:475:ARG:CZ    | 2:B:1061:LYS:HB2  | 2.14                     | 0.77              |
| 2:B:467:THR:HB    | 2:B:469:ASN:ND2   | 2.00                     | 0.77              |
| 15:O:186:SER:O    | 15:O:190:ILE:HG22 | 1.84                     | 0.77              |
| 15:O:414:ALA:O    | 15:O:418:ILE:HD12 | 1.85                     | 0.77              |
| 1:A:1028:GLU:HG3  | 1:A:1029:GLY:N    | 2.00                     | 0.77              |
| 15:O:234:ILE:CG2  | 15:O:371:HIS:CD2  | 2.66                     | 0.77              |
| 15:O:386:PHE:CD2  | 15:O:606:MET:HE1  | 2.20                     | 0.77              |
| 1:A:1603:MET:CE   | 1:A:1615:TYR:CD2  | 2.68                     | 0.76              |
| 1:A:1662:ASN:CA   | 7:G:101:SER:HB2   | 2.13                     | 0.76              |
| 3:C:75:VAL:HG12   | 3:C:221:PRO:HG3   | 1.63                     | 0.76              |
| 9:I:60:LEU:HA     | 9:I:63:LYS:HG3    | 1.65                     | 0.76              |
| 15:O:359:GLY:O    | 15:O:363:THR:HG22 | 1.85                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:425:GLY:HA2  | 15:O:483:ILE:CD1  | 2.13                     | 0.76              |
| 2:B:878:GLU:OE2   | 2:B:909:ARG:NH1   | 2.17                     | 0.76              |
| 15:O:174:ASP:O    | 15:O:177:LYS:HG2  | 1.85                     | 0.76              |
| 15:O:240:ILE:HB   | 15:O:332:LEU:HD13 | 1.66                     | 0.76              |
| 1:A:437:PHE:HZ    | 1:A:456:VAL:CG2   | 1.98                     | 0.76              |
| 3:C:56:LEU:CD1    | 3:C:300:PHE:HE1   | 1.95                     | 0.76              |
| 15:O:360:VAL:O    | 15:O:364:LEU:HG   | 1.83                     | 0.76              |
| 3:C:75:VAL:CG1    | 3:C:221:PRO:HD3   | 2.10                     | 0.76              |
| 2:B:328:GLN:HE22  | 13:M:109:ARG:HH21 | 1.31                     | 0.76              |
| 15:O:62:ASP:HB3   | 15:O:67:ASP:OD2   | 1.86                     | 0.76              |
| 1:A:438:ILE:HG23  | 2:B:1192:MET:HG2  | 1.68                     | 0.76              |
| 3:C:55:ASP:OD1    | 3:C:299:ILE:CG1   | 2.34                     | 0.76              |
| 15:O:432:LYS:CB   | 15:O:609:TYR:C    | 2.54                     | 0.76              |
| 15:O:484:PHE:CE1  | 15:O:502:LEU:CD1  | 2.69                     | 0.76              |
| 1:A:502:ALA:HB1   | 1:A:581:ILE:HG22  | 1.64                     | 0.76              |
| 2:B:1069:ILE:HG22 | 2:B:1070:ARG:H    | 1.50                     | 0.76              |
| 1:A:641:GLU:HB2   | 6:F:99:LEU:HD13   | 1.68                     | 0.76              |
| 15:O:158:LEU:CD2  | 15:O:172:HIS:CD2  | 2.67                     | 0.76              |
| 1:A:478:TYR:CE2   | 2:B:1049:THR:CG2  | 2.68                     | 0.76              |
| 15:O:454:VAL:CA   | 15:O:514:PHE:CZ   | 2.67                     | 0.76              |
| 3:C:131:THR:HG23  | 3:C:209:ILE:HG23  | 1.68                     | 0.76              |
| 7:G:159:LYS:H     | 15:O:105:ASN:HD22 | 1.32                     | 0.76              |
| 1:A:1055:ILE:CG2  | 1:A:1060:GLU:HG3  | 2.16                     | 0.76              |
| 3:C:70:ILE:HD11   | 11:K:71:THR:HG21  | 1.67                     | 0.76              |
| 7:G:154:ASN:OD1   | 15:O:183:ILE:HG12 | 1.85                     | 0.76              |
| 1:A:1052:GLY:O    | 5:E:205:SER:HB2   | 1.85                     | 0.76              |
| 1:A:1050:TYR:CD1  | 1:A:1185:VAL:HG11 | 2.20                     | 0.75              |
| 1:A:878:ARG:NE    | 9:I:67:VAL:CG1    | 2.48                     | 0.75              |
| 2:B:769:PHE:HE1   | 2:B:798:PHE:CZ    | 2.03                     | 0.75              |
| 15:O:219:ARG:HH22 | 15:O:360:VAL:HG21 | 1.47                     | 0.75              |
| 15:O:371:HIS:C    | 15:O:374:PRO:HD2  | 2.06                     | 0.75              |
| 6:F:66:ARG:NH2    | 7:G:90:LEU:HD13   | 2.01                     | 0.75              |
| 15:O:359:GLY:HA2  | 15:O:362:ASN:ND2  | 2.01                     | 0.75              |
| 1:A:1019:LEU:CD1  | 1:A:1227:MET:HG3  | 2.17                     | 0.75              |
| 15:O:166:ILE:HD13 | 15:O:213:SER:OG   | 1.86                     | 0.75              |
| 1:A:891:ILE:HD13  | 9:I:71:LEU:HB2    | 1.68                     | 0.75              |
| 1:A:1048:PHE:HE2  | 5:E:211:TYR:N     | 1.83                     | 0.75              |
| 15:O:428:ILE:HD12 | 15:O:439:ILE:CG2  | 2.16                     | 0.75              |
| 1:A:1048:PHE:CE2  | 5:E:211:TYR:N     | 2.53                     | 0.75              |
| 2:B:42:VAL:HB     | 2:B:46:ILE:HD11   | 1.51                     | 0.75              |
| 2:B:207:ILE:CG1   | 2:B:503:VAL:HG22  | 2.04                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:131:THR:HG22  | 3:C:208:CYS:O     | 1.86                     | 0.75              |
| 4:D:44:ILE:HG21   | 4:D:90:LYS:HE3    | 1.69                     | 0.75              |
| 15:O:230:TRP:CE2  | 15:O:364:LEU:HD21 | 2.20                     | 0.75              |
| 7:G:154:ASN:HD21  | 15:O:182:MET:HE1  | 1.51                     | 0.75              |
| 15:O:198:PHE:CE2  | 15:O:232:LEU:HG   | 2.22                     | 0.75              |
| 15:O:342:HIS:NE2  | 15:O:346:GLN:NE2  | 2.34                     | 0.75              |
| 3:C:31:TRP:CB     | 11:K:82:LYS:CD    | 2.51                     | 0.74              |
| 1:A:437:PHE:CE1   | 1:A:456:VAL:CG2   | 2.58                     | 0.74              |
| 15:O:101:SER:HB3  | 15:O:142:ILE:HD12 | 1.69                     | 0.74              |
| 15:O:484:PHE:CE1  | 15:O:502:LEU:HD12 | 2.21                     | 0.74              |
| 15:O:440:ILE:CG2  | 15:O:491:PHE:HE1  | 2.01                     | 0.74              |
| 1:A:1348:VAL:CG1  | 2:B:268:GLU:HB2   | 2.18                     | 0.74              |
| 3:C:45:SER:CB     | 3:C:271:ARG:NH2   | 2.49                     | 0.74              |
| 4:D:96:PHE:HE1    | 7:G:150:HIS:CG    | 2.04                     | 0.74              |
| 1:A:1575:ILE:HG12 | 9:I:122:ARG:HH12  | 1.52                     | 0.74              |
| 15:O:241:ASP:OD1  | 15:O:378:THR:CG2  | 2.33                     | 0.74              |
| 1:A:556:ALA:HB1   | 15:O:243:GLU:OE2  | 1.88                     | 0.74              |
| 3:C:64:ALA:O      | 3:C:227:TYR:HE2   | 1.69                     | 0.74              |
| 15:O:369:LYS:HE2  | 15:O:370:THR:HG23 | 1.67                     | 0.74              |
| 4:D:25:THR:HG22   | 6:F:59:GLN:NE2    | 1.93                     | 0.74              |
| 15:O:143:LEU:HD11 | 15:O:150:TRP:CD1  | 2.22                     | 0.74              |
| 15:O:374:PRO:HG2  | 15:O:375:THR:HG23 | 1.69                     | 0.74              |
| 15:O:484:PHE:HE1  | 15:O:502:LEU:HD12 | 1.52                     | 0.74              |
| 3:C:82:TYR:CD1    | 12:L:68:GLU:HG3   | 2.22                     | 0.74              |
| 15:O:238:ILE:HD11 | 15:O:371:HIS:HB3  | 1.70                     | 0.74              |
| 15:O:390:GLN:HE22 | 15:O:432:LYS:N    | 1.86                     | 0.74              |
| 15:O:421:LEU:CD1  | 15:O:476:ALA:HB2  | 2.18                     | 0.74              |
| 2:B:401:GLU:HG3   | 2:B:402:VAL:N     | 2.03                     | 0.74              |
| 15:O:407:SER:HB2  | 15:O:408:PHE:CD1  | 2.22                     | 0.74              |
| 1:A:411:VAL:HG22  | 1:A:412:SER:H     | 1.52                     | 0.73              |
| 2:B:42:VAL:HB     | 2:B:46:ILE:HD12   | 1.59                     | 0.73              |
| 2:B:518:ARG:NH2   | 2:B:537:SER:O     | 2.21                     | 0.73              |
| 15:O:371:HIS:O    | 15:O:374:PRO:HD2  | 1.88                     | 0.73              |
| 4:D:37:LEU:HD22   | 4:D:97:LYS:HE3    | 1.70                     | 0.73              |
| 1:A:1048:PHE:HB2  | 5:E:208:TYR:OH    | 1.89                     | 0.73              |
| 15:O:245:GLN:HA   | 15:O:245:GLN:HE21 | 1.51                     | 0.73              |
| 15:O:423:TYR:CD1  | 15:O:594:TYR:CE2  | 2.72                     | 0.73              |
| 1:A:527:PRO:O     | 1:A:580:HIS:CE1   | 2.41                     | 0.73              |
| 3:C:64:ALA:C      | 3:C:227:TYR:CE2   | 2.60                     | 0.73              |
| 4:D:25:THR:HB     | 6:F:59:GLN:CG     | 2.19                     | 0.73              |
| 15:O:432:LYS:HG2  | 15:O:608:GLU:C    | 2.07                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:478:LEU:HD13  | 2:B:484:TYR:HE1   | 1.50                     | 0.73              |
| 3:C:55:ASP:OD1    | 3:C:299:ILE:HG23  | 1.88                     | 0.73              |
| 2:B:1020:GLU:HG2  | 3:C:61:THR:HG21   | 1.70                     | 0.73              |
| 3:C:253:PRO:O     | 14:N:180:PHE:CE1  | 2.41                     | 0.73              |
| 7:G:143:SER:OG    | 15:O:101:SER:O    | 2.06                     | 0.73              |
| 7:G:144:HIS:NE2   | 15:O:145:SER:CB   | 2.51                     | 0.73              |
| 15:O:120:ILE:CD1  | 15:O:150:TRP:CE3  | 2.71                     | 0.73              |
| 15:O:194:LEU:CD2  | 15:O:225:LEU:HD11 | 2.19                     | 0.73              |
| 7:G:28:ILE:CG2    | 7:G:29:ASP:H      | 1.89                     | 0.73              |
| 15:O:201:LYS:HD3  | 15:O:239:SER:OG   | 1.88                     | 0.73              |
| 15:O:241:ASP:C    | 15:O:378:THR:HG21 | 2.08                     | 0.73              |
| 15:O:373:LEU:HD11 | 15:O:416:LYS:HG2  | 1.65                     | 0.73              |
| 15:O:237:ILE:HG22 | 15:O:381:ILE:HB   | 1.71                     | 0.73              |
| 15:O:356:GLU:O    | 15:O:360:VAL:HG23 | 1.88                     | 0.73              |
| 3:C:56:LEU:HG     | 3:C:300:PHE:HD1   | 1.53                     | 0.73              |
| 4:D:92:ILE:HG12   | 7:G:152:ALA:CB    | 2.16                     | 0.73              |
| 1:A:1305:GLU:OE2  | 9:I:63:LYS:NZ     | 2.16                     | 0.72              |
| 2:B:552:SER:O     | 2:B:647:SER:N     | 2.21                     | 0.72              |
| 15:O:152:GLN:HG3  | 15:O:193:TYR:OH   | 1.89                     | 0.72              |
| 15:O:156:MET:SD   | 15:O:197:PHE:CE2  | 2.82                     | 0.72              |
| 15:O:348:THR:CG2  | 15:O:351:SER:HB3  | 2.19                     | 0.72              |
| 1:A:50:TYR:CE1    | 1:A:368:ARG:O     | 2.42                     | 0.72              |
| 15:O:162:PHE:O    | 15:O:210:ASN:C    | 2.27                     | 0.72              |
| 15:O:234:ILE:HG22 | 15:O:371:HIS:HD2  | 1.53                     | 0.72              |
| 15:O:447:THR:O    | 15:O:450:LEU:CB   | 2.33                     | 0.72              |
| 15:O:390:GLN:HE21 | 15:O:432:LYS:H    | 1.38                     | 0.72              |
| 1:A:509:GLU:CD    | 1:A:579:ARG:HE    | 1.92                     | 0.72              |
| 2:B:207:ILE:CD1   | 2:B:503:VAL:CG2   | 2.68                     | 0.72              |
| 15:O:352:LEU:CA   | 15:O:358:VAL:HG23 | 2.19                     | 0.72              |
| 4:D:23:HIS:CD2    | 6:F:58:PHE:CZ     | 2.78                     | 0.72              |
| 1:A:413:LEU:CB    | 1:A:417:ARG:HH21  | 2.03                     | 0.72              |
| 14:N:85:HIS:CE1   | 14:N:141:GLU:CD   | 2.60                     | 0.72              |
| 15:O:488:HIS:CD2  | 15:O:489:ASN:OD1  | 2.42                     | 0.72              |
| 1:A:1056:ASP:OD1  | 1:A:1179:ILE:HD13 | 1.90                     | 0.72              |
| 2:B:938:PHE:CE1   | 3:C:68:ARG:CZ     | 2.73                     | 0.72              |
| 2:B:938:PHE:CZ    | 3:C:68:ARG:HD2    | 2.24                     | 0.72              |
| 1:A:878:ARG:HE    | 9:I:67:VAL:HG12   | 1.53                     | 0.72              |
| 2:B:207:ILE:CD1   | 2:B:503:VAL:HG21  | 2.20                     | 0.72              |
| 3:C:56:LEU:CB     | 3:C:298:PHE:HB2   | 2.17                     | 0.72              |
| 4:D:23:HIS:HD2    | 6:F:58:PHE:CZ     | 2.07                     | 0.72              |
| 15:O:225:LEU:HD13 | 15:O:225:LEU:O    | 1.89                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:478:TYR:CA    | 2:B:1048:SER:CA   | 2.34                     | 0.71              |
| 3:C:45:SER:CB     | 3:C:271:ARG:HH22  | 2.03                     | 0.71              |
| 12:L:68:GLU:HG2   | 12:L:69:ALA:N     | 2.01                     | 0.71              |
| 15:O:432:LYS:HB3  | 15:O:609:TYR:HA   | 0.81                     | 0.71              |
| 1:A:1055:ILE:CD1  | 1:A:1063:MET:CE   | 2.67                     | 0.71              |
| 2:B:152:LEU:HD13  | 2:B:443:LYS:HG3   | 1.71                     | 0.71              |
| 3:C:54:PHE:O      | 3:C:299:ILE:HA    | 1.90                     | 0.71              |
| 15:O:158:LEU:HD22 | 15:O:172:HIS:HA   | 1.71                     | 0.71              |
| 1:A:411:VAL:HG22  | 1:A:412:SER:N     | 2.05                     | 0.71              |
| 1:A:1003:ARG:HD2  | 2:B:520:LEU:H     | 1.56                     | 0.71              |
| 1:A:527:PRO:O     | 1:A:580:HIS:HE1   | 1.73                     | 0.71              |
| 2:B:1069:ILE:HD12 | 2:B:1069:ILE:N    | 2.05                     | 0.71              |
| 2:B:281:CYS:HA    | 2:B:323:ARG:HD2   | 1.72                     | 0.71              |
| 15:O:361:PHE:CE1  | 15:O:365:THR:HG21 | 2.24                     | 0.71              |
| 1:A:524:ILE:O     | 1:A:554:ARG:NH1   | 2.23                     | 0.71              |
| 2:B:1069:ILE:HG22 | 2:B:1070:ARG:N    | 2.03                     | 0.71              |
| 3:C:52:ALA:O      | 3:C:301:ASN:OD1   | 2.07                     | 0.71              |
| 1:A:478:TYR:CD1   | 2:B:1048:SER:HB2  | 2.25                     | 0.71              |
| 1:A:1048:PHE:CD2  | 5:E:210:SER:HA    | 2.26                     | 0.71              |
| 4:D:92:ILE:CG1    | 7:G:152:ALA:HB2   | 2.16                     | 0.71              |
| 15:O:128:LEU:HB3  | 15:O:129:PRO:CD   | 2.21                     | 0.71              |
| 15:O:163:ILE:HA   | 15:O:211:TYR:N    | 1.97                     | 0.71              |
| 1:A:468:ARG:NE    | 1:A:1021:ARG:HH12 | 1.89                     | 0.71              |
| 1:A:1038:ILE:HD11 | 1:A:1050:TYR:HA   | 1.71                     | 0.71              |
| 3:C:62:SER:HB2    | 11:K:74:ASN:CG    | 2.10                     | 0.71              |
| 1:A:83:VAL:CG2    | 1:A:427:PHE:HE2   | 2.03                     | 0.71              |
| 2:B:211:ARG:NH2   | 2:B:239:VAL:HG21  | 2.06                     | 0.71              |
| 3:C:31:TRP:CE3    | 11:K:82:LYS:CG    | 2.69                     | 0.71              |
| 3:C:70:ILE:HD11   | 11:K:71:THR:HG23  | 1.71                     | 0.71              |
| 6:F:106:PRO:HG2   | 7:G:55:GLU:HG3    | 1.73                     | 0.71              |
| 15:O:352:LEU:O    | 15:O:358:VAL:CG2  | 2.39                     | 0.71              |
| 1:A:990:ILE:HB    | 1:A:994:GLU:CB    | 2.21                     | 0.70              |
| 2:B:1165:ASN:N    | 2:B:1165:ASN:OD1  | 2.24                     | 0.70              |
| 2:B:470:LEU:HB2   | 2:B:484:TYR:CE2   | 2.26                     | 0.70              |
| 3:C:54:PHE:CE2    | 3:C:300:PHE:CG    | 2.78                     | 0.70              |
| 15:O:198:PHE:CE1  | 15:O:236:LYS:HG3  | 2.25                     | 0.70              |
| 15:O:152:GLN:HG2  | 15:O:193:TYR:HH   | 1.53                     | 0.70              |
| 15:O:459:GLU:O    | 15:O:463:GLN:CG   | 2.37                     | 0.70              |
| 3:C:64:ALA:CB     | 3:C:298:PHE:CE2   | 2.73                     | 0.70              |
| 9:I:2:SER:HB2     | 9:I:11:LEU:HD21   | 1.72                     | 0.70              |
| 15:O:373:LEU:N    | 15:O:374:PRO:CD   | 2.54                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:447:THR:CG2  | 15:O:480:LEU:HD22 | 2.21                     | 0.70              |
| 1:A:891:ILE:HD12  | 9:I:71:LEU:HB2    | 1.71                     | 0.70              |
| 3:C:71:MET:HE1    | 3:C:225:ALA:CB    | 2.21                     | 0.70              |
| 7:G:158:LYS:HD3   | 15:O:105:ASN:HB3  | 1.72                     | 0.70              |
| 1:A:438:ILE:HG23  | 2:B:1192:MET:HE3  | 1.73                     | 0.70              |
| 2:B:894:LYS:N     | 12:L:54:ARG:NH2   | 2.34                     | 0.70              |
| 7:G:159:LYS:H     | 15:O:105:ASN:ND2  | 1.89                     | 0.70              |
| 15:O:225:LEU:O    | 15:O:227:PHE:N    | 2.24                     | 0.70              |
| 4:D:80:THR:HG21   | 15:O:227:PHE:HD2  | 1.56                     | 0.70              |
| 15:O:428:ILE:O    | 15:O:487:ARG:NE   | 2.24                     | 0.70              |
| 1:A:1246:VAL:O    | 1:A:1517:ARG:NH2  | 2.25                     | 0.70              |
| 15:O:373:LEU:O    | 15:O:373:LEU:HD12 | 1.91                     | 0.70              |
| 1:A:436:ALA:HB1   | 1:A:443:ALA:CB    | 2.19                     | 0.70              |
| 1:A:478:TYR:CE2   | 2:B:1049:THR:HG22 | 2.27                     | 0.70              |
| 15:O:426:SER:HG   | 15:O:594:TYR:HB2  | 1.54                     | 0.70              |
| 3:C:223:SER:O     | 3:C:224:THR:HB    | 1.92                     | 0.70              |
| 2:B:291:GLY:HA3   | 2:B:375:LEU:HD13  | 1.74                     | 0.70              |
| 1:A:1055:ILE:CD1  | 1:A:1063:MET:HE3  | 2.20                     | 0.69              |
| 1:A:436:ALA:O     | 1:A:440:SER:HA    | 1.91                     | 0.69              |
| 2:B:64:GLY:O      | 2:B:68:ILE:HG13   | 1.92                     | 0.69              |
| 3:C:54:PHE:N      | 3:C:300:PHE:O     | 2.21                     | 0.69              |
| 13:M:38:PHE:HB3   | 13:M:53:LEU:HD11  | 1.73                     | 0.69              |
| 15:O:369:LYS:HB3  | 15:O:369:LYS:NZ   | 2.04                     | 0.69              |
| 1:A:1348:VAL:HG23 | 2:B:268:GLU:O     | 1.91                     | 0.69              |
| 1:A:406:LEU:CD1   | 1:A:411:VAL:CB    | 2.71                     | 0.69              |
| 1:A:438:ILE:CG2   | 2:B:1192:MET:HG2  | 2.23                     | 0.69              |
| 1:A:782:ASP:OD1   | 1:A:931:SER:O     | 2.10                     | 0.69              |
| 1:A:1049:MET:HG2  | 1:A:1050:TYR:H    | 1.55                     | 0.69              |
| 2:B:211:ARG:CG    | 2:B:401:GLU:OE1   | 2.39                     | 0.69              |
| 2:B:42:VAL:HG12   | 2:B:46:ILE:HG13   | 1.73                     | 0.69              |
| 1:A:99:ARG:O      | 1:A:109:ARG:NH2   | 2.24                     | 0.69              |
| 2:B:300:SER:OG    | 9:I:49:THR:HG22   | 1.92                     | 0.69              |
| 7:G:156:SER:CB    | 15:O:146:SER:HA   | 2.22                     | 0.69              |
| 15:O:220:GLY:O    | 15:O:221:TYR:CD1  | 2.46                     | 0.69              |
| 1:A:1:MET:CA      | 2:B:1098:TYR:CD1  | 2.75                     | 0.69              |
| 4:D:99:LEU:HB3    | 4:D:100:PRO:CD    | 2.22                     | 0.69              |
| 15:O:369:LYS:O    | 15:O:373:LEU:CB   | 2.41                     | 0.69              |
| 3:C:31:TRP:CG     | 11:K:82:LYS:CD    | 2.76                     | 0.69              |
| 1:A:478:TYR:CA    | 2:B:1047:ARG:O    | 2.41                     | 0.69              |
| 3:C:41:GLU:HB3    | 3:C:57:ILE:HG22   | 1.74                     | 0.69              |
| 3:C:253:PRO:HB2   | 14:N:180:PHE:CB   | 2.22                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:982:VAL:HG13  | 1:A:994:GLU:OE2   | 1.92                     | 0.69              |
| 1:A:1573:TYR:O    | 9:I:122:ARG:NH2   | 2.26                     | 0.69              |
| 15:O:417:LYS:HD3  | 15:O:472:HIS:HE1  | 1.57                     | 0.69              |
| 1:A:1348:VAL:HG23 | 2:B:269:TYR:HA    | 1.75                     | 0.68              |
| 4:D:48:GLU:CG     | 4:D:86:ILE:CD1    | 2.71                     | 0.68              |
| 2:B:1002:LYS:HD2  | 14:N:166:LEU:HB2  | 1.74                     | 0.68              |
| 2:B:769:PHE:CD1   | 2:B:798:PHE:CE1   | 2.68                     | 0.68              |
| 4:D:25:THR:CB     | 6:F:59:GLN:CG     | 2.71                     | 0.68              |
| 15:O:174:ASP:HA   | 15:O:177:LYS:CE   | 2.22                     | 0.68              |
| 2:B:566:TYR:HB3   | 13:M:74:ASN:OD1   | 1.94                     | 0.68              |
| 15:O:390:GLN:CB   | 15:O:609:TYR:CD1  | 2.76                     | 0.68              |
| 1:A:432:ASN:HD21  | 1:A:444:GLN:H     | 1.38                     | 0.68              |
| 3:C:71:MET:CE     | 3:C:225:ALA:CB    | 2.71                     | 0.68              |
| 3:C:64:ALA:HB1    | 3:C:227:TYR:CE2   | 2.29                     | 0.68              |
| 15:O:430:ARG:HH21 | 15:O:596:PRO:HD3  | 1.55                     | 0.68              |
| 2:B:934:ILE:CG2   | 3:C:73:SER:HB3    | 2.24                     | 0.68              |
| 3:C:55:ASP:HB3    | 3:C:297:HIS:CD2   | 2.28                     | 0.68              |
| 2:B:1043:LYS:HG3  | 2:B:1063:ARG:NE   | 2.09                     | 0.68              |
| 4:D:80:THR:CG2    | 15:O:227:PHE:CD2  | 2.76                     | 0.68              |
| 15:O:241:ASP:CG   | 15:O:380:SER:HB2  | 2.14                     | 0.68              |
| 15:O:430:ARG:HH22 | 15:O:596:PRO:HD3  | 1.58                     | 0.68              |
| 1:A:35:PRO:HA     | 1:A:390:LEU:CD1   | 2.24                     | 0.68              |
| 3:C:54:PHE:O      | 3:C:299:ILE:C     | 2.32                     | 0.68              |
| 1:A:209:THR:HG21  | 5:E:173:SER:OG    | 1.93                     | 0.68              |
| 15:O:343:VAL:CG1  | 15:O:388:VAL:CG2  | 2.71                     | 0.68              |
| 2:B:207:ILE:HD11  | 2:B:503:VAL:CG1   | 2.25                     | 0.68              |
| 3:C:52:ALA:O      | 3:C:301:ASN:CG    | 2.31                     | 0.68              |
| 15:O:237:ILE:CB   | 15:O:381:ILE:CD1  | 2.57                     | 0.68              |
| 2:B:938:PHE:CE1   | 3:C:68:ARG:NE     | 2.61                     | 0.67              |
| 1:A:572:THR:HA    | 7:G:52:MET:CE     | 2.23                     | 0.67              |
| 15:O:368:PHE:O    | 15:O:372:VAL:HG23 | 1.94                     | 0.67              |
| 3:C:57:ILE:HD12   | 3:C:297:HIS:CE1   | 2.29                     | 0.67              |
| 15:O:474:TYR:HB3  | 15:O:520:CYS:SG   | 2.33                     | 0.67              |
| 2:B:566:TYR:CE2   | 13:M:70:SER:HA    | 2.30                     | 0.67              |
| 3:C:57:ILE:CD1    | 3:C:297:HIS:ND1   | 2.56                     | 0.67              |
| 5:E:76:GLY:HA3    | 5:E:106:GLN:HB2   | 1.76                     | 0.67              |
| 15:O:458:GLU:HG3  | 15:O:514:PHE:CZ   | 2.28                     | 0.67              |
| 3:C:71:MET:HE1    | 3:C:225:ALA:HB2   | 1.75                     | 0.67              |
| 15:O:66:ASN:N     | 15:O:66:ASN:HD22  | 1.89                     | 0.67              |
| 1:A:436:ALA:HB2   | 1:A:443:ALA:HB1   | 1.66                     | 0.67              |
| 1:A:381:SER:HB2   | 1:A:453:ILE:CG2   | 2.24                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1043:LYS:CG   | 2:B:1063:ARG:CZ   | 2.68                     | 0.67              |
| 15:O:241:ASP:C    | 15:O:378:THR:CG2  | 2.63                     | 0.67              |
| 15:O:431:ALA:HB1  | 15:O:434:LEU:CD1  | 2.20                     | 0.67              |
| 1:A:81:LEU:HB2    | 1:A:358:ASP:O     | 1.94                     | 0.67              |
| 4:D:48:GLU:HG2    | 4:D:86:ILE:HD11   | 1.76                     | 0.67              |
| 1:A:1006:LEU:HB3  | 2:B:539:CYS:SG    | 2.34                     | 0.67              |
| 15:O:471:LYS:HB2  | 15:O:585:PHE:CZ   | 2.25                     | 0.67              |
| 1:A:1344:ILE:HG21 | 2:B:333:LYS:HG3   | 1.76                     | 0.67              |
| 3:C:71:MET:O      | 3:C:222:VAL:HG21  | 1.94                     | 0.67              |
| 1:A:1556:GLU:OE2  | 5:E:212:ARG:NH1   | 2.28                     | 0.67              |
| 15:O:371:HIS:O    | 15:O:374:PRO:HG2  | 1.95                     | 0.67              |
| 1:A:1011:VAL:C    | 1:A:1201:THR:HG21 | 2.15                     | 0.67              |
| 1:A:356:PHE:C     | 1:A:357:MET:HG3   | 2.14                     | 0.67              |
| 1:A:406:LEU:HD12  | 1:A:406:LEU:O     | 1.94                     | 0.67              |
| 3:C:84:TYR:HD2    | 12:L:66:GLN:HB2   | 1.59                     | 0.67              |
| 15:O:108:GLU:HB2  | 15:O:147:ILE:HD11 | 1.76                     | 0.67              |
| 1:A:1027:LEU:O    | 1:A:1028:GLU:HG2  | 1.95                     | 0.66              |
| 2:B:470:LEU:HD22  | 2:B:484:TYR:OH    | 1.95                     | 0.66              |
| 3:C:253:PRO:CG    | 14:N:180:PHE:HB3  | 2.25                     | 0.66              |
| 3:C:86:PHE:HE1    | 12:L:64:LEU:CD1   | 2.08                     | 0.66              |
| 15:O:371:HIS:O    | 15:O:374:PRO:CG   | 2.43                     | 0.66              |
| 2:B:207:ILE:HD11  | 2:B:503:VAL:HG11  | 1.76                     | 0.66              |
| 15:O:240:ILE:CG2  | 15:O:332:LEU:CD1  | 2.67                     | 0.66              |
| 15:O:390:GLN:CD   | 15:O:609:TYR:HB3  | 2.15                     | 0.66              |
| 1:A:1050:TYR:CE1  | 1:A:1185:VAL:HG12 | 2.29                     | 0.66              |
| 3:C:131:THR:CG2   | 3:C:209:ILE:HG23  | 2.25                     | 0.66              |
| 4:D:25:THR:CA     | 6:F:59:GLN:HG3    | 2.24                     | 0.66              |
| 13:M:101:VAL:HG12 | 13:M:106:LYS:HG3  | 1.72                     | 0.66              |
| 15:O:390:GLN:HB3  | 15:O:609:TYR:CD1  | 2.30                     | 0.66              |
| 1:A:113:VAL:HG21  | 1:A:178:LEU:HD13  | 1.77                     | 0.66              |
| 3:C:223:SER:HB2   | 3:C:303:GLU:HB3   | 1.76                     | 0.66              |
| 4:D:96:PHE:CE1    | 7:G:150:HIS:CG    | 2.83                     | 0.66              |
| 1:A:863:ASN:HD22  | 9:I:67:VAL:CA     | 2.07                     | 0.66              |
| 15:O:240:ILE:CG2  | 15:O:332:LEU:CD2  | 2.63                     | 0.66              |
| 1:A:437:PHE:O     | 1:A:455:GLY:HA3   | 1.96                     | 0.66              |
| 7:G:242:VAL:HG21  | 15:O:183:ILE:CG2  | 2.26                     | 0.66              |
| 15:O:434:LEU:HD12 | 15:O:434:LEU:N    | 2.10                     | 0.66              |
| 1:A:403:LEU:HD12  | 1:A:419:ILE:HG21  | 1.77                     | 0.66              |
| 15:O:428:ILE:HG23 | 15:O:439:ILE:CG2  | 2.23                     | 0.66              |
| 1:A:1000:MET:CG   | 2:B:520:LEU:HD23  | 2.26                     | 0.66              |
| 1:A:1344:ILE:CG2  | 2:B:333:LYS:HG3   | 2.26                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:109:ARG:NH1   | 1:A:230:ARG:O     | 2.29                     | 0.66              |
| 15:O:454:VAL:HG23 | 15:O:458:GLU:HG3  | 1.77                     | 0.66              |
| 1:A:403:LEU:CD1   | 1:A:419:ILE:CG2   | 2.74                     | 0.66              |
| 15:O:247:GLU:OE1  | 15:O:325:ILE:HG13 | 1.95                     | 0.66              |
| 2:B:209:GLN:HG2   | 2:B:210:ARG:N     | 2.07                     | 0.65              |
| 2:B:209:GLN:O     | 2:B:401:GLU:N     | 2.27                     | 0.65              |
| 1:A:1000:MET:HG2  | 2:B:520:LEU:CD2   | 2.25                     | 0.65              |
| 3:C:52:ALA:O      | 3:C:301:ASN:CA    | 2.42                     | 0.65              |
| 15:O:422:GLN:NE2  | 15:O:592:PHE:CD2  | 2.65                     | 0.65              |
| 1:A:756:LYS:HD3   | 9:I:85:LYS:HZ2    | 1.32                     | 0.65              |
| 1:A:478:TYR:CA    | 2:B:1048:SER:O    | 2.44                     | 0.65              |
| 2:B:300:SER:OG    | 9:I:49:THR:CG2    | 2.44                     | 0.65              |
| 2:B:711:GLN:HG2   | 2:B:713:PRO:HD2   | 1.78                     | 0.65              |
| 3:C:230:LEU:CG    | 3:C:294:VAL:HG21  | 2.26                     | 0.65              |
| 15:O:108:GLU:O    | 15:O:108:GLU:HG3  | 1.96                     | 0.65              |
| 15:O:146:SER:O    | 15:O:148:PRO:HD3  | 1.95                     | 0.65              |
| 15:O:219:ARG:HH21 | 15:O:360:VAL:HG22 | 1.60                     | 0.65              |
| 4:D:48:GLU:HG3    | 4:D:86:ILE:HD12   | 1.78                     | 0.65              |
| 2:B:891:GLU:HA    | 12:L:54:ARG:NE    | 2.12                     | 0.65              |
| 3:C:272:LYS:HG2   | 14:N:175:TYR:CD1  | 2.32                     | 0.65              |
| 15:O:458:GLU:CG   | 15:O:514:PHE:CZ   | 2.79                     | 0.65              |
| 1:A:1034:TYR:CD1  | 1:A:1181:PRO:HG2  | 2.32                     | 0.65              |
| 1:A:799:GLU:HG3   | 1:A:1062:HIS:CE1  | 2.32                     | 0.65              |
| 2:B:566:TYR:CD2   | 13:M:73:SER:OG    | 2.48                     | 0.65              |
| 2:B:938:PHE:CZ    | 3:C:68:ARG:CD     | 2.80                     | 0.65              |
| 4:D:99:LEU:HB3    | 4:D:100:PRO:HD3   | 1.78                     | 0.65              |
| 15:O:343:VAL:CG1  | 15:O:388:VAL:HG23 | 2.27                     | 0.65              |
| 1:A:406:LEU:CD1   | 1:A:411:VAL:CG2   | 2.74                     | 0.65              |
| 2:B:341:SER:OG    | 2:B:343:ASP:OD1   | 2.13                     | 0.65              |
| 4:D:25:THR:HG21   | 6:F:59:GLN:NE2    | 2.12                     | 0.65              |
| 1:A:502:ALA:CB    | 1:A:581:ILE:CG2   | 2.63                     | 0.65              |
| 3:C:222:VAL:C     | 3:C:224:THR:N     | 2.49                     | 0.65              |
| 15:O:241:ASP:CB   | 15:O:380:SER:HB2  | 2.26                     | 0.65              |
| 15:O:488:HIS:NE2  | 15:O:489:ASN:OD1  | 2.29                     | 0.65              |
| 1:A:1651:THR:OG1  | 2:B:1085:SER:OG   | 2.14                     | 0.65              |
| 1:A:782:ASP:CG    | 1:A:783:LYS:N     | 2.50                     | 0.65              |
| 3:C:59:ILE:HG23   | 3:C:298:PHE:HE1   | 1.54                     | 0.65              |
| 7:G:144:HIS:NE2   | 15:O:145:SER:HB2  | 2.12                     | 0.65              |
| 15:O:241:ASP:HA   | 15:O:380:SER:HB2  | 1.78                     | 0.65              |
| 1:A:1053:ASP:O    | 1:A:1054:ALA:HB3  | 1.97                     | 0.65              |
| 1:A:406:LEU:HD11  | 1:A:411:VAL:HG21  | 1.78                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:438:ILE:HG23  | 2:B:1192:MET:CE   | 2.26                     | 0.65              |
| 2:B:915:ASP:OD1   | 2:B:1038:HIS:HD2  | 1.78                     | 0.65              |
| 2:B:923:GLN:NE2   | 2:B:953:ALA:O     | 2.30                     | 0.65              |
| 15:O:343:VAL:HG11 | 15:O:388:VAL:CG2  | 2.27                     | 0.65              |
| 1:A:953:GLU:C     | 1:A:1205:PHE:CB   | 2.66                     | 0.64              |
| 7:G:156:SER:HB2   | 15:O:146:SER:HA   | 1.78                     | 0.64              |
| 15:O:417:LYS:CD   | 15:O:472:HIS:HE1  | 2.10                     | 0.64              |
| 15:O:428:ILE:HD12 | 15:O:439:ILE:HD12 | 1.79                     | 0.64              |
| 1:A:1575:ILE:HG13 | 9:I:122:ARG:HH12  | 1.60                     | 0.64              |
| 15:O:374:PRO:CG   | 15:O:375:THR:HG23 | 2.27                     | 0.64              |
| 1:A:1262:LEU:CD2  | 1:A:1497:ILE:HG12 | 2.28                     | 0.64              |
| 1:A:834:ARG:NH2   | 2:B:994:ASP:OD1   | 2.30                     | 0.64              |
| 3:C:54:PHE:CE1    | 3:C:300:PHE:HB3   | 2.31                     | 0.64              |
| 7:G:159:LYS:HB3   | 15:O:103:ASN:OD1  | 1.98                     | 0.64              |
| 2:B:1120:ILE:HD12 | 15:O:117:GLN:HE22 | 1.63                     | 0.64              |
| 15:O:510:VAL:HG13 | 15:O:517:LEU:HD11 | 1.79                     | 0.64              |
| 2:B:623:ASP:O     | 2:B:648:ARG:NH1   | 2.25                     | 0.64              |
| 1:A:1344:ILE:CD1  | 2:B:329:TYR:CE2   | 2.71                     | 0.64              |
| 1:A:1023:LEU:HD23 | 1:A:1598:PHE:CD1  | 2.32                     | 0.64              |
| 2:B:469:ASN:HA    | 2:B:481:VAL:O     | 1.97                     | 0.64              |
| 3:C:86:PHE:CE1    | 12:L:64:LEU:CD1   | 2.79                     | 0.64              |
| 1:A:1036:ASN:HB3  | 1:A:1049:MET:HG3  | 1.78                     | 0.64              |
| 1:A:413:LEU:O     | 1:A:417:ARG:NH2   | 2.30                     | 0.64              |
| 1:A:83:VAL:CB     | 1:A:427:PHE:CE2   | 2.81                     | 0.64              |
| 1:A:480:ALA:CB    | 2:B:1046:VAL:CG2  | 2.63                     | 0.64              |
| 7:G:144:HIS:NE2   | 15:O:145:SER:HB3  | 2.13                     | 0.64              |
| 3:C:82:TYR:HE1    | 12:L:68:GLU:OE1   | 1.80                     | 0.64              |
| 1:A:1038:ILE:CG1  | 1:A:1049:MET:O    | 2.44                     | 0.64              |
| 1:A:1273:THR:HG23 | 9:I:48:VAL:HG22   | 1.79                     | 0.64              |
| 2:B:699:ILE:HD13  | 2:B:760:TYR:CE1   | 2.32                     | 0.64              |
| 15:O:240:ILE:CG2  | 15:O:332:LEU:CG   | 2.76                     | 0.64              |
| 1:A:1055:ILE:CG2  | 1:A:1063:MET:SD   | 2.85                     | 0.64              |
| 1:A:995:TYR:O     | 1:A:999:CYS:HB2   | 1.98                     | 0.64              |
| 3:C:73:SER:O      | 3:C:214:GLY:N     | 2.31                     | 0.64              |
| 5:E:20:LYS:HE2    | 5:E:34:GLU:HG2    | 1.80                     | 0.64              |
| 15:O:170:VAL:HG13 | 15:O:171:CYS:N    | 2.12                     | 0.64              |
| 1:A:478:TYR:OH    | 2:B:1049:THR:HG21 | 1.97                     | 0.64              |
| 3:C:54:PHE:O      | 3:C:299:ILE:CA    | 2.45                     | 0.64              |
| 1:A:399:LEU:CD2   | 1:A:423:LEU:HA    | 2.28                     | 0.64              |
| 1:A:953:GLU:C     | 1:A:1205:PHE:HB3  | 2.18                     | 0.64              |
| 1:A:1021:ARG:HD3  | 2:B:1073:GLU:OE1  | 1.98                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:368:PHE:CE2  | 15:O:382:GLN:HA   | 2.33                     | 0.64              |
| 15:O:383:TYR:CE2  | 15:O:597:LEU:HD22 | 2.33                     | 0.64              |
| 1:A:1055:ILE:HD12 | 1:A:1063:MET:HE3  | 1.74                     | 0.63              |
| 4:D:25:THR:CB     | 6:F:59:GLN:HE21   | 2.06                     | 0.63              |
| 1:A:1322:ILE:HD12 | 1:A:1457:ILE:HD11 | 1.79                     | 0.63              |
| 8:H:44:VAL:HG22   | 8:H:48:PRO:HA     | 1.81                     | 0.63              |
| 15:O:454:VAL:HG23 | 15:O:458:GLU:CG   | 2.28                     | 0.63              |
| 1:A:476:VAL:HG11  | 2:B:1071:VAL:CG2  | 2.25                     | 0.63              |
| 1:A:478:TYR:N     | 2:B:1048:SER:C    | 2.52                     | 0.63              |
| 3:C:41:GLU:CB     | 3:C:57:ILE:CG2    | 2.70                     | 0.63              |
| 1:A:1654:PHE:CE2  | 6:F:92:ARG:HD3    | 2.33                     | 0.63              |
| 15:O:392:GLN:HB2  | 15:O:395:LEU:HD22 | 1.79                     | 0.63              |
| 15:O:426:SER:OG   | 15:O:594:TYR:CA   | 2.46                     | 0.63              |
| 1:A:1026:GLN:HE22 | 1:A:1603:MET:HA   | 1.61                     | 0.63              |
| 15:O:454:VAL:HG23 | 15:O:458:GLU:OE2  | 1.98                     | 0.63              |
| 2:B:281:CYS:HA    | 2:B:323:ARG:CD    | 2.29                     | 0.63              |
| 3:C:75:VAL:CG1    | 3:C:221:PRO:HD2   | 2.06                     | 0.63              |
| 7:G:141:SER:CB    | 15:O:138:TYR:CZ   | 2.81                     | 0.63              |
| 1:A:1600:ARG:NE   | 1:A:1616:GLU:OE1  | 2.30                     | 0.63              |
| 1:A:888:LYS:HE2   | 9:I:69:THR:HG22   | 1.79                     | 0.63              |
| 2:B:475:GLY:O     | 2:B:476:LEU:HB2   | 1.98                     | 0.63              |
| 15:O:155:SER:HA   | 15:O:158:LEU:HD12 | 1.81                     | 0.63              |
| 15:O:379:ARG:CB   | 15:O:382:GLN:HE22 | 2.12                     | 0.63              |
| 1:A:402:ASP:O     | 1:A:406:LEU:HD23  | 1.99                     | 0.63              |
| 1:A:401:ASP:OD2   | 1:A:405:LYS:NZ    | 2.32                     | 0.63              |
| 1:A:408:LYS:HA    | 1:A:411:VAL:HG11  | 1.79                     | 0.63              |
| 4:D:80:THR:CG2    | 15:O:227:PHE:CB   | 2.75                     | 0.63              |
| 1:A:1655:ASP:N    | 6:F:135:ARG:O     | 2.28                     | 0.63              |
| 6:F:70:LYS:HG3    | 7:G:94:PRO:HB2    | 1.80                     | 0.63              |
| 15:O:373:LEU:N    | 15:O:374:PRO:HD2  | 2.14                     | 0.63              |
| 1:A:1060:GLU:O    | 1:A:1060:GLU:HG2  | 1.98                     | 0.63              |
| 4:D:23:HIS:HD2    | 6:F:58:PHE:CE2    | 2.16                     | 0.63              |
| 7:G:158:LYS:CE    | 15:O:105:ASN:OD1  | 2.47                     | 0.63              |
| 15:O:245:GLN:HA   | 15:O:245:GLN:NE2  | 2.14                     | 0.63              |
| 15:O:471:LYS:HG3  | 15:O:472:HIS:N    | 2.14                     | 0.63              |
| 1:A:436:ALA:O     | 1:A:440:SER:CA    | 2.46                     | 0.62              |
| 1:A:509:GLU:HG2   | 1:A:579:ARG:HG2   | 1.81                     | 0.62              |
| 3:C:75:VAL:HG12   | 3:C:76:PRO:O      | 1.98                     | 0.62              |
| 7:G:142:ALA:O     | 15:O:102:SER:O    | 2.16                     | 0.62              |
| 12:L:68:GLU:CG    | 12:L:69:ALA:H     | 2.05                     | 0.62              |
| 1:A:83:VAL:CG2    | 1:A:427:PHE:HZ    | 2.01                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:991:LYS:N     | 1:A:994:GLU:OE1   | 2.31                     | 0.62              |
| 15:O:181:ARG:HH11 | 15:O:181:ARG:CG   | 2.12                     | 0.62              |
| 1:A:1050:TYR:HB2  | 1:A:1179:ILE:HG21 | 1.81                     | 0.62              |
| 2:B:42:VAL:CA     | 2:B:46:ILE:HD12   | 2.29                     | 0.62              |
| 15:O:151:TRP:CZ2  | 15:O:176:LEU:HD23 | 2.35                     | 0.62              |
| 1:A:572:THR:HA    | 7:G:52:MET:HE1    | 1.80                     | 0.62              |
| 3:C:41:GLU:O      | 3:C:57:ILE:HG22   | 1.99                     | 0.62              |
| 15:O:386:PHE:CD2  | 15:O:606:MET:HE2  | 2.34                     | 0.62              |
| 15:O:98:ASP:OD2   | 15:O:135:LYS:HD3  | 1.99                     | 0.62              |
| 15:O:225:LEU:C    | 15:O:225:LEU:HD13 | 2.19                     | 0.62              |
| 15:O:457:ARG:HA   | 15:O:460:GLU:CB   | 2.30                     | 0.62              |
| 2:B:40:GLU:OE1    | 2:B:550:ARG:NH2   | 2.32                     | 0.62              |
| 7:G:142:ALA:C     | 15:O:102:SER:O    | 2.38                     | 0.62              |
| 15:O:447:THR:HA   | 15:O:450:LEU:HD12 | 1.80                     | 0.62              |
| 1:A:1011:VAL:C    | 1:A:1201:THR:CG2  | 2.68                     | 0.62              |
| 1:A:406:LEU:HD12  | 1:A:411:VAL:HB    | 1.82                     | 0.62              |
| 5:E:197:LYS:HD3   | 5:E:199:ILE:HD11  | 1.79                     | 0.62              |
| 1:A:1028:GLU:CG   | 1:A:1029:GLY:N    | 2.62                     | 0.62              |
| 1:A:1657:LEU:HD21 | 6:F:135:ARG:CZ    | 2.30                     | 0.62              |
| 2:B:1043:LYS:HG3  | 2:B:1063:ARG:CD   | 2.29                     | 0.62              |
| 2:B:554:GLN:HA    | 2:B:646:HIS:CD2   | 2.34                     | 0.62              |
| 3:C:58:ASN:N      | 3:C:296:ASN:O     | 2.30                     | 0.62              |
| 15:O:460:GLU:O    | 15:O:469:ARG:NH1  | 2.32                     | 0.62              |
| 1:A:891:ILE:CD1   | 9:I:71:LEU:CB     | 2.77                     | 0.62              |
| 3:C:222:VAL:C     | 3:C:224:THR:H     | 2.03                     | 0.62              |
| 3:C:59:ILE:O      | 3:C:298:PHE:HE1   | 1.83                     | 0.62              |
| 15:O:343:VAL:HG12 | 15:O:388:VAL:HG23 | 1.82                     | 0.62              |
| 15:O:435:SER:HB3  | 15:O:438:GLN:CG   | 2.23                     | 0.62              |
| 3:C:62:SER:CB     | 11:K:74:ASN:HD21  | 2.12                     | 0.62              |
| 15:O:368:PHE:CE2  | 15:O:385:MET:HB2  | 2.34                     | 0.62              |
| 15:O:581:THR:HA   | 15:O:584:GLN:NE2  | 2.15                     | 0.62              |
| 2:B:934:ILE:HG23  | 3:C:73:SER:HB3    | 1.82                     | 0.61              |
| 3:C:55:ASP:OD2    | 3:C:299:ILE:HG12  | 1.97                     | 0.61              |
| 4:D:47:LYS:HD2    | 4:D:82:LEU:HD21   | 1.82                     | 0.61              |
| 15:O:100:LEU:HD22 | 15:O:107:ILE:HD11 | 1.82                     | 0.61              |
| 15:O:144:CYS:O    | 15:O:148:PRO:HG3  | 2.00                     | 0.61              |
| 12:L:30:ILE:CD1   | 12:L:59:ALA:HB2   | 2.29                     | 0.61              |
| 15:O:431:ALA:HB3  | 15:O:434:LEU:CD1  | 2.23                     | 0.61              |
| 15:O:447:THR:CG2  | 15:O:480:LEU:CD2  | 2.79                     | 0.61              |
| 15:O:450:LEU:O    | 15:O:454:VAL:HG12 | 1.99                     | 0.61              |
| 3:C:131:THR:CG2   | 3:C:208:CYS:O     | 2.48                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:71:MET:CE     | 3:C:302:VAL:HG22  | 2.29                     | 0.61              |
| 15:O:158:LEU:HB3  | 15:O:172:HIS:HB3  | 1.82                     | 0.61              |
| 1:A:1025:LYS:HZ2  | 2:B:1076:ARG:NH1  | 1.98                     | 0.61              |
| 1:A:406:LEU:HD13  | 1:A:411:VAL:CB    | 2.27                     | 0.61              |
| 2:B:481:VAL:HG12  | 2:B:481:VAL:O     | 2.01                     | 0.61              |
| 2:B:769:PHE:HE1   | 2:B:798:PHE:HZ    | 1.48                     | 0.61              |
| 1:A:1662:ASN:N    | 7:G:101:SER:O     | 2.32                     | 0.61              |
| 7:G:141:SER:HB3   | 15:O:138:TYR:OH   | 1.95                     | 0.61              |
| 15:O:447:THR:HG22 | 15:O:480:LEU:CD2  | 2.28                     | 0.61              |
| 1:A:413:LEU:O     | 1:A:417:ARG:CZ    | 2.47                     | 0.61              |
| 1:A:478:TYR:H     | 2:B:1048:SER:C    | 2.03                     | 0.61              |
| 2:B:1069:ILE:O    | 2:B:1070:ARG:HB2  | 2.00                     | 0.61              |
| 6:F:73:ALA:HB2    | 6:F:143:PHE:CZ    | 2.36                     | 0.61              |
| 15:O:181:ARG:HB2  | 15:O:181:ARG:NH1  | 2.12                     | 0.61              |
| 15:O:369:LYS:HG3  | 15:O:406:ILE:HD11 | 1.83                     | 0.61              |
| 15:O:396:MET:SD   | 15:O:434:LEU:HA   | 2.41                     | 0.61              |
| 1:A:1050:TYR:CB   | 1:A:1179:ILE:HG21 | 2.31                     | 0.61              |
| 2:B:923:GLN:NE2   | 2:B:957:ARG:HD2   | 2.16                     | 0.61              |
| 3:C:71:MET:CE     | 3:C:225:ALA:HB1   | 2.30                     | 0.61              |
| 12:L:30:ILE:HD11  | 12:L:59:ALA:HB2   | 1.82                     | 0.61              |
| 15:O:67:ASP:OD1   | 15:O:69:THR:HB    | 2.00                     | 0.61              |
| 1:A:1660:VAL:CG2  | 7:G:103:LYS:HB2   | 2.30                     | 0.61              |
| 1:A:509:GLU:HG3   | 1:A:579:ARG:HD3   | 1.81                     | 0.61              |
| 3:C:71:MET:SD     | 3:C:225:ALA:CB    | 2.88                     | 0.61              |
| 4:D:44:ILE:HD13   | 4:D:90:LYS:HG3    | 1.82                     | 0.61              |
| 15:O:408:PHE:CE1  | 15:O:446:LEU:HD13 | 2.35                     | 0.61              |
| 15:O:454:VAL:HG23 | 15:O:458:GLU:CD   | 2.20                     | 0.61              |
| 1:A:564:PRO:HB2   | 15:O:371:HIS:CE1  | 2.36                     | 0.61              |
| 15:O:371:HIS:O    | 15:O:374:PRO:CD   | 2.49                     | 0.61              |
| 15:O:56:VAL:HG21  | 15:O:99:ILE:HD12  | 1.82                     | 0.61              |
| 1:A:479:ALA:HB2   | 2:B:1091:ARG:HH22 | 1.65                     | 0.60              |
| 2:B:552:SER:OG    | 2:B:647:SER:N     | 2.35                     | 0.60              |
| 8:H:25:ARG:NH1    | 8:H:27:GLU:OE2    | 2.34                     | 0.60              |
| 15:O:457:ARG:O    | 15:O:460:GLU:CB   | 2.47                     | 0.60              |
| 15:O:467:MET:HG3  | 15:O:519:PHE:CE2  | 2.36                     | 0.60              |
| 15:O:582:ARG:O    | 15:O:586:ILE:HG13 | 2.01                     | 0.60              |
| 1:A:932:GLY:O     | 9:I:125:ASN:ND2   | 2.34                     | 0.60              |
| 1:A:1651:THR:OG1  | 2:B:1085:SER:CB   | 2.49                     | 0.60              |
| 1:A:1344:ILE:HG22 | 2:B:333:LYS:CG    | 2.31                     | 0.60              |
| 1:A:1052:GLY:O    | 5:E:205:SER:CB    | 2.48                     | 0.60              |
| 5:E:93:MET:HG3    | 5:E:120:ALA:HB1   | 1.82                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:487:ARG:HH11 | 15:O:487:ARG:CG   | 2.14                     | 0.60              |
| 1:A:799:GLU:OE2   | 1:A:1062:HIS:HB2  | 2.01                     | 0.60              |
| 2:B:938:PHE:CD1   | 3:C:68:ARG:CZ     | 2.83                     | 0.60              |
| 1:A:1261:VAL:HG13 | 1:A:1265:GLU:CD   | 2.22                     | 0.60              |
| 1:A:1261:VAL:HG13 | 1:A:1265:GLU:OE1  | 2.01                     | 0.60              |
| 2:B:1020:GLU:CG   | 3:C:61:THR:HG21   | 2.32                     | 0.60              |
| 4:D:80:THR:HG21   | 15:O:227:PHE:CB   | 2.28                     | 0.60              |
| 3:C:272:LYS:CG    | 14:N:175:TYR:CE1  | 2.83                     | 0.60              |
| 7:G:143:SER:CB    | 15:O:101:SER:O    | 2.48                     | 0.60              |
| 1:A:1034:TYR:HA   | 1:A:1181:PRO:CG   | 2.32                     | 0.60              |
| 2:B:1090:ASP:O    | 2:B:1095:SER:N    | 2.34                     | 0.60              |
| 1:A:1226:VAL:HG12 | 1:A:1227:MET:HG2  | 1.83                     | 0.60              |
| 1:A:246:ASP:HB3   | 1:A:248:PHE:H     | 1.66                     | 0.60              |
| 1:A:996:TYR:HE1   | 1:A:1000:MET:CE   | 2.14                     | 0.60              |
| 1:A:449:GLY:O     | 1:A:451:VAL:N     | 2.34                     | 0.60              |
| 2:B:228:SER:HB2   | 2:B:253:LEU:HD23  | 1.84                     | 0.60              |
| 15:O:241:ASP:OD1  | 15:O:379:ARG:C    | 2.39                     | 0.60              |
| 1:A:84:PRO:HG2    | 1:A:318:THR:HG22  | 1.84                     | 0.60              |
| 1:A:477:ASN:O     | 1:A:478:TYR:HB2   | 2.01                     | 0.60              |
| 2:B:699:ILE:CD1   | 2:B:760:TYR:CE1   | 2.85                     | 0.60              |
| 1:A:87:ASN:HB2    | 1:A:357:MET:SD    | 2.42                     | 0.60              |
| 15:O:98:ASP:OD2   | 15:O:135:LYS:NZ   | 2.35                     | 0.60              |
| 1:A:1026:GLN:OE1  | 1:A:1603:MET:CB   | 2.48                     | 0.59              |
| 3:C:55:ASP:HB3    | 3:C:297:HIS:NE2   | 2.17                     | 0.59              |
| 1:A:1008:ASP:O    | 1:A:1011:VAL:CG2  | 2.41                     | 0.59              |
| 1:A:1034:TYR:HA   | 1:A:1181:PRO:HG3  | 1.84                     | 0.59              |
| 1:A:1054:ALA:O    | 1:A:1178:LEU:HD23 | 2.02                     | 0.59              |
| 2:B:1019:GLY:HA3  | 3:C:65:ASN:CB     | 2.27                     | 0.59              |
| 15:O:198:PHE:CD1  | 15:O:236:LYS:CE   | 2.78                     | 0.59              |
| 1:A:406:LEU:HD13  | 1:A:411:VAL:CG2   | 2.31                     | 0.59              |
| 6:F:106:PRO:HG2   | 7:G:55:GLU:CG     | 2.30                     | 0.59              |
| 1:A:699:CYS:O     | 1:A:815:ARG:NH1   | 2.35                     | 0.59              |
| 2:B:207:ILE:O     | 2:B:207:ILE:HG22  | 2.02                     | 0.59              |
| 1:A:1027:LEU:HD21 | 1:A:1588:MET:HG2  | 1.84                     | 0.59              |
| 1:A:35:PRO:HA     | 1:A:390:LEU:HD12  | 1.84                     | 0.59              |
| 1:A:878:ARG:HG2   | 9:I:67:VAL:CG1    | 2.29                     | 0.59              |
| 2:B:211:ARG:HB3   | 2:B:239:VAL:CG1   | 2.32                     | 0.59              |
| 2:B:551:ILE:HA    | 2:B:648:ARG:O     | 2.02                     | 0.59              |
| 2:B:566:TYR:HB2   | 13:M:73:SER:OG    | 2.03                     | 0.59              |
| 4:D:80:THR:OG1    | 15:O:227:PHE:CD1  | 2.55                     | 0.59              |
| 5:E:55:ARG:NH2    | 5:E:113:GLN:OE1   | 2.36                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:720:PHE:CE2   | 8:H:141:TYR:HE2   | 2.21                     | 0.59              |
| 15:O:374:PRO:HB2  | 15:O:375:THR:HG23 | 1.85                     | 0.59              |
| 15:O:390:GLN:HB2  | 15:O:609:TYR:CD1  | 2.37                     | 0.59              |
| 1:A:509:GLU:O     | 1:A:576:LYS:HA    | 2.03                     | 0.59              |
| 1:A:863:ASN:ND2   | 9:I:68:LYS:H      | 2.01                     | 0.59              |
| 15:O:101:SER:HB3  | 15:O:142:ILE:CD1  | 2.33                     | 0.59              |
| 1:A:516:ILE:HG21  | 15:O:376:TYR:CZ   | 2.38                     | 0.59              |
| 1:A:581:ILE:HG13  | 1:A:582:LYS:H     | 1.68                     | 0.59              |
| 2:B:829:ASN:N     | 2:B:829:ASN:OD1   | 2.36                     | 0.59              |
| 2:B:328:GLN:NE2   | 13:M:109:ARG:HH21 | 1.99                     | 0.59              |
| 2:B:110:ASN:O     | 2:B:112:GLY:N     | 2.35                     | 0.59              |
| 2:B:209:GLN:O     | 2:B:401:GLU:HG2   | 2.03                     | 0.59              |
| 3:C:231:PRO:HG2   | 3:C:270:ALA:HB1   | 1.83                     | 0.59              |
| 2:B:563:SER:CB    | 13:M:73:SER:HB3   | 2.33                     | 0.59              |
| 3:C:272:LYS:HG2   | 14:N:175:TYR:CE1  | 2.38                     | 0.59              |
| 15:O:369:LYS:HD3  | 15:O:373:LEU:HD22 | 1.85                     | 0.59              |
| 15:O:428:ILE:CD1  | 15:O:439:ILE:HD12 | 2.33                     | 0.59              |
| 1:A:990:ILE:CB    | 1:A:994:GLU:OE1   | 2.51                     | 0.58              |
| 2:B:538:PRO:HB2   | 2:B:542:LEU:HG    | 1.84                     | 0.58              |
| 15:O:348:THR:HG23 | 15:O:351:SER:H    | 1.67                     | 0.58              |
| 15:O:241:ASP:O    | 15:O:378:THR:CG2  | 2.51                     | 0.58              |
| 15:O:607:LYS:HG3  | 15:O:608:GLU:N    | 2.17                     | 0.58              |
| 3:C:253:PRO:CB    | 14:N:180:PHE:HB3  | 2.33                     | 0.58              |
| 1:A:1048:PHE:HZ   | 5:E:211:TYR:CD1   | 2.18                     | 0.58              |
| 7:G:159:LYS:N     | 15:O:105:ASN:HD22 | 2.01                     | 0.58              |
| 1:A:827:THR:OG1   | 1:A:828:CYS:N     | 2.36                     | 0.58              |
| 7:G:30:GLU:HA     | 7:G:32:ASN:N      | 2.18                     | 0.58              |
| 15:O:129:PRO:CG   | 15:O:132:THR:CB   | 2.74                     | 0.58              |
| 15:O:164:LEU:O    | 15:O:165:PRO:O    | 2.20                     | 0.58              |
| 15:O:369:LYS:CE   | 15:O:370:THR:HG22 | 2.33                     | 0.58              |
| 1:A:1074:TYR:HE2  | 1:A:1159:ASP:HB3  | 1.68                     | 0.58              |
| 1:A:1055:ILE:HD11 | 1:A:1174:TYR:CD2  | 2.39                     | 0.58              |
| 1:A:1660:VAL:HG23 | 7:G:103:LYS:HB2   | 1.85                     | 0.58              |
| 1:A:415:ASP:HA    | 1:A:418:VAL:HG12  | 1.84                     | 0.58              |
| 2:B:415:GLU:OE2   | 2:B:474:SER:OG    | 2.21                     | 0.58              |
| 2:B:328:GLN:HE22  | 13:M:109:ARG:NH2  | 1.99                     | 0.58              |
| 1:A:437:PHE:CZ    | 1:A:456:VAL:HG22  | 2.28                     | 0.58              |
| 4:D:48:GLU:HG3    | 4:D:86:ILE:CD1    | 2.32                     | 0.58              |
| 11:K:68:GLU:HG2   | 11:K:72:LEU:HD23  | 1.86                     | 0.58              |
| 15:O:454:VAL:CG2  | 15:O:458:GLU:OE2  | 2.51                     | 0.58              |
| 1:A:468:ARG:HE    | 1:A:1021:ARG:NH1  | 2.00                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:221:PRO:O     | 3:C:222:VAL:HG13  | 2.04                     | 0.58              |
| 2:B:1019:GLY:CA   | 3:C:65:ASN:HB2    | 2.28                     | 0.58              |
| 4:D:27:LEU:HD22   | 7:G:23:GLN:O      | 2.03                     | 0.58              |
| 4:D:25:THR:HG21   | 6:F:59:GLN:HE21   | 1.57                     | 0.58              |
| 3:C:253:PRO:HB2   | 14:N:180:PHE:HB3  | 1.85                     | 0.58              |
| 15:O:386:PHE:HD2  | 15:O:606:MET:HE2  | 1.62                     | 0.58              |
| 15:O:484:PHE:CD1  | 15:O:502:LEU:HD13 | 2.38                     | 0.58              |
| 7:G:159:LYS:N     | 15:O:105:ASN:ND2  | 2.51                     | 0.58              |
| 2:B:1016:GLY:O    | 3:C:69:ARG:HD2    | 2.04                     | 0.58              |
| 2:B:923:GLN:HG2   | 2:B:949:ILE:HD11  | 1.84                     | 0.58              |
| 13:M:10:ILE:HB    | 14:N:70:LEU:HB3   | 1.86                     | 0.58              |
| 1:A:406:LEU:CD1   | 1:A:411:VAL:HG21  | 2.34                     | 0.58              |
| 2:B:117:VAL:HG13  | 2:B:117:VAL:O     | 2.03                     | 0.58              |
| 4:D:48:GLU:OE1    | 4:D:90:LYS:NZ     | 2.37                     | 0.58              |
| 4:D:25:THR:C      | 6:F:59:GLN:HG3    | 2.24                     | 0.58              |
| 12:L:38:LEU:HD12  | 12:L:49:LYS:HG3   | 1.85                     | 0.58              |
| 15:O:421:LEU:HD13 | 15:O:476:ALA:CB   | 2.31                     | 0.58              |
| 15:O:423:TYR:HD1  | 15:O:594:TYR:CZ   | 2.20                     | 0.58              |
| 12:L:33:GLU:HG3   | 12:L:53:HIS:CE1   | 2.39                     | 0.57              |
| 14:N:69:SER:OG    | 14:N:70:LEU:N     | 2.37                     | 0.57              |
| 15:O:174:ASP:O    | 15:O:177:LYS:CG   | 2.52                     | 0.57              |
| 1:A:407:GLN:O     | 1:A:411:VAL:HG12  | 2.04                     | 0.57              |
| 1:A:581:ILE:HG13  | 1:A:582:LYS:N     | 2.19                     | 0.57              |
| 14:N:89:ILE:HG12  | 14:N:139:VAL:HG22 | 1.85                     | 0.57              |
| 3:C:56:LEU:CG     | 3:C:300:PHE:CD1   | 2.86                     | 0.57              |
| 15:O:369:LYS:O    | 15:O:373:LEU:HB3  | 2.04                     | 0.57              |
| 1:A:1055:ILE:HG22 | 1:A:1060:GLU:HB2  | 1.87                     | 0.57              |
| 1:A:476:VAL:CG1   | 2:B:1071:VAL:HG23 | 2.30                     | 0.57              |
| 2:B:467:THR:C     | 2:B:469:ASN:H     | 2.07                     | 0.57              |
| 15:O:247:GLU:HB3  | 15:O:325:ILE:HD11 | 1.86                     | 0.57              |
| 15:O:471:LYS:CB   | 15:O:585:PHE:HE1  | 1.94                     | 0.57              |
| 3:C:51:GLU:CB     | 3:C:303:GLU:CG    | 2.80                     | 0.57              |
| 2:B:848:ILE:HB    | 12:L:60:ARG:HG3   | 1.86                     | 0.57              |
| 15:O:487:ARG:O    | 15:O:490:ILE:HB   | 2.03                     | 0.57              |
| 1:A:953:GLU:HA    | 1:A:1205:PHE:CG   | 2.40                     | 0.57              |
| 1:A:493:ASN:HB3   | 1:A:654:ASP:OD1   | 2.04                     | 0.57              |
| 1:A:782:ASP:O     | 1:A:784:SER:N     | 2.38                     | 0.57              |
| 2:B:207:ILE:HD11  | 2:B:503:VAL:CG2   | 2.34                     | 0.57              |
| 2:B:893:ASN:HA    | 12:L:54:ARG:NH2   | 2.20                     | 0.57              |
| 6:F:66:ARG:CZ     | 7:G:90:LEU:CD1    | 2.80                     | 0.57              |
| 7:G:143:SER:HB3   | 15:O:103:ASN:N    | 2.20                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:173:HIS:CD2  | 15:O:217:LYS:HG2  | 2.39                     | 0.57              |
| 15:O:391:GLN:OE1  | 15:O:609:TYR:OH   | 2.23                     | 0.57              |
| 1:A:1003:ARG:NE   | 2:B:520:LEU:CB    | 2.61                     | 0.57              |
| 1:A:1348:VAL:CG2  | 2:B:268:GLU:C     | 2.72                     | 0.57              |
| 15:O:128:LEU:HD22 | 15:O:129:PRO:HD3  | 1.86                     | 0.57              |
| 15:O:190:ILE:HA   | 15:O:193:TYR:CD2  | 2.39                     | 0.57              |
| 15:O:417:LYS:HB3  | 15:O:472:HIS:CE1  | 2.39                     | 0.57              |
| 15:O:484:PHE:CE1  | 15:O:502:LEU:HD13 | 2.39                     | 0.57              |
| 1:A:1235:THR:O    | 1:A:1544:ASN:ND2  | 2.38                     | 0.57              |
| 1:A:468:ARG:NE    | 1:A:1021:ARG:CZ   | 2.63                     | 0.57              |
| 2:B:833:PRO:HG2   | 2:B:836:TRP:CE2   | 2.40                     | 0.57              |
| 15:O:230:TRP:CZ2  | 15:O:364:LEU:HD11 | 2.39                     | 0.57              |
| 15:O:422:GLN:NE2  | 15:O:592:PHE:CZ   | 2.69                     | 0.57              |
| 1:A:18:ILE:HD12   | 1:A:354:SER:HB3   | 1.85                     | 0.57              |
| 1:A:478:TYR:HA    | 2:B:1048:SER:C    | 2.18                     | 0.57              |
| 1:A:988:SER:HB2   | 2:B:988:GLU:HG2   | 1.87                     | 0.57              |
| 2:B:1043:LYS:HG3  | 2:B:1063:ARG:HD2  | 1.85                     | 0.57              |
| 1:A:727:THR:HG21  | 8:H:119:GLY:O     | 2.05                     | 0.57              |
| 1:A:1048:PHE:O    | 1:A:1049:MET:HB2  | 2.04                     | 0.57              |
| 3:C:56:LEU:CG     | 3:C:300:PHE:CE1   | 2.88                     | 0.57              |
| 4:D:48:GLU:CG     | 4:D:86:ILE:HD11   | 2.35                     | 0.57              |
| 15:O:158:LEU:HD22 | 15:O:172:HIS:CB   | 2.35                     | 0.57              |
| 1:A:563:THR:HA    | 15:O:375:THR:HG21 | 1.87                     | 0.56              |
| 2:B:1020:GLU:CG   | 3:C:61:THR:OG1    | 2.53                     | 0.56              |
| 2:B:894:LYS:HG2   | 12:L:47:ARG:HD2   | 1.86                     | 0.56              |
| 2:B:894:LYS:HG2   | 12:L:47:ARG:NE    | 2.19                     | 0.56              |
| 15:O:154:VAL:O    | 15:O:158:LEU:HG   | 2.04                     | 0.56              |
| 1:A:412:SER:HB3   | 1:A:414:GLU:H     | 1.70                     | 0.56              |
| 1:A:799:GLU:CD    | 1:A:1062:HIS:HB2  | 2.25                     | 0.56              |
| 2:B:207:ILE:HD11  | 2:B:503:VAL:HG21  | 1.87                     | 0.56              |
| 2:B:800:TYR:CD1   | 2:B:801:GLY:N     | 2.73                     | 0.56              |
| 4:D:28:PRO:HD2    | 7:G:24:VAL:CG1    | 2.35                     | 0.56              |
| 5:E:145:THR:C     | 5:E:147:HIS:H     | 2.08                     | 0.56              |
| 6:F:75:PRO:HG2    | 6:F:78:GLN:CG     | 2.34                     | 0.56              |
| 7:G:20:HIS:O      | 7:G:20:HIS:ND1    | 2.38                     | 0.56              |
| 3:C:82:TYR:CE1    | 12:L:68:GLU:OE1   | 2.58                     | 0.56              |
| 1:A:1050:TYR:CG   | 1:A:1179:ILE:HG21 | 2.40                     | 0.56              |
| 2:B:1013:MET:SD   | 2:B:1026:ILE:HG12 | 2.45                     | 0.56              |
| 2:B:338:PHE:HZ    | 2:B:357:ILE:HD12  | 1.70                     | 0.56              |
| 3:C:223:SER:HB2   | 3:C:303:GLU:CB    | 2.35                     | 0.56              |
| 7:G:143:SER:CB    | 15:O:104:ILE:N    | 2.57                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:O:109:SER:OG  | 15:O:111:ARG:HG3  | 2.05                     | 0.56              |
| 15:O:66:ASN:N    | 15:O:66:ASN:ND2   | 2.53                     | 0.56              |
| 2:B:890:ASP:O    | 12:L:54:ARG:NE    | 2.38                     | 0.56              |
| 5:E:90:VAL:HG13  | 5:E:120:ALA:HA    | 1.88                     | 0.56              |
| 7:G:56:ASN:HB3   | 7:G:59:GLN:HB3    | 1.86                     | 0.56              |
| 1:A:966:LEU:CD2  | 1:A:997:PHE:CZ    | 2.83                     | 0.56              |
| 3:C:56:LEU:HD12  | 3:C:300:PHE:CE1   | 2.23                     | 0.56              |
| 11:K:49:LEU:HD23 | 11:K:51:THR:HG23  | 1.86                     | 0.56              |
| 15:O:458:GLU:HG2 | 15:O:514:PHE:CZ   | 2.40                     | 0.56              |
| 2:B:1020:GLU:HG2 | 3:C:61:THR:OG1    | 2.06                     | 0.56              |
| 3:C:86:PHE:HE2   | 3:C:205:LYS:HG3   | 1.69                     | 0.56              |
| 12:L:63:ARG:HG3  | 12:L:64:LEU:H     | 1.69                     | 0.56              |
| 1:A:477:ASN:OD1  | 2:B:1047:ARG:NH1  | 2.39                     | 0.56              |
| 2:B:208:VAL:HG23 | 2:B:401:GLU:CG    | 2.35                     | 0.56              |
| 2:B:554:GLN:CA   | 2:B:646:HIS:CD2   | 2.89                     | 0.56              |
| 7:G:141:SER:HB3  | 15:O:138:TYR:CZ   | 2.41                     | 0.56              |
| 15:O:396:MET:HE1 | 15:O:434:LEU:CD1  | 2.32                     | 0.56              |
| 15:O:447:THR:HA  | 15:O:450:LEU:CG   | 2.35                     | 0.56              |
| 15:O:432:LYS:HG3 | 15:O:608:GLU:O    | 1.96                     | 0.56              |
| 15:O:98:ASP:CG   | 15:O:135:LYS:HD3  | 2.26                     | 0.56              |
| 1:A:990:ILE:HB   | 1:A:994:GLU:OE1   | 2.06                     | 0.56              |
| 15:O:191:ASP:O   | 15:O:194:LEU:HB2  | 2.06                     | 0.56              |
| 15:O:205:ARG:O   | 15:O:209:VAL:HG12 | 2.05                     | 0.56              |
| 2:B:480:GLN:HB3  | 2:B:507:SER:OG    | 2.05                     | 0.56              |
| 3:C:71:MET:CE    | 3:C:225:ALA:HB2   | 2.33                     | 0.56              |
| 13:M:15:VAL:HG22 | 13:M:90:LEU:HB2   | 1.88                     | 0.56              |
| 15:O:63:LEU:HD23 | 15:O:111:ARG:HD2  | 1.87                     | 0.56              |
| 1:A:1655:ASP:CG  | 6:F:137:TYR:CE2   | 2.76                     | 0.56              |
| 1:A:35:PRO:HA    | 1:A:390:LEU:HD13  | 1.88                     | 0.56              |
| 1:A:797:LEU:HD13 | 1:A:809:VAL:HG21  | 1.87                     | 0.56              |
| 15:O:129:PRO:HG2 | 15:O:132:THR:OG1  | 2.06                     | 0.56              |
| 15:O:447:THR:C   | 15:O:450:LEU:H    | 2.09                     | 0.56              |
| 15:O:458:GLU:CB  | 15:O:461:VAL:CG2  | 2.80                     | 0.56              |
| 15:O:484:PHE:CD1 | 15:O:502:LEU:CD1  | 2.89                     | 0.56              |
| 15:O:440:ILE:CG2 | 15:O:491:PHE:CE1  | 2.82                     | 0.56              |
| 1:A:468:ARG:CZ   | 1:A:1021:ARG:NH1  | 2.65                     | 0.56              |
| 1:A:1482:LYS:HE2 | 2:B:304:ASP:CG    | 2.26                     | 0.56              |
| 2:B:470:LEU:HB3  | 2:B:481:VAL:HG13  | 1.87                     | 0.56              |
| 3:C:64:ALA:CB    | 3:C:298:PHE:CD2   | 2.89                     | 0.56              |
| 1:A:1655:ASP:CB  | 6:F:135:ARG:HB3   | 2.36                     | 0.56              |
| 1:A:87:ASN:CB    | 1:A:357:MET:SD    | 2.94                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:478:TYR:OH    | 2:B:1049:THR:CG2  | 2.51                     | 0.55              |
| 2:B:1020:GLU:HG2  | 3:C:61:THR:CG2    | 2.34                     | 0.55              |
| 1:A:1:MET:CG      | 2:B:1098:TYR:CE2  | 2.88                     | 0.55              |
| 2:B:470:LEU:HB2   | 2:B:484:TYR:HE2   | 1.66                     | 0.55              |
| 15:O:166:ILE:HD11 | 15:O:213:SER:OG   | 2.06                     | 0.55              |
| 15:O:369:LYS:HE2  | 15:O:370:THR:HG22 | 1.87                     | 0.55              |
| 15:O:343:VAL:CG1  | 15:O:388:VAL:HG21 | 2.36                     | 0.55              |
| 1:A:1162:ASN:HD21 | 1:A:1164:LYS:HB2  | 1.71                     | 0.55              |
| 1:A:1038:ILE:HG12 | 1:A:1049:MET:C    | 2.27                     | 0.55              |
| 1:A:1049:MET:C    | 1:A:1051:GLY:H    | 2.09                     | 0.55              |
| 1:A:1575:ILE:HG13 | 9:I:122:ARG:HH22  | 1.71                     | 0.55              |
| 1:A:916:THR:O     | 1:A:919:LYS:NZ    | 2.40                     | 0.55              |
| 2:B:236:ILE:HD13  | 2:B:377:MET:HE1   | 1.88                     | 0.55              |
| 2:B:934:ILE:CG2   | 3:C:72:ILE:HB     | 2.35                     | 0.55              |
| 3:C:84:TYR:CE2    | 12:L:66:GLN:CD    | 2.77                     | 0.55              |
| 15:O:359:GLY:CA   | 15:O:362:ASN:HD22 | 2.16                     | 0.55              |
| 15:O:447:THR:HA   | 15:O:450:LEU:HG   | 1.88                     | 0.55              |
| 15:O:447:THR:O    | 15:O:450:LEU:N    | 2.39                     | 0.55              |
| 1:A:1050:TYR:CD2  | 1:A:1179:ILE:HG21 | 2.41                     | 0.55              |
| 1:A:1348:VAL:N    | 2:B:268:GLU:O     | 2.37                     | 0.55              |
| 1:A:389:VAL:HA    | 1:A:430:ILE:HD11  | 1.88                     | 0.55              |
| 2:B:859:CYS:HB3   | 2:B:872:LYS:HB2   | 1.88                     | 0.55              |
| 10:J:10:CYS:HB3   | 10:J:43:ARG:NH1   | 2.21                     | 0.55              |
| 13:M:11:GLU:N     | 13:M:86:LYS:O     | 2.36                     | 0.55              |
| 15:O:432:LYS:HB2  | 15:O:610:TYR:N    | 2.20                     | 0.55              |
| 1:A:437:PHE:CE2   | 1:A:456:VAL:CG2   | 2.85                     | 0.55              |
| 3:C:139:LYS:HG2   | 3:C:201:GLU:HB3   | 1.89                     | 0.55              |
| 5:E:144:ILE:O     | 5:E:147:HIS:HB2   | 2.07                     | 0.55              |
| 1:A:1657:LEU:HD22 | 7:G:104:LEU:HD13  | 1.89                     | 0.55              |
| 15:O:343:VAL:HG11 | 15:O:388:VAL:HG21 | 1.89                     | 0.55              |
| 15:O:447:THR:HA   | 15:O:450:LEU:CD1  | 2.36                     | 0.55              |
| 15:O:517:LEU:HD12 | 15:O:543:ILE:HG21 | 1.88                     | 0.55              |
| 1:A:405:LYS:O     | 1:A:405:LYS:HG2   | 2.07                     | 0.55              |
| 5:E:159:ASP:OD1   | 5:E:162:ARG:NH1   | 2.38                     | 0.55              |
| 7:G:143:SER:HB3   | 15:O:101:SER:O    | 2.06                     | 0.55              |
| 1:A:1024:THR:O    | 1:A:1028:GLU:HB3  | 2.07                     | 0.55              |
| 1:A:1162:ASN:HD22 | 1:A:1165:LYS:HG3  | 1.71                     | 0.55              |
| 2:B:322:ASN:HB3   | 2:B:325:GLN:H     | 1.71                     | 0.55              |
| 3:C:56:LEU:HG     | 3:C:300:PHE:CE1   | 2.41                     | 0.55              |
| 15:O:164:LEU:HB3  | 15:O:165:PRO:HD2  | 1.89                     | 0.55              |
| 15:O:432:LYS:CB   | 15:O:608:GLU:O    | 2.55                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:25:THR:HG22   | 7:G:26:ASN:N      | 2.17                     | 0.55              |
| 7:G:28:ILE:CG2    | 7:G:29:ASP:N      | 2.56                     | 0.55              |
| 1:A:1596:LEU:HD22 | 1:A:1602:GLY:HA2  | 1.89                     | 0.55              |
| 2:B:373:MET:O     | 2:B:377:MET:HG3   | 2.08                     | 0.55              |
| 3:C:57:ILE:CG1    | 3:C:297:HIS:ND1   | 2.70                     | 0.55              |
| 3:C:45:SER:HB2    | 3:C:271:ARG:CZ    | 2.35                     | 0.55              |
| 15:O:158:LEU:HD22 | 15:O:172:HIS:CA   | 2.36                     | 0.55              |
| 15:O:369:LYS:HD2  | 15:O:369:LYS:C    | 2.27                     | 0.55              |
| 1:A:863:ASN:HD21  | 9:I:68:LYS:N      | 2.05                     | 0.54              |
| 15:O:147:ILE:HG22 | 15:O:147:ILE:O    | 2.07                     | 0.54              |
| 1:A:996:TYR:CE1   | 1:A:1000:MET:CE   | 2.90                     | 0.54              |
| 2:B:42:VAL:HG21   | 2:B:190:ILE:HB    | 1.89                     | 0.54              |
| 7:G:143:SER:HA    | 15:O:103:ASN:HA   | 1.90                     | 0.54              |
| 1:A:800:VAL:HG23  | 1:A:1068:PHE:CZ   | 2.41                     | 0.54              |
| 1:A:479:ALA:HB2   | 2:B:1091:ARG:NH2  | 2.22                     | 0.54              |
| 3:C:253:PRO:HB2   | 14:N:180:PHE:CG   | 2.42                     | 0.54              |
| 1:A:412:SER:C     | 1:A:414:GLU:N     | 2.56                     | 0.54              |
| 15:O:158:LEU:CD2  | 15:O:172:HIS:HD2  | 2.01                     | 0.54              |
| 15:O:488:HIS:C    | 15:O:490:ILE:H    | 2.10                     | 0.54              |
| 15:O:487:ARG:NH2  | 15:O:611:ILE:HD12 | 2.22                     | 0.54              |
| 1:A:402:ASP:HA    | 1:A:405:LYS:HB3   | 1.88                     | 0.54              |
| 1:A:399:LEU:HD11  | 1:A:423:LEU:HG    | 1.89                     | 0.54              |
| 2:B:401:GLU:HG3   | 2:B:402:VAL:H     | 1.69                     | 0.54              |
| 2:B:799:GLY:O     | 2:B:1035:ARG:NH1  | 2.39                     | 0.54              |
| 4:D:48:GLU:HG2    | 4:D:86:ILE:CD1    | 2.36                     | 0.54              |
| 7:G:229:LEU:HD12  | 7:G:230:ARG:H     | 1.72                     | 0.54              |
| 7:G:158:LYS:HZ2   | 15:O:108:GLU:CG   | 2.03                     | 0.54              |
| 15:O:360:VAL:O    | 15:O:363:THR:HG23 | 2.06                     | 0.54              |
| 15:O:372:VAL:C    | 15:O:374:PRO:CD   | 2.76                     | 0.54              |
| 15:O:241:ASP:CA   | 15:O:380:SER:HB2  | 2.38                     | 0.54              |
| 1:A:1008:ASP:OD1  | 1:A:1202:LEU:HB3  | 2.07                     | 0.54              |
| 1:A:1446:ARG:O    | 1:A:1450:ILE:HG13 | 2.08                     | 0.54              |
| 1:A:478:TYR:CA    | 2:B:1048:SER:C    | 2.74                     | 0.54              |
| 2:B:284:SER:OG    | 2:B:287:GLU:HG3   | 2.07                     | 0.54              |
| 3:C:58:ASN:HA     | 3:C:296:ASN:HB2   | 0.84                     | 0.54              |
| 3:C:253:PRO:CA    | 14:N:180:PHE:HD1  | 2.20                     | 0.54              |
| 1:A:589:MET:HE1   | 1:A:614:LEU:HD13  | 1.89                     | 0.54              |
| 1:A:878:ARG:CZ    | 9:I:66:VAL:HG23   | 2.38                     | 0.54              |
| 1:A:1347:ALA:HA   | 2:B:269:TYR:CE1   | 2.43                     | 0.54              |
| 3:C:59:ILE:HG22   | 3:C:298:PHE:CE1   | 2.31                     | 0.54              |
| 15:O:169:THR:HA   | 15:O:172:HIS:ND1  | 2.22                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:426:SER:HB3  | 15:O:594:TYR:HD2  | 1.72                     | 0.54              |
| 1:A:1344:ILE:CG2  | 2:B:333:LYS:CG    | 2.86                     | 0.54              |
| 9:I:71:LEU:HG     | 9:I:72:LYS:O      | 2.08                     | 0.54              |
| 1:A:1651:THR:OG1  | 2:B:1085:SER:HB2  | 2.07                     | 0.54              |
| 3:C:253:PRO:CB    | 14:N:180:PHE:CD1  | 2.79                     | 0.54              |
| 15:O:100:LEU:HD22 | 15:O:107:ILE:CD1  | 2.38                     | 0.54              |
| 15:O:423:TYR:CD1  | 15:O:594:TYR:CZ   | 2.95                     | 0.54              |
| 2:B:1043:LYS:CG   | 2:B:1063:ARG:NE   | 2.70                     | 0.54              |
| 2:B:21:ARG:NH1    | 2:B:22:GLU:OE1    | 2.40                     | 0.54              |
| 7:G:132:VAL:HG22  | 7:G:232:THR:HG22  | 1.90                     | 0.54              |
| 1:A:556:ALA:CA    | 15:O:246:ASN:HD22 | 2.20                     | 0.54              |
| 15:O:391:GLN:NE2  | 15:O:609:TYR:CE2  | 2.76                     | 0.54              |
| 2:B:788:ILE:HB    | 2:B:948:ILE:HB    | 1.89                     | 0.53              |
| 1:A:1136:VAL:HG22 | 1:A:1174:TYR:CG   | 2.44                     | 0.53              |
| 1:A:413:LEU:C     | 1:A:417:ARG:NH2   | 2.56                     | 0.53              |
| 1:A:389:VAL:HA    | 1:A:430:ILE:CD1   | 2.38                     | 0.53              |
| 3:C:55:ASP:CB     | 3:C:297:HIS:HE2   | 2.21                     | 0.53              |
| 3:C:97:LEU:HD11   | 3:C:202:ILE:HD13  | 1.90                     | 0.53              |
| 15:O:368:PHE:CZ   | 15:O:385:MET:HB2  | 2.43                     | 0.53              |
| 1:A:641:GLU:HB2   | 6:F:99:LEU:CD1    | 2.36                     | 0.53              |
| 3:C:55:ASP:OD1    | 3:C:299:ILE:CG2   | 2.56                     | 0.53              |
| 1:A:1660:VAL:HG22 | 7:G:103:LYS:C     | 2.28                     | 0.53              |
| 9:I:96:TYR:HA     | 9:I:111:PHE:O     | 2.09                     | 0.53              |
| 15:O:69:THR:O     | 15:O:73:ILE:HG13  | 2.07                     | 0.53              |
| 1:A:572:THR:HA    | 7:G:52:MET:HE3    | 1.90                     | 0.53              |
| 2:B:398:GLN:O     | 2:B:398:GLN:HG2   | 2.06                     | 0.53              |
| 15:O:147:ILE:HG22 | 15:O:149:LYS:HB3  | 1.90                     | 0.53              |
| 1:A:1655:ASP:HB2  | 6:F:135:ARG:CB    | 2.38                     | 0.53              |
| 1:A:91:PHE:CD2    | 1:A:249:THR:HG22  | 2.43                     | 0.53              |
| 1:A:1482:LYS:HE2  | 2:B:304:ASP:OD2   | 2.08                     | 0.53              |
| 2:B:470:LEU:O     | 2:B:481:VAL:CG1   | 2.56                     | 0.53              |
| 4:D:37:LEU:CD2    | 4:D:97:LYS:HE3    | 2.38                     | 0.53              |
| 13:M:75:GLN:HB2   | 14:N:60:SER:HA    | 1.91                     | 0.53              |
| 15:O:342:HIS:O    | 15:O:346:GLN:CG   | 2.51                     | 0.53              |
| 15:O:63:LEU:CD2   | 15:O:111:ARG:HD2  | 2.38                     | 0.53              |
| 1:A:1008:ASP:OD1  | 1:A:1202:LEU:CG   | 2.56                     | 0.53              |
| 2:B:563:SER:HA    | 13:M:73:SER:OG    | 2.08                     | 0.53              |
| 3:C:67:PHE:O      | 3:C:71:MET:HG3    | 2.08                     | 0.53              |
| 2:B:934:ILE:HG21  | 3:C:73:SER:HB3    | 1.91                     | 0.53              |
| 15:O:156:MET:HE2  | 15:O:193:TYR:CE1  | 2.44                     | 0.53              |
| 15:O:218:LEU:HD23 | 15:O:229:ILE:HD11 | 1.90                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:O:238:ILE:CD1 | 15:O:371:HIS:HB3  | 2.37                     | 0.53              |
| 15:O:390:GLN:HB2 | 15:O:609:TYR:CG   | 2.43                     | 0.53              |
| 1:A:1289:SER:HB3 | 1:A:1475:GLU:HG2  | 1.91                     | 0.53              |
| 1:A:1344:ILE:CG2 | 2:B:333:LYS:CB    | 2.86                     | 0.53              |
| 1:A:248:PHE:CD1  | 1:A:442:LYS:O     | 2.62                     | 0.53              |
| 2:B:317:TYR:HB3  | 2:B:320:LEU:HD12  | 1.89                     | 0.53              |
| 4:D:28:PRO:CD    | 7:G:24:VAL:HG13   | 2.35                     | 0.53              |
| 4:D:92:ILE:HG22  | 4:D:96:PHE:CE2    | 2.41                     | 0.53              |
| 11:K:48:LYS:HE2  | 11:K:64:GLN:NE2   | 2.23                     | 0.53              |
| 15:O:374:PRO:CB  | 15:O:375:THR:HG23 | 2.39                     | 0.53              |
| 1:A:408:LYS:C    | 1:A:411:VAL:HG12  | 2.29                     | 0.53              |
| 2:B:472:SER:O    | 2:B:474:SER:N     | 2.41                     | 0.53              |
| 3:C:131:THR:HG21 | 3:C:207:HIS:HB3   | 1.91                     | 0.53              |
| 4:D:23:HIS:CD2   | 6:F:58:PHE:CD2    | 2.97                     | 0.53              |
| 7:G:30:GLU:HA    | 7:G:32:ASN:H      | 1.74                     | 0.53              |
| 13:M:12:ILE:HD12 | 14:N:67:LEU:HB2   | 1.90                     | 0.53              |
| 15:O:189:PHE:CD1 | 15:O:190:ILE:N    | 2.76                     | 0.53              |
| 15:O:520:CYS:O   | 15:O:521:ASN:O    | 2.27                     | 0.53              |
| 1:A:1317:ILE:HA  | 1:A:1321:PHE:HB3  | 1.90                     | 0.53              |
| 2:B:207:ILE:CD1  | 2:B:503:VAL:HG22  | 2.36                     | 0.53              |
| 2:B:211:ARG:NH2  | 2:B:243:GLN:OE1   | 2.42                     | 0.53              |
| 2:B:566:TYR:HD2  | 13:M:73:SER:HG    | 1.56                     | 0.53              |
| 3:C:272:LYS:HG3  | 14:N:175:TYR:CE1  | 2.44                     | 0.53              |
| 2:B:555:GLN:HB2  | 2:B:646:HIS:CE1   | 2.44                     | 0.52              |
| 1:A:800:VAL:HG23 | 1:A:1068:PHE:HZ   | 1.73                     | 0.52              |
| 1:A:477:ASN:OD1  | 2:B:1059:PRO:HG2  | 1.99                     | 0.52              |
| 2:B:894:LYS:HG2  | 12:L:47:ARG:HD3   | 1.89                     | 0.52              |
| 3:C:64:ALA:CB    | 3:C:227:TYR:CE2   | 2.92                     | 0.52              |
| 15:O:459:GLU:C   | 15:O:461:VAL:N    | 2.61                     | 0.52              |
| 2:B:33:SER:C     | 2:B:35:PHE:H      | 2.12                     | 0.52              |
| 3:C:64:ALA:HB3   | 3:C:298:PHE:CE2   | 2.44                     | 0.52              |
| 15:O:371:HIS:C   | 15:O:374:PRO:CD   | 2.78                     | 0.52              |
| 15:O:499:GLU:O   | 15:O:502:LEU:HG   | 2.09                     | 0.52              |
| 3:C:127:THR:H    | 3:C:130:ASN:HB2   | 1.74                     | 0.52              |
| 7:G:142:ALA:HB3  | 15:O:102:SER:HA   | 1.91                     | 0.52              |
| 9:I:59:SER:O     | 9:I:63:LYS:HG3    | 2.09                     | 0.52              |
| 15:O:337:THR:O   | 15:O:341:THR:OG1  | 2.27                     | 0.52              |
| 2:B:22:GLU:O     | 2:B:26:ILE:HG13   | 2.10                     | 0.52              |
| 7:G:242:VAL:HG21 | 15:O:183:ILE:HG21 | 1.91                     | 0.52              |
| 9:I:59:SER:O     | 9:I:63:LYS:CG     | 2.57                     | 0.52              |
| 1:A:509:GLU:HG3  | 1:A:579:ARG:CD    | 2.39                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:969:PHE:CE2   | 1:A:978:ALA:HA    | 2.44                     | 0.52              |
| 2:B:915:ASP:OD1   | 2:B:1038:HIS:CD2  | 2.61                     | 0.52              |
| 2:B:527:PHE:CE1   | 2:B:666:PRO:HG3   | 2.45                     | 0.52              |
| 15:O:348:THR:HG22 | 15:O:351:SER:CB   | 2.26                     | 0.52              |
| 2:B:833:PRO:O     | 2:B:834:LYS:HB3   | 2.10                     | 0.52              |
| 3:C:82:TYR:CE1    | 12:L:68:GLU:HG3   | 2.44                     | 0.52              |
| 15:O:156:MET:HG3  | 15:O:197:PHE:HE2  | 1.60                     | 0.52              |
| 15:O:155:SER:HB2  | 15:O:176:LEU:HD21 | 1.91                     | 0.52              |
| 15:O:373:LEU:CD1  | 15:O:416:LYS:CG   | 2.62                     | 0.52              |
| 1:A:441:THR:HG22  | 1:A:441:THR:O     | 2.10                     | 0.52              |
| 2:B:134:ARG:HD2   | 2:B:160:GLY:HA3   | 1.91                     | 0.52              |
| 2:B:42:VAL:O      | 2:B:46:ILE:CD1    | 2.52                     | 0.52              |
| 4:D:37:LEU:HD22   | 4:D:97:LYS:CE     | 2.39                     | 0.52              |
| 13:M:105:SER:HA   | 13:M:108:LEU:CG   | 2.29                     | 0.52              |
| 15:O:175:MET:HA   | 15:O:175:MET:HE2  | 1.92                     | 0.52              |
| 15:O:206:ARG:HA   | 15:O:209:VAL:HG12 | 1.90                     | 0.52              |
| 15:O:402:THR:O    | 15:O:406:ILE:HG13 | 2.10                     | 0.52              |
| 15:O:458:GLU:CG   | 15:O:514:PHE:CE2  | 2.92                     | 0.52              |
| 3:C:51:GLU:CB     | 3:C:303:GLU:HG3   | 2.40                     | 0.52              |
| 7:G:26:ASN:HD21   | 7:G:126:GLN:HE21  | 1.56                     | 0.52              |
| 15:O:459:GLU:HG3  | 15:O:460:GLU:N    | 2.25                     | 0.52              |
| 1:A:497:VAL:HG21  | 1:A:605:VAL:HG13  | 1.92                     | 0.51              |
| 1:A:722:PRO:HG2   | 8:H:46:LEU:HD13   | 1.90                     | 0.51              |
| 2:B:37:LEU:CD1    | 2:B:760:TYR:CZ    | 2.90                     | 0.51              |
| 15:O:415:GLU:O    | 15:O:419:LYS:HG3  | 2.10                     | 0.51              |
| 15:O:518:LYS:HD3  | 15:O:519:PHE:CZ   | 2.45                     | 0.51              |
| 1:A:636:HIS:CE1   | 2:B:1091:ARG:HH21 | 2.28                     | 0.51              |
| 2:B:1069:ILE:CD1  | 2:B:1069:ILE:N    | 2.73                     | 0.51              |
| 2:B:307:GLU:OE2   | 2:B:311:ARG:NH1   | 2.43                     | 0.51              |
| 2:B:938:PHE:CD1   | 3:C:68:ARG:NE     | 2.78                     | 0.51              |
| 3:C:47:LEU:HD23   | 3:C:48:ASP:N      | 2.25                     | 0.51              |
| 2:B:1120:ILE:CD1  | 15:O:117:GLN:HE22 | 2.23                     | 0.51              |
| 15:O:241:ASP:O    | 15:O:378:THR:HG23 | 2.10                     | 0.51              |
| 15:O:478:GLN:OE1  | 15:O:521:ASN:HB2  | 2.10                     | 0.51              |
| 15:O:426:SER:HB3  | 15:O:594:TYR:HB2  | 1.88                     | 0.51              |
| 15:O:377:TYR:O    | 15:O:378:THR:OG1  | 2.20                     | 0.51              |
| 1:A:87:ASN:HA     | 1:A:357:MET:SD    | 2.50                     | 0.51              |
| 15:O:457:ARG:O    | 15:O:461:VAL:HG23 | 2.10                     | 0.51              |
| 15:O:98:ASP:OD2   | 15:O:135:LYS:CE   | 2.58                     | 0.51              |
| 1:A:1003:ARG:CD   | 2:B:520:LEU:N     | 2.73                     | 0.51              |
| 1:A:1603:MET:HE1  | 1:A:1615:TYR:CD2  | 2.43                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1657:LEU:HB3  | 7:G:104:LEU:HB3  | 1.93                     | 0.51              |
| 2:B:1047:ARG:NH2  | 2:B:1051:PRO:O   | 2.43                     | 0.51              |
| 3:C:64:ALA:O      | 3:C:227:TYR:CE2  | 2.58                     | 0.51              |
| 15:O:158:LEU:HD22 | 15:O:172:HIS:CD2 | 2.46                     | 0.51              |
| 15:O:383:TYR:CZ   | 15:O:597:LEU:HB2 | 2.46                     | 0.51              |
| 1:A:392:THR:CB    | 1:A:430:ILE:HD13 | 2.37                     | 0.51              |
| 2:B:527:PHE:CD1   | 2:B:666:PRO:HG3  | 2.46                     | 0.51              |
| 4:D:95:ASP:OD2    | 7:G:150:HIS:CA   | 2.56                     | 0.51              |
| 15:O:151:TRP:HZ2  | 15:O:176:LEU:HA  | 1.76                     | 0.51              |
| 15:O:379:ARG:CB   | 15:O:382:GLN:NE2 | 2.74                     | 0.51              |
| 15:O:487:ARG:CG   | 15:O:487:ARG:NH1 | 2.73                     | 0.51              |
| 1:A:1028:GLU:CG   | 1:A:1029:GLY:H   | 2.24                     | 0.51              |
| 1:A:1056:ASP:OD2  | 1:A:1179:ILE:HA  | 2.11                     | 0.51              |
| 1:A:401:ASP:O     | 1:A:405:LYS:HB3  | 2.09                     | 0.51              |
| 2:B:472:SER:O     | 2:B:473:GLN:C    | 2.48                     | 0.51              |
| 3:C:31:TRP:CD2    | 11:K:82:LYS:CG   | 2.91                     | 0.51              |
| 15:O:247:GLU:OE1  | 15:O:325:ILE:CD1 | 2.57                     | 0.51              |
| 1:A:954:GLY:N     | 1:A:1205:PHE:HB3 | 2.25                     | 0.51              |
| 2:B:819:ASP:CG    | 2:B:820:PRO:HD2  | 2.31                     | 0.51              |
| 3:C:229:LEU:HD22  | 3:C:295:ARG:O    | 2.11                     | 0.51              |
| 1:A:1655:ASP:CG   | 6:F:137:TYR:HE2  | 2.14                     | 0.51              |
| 2:B:300:SER:CB    | 9:I:49:THR:HG22  | 2.41                     | 0.51              |
| 15:O:369:LYS:CE   | 15:O:370:THR:CG2 | 2.86                     | 0.51              |
| 1:A:475:ARG:HB3   | 2:B:1059:PRO:HB2 | 1.90                     | 0.51              |
| 1:A:840:ASN:O     | 1:A:844:THR:HG23 | 2.11                     | 0.51              |
| 2:B:769:PHE:CZ    | 2:B:798:PHE:CE1  | 2.91                     | 0.51              |
| 3:C:131:THR:HG22  | 3:C:208:CYS:N    | 2.26                     | 0.51              |
| 7:G:244:SER:HB2   | 15:O:148:PRO:HD2 | 1.91                     | 0.51              |
| 15:O:198:PHE:CD2  | 15:O:232:LEU:CG  | 2.60                     | 0.51              |
| 1:A:1003:ARG:CD   | 2:B:520:LEU:H    | 2.23                     | 0.51              |
| 1:A:1450:ILE:HD12 | 1:A:1460:TYR:CD2 | 2.46                     | 0.51              |
| 1:A:527:PRO:C     | 1:A:580:HIS:HE1  | 2.14                     | 0.51              |
| 2:B:934:ILE:HG21  | 3:C:69:ARG:O     | 2.10                     | 0.51              |
| 15:O:248:LEU:HD23 | 15:O:248:LEU:O   | 2.10                     | 0.51              |
| 1:A:509:GLU:OE2   | 1:A:579:ARG:CZ   | 2.58                     | 0.50              |
| 1:A:991:LYS:HB3   | 1:A:993:GLN:OE1  | 2.11                     | 0.50              |
| 1:A:880:GLN:OE1   | 2:B:633:THR:O    | 2.27                     | 0.50              |
| 2:B:934:ILE:HG21  | 3:C:73:SER:CB    | 2.41                     | 0.50              |
| 3:C:296:ASN:O     | 3:C:297:HIS:HB2  | 2.11                     | 0.50              |
| 3:C:57:ILE:O      | 3:C:58:ASN:HB2   | 2.12                     | 0.50              |
| 1:A:1048:PHE:CE2  | 5:E:211:TYR:HD1  | 2.21                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1660:VAL:O    | 7:G:103:LYS:N     | 2.39                     | 0.50              |
| 4:D:28:PRO:CD     | 7:G:24:VAL:CG1    | 2.89                     | 0.50              |
| 15:O:444:SER:O    | 15:O:447:THR:OG1  | 2.23                     | 0.50              |
| 15:O:446:LEU:O    | 15:O:449:TRP:CB   | 2.42                     | 0.50              |
| 1:A:478:TYR:HD1   | 2:B:1048:SER:HB2  | 1.76                     | 0.50              |
| 1:A:1660:VAL:N    | 7:G:103:LYS:O     | 2.41                     | 0.50              |
| 10:J:1:MET:HG2    | 10:J:57:ILE:HB    | 1.93                     | 0.50              |
| 4:D:80:THR:HG23   | 15:O:227:PHE:HB3  | 1.88                     | 0.50              |
| 1:A:564:PRO:HB2   | 15:O:371:HIS:HE1  | 1.76                     | 0.50              |
| 1:A:1326:GLU:OE2  | 1:A:1454:HIS:HB3  | 2.11                     | 0.50              |
| 2:B:1010:ASN:HB3  | 2:B:1025:ASP:HB3  | 1.93                     | 0.50              |
| 2:B:894:LYS:HD3   | 12:L:47:ARG:NH1   | 2.26                     | 0.50              |
| 15:O:591:TYR:CE2  | 15:O:593:PRO:HG3  | 2.46                     | 0.50              |
| 1:A:970:LYS:HG2   | 1:A:973:GLU:HG2   | 1.92                     | 0.50              |
| 2:B:469:ASN:CA    | 2:B:481:VAL:O     | 2.60                     | 0.50              |
| 6:F:74:ILE:CG2    | 6:F:75:PRO:CD     | 2.87                     | 0.50              |
| 2:B:1002:LYS:CD   | 14:N:166:LEU:HB2  | 2.40                     | 0.50              |
| 1:A:437:PHE:CE2   | 1:A:456:VAL:HG23  | 2.36                     | 0.50              |
| 2:B:293:ILE:HG12  | 2:B:306:LEU:HD13  | 1.94                     | 0.50              |
| 2:B:472:SER:HB3   | 2:B:476:LEU:HD11  | 1.92                     | 0.50              |
| 1:A:1003:ARG:CD   | 2:B:520:LEU:HB2   | 2.41                     | 0.50              |
| 2:B:68:ILE:HD11   | 2:B:414:LYS:CG    | 2.39                     | 0.50              |
| 8:H:26:ILE:HD12   | 8:H:42:ILE:HD12   | 1.93                     | 0.50              |
| 15:O:242:VAL:HA   | 15:O:378:THR:CG2  | 2.37                     | 0.50              |
| 15:O:352:LEU:HD22 | 15:O:358:VAL:HG22 | 1.81                     | 0.50              |
| 2:B:203:ILE:HG21  | 2:B:405:GLY:HA2   | 1.93                     | 0.50              |
| 2:B:284:SER:HB2   | 9:I:14:GLY:HA3    | 1.93                     | 0.50              |
| 3:C:230:LEU:HD11  | 3:C:231:PRO:HD2   | 1.92                     | 0.50              |
| 4:D:44:ILE:CG2    | 4:D:90:LYS:HE3    | 2.40                     | 0.50              |
| 5:E:145:THR:C     | 5:E:147:HIS:N     | 2.65                     | 0.50              |
| 14:N:87:TYR:CE1   | 14:N:141:GLU:OE1  | 2.64                     | 0.50              |
| 15:O:359:GLY:CA   | 15:O:362:ASN:ND2  | 2.73                     | 0.50              |
| 15:O:488:HIS:O    | 15:O:491:PHE:N    | 2.37                     | 0.50              |
| 1:A:505:LEU:HD12  | 1:A:581:ILE:HD13  | 1.93                     | 0.50              |
| 3:C:100:ARG:NH2   | 10:J:3:VAL:O      | 2.44                     | 0.50              |
| 15:O:208:LEU:O    | 15:O:212:THR:HG23 | 2.12                     | 0.50              |
| 1:A:953:GLU:CA    | 1:A:1205:PHE:CG   | 2.95                     | 0.50              |
| 3:C:222:VAL:O     | 3:C:224:THR:N     | 2.44                     | 0.50              |
| 3:C:231:PRO:HG2   | 3:C:270:ALA:CB    | 2.42                     | 0.50              |
| 3:C:47:LEU:HD23   | 3:C:48:ASP:H      | 1.77                     | 0.50              |
| 2:B:328:GLN:NE2   | 13:M:109:ARG:NH2  | 2.59                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1025:LYS:NZ   | 2:B:1076:ARG:NH1  | 2.59                     | 0.50              |
| 1:A:1048:PHE:CE2  | 5:E:210:SER:HA    | 2.46                     | 0.50              |
| 1:A:1056:ASP:HB2  | 1:A:1177:SER:O    | 2.11                     | 0.50              |
| 2:B:858:ILE:HD13  | 2:B:872:LYS:O     | 2.11                     | 0.50              |
| 15:O:352:LEU:CA   | 15:O:358:VAL:CG2  | 2.90                     | 0.50              |
| 1:A:863:ASN:HD22  | 9:I:67:VAL:C      | 2.15                     | 0.49              |
| 1:A:1003:ARG:HD2  | 2:B:520:LEU:N     | 2.23                     | 0.49              |
| 7:G:47:VAL:HB     | 7:G:65:HIS:CD2    | 2.47                     | 0.49              |
| 14:N:85:HIS:CE1   | 14:N:141:GLU:OE1  | 2.64                     | 0.49              |
| 15:O:368:PHE:C    | 15:O:368:PHE:CD1  | 2.85                     | 0.49              |
| 15:O:453:TYR:CE1  | 15:O:473:PHE:HB2  | 2.47                     | 0.49              |
| 1:A:1006:LEU:HD21 | 2:B:535:ASP:CB    | 2.42                     | 0.49              |
| 7:G:143:SER:HB3   | 15:O:103:ASN:CA   | 2.42                     | 0.49              |
| 15:O:324:GLY:O    | 15:O:326:LYS:N    | 2.44                     | 0.49              |
| 15:O:368:PHE:CD2  | 15:O:385:MET:HG2  | 2.47                     | 0.49              |
| 15:O:468:GLU:C    | 15:O:470:PHE:N    | 2.65                     | 0.49              |
| 1:A:381:SER:HB2   | 1:A:453:ILE:HG21  | 1.93                     | 0.49              |
| 2:B:1019:GLY:CA   | 3:C:65:ASN:CG     | 2.81                     | 0.49              |
| 2:B:338:PHE:CE1   | 2:B:353:VAL:HG22  | 2.47                     | 0.49              |
| 4:D:23:HIS:CG     | 6:F:58:PHE:CD2    | 3.00                     | 0.49              |
| 7:G:242:VAL:HG21  | 15:O:183:ILE:HG23 | 1.93                     | 0.49              |
| 9:I:91:ASN:OD1    | 9:I:92:GLU:N      | 2.45                     | 0.49              |
| 1:A:1622:LEU:HD21 | 2:B:1189:LEU:HD22 | 1.94                     | 0.49              |
| 1:A:412:SER:H     | 1:A:415:ASP:HB2   | 1.76                     | 0.49              |
| 1:A:507:TYR:HB2   | 1:A:637:PHE:CE2   | 2.47                     | 0.49              |
| 2:B:1043:LYS:HE2  | 2:B:1063:ARG:CD   | 2.42                     | 0.49              |
| 3:C:71:MET:HE1    | 3:C:225:ALA:HB1   | 1.90                     | 0.49              |
| 3:C:71:MET:CE     | 3:C:302:VAL:CG2   | 2.90                     | 0.49              |
| 1:A:1053:ASP:HB2  | 5:E:204:THR:CG2   | 2.43                     | 0.49              |
| 2:B:1120:ILE:HD12 | 15:O:117:GLN:NE2  | 2.27                     | 0.49              |
| 15:O:430:ARG:O    | 15:O:431:ALA:O    | 2.31                     | 0.49              |
| 1:A:1148:LEU:HD22 | 1:A:1163:GLU:HG3  | 1.92                     | 0.49              |
| 1:A:995:TYR:O     | 1:A:999:CYS:N     | 2.35                     | 0.49              |
| 2:B:211:ARG:HH11  | 2:B:211:ARG:HG2   | 1.77                     | 0.49              |
| 4:D:30:HIS:HE2    | 7:G:26:ASN:CG     | 2.11                     | 0.49              |
| 12:L:45:ALA:O     | 12:L:47:ARG:N     | 2.46                     | 0.49              |
| 15:O:173:HIS:CE1  | 15:O:217:LYS:HB3  | 2.47                     | 0.49              |
| 1:A:1034:TYR:HA   | 1:A:1181:PRO:HB3  | 1.95                     | 0.49              |
| 1:A:1500:GLN:HG2  | 1:A:1501:ILE:N    | 2.28                     | 0.49              |
| 15:O:173:HIS:CD2  | 15:O:217:LYS:CG   | 2.95                     | 0.49              |
| 15:O:488:HIS:C    | 15:O:490:ILE:N    | 2.59                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:488:HIS:CE1  | 15:O:489:ASN:H    | 2.27                     | 0.49              |
| 1:A:1026:GLN:NE2  | 1:A:1603:MET:HA   | 2.26                     | 0.49              |
| 15:O:177:LYS:HG3  | 15:O:178:TYR:N    | 2.26                     | 0.49              |
| 15:O:443:ALA:O    | 15:O:447:THR:HG23 | 2.12                     | 0.49              |
| 2:B:211:ARG:NH1   | 2:B:211:ARG:HG2   | 2.28                     | 0.49              |
| 6:F:75:PRO:HG3    | 6:F:78:GLN:NE2    | 2.27                     | 0.49              |
| 15:O:361:PHE:CD1  | 15:O:361:PHE:C    | 2.86                     | 0.49              |
| 15:O:507:GLN:O    | 15:O:511:ILE:HG23 | 2.12                     | 0.49              |
| 1:A:795:HIS:NE2   | 1:A:1062:HIS:HE1  | 2.11                     | 0.49              |
| 1:A:1661:PRO:CA   | 7:G:101:SER:O     | 2.61                     | 0.49              |
| 1:A:249:THR:HG1   | 1:A:435:ASN:HD21  | 1.58                     | 0.49              |
| 1:A:476:VAL:O     | 2:B:1059:PRO:HG2  | 2.13                     | 0.49              |
| 1:A:982:VAL:HG13  | 1:A:994:GLU:CD    | 2.33                     | 0.49              |
| 2:B:252:TYR:OH    | 2:B:305:ARG:NH1   | 2.44                     | 0.49              |
| 2:B:262:PHE:CD1   | 2:B:357:ILE:HD13  | 2.48                     | 0.49              |
| 13:M:65:TYR:CE1   | 13:M:97:VAL:HB    | 2.48                     | 0.49              |
| 15:O:234:ILE:O    | 15:O:238:ILE:HG13 | 2.12                     | 0.49              |
| 1:A:582:LYS:O     | 1:A:585:ASP:HB2   | 2.12                     | 0.49              |
| 1:A:91:PHE:CZ     | 1:A:249:THR:HA    | 2.46                     | 0.49              |
| 1:A:1662:ASN:N    | 7:G:101:SER:HB2   | 2.28                     | 0.49              |
| 15:O:163:ILE:HG22 | 15:O:207:LYS:O    | 2.12                     | 0.49              |
| 15:O:434:LEU:CD1  | 15:O:434:LEU:N    | 2.75                     | 0.49              |
| 2:B:281:CYS:HA    | 2:B:323:ARG:NE    | 2.28                     | 0.48              |
| 1:A:1053:ASP:HB2  | 5:E:204:THR:HG22  | 1.95                     | 0.48              |
| 15:O:396:MET:HE1  | 15:O:433:LYS:C    | 2.34                     | 0.48              |
| 15:O:468:GLU:C    | 15:O:470:PHE:H    | 2.15                     | 0.48              |
| 15:O:390:GLN:C    | 15:O:609:TYR:CE1  | 2.81                     | 0.48              |
| 1:A:475:ARG:NH1   | 2:B:1061:LYS:HB2  | 2.28                     | 0.48              |
| 2:B:225:ARG:NH2   | 2:B:261:ARG:HD3   | 2.27                     | 0.48              |
| 4:D:95:ASP:OD1    | 7:G:151:ASP:HB2   | 2.12                     | 0.48              |
| 7:G:137:ILE:HG13  | 7:G:227:GLY:O     | 2.13                     | 0.48              |
| 8:H:112:ILE:HD12  | 8:H:129:TYR:HB2   | 1.93                     | 0.48              |
| 15:O:591:TYR:HE2  | 15:O:593:PRO:HG3  | 1.77                     | 0.48              |
| 1:A:996:TYR:HE1   | 1:A:1000:MET:HE1  | 1.78                     | 0.48              |
| 1:A:1050:TYR:HE1  | 1:A:1185:VAL:HG12 | 1.67                     | 0.48              |
| 1:A:1055:ILE:CG2  | 1:A:1060:GLU:HB2  | 2.43                     | 0.48              |
| 1:A:1260:LYS:HE2  | 1:A:1262:LEU:HD11 | 1.95                     | 0.48              |
| 2:B:1043:LYS:HG3  | 2:B:1063:ARG:CZ   | 2.43                     | 0.48              |
| 2:B:209:GLN:CG    | 2:B:210:ARG:H     | 2.08                     | 0.48              |
| 15:O:391:GLN:HE22 | 15:O:609:TYR:HE2  | 1.61                     | 0.48              |
| 1:A:440:SER:C     | 1:A:442:LYS:H     | 2.17                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:50:TYR:CD1    | 1:A:365:THR:HG23  | 2.47                     | 0.48              |
| 5:E:145:THR:O     | 5:E:147:HIS:N     | 2.46                     | 0.48              |
| 15:O:597:LEU:HD12 | 15:O:598:PHE:H    | 1.77                     | 0.48              |
| 15:O:383:TYR:CG   | 15:O:597:LEU:HD22 | 2.47                     | 0.48              |
| 15:O:91:LYS:HG3   | 15:O:92:ASN:N     | 2.28                     | 0.48              |
| 1:A:1606:SER:HB3  | 1:A:1611:MET:HE2  | 1.96                     | 0.48              |
| 2:B:471:VAL:O     | 2:B:471:VAL:HG12  | 2.13                     | 0.48              |
| 2:B:929:ARG:HH22  | 11:K:96:PRO:HB2   | 1.77                     | 0.48              |
| 15:O:199:PRO:HB2  | 15:O:208:LEU:HD23 | 1.95                     | 0.48              |
| 1:A:365:THR:O     | 1:A:368:ARG:N     | 2.37                     | 0.48              |
| 1:A:413:LEU:CA    | 1:A:417:ARG:HH21  | 2.27                     | 0.48              |
| 1:A:721:LYS:HB3   | 8:H:96:VAL:HB     | 1.95                     | 0.48              |
| 2:B:550:ARG:O     | 2:B:649:MET:HA    | 2.14                     | 0.48              |
| 2:B:800:TYR:CD1   | 2:B:800:TYR:C     | 2.87                     | 0.48              |
| 4:D:48:GLU:CD     | 4:D:90:LYS:NZ     | 2.66                     | 0.48              |
| 1:A:932:GLY:C     | 9:I:125:ASN:HD21  | 2.16                     | 0.48              |
| 14:N:111:VAL:HG13 | 14:N:122:ALA:HB2  | 1.96                     | 0.48              |
| 15:O:241:ASP:OD1  | 15:O:380:SER:HB2  | 2.13                     | 0.48              |
| 15:O:408:PHE:CD2  | 15:O:449:TRP:CE2  | 3.02                     | 0.48              |
| 15:O:484:PHE:O    | 15:O:488:HIS:HB3  | 2.14                     | 0.48              |
| 15:O:440:ILE:HD13 | 15:O:491:PHE:CD1  | 2.48                     | 0.48              |
| 1:A:399:LEU:HD22  | 1:A:423:LEU:HA    | 1.95                     | 0.48              |
| 1:A:597:LYS:HB2   | 2:B:1082:HIS:CE1  | 2.48                     | 0.48              |
| 1:A:1003:ARG:HD2  | 2:B:520:LEU:CB    | 2.43                     | 0.48              |
| 1:A:40:ASN:OD1    | 1:A:40:ASN:N      | 2.44                     | 0.48              |
| 1:A:747:ILE:HD13  | 1:A:748:ASN:H     | 1.77                     | 0.48              |
| 1:A:480:ALA:CA    | 2:B:1046:VAL:HG23 | 2.42                     | 0.48              |
| 3:C:157:TYR:HB2   | 3:C:160:ALA:HB2   | 1.94                     | 0.48              |
| 4:D:92:ILE:CD1    | 7:G:152:ALA:CB    | 2.92                     | 0.48              |
| 5:E:61:GLN:HE21   | 5:E:105:PHE:HE1   | 1.61                     | 0.48              |
| 1:A:684:ASP:OD1   | 8:H:20:TYR:HB3    | 2.13                     | 0.48              |
| 15:O:369:LYS:HE2  | 15:O:370:THR:N    | 2.28                     | 0.48              |
| 15:O:477:PHE:CE2  | 15:O:481:CYS:SG   | 3.07                     | 0.48              |
| 1:A:1006:LEU:CD2  | 2:B:535:ASP:HB2   | 2.43                     | 0.48              |
| 1:A:1023:LEU:CD2  | 1:A:1598:PHE:CD1  | 2.97                     | 0.48              |
| 1:A:1162:ASN:ND2  | 1:A:1165:LYS:HG3  | 2.29                     | 0.48              |
| 1:A:869:PRO:HG2   | 1:A:872:ASP:HB2   | 1.96                     | 0.48              |
| 2:B:1133:MET:CE   | 7:G:17:ILE:HD13   | 2.44                     | 0.48              |
| 2:B:552:SER:O     | 2:B:647:SER:CA    | 2.61                     | 0.48              |
| 15:O:369:LYS:HD2  | 15:O:370:THR:HA   | 1.95                     | 0.48              |
| 15:O:446:LEU:C    | 15:O:449:TRP:HB3  | 2.31                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1055:ILE:CG2  | 1:A:1060:GLU:CG   | 2.90                     | 0.48              |
| 1:A:1312:GLU:O    | 1:A:1316:VAL:HG23 | 2.13                     | 0.48              |
| 2:B:1045:GLN:HB3  | 2:B:1063:ARG:HG3  | 1.95                     | 0.48              |
| 2:B:894:LYS:HD3   | 12:L:47:ARG:CZ    | 2.44                     | 0.48              |
| 2:B:70:GLU:CB     | 2:B:97:VAL:O      | 2.62                     | 0.48              |
| 15:O:146:SER:C    | 15:O:148:PRO:HD3  | 2.34                     | 0.48              |
| 1:A:747:ILE:HD13  | 1:A:748:ASN:N     | 2.29                     | 0.47              |
| 4:D:92:ILE:HD11   | 7:G:152:ALA:HB1   | 1.95                     | 0.47              |
| 7:G:158:LYS:HE2   | 15:O:105:ASN:OD1  | 2.14                     | 0.47              |
| 15:O:151:TRP:CZ2  | 15:O:176:LEU:HA   | 2.49                     | 0.47              |
| 15:O:225:LEU:HD12 | 15:O:229:ILE:HG13 | 1.96                     | 0.47              |
| 1:A:960:MET:SD    | 2:B:522:PRO:HB2   | 2.54                     | 0.47              |
| 1:A:959:VAL:HG22  | 1:A:965:THR:HG22  | 1.95                     | 0.47              |
| 2:B:73:ILE:HB     | 2:B:425:ILE:HD12  | 1.96                     | 0.47              |
| 4:D:80:THR:HG21   | 15:O:227:PHE:CG   | 2.48                     | 0.47              |
| 15:O:369:LYS:O    | 15:O:373:LEU:CA   | 2.60                     | 0.47              |
| 15:O:478:GLN:NE2  | 15:O:592:PHE:CZ   | 2.69                     | 0.47              |
| 2:B:208:VAL:CG2   | 2:B:401:GLU:CG    | 2.92                     | 0.47              |
| 2:B:73:ILE:HD12   | 2:B:425:ILE:HG23  | 1.95                     | 0.47              |
| 3:C:230:LEU:CG    | 3:C:294:VAL:CG2   | 2.92                     | 0.47              |
| 15:O:120:ILE:HD13 | 15:O:150:TRP:CE3  | 2.49                     | 0.47              |
| 1:A:1348:VAL:HB   | 2:B:268:GLU:CA    | 2.43                     | 0.47              |
| 2:B:552:SER:O     | 2:B:647:SER:HA    | 2.14                     | 0.47              |
| 2:B:584:CYS:HB3   | 2:B:596:VAL:HG23  | 1.95                     | 0.47              |
| 10:J:6:ARG:HD2    | 10:J:11:GLY:O     | 2.13                     | 0.47              |
| 1:A:1261:VAL:HG12 | 1:A:1262:LEU:N    | 2.28                     | 0.47              |
| 1:A:1605:THR:C    | 1:A:1606:SER:O    | 2.37                     | 0.47              |
| 1:A:1482:LYS:HE2  | 2:B:304:ASP:OD1   | 2.15                     | 0.47              |
| 1:A:1048:PHE:CE1  | 5:E:211:TYR:CD1   | 3.01                     | 0.47              |
| 5:E:48:ASP:OD1    | 5:E:50:MET:HB3    | 2.13                     | 0.47              |
| 1:A:258:GLU:HA    | 1:A:261:ILE:HD12  | 1.97                     | 0.47              |
| 2:B:338:PHE:CZ    | 2:B:357:ILE:HD12  | 2.49                     | 0.47              |
| 2:B:470:LEU:O     | 2:B:481:VAL:HG13  | 2.15                     | 0.47              |
| 15:O:107:ILE:O    | 15:O:109:SER:N    | 2.46                     | 0.47              |
| 1:A:439:ASP:HB3   | 1:A:442:LYS:HD2   | 1.96                     | 0.47              |
| 1:A:741:PRO:HA    | 1:A:742:PRO:HD3   | 1.68                     | 0.47              |
| 2:B:1020:GLU:HG2  | 3:C:61:THR:CB     | 2.44                     | 0.47              |
| 15:O:460:GLU:O    | 15:O:469:ARG:NH2  | 2.47                     | 0.47              |
| 15:O:521:ASN:ND2  | 15:O:523:ASN:N    | 2.54                     | 0.47              |
| 2:B:812:ALA:HA    | 2:B:815:ARG:HD3   | 1.95                     | 0.47              |
| 3:C:126:PHE:HD1   | 3:C:131:THR:HG1   | 1.62                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1573:TYR:HB3  | 9:I:122:ARG:NH2   | 2.30                     | 0.47              |
| 15:O:237:ILE:CG2  | 15:O:381:ILE:CG1  | 2.93                     | 0.47              |
| 15:O:471:LYS:CG   | 15:O:472:HIS:N    | 2.75                     | 0.47              |
| 1:A:19:LEU:HD11   | 2:B:1190:SER:HB2  | 1.96                     | 0.47              |
| 2:B:396:ALA:HB1   | 2:B:523:GLU:HG3   | 1.96                     | 0.47              |
| 3:C:247:PHE:HE1   | 3:C:289:VAL:HG21  | 1.80                     | 0.47              |
| 1:A:479:ALA:HB2   | 1:A:636:HIS:ND1   | 2.29                     | 0.47              |
| 3:C:86:PHE:CD1    | 12:L:64:LEU:HD13  | 2.46                     | 0.47              |
| 3:C:31:TRP:NE1    | 11:K:82:LYS:NZ    | 2.54                     | 0.47              |
| 13:M:109:ARG:HH22 | 13:M:112:LYS:HG3  | 1.79                     | 0.47              |
| 15:O:170:VAL:CG1  | 15:O:171:CYS:N    | 2.78                     | 0.47              |
| 15:O:176:LEU:HD13 | 15:O:218:LEU:HD13 | 1.96                     | 0.47              |
| 1:A:55:GLY:HA2    | 1:A:62:CYS:SG     | 2.56                     | 0.47              |
| 2:B:413:LEU:O     | 2:B:417:ILE:HG13  | 2.14                     | 0.47              |
| 15:O:129:PRO:O    | 15:O:133:LEU:CB   | 2.62                     | 0.47              |
| 15:O:602:TYR:O    | 15:O:606:MET:HG2  | 2.15                     | 0.47              |
| 2:B:1103:VAL:HG22 | 2:B:1176:VAL:HG22 | 1.97                     | 0.46              |
| 2:B:203:ILE:CG2   | 2:B:405:GLY:HA2   | 2.45                     | 0.46              |
| 2:B:470:LEU:N     | 2:B:481:VAL:O     | 2.47                     | 0.46              |
| 2:B:569:GLY:HA2   | 14:N:140:SER:OG   | 2.15                     | 0.46              |
| 3:C:231:PRO:CG    | 3:C:270:ALA:O     | 2.62                     | 0.46              |
| 3:C:239:ILE:HG23  | 3:C:243:SER:HB3   | 1.96                     | 0.46              |
| 1:A:863:ASN:HD22  | 9:I:68:LYS:N      | 2.08                     | 0.46              |
| 15:O:138:TYR:CD2  | 15:O:142:ILE:CD1  | 2.92                     | 0.46              |
| 15:O:488:HIS:O    | 15:O:489:ASN:C    | 2.54                     | 0.46              |
| 1:A:1320:GLN:HB2  | 1:A:1320:GLN:HE21 | 1.56                     | 0.46              |
| 1:A:364:PRO:HB2   | 1:A:367:PHE:CD2   | 2.51                     | 0.46              |
| 1:A:403:LEU:CD2   | 1:A:423:LEU:HD11  | 2.45                     | 0.46              |
| 2:B:681:ILE:O     | 14:N:154:ARG:NE   | 2.36                     | 0.46              |
| 2:B:736:ARG:HD3   | 2:B:738:ASP:OD2   | 2.15                     | 0.46              |
| 4:D:46:GLU:OE1    | 4:D:47:LYS:HE2    | 2.15                     | 0.46              |
| 4:D:95:ASP:HB2    | 7:G:151:ASP:HB3   | 1.97                     | 0.46              |
| 15:O:170:VAL:HG13 | 15:O:171:CYS:H    | 1.79                     | 0.46              |
| 15:O:206:ARG:HA   | 15:O:209:VAL:CG1  | 2.44                     | 0.46              |
| 15:O:388:VAL:HG13 | 15:O:389:SER:N    | 2.31                     | 0.46              |
| 1:A:1053:ASP:O    | 1:A:1054:ALA:CB   | 2.62                     | 0.46              |
| 1:A:1060:GLU:HA   | 1:A:1063:MET:CG   | 2.37                     | 0.46              |
| 1:A:1258:ILE:HB   | 1:A:1501:ILE:HD12 | 1.97                     | 0.46              |
| 1:A:1440:ASN:HA   | 1:A:1443:GLN:HB2  | 1.96                     | 0.46              |
| 1:A:412:SER:C     | 1:A:414:GLU:H     | 2.17                     | 0.46              |
| 1:A:492:THR:HG23  | 1:A:811:SER:OG    | 2.14                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:996:TYR:CE1   | 1:A:1000:MET:HE3  | 2.51                     | 0.46              |
| 3:C:231:PRO:HG3   | 3:C:270:ALA:O     | 2.16                     | 0.46              |
| 15:O:181:ARG:NH1  | 15:O:181:ARG:CG   | 2.77                     | 0.46              |
| 2:B:679:GLN:HG3   | 14:N:155:VAL:O    | 2.14                     | 0.46              |
| 3:C:71:MET:HE1    | 3:C:302:VAL:CG2   | 2.40                     | 0.46              |
| 9:I:23:VAL:O      | 9:I:39:LYS:NZ     | 2.48                     | 0.46              |
| 11:K:93:ILE:HA    | 11:K:94:PRO:HD2   | 1.75                     | 0.46              |
| 15:O:148:PRO:HB3  | 15:O:183:ILE:HD13 | 1.98                     | 0.46              |
| 15:O:433:LYS:HG3  | 15:O:433:LYS:O    | 2.16                     | 0.46              |
| 15:O:74:ILE:O     | 15:O:78:VAL:HG13  | 2.16                     | 0.46              |
| 2:B:280:LEU:HD13  | 2:B:371:PHE:N     | 2.30                     | 0.46              |
| 4:D:95:ASP:HB2    | 7:G:151:ASP:CB    | 2.46                     | 0.46              |
| 1:A:211:THR:HG23  | 5:E:177:ARG:CZ    | 2.45                     | 0.46              |
| 15:O:506:PHE:HD2  | 15:O:537:VAL:CG1  | 2.28                     | 0.46              |
| 1:A:411:VAL:CG2   | 1:A:412:SER:N     | 2.76                     | 0.46              |
| 1:A:507:TYR:HB2   | 1:A:637:PHE:CZ    | 2.51                     | 0.46              |
| 2:B:467:THR:O     | 2:B:469:ASN:N     | 2.49                     | 0.46              |
| 7:G:141:SER:HB2   | 15:O:138:TYR:CZ   | 2.43                     | 0.46              |
| 7:G:143:SER:HB3   | 15:O:102:SER:C    | 2.35                     | 0.46              |
| 15:O:352:LEU:HA   | 15:O:358:VAL:CG2  | 2.31                     | 0.46              |
| 1:A:1028:GLU:HG3  | 1:A:1637:PRO:HG2  | 1.97                     | 0.46              |
| 1:A:94:LEU:HD11   | 1:A:356:PHE:CZ    | 2.51                     | 0.46              |
| 2:B:265:ARG:NH2   | 2:B:339:GLN:OE1   | 2.48                     | 0.46              |
| 1:A:1003:ARG:CD   | 2:B:520:LEU:CB    | 2.93                     | 0.46              |
| 2:B:822:THR:HB    | 2:B:823:GLN:HG3   | 1.98                     | 0.46              |
| 4:D:48:GLU:CG     | 4:D:86:ILE:HD12   | 2.39                     | 0.46              |
| 2:B:202:LEU:HD13  | 2:B:500:PHE:CE1   | 2.51                     | 0.46              |
| 3:C:57:ILE:CA     | 3:C:297:HIS:HA    | 2.09                     | 0.46              |
| 3:C:50:ARG:O      | 3:C:303:GLU:CA    | 2.58                     | 0.46              |
| 4:D:25:THR:CB     | 6:F:59:GLN:HG2    | 2.39                     | 0.46              |
| 15:O:459:GLU:O    | 15:O:463:GLN:CB   | 2.63                     | 0.46              |
| 15:O:447:THR:HB   | 15:O:505:PHE:CE2  | 2.51                     | 0.46              |
| 1:A:1575:ILE:HG13 | 9:I:122:ARG:NH1   | 2.29                     | 0.46              |
| 1:A:184:LYS:HA    | 1:A:187:GLU:HG2   | 1.98                     | 0.46              |
| 1:A:5:LYS:HE2     | 1:A:5:LYS:HB3     | 1.68                     | 0.46              |
| 2:B:774:ALA:HB1   | 2:B:1026:ILE:HD11 | 1.97                     | 0.46              |
| 2:B:1120:ILE:CD1  | 15:O:117:GLN:NE2  | 2.79                     | 0.46              |
| 1:A:438:ILE:CG2   | 2:B:1192:MET:CE   | 2.92                     | 0.46              |
| 2:B:890:ASP:HB3   | 2:B:896:GLN:OE1   | 2.15                     | 0.46              |
| 3:C:31:TRP:NE1    | 11:K:78:TYR:OH    | 2.46                     | 0.46              |
| 5:E:131:THR:HG21  | 5:E:191:LYS:CE    | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:239:SER:O    | 15:O:243:GLU:HG2  | 2.16                     | 0.46              |
| 1:A:412:SER:HB3   | 1:A:414:GLU:HB3   | 1.96                     | 0.46              |
| 2:B:293:ILE:CD1   | 2:B:302:LEU:HB3   | 2.46                     | 0.46              |
| 2:B:554:GLN:C     | 2:B:646:HIS:CD2   | 2.90                     | 0.46              |
| 1:A:618:TYR:CE1   | 2:B:783:MET:HB2   | 2.50                     | 0.46              |
| 4:D:92:ILE:CD1    | 7:G:152:ALA:HB1   | 2.45                     | 0.46              |
| 15:O:467:MET:HE1  | 15:O:470:PHE:HE2  | 1.81                     | 0.46              |
| 1:A:1019:LEU:CD1  | 1:A:1227:MET:CG   | 2.91                     | 0.45              |
| 1:A:1608:SER:OG   | 1:A:1632:GLU:OE2  | 2.20                     | 0.45              |
| 2:B:724:GLN:O     | 2:B:1037:ARG:HG3  | 2.17                     | 0.45              |
| 2:B:292:ILE:HB    | 2:B:306:LEU:HD11  | 1.98                     | 0.45              |
| 4:D:28:PRO:CB     | 7:G:24:VAL:HG11   | 2.46                     | 0.45              |
| 13:M:26:PHE:CE1   | 13:M:98:SER:HB2   | 2.51                     | 0.45              |
| 15:O:428:ILE:CG2  | 15:O:439:ILE:CG2  | 2.86                     | 0.45              |
| 15:O:506:PHE:CG   | 15:O:528:PHE:HZ   | 2.34                     | 0.45              |
| 1:A:954:GLY:N     | 1:A:1205:PHE:CB   | 2.79                     | 0.45              |
| 1:A:436:ALA:O     | 1:A:440:SER:N     | 2.49                     | 0.45              |
| 2:B:552:SER:C     | 2:B:647:SER:H     | 2.16                     | 0.45              |
| 4:D:40:LEU:HD13   | 4:D:93:GLN:HB2    | 1.98                     | 0.45              |
| 9:I:89:CYS:SG     | 9:I:91:ASN:HB2    | 2.56                     | 0.45              |
| 11:K:80:ILE:HD13  | 11:K:105:ILE:HD11 | 1.98                     | 0.45              |
| 15:O:485:CYS:SG   | 15:O:531:ILE:HD12 | 2.56                     | 0.45              |
| 15:O:458:GLU:HG3  | 15:O:514:PHE:CE2  | 2.51                     | 0.45              |
| 2:B:68:ILE:CD1    | 2:B:414:LYS:HG3   | 2.41                     | 0.45              |
| 2:B:480:GLN:CB    | 2:B:507:SER:OG    | 2.64                     | 0.45              |
| 3:C:228:ARG:HG3   | 3:C:299:ILE:HB    | 1.98                     | 0.45              |
| 3:C:54:PHE:CD1    | 3:C:300:PHE:O     | 2.69                     | 0.45              |
| 15:O:190:ILE:HD13 | 15:O:190:ILE:C    | 2.37                     | 0.45              |
| 15:O:245:GLN:O    | 15:O:248:LEU:N    | 2.39                     | 0.45              |
| 15:O:370:THR:O    | 15:O:374:PRO:CG   | 2.63                     | 0.45              |
| 15:O:459:GLU:O    | 15:O:463:GLN:N    | 2.50                     | 0.45              |
| 15:O:69:THR:HG22  | 15:O:70:GLN:N     | 2.31                     | 0.45              |
| 1:A:1237:GLN:H    | 1:A:1544:ASN:HB2  | 1.81                     | 0.45              |
| 2:B:841:ASP:OD1   | 2:B:842:GLU:N     | 2.40                     | 0.45              |
| 3:C:294:VAL:HG12  | 3:C:294:VAL:O     | 2.15                     | 0.45              |
| 3:C:295:ARG:HD3   | 3:C:295:ARG:HA    | 1.66                     | 0.45              |
| 2:B:1020:GLU:HG3  | 3:C:61:THR:OG1    | 2.17                     | 0.45              |
| 7:G:143:SER:CB    | 15:O:103:ASN:HA   | 2.46                     | 0.45              |
| 15:O:169:THR:O    | 15:O:170:VAL:C    | 2.54                     | 0.45              |
| 1:A:1006:LEU:HD21 | 2:B:535:ASP:HB2   | 1.98                     | 0.45              |
| 1:A:1657:LEU:HD22 | 7:G:104:LEU:CD1   | 2.45                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:782:ASP:O     | 1:A:785:GLN:N     | 2.27                     | 0.45              |
| 1:A:863:ASN:ND2   | 9:I:67:VAL:C      | 2.70                     | 0.45              |
| 1:A:953:GLU:HG2   | 1:A:1205:PHE:CD2  | 2.50                     | 0.45              |
| 2:B:61:LEU:HA     | 2:B:61:LEU:HD23   | 1.76                     | 0.45              |
| 2:B:646:HIS:O     | 2:B:647:SER:HB2   | 2.16                     | 0.45              |
| 1:A:1048:PHE:HZ   | 5:E:211:TYR:HB2   | 1.81                     | 0.45              |
| 7:G:242:VAL:HG12  | 15:O:185:SER:CB   | 2.46                     | 0.45              |
| 15:O:372:VAL:CG1  | 15:O:423:TYR:OH   | 2.64                     | 0.45              |
| 1:A:1348:VAL:CA   | 2:B:268:GLU:O     | 2.63                     | 0.45              |
| 2:B:585:CYS:HB2   | 2:B:595:TRP:CZ3   | 2.51                     | 0.45              |
| 4:D:80:THR:CG2    | 15:O:227:PHE:CG   | 2.99                     | 0.45              |
| 6:F:75:PRO:HG3    | 6:F:78:GLN:CD     | 2.37                     | 0.45              |
| 1:A:891:ILE:CD1   | 9:I:71:LEU:N      | 2.80                     | 0.45              |
| 15:O:148:PRO:HB3  | 15:O:183:ILE:CD1  | 2.46                     | 0.45              |
| 15:O:407:SER:CB   | 15:O:408:PHE:CD1  | 2.95                     | 0.45              |
| 15:O:521:ASN:HD22 | 15:O:523:ASN:H    | 1.59                     | 0.45              |
| 1:A:799:GLU:CG    | 1:A:1062:HIS:CG   | 2.85                     | 0.45              |
| 1:A:799:GLU:CG    | 1:A:1062:HIS:ND1  | 2.69                     | 0.45              |
| 1:A:1154:LEU:O    | 1:A:1158:SER:HB2  | 2.17                     | 0.45              |
| 1:A:1291:VAL:HG22 | 1:A:1473:LYS:HG3  | 1.99                     | 0.45              |
| 1:A:1657:LEU:HD11 | 6:F:135:ARG:HB2   | 1.98                     | 0.45              |
| 2:B:205:MET:HE1   | 2:B:500:PHE:O     | 2.16                     | 0.45              |
| 3:C:117:ASP:OD1   | 3:C:119:ASN:ND2   | 2.44                     | 0.45              |
| 3:C:176:SER:O     | 3:C:180:ALA:HB2   | 2.16                     | 0.45              |
| 13:M:65:TYR:HE1   | 13:M:97:VAL:HB    | 1.81                     | 0.45              |
| 15:O:369:LYS:HE3  | 15:O:370:THR:HG22 | 1.99                     | 0.45              |
| 15:O:384:ILE:HA   | 15:O:602:TYR:OH   | 2.16                     | 0.45              |
| 15:O:408:PHE:HZ   | 15:O:446:LEU:CD2  | 2.30                     | 0.45              |
| 15:O:468:GLU:O    | 15:O:470:PHE:N    | 2.49                     | 0.45              |
| 1:A:878:ARG:NE    | 9:I:67:VAL:HG13   | 2.30                     | 0.45              |
| 2:B:1158:ILE:HA   | 2:B:1167:PHE:O    | 2.17                     | 0.45              |
| 5:E:7:ARG:O       | 5:E:11:ARG:HG3    | 2.17                     | 0.45              |
| 15:O:237:ILE:HG22 | 15:O:381:ILE:CB   | 2.44                     | 0.45              |
| 15:O:98:ASP:OD2   | 15:O:135:LYS:CD   | 2.64                     | 0.45              |
| 1:A:1463:ASP:HB2  | 1:A:1469:TRP:CE2  | 2.52                     | 0.45              |
| 3:C:57:ILE:HG13   | 3:C:296:ASN:O     | 2.17                     | 0.45              |
| 11:K:49:LEU:HG    | 11:K:54:THR:HG21  | 1.98                     | 0.45              |
| 3:C:71:MET:CB     | 3:C:225:ALA:HB3   | 2.47                     | 0.45              |
| 5:E:144:ILE:HG13  | 5:E:145:THR:N     | 2.32                     | 0.45              |
| 4:D:22:ILE:O      | 7:G:76:LYS:HG2    | 2.17                     | 0.45              |
| 13:M:61:GLU:OE2   | 13:M:106:LYS:NZ   | 2.43                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1054:ALA:HB1  | 1:A:1178:LEU:HD22 | 1.98                     | 0.44              |
| 3:C:231:PRO:HG2   | 3:C:270:ALA:C     | 2.37                     | 0.44              |
| 7:G:163:PRO:HG2   | 7:G:166:TRP:CD1   | 2.53                     | 0.44              |
| 1:A:878:ARG:NH2   | 9:I:66:VAL:HG23   | 2.32                     | 0.44              |
| 15:O:426:SER:HB3  | 15:O:594:TYR:CD2  | 2.50                     | 0.44              |
| 15:O:426:SER:OG   | 15:O:594:TYR:C    | 2.54                     | 0.44              |
| 1:A:54:LEU:HD13   | 1:A:368:ARG:NH2   | 2.33                     | 0.44              |
| 1:A:799:GLU:HG3   | 1:A:1062:HIS:CD2  | 2.49                     | 0.44              |
| 2:B:470:LEU:HD22  | 2:B:478:LEU:HD12  | 1.99                     | 0.44              |
| 2:B:683:ASN:HA    | 14:N:150:TYR:CZ   | 2.53                     | 0.44              |
| 15:O:143:LEU:HD11 | 15:O:150:TRP:HD1  | 1.77                     | 0.44              |
| 15:O:156:MET:CE   | 15:O:193:TYR:CE1  | 3.00                     | 0.44              |
| 1:A:437:PHE:CE2   | 1:A:456:VAL:HG21  | 2.52                     | 0.44              |
| 1:A:480:ALA:HA    | 2:B:1046:VAL:HA   | 1.97                     | 0.44              |
| 2:B:833:PRO:HG2   | 2:B:836:TRP:CZ2   | 2.52                     | 0.44              |
| 5:E:78:LEU:HD13   | 5:E:107:THR:HB    | 1.98                     | 0.44              |
| 5:E:177:ARG:HD3   | 5:E:215:MET:HB2   | 1.99                     | 0.44              |
| 7:G:154:ASN:ND2   | 15:O:182:MET:HE1  | 2.26                     | 0.44              |
| 15:O:488:HIS:CE1  | 15:O:489:ASN:OD1  | 2.71                     | 0.44              |
| 1:A:1441:LYS:HB3  | 1:A:1441:LYS:HE2  | 1.75                     | 0.44              |
| 1:A:257:ASN:OD1   | 1:A:258:GLU:N     | 2.51                     | 0.44              |
| 1:A:35:PRO:CA     | 1:A:390:LEU:HD13  | 2.47                     | 0.44              |
| 2:B:107:PRO:HG2   | 2:B:133:TYR:CZ    | 2.52                     | 0.44              |
| 2:B:468:GLY:O     | 2:B:484:TYR:HD2   | 2.01                     | 0.44              |
| 2:B:786:ALA:HB1   | 2:B:928:SER:HB2   | 1.98                     | 0.44              |
| 3:C:131:THR:HG22  | 3:C:208:CYS:C     | 2.35                     | 0.44              |
| 3:C:230:LEU:CG    | 3:C:231:PRO:HD2   | 2.48                     | 0.44              |
| 2:B:1020:GLU:OE2  | 3:C:61:THR:HG21   | 2.18                     | 0.44              |
| 3:C:272:LYS:HA    | 14:N:175:TYR:CE2  | 2.53                     | 0.44              |
| 1:A:1229:ALA:HB3  | 1:A:1597:ALA:HB2  | 1.99                     | 0.44              |
| 1:A:1600:ARG:NH2  | 1:A:1617:THR:OG1  | 2.48                     | 0.44              |
| 1:A:37:VAL:HG12   | 1:A:38:LEU:HG     | 2.00                     | 0.44              |
| 1:A:891:ILE:HD13  | 9:I:71:LEU:CB     | 2.44                     | 0.44              |
| 1:A:920:PHE:CD1   | 1:A:921:PRO:HA    | 2.52                     | 0.44              |
| 2:B:399:HIS:C     | 2:B:400:GLN:CG    | 2.86                     | 0.44              |
| 3:C:252:PRO:HD2   | 3:C:255:VAL:HG21  | 1.99                     | 0.44              |
| 4:D:48:GLU:OE2    | 4:D:90:LYS:NZ     | 2.51                     | 0.44              |
| 10:J:36:LEU:HD13  | 10:J:47:ARG:HB3   | 1.98                     | 0.44              |
| 15:O:163:ILE:CG2  | 15:O:211:TYR:HB2  | 2.38                     | 0.44              |
| 15:O:368:PHE:HE2  | 15:O:382:GLN:HA   | 1.81                     | 0.44              |
| 15:O:391:GLN:CD   | 15:O:609:TYR:OH   | 2.55                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1313:LEU:O    | 1:A:1317:ILE:HD12 | 2.18                     | 0.44              |
| 1:A:1654:PHE:HA   | 6:F:135:ARG:O     | 2.17                     | 0.44              |
| 2:B:190:ILE:HG13  | 2:B:191:GLY:N     | 2.32                     | 0.44              |
| 2:B:910:THR:OG1   | 2:B:912:GLN:NE2   | 2.51                     | 0.44              |
| 2:B:954:PHE:H     | 2:B:955:PRO:HD2   | 1.83                     | 0.44              |
| 2:B:974:LEU:O     | 10:J:47:ARG:NH1   | 2.50                     | 0.44              |
| 12:L:63:ARG:HD2   | 12:L:63:ARG:HA    | 1.74                     | 0.44              |
| 15:O:158:LEU:HD22 | 15:O:172:HIS:CG   | 2.52                     | 0.44              |
| 15:O:237:ILE:HG22 | 15:O:381:ILE:CD1  | 2.34                     | 0.44              |
| 15:O:581:THR:HA   | 15:O:584:GLN:CD   | 2.37                     | 0.44              |
| 1:A:1023:LEU:CD2  | 1:A:1598:PHE:CE1  | 3.01                     | 0.44              |
| 1:A:509:GLU:CG    | 1:A:579:ARG:HE    | 2.31                     | 0.44              |
| 1:A:1:MET:CB      | 2:B:1098:TYR:CG   | 2.98                     | 0.44              |
| 2:B:938:PHE:CD1   | 3:C:68:ARG:NH2    | 2.86                     | 0.44              |
| 4:D:28:PRO:HB2    | 7:G:24:VAL:CG1    | 2.47                     | 0.44              |
| 5:E:93:MET:CG     | 5:E:120:ALA:HB1   | 2.46                     | 0.44              |
| 15:O:78:VAL:HA    | 15:O:88:ILE:HG22  | 2.00                     | 0.44              |
| 1:A:1660:VAL:O    | 7:G:102:GLU:CA    | 2.50                     | 0.44              |
| 1:A:782:ASP:O     | 1:A:783:LYS:C     | 2.56                     | 0.44              |
| 2:B:78:PRO:O      | 2:B:79:LEU:HB3    | 2.17                     | 0.44              |
| 15:O:128:LEU:HB3  | 15:O:129:PRO:HD2  | 1.97                     | 0.44              |
| 15:O:237:ILE:HD13 | 15:O:384:ILE:HD11 | 2.00                     | 0.44              |
| 1:A:507:TYR:CD2   | 1:A:508:PRO:O     | 2.70                     | 0.44              |
| 3:C:55:ASP:CG     | 3:C:299:ILE:CG1   | 2.47                     | 0.44              |
| 15:O:412:GLU:OE1  | 15:O:412:GLU:HA   | 2.18                     | 0.44              |
| 15:O:458:GLU:CB   | 15:O:461:VAL:HG21 | 2.47                     | 0.44              |
| 15:O:515:ASN:N    | 15:O:516:PRO:HD3  | 2.33                     | 0.44              |
| 15:O:76:ASN:O     | 15:O:80:LEU:HD13  | 2.18                     | 0.44              |
| 1:A:1:MET:CB      | 2:B:1098:TYR:CD1  | 3.01                     | 0.43              |
| 1:A:34:ASN:C      | 1:A:390:LEU:HD13  | 2.38                     | 0.43              |
| 1:A:509:GLU:OE2   | 1:A:579:ARG:NH2   | 2.51                     | 0.43              |
| 1:A:677:GLY:HA3   | 1:A:786:TYR:OH    | 2.18                     | 0.43              |
| 3:C:230:LEU:CG    | 3:C:231:PRO:CD    | 2.96                     | 0.43              |
| 6:F:76:LYS:C      | 6:F:78:GLN:H      | 2.22                     | 0.43              |
| 6:F:75:PRO:CG     | 6:F:78:GLN:CD     | 2.87                     | 0.43              |
| 4:D:96:PHE:CE1    | 7:G:150:HIS:CD2   | 3.06                     | 0.43              |
| 15:O:174:ASP:C    | 15:O:177:LYS:HG2  | 2.36                     | 0.43              |
| 15:O:607:LYS:HE2  | 15:O:607:LYS:HB2  | 1.88                     | 0.43              |
| 15:O:56:VAL:CG2   | 15:O:99:ILE:HD12  | 2.48                     | 0.43              |
| 1:A:1028:GLU:HA   | 1:A:1187:ILE:HG12 | 2.00                     | 0.43              |
| 1:A:1261:VAL:HG21 | 1:A:1306:TYR:HB3  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:26:SER:O      | 9:I:39:LYS:HB2    | 2.18                     | 0.43              |
| 2:B:563:SER:HB2   | 13:M:73:SER:HB3   | 2.00                     | 0.43              |
| 15:O:194:LEU:HD21 | 15:O:225:LEU:HD11 | 1.96                     | 0.43              |
| 15:O:458:GLU:HA   | 15:O:461:VAL:HG23 | 0.48                     | 0.43              |
| 1:A:36:THR:HG22   | 1:A:45:VAL:HG21   | 2.00                     | 0.43              |
| 1:A:403:LEU:HA    | 1:A:403:LEU:HD12  | 1.79                     | 0.43              |
| 1:A:436:ALA:HA    | 1:A:443:ALA:HB2   | 1.99                     | 0.43              |
| 1:A:509:GLU:HA    | 1:A:509:GLU:OE1   | 2.18                     | 0.43              |
| 1:A:782:ASP:C     | 1:A:784:SER:N     | 2.71                     | 0.43              |
| 2:B:1069:ILE:CG2  | 2:B:1070:ARG:N    | 2.73                     | 0.43              |
| 2:B:203:ILE:HB    | 2:B:405:GLY:HA3   | 2.00                     | 0.43              |
| 1:A:718:THR:HG21  | 8:H:118:PHE:O     | 2.18                     | 0.43              |
| 14:N:87:TYR:CD1   | 14:N:141:GLU:HA   | 2.53                     | 0.43              |
| 15:O:413:ALA:HB1  | 15:O:415:GLU:OE1  | 2.18                     | 0.43              |
| 1:A:535:GLN:HA    | 1:A:546:LEU:HG    | 1.99                     | 0.43              |
| 3:C:64:ALA:HB2    | 3:C:298:PHE:CE2   | 2.51                     | 0.43              |
| 15:O:245:GLN:CG   | 15:O:378:THR:HG23 | 2.48                     | 0.43              |
| 15:O:383:TYR:O    | 15:O:386:PHE:N    | 2.51                     | 0.43              |
| 15:O:460:GLU:O    | 15:O:469:ARG:CZ   | 2.66                     | 0.43              |
| 1:A:1606:SER:HB3  | 1:A:1611:MET:CE   | 2.47                     | 0.43              |
| 2:B:209:GLN:CG    | 2:B:210:ARG:N     | 2.76                     | 0.43              |
| 3:C:84:TYR:CZ     | 12:L:66:GLN:OE1   | 2.60                     | 0.43              |
| 13:M:8:SER:O      | 14:N:71:PRO:HA    | 2.19                     | 0.43              |
| 14:N:40:LEU:HD12  | 14:N:40:LEU:HA    | 1.84                     | 0.43              |
| 14:N:94:ASP:HB3   | 14:N:99:LEU:HG    | 2.00                     | 0.43              |
| 15:O:173:HIS:HE1  | 15:O:214:ASN:O    | 2.02                     | 0.43              |
| 15:O:431:ALA:HB3  | 15:O:434:LEU:HD21 | 2.00                     | 0.43              |
| 15:O:434:LEU:HD23 | 15:O:439:ILE:HG13 | 2.00                     | 0.43              |
| 2:B:236:ILE:HG21  | 2:B:377:MET:HE1   | 1.99                     | 0.43              |
| 2:B:893:ASN:O     | 2:B:895:PHE:HD1   | 2.01                     | 0.43              |
| 15:O:66:ASN:CG    | 15:O:111:ARG:NH1  | 2.72                     | 0.43              |
| 15:O:189:PHE:HA   | 15:O:192:THR:HG23 | 1.99                     | 0.43              |
| 15:O:232:LEU:HA   | 15:O:232:LEU:HD12 | 1.74                     | 0.43              |
| 15:O:352:LEU:HD23 | 15:O:358:VAL:HG23 | 1.85                     | 0.43              |
| 1:A:399:LEU:CD1   | 1:A:423:LEU:HG    | 2.44                     | 0.43              |
| 15:O:377:TYR:CD2  | 15:O:377:TYR:O    | 2.70                     | 0.43              |
| 1:A:1600:ARG:NH2  | 1:A:1621:PHE:CE2  | 2.86                     | 0.43              |
| 2:B:29:PRO:O      | 2:B:177:PRO:HD2   | 2.18                     | 0.43              |
| 2:B:699:ILE:O     | 2:B:703:LEU:HG    | 2.19                     | 0.43              |
| 2:B:923:GLN:HG2   | 2:B:949:ILE:CD1   | 2.47                     | 0.43              |
| 7:G:29:ASP:OD1    | 7:G:30:GLU:N      | 2.52                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 15:O:356:GLU:HA   | 15:O:356:GLU:OE1 | 2.19                     | 0.43              |
| 15:O:412:GLU:O    | 15:O:413:ALA:C   | 2.57                     | 0.43              |
| 15:O:487:ARG:HG3  | 15:O:487:ARG:NH1 | 2.34                     | 0.43              |
| 1:A:1305:GLU:CD   | 9:I:63:LYS:HE3   | 2.39                     | 0.43              |
| 2:B:399:HIS:O     | 2:B:400:GLN:HG2  | 2.18                     | 0.43              |
| 2:B:555:GLN:N     | 2:B:646:HIS:NE2  | 2.67                     | 0.43              |
| 2:B:1017:ALA:C    | 3:C:65:ASN:ND2   | 2.72                     | 0.43              |
| 15:O:169:THR:O    | 15:O:172:HIS:N   | 2.52                     | 0.43              |
| 4:D:80:THR:HB     | 15:O:227:PHE:CD2 | 2.50                     | 0.43              |
| 15:O:48:SER:O     | 15:O:49:ALA:C    | 2.57                     | 0.43              |
| 1:A:1575:ILE:HG12 | 9:I:122:ARG:NH1  | 2.28                     | 0.43              |
| 1:A:407:GLN:HB3   | 1:A:409:ASP:OD2  | 2.19                     | 0.43              |
| 2:B:742:TYR:CE2   | 2:B:1037:ARG:HD3 | 2.54                     | 0.43              |
| 1:A:1657:LEU:HD21 | 6:F:135:ARG:NH2  | 2.34                     | 0.43              |
| 15:O:124:LYS:O    | 15:O:127:GLU:HB2 | 2.18                     | 0.43              |
| 15:O:225:LEU:CD1  | 15:O:225:LEU:C   | 2.86                     | 0.43              |
| 1:A:1070:LEU:C    | 1:A:1072:ASN:H   | 2.21                     | 0.42              |
| 1:A:1172:LEU:O    | 1:A:1176:ARG:HG2 | 2.19                     | 0.42              |
| 2:B:883:GLU:HG3   | 2:B:906:ARG:HB2  | 2.01                     | 0.42              |
| 14:N:63:ASP:OD2   | 14:N:66:LYS:NZ   | 2.35                     | 0.42              |
| 15:O:390:GLN:NE2  | 15:O:431:ALA:HA  | 2.34                     | 0.42              |
| 2:B:550:ARG:HD3   | 2:B:550:ARG:HA   | 1.80                     | 0.42              |
| 6:F:66:ARG:NH1    | 7:G:90:LEU:CD1   | 2.82                     | 0.42              |
| 12:L:32:ALA:HB3   | 12:L:55:ILE:HG23 | 2.01                     | 0.42              |
| 15:O:156:MET:HG2  | 15:O:197:PHE:CZ  | 2.53                     | 0.42              |
| 15:O:199:PRO:HD3  | 15:O:211:TYR:CG  | 2.54                     | 0.42              |
| 15:O:457:ARG:HA   | 15:O:460:GLU:CG  | 2.49                     | 0.42              |
| 15:O:96:LEU:O     | 15:O:100:LEU:HG  | 2.20                     | 0.42              |
| 1:A:953:GLU:CA    | 1:A:1205:PHE:CD2 | 2.97                     | 0.42              |
| 1:A:550:SER:OG    | 1:A:553:GLN:HG3  | 2.19                     | 0.42              |
| 1:A:938:VAL:HG22  | 9:I:82:ILE:HD13  | 2.00                     | 0.42              |
| 2:B:300:SER:OG    | 9:I:49:THR:HG23  | 2.17                     | 0.42              |
| 2:B:569:GLY:CA    | 14:N:140:SER:OG  | 2.66                     | 0.42              |
| 3:C:55:ASP:HB3    | 3:C:297:HIS:HE2  | 1.80                     | 0.42              |
| 15:O:173:HIS:NE2  | 15:O:217:LYS:HB3 | 2.35                     | 0.42              |
| 15:O:336:LEU:HD11 | 15:O:380:SER:O   | 2.19                     | 0.42              |
| 1:A:1034:TYR:HA   | 1:A:1181:PRO:CB  | 2.49                     | 0.42              |
| 1:A:998:HIS:NE2   | 2:B:712:SER:N    | 2.55                     | 0.42              |
| 3:C:57:ILE:HB     | 3:C:297:HIS:CE1  | 2.55                     | 0.42              |
| 6:F:93:ILE:HA     | 6:F:93:ILE:HD13  | 1.70                     | 0.42              |
| 14:N:70:LEU:HA    | 14:N:71:PRO:HD3  | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:404:ILE:CD1  | 15:O:442:VAL:HG11 | 2.49                     | 0.42              |
| 15:O:430:ARG:HH22 | 15:O:596:PRO:CD   | 2.25                     | 0.42              |
| 15:O:515:ASN:HD21 | 15:O:547:ASN:HD21 | 1.67                     | 0.42              |
| 2:B:1082:HIS:HB3  | 2:B:1084:THR:HG23 | 2.01                     | 0.42              |
| 2:B:211:ARG:CB    | 2:B:239:VAL:CG1   | 2.98                     | 0.42              |
| 2:B:809:VAL:HG13  | 2:B:901:VAL:HB    | 2.01                     | 0.42              |
| 3:C:31:TRP:CE3    | 11:K:82:LYS:CB    | 3.02                     | 0.42              |
| 4:D:44:ILE:HG21   | 4:D:90:LYS:CE     | 2.45                     | 0.42              |
| 7:G:160:ASN:OD1   | 7:G:160:ASN:N     | 2.52                     | 0.42              |
| 9:I:60:LEU:CA     | 9:I:63:LYS:HG3    | 2.45                     | 0.42              |
| 15:O:369:LYS:CD   | 15:O:369:LYS:C    | 2.86                     | 0.42              |
| 1:A:990:ILE:CB    | 1:A:994:GLU:HB2   | 2.41                     | 0.42              |
| 1:A:475:ARG:NH1   | 2:B:1061:LYS:HA   | 2.35                     | 0.42              |
| 2:B:399:HIS:C     | 2:B:400:GLN:HG3   | 2.40                     | 0.42              |
| 2:B:57:ASP:N      | 2:B:57:ASP:OD1    | 2.52                     | 0.42              |
| 1:A:1655:ASP:HB2  | 6:F:135:ARG:CG    | 2.49                     | 0.42              |
| 2:B:890:ASP:O     | 12:L:54:ARG:CD    | 2.68                     | 0.42              |
| 15:O:124:LYS:HD3  | 15:O:127:GLU:OE2  | 2.20                     | 0.42              |
| 15:O:202:ASN:N    | 15:O:202:ASN:OD1  | 2.52                     | 0.42              |
| 15:O:234:ILE:HD13 | 15:O:234:ILE:HA   | 1.74                     | 0.42              |
| 15:O:468:GLU:HG2  | 15:O:469:ARG:N    | 2.33                     | 0.42              |
| 1:A:999:CYS:SG    | 2:B:531:VAL:HG22  | 2.59                     | 0.42              |
| 11:K:50:LEU:O     | 11:K:54:THR:HG23  | 2.20                     | 0.42              |
| 13:M:102:SER:O    | 13:M:106:LYS:CB   | 2.56                     | 0.42              |
| 7:G:159:LYS:HD2   | 15:O:103:ASN:CG   | 2.39                     | 0.42              |
| 15:O:413:ALA:C    | 15:O:415:GLU:N    | 2.72                     | 0.42              |
| 1:A:1003:ARG:HD2  | 2:B:520:LEU:HB3   | 2.02                     | 0.42              |
| 1:A:478:TYR:HA    | 2:B:1048:SER:HA   | 0.57                     | 0.42              |
| 2:B:469:ASN:HA    | 2:B:482:SER:HA    | 2.00                     | 0.42              |
| 2:B:478:LEU:HB3   | 2:B:484:TYR:OH    | 2.20                     | 0.42              |
| 2:B:697:LEU:HB2   | 2:B:702:ASN:ND2   | 2.35                     | 0.42              |
| 2:B:938:PHE:CE2   | 3:C:68:ARG:HD2    | 2.54                     | 0.42              |
| 1:A:1575:ILE:CG1  | 9:I:122:ARG:HH22  | 2.32                     | 0.42              |
| 15:O:447:THR:HG21 | 15:O:480:LEU:HD21 | 2.02                     | 0.42              |
| 15:O:447:THR:HB   | 15:O:505:PHE:CZ   | 2.55                     | 0.42              |
| 1:A:660:PRO:O     | 1:A:1057:ILE:HG21 | 2.20                     | 0.42              |
| 3:C:116:VAL:HG11  | 3:C:125:LYS:HE3   | 2.01                     | 0.42              |
| 2:B:881:TYR:CZ    | 12:L:67:PHE:HE1   | 2.37                     | 0.42              |
| 15:O:66:ASN:ND2   | 15:O:111:ARG:CZ   | 2.83                     | 0.42              |
| 15:O:129:PRO:HD2  | 15:O:132:THR:CB   | 2.25                     | 0.42              |
| 15:O:409:ALA:O    | 15:O:417:LYS:HE2  | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:467:MET:CG   | 15:O:519:PHE:CZ   | 2.96                     | 0.42              |
| 15:O:77:GLN:HG2   | 15:O:88:ILE:HB    | 2.01                     | 0.42              |
| 1:A:953:GLU:C     | 1:A:1205:PHE:CG   | 2.94                     | 0.42              |
| 2:B:1017:ALA:O    | 3:C:65:ASN:ND2    | 2.53                     | 0.42              |
| 3:C:57:ILE:HG13   | 3:C:297:HIS:HB2   | 2.02                     | 0.42              |
| 2:B:938:PHE:CE1   | 3:C:68:ARG:CD     | 3.03                     | 0.42              |
| 5:E:67:GLU:CD     | 5:E:67:GLU:H      | 2.23                     | 0.42              |
| 4:D:28:PRO:CB     | 7:G:24:VAL:CG1    | 2.98                     | 0.42              |
| 15:O:370:THR:O    | 15:O:374:PRO:HG3  | 2.19                     | 0.42              |
| 1:A:1648:ASN:O    | 1:A:1652:GLY:O    | 2.38                     | 0.41              |
| 1:A:365:THR:C     | 1:A:367:PHE:N     | 2.73                     | 0.41              |
| 1:A:692:TYR:O     | 1:A:696:ILE:HG12  | 2.19                     | 0.41              |
| 1:A:478:TYR:O     | 2:B:1047:ARG:O    | 2.37                     | 0.41              |
| 2:B:211:ARG:HH21  | 2:B:239:VAL:HG21  | 1.81                     | 0.41              |
| 3:C:236:LEU:HD11  | 3:C:290:LYS:HG3   | 2.02                     | 0.41              |
| 15:O:173:HIS:CG   | 15:O:217:LYS:HG3  | 2.55                     | 0.41              |
| 15:O:417:LYS:HD3  | 15:O:472:HIS:CE1  | 2.33                     | 0.41              |
| 1:A:385:LEU:HD23  | 1:A:385:LEU:HA    | 1.88                     | 0.41              |
| 1:A:437:PHE:C     | 1:A:439:ASP:H     | 2.22                     | 0.41              |
| 1:A:507:TYR:CE2   | 1:A:508:PRO:O     | 2.73                     | 0.41              |
| 1:A:874:GLU:OE2   | 1:A:878:ARG:HD2   | 2.20                     | 0.41              |
| 2:B:1090:ASP:HA   | 2:B:1094:ASN:HB2  | 2.02                     | 0.41              |
| 2:B:1020:GLU:CD   | 3:C:61:THR:HG21   | 2.40                     | 0.41              |
| 8:H:105:GLU:HG2   | 8:H:115:TYR:HE1   | 1.84                     | 0.41              |
| 14:N:81:THR:HG22  | 14:N:86:ASP:HB3   | 2.01                     | 0.41              |
| 15:O:56:VAL:HG23  | 15:O:57:LYS:N     | 2.35                     | 0.41              |
| 15:O:430:ARG:O    | 15:O:610:TYR:HA   | 2.20                     | 0.41              |
| 1:A:451:VAL:HA    | 1:A:452:PRO:HD3   | 1.95                     | 0.41              |
| 1:A:680:LEU:O     | 1:A:728:GLY:HA3   | 2.21                     | 0.41              |
| 2:B:478:LEU:CB    | 2:B:484:TYR:OH    | 2.69                     | 0.41              |
| 2:B:656:LEU:HD21  | 2:B:689:VAL:HG12  | 2.01                     | 0.41              |
| 3:C:64:ALA:HB1    | 3:C:298:PHE:CD2   | 2.56                     | 0.41              |
| 15:O:150:TRP:O    | 15:O:154:VAL:HG23 | 2.21                     | 0.41              |
| 15:O:234:ILE:HG22 | 15:O:371:HIS:CD2  | 2.42                     | 0.41              |
| 15:O:458:GLU:HG2  | 15:O:461:VAL:HG21 | 2.02                     | 0.41              |
| 15:O:592:PHE:HA   | 15:O:593:PRO:HD3  | 1.91                     | 0.41              |
| 1:A:1248:ASP:OD1  | 1:A:1517:ARG:NH1  | 2.49                     | 0.41              |
| 1:A:1499:ARG:HG2  | 1:A:1500:GLN:N    | 2.35                     | 0.41              |
| 1:A:854:GLY:HA3   | 1:A:974:THR:O     | 2.21                     | 0.41              |
| 1:A:891:ILE:HD12  | 9:I:71:LEU:N      | 2.35                     | 0.41              |
| 2:B:1094:ASN:O    | 2:B:1096:SER:N    | 2.41                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:321:GLN:HB3   | 9:I:32:GLN:HE21   | 1.84                     | 0.41              |
| 2:B:401:GLU:C     | 2:B:402:VAL:HG23  | 2.41                     | 0.41              |
| 2:B:143:TRP:CE3   | 2:B:446:MET:HG3   | 2.54                     | 0.41              |
| 2:B:553:THR:C     | 2:B:646:HIS:HD2   | 2.23                     | 0.41              |
| 3:C:41:GLU:C      | 3:C:57:ILE:HG22   | 2.41                     | 0.41              |
| 7:G:223:GLU:HG3   | 7:G:223:GLU:H     | 1.71                     | 0.41              |
| 15:O:108:GLU:HB2  | 15:O:147:ILE:CD1  | 2.47                     | 0.41              |
| 15:O:201:LYS:HG3  | 15:O:201:LYS:H    | 1.59                     | 0.41              |
| 15:O:352:LEU:CD2  | 15:O:358:VAL:CG2  | 2.56                     | 0.41              |
| 15:O:423:TYR:CE1  | 15:O:593:PRO:HB2  | 2.55                     | 0.41              |
| 1:A:1348:VAL:HA   | 1:A:1349:PRO:HD3  | 1.93                     | 0.41              |
| 1:A:1242:ILE:HG22 | 1:A:1536:ILE:HG22 | 2.01                     | 0.41              |
| 2:B:464:PHE:O     | 2:B:468:GLY:N     | 2.49                     | 0.41              |
| 3:C:84:TYR:HD2    | 12:L:66:GLN:CB    | 2.30                     | 0.41              |
| 4:D:82:LEU:O      | 4:D:86:ILE:HG23   | 2.20                     | 0.41              |
| 7:G:24:VAL:O      | 7:G:25:THR:O      | 2.39                     | 0.41              |
| 3:C:84:TYR:CE2    | 12:L:66:GLN:HB2   | 2.47                     | 0.41              |
| 7:G:154:ASN:ND2   | 15:O:182:MET:HE3  | 2.27                     | 0.41              |
| 1:A:1056:ASP:HB3  | 1:A:1059:LYS:HB2  | 2.02                     | 0.41              |
| 1:A:1:MET:HB2     | 2:B:1098:TYR:CD2  | 2.54                     | 0.41              |
| 1:A:248:PHE:HD1   | 1:A:442:LYS:O     | 2.01                     | 0.41              |
| 2:B:211:ARG:O     | 2:B:212:ASN:HB2   | 2.21                     | 0.41              |
| 2:B:286:ARG:HD2   | 2:B:286:ARG:HA    | 1.88                     | 0.41              |
| 7:G:139:ILE:CD1   | 15:O:178:TYR:OH   | 2.68                     | 0.41              |
| 1:A:1305:GLU:HG3  | 9:I:60:LEU:HG     | 2.03                     | 0.41              |
| 3:C:272:LYS:HG3   | 14:N:175:TYR:CZ   | 2.55                     | 0.41              |
| 14:N:25:ILE:HA    | 14:N:26:PRO:HD3   | 1.84                     | 0.41              |
| 1:A:1063:MET:HB3  | 1:A:1063:MET:HE2  | 1.85                     | 0.41              |
| 2:B:206:LEU:HD23  | 2:B:206:LEU:HA    | 1.81                     | 0.41              |
| 3:C:80:ALA:HB3    | 3:C:102:GLY:HA2   | 2.03                     | 0.41              |
| 7:G:28:ILE:HG23   | 7:G:34:THR:O      | 2.20                     | 0.41              |
| 8:H:95:TYR:HD2    | 8:H:144:ILE:HD12  | 1.86                     | 0.41              |
| 12:L:33:GLU:HG3   | 12:L:53:HIS:ND1   | 2.36                     | 0.41              |
| 15:O:241:ASP:HA   | 15:O:380:SER:CB   | 2.46                     | 0.41              |
| 1:A:1049:MET:C    | 1:A:1051:GLY:N    | 2.74                     | 0.41              |
| 1:A:1179:ILE:HD11 | 1:A:1183:GLU:CD   | 2.40                     | 0.41              |
| 3:C:57:ILE:HB     | 3:C:297:HIS:ND1   | 2.35                     | 0.41              |
| 4:D:23:HIS:CD2    | 6:F:58:PHE:CE1    | 3.08                     | 0.41              |
| 11:K:54:THR:HG22  | 11:K:62:SER:H     | 1.86                     | 0.41              |
| 15:O:107:ILE:CG2  | 15:O:107:ILE:O    | 2.69                     | 0.41              |
| 15:O:115:LEU:O    | 15:O:119:ILE:HG13 | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:237:ILE:HG21 | 15:O:381:ILE:CG1  | 2.51                     | 0.41              |
| 1:A:1195:GLU:HB3  | 1:A:1196:PRO:HD3  | 2.03                     | 0.41              |
| 1:A:1317:ILE:O    | 1:A:1322:ILE:HG12 | 2.21                     | 0.41              |
| 1:A:1262:LEU:HD22 | 1:A:1497:ILE:HG12 | 2.03                     | 0.41              |
| 1:A:1575:ILE:HG13 | 9:I:122:ARG:NH2   | 2.36                     | 0.41              |
| 2:B:1043:LYS:HE2  | 2:B:1063:ARG:HD2  | 2.01                     | 0.41              |
| 2:B:262:PHE:CE1   | 2:B:357:ILE:HD13  | 2.56                     | 0.41              |
| 2:B:527:PHE:CE2   | 2:B:666:PRO:HA    | 2.55                     | 0.41              |
| 8:H:41:ASP:HB2    | 8:H:121:LEU:HB3   | 2.02                     | 0.41              |
| 9:I:2:SER:HA      | 9:I:9:PHE:O       | 2.21                     | 0.41              |
| 15:O:107:ILE:CD1  | 15:O:115:LEU:HD23 | 2.51                     | 0.41              |
| 15:O:147:ILE:HG22 | 15:O:149:LYS:CB   | 2.51                     | 0.41              |
| 15:O:163:ILE:HD12 | 15:O:207:LYS:HG2  | 2.02                     | 0.41              |
| 1:A:1074:TYR:CE2  | 1:A:1159:ASP:HB3  | 2.54                     | 0.41              |
| 1:A:315:ILE:HG13  | 1:A:319:GLU:HB2   | 2.03                     | 0.41              |
| 1:A:440:SER:C     | 1:A:442:LYS:N     | 2.74                     | 0.41              |
| 1:A:509:GLU:CG    | 1:A:579:ARG:CD    | 2.99                     | 0.41              |
| 2:B:1094:ASN:C    | 2:B:1096:SER:H    | 2.24                     | 0.41              |
| 2:B:279:ALA:HB2   | 2:B:326:VAL:HG12  | 2.03                     | 0.41              |
| 2:B:545:PHE:CZ    | 2:B:551:ILE:HD11  | 2.56                     | 0.41              |
| 7:G:50:ALA:HA     | 7:G:113:PHE:CD2   | 2.56                     | 0.41              |
| 15:O:369:LYS:CB   | 15:O:369:LYS:HZ3  | 2.21                     | 0.41              |
| 1:A:1037:SER:HA   | 1:A:1049:MET:HA   | 2.03                     | 0.41              |
| 1:A:700:ILE:HA    | 1:A:700:ILE:HD13  | 1.81                     | 0.41              |
| 1:A:964:LYS:HE2   | 1:A:964:LYS:HB3   | 1.83                     | 0.41              |
| 2:B:1069:ILE:CG2  | 2:B:1070:ARG:H    | 2.20                     | 0.41              |
| 2:B:371:PHE:CE2   | 2:B:375:LEU:HD11  | 2.56                     | 0.41              |
| 2:B:401:GLU:CG    | 2:B:402:VAL:N     | 2.73                     | 0.41              |
| 2:B:42:VAL:O      | 2:B:46:ILE:CG1    | 2.69                     | 0.41              |
| 2:B:699:ILE:HD13  | 2:B:760:TYR:CD1   | 2.55                     | 0.41              |
| 2:B:736:ARG:NH1   | 2:B:738:ASP:OD1   | 2.54                     | 0.41              |
| 15:O:194:LEU:O    | 15:O:232:LEU:CD2  | 2.57                     | 0.41              |
| 15:O:447:THR:O    | 15:O:450:LEU:CA   | 2.68                     | 0.41              |
| 1:A:411:VAL:CG2   | 1:A:412:SER:H     | 2.26                     | 0.40              |
| 2:B:416:LYS:HD3   | 2:B:416:LYS:HA    | 1.87                     | 0.40              |
| 1:A:1006:LEU:CD2  | 2:B:535:ASP:CB    | 2.99                     | 0.40              |
| 15:O:198:PHE:HD2  | 15:O:232:LEU:CD2  | 2.32                     | 0.40              |
| 1:A:1055:ILE:HG21 | 1:A:1060:GLU:CG   | 2.34                     | 0.40              |
| 1:A:1229:ALA:HB1  | 1:A:1595:TYR:CE2  | 2.56                     | 0.40              |
| 1:A:356:PHE:C     | 1:A:357:MET:CG    | 2.86                     | 0.40              |
| 1:A:365:THR:O     | 1:A:367:PHE:N     | 2.54                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:516:ILE:HG12  | 15:O:376:TYR:HE2  | 1.73                     | 0.40              |
| 1:A:556:ALA:HA    | 15:O:246:ASN:HD22 | 1.85                     | 0.40              |
| 2:B:219:ARG:HA    | 2:B:220:PRO:HD2   | 1.73                     | 0.40              |
| 2:B:427:GLN:OE1   | 2:B:452:ARG:NH1   | 2.54                     | 0.40              |
| 2:B:555:GLN:CB    | 2:B:646:HIS:CE1   | 3.04                     | 0.40              |
| 7:G:41:VAL:HA     | 7:G:42:PRO:HD3    | 1.92                     | 0.40              |
| 8:H:7:ASP:HA      | 8:H:57:VAL:O      | 2.21                     | 0.40              |
| 11:K:135:PHE:CE2  | 11:K:139:ILE:HD11 | 2.56                     | 0.40              |
| 12:L:68:GLU:CG    | 12:L:69:ALA:N     | 2.73                     | 0.40              |
| 15:O:128:LEU:HD13 | 15:O:132:THR:HG22 | 2.02                     | 0.40              |
| 15:O:244:LEU:O    | 15:O:244:LEU:HD23 | 2.20                     | 0.40              |
| 1:A:1008:ASP:OD1  | 1:A:1202:LEU:HD13 | 2.19                     | 0.40              |
| 1:A:1661:PRO:HA   | 7:G:101:SER:O     | 2.21                     | 0.40              |
| 1:A:487:ASP:HB2   | 1:A:615:ARG:HB3   | 2.02                     | 0.40              |
| 3:C:128:ASP:OD1   | 3:C:128:ASP:N     | 2.54                     | 0.40              |
| 4:D:25:THR:HB     | 6:F:59:GLN:HG3    | 2.02                     | 0.40              |
| 1:A:756:LYS:HD2   | 9:I:85:LYS:HZ2    | 1.61                     | 0.40              |
| 15:O:505:PHE:O    | 15:O:509:MET:HG2  | 2.21                     | 0.40              |
| 1:A:601:MET:HE1   | 1:A:656:GLN:HB2   | 2.03                     | 0.40              |
| 2:B:467:THR:HB    | 2:B:469:ASN:HD21  | 1.81                     | 0.40              |
| 2:B:491:ILE:HB    | 2:B:495:ARG:HD2   | 2.03                     | 0.40              |
| 3:C:45:SER:HB3    | 3:C:271:ARG:HH22  | 1.80                     | 0.40              |
| 15:O:237:ILE:HB   | 15:O:381:ILE:HD11 | 1.92                     | 0.40              |
| 15:O:422:GLN:HB3  | 15:O:593:PRO:HD3  | 2.02                     | 0.40              |
| 1:A:389:VAL:O     | 1:A:393:SER:HB2   | 2.22                     | 0.40              |
| 1:A:498:PRO:HA    | 1:A:499:PRO:HD3   | 1.81                     | 0.40              |
| 2:B:168:ASN:O     | 2:B:169:ARG:HD3   | 2.21                     | 0.40              |
| 4:D:23:HIS:CB     | 6:F:58:PHE:CD2    | 3.04                     | 0.40              |
| 1:A:1048:PHE:HD2  | 5:E:210:SER:HG    | 1.69                     | 0.40              |
| 7:G:17:ILE:C      | 7:G:19:LYS:H      | 2.25                     | 0.40              |
| 8:H:39:THR:O      | 8:H:123:MET:HA    | 2.22                     | 0.40              |
| 9:I:87:PRO:HG2    | 9:I:119:TYR:CE2   | 2.56                     | 0.40              |
| 15:O:342:HIS:NE2  | 15:O:346:GLN:HG3  | 2.34                     | 0.40              |
| 15:O:376:TYR:O    | 15:O:377:TYR:HB3  | 2.22                     | 0.40              |

There are no symmetry-related clashes.



## 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 PDB entries followed by that with respect to all EM entries.

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     | 1464/1664 (88%) | 1370 (94%) | 82 (6%)  | 12 (1%)  | 22          | 66  |
| 2   | B     | 1166/1203 (97%) | 1086 (93%) | 56 (5%)  | 24 (2%)  | 8           | 46  |
| 3   | C     | 303/335 (90%)   | 278 (92%)  | 18 (6%)  | 7 (2%)   | 7           | 44  |
| 4   | D     | 54/137 (39%)    | 50 (93%)   | 2 (4%)   | 2 (4%)   | 4           | 34  |
| 5   | E     | 210/215 (98%)   | 197 (94%)  | 11 (5%)  | 2 (1%)   | 18          | 61  |
| 6   | F     | 98/155 (63%)    | 94 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 7   | G     | 189/326 (58%)   | 171 (90%)  | 13 (7%)  | 5 (3%)   | 6           | 42  |
| 8   | H     | 127/146 (87%)   | 121 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 9   | I     | 101/125 (81%)   | 89 (88%)   | 9 (9%)   | 3 (3%)   | 5           | 38  |
| 10  | J     | 67/70 (96%)     | 63 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 11  | K     | 99/142 (70%)    | 92 (93%)   | 7 (7%)   | 0        | 100         | 100 |
| 12  | L     | 41/70 (59%)     | 32 (78%)   | 6 (15%)  | 3 (7%)   | 1           | 19  |
| 13  | M     | 103/415 (25%)   | 93 (90%)   | 8 (8%)   | 2 (2%)   | 9           | 48  |
| 14  | N     | 139/233 (60%)   | 123 (88%)  | 13 (9%)  | 3 (2%)   | 8           | 45  |
| 15  | O     | 457/627 (73%)   | 400 (88%)  | 38 (8%)  | 19 (4%)  | 3           | 31  |
| All | All   | 4618/5863 (79%) | 4259 (92%) | 277 (6%) | 82 (2%)  | 14          | 50  |

All (82) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1606 | SER  |
| 2   | B     | 111  | ASP  |
| 2   | B     | 117  | VAL  |
| 2   | B     | 895  | PHE  |
| 2   | B     | 1069 | ILE  |
| 3   | C     | 224  | THR  |
| 4   | D     | 99   | LEU  |
| 7   | G     | 25   | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | I     | 41   | GLN  |
| 15  | O     | 165  | PRO  |
| 15  | O     | 226  | GLY  |
| 15  | O     | 325  | ILE  |
| 15  | O     | 380  | SER  |
| 15  | O     | 431  | ALA  |
| 15  | O     | 489  | ASN  |
| 15  | O     | 521  | ASN  |
| 1   | A     | 448  | SER  |
| 1   | A     | 783  | LYS  |
| 1   | A     | 1533 | GLU  |
| 2   | B     | 473  | GLN  |
| 2   | B     | 817  | ARG  |
| 2   | B     | 1140 | LYS  |
| 4   | D     | 98   | GLY  |
| 5   | E     | 50   | MET  |
| 7   | G     | 27   | PRO  |
| 9   | I     | 5    | GLY  |
| 12  | L     | 62   | LYS  |
| 15  | O     | 374  | PRO  |
| 15  | O     | 488  | HIS  |
| 15  | O     | 540  | CYS  |
| 1   | A     | 450  | LYS  |
| 1   | A     | 1050 | TYR  |
| 2   | B     | 34   | ALA  |
| 2   | B     | 78   | PRO  |
| 2   | B     | 208  | VAL  |
| 2   | B     | 209  | GLN  |
| 2   | B     | 1044 | PHE  |
| 2   | B     | 1070 | ARG  |
| 2   | B     | 1095 | SER  |
| 2   | B     | 1098 | TYR  |
| 3   | C     | 297  | HIS  |
| 5   | E     | 146  | HIS  |
| 7   | G     | 99   | ASP  |
| 9   | I     | 21   | ASN  |
| 12  | L     | 46   | VAL  |
| 13  | M     | 85   | LYS  |
| 15  | O     | 82   | SER  |
| 15  | O     | 130  | PRO  |
| 15  | O     | 457  | ARG  |
| 15  | O     | 469  | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 834  | LYS  |
| 2   | B     | 1094 | ASN  |
| 3   | C     | 295  | ARG  |
| 7   | G     | 100  | THR  |
| 12  | L     | 43   | THR  |
| 13  | M     | 36   | THR  |
| 14  | N     | 115  | SER  |
| 15  | O     | 148  | PRO  |
| 15  | O     | 187  | MET  |
| 1   | A     | 439  | ASP  |
| 1   | A     | 451  | VAL  |
| 1   | A     | 564  | PRO  |
| 1   | A     | 581  | ILE  |
| 1   | A     | 1049 | MET  |
| 2   | B     | 80   | ASN  |
| 2   | B     | 1062 | GLY  |
| 2   | B     | 1096 | SER  |
| 3   | C     | 32   | ASN  |
| 3   | C     | 296  | ASN  |
| 15  | O     | 377  | TYR  |
| 1   | A     | 1512 | PRO  |
| 2   | B     | 1063 | ARG  |
| 3   | C     | 222  | VAL  |
| 15  | O     | 147  | ILE  |
| 3   | C     | 221  | PRO  |
| 14  | N     | 70   | LEU  |
| 15  | O     | 128  | LEU  |
| 2   | B     | 468  | GLY  |
| 14  | N     | 39   | PRO  |
| 7   | G     | 28   | ILE  |
| 2   | B     | 833  | PRO  |
| 2   | B     | 954  | PHE  |

### 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 PDB entries followed by that with respect to all EM entries.

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     | 1307/1465 (89%) | 1221 (93%) | 86 (7%)  | 19          | 53 |
| 2   | B     | 1027/1053 (98%) | 956 (93%)  | 71 (7%)  | 18          | 52 |
| 3   | C     | 269/296 (91%)   | 249 (93%)  | 20 (7%)  | 16          | 49 |
| 4   | D     | 55/116 (47%)    | 49 (89%)   | 6 (11%)  | 7           | 32 |
| 5   | E     | 194/197 (98%)   | 180 (93%)  | 14 (7%)  | 17          | 50 |
| 6   | F     | 90/137 (66%)    | 86 (96%)   | 4 (4%)   | 33          | 64 |
| 7   | G     | 170/291 (58%)   | 158 (93%)  | 12 (7%)  | 17          | 51 |
| 8   | H     | 115/128 (90%)   | 111 (96%)  | 4 (4%)   | 41          | 70 |
| 9   | I     | 97/110 (88%)    | 91 (94%)   | 6 (6%)   | 21          | 55 |
| 10  | J     | 64/65 (98%)     | 57 (89%)   | 7 (11%)  | 7           | 32 |
| 11  | K     | 91/130 (70%)    | 84 (92%)   | 7 (8%)   | 15          | 48 |
| 12  | L     | 38/57 (67%)     | 34 (90%)   | 4 (10%)  | 8           | 34 |
| 13  | M     | 95/371 (26%)    | 85 (90%)   | 10 (10%) | 8           | 34 |
| 14  | N     | 135/220 (61%)   | 129 (96%)  | 6 (4%)   | 33          | 64 |
| 15  | O     | 427/576 (74%)   | 378 (88%)  | 49 (12%) | 6           | 30 |
| All | All   | 4174/5212 (80%) | 3868 (93%) | 306 (7%) | 21          | 50 |

All (306) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | GLU  |
| 1   | A     | 40  | ASN  |
| 1   | A     | 83  | VAL  |
| 1   | A     | 90  | PHE  |
| 1   | A     | 117 | ARG  |
| 1   | A     | 136 | LEU  |
| 1   | A     | 174 | SER  |
| 1   | A     | 186 | SER  |
| 1   | A     | 202 | THR  |
| 1   | A     | 230 | ARG  |
| 1   | A     | 257 | ASN  |
| 1   | A     | 271 | ARG  |
| 1   | A     | 272 | GLN  |
| 1   | A     | 273 | ASP  |
| 1   | A     | 312 | SER  |
| 1   | A     | 315 | ILE  |
| 1   | A     | 346 | SER  |
| 1   | A     | 357 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 373  | LEU  |
| 1   | A     | 379  | GLU  |
| 1   | A     | 393  | SER  |
| 1   | A     | 409  | ASP  |
| 1   | A     | 412  | SER  |
| 1   | A     | 413  | LEU  |
| 1   | A     | 439  | ASP  |
| 1   | A     | 446  | ARG  |
| 1   | A     | 447  | THR  |
| 1   | A     | 451  | VAL  |
| 1   | A     | 503  | VAL  |
| 1   | A     | 555  | LYS  |
| 1   | A     | 582  | LYS  |
| 1   | A     | 611  | GLU  |
| 1   | A     | 627  | ASP  |
| 1   | A     | 656  | GLN  |
| 1   | A     | 661  | THR  |
| 1   | A     | 666  | VAL  |
| 1   | A     | 670  | ILE  |
| 1   | A     | 684  | ASP  |
| 1   | A     | 708  | THR  |
| 1   | A     | 709  | ARG  |
| 1   | A     | 739  | VAL  |
| 1   | A     | 747  | ILE  |
| 1   | A     | 758  | GLU  |
| 1   | A     | 783  | LYS  |
| 1   | A     | 957  | VAL  |
| 1   | A     | 966  | LEU  |
| 1   | A     | 988  | SER  |
| 1   | A     | 999  | CYS  |
| 1   | A     | 1004 | GLU  |
| 1   | A     | 1026 | GLN  |
| 1   | A     | 1033 | SER  |
| 1   | A     | 1056 | ASP  |
| 1   | A     | 1085 | LEU  |
| 1   | A     | 1098 | SER  |
| 1   | A     | 1118 | VAL  |
| 1   | A     | 1123 | VAL  |
| 1   | A     | 1131 | LYS  |
| 1   | A     | 1159 | ASP  |
| 1   | A     | 1162 | ASN  |
| 1   | A     | 1204 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1215 | VAL  |
| 1   | A     | 1226 | VAL  |
| 1   | A     | 1273 | THR  |
| 1   | A     | 1275 | THR  |
| 1   | A     | 1276 | THR  |
| 1   | A     | 1304 | GLU  |
| 1   | A     | 1310 | LYS  |
| 1   | A     | 1314 | GLN  |
| 1   | A     | 1320 | GLN  |
| 1   | A     | 1441 | LYS  |
| 1   | A     | 1455 | ARG  |
| 1   | A     | 1509 | HIS  |
| 1   | A     | 1531 | ASP  |
| 1   | A     | 1533 | GLU  |
| 1   | A     | 1536 | ILE  |
| 1   | A     | 1571 | SER  |
| 1   | A     | 1601 | GLN  |
| 1   | A     | 1604 | GLU  |
| 1   | A     | 1605 | THR  |
| 1   | A     | 1607 | THR  |
| 1   | A     | 1609 | SER  |
| 1   | A     | 1611 | MET  |
| 1   | A     | 1632 | GLU  |
| 1   | A     | 1633 | GLN  |
| 1   | A     | 1635 | ASP  |
| 1   | A     | 1645 | LYS  |
| 2   | B     | 13   | THR  |
| 2   | B     | 17   | ARG  |
| 2   | B     | 22   | GLU  |
| 2   | B     | 53   | THR  |
| 2   | B     | 57   | ASP  |
| 2   | B     | 65   | VAL  |
| 2   | B     | 70   | GLU  |
| 2   | B     | 79   | LEU  |
| 2   | B     | 81   | SER  |
| 2   | B     | 87   | ASN  |
| 2   | B     | 150  | GLU  |
| 2   | B     | 187  | SER  |
| 2   | B     | 202  | LEU  |
| 2   | B     | 211  | ARG  |
| 2   | B     | 221  | SER  |
| 2   | B     | 225  | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 228  | SER  |
| 2   | B     | 231  | HIS  |
| 2   | B     | 239  | VAL  |
| 2   | B     | 281  | CYS  |
| 2   | B     | 300  | SER  |
| 2   | B     | 305  | ARG  |
| 2   | B     | 306  | LEU  |
| 2   | B     | 311  | ARG  |
| 2   | B     | 315  | LYS  |
| 2   | B     | 379  | ARG  |
| 2   | B     | 459  | SER  |
| 2   | B     | 486  | VAL  |
| 2   | B     | 537  | SER  |
| 2   | B     | 583  | LEU  |
| 2   | B     | 622  | ILE  |
| 2   | B     | 658  | LEU  |
| 2   | B     | 720  | GLN  |
| 2   | B     | 724  | GLN  |
| 2   | B     | 725  | THR  |
| 2   | B     | 731  | VAL  |
| 2   | B     | 753  | LYS  |
| 2   | B     | 782  | ASP  |
| 2   | B     | 811  | LEU  |
| 2   | B     | 813  | LEU  |
| 2   | B     | 819  | ASP  |
| 2   | B     | 822  | THR  |
| 2   | B     | 824  | HIS  |
| 2   | B     | 829  | ASN  |
| 2   | B     | 833  | PRO  |
| 2   | B     | 835  | GLU  |
| 2   | B     | 839  | LYS  |
| 2   | B     | 858  | ILE  |
| 2   | B     | 871  | ILE  |
| 2   | B     | 883  | GLU  |
| 2   | B     | 894  | LYS  |
| 2   | B     | 897  | GLU  |
| 2   | B     | 977  | ILE  |
| 2   | B     | 998  | GLU  |
| 2   | B     | 1026 | ILE  |
| 2   | B     | 1033 | TYR  |
| 2   | B     | 1037 | ARG  |
| 2   | B     | 1043 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1047 | ARG  |
| 2   | B     | 1060 | VAL  |
| 2   | B     | 1070 | ARG  |
| 2   | B     | 1075 | GLU  |
| 2   | B     | 1097 | ASP  |
| 2   | B     | 1100 | GLN  |
| 2   | B     | 1103 | VAL  |
| 2   | B     | 1125 | THR  |
| 2   | B     | 1136 | GLU  |
| 2   | B     | 1141 | LEU  |
| 2   | B     | 1163 | GLN  |
| 2   | B     | 1165 | ASN  |
| 2   | B     | 1174 | THR  |
| 3   | C     | 38   | LYS  |
| 3   | C     | 43   | ASN  |
| 3   | C     | 50   | ARG  |
| 3   | C     | 61   | THR  |
| 3   | C     | 77   | SER  |
| 3   | C     | 91   | VAL  |
| 3   | C     | 97   | LEU  |
| 3   | C     | 118  | SER  |
| 3   | C     | 131  | THR  |
| 3   | C     | 142  | ARG  |
| 3   | C     | 181  | ASP  |
| 3   | C     | 222  | VAL  |
| 3   | C     | 224  | THR  |
| 3   | C     | 228  | ARG  |
| 3   | C     | 232  | GLN  |
| 3   | C     | 243  | SER  |
| 3   | C     | 245  | ARG  |
| 3   | C     | 277  | ARG  |
| 3   | C     | 279  | VAL  |
| 3   | C     | 295  | ARG  |
| 4   | D     | 15   | THR  |
| 4   | D     | 29   | GLN  |
| 4   | D     | 38   | GLN  |
| 4   | D     | 46   | GLU  |
| 4   | D     | 80   | THR  |
| 4   | D     | 99   | LEU  |
| 5   | E     | 31   | THR  |
| 5   | E     | 33   | GLU  |
| 5   | E     | 41   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 74  | ASP  |
| 5   | E     | 77  | SER  |
| 5   | E     | 90  | VAL  |
| 5   | E     | 92  | THR  |
| 5   | E     | 93  | MET  |
| 5   | E     | 107 | THR  |
| 5   | E     | 131 | THR  |
| 5   | E     | 136 | ASN  |
| 5   | E     | 142 | VAL  |
| 5   | E     | 162 | ARG  |
| 5   | E     | 177 | ARG  |
| 6   | F     | 59  | GLN  |
| 6   | F     | 87  | LYS  |
| 6   | F     | 99  | LEU  |
| 6   | F     | 109 | VAL  |
| 7   | G     | 18  | LYS  |
| 7   | G     | 24  | VAL  |
| 7   | G     | 35  | SER  |
| 7   | G     | 39  | VAL  |
| 7   | G     | 139 | ILE  |
| 7   | G     | 147 | LEU  |
| 7   | G     | 167 | THR  |
| 7   | G     | 169 | VAL  |
| 7   | G     | 223 | GLU  |
| 7   | G     | 230 | ARG  |
| 7   | G     | 239 | THR  |
| 7   | G     | 243 | VAL  |
| 8   | H     | 3   | ASN  |
| 8   | H     | 39  | THR  |
| 8   | H     | 108 | SER  |
| 8   | H     | 112 | ILE  |
| 9   | I     | 2   | SER  |
| 9   | I     | 15  | ASP  |
| 9   | I     | 45  | LEU  |
| 9   | I     | 70  | SER  |
| 9   | I     | 74  | ASN  |
| 9   | I     | 81  | THR  |
| 10  | J     | 3   | VAL  |
| 10  | J     | 9   | SER  |
| 10  | J     | 10  | CYS  |
| 10  | J     | 14  | VAL  |
| 10  | J     | 27  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 45  | CYS  |
| 10  | J     | 48  | ARG  |
| 11  | K     | 45  | GLU  |
| 11  | K     | 51  | THR  |
| 11  | K     | 68  | GLU  |
| 11  | K     | 99  | ASN  |
| 11  | K     | 118 | GLN  |
| 11  | K     | 123 | ASP  |
| 11  | K     | 133 | SER  |
| 12  | L     | 38  | LEU  |
| 12  | L     | 55  | ILE  |
| 12  | L     | 60  | ARG  |
| 12  | L     | 66  | GLN  |
| 13  | M     | 17  | ASP  |
| 13  | M     | 18  | GLN  |
| 13  | M     | 31  | ARG  |
| 13  | M     | 44  | LYS  |
| 13  | M     | 48  | LYS  |
| 13  | M     | 65  | TYR  |
| 13  | M     | 77  | VAL  |
| 13  | M     | 84  | GLU  |
| 13  | M     | 98  | SER  |
| 13  | M     | 109 | ARG  |
| 14  | N     | 51  | GLN  |
| 14  | N     | 124 | THR  |
| 14  | N     | 135 | LYS  |
| 14  | N     | 153 | VAL  |
| 14  | N     | 167 | LYS  |
| 14  | N     | 178 | GLU  |
| 15  | O     | 66  | ASN  |
| 15  | O     | 67  | ASP  |
| 15  | O     | 69  | THR  |
| 15  | O     | 78  | VAL  |
| 15  | O     | 80  | LEU  |
| 15  | O     | 87  | ARG  |
| 15  | O     | 101 | SER  |
| 15  | O     | 111 | ARG  |
| 15  | O     | 117 | GLN  |
| 15  | O     | 149 | LYS  |
| 15  | O     | 171 | CYS  |
| 15  | O     | 175 | MET  |
| 15  | O     | 180 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | O     | 181 | ARG  |
| 15  | O     | 190 | ILE  |
| 15  | O     | 192 | THR  |
| 15  | O     | 202 | ASN  |
| 15  | O     | 203 | ASP  |
| 15  | O     | 204 | THR  |
| 15  | O     | 205 | ARG  |
| 15  | O     | 212 | THR  |
| 15  | O     | 213 | SER  |
| 15  | O     | 215 | LEU  |
| 15  | O     | 228 | GLN  |
| 15  | O     | 232 | LEU  |
| 15  | O     | 234 | ILE  |
| 15  | O     | 245 | GLN  |
| 15  | O     | 248 | LEU  |
| 15  | O     | 341 | THR  |
| 15  | O     | 350 | GLU  |
| 15  | O     | 354 | SER  |
| 15  | O     | 363 | THR  |
| 15  | O     | 368 | PHE  |
| 15  | O     | 369 | LYS  |
| 15  | O     | 395 | LEU  |
| 15  | O     | 437 | THR  |
| 15  | O     | 454 | VAL  |
| 15  | O     | 457 | ARG  |
| 15  | O     | 487 | ARG  |
| 15  | O     | 489 | ASN  |
| 15  | O     | 494 | THR  |
| 15  | O     | 495 | ASP  |
| 15  | O     | 522 | GLU  |
| 15  | O     | 526 | LEU  |
| 15  | O     | 540 | CYS  |
| 15  | O     | 581 | THR  |
| 15  | O     | 584 | GLN  |
| 15  | O     | 597 | LEU  |
| 15  | O     | 602 | TYR  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 432 | ASN  |
| 1   | A     | 580 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 863  | ASN  |
| 1   | A     | 1162 | ASN  |
| 2   | B     | 328  | GLN  |
| 2   | B     | 462  | GLN  |
| 2   | B     | 646  | HIS  |
| 2   | B     | 912  | GLN  |
| 2   | B     | 1038 | HIS  |
| 2   | B     | 1163 | GLN  |
| 4   | D     | 23   | HIS  |
| 4   | D     | 93   | GLN  |
| 6   | F     | 59   | GLN  |
| 6   | F     | 78   | GLN  |
| 7   | G     | 126  | GLN  |
| 7   | G     | 150  | HIS  |
| 7   | G     | 154  | ASN  |
| 9   | I     | 32   | GLN  |
| 12  | L     | 66   | GLN  |
| 14  | N     | 85   | HIS  |
| 15  | O     | 66   | ASN  |
| 15  | O     | 70   | GLN  |
| 15  | O     | 105  | ASN  |
| 15  | O     | 117  | GLN  |
| 15  | O     | 172  | HIS  |
| 15  | O     | 173  | HIS  |
| 15  | O     | 245  | GLN  |
| 15  | O     | 346  | GLN  |
| 15  | O     | 362  | ASN  |
| 15  | O     | 371  | HIS  |
| 15  | O     | 390  | GLN  |
| 15  | O     | 472  | HIS  |
| 15  | O     | 497  | ASN  |
| 15  | O     | 507  | GLN  |
| 15  | O     | 521  | ASN  |
| 15  | O     | 547  | ASN  |
| 15  | O     | 549  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.