



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:43 PM UTC

PDB ID : 1IW7 / pdb\_00001iw7  
Title : Crystal structure of the RNA polymerase holoenzyme from *Thermus thermophilus* at 2.6Å resolution  
Authors : RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2002-04-22  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

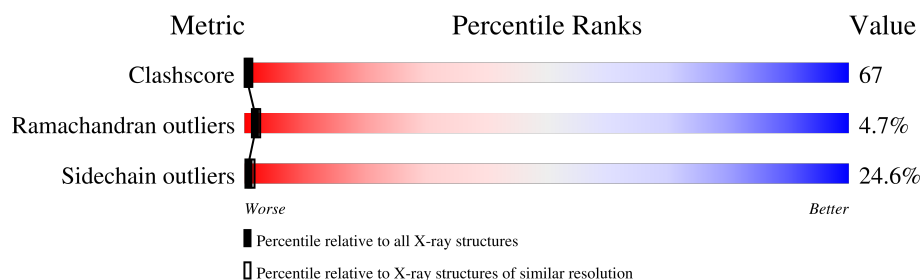
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 4347 (2.60-2.60)                                      |
| Ramachandran outliers | 187476                      | 4277 (2.60-2.60)                                      |
| Sidechain outliers    | 187428                      | 4277 (2.60-2.60)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|-------------------|
| 1   | A     | 315    | 17% 43% 12% • 27% |
| 1   | B     | 315    | 19% 43% 11% • 27% |
| 1   | K     | 315    | 17% 43% 11% • 27% |
| 1   | L     | 315    | 19% 42% 11% • 27% |
| 2   | C     | 1119   | 21% 56% 21% •     |
| 2   | M     | 1119   | 20% 56% 21% •     |
| 3   | D     | 1524   | 20% 50% 19% • 9%  |
| 3   | N     | 1524   | 21% 48% 20% • 9%  |

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| Mol | Chain | Length | Quality of chain                                |
|-----|-------|--------|-------------------------------------------------|
| 4   | E     | 99     | <div><div></div><div>23%51%19%••</div></div>    |
| 4   | O     | 99     | <div><div></div><div>24%59%10%••</div></div>    |
| 5   | F     | 423    | <div><div></div><div>19%44%13%5%18%</div></div> |
| 5   | P     | 423    | <div><div></div><div>19%44%15%•18%</div></div>  |

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 59529 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RNA polymerase alpha subunit.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1806  | 1153 | 313 | 337 | 3 |         |         |       |
| 1   | B     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1806  | 1153 | 313 | 337 | 3 |         |         |       |
| 1   | K     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1806  | 1153 | 313 | 337 | 3 |         |         |       |
| 1   | L     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1806  | 1153 | 313 | 337 | 3 |         |         |       |

- Molecule 2 is a protein called RNA polymerase beta subunit.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | C     | 1119     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8829  | 5581 | 1577 | 1647 | 24 |         |         |       |
| 2   | M     | 1119     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8829  | 5581 | 1577 | 1647 | 24 |         |         |       |

- Molecule 3 is a protein called RNA polymerase beta subunit.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | D     | 1392     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10801 | 6823 | 1925 | 2020 | 33 |         |         |       |
| 3   | N     | 1392     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10801 | 6823 | 1925 | 2020 | 33 |         |         |       |

- Molecule 4 is a protein called RNA polymerase omega subunit.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | E     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 488 | 133 | 144 | 4 |         |         |       |
| 4   | O     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 488 | 133 | 144 | 4 |         |         |       |

- Molecule 5 is a protein called RNA polymerase sigma-70 subunit.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | F     | 345      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2771  | 1744 | 504 | 519 | 4 |         |         |       |
| 5   | P     | 345      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2771  | 1744 | 504 | 519 | 4 |         |         |       |

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 6   | A     | 18       | Total | Mg  | 0       | 0       |
|     |       |          | 18    | 18  |         |         |
| 6   | B     | 24       | Total | Mg  | 0       | 0       |
|     |       |          | 24    | 24  |         |         |
| 6   | C     | 63       | Total | Mg  | 0       | 0       |
|     |       |          | 63    | 63  |         |         |
| 6   | D     | 118      | Total | Mg  | 0       | 0       |
|     |       |          | 118   | 118 |         |         |
| 6   | E     | 6        | Total | Mg  | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 6   | F     | 31       | Total | Mg  | 0       | 0       |
|     |       |          | 31    | 31  |         |         |
| 6   | K     | 20       | Total | Mg  | 0       | 0       |
|     |       |          | 20    | 20  |         |         |
| 6   | L     | 19       | Total | Mg  | 0       | 0       |
|     |       |          | 19    | 19  |         |         |
| 6   | M     | 64       | Total | Mg  | 0       | 0       |
|     |       |          | 64    | 64  |         |         |
| 6   | N     | 92       | Total | Mg  | 0       | 0       |
|     |       |          | 92    | 92  |         |         |
| 6   | O     | 8        | Total | Mg  | 0       | 0       |
|     |       |          | 8     | 8   |         |         |
| 6   | P     | 22       | Total | Mg  | 0       | 0       |
|     |       |          | 22    | 22  |         |         |

- Molecule 7 is LEAD (II) ION (CCD ID: PB) (formula: Pb).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | D     | 2        | Total | Pb | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 7   | N     | 2        | Total | Pb | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 8 is water.

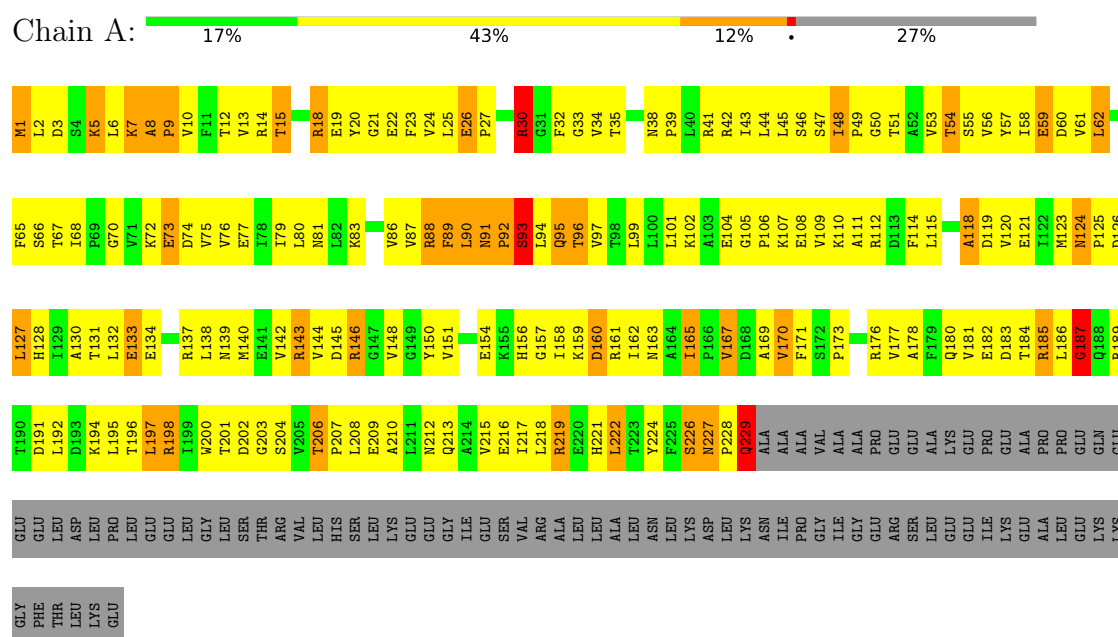
| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 8   | A     | 194      | Total<br>194  | O<br>194  | 0       | 0       |
| 8   | B     | 193      | Total<br>193  | O<br>193  | 0       | 0       |
| 8   | C     | 869      | Total<br>869  | O<br>869  | 0       | 0       |
| 8   | D     | 1163     | Total<br>1163 | O<br>1163 | 0       | 0       |
| 8   | E     | 114      | Total<br>114  | O<br>114  | 0       | 0       |
| 8   | F     | 381      | Total<br>381  | O<br>381  | 0       | 0       |
| 8   | K     | 161      | Total<br>161  | O<br>161  | 0       | 0       |
| 8   | L     | 157      | Total<br>157  | O<br>157  | 0       | 0       |
| 8   | M     | 822      | Total<br>822  | O<br>822  | 0       | 0       |
| 8   | N     | 983      | Total<br>983  | O<br>983  | 0       | 0       |
| 8   | O     | 114      | Total<br>114  | O<br>114  | 0       | 0       |
| 8   | P     | 325      | Total<br>325  | O<br>325  | 0       | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

Note EDS was not executed.

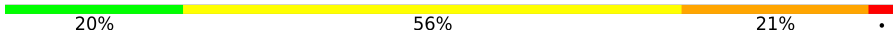
#### • Molecule 1: RNA polymerase alpha subunit







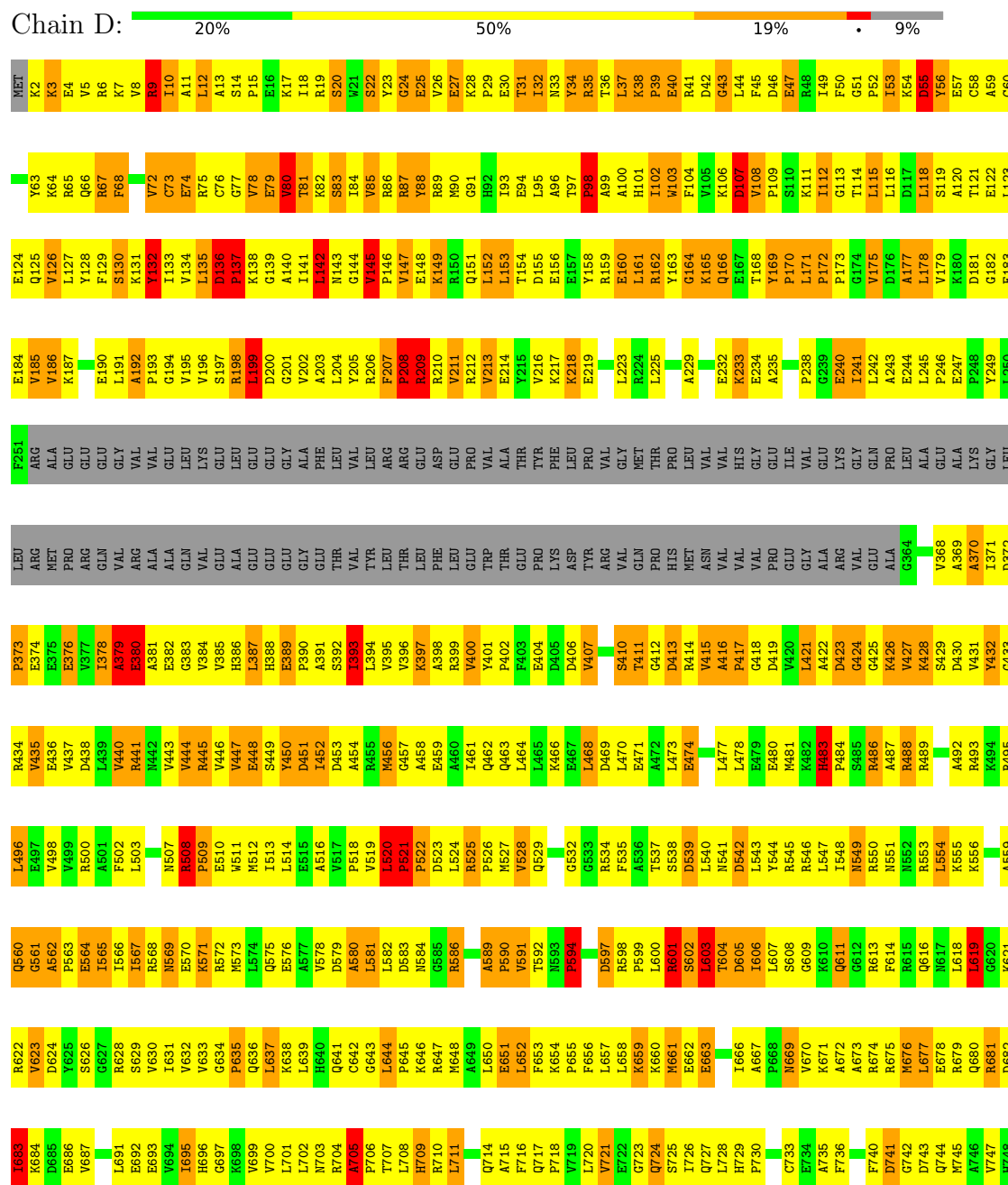
● Molecule 2: RNA polymerase beta subunit

Chain M:  20% 56% 21%

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| M1   | G62  | T122 | K185 | R250 | F311 | V373 | Y435 | I496 | R557 | Y682 | G809 | P873 | L874 | R879 | M881 | Q884 | L885 | L886 | E887 | T888 | H889 | L890 | G891 | L892 | A893 | G894 | Y895 | F896 | L897 | G898 | Q899 | R900 | Y901 | I902 | S903 | P904 | I905 | F906 | D907 | K908 | A909 | K910 | E911 | P912 | E913 | L914 | R915 | E916 | L917 | L918 | A919 | Q920 | A921 | Y925 | G926 | K927 | R928 | R929 | K930 | G931 | E932 | G933 | F934 |      |
| G63  | G64  | D124 | V65  | L66  | D67  | F68  | L69  | E70  | E71  | R72  | L73  | P14  | L15  | P16  | P17  | L18  | T19  | E20  | D81  | I21  | Q22  | V23  | E24  | S25  | Y26  | R27  | R28  | A29  | L30  | Q31  | A32  | D33  | V34  | P35  | P36  | E37  | K38  | Q39  | E40  | N41  | V42  | K43  | I44  | Q45  | A46  | A47  | F48  | R49  | E50  | T51  | P52  | P53  | F54  | E55  | E56  | E57  | D58  | K59  | G60  | M61  |      |      |      |      |
| D251 | K186 | K187 | K188 | R189 | K190 | F191 | P192 | L193 | V194 | L195 | L196 | L197 | D263 | P264 | R265 | R266 | Y267 | D268 | L269 | E270 | E271 | A272 | G273 | R274 | Y275 | G276 | A277 | E278 | E279 | K280 | L281 | G282 | I283 | R284 | L285 | S286 | G287 | R288 | T289 | L290 | A291 | R292 | F293 | G296 | E297 | R298 | G299 | D300 | E301 | V302 | F303 | L304 | P305 | T306 | L307 | R308 | Y309 | L310 | K311 | L312 |      |      |      |      |
| A312 | A313 | T314 | A315 | G316 | P317 | P318 | G319 | H320 | E321 | V322 | D323 | D324 | I325 | D326 | H327 | L328 | G329 | N330 | R331 | G332 | I333 | R334 | T335 | V336 | G337 | E338 | L339 | M340 | T341 | D342 | G343 | F344 | R345 | G346 | G347 | L348 | A349 | R350 | L351 | A352 | R353 | G354 | V355 | R356 | E357 | R358 | M359 | L360 | E364 | D365 | S366 | L367 | T368 | P369 | A370 | R371 | L372 |      |      |      |      |      |      |      |
| N374 | S375 | R376 | P377 | L378 | E379 | A380 | R383 | E384 | F385 | F386 | S387 | R388 | S389 | S392 | L392 | G393 | F394 | K395 | D396 | E397 | L398 | T399 | P400 | L401 | S402 | L403 | L404 | R405 | H406 | R407 | R408 | R409 | I410 | S411 | A412 | L413 | G414 | P415 | G416 | G417 | G418 | T419 | R420 | R421 | A422 | A423 | G424 | F425 | D426 | V427 | R428 | D429 | E430 | H431 | R432 | T433 | H434 |      |      |      |      |      |      |      |
| Y436 | G437 | R438 | C439 | P440 | V441 | E442 | T443 | E445 | N448 | I449 | G450 | L451 | I452 | I453 | S454 | L455 | A456 | R457 | A458 | G459 | R460 | V461 | D462 | E463 | L464 | G465 | F466 | I467 | R468 | T469 | P470 | Y471 | R472 | S473 | R474 | V475 | G476 | G477 | V478 | V479 | T480 | D481 | E482 | V483 | N484 | V485 | V486 | T487 | F488 | L489 | L490 | E491 | D492 | R493 | Y494 | T495 |      |      |      |      |      |      |      |      |
| I497 | A498 | Q499 | A500 | T501 | P502 | P503 | L504 | E505 | P506 | R507 | L508 | A509 | E510 | R511 | E512 | V513 | A514 | A515 | R516 | V517 | K518 | G519 | E520 | P521 | V522 | I523 | V524 | S525 | P526 | E527 | E528 | V529 | F530 | F531 | M532 | V533 | V534 | S535 | P536 | K537 | Q538 | S541 | V542 | N543 | T544 | N545 | V546 | I547 | N548 | P549 | L550 | I551 | V552 | V553 | H554 | E555 | N556 |      |      |      |      |      |      |      |
| R558 | A559 | L560 | M561 | N562 | N563 | M564 | Q565 | T566 | A567 | A568 | Q569 | P570 | L571 | P572 | R573 | A574 | Q575 | A576 | P577 | V578 | V579 | M580 | T581 | G582 | L583 | E584 | E585 | R586 | V587 | R588 | R589 | D590 | S591 | A592 | L593 | T594 | S595 | E596 | A597 | E598 | E599 | D600 | G601 | E602 | V603 | A604 | K605 | V606 | D607 | G608 | N609 | R610 | I611 | V612 | V613 | R614 | E615 | D616 |      |      |      |      |      |      |
| E622 | Y623 | P624 | L625 | G626 | R627 | R628 | R629 | S630 | S631 | N632 | Q633 | G634 | T635 | A636 | D637 | Q638 | Q639 | R640 | P641 | R642 | G643 | V644 | V645 | G646 | Q647 | R648 | V649 | R650 | K651 | G652 | D653 | L654 | L655 | D656 | D657 | G658 | P659 | A660 | S661 | E662 | N663 | G664 | F665 | L666 | A667 | L668 | G669 | Q670 | N671 | V672 | L673 | V674 | A675 | V676 | M677 | F678 | F679 | D680 | G681 |      |      |      |      |      |
| Y682 | N683 | E684 | E685 | P686 | A687 | L688 | V689 | S690 | E691 | E692 | E693 | L694 | L695 | K696 | R697 | D698 | F699 | Y700 | T701 | E702 | E703 | E704 | E705 | E706 | E707 | E708 | E709 | E710 | E711 | A712 | R713 | R714 | T715 | T716 | L717 | P718 | G719 | A720 | E721 | R722 | T723 | R724 | D725 | T726 | R727 | R728 | L729 | S730 | E731 | A732 | A733 | L734 | R735 | D736 | L737 | D738 | E739 | E740 | E741 | V742 | V743 | R744 |      |      |
| A745 | V746 | V747 | K748 | P749 | G750 | D751 | L752 | L753 | V754 | G755 | R756 | T757 | S758 | F759 | F760 | R761 | R762 | G763 | E764 | P765 | T766 | P767 | E768 | E769 | E770 | E771 | R772 | L773 | L774 | R775 | T776 | T777 | F778 | G779 | K780 | A781 | R782 | R783 | D784 | V785 | K786 | L787 | T788 | R789 | L790 | R791 | V792 | G793 | L794 | G795 | L796 | G797 | G798 | V799 | R800 | T801 | V802 | R803 | G804 | K805 | P806 | R807 | G808 | R809 |
| G809 | D810 | P811 | G812 | R813 | E814 | L815 | K816 | P817 | G818 | R819 | E820 | R821 | V822 | V823 | R824 | V825 | R826 | E827 | A828 | K829 | Y830 | R831 | L832 | A833 | G834 | Y835 | F836 | L837 | L838 | P839 | R840 | V841 | R842 | H843 | K844 | V845 | R846 | V847 | R848 | R849 | A850 | K851 | L852 | L853 | P854 | V855 | E856 | D857 | P858 | P859 | H860 | L861 | P862 | D863 | G864 | K865 | P866 | R867 | G868 | V869 | L870 | L871 | G872 | P873 |
| P873 | L874 | G875 | V876 | P877 | S878 | L879 | M880 | N881 | Q882 | L883 | L884 | E885 | L886 | E887 | T888 | H889 | L890 | G891 | L892 | A893 | G894 | Y895 | F896 | L897 | G898 | Q899 | R900 | Y901 | I902 | S903 | P904 | I905 | F906 | D907 | A908 | K909 | K910 | E911 | P912 | E913 | I914 | K915 | E916 | L917 | L918 | A919 | Q920 | A921 | Y925 | G926 | K927 | R928 | R929 | K930 | G931 | E932 | G933 | F934 |      |      |      |      |      |      |

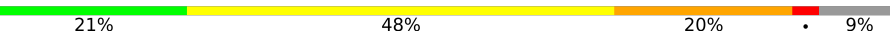


### • Molecule 3: RNA polymerase beta subunit



|     |       |       |       |       |       |       |       |       |       |      |      |      |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|
| GLN | K1463 | E1401 | G1340 | V1273 | S1210 | L1144 | G1081 | F1017 | A954  | A889 | R818 | V749 |
| ALA | E1464 | A1402 | P1341 | I1274 | M1211 | Y1145 | A1082 | M1018 | V955  | V890 | G819 | P750 |
|     | N1465 | L1403 | E1342 | S1275 | A1212 | G1146 | D1083 | P1019 | I956  | E891 | E820 | L751 |
|     | I1466 | N1404 | A1343 | E1276 | R1213 | R1147 | T1084 | L1020 | P957  | D892 | V821 | S752 |
|     | L1467 | E1405 | V1344 | I1277 | P1214 | V1148 | A1085 | Y1021 | E958  | K894 | L823 | Q756 |
|     | L1468 | R1406 | E1345 | D1278 | V1215 | L1149 | L1086 | Y1022 | E959  | K895 | L824 | A769 |
|     | G1469 | L1407 | R1346 | G1279 | S1216 | A1150 | E1087 | M1023 | K960  | V895 | N824 | R760 |
|     | L1470 | T1408 | Y1347 | V1280 | I1217 | R1151 | T1088 | S1026 | K961  | W897 | A825 | I761 |
|     | R1471 | A1409 | L1348 | V1281 | G1218 | E1152 | A1089 | G1027 | G962  | E898 | K828 | Q762 |
|     | P1472 | E1410 | E1349 | I1282 | E1219 | V1153 | S1091 | A1028 | L964  | L899 | V829 | M763 |
|     | A1473 | G1411 | E1350 | I1283 | A1220 | E1154 | G1092 | R1029 | L964  | I900 | A830 | L764 |
|     | A1474 | E1351 | E1284 | E1285 | V1221 | V1155 | G1092 | G1030 | A967  | Q901 | A830 | S765 |
|     | G1475 | I1352 | E1286 | E1286 | G1222 | L1156 | T1095 | M1031 | D963  | L902 | G831 |      |
|     | T1476 | Q1353 | T1287 | T1286 | I1223 | G1157 | T1096 | P1032 | R969  | D903 | T834 | L770 |
|     | G1477 | L1354 | E1288 | E1287 | V1224 | V1158 | R1096 | Q1033 | K970  | P905 | S835 | S771 |
|     | S1478 | V1355 | E1288 | E1288 | A1225 | R1159 | K1097 | L1038 | L971  | Q906 | V836 | P772 |
|     | D1479 | K1356 | L1289 | K1289 | A1226 | L1160 | L1098 | Q1034 | L971  | E907 | G837 | A773 |
|     | F1480 | R1357 | L1290 | L1290 | Q1227 | E1161 | V1099 | I1035 | L972  | K908 | S774 | S774 |
|     | V1481 | A1358 | S1228 | S1228 | S1228 | E1162 | D1100 | R1036 | Q973  | N909 | V842 | L778 |
|     | R1482 | Q1359 | L1229 | L1229 | G1230 | G1163 | V1101 | Q1037 | Q976  | S910 | F843 |      |
|     | F1483 | G1360 | G1230 | G1230 | G1230 | R1164 | T1102 | L1038 | A977  | L911 | A844 |      |
|     | T1484 | V1361 | E1231 | E1231 | E1231 | Y1165 | H1103 | M1045 | L983  | L914 | P781 |      |
|     | Q1485 | K1362 | P1232 | P1232 | P1232 | L1166 | E1109 | Q1046 | T984  | Y916 | S782 |      |
|     | V1486 | T1425 | L1363 | L1363 | L1363 | S1167 | A1110 | K1047 | D985  | Q917 | R783 |      |
|     | L1487 | H1364 | G1234 | G1234 | G1234 | M1168 | D1111 | E987  | L986  | A918 | D784 |      |
|     | D1488 | D1365 | Q1235 | Q1235 | Q1235 | D1169 | C1112 | P1048 | R987  | F919 | I785 |      |
|     | Q1489 | K1366 | T1236 | T1236 | T1236 | D1170 | G1113 | S1049 | R988  | L920 | I786 |      |
|     | K1490 | H1367 | L1237 | L1237 | L1237 | V1171 | E1109 | G1050 | Y989  | R921 | L787 |      |
|     | L1491 | E1368 | R1238 | R1238 | R1238 | H1172 | T1115 | T1052 | D990  | L922 | G788 |      |
|     | K1492 | L1369 | A1240 | A1240 | A1240 | L1173 | M1116 | F1053 | Q991  | M924 | L860 |      |
|     | A1493 | S1370 | T1372 | T1372 | T1372 | A1177 | I1118 | P1056 | I992  | E925 | Q861 |      |
|     | L1494 | R1373 | R1372 | R1372 | R1372 | A1178 | G1119 | L930  | L993  | K926 | I792 |      |
|     | L1495 | Q1374 | E1308 | E1308 | E1308 | E1179 | S1120 | V1057 | Q994  | K926 | T793 |      |
|     | E1496 | M1375 | T1243 | T1243 | T1243 | E1179 | V1120 | R1058 | L995  | L930 | Q794 |      |
|     | A1498 | K1376 | L1312 | L1312 | L1312 | V1188 | L1121 | L931  | W996  | V795 | V795 |      |
|     | R1499 | K1377 | L1312 | L1312 | L1312 | V1188 | L1122 | S1069 | T997  | L865 | R785 |      |
|     | S1439 | Y1378 | V1313 | V1313 | V1313 | R1189 | F1123 | S1060 | E998  | V866 | K797 |      |
|     | F1440 | V1379 | K1314 | K1314 | K1314 | S1190 | Q1124 | F1061 | T999  | R867 | E798 |      |
|     | Q1441 | E1380 | D1251 | D1251 | D1251 | L1192 | E1125 | R1062 | T1000 | Y868 | K799 |      |
|     | M1442 | V1381 | I1252 | I1252 | I1252 | L1193 | E1127 | L1065 | E1001 | M869 | K800 |      |
|     | T1443 | T1382 | G1316 | G1316 | G1316 | C1194 | V1128 | T1066 | K1002 | G870 | G803 |      |
|     | T1444 | D1383 | D1317 | D1317 | D1317 | Q1195 | T1129 | V1067 | T1004 | R872 | L804 |      |
|     | H1445 | P1384 | V1319 | V1319 | V1319 | T1196 | R1130 | L1068 | Q1005 | T940 | E805 |      |
|     | V1446 | G1385 | L1256 | L1256 | L1256 | E1197 | S1131 | E1069 | A1006 | F941 | F806 |      |
|     | L1447 | D1386 | P1257 | P1257 | P1257 | L1192 | D1126 | Y1070 | V1007 | S942 | A807 |      |
|     | T1448 | S1387 | R1258 | R1258 | R1258 | T1193 | E1127 | L1065 | K1002 | G946 | T808 |      |
|     | A1451 | L1389 | E1261 | E1261 | E1261 | Q1196 | R1130 | V1067 | T1004 | P877 | P809 |      |
|     | T1452 | E1391 | L1262 | L1262 | L1262 | V1198 | L1132 | E1069 | A1006 | L874 | E810 |      |
|     | G1454 | G1392 | E1264 | E1264 | E1264 | G1199 | R1133 | S1073 | K1009 | T876 | R879 |      |
|     | K1455 | Q1393 | A1265 | A1265 | A1265 | V1200 | L1134 | S1074 | I1009 | P877 | E811 |      |
|     | L1456 | V1394 | R1266 | R1266 | R1266 | C1201 | R1135 | S1074 | N1010 | R877 | E810 |      |
|     | D1457 | E1395 | R1267 | R1267 | R1267 | Q1202 | K1136 | G1075 | F1011 | T876 | E811 |      |
|     | E1458 | L1396 | P1268 | P1268 | P1268 | K1203 | R1137 | G1075 | E1012 | I880 | A812 |      |
|     | L1459 | K1397 | K1269 | K1269 | K1269 | A1138 | A1138 | A1077 | E1013 | G950 | L813 |      |
|     | I1460 | W1398 | A1270 | A1270 | A1270 | Y1207 | E1141 | R1078 | N1014 | P951 | A814 |      |
|     | G1461 | D1399 | K1271 | K1271 | K1271 | D1208 | E1141 | K1079 | Y1015 | D952 | A814 |      |
|     | L1462 | V1400 | K1339 | K1339 | K1339 | L1209 | E1141 | G1080 | P1016 | D953 | E817 |      |

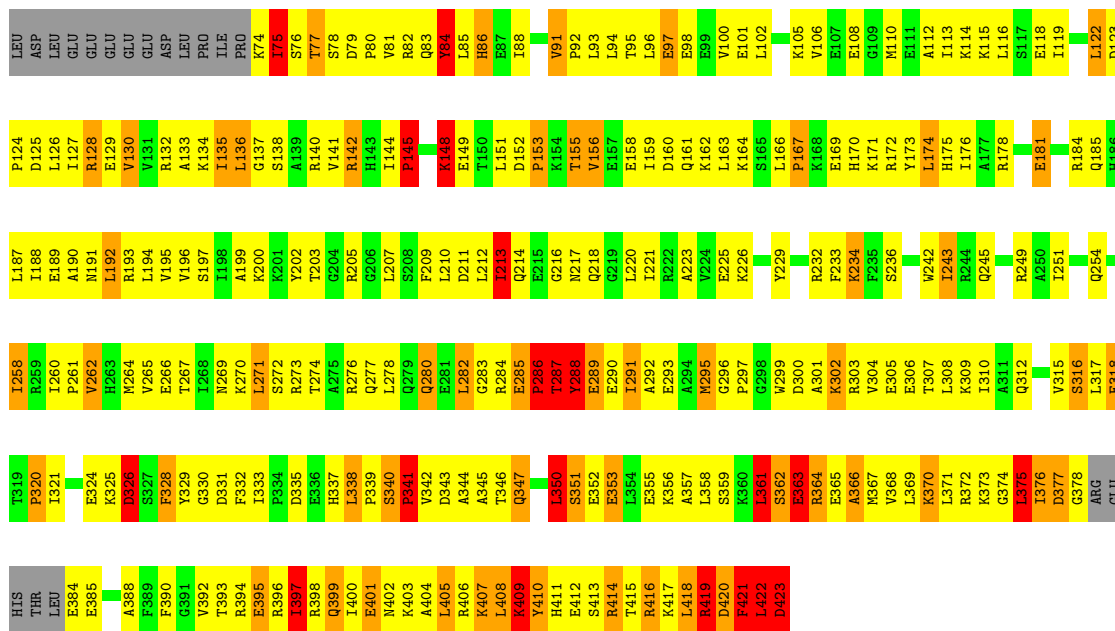
● Molecule 3: RNA polymerase beta subunit

Chain N:  21% 48% 20% 9%

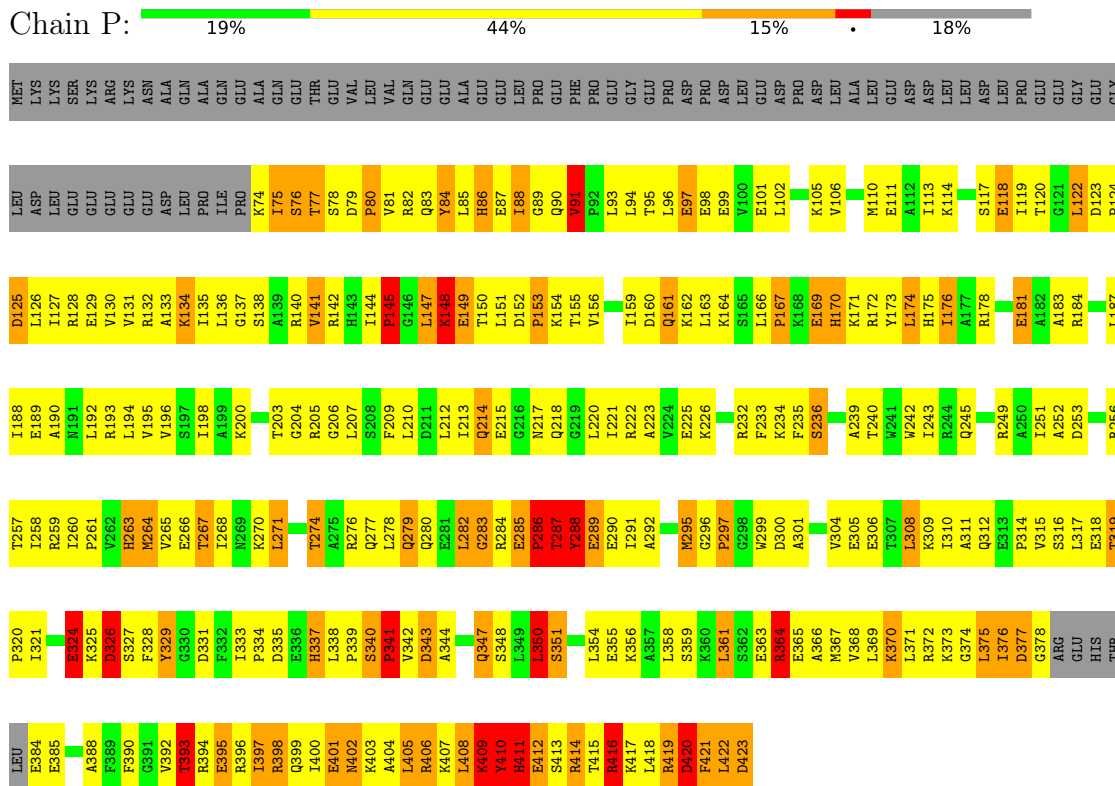
|     |    |    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | K2 | K3 | E4 | V5 | R6 | K7 | V8 | R9 | I10 | A11 | L12 | A13 | S14 | P15 | E16 | K17 | I18 | R19 | S22 | Y23 | G24 | E25 | V26 | E27 | K28 | P29 | E30 | T31 | I32 | K33 | Y34 | R35 | T36 | L37 | K38 | P39 | E40 | R41 | D42 | G43 | L44 | F45 | D46 | E47 | I49 | F50 | G51 | P52 | I53 | K54 | D55 | L56 | ARG | GLY | ALA | ALA | ARG | ARG | GLY | VAL | LYS | ARG | GLY | GLN | GLN | PRO | GLY | C50 | G61 |
|-----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

|       |      |      |      |      |      |      |      |      |      |     |     |      |      |      |
|-------|------|------|------|------|------|------|------|------|------|-----|-----|------|------|------|
| F1008 | G938 | T875 | E811 | H748 | K621 | A559 | V499 | L439 | A379 | GLN | GLY | E190 | Q125 | K62  |
| F939  | F939 | S876 | A812 | V749 | R622 | Q560 | R500 | V440 | E380 | VAL | GLY | L191 | V126 | K65  |
| T940  | T940 | P877 | L813 | P750 | G623 | G561 | A501 | R441 | E381 | ALA | VAL | L192 | L127 | R66  |
| F941  | F941 | G878 | A814 | L751 | D624 | A562 | F502 | R442 | E382 | ALA | VAL | F193 | Y128 | Q66  |
| S942  | S942 | R879 | A815 | S752 | Y625 | E563 | L503 | V443 | G383 | ALA | GLU | G194 | F129 | R67  |
| T943  | T943 | I880 | E817 | S753 | S626 | E564 | D504 | V444 | V384 | GLN | LEU | V195 | S130 | F68  |
| T944  | T944 | L881 | R818 | F754 | G627 | I565 | S505 | R445 | V385 | VAL | LYS | V196 | K131 | E69  |
|       |      | F882 | G819 | A755 | R628 | I566 | G506 | V446 | H386 | GLU | LYS | S197 | Y132 |      |
|       |      | A883 | E820 | A756 | S629 | I567 | M507 | V447 | L387 | GLU | GLU | L198 | I133 | V72  |
|       |      | R884 | R821 | A757 | F630 | R568 | R508 | S448 | H388 | GLU | GLU | L199 | V134 | C73  |
|       |      | L885 | H696 | A758 | G631 | R569 | P509 | S449 | H389 | GLU | GLU | D200 | L135 | E74  |
|       |      | V886 | G697 | A759 | F632 | E570 | E510 | Y450 | P390 | GLY | GLY | G201 | D136 | E75  |
|       |      | N824 | K698 | R760 | V633 | K571 | M511 | D451 | A391 | ALA | ALA | V202 | P137 | C76  |
|       |      | A825 | V699 | I761 | G634 | R572 | M512 | I452 | S392 | GLU | PHE | A203 | K138 | C77  |
|       |      | R826 | V700 | Q762 | P635 | M573 | I513 | D453 | I393 | THR | LEU | L204 | G139 | V78  |
|       |      | R827 | L701 | Q763 | Q636 | L574 | L514 | A454 | L394 | VAL | VAL | Y205 | A140 | V79  |
|       |      | K828 | L702 | L764 | L637 | E575 | E515 | R455 | V395 | THR | LEU | R206 | L141 | V80  |
|       |      | R829 | N703 | S765 | K638 | E576 | A516 | M456 | V396 | LEU | ARG | F207 | I142 | T81  |
|       |      | A830 | R704 | A766 | L639 | A577 | V517 | G457 | K397 | THR | ARG | P208 | N143 | K82  |
|       |      | Q831 | A705 | H767 | H640 | V578 | P518 | A458 | A398 | GLU | GLU | R209 | G144 | S83  |
|       |      | R832 | P706 | N768 | Q641 | V579 | V519 | E458 | A399 | ASP | ASP | R210 | V145 | I84  |
|       |      | E833 | L707 | L769 | C642 | A580 | L520 | A460 | Y401 | GLU | GLU | V211 | P146 | V85  |
|       |      | T834 | L708 | L770 |      | L581 | P521 | I461 | Y401 | PRO | PRO | R212 | P147 | R86  |
|       |      | S835 | H709 | S771 | P645 | L582 | P522 | Q462 | P402 | VAL | VAL | Y213 | E148 | R87  |
|       |      | V836 | R710 |      | K646 | D583 | D523 | Q463 | F403 | THR | ALA | E214 | K149 | Y88  |
|       |      | G837 | L711 | S774 | R647 | N584 | L524 | L464 | E404 | GLU | THR | Y215 | R150 | R89  |
|       |      | R838 | G712 | G775 | M648 | R587 | R525 | L465 | D405 | PRO | THR | V216 | Q151 | M90  |
|       |      | L839 | I713 | E776 | A649 | P526 | K466 | K466 | D406 | LYS | PHE | K217 | L152 | G91  |
|       |      | K840 | Q714 | P777 | L650 | G588 | M527 | E467 | A407 | ASP | LEU | K218 | L153 | H92  |
|       |      | R841 | A715 | L778 | E651 | A589 | V528 | L468 | E408 | THR | PRO | E219 | T154 | I93  |
|       |      | V842 | F716 | A779 | L652 | P590 | Q529 | D469 | V409 | ARG | VAL | R220 | D155 | E94  |
|       |      | F843 | Q717 | K780 | F653 | V591 | V530 | L470 | S410 | VAL | GLY | A221 | E156 | L95  |
|       |      | A844 | P718 | R781 | K654 | T592 | D531 | E471 | T411 | GLN | MET | L225 | E157 | A96  |
|       |      | N845 | S782 | S782 | P655 | N593 | G532 | A472 | G412 | THR | THR | L226 | Y158 | T97  |
|       |      | R846 | L720 | F656 | F656 | P594 | G533 | L473 | D413 | PRO | PRO | L227 | A99  | P98  |
|       |      | D847 | V721 | L657 | L657 |      | R534 | E474 | R414 | LEU | LEU | A228 | L161 | A99  |
|       |      | E848 | E722 | I785 | L658 | D597 | F535 | K475 | V415 | ASN | VAL | A228 | R162 | A100 |
|       |      | A849 | G723 | I786 | K659 | R598 | A536 | E476 | A416 | VAL | VAL |      | Y163 | H101 |
|       |      | L850 | Q724 | L787 | M660 | P599 | T537 | L477 | P417 | VAL | HIS | E232 | G164 | I102 |
|       |      | A851 |      | G788 | M661 | L600 | S538 | L478 | G418 | VAL | GLY | R233 | K165 | W103 |
|       |      | V853 |      | L789 | E662 | R601 | D539 | E479 | D419 | PRO | GLU | E234 | Q166 | F104 |
|       |      |      | Q727 |      | E663 | S602 | L540 | E480 | V420 | GLY | ILE |      | E167 |      |
|       |      |      | L728 |      | K664 | L603 | N541 | M481 | L421 | GLY | VAL | P238 | T168 | D107 |
|       |      |      | H729 |      |      | T604 | D542 | K482 | A422 | ALA | GLU | G239 | Y169 | V108 |
|       |      |      | P730 |      |      | D605 | L543 | R483 | D423 | ARG | LYS | E240 | P170 | P109 |
|       |      |      | L731 |      | N669 | D605 | L543 | R483 | D423 | ARG | LYS | E240 | P170 | P109 |
|       |      |      | V732 |      | V670 | I606 | Y544 | P484 | G424 | VAL | GLY | I241 | L171 | S110 |
|       |      |      | C733 |      | K671 | L607 | R545 | S485 | G425 | GLU | GLN | L242 | P172 | K111 |
|       |      |      | E734 |      | A672 | S608 | R546 | R486 | K426 | ALA | PRO | A243 | P173 | I112 |
|       |      |      | A735 |      | A673 | G609 | L547 | A487 | V427 | LEU | LEU | E244 | G113 | G113 |
|       |      |      | F736 |      | R674 | K610 | I548 | R488 | K428 | ALA | ALA | L245 | A177 | T114 |
|       |      |      | N737 |      | R675 | Q611 | N549 | R489 | S429 | GLU | GLU | P246 | L178 | L115 |
|       |      |      | A738 |      | M676 | G612 | R550 | A490 | S429 | ALA | ALA | E247 | V179 | L116 |
|       |      |      | D739 |      | L677 | R613 | N551 | K491 | V431 | LYS | LYS | P248 | K180 | D117 |
|       |      |      | F740 |      | E678 | F614 | N552 | A492 | Y432 | GLY | GLY | Y249 | L181 | L118 |
|       |      |      | D741 |      | R679 | R615 | R553 | K493 | G434 | LEU | LEU | L250 | G182 | G182 |
|       |      |      | G742 |      | Q680 | Q616 | L554 | K494 | R433 | LEU | LEU | F251 | V185 | A120 |
|       |      |      |      |      | R681 | N617 | K555 | R495 | V435 | ARG | ARG |      | V185 | T121 |
|       |      |      | M745 |      | D682 | L618 | K556 | L496 | E436 | MET | MET |      | V186 | E122 |
|       |      |      | A746 |      | I683 | L619 | L557 | E497 | V377 | GLU | GLU |      | K187 | L123 |
|       |      |      | V747 |      | K684 | G620 | L558 | V498 | I378 | ARG | ARG |      |      | E124 |





- Molecule 5: RNA polymerase sigma-70 subunit



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                            | Source    |
|----------------------------------------------------------|--------------------------------------------------|-----------|
| Space group                                              | P 32                                             | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 236.35Å 236.35Å 249.04Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å)                                           | 40.00 – 2.60                                     | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (40.00-2.60)                     | Depositor |
| $R_{merge}$                                              | 0.13                                             | Depositor |
| $R_{sym}$                                                | (Not available)                                  | Depositor |
| Refinement program                                       | CNS 1.0                                          | Depositor |
| R, $R_{free}$                                            | 0.228 , 0.274                                    | Depositor |
| Estimated twinning fraction                              | No twinning to report.                           | Xtriage   |
| Total number of atoms                                    | 59529                                            | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 58.0                                             | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.76         | 2/1838 (0.1%)   | 1.29        | 19/2498 (0.8%)   |
| 1   | B     | 0.74         | 0/1838          | 1.19        | 20/2498 (0.8%)   |
| 1   | K     | 0.71         | 1/1838 (0.1%)   | 1.21        | 17/2498 (0.7%)   |
| 1   | L     | 0.73         | 0/1838          | 1.24        | 15/2498 (0.6%)   |
| 2   | C     | 0.82         | 8/8997 (0.1%)   | 1.45        | 129/12164 (1.1%) |
| 2   | M     | 0.82         | 9/8997 (0.1%)   | 1.44        | 119/12164 (1.0%) |
| 3   | D     | 0.84         | 18/10979 (0.2%) | 1.47        | 168/14844 (1.1%) |
| 3   | N     | 0.84         | 20/10979 (0.2%) | 1.48        | 167/14844 (1.1%) |
| 4   | E     | 0.84         | 0/783           | 1.47        | 11/1054 (1.0%)   |
| 4   | O     | 0.81         | 0/783           | 1.50        | 9/1054 (0.9%)    |
| 5   | F     | 1.00         | 13/2812 (0.5%)  | 1.44        | 47/3781 (1.2%)   |
| 5   | P     | 0.92         | 9/2812 (0.3%)   | 1.44        | 38/3781 (1.0%)   |
| All | All   | 0.83         | 80/54494 (0.1%) | 1.43        | 759/73678 (1.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | D     | 0                   | 3                   |
| 3   | N     | 0                   | 3                   |
| 5   | F     | 0                   | 1                   |
| All | All   | 0                   | 7                   |

All (80) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 3   | D     | 380 | GLU  | C-N   | -11.84 | 1.17        | 1.33     |
| 2   | C     | 58  | ASP  | CA-C  | -11.64 | 1.39        | 1.52     |
| 3   | N     | 380 | GLU  | C-N   | -11.54 | 1.17        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5   | F     | 423  | ASP  | C-OXT  | 10.80 | 1.45        | 1.23     |
| 5   | F     | 420  | ASP  | CA-C   | -9.97 | 1.40        | 1.52     |
| 5   | F     | 419  | ARG  | CA-C   | -9.38 | 1.40        | 1.52     |
| 3   | D     | 378  | ILE  | C-O    | 9.36  | 1.35        | 1.24     |
| 3   | N     | 207  | PHE  | CA-C   | 8.73  | 1.63        | 1.52     |
| 3   | D     | 379  | ALA  | C-N    | -8.43 | 1.21        | 1.33     |
| 5   | F     | 350  | LEU  | CG-CD1 | -8.31 | 1.25        | 1.52     |
| 5   | F     | 401  | GLU  | CB-CG  | 8.30  | 1.77        | 1.52     |
| 3   | D     | 380  | GLU  | C-O    | 8.30  | 1.34        | 1.24     |
| 3   | N     | 378  | ILE  | C-O    | 8.14  | 1.33        | 1.24     |
| 3   | N     | 177  | ALA  | CA-CB  | -8.11 | 1.39        | 1.53     |
| 5   | P     | 401  | GLU  | CB-CG  | 8.10  | 1.76        | 1.52     |
| 3   | D     | 207  | PHE  | CA-C   | 8.04  | 1.62        | 1.52     |
| 5   | F     | 419  | ARG  | CB-CG  | 8.03  | 1.76        | 1.52     |
| 5   | F     | 401  | GLU  | CG-CD  | 8.01  | 1.72        | 1.52     |
| 3   | N     | 388  | HIS  | C-N    | 8.01  | 1.44        | 1.33     |
| 3   | N     | 380  | GLU  | C-O    | 8.00  | 1.33        | 1.23     |
| 5   | P     | 423  | ASP  | C-OXT  | 8.00  | 1.39        | 1.23     |
| 5   | F     | 421  | PHE  | CA-C   | -7.77 | 1.41        | 1.52     |
| 5   | P     | 401  | GLU  | CG-CD  | 7.77  | 1.71        | 1.52     |
| 5   | P     | 410  | TYR  | N-CA   | -7.70 | 1.37        | 1.46     |
| 2   | M     | 686  | ASP  | CA-C   | -7.64 | 1.46        | 1.53     |
| 3   | N     | 1007 | VAL  | CA-CB  | 7.54  | 1.62        | 1.54     |
| 3   | D     | 208  | PRO  | CA-C   | 7.50  | 1.63        | 1.52     |
| 2   | M     | 291  | ALA  | CA-CB  | -7.45 | 1.41        | 1.53     |
| 5   | F     | 366  | ALA  | CA-CB  | -7.36 | 1.41        | 1.53     |
| 2   | C     | 291  | ALA  | CA-CB  | -7.16 | 1.41        | 1.53     |
| 2   | C     | 686  | ASP  | CA-C   | -7.15 | 1.46        | 1.53     |
| 2   | M     | 687  | ALA  | CA-C   | -7.15 | 1.44        | 1.52     |
| 5   | F     | 410  | TYR  | N-CA   | -7.09 | 1.37        | 1.46     |
| 3   | N     | 386  | HIS  | C-N    | 6.98  | 1.43        | 1.33     |
| 3   | N     | 379  | ALA  | C-N    | -6.96 | 1.23        | 1.33     |
| 3   | N     | 371  | ILE  | C-O    | 6.78  | 1.30        | 1.24     |
| 3   | N     | 208  | PRO  | CA-C   | 6.70  | 1.61        | 1.52     |
| 2   | C     | 57   | GLU  | CA-C   | -6.62 | 1.46        | 1.52     |
| 5   | F     | 421  | PHE  | N-CA   | -6.57 | 1.37        | 1.46     |
| 1   | A     | 165  | ILE  | CA-CB  | 6.28  | 1.59        | 1.54     |
| 3   | D     | 218  | LYS  | C-O    | 6.18  | 1.30        | 1.23     |
| 5   | P     | 409  | LYS  | CA-C   | -6.10 | 1.45        | 1.52     |
| 3   | N     | 209  | ARG  | N-CA   | 6.09  | 1.53        | 1.46     |
| 2   | M     | 264  | PRO  | CB-CG  | -6.07 | 1.19        | 1.49     |
| 3   | D     | 371  | ILE  | C-O    | 6.05  | 1.30        | 1.24     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | M     | 58   | ASP  | CA-C   | -6.05 | 1.45        | 1.52     |
| 2   | C     | 687  | ALA  | CA-C   | -5.99 | 1.45        | 1.52     |
| 3   | D     | 386  | HIS  | C-N    | 5.98  | 1.42        | 1.33     |
| 3   | N     | 387  | LEU  | C-N    | 5.98  | 1.41        | 1.33     |
| 2   | C     | 253  | ALA  | CA-CB  | -5.98 | 1.43        | 1.53     |
| 3   | D     | 389  | GLU  | N-CA   | -5.98 | 1.41        | 1.46     |
| 1   | K     | 229  | GLN  | C-O    | 5.97  | 1.35        | 1.23     |
| 1   | A     | 48   | ILE  | C-N    | 5.96  | 1.41        | 1.33     |
| 3   | D     | 1177 | ALA  | CA-CB  | -5.94 | 1.44        | 1.53     |
| 2   | M     | 59   | LYS  | N-CA   | -5.86 | 1.41        | 1.46     |
| 5   | F     | 401  | GLU  | CA-CB  | 5.86  | 1.62        | 1.53     |
| 3   | D     | 209  | ARG  | N-CA   | 5.76  | 1.53        | 1.46     |
| 3   | N     | 218  | LYS  | C-O    | 5.74  | 1.29        | 1.24     |
| 5   | P     | 401  | GLU  | CA-CB  | 5.64  | 1.63        | 1.53     |
| 3   | D     | 1007 | VAL  | CA-CB  | 5.63  | 1.60        | 1.54     |
| 3   | N     | 132  | TYR  | CA-C   | -5.63 | 1.45        | 1.52     |
| 3   | D     | 1284 | GLU  | CA-C   | 5.61  | 1.59        | 1.52     |
| 5   | F     | 376  | ILE  | CA-C   | -5.59 | 1.45        | 1.52     |
| 5   | P     | 420  | ASP  | CA-C   | -5.56 | 1.45        | 1.52     |
| 2   | M     | 368  | THR  | CA-C   | 5.52  | 1.59        | 1.52     |
| 3   | N     | 761  | ILE  | CA-CB  | 5.47  | 1.60        | 1.55     |
| 5   | P     | 421  | PHE  | N-CA   | -5.29 | 1.39        | 1.46     |
| 2   | C     | 905  | ILE  | N-CA   | -5.22 | 1.39        | 1.46     |
| 3   | D     | 247  | GLU  | C-O    | 5.14  | 1.30        | 1.24     |
| 3   | D     | 581  | LEU  | CB-CG  | -5.13 | 1.43        | 1.53     |
| 3   | D     | 136  | ASP  | CA-C   | 5.12  | 1.59        | 1.52     |
| 2   | M     | 905  | ILE  | N-CA   | -5.11 | 1.40        | 1.46     |
| 2   | C     | 58   | ASP  | N-CA   | -5.08 | 1.40        | 1.46     |
| 3   | N     | 372  | ASP  | C-N    | 5.07  | 1.45        | 1.33     |
| 3   | N     | 186  | VAL  | CA-CB  | 5.07  | 1.60        | 1.55     |
| 5   | P     | 350  | LEU  | CG-CD1 | -5.05 | 1.35        | 1.52     |
| 2   | M     | 54   | ILE  | CA-CB  | 5.04  | 1.59        | 1.53     |
| 3   | D     | 145  | VAL  | CA-CB  | 5.02  | 1.60        | 1.54     |
| 3   | N     | 87   | ARG  | C-O    | -5.01 | 1.18        | 1.24     |
| 3   | N     | 247  | GLU  | C-O    | 5.01  | 1.30        | 1.24     |

All (759) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3   | D     | 380 | GLU  | CA-C-O | -21.63 | 96.85       | 120.43   |
| 1   | L     | 229 | GLN  | CA-C-O | 21.37  | 157.12      | 120.80   |
| 3   | N     | 380 | GLU  | CA-C-O | -20.66 | 97.86       | 120.80   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 2   | C     | 243  | ARG  | CA-C-N | 19.93  | 144.75      | 119.84   |
| 2   | C     | 243  | ARG  | C-N-CA | 19.93  | 144.75      | 119.84   |
| 3   | N     | 207  | PHE  | CA-C-N | 19.21  | 143.86      | 119.84   |
| 3   | N     | 207  | PHE  | C-N-CA | 19.21  | 143.86      | 119.84   |
| 3   | D     | 508  | ARG  | CA-C-N | 18.65  | 143.16      | 119.84   |
| 3   | D     | 508  | ARG  | C-N-CA | 18.65  | 143.16      | 119.84   |
| 2   | M     | 243  | ARG  | CA-C-N | 18.20  | 142.59      | 119.84   |
| 2   | M     | 243  | ARG  | C-N-CA | 18.20  | 142.59      | 119.84   |
| 3   | N     | 508  | ARG  | CA-C-N | 18.02  | 142.36      | 119.84   |
| 3   | N     | 508  | ARG  | C-N-CA | 18.02  | 142.36      | 119.84   |
| 3   | D     | 207  | PHE  | CA-C-N | 17.58  | 141.82      | 119.84   |
| 3   | D     | 207  | PHE  | C-N-CA | 17.58  | 141.82      | 119.84   |
| 2   | M     | 177  | GLU  | CA-C-N | 17.03  | 141.13      | 119.84   |
| 2   | M     | 177  | GLU  | C-N-CA | 17.03  | 141.13      | 119.84   |
| 2   | C     | 177  | GLU  | CA-C-N | 16.89  | 140.95      | 119.84   |
| 2   | C     | 177  | GLU  | C-N-CA | 16.89  | 140.95      | 119.84   |
| 2   | M     | 230  | ARG  | CA-C-N | 14.94  | 138.52      | 119.84   |
| 2   | M     | 230  | ARG  | C-N-CA | 14.94  | 138.52      | 119.84   |
| 3   | D     | 245  | LEU  | CA-C-O | -14.35 | 107.65      | 119.71   |
| 2   | C     | 230  | ARG  | CA-C-N | 14.28  | 137.69      | 119.84   |
| 2   | C     | 230  | ARG  | C-N-CA | 14.28  | 137.69      | 119.84   |
| 2   | M     | 810  | ASP  | CA-C-N | 14.18  | 133.71      | 118.97   |
| 2   | M     | 810  | ASP  | C-N-CA | 14.18  | 133.71      | 118.97   |
| 3   | D     | 1389 | LEU  | N-CA-C | 14.15  | 126.42      | 111.14   |
| 3   | N     | 1389 | LEU  | N-CA-C | 14.07  | 126.13      | 111.07   |
| 2   | C     | 810  | ASP  | CA-C-N | 13.71  | 133.22      | 118.97   |
| 2   | C     | 810  | ASP  | C-N-CA | 13.71  | 133.22      | 118.97   |
| 4   | O     | 49   | GLN  | N-CA-C | 13.65  | 129.40      | 113.02   |
| 3   | D     | 171  | LEU  | CA-C-N | 13.57  | 134.36      | 120.38   |
| 3   | D     | 171  | LEU  | C-N-CA | 13.57  | 134.36      | 120.38   |
| 3   | N     | 171  | LEU  | CA-C-N | 13.44  | 134.22      | 120.38   |
| 3   | N     | 171  | LEU  | C-N-CA | 13.44  | 134.22      | 120.38   |
| 4   | E     | 49   | GLN  | N-CA-C | 13.24  | 128.91      | 113.15   |
| 1   | A     | 2    | LEU  | N-CA-C | 12.95  | 127.20      | 111.40   |
| 3   | N     | 209  | ARG  | N-CA-C | 12.90  | 129.84      | 112.68   |
| 3   | D     | 209  | ARG  | N-CA-C | 12.88  | 129.82      | 112.68   |
| 2   | M     | 728  | HIS  | N-CA-C | 11.99  | 125.73      | 111.82   |
| 1   | A     | 48   | ILE  | CA-C-N | 11.96  | 131.69      | 120.21   |
| 1   | A     | 48   | ILE  | C-N-CA | 11.96  | 131.69      | 120.21   |
| 2   | C     | 414  | GLY  | CA-C-N | 11.96  | 134.79      | 119.84   |
| 2   | C     | 414  | GLY  | C-N-CA | 11.96  | 134.79      | 119.84   |
| 1   | K     | 2    | LEU  | N-CA-C | 11.95  | 125.98      | 111.40   |

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| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 2   | C     | 728  | HIS  | N-CA-C   | 11.81  | 125.52      | 111.82   |
| 2   | M     | 414  | GLY  | CA-C-N   | 11.59  | 134.33      | 119.84   |
| 2   | M     | 414  | GLY  | C-N-CA   | 11.59  | 134.33      | 119.84   |
| 3   | N     | 199  | LEU  | CA-C-N   | -11.57 | 106.75      | 122.72   |
| 3   | N     | 199  | LEU  | C-N-CA   | -11.57 | 106.75      | 122.72   |
| 3   | N     | 245  | LEU  | CA-C-O   | -11.36 | 109.71      | 119.59   |
| 5   | F     | 91   | VAL  | CA-C-N   | -10.90 | 109.32      | 120.98   |
| 5   | F     | 91   | VAL  | C-N-CA   | -10.90 | 109.32      | 120.98   |
| 2   | M     | 260  | LEU  | N-CA-C   | 10.88  | 127.70      | 112.04   |
| 3   | D     | 1126 | ASP  | N-CA-C   | 10.69  | 127.64      | 107.75   |
| 5   | P     | 91   | VAL  | CA-C-N   | -10.50 | 109.75      | 120.98   |
| 5   | P     | 91   | VAL  | C-N-CA   | -10.50 | 109.75      | 120.98   |
| 2   | C     | 260  | LEU  | N-CA-C   | 10.21  | 127.18      | 111.56   |
| 3   | D     | 1287 | GLU  | N-CA-C   | 10.17  | 122.05      | 110.97   |
| 3   | N     | 1124 | GLN  | CA-C-N   | 10.15  | 132.52      | 119.84   |
| 3   | N     | 1124 | GLN  | C-N-CA   | 10.15  | 132.52      | 119.84   |
| 2   | C     | 547  | ILE  | CA-C-N   | 10.05  | 132.40      | 119.84   |
| 2   | C     | 547  | ILE  | C-N-CA   | 10.05  | 132.40      | 119.84   |
| 5   | P     | 411  | HIS  | CA-CB-CG | 10.02  | 123.82      | 113.80   |
| 3   | D     | 208  | PRO  | N-CA-C   | 9.97   | 133.01      | 112.47   |
| 1   | L     | 2    | LEU  | N-CA-C   | 9.89   | 126.29      | 112.04   |
| 3   | D     | 199  | LEU  | CA-C-N   | -9.74  | 109.28      | 122.72   |
| 3   | D     | 199  | LEU  | C-N-CA   | -9.74  | 109.28      | 122.72   |
| 3   | D     | 1209 | LEU  | N-CA-C   | -9.70  | 95.53       | 110.17   |
| 3   | D     | 705  | ALA  | CA-C-N   | -9.68  | 107.74      | 119.84   |
| 3   | D     | 705  | ALA  | C-N-CA   | -9.68  | 107.74      | 119.84   |
| 3   | N     | 1209 | LEU  | N-CA-C   | -9.68  | 95.36       | 110.36   |
| 1   | B     | 2    | LEU  | N-CA-C   | 9.66   | 125.95      | 112.04   |
| 3   | D     | 225  | LEU  | CA-C-N   | 9.65   | 131.91      | 119.84   |
| 3   | D     | 225  | LEU  | C-N-CA   | 9.65   | 131.91      | 119.84   |
| 3   | N     | 225  | LEU  | CA-C-N   | 9.56   | 131.79      | 119.84   |
| 3   | N     | 225  | LEU  | C-N-CA   | 9.56   | 131.79      | 119.84   |
| 3   | N     | 589  | ALA  | CA-C-N   | 9.55   | 129.49      | 119.85   |
| 3   | N     | 589  | ALA  | C-N-CA   | 9.55   | 129.49      | 119.85   |
| 4   | E     | 93   | TYR  | CA-C-N   | 9.54   | 131.77      | 119.84   |
| 4   | E     | 93   | TYR  | C-N-CA   | 9.54   | 131.77      | 119.84   |
| 3   | D     | 199  | LEU  | N-CA-C   | 9.51   | 125.33      | 112.68   |
| 2   | M     | 1078 | GLU  | CA-C-N   | 9.51   | 131.73      | 119.84   |
| 2   | M     | 1078 | GLU  | C-N-CA   | 9.51   | 131.73      | 119.84   |
| 4   | O     | 93   | TYR  | CA-C-N   | 9.43   | 131.63      | 119.84   |
| 4   | O     | 93   | TYR  | C-N-CA   | 9.43   | 131.63      | 119.84   |
| 2   | M     | 729  | LEU  | N-CA-C   | 9.38   | 125.31      | 114.62   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | N     | 208  | PRO  | N-CA-C   | 9.34  | 131.72      | 112.47   |
| 2   | M     | 441  | VAL  | N-CA-C   | 9.32  | 119.29      | 110.53   |
| 3   | D     | 1208 | ASP  | N-CA-C   | 9.31  | 123.53      | 108.63   |
| 2   | M     | 1118 | LYS  | N-CA-C   | 9.27  | 124.51      | 109.40   |
| 3   | N     | 199  | LEU  | N-CA-C   | 9.24  | 124.97      | 112.68   |
| 3   | D     | 448  | GLU  | N-CA-C   | 9.22  | 125.66      | 113.30   |
| 3   | N     | 1287 | GLU  | N-CA-C   | 9.13  | 122.16      | 111.02   |
| 2   | C     | 729  | LEU  | N-CA-C   | 9.10  | 124.99      | 114.62   |
| 2   | M     | 726  | ILE  | CA-C-N   | 9.09  | 131.20      | 119.84   |
| 2   | M     | 726  | ILE  | C-N-CA   | 9.09  | 131.20      | 119.84   |
| 5   | P     | 410  | TYR  | CA-CB-CG | -9.08 | 97.56       | 113.90   |
| 2   | M     | 113  | VAL  | CA-C-N   | -9.07 | 110.36      | 122.42   |
| 2   | M     | 113  | VAL  | C-N-CA   | -9.07 | 110.36      | 122.42   |
| 5   | F     | 377  | ASP  | N-CA-C   | -9.06 | 94.45       | 108.76   |
| 3   | N     | 132  | TYR  | CA-CB-CG | -9.00 | 97.70       | 113.90   |
| 3   | D     | 172  | PRO  | CA-C-N   | 8.99  | 131.83      | 120.51   |
| 3   | D     | 172  | PRO  | C-N-CA   | 8.99  | 131.83      | 120.51   |
| 2   | C     | 1078 | GLU  | CA-C-N   | 8.95  | 131.03      | 119.84   |
| 2   | C     | 1078 | GLU  | C-N-CA   | 8.95  | 131.03      | 119.84   |
| 3   | N     | 525  | ARG  | CA-C-N   | 8.95  | 129.01      | 119.89   |
| 3   | N     | 525  | ARG  | C-N-CA   | 8.95  | 129.01      | 119.89   |
| 5   | F     | 84   | TYR  | CA-CB-CG | 8.94  | 129.98      | 113.90   |
| 3   | N     | 448  | GLU  | N-CA-C   | 8.92  | 125.25      | 113.30   |
| 2   | C     | 1118 | LYS  | N-CA-C   | 8.90  | 123.91      | 109.40   |
| 3   | D     | 1243 | THR  | N-CA-C   | 8.80  | 121.68      | 110.33   |
| 1   | A     | 229  | GLN  | CA-C-O   | 8.77  | 135.71      | 120.80   |
| 3   | D     | 525  | ARG  | CA-C-N   | 8.77  | 128.84      | 119.89   |
| 3   | D     | 525  | ARG  | C-N-CA   | 8.77  | 128.84      | 119.89   |
| 3   | N     | 1126 | ASP  | N-CA-C   | 8.77  | 129.48      | 110.80   |
| 5   | P     | 363  | GLU  | N-CA-C   | 8.71  | 120.77      | 111.28   |
| 1   | B     | 229  | GLN  | CA-C-O   | 8.62  | 135.45      | 120.80   |
| 3   | N     | 172  | PRO  | CA-C-N   | 8.61  | 131.36      | 120.51   |
| 3   | N     | 172  | PRO  | C-N-CA   | 8.61  | 131.36      | 120.51   |
| 3   | D     | 1116 | ASN  | N-CA-C   | -8.46 | 95.89       | 109.76   |
| 2   | M     | 547  | ILE  | CA-C-N   | 8.45  | 130.40      | 119.84   |
| 2   | M     | 547  | ILE  | C-N-CA   | 8.45  | 130.40      | 119.84   |
| 2   | M     | 151  | ASP  | CA-C-N   | 8.45  | 130.40      | 119.84   |
| 2   | M     | 151  | ASP  | C-N-CA   | 8.45  | 130.40      | 119.84   |
| 2   | M     | 1117 | SER  | CA-C-N   | -8.45 | 110.27      | 122.94   |
| 2   | M     | 1117 | SER  | C-N-CA   | -8.45 | 110.27      | 122.94   |
| 3   | D     | 1127 | GLU  | N-CA-C   | -8.42 | 98.23       | 111.02   |
| 3   | N     | 1128 | VAL  | N-CA-C   | -8.40 | 98.74       | 109.58   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | C     | 57   | GLU  | CA-C-N   | -8.40 | 107.98      | 121.58   |
| 2   | C     | 57   | GLU  | C-N-CA   | -8.40 | 107.98      | 121.58   |
| 3   | D     | 143  | ASN  | N-CA-C   | -8.35 | 103.61      | 113.88   |
| 3   | N     | 218  | LYS  | CA-C-O   | -8.33 | 113.53      | 121.02   |
| 3   | D     | 831  | GLY  | N-CA-C   | -8.32 | 93.47       | 113.18   |
| 3   | N     | 831  | GLY  | N-CA-C   | -8.27 | 93.58       | 113.18   |
| 2   | C     | 726  | ILE  | CA-C-N   | 8.24  | 130.14      | 119.84   |
| 2   | C     | 726  | ILE  | C-N-CA   | 8.24  | 130.14      | 119.84   |
| 2   | C     | 113  | VAL  | CA-C-N   | -8.23 | 111.48      | 122.42   |
| 2   | C     | 113  | VAL  | C-N-CA   | -8.23 | 111.48      | 122.42   |
| 2   | C     | 266  | ARG  | N-CA-C   | -8.21 | 97.23       | 110.20   |
| 3   | D     | 589  | ALA  | CA-C-N   | 8.19  | 128.12      | 119.85   |
| 3   | D     | 589  | ALA  | C-N-CA   | 8.19  | 128.12      | 119.85   |
| 2   | M     | 266  | ARG  | N-CA-C   | -8.18 | 97.28       | 110.20   |
| 2   | C     | 151  | ASP  | CA-C-N   | 8.16  | 130.04      | 119.84   |
| 2   | C     | 151  | ASP  | C-N-CA   | 8.16  | 130.04      | 119.84   |
| 3   | D     | 217  | LYS  | CA-C-N   | -8.14 | 111.14      | 122.87   |
| 3   | D     | 217  | LYS  | C-N-CA   | -8.14 | 111.14      | 122.87   |
| 3   | D     | 244  | GLU  | CA-C-N   | -8.14 | 109.19      | 120.83   |
| 3   | D     | 244  | GLU  | C-N-CA   | -8.14 | 109.19      | 120.83   |
| 5   | F     | 287  | THR  | N-CA-C   | -8.12 | 99.05       | 110.50   |
| 3   | N     | 1317 | ASP  | CA-C-N   | 8.04  | 133.29      | 121.31   |
| 3   | N     | 1317 | ASP  | C-N-CA   | 8.04  | 133.29      | 121.31   |
| 5   | F     | 410  | TYR  | CA-CB-CG | -8.04 | 99.43       | 113.90   |
| 3   | N     | 108  | VAL  | CA-C-N   | -8.02 | 110.37      | 120.23   |
| 3   | N     | 108  | VAL  | C-N-CA   | -8.02 | 110.37      | 120.23   |
| 2   | M     | 163  | ILE  | CA-C-N   | 7.99  | 129.83      | 119.84   |
| 2   | M     | 163  | ILE  | C-N-CA   | 7.99  | 129.83      | 119.84   |
| 3   | N     | 634  | GLY  | CA-C-N   | 7.98  | 129.82      | 119.84   |
| 3   | N     | 634  | GLY  | C-N-CA   | 7.98  | 129.82      | 119.84   |
| 2   | M     | 319  | GLY  | N-CA-C   | -7.98 | 94.28       | 113.18   |
| 3   | D     | 1317 | ASP  | CA-C-N   | 7.97  | 133.19      | 121.31   |
| 3   | D     | 1317 | ASP  | C-N-CA   | 7.97  | 133.19      | 121.31   |
| 2   | C     | 441  | VAL  | N-CA-C   | 7.94  | 119.65      | 111.00   |
| 3   | D     | 81   | THR  | N-CA-C   | -7.93 | 97.36       | 109.41   |
| 5   | P     | 287  | THR  | N-CA-C   | -7.90 | 99.36       | 110.50   |
| 2   | M     | 261  | ILE  | N-CA-C   | 7.89  | 125.75      | 109.34   |
| 2   | C     | 261  | ILE  | N-CA-C   | 7.88  | 125.73      | 109.34   |
| 2   | C     | 1019 | GLN  | CA-C-N   | 7.83  | 129.63      | 119.84   |
| 2   | C     | 1019 | GLN  | C-N-CA   | 7.83  | 129.63      | 119.84   |
| 5   | P     | 411  | HIS  | CB-CA-C  | 7.79  | 125.45      | 109.95   |
| 4   | O     | 51   | LEU  | N-CA-C   | -7.78 | 97.97       | 108.24   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | N     | 143  | ASN  | N-CA-C   | -7.75 | 103.95      | 113.41   |
| 3   | N     | 393  | ILE  | CB-CA-C  | -7.69 | 101.03      | 111.33   |
| 2   | C     | 319  | GLY  | N-CA-C   | -7.67 | 95.00       | 113.18   |
| 3   | N     | 521  | PRO  | CA-C-N   | 7.66  | 129.41      | 119.84   |
| 3   | N     | 521  | PRO  | C-N-CA   | 7.66  | 129.41      | 119.84   |
| 3   | D     | 634  | GLY  | CA-C-N   | 7.66  | 129.41      | 119.84   |
| 3   | D     | 634  | GLY  | C-N-CA   | 7.66  | 129.41      | 119.84   |
| 2   | M     | 251  | ASP  | N-CA-C   | 7.65  | 120.35      | 111.02   |
| 2   | C     | 1117 | SER  | CA-C-N   | -7.64 | 111.49      | 122.94   |
| 2   | C     | 1117 | SER  | C-N-CA   | -7.64 | 111.49      | 122.94   |
| 3   | D     | 1124 | GLN  | CA-C-N   | 7.63  | 129.38      | 119.84   |
| 3   | D     | 1124 | GLN  | C-N-CA   | 7.63  | 129.38      | 119.84   |
| 2   | M     | 188  | LYS  | N-CA-C   | 7.63  | 121.08      | 111.24   |
| 3   | N     | 561  | GLY  | CA-C-N   | -7.62 | 113.11      | 122.64   |
| 3   | N     | 561  | GLY  | C-N-CA   | -7.62 | 113.11      | 122.64   |
| 2   | M     | 1019 | GLN  | CA-C-N   | 7.60  | 129.34      | 119.84   |
| 2   | M     | 1019 | GLN  | C-N-CA   | 7.60  | 129.34      | 119.84   |
| 2   | C     | 591  | SER  | N-CA-C   | -7.59 | 101.08      | 110.41   |
| 3   | D     | 561  | GLY  | CA-C-N   | -7.59 | 113.16      | 122.64   |
| 3   | D     | 561  | GLY  | C-N-CA   | -7.59 | 113.16      | 122.64   |
| 3   | D     | 142  | LEU  | N-CA-C   | 7.58  | 120.78      | 110.55   |
| 3   | N     | 81   | THR  | N-CA-C   | -7.56 | 97.91       | 109.41   |
| 3   | D     | 1251 | ASP  | N-CA-C   | 7.54  | 122.93      | 112.45   |
| 5   | F     | 419  | ARG  | CB-CG-CD | 7.53  | 128.62      | 111.30   |
| 3   | N     | 217  | LYS  | CA-C-N   | -7.52 | 110.03      | 121.53   |
| 3   | N     | 217  | LYS  | C-N-CA   | -7.52 | 110.03      | 121.53   |
| 2   | C     | 243  | ARG  | C-N-CD   | -7.51 | 94.19       | 125.00   |
| 2   | M     | 52   | PHE  | CA-C-N   | -7.51 | 110.45      | 119.84   |
| 2   | M     | 52   | PHE  | C-N-CA   | -7.51 | 110.45      | 119.84   |
| 5   | P     | 377  | ASP  | N-CA-C   | -7.51 | 96.90       | 108.76   |
| 2   | C     | 188  | LYS  | N-CA-C   | 7.50  | 120.92      | 111.24   |
| 3   | N     | 371  | ILE  | O-C-N    | -7.50 | 114.02      | 122.04   |
| 5   | F     | 296  | GLY  | CA-C-N   | 7.49  | 129.20      | 119.84   |
| 5   | F     | 296  | GLY  | C-N-CA   | 7.49  | 129.20      | 119.84   |
| 2   | M     | 263  | ASP  | CA-C-N   | 7.49  | 129.20      | 119.84   |
| 2   | M     | 263  | ASP  | C-N-CA   | 7.49  | 129.20      | 119.84   |
| 3   | N     | 1251 | ASP  | N-CA-C   | 7.48  | 122.84      | 112.45   |
| 3   | D     | 378  | ILE  | CA-C-O   | -7.44 | 111.48      | 120.78   |
| 2   | C     | 768  | THR  | CA-C-N   | 7.41  | 126.95      | 119.24   |
| 2   | C     | 768  | THR  | C-N-CA   | 7.41  | 126.95      | 119.24   |
| 3   | D     | 378  | ILE  | O-C-N    | -7.41 | 113.30      | 122.57   |
| 2   | C     | 608  | GLY  | N-CA-C   | -7.40 | 105.62      | 115.32   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | D     | 201  | GLY  | N-CA-C     | -7.40 | 97.26       | 111.02   |
| 3   | N     | 1116 | ASN  | N-CA-C     | -7.40 | 97.63       | 109.76   |
| 3   | N     | 1388 | ARG  | CA-C-N     | 7.39  | 130.05      | 120.44   |
| 3   | N     | 1388 | ARG  | C-N-CA     | 7.39  | 130.05      | 120.44   |
| 3   | D     | 1285 | GLU  | N-CA-C     | 7.39  | 122.33      | 113.16   |
| 2   | M     | 1118 | LYS  | CA-C-N     | 7.38  | 134.99      | 121.70   |
| 2   | M     | 1118 | LYS  | C-N-CA     | 7.38  | 134.99      | 121.70   |
| 3   | N     | 378  | ILE  | CA-C-O     | -7.37 | 111.56      | 120.78   |
| 3   | D     | 198  | ARG  | CA-C-N     | -7.37 | 108.75      | 122.60   |
| 3   | D     | 198  | ARG  | C-N-CA     | -7.37 | 108.75      | 122.60   |
| 2   | C     | 1118 | LYS  | CA-C-N     | 7.36  | 134.94      | 121.70   |
| 2   | C     | 1118 | LYS  | C-N-CA     | 7.36  | 134.94      | 121.70   |
| 3   | N     | 201  | GLY  | N-CA-C     | -7.32 | 97.40       | 111.02   |
| 4   | E     | 51   | LEU  | N-CA-C     | -7.32 | 97.92       | 107.73   |
| 3   | D     | 108  | VAL  | CA-C-N     | -7.30 | 111.25      | 120.23   |
| 3   | D     | 108  | VAL  | C-N-CA     | -7.30 | 111.25      | 120.23   |
| 3   | D     | 132  | TYR  | CA-CB-CG   | -7.30 | 100.77      | 113.90   |
| 3   | D     | 1110 | ALA  | N-CA-C     | -7.30 | 98.21       | 109.52   |
| 3   | D     | 682  | ASP  | CA-C-N     | -7.26 | 113.42      | 122.93   |
| 3   | D     | 682  | ASP  | C-N-CA     | -7.26 | 113.42      | 122.93   |
| 3   | D     | 1190 | SER  | N-CA-C     | 7.25  | 114.65      | 108.13   |
| 5   | F     | 75   | ILE  | CA-C-N     | 7.25  | 135.38      | 121.54   |
| 5   | F     | 75   | ILE  | C-N-CA     | 7.25  | 135.38      | 121.54   |
| 3   | N     | 378  | ILE  | O-C-N      | -7.24 | 113.52      | 122.57   |
| 2   | M     | 440  | PRO  | CA-C-N     | 7.24  | 129.82      | 120.56   |
| 2   | M     | 440  | PRO  | C-N-CA     | 7.24  | 129.82      | 120.56   |
| 3   | N     | 1127 | GLU  | N-CA-C     | -7.22 | 100.04      | 111.02   |
| 5   | F     | 376  | ILE  | N-CA-C     | 7.21  | 124.35      | 109.34   |
| 3   | N     | 1190 | SER  | N-CA-C     | 7.17  | 114.58      | 108.13   |
| 5   | F     | 377  | ASP  | CA-C-O     | -7.17 | 113.00      | 120.89   |
| 3   | D     | 198  | ARG  | N-CA-C     | 7.16  | 122.10      | 113.23   |
| 5   | F     | 350  | LEU  | CD1-CG-CD2 | -7.14 | 95.08       | 110.80   |
| 2   | C     | 163  | ILE  | CA-C-N     | 7.14  | 128.76      | 119.84   |
| 2   | C     | 163  | ILE  | C-N-CA     | 7.14  | 128.76      | 119.84   |
| 5   | F     | 419  | ARG  | CB-CA-C    | -7.14 | 99.39       | 110.81   |
| 3   | N     | 198  | ARG  | N-CA-C     | 7.14  | 122.08      | 113.23   |
| 1   | K     | 91   | ASN  | CA-C-N     | 7.13  | 128.76      | 119.84   |
| 1   | K     | 91   | ASN  | C-N-CA     | 7.13  | 128.76      | 119.84   |
| 3   | D     | 371  | ILE  | O-C-N      | -7.13 | 114.41      | 122.04   |
| 5   | F     | 363  | GLU  | N-CA-C     | 7.12  | 118.69      | 111.07   |
| 5   | F     | 419  | ARG  | CA-C-N     | -7.12 | 110.56      | 121.66   |
| 5   | F     | 419  | ARG  | C-N-CA     | -7.12 | 110.56      | 121.66   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | N     | 1109 | GLU  | N-CA-C   | 7.11  | 118.56      | 108.74   |
| 3   | D     | 603  | LEU  | CA-CB-CG | -7.11 | 91.41       | 116.30   |
| 3   | N     | 1285 | GLU  | N-CA-C   | 7.09  | 122.11      | 113.17   |
| 5   | P     | 296  | GLY  | CA-C-N   | 7.05  | 128.66      | 119.84   |
| 5   | P     | 296  | GLY  | C-N-CA   | 7.05  | 128.66      | 119.84   |
| 3   | N     | 199  | LEU  | CA-CB-CG | -7.05 | 91.64       | 116.30   |
| 3   | N     | 705  | ALA  | CA-C-N   | -7.04 | 111.03      | 119.84   |
| 3   | N     | 705  | ALA  | C-N-CA   | -7.04 | 111.03      | 119.84   |
| 2   | M     | 258  | TYR  | N-CA-C   | -7.04 | 104.68      | 113.20   |
| 2   | M     | 163  | ILE  | C-N-CD   | -7.04 | 96.14       | 125.00   |
| 5   | P     | 75   | ILE  | CA-C-N   | 7.02  | 134.95      | 121.54   |
| 5   | P     | 75   | ILE  | C-N-CA   | 7.02  | 134.95      | 121.54   |
| 2   | C     | 258  | TYR  | N-CA-C   | -7.00 | 104.72      | 113.20   |
| 3   | N     | 172  | PRO  | N-CA-C   | 6.98  | 119.22      | 110.70   |
| 5   | F     | 419  | ARG  | N-CA-CB  | 6.96  | 120.31      | 109.94   |
| 3   | N     | 406  | ASP  | N-CA-C   | 6.95  | 121.46      | 113.19   |
| 2   | C     | 263  | ASP  | CA-C-N   | 6.93  | 128.50      | 119.84   |
| 2   | C     | 263  | ASP  | C-N-CA   | 6.93  | 128.50      | 119.84   |
| 5   | P     | 283  | GLY  | N-CA-C   | -6.91 | 105.69      | 115.30   |
| 3   | D     | 164  | GLY  | CA-C-O   | -6.90 | 117.48      | 122.45   |
| 3   | D     | 172  | PRO  | N-CA-C   | 6.88  | 119.10      | 110.70   |
| 2   | C     | 163  | ILE  | C-N-CD   | -6.88 | 96.81       | 125.00   |
| 2   | C     | 56   | GLU  | CA-C-N   | -6.87 | 111.11      | 122.79   |
| 2   | C     | 56   | GLU  | C-N-CA   | -6.87 | 111.11      | 122.79   |
| 3   | D     | 1109 | GLU  | N-CA-C   | 6.86  | 118.21      | 108.74   |
| 1   | A     | 91   | ASN  | CA-C-N   | 6.84  | 128.40      | 119.84   |
| 1   | A     | 91   | ASN  | C-N-CA   | 6.84  | 128.40      | 119.84   |
| 3   | N     | 1477 | GLY  | N-CA-C   | -6.84 | 107.15      | 114.67   |
| 3   | N     | 244  | GLU  | CA-C-N   | -6.82 | 109.29      | 121.69   |
| 3   | N     | 244  | GLU  | C-N-CA   | -6.82 | 109.29      | 121.69   |
| 1   | L     | 90   | LEU  | N-CA-C   | 6.81  | 120.07      | 111.69   |
| 3   | N     | 1110 | ALA  | N-CA-C   | -6.81 | 98.74       | 109.50   |
| 2   | C     | 244  | PRO  | CA-N-CD  | -6.80 | 102.47      | 112.00   |
| 3   | N     | 682  | ASP  | CA-C-N   | -6.79 | 114.03      | 122.93   |
| 3   | N     | 682  | ASP  | C-N-CA   | -6.79 | 114.03      | 122.93   |
| 2   | C     | 52   | PHE  | CA-C-N   | -6.78 | 111.37      | 119.84   |
| 2   | C     | 52   | PHE  | C-N-CA   | -6.78 | 111.37      | 119.84   |
| 3   | N     | 198  | ARG  | CA-C-N   | -6.77 | 109.87      | 122.60   |
| 3   | N     | 198  | ARG  | C-N-CA   | -6.77 | 109.87      | 122.60   |
| 2   | M     | 15   | LEU  | CA-C-N   | -6.77 | 113.41      | 120.38   |
| 2   | M     | 15   | LEU  | C-N-CA   | -6.77 | 113.41      | 120.38   |
| 1   | B     | 90   | LEU  | N-CA-C   | 6.76  | 120.01      | 111.69   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | C     | 514  | VAL  | N-CA-C   | 6.75  | 118.29      | 109.58   |
| 3   | D     | 520  | LEU  | CA-C-N   | 6.75  | 127.33      | 120.38   |
| 3   | D     | 520  | LEU  | C-N-CA   | 6.75  | 127.33      | 120.38   |
| 3   | D     | 521  | PRO  | CA-C-N   | 6.75  | 128.28      | 119.84   |
| 3   | D     | 521  | PRO  | C-N-CA   | 6.75  | 128.28      | 119.84   |
| 1   | A     | 8    | ALA  | CA-C-N   | 6.74  | 128.26      | 119.84   |
| 1   | A     | 8    | ALA  | C-N-CA   | 6.74  | 128.26      | 119.84   |
| 3   | N     | 165  | LYS  | CA-C-N   | -6.74 | 112.42      | 122.39   |
| 3   | N     | 165  | LYS  | C-N-CA   | -6.74 | 112.42      | 122.39   |
| 2   | M     | 189  | ARG  | N-CA-C   | 6.72  | 120.43      | 110.48   |
| 3   | N     | 166  | GLN  | N-CA-C   | 6.72  | 119.42      | 108.26   |
| 4   | E     | 51   | LEU  | CA-C-N   | -6.72 | 111.91      | 122.73   |
| 4   | E     | 51   | LEU  | C-N-CA   | -6.72 | 111.91      | 122.73   |
| 3   | D     | 199  | LEU  | CA-CB-CG | -6.70 | 92.84       | 116.30   |
| 3   | D     | 165  | LYS  | CA-C-N   | -6.70 | 112.47      | 122.39   |
| 3   | D     | 165  | LYS  | C-N-CA   | -6.70 | 112.47      | 122.39   |
| 2   | M     | 9    | ILE  | N-CA-C   | -6.70 | 97.97       | 107.75   |
| 2   | C     | 223  | ASP  | N-CA-C   | 6.69  | 119.19      | 111.02   |
| 4   | O     | 51   | LEU  | CA-C-N   | -6.67 | 111.99      | 122.73   |
| 4   | O     | 51   | LEU  | C-N-CA   | -6.67 | 111.99      | 122.73   |
| 3   | D     | 1389 | LEU  | CA-C-N   | -6.65 | 111.62      | 122.26   |
| 3   | D     | 1389 | LEU  | C-N-CA   | -6.65 | 111.62      | 122.26   |
| 3   | N     | 387  | LEU  | CA-C-N   | 6.65  | 131.38      | 120.94   |
| 3   | N     | 387  | LEU  | C-N-CA   | 6.65  | 131.38      | 120.94   |
| 2   | M     | 591  | SER  | N-CA-C   | -6.64 | 102.24      | 110.41   |
| 3   | N     | 1242 | HIS  | CA-C-N   | 6.61  | 134.17      | 121.54   |
| 3   | N     | 1242 | HIS  | C-N-CA   | 6.61  | 134.17      | 121.54   |
| 1   | B     | 187  | GLY  | CA-C-N   | 6.58  | 129.09      | 120.28   |
| 1   | B     | 187  | GLY  | C-N-CA   | 6.58  | 129.09      | 120.28   |
| 3   | D     | 406  | ASP  | N-CA-C   | 6.58  | 121.16      | 113.20   |
| 1   | A     | 90   | LEU  | N-CA-C   | 6.55  | 118.50      | 111.36   |
| 3   | N     | 683  | ILE  | N-CA-C   | 6.55  | 117.27      | 107.51   |
| 2   | C     | 728  | HIS  | CA-C-O   | -6.55 | 112.44      | 119.97   |
| 3   | D     | 387  | LEU  | CA-C-O   | 6.52  | 129.84      | 120.51   |
| 5   | F     | 423  | ASP  | CA-CB-CG | 6.51  | 119.11      | 112.60   |
| 2   | C     | 178  | PRO  | N-CA-C   | 6.51  | 125.88      | 112.47   |
| 2   | M     | 792  | VAL  | CA-C-N   | 6.49  | 124.33      | 119.66   |
| 2   | M     | 792  | VAL  | C-N-CA   | 6.49  | 124.33      | 119.66   |
| 3   | D     | 166  | GLN  | N-CA-C   | 6.49  | 119.03      | 108.26   |
| 1   | K     | 48   | ILE  | CA-C-N   | 6.47  | 126.84      | 119.92   |
| 1   | K     | 48   | ILE  | C-N-CA   | 6.47  | 126.84      | 119.92   |
| 2   | C     | 118  | ILE  | CA-C-N   | 6.47  | 126.49      | 119.89   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | C     | 118  | ILE  | C-N-CA   | 6.47  | 126.49      | 119.89   |
| 2   | C     | 213  | ALA  | N-CA-C   | -6.46 | 103.47      | 112.45   |
| 5   | P     | 376  | ILE  | N-CA-C   | 6.45  | 122.76      | 109.34   |
| 3   | N     | 1389 | LEU  | CA-C-O   | -6.45 | 114.05      | 120.82   |
| 2   | M     | 16   | PRO  | CA-C-N   | -6.45 | 113.13      | 119.90   |
| 2   | M     | 16   | PRO  | C-N-CA   | -6.45 | 113.13      | 119.90   |
| 3   | N     | 520  | LEU  | CA-C-N   | 6.43  | 127.01      | 120.38   |
| 3   | N     | 520  | LEU  | C-N-CA   | 6.43  | 127.01      | 120.38   |
| 2   | M     | 608  | GLY  | N-CA-C   | -6.43 | 105.50      | 115.73   |
| 5   | F     | 423  | ASP  | CA-C-O   | 6.43  | 140.29      | 121.00   |
| 2   | C     | 399  | ASN  | CA-C-N   | 6.43  | 127.87      | 119.84   |
| 2   | C     | 399  | ASN  | C-N-CA   | 6.43  | 127.87      | 119.84   |
| 3   | N     | 233  | LYS  | CA-C-N   | 6.42  | 133.81      | 121.54   |
| 3   | N     | 233  | LYS  | C-N-CA   | 6.42  | 133.81      | 121.54   |
| 2   | M     | 57   | GLU  | N-CA-C   | 6.41  | 124.46      | 110.80   |
| 3   | N     | 771  | SER  | CA-C-N   | 6.41  | 126.54      | 119.87   |
| 3   | N     | 771  | SER  | C-N-CA   | 6.41  | 126.54      | 119.87   |
| 3   | N     | 372  | ASP  | O-C-N    | -6.40 | 116.53      | 121.14   |
| 3   | N     | 1209 | LEU  | CA-C-O   | -6.40 | 114.08      | 121.82   |
| 5   | P     | 340  | SER  | CA-C-N   | 6.40  | 127.84      | 119.84   |
| 5   | P     | 340  | SER  | C-N-CA   | 6.40  | 127.84      | 119.84   |
| 2   | C     | 9    | ILE  | N-CA-C   | -6.40 | 98.53       | 107.80   |
| 2   | M     | 213  | ALA  | N-CA-C   | -6.38 | 103.58      | 112.45   |
| 3   | D     | 683  | ILE  | N-CA-C   | 6.38  | 117.01      | 107.51   |
| 2   | M     | 243  | ARG  | C-N-CD   | -6.36 | 98.92       | 125.00   |
| 2   | C     | 165  | LEU  | CA-C-N   | 6.33  | 142.19      | 127.00   |
| 2   | C     | 165  | LEU  | C-N-CA   | 6.33  | 142.19      | 127.00   |
| 3   | N     | 1389 | LEU  | CA-C-N   | -6.33 | 112.13      | 122.26   |
| 3   | N     | 1389 | LEU  | C-N-CA   | -6.33 | 112.13      | 122.26   |
| 1   | K     | 90   | LEU  | N-CA-C   | 6.32  | 118.25      | 111.36   |
| 5   | F     | 283  | GLY  | N-CA-C   | -6.31 | 105.36      | 115.08   |
| 5   | F     | 361  | LEU  | CA-CB-CG | 6.31  | 138.40      | 116.30   |
| 3   | N     | 1288 | GLU  | N-CA-C   | 6.31  | 119.10      | 111.40   |
| 3   | D     | 619  | LEU  | N-CA-C   | -6.31 | 105.07      | 112.89   |
| 3   | D     | 1317 | ASP  | N-CA-C   | 6.31  | 119.41      | 110.14   |
| 2   | C     | 169  | GLY  | CA-C-N   | 6.29  | 127.70      | 119.84   |
| 2   | C     | 169  | GLY  | C-N-CA   | 6.29  | 127.70      | 119.84   |
| 2   | M     | 178  | PRO  | N-CA-C   | 6.29  | 125.42      | 112.47   |
| 2   | M     | 118  | ILE  | CA-C-N   | 6.26  | 126.28      | 119.89   |
| 2   | M     | 118  | ILE  | C-N-CA   | 6.26  | 126.28      | 119.89   |
| 5   | F     | 340  | SER  | CA-C-N   | 6.25  | 127.66      | 119.84   |
| 5   | F     | 340  | SER  | C-N-CA   | 6.25  | 127.66      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | L     | 91   | ASN  | N-CA-C     | 6.22  | 115.47      | 108.25   |
| 1   | K     | 91   | ASN  | N-CA-C     | 6.22  | 115.46      | 108.25   |
| 3   | N     | 192  | ALA  | CA-C-N     | -6.22 | 114.22      | 120.31   |
| 3   | N     | 192  | ALA  | C-N-CA     | -6.22 | 114.22      | 120.31   |
| 2   | M     | 761  | PHE  | CA-C-N     | 6.21  | 133.40      | 121.54   |
| 2   | M     | 761  | PHE  | C-N-CA     | 6.21  | 133.40      | 121.54   |
| 1   | A     | 187  | GLY  | N-CA-C     | 6.20  | 127.88      | 113.18   |
| 3   | N     | 142  | LEU  | N-CA-C     | 6.20  | 119.70      | 110.52   |
| 2   | M     | 728  | HIS  | CA-C-O     | -6.20 | 112.84      | 119.97   |
| 3   | N     | 1331 | ASP  | CA-C-N     | 6.20  | 127.59      | 119.84   |
| 3   | N     | 1331 | ASP  | C-N-CA     | 6.20  | 127.59      | 119.84   |
| 1   | A     | 105  | GLY  | CA-C-N     | 6.20  | 127.58      | 119.84   |
| 1   | A     | 105  | GLY  | C-N-CA     | 6.20  | 127.58      | 119.84   |
| 5   | F     | 410  | TYR  | CA-C-N     | -6.18 | 110.17      | 120.68   |
| 5   | F     | 410  | TYR  | C-N-CA     | -6.18 | 110.17      | 120.68   |
| 3   | D     | 132  | TYR  | CA-C-N     | 6.18  | 129.01      | 120.49   |
| 3   | D     | 132  | TYR  | C-N-CA     | 6.18  | 129.01      | 120.49   |
| 2   | C     | 57   | GLU  | N-CA-C     | 6.17  | 121.14      | 112.93   |
| 3   | D     | 1288 | GLU  | N-CA-C     | 6.17  | 117.88      | 111.03   |
| 1   | K     | 187  | GLY  | N-CA-C     | 6.17  | 127.79      | 113.18   |
| 2   | C     | 938  | LYS  | N-CA-C     | -6.14 | 104.67      | 111.36   |
| 5   | F     | 375  | LEU  | CD1-CG-CD2 | -6.13 | 97.31       | 110.80   |
| 3   | N     | 1091 | SER  | N-CA-C     | -6.10 | 104.94      | 112.38   |
| 3   | D     | 1087 | ARG  | CA-CB-CG   | -6.10 | 101.91      | 114.10   |
| 2   | M     | 242  | LEU  | CA-C-O     | -6.09 | 115.61      | 122.01   |
| 3   | N     | 53   | ILE  | CA-C-O     | 6.09  | 124.41      | 119.29   |
| 2   | M     | 86   | LYS  | N-CA-C     | -6.08 | 101.77      | 110.59   |
| 3   | N     | 164  | GLY  | N-CA-C     | -6.06 | 105.96      | 112.08   |
| 3   | N     | 186  | VAL  | N-CA-C     | 6.05  | 117.42      | 111.67   |
| 4   | O     | 50   | THR  | CA-C-N     | 6.05  | 132.98      | 122.32   |
| 4   | O     | 50   | THR  | C-N-CA     | 6.05  | 132.98      | 122.32   |
| 3   | D     | 10   | ILE  | CB-CA-C    | -6.05 | 103.28      | 111.15   |
| 1   | L     | 226  | SER  | N-CA-C     | 6.04  | 120.71      | 112.68   |
| 3   | N     | 38   | LYS  | CA-C-N     | 6.04  | 126.06      | 119.90   |
| 3   | N     | 38   | LYS  | C-N-CA     | 6.04  | 126.06      | 119.90   |
| 3   | D     | 592  | THR  | N-CA-C     | -6.03 | 102.57      | 110.53   |
| 3   | D     | 186  | VAL  | N-CA-C     | 6.03  | 117.40      | 111.67   |
| 2   | M     | 341  | THR  | CB-CA-C    | -6.03 | 101.42      | 110.88   |
| 3   | D     | 441  | ARG  | N-CA-C     | -6.02 | 101.61      | 110.52   |
| 3   | N     | 371  | ILE  | CA-C-O     | -6.02 | 114.24      | 119.29   |
| 2   | C     | 268  | ASP  | N-CA-C     | 6.01  | 119.26      | 109.59   |
| 2   | M     | 244  | PRO  | CA-N-CD    | -6.01 | 103.59      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | D     | 637  | LEU  | CA-CB-CG   | 6.00  | 137.29      | 116.30   |
| 5   | P     | 419  | ARG  | NH1-CZ-NH2 | -6.00 | 111.50      | 119.30   |
| 2   | M     | 417  | GLY  | N-CA-C     | -5.99 | 105.34      | 113.37   |
| 5   | P     | 401  | GLU  | CB-CG-CD   | 5.99  | 122.79      | 112.60   |
| 2   | C     | 1117 | SER  | CA-C-O     | -5.98 | 115.29      | 121.87   |
| 2   | M     | 795  | GLY  | N-CA-C     | -5.98 | 99.02       | 113.18   |
| 2   | C     | 243  | ARG  | N-CA-C     | 5.97  | 123.01      | 109.81   |
| 2   | M     | 768  | THR  | CA-C-N     | 5.97  | 126.13      | 119.32   |
| 2   | M     | 768  | THR  | C-N-CA     | 5.97  | 126.13      | 119.32   |
| 3   | N     | 408  | GLU  | N-CA-C     | -5.96 | 102.83      | 110.53   |
| 2   | C     | 463  | GLU  | CA-C-N     | -5.96 | 114.37      | 122.95   |
| 2   | C     | 463  | GLU  | C-N-CA     | -5.96 | 114.37      | 122.95   |
| 1   | K     | 186  | LEU  | N-CA-C     | -5.96 | 99.95       | 109.96   |
| 3   | N     | 387  | LEU  | CA-C-O     | 5.96  | 129.03      | 120.51   |
| 2   | M     | 728  | HIS  | CA-C-N     | -5.95 | 110.26      | 121.63   |
| 2   | M     | 728  | HIS  | C-N-CA     | -5.95 | 110.26      | 121.63   |
| 3   | N     | 592  | THR  | N-CA-C     | -5.94 | 102.69      | 110.53   |
| 2   | M     | 243  | ARG  | N-CA-C     | 5.94  | 122.94      | 109.81   |
| 5   | P     | 377  | ASP  | CA-C-O     | -5.93 | 114.36      | 120.89   |
| 2   | C     | 728  | HIS  | CA-C-N     | -5.92 | 110.31      | 121.63   |
| 2   | C     | 728  | HIS  | C-N-CA     | -5.92 | 110.31      | 121.63   |
| 5   | P     | 319  | THR  | CA-C-N     | -5.92 | 113.68      | 119.78   |
| 5   | P     | 319  | THR  | C-N-CA     | -5.92 | 113.68      | 119.78   |
| 2   | M     | 114  | PHE  | CA-CB-CG   | 5.92  | 119.72      | 113.80   |
| 2   | C     | 655  | LEU  | N-CA-C     | -5.91 | 106.19      | 113.41   |
| 3   | D     | 1388 | ARG  | CA-C-N     | 5.91  | 128.48      | 120.44   |
| 3   | D     | 1388 | ARG  | C-N-CA     | 5.91  | 128.48      | 120.44   |
| 5   | P     | 397  | ILE  | CB-CA-C    | -5.91 | 101.60      | 111.29   |
| 2   | M     | 246  | ASP  | CA-C-N     | 5.91  | 126.46      | 120.38   |
| 2   | M     | 246  | ASP  | C-N-CA     | 5.91  | 126.46      | 120.38   |
| 2   | C     | 291  | ALA  | N-CA-C     | 5.90  | 118.84      | 108.75   |
| 3   | N     | 1116 | ASN  | CA-C-N     | -5.90 | 112.92      | 122.36   |
| 3   | N     | 1116 | ASN  | C-N-CA     | -5.90 | 112.92      | 122.36   |
| 3   | N     | 724  | GLN  | N-CA-C     | 5.89  | 118.59      | 111.40   |
| 1   | B     | 91   | ASN  | N-CA-C     | 5.89  | 115.08      | 108.25   |
| 3   | D     | 806  | PHE  | N-CA-C     | 5.89  | 119.57      | 112.38   |
| 3   | N     | 1317 | ASP  | N-CA-C     | 5.89  | 119.18      | 110.46   |
| 5   | P     | 402  | ASN  | CA-C-N     | -5.89 | 111.55      | 122.09   |
| 5   | P     | 402  | ASN  | C-N-CA     | -5.89 | 111.55      | 122.09   |
| 2   | C     | 86   | LYS  | N-CA-C     | -5.88 | 102.06      | 110.59   |
| 3   | D     | 164  | GLY  | N-CA-C     | -5.88 | 106.04      | 112.04   |
| 3   | N     | 441  | ARG  | N-CA-C     | -5.88 | 101.82      | 110.52   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | D     | 38   | LYS  | CA-C-N  | 5.88  | 125.89      | 119.90   |
| 3   | D     | 38   | LYS  | C-N-CA  | 5.88  | 125.89      | 119.90   |
| 2   | M     | 165  | LEU  | CA-C-N  | 5.88  | 141.10      | 127.00   |
| 2   | M     | 165  | LEU  | C-N-CA  | 5.88  | 141.10      | 127.00   |
| 2   | C     | 15   | LEU  | CA-C-N  | -5.87 | 114.33      | 120.38   |
| 2   | C     | 15   | LEU  | C-N-CA  | -5.87 | 114.33      | 120.38   |
| 2   | C     | 535  | SER  | N-CA-C  | 5.87  | 113.41      | 108.13   |
| 3   | N     | 1208 | ASP  | N-CA-C  | 5.87  | 123.30      | 110.80   |
| 3   | N     | 1418 | LYS  | CA-C-N  | -5.86 | 113.72      | 119.76   |
| 3   | N     | 1418 | LYS  | C-N-CA  | -5.86 | 113.72      | 119.76   |
| 3   | N     | 34   | TYR  | N-CA-C  | 5.86  | 120.98      | 111.37   |
| 2   | C     | 189  | ARG  | N-CA-C  | 5.85  | 119.45      | 110.20   |
| 5   | F     | 397  | ILE  | CB-CA-C | -5.85 | 101.69      | 111.29   |
| 3   | D     | 388  | HIS  | CA-C-O  | 5.85  | 128.15      | 122.01   |
| 3   | D     | 233  | LYS  | CA-C-N  | 5.83  | 132.67      | 121.54   |
| 3   | D     | 233  | LYS  | C-N-CA  | 5.83  | 132.67      | 121.54   |
| 2   | C     | 761  | PHE  | CA-C-N  | 5.83  | 132.66      | 121.54   |
| 2   | C     | 761  | PHE  | C-N-CA  | 5.83  | 132.66      | 121.54   |
| 1   | A     | 7    | LYS  | N-CA-C  | -5.82 | 106.52      | 113.21   |
| 3   | N     | 1109 | GLU  | CA-C-N  | 5.82  | 131.70      | 122.62   |
| 3   | N     | 1109 | GLU  | C-N-CA  | 5.82  | 131.70      | 122.62   |
| 5   | F     | 148  | LYS  | N-CA-C  | 5.81  | 123.17      | 110.80   |
| 1   | L     | 91   | ASN  | CA-C-N  | 5.81  | 127.10      | 119.84   |
| 1   | L     | 91   | ASN  | C-N-CA  | 5.81  | 127.10      | 119.84   |
| 3   | N     | 132  | TYR  | CA-C-N  | 5.80  | 129.16      | 120.69   |
| 3   | N     | 132  | TYR  | C-N-CA  | 5.80  | 129.16      | 120.69   |
| 1   | K     | 105  | GLY  | CA-C-N  | 5.80  | 127.09      | 119.84   |
| 1   | K     | 105  | GLY  | C-N-CA  | 5.80  | 127.09      | 119.84   |
| 2   | M     | 319  | GLY  | CA-C-N  | -5.79 | 114.94      | 123.05   |
| 2   | M     | 319  | GLY  | C-N-CA  | -5.79 | 114.94      | 123.05   |
| 3   | D     | 1209 | LEU  | CA-C-O  | -5.79 | 114.35      | 121.88   |
| 5   | F     | 421  | PHE  | CB-CA-C | 5.79  | 118.10      | 110.06   |
| 1   | L     | 8    | ALA  | CA-C-N  | 5.79  | 127.07      | 119.84   |
| 1   | L     | 8    | ALA  | C-N-CA  | 5.79  | 127.07      | 119.84   |
| 2   | C     | 465  | GLY  | CA-C-N  | -5.78 | 115.08      | 122.77   |
| 2   | C     | 465  | GLY  | C-N-CA  | -5.78 | 115.08      | 122.77   |
| 5   | F     | 419  | ARG  | CA-C-O  | -5.78 | 114.71      | 120.90   |
| 3   | D     | 1109 | GLU  | CA-C-N  | 5.78  | 131.67      | 122.59   |
| 3   | D     | 1109 | GLU  | C-N-CA  | 5.78  | 131.67      | 122.59   |
| 2   | C     | 792  | VAL  | CA-C-N  | 5.75  | 123.80      | 119.66   |
| 2   | C     | 792  | VAL  | C-N-CA  | 5.75  | 123.80      | 119.66   |
| 3   | D     | 1116 | ASN  | CA-C-N  | -5.75 | 113.28      | 122.53   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | D     | 1116 | ASN  | C-N-CA    | -5.75 | 113.28      | 122.53   |
| 1   | B     | 185  | ARG  | N-CA-C    | 5.74  | 117.88      | 108.52   |
| 3   | N     | 240  | GLU  | CA-C-N    | 5.74  | 132.31      | 121.97   |
| 3   | N     | 240  | GLU  | C-N-CA    | 5.74  | 132.31      | 121.97   |
| 5   | P     | 148  | LYS  | N-CA-C    | 5.74  | 123.02      | 110.80   |
| 2   | M     | 465  | GLY  | CA-C-N    | -5.73 | 115.15      | 122.77   |
| 2   | M     | 465  | GLY  | C-N-CA    | -5.73 | 115.15      | 122.77   |
| 3   | D     | 371  | ILE  | CA-C-O    | -5.73 | 114.48      | 119.29   |
| 5   | F     | 409  | LYS  | CA-C-N    | -5.73 | 111.60      | 120.31   |
| 5   | F     | 409  | LYS  | C-N-CA    | -5.73 | 111.60      | 120.31   |
| 3   | D     | 1190 | SER  | CA-C-N    | 5.72  | 125.58      | 119.28   |
| 3   | D     | 1190 | SER  | C-N-CA    | 5.72  | 125.58      | 119.28   |
| 3   | N     | 564  | GLU  | N-CA-C    | 5.72  | 117.19      | 111.07   |
| 1   | A     | 91   | ASN  | N-CA-C    | 5.72  | 114.88      | 108.25   |
| 3   | D     | 171  | LEU  | CA-CB-CG  | 5.72  | 136.31      | 116.30   |
| 2   | M     | 367  | LEU  | N-CA-C    | 5.71  | 120.24      | 113.16   |
| 2   | M     | 291  | ALA  | N-CA-C    | 5.70  | 118.50      | 108.75   |
| 3   | D     | 175  | VAL  | CA-C-N    | -5.68 | 114.04      | 122.56   |
| 3   | D     | 175  | VAL  | C-N-CA    | -5.68 | 114.04      | 122.56   |
| 2   | M     | 514  | VAL  | N-CA-C    | 5.67  | 117.80      | 109.63   |
| 1   | B     | 91   | ASN  | CA-C-N    | 5.67  | 126.93      | 119.84   |
| 1   | B     | 91   | ASN  | C-N-CA    | 5.67  | 126.93      | 119.84   |
| 2   | M     | 264  | PRO  | CA-N-CD   | -5.67 | 104.07      | 112.00   |
| 3   | D     | 580  | ALA  | CA-C-N    | -5.66 | 111.27      | 120.72   |
| 3   | D     | 580  | ALA  | C-N-CA    | -5.66 | 111.27      | 120.72   |
| 1   | B     | 188  | GLN  | N-CA-C    | 5.66  | 117.45      | 111.28   |
| 4   | E     | 51   | LEU  | CA-C-O    | -5.65 | 115.06      | 120.94   |
| 5   | P     | 416  | ARG  | NE-CZ-NH1 | 5.64  | 127.14      | 121.50   |
| 3   | N     | 393  | ILE  | N-CA-CB   | 5.64  | 117.08      | 110.82   |
| 3   | N     | 232  | GLU  | CA-C-N    | 5.63  | 132.30      | 121.54   |
| 3   | N     | 232  | GLU  | C-N-CA    | 5.63  | 132.30      | 121.54   |
| 3   | N     | 1026 | SER  | N-CA-C    | -5.63 | 102.69      | 110.35   |
| 3   | N     | 1476 | THR  | N-CA-C    | -5.63 | 106.36      | 113.18   |
| 2   | C     | 75   | GLU  | CA-C-N    | 5.63  | 126.18      | 120.38   |
| 2   | C     | 75   | GLU  | C-N-CA    | 5.63  | 126.18      | 120.38   |
| 1   | K     | 8    | ALA  | CA-C-N    | 5.63  | 126.88      | 119.84   |
| 1   | K     | 8    | ALA  | C-N-CA    | 5.63  | 126.88      | 119.84   |
| 1   | K     | 30   | ARG  | N-CA-C    | 5.63  | 118.35      | 109.96   |
| 2   | C     | 242  | LEU  | CA-C-O    | -5.62 | 116.10      | 122.01   |
| 3   | N     | 213  | VAL  | CA-C-N    | -5.61 | 115.76      | 122.44   |
| 3   | N     | 213  | VAL  | C-N-CA    | -5.61 | 115.76      | 122.44   |
| 3   | N     | 1125 | PRO  | CA-C-N    | 5.61  | 132.26      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | N     | 1125 | PRO  | C-N-CA   | 5.61  | 132.26      | 121.54   |
| 3   | D     | 724  | GLN  | N-CA-C   | 5.61  | 118.24      | 111.40   |
| 5   | F     | 401  | GLU  | CB-CG-CD | 5.61  | 122.13      | 112.60   |
| 5   | P     | 203  | THR  | N-CA-C   | 5.60  | 117.25      | 111.03   |
| 3   | D     | 34   | TYR  | N-CA-C   | 5.60  | 120.55      | 111.37   |
| 3   | N     | 80   | VAL  | N-CA-C   | 5.59  | 120.96      | 109.34   |
| 1   | L     | 30   | ARG  | N-CA-C   | 5.58  | 118.67      | 110.30   |
| 3   | D     | 1114 | THR  | CA-C-N   | -5.58 | 114.64      | 123.12   |
| 3   | D     | 1114 | THR  | C-N-CA   | -5.58 | 114.64      | 123.12   |
| 2   | C     | 165  | LEU  | C-N-CD   | -5.57 | 108.35      | 120.60   |
| 2   | M     | 268  | ASP  | N-CA-C   | 5.57  | 118.55      | 109.59   |
| 2   | C     | 762  | LYS  | N-CA-C   | 5.56  | 122.64      | 110.80   |
| 3   | N     | 806  | PHE  | N-CA-C   | 5.55  | 119.16      | 112.38   |
| 3   | D     | 1414 | PRO  | CA-C-N   | -5.55 | 116.06      | 122.95   |
| 3   | D     | 1414 | PRO  | C-N-CA   | -5.55 | 116.06      | 122.95   |
| 3   | D     | 1125 | PRO  | N-CA-C   | 5.54  | 123.89      | 112.47   |
| 3   | D     | 22   | SER  | N-CA-C   | 5.54  | 118.63      | 110.59   |
| 3   | D     | 192  | ALA  | CA-C-N   | -5.53 | 114.89      | 120.31   |
| 3   | D     | 192  | ALA  | C-N-CA   | -5.53 | 114.89      | 120.31   |
| 2   | C     | 110  | GLU  | CA-C-N   | 5.53  | 132.10      | 121.54   |
| 2   | C     | 110  | GLU  | C-N-CA   | 5.53  | 132.10      | 121.54   |
| 5   | F     | 361  | LEU  | CB-CA-C  | -5.52 | 100.53      | 110.36   |
| 2   | M     | 938  | LYS  | N-CA-C   | -5.51 | 105.35      | 111.36   |
| 3   | N     | 376  | GLU  | CA-C-N   | 5.51  | 130.28      | 123.12   |
| 3   | N     | 376  | GLU  | C-N-CA   | 5.51  | 130.28      | 123.12   |
| 2   | C     | 367  | LEU  | N-CA-C   | 5.50  | 119.99      | 113.16   |
| 3   | D     | 379  | ALA  | CA-C-N   | 5.49  | 130.30      | 122.72   |
| 3   | D     | 379  | ALA  | C-N-CA   | 5.49  | 130.30      | 122.72   |
| 3   | D     | 863  | VAL  | CB-CA-C  | -5.49 | 105.30      | 111.23   |
| 2   | C     | 193  | LEU  | N-CA-C   | -5.49 | 105.68      | 112.38   |
| 2   | C     | 795  | GLY  | N-CA-C   | -5.49 | 100.18      | 113.18   |
| 3   | N     | 1124 | GLN  | C-N-CD   | -5.49 | 102.51      | 125.00   |
| 5   | F     | 287  | THR  | CA-C-O   | -5.48 | 115.58      | 121.56   |
| 5   | P     | 421  | PHE  | CA-CB-CG | -5.48 | 108.32      | 113.80   |
| 4   | E     | 50   | THR  | CA-C-N   | 5.48  | 132.76      | 122.84   |
| 4   | E     | 50   | THR  | C-N-CA   | 5.48  | 132.76      | 122.84   |
| 3   | N     | 1399 | ASP  | N-CA-C   | -5.48 | 105.85      | 112.54   |
| 2   | M     | 7    | GLY  | CA-C-N   | -5.48 | 115.06      | 122.95   |
| 2   | M     | 7    | GLY  | C-N-CA   | -5.48 | 115.06      | 122.95   |
| 2   | M     | 187  | ASN  | CA-C-N   | -5.46 | 112.03      | 120.88   |
| 2   | M     | 187  | ASN  | C-N-CA   | -5.46 | 112.03      | 120.88   |
| 2   | M     | 484  | VAL  | CB-CA-C  | -5.46 | 103.66      | 111.31   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | N     | 22   | SER  | N-CA-C   | 5.46  | 118.51      | 110.59   |
| 2   | M     | 762  | LYS  | N-CA-C   | 5.46  | 122.42      | 110.80   |
| 4   | O     | 51   | LEU  | CA-C-O   | -5.45 | 115.32      | 121.05   |
| 3   | D     | 603  | LEU  | N-CA-C   | 5.45  | 117.92      | 111.33   |
| 2   | M     | 282  | GLY  | CA-C-N   | -5.45 | 117.05      | 122.77   |
| 2   | M     | 282  | GLY  | C-N-CA   | -5.45 | 117.05      | 122.77   |
| 3   | N     | 73   | CYS  | N-CA-C   | 5.45  | 118.51      | 109.46   |
| 3   | N     | 1190 | SER  | CA-C-N   | 5.45  | 125.79      | 119.47   |
| 3   | N     | 1190 | SER  | C-N-CA   | 5.45  | 125.79      | 119.47   |
| 3   | D     | 240  | GLU  | CA-C-N   | 5.44  | 131.76      | 121.97   |
| 3   | D     | 240  | GLU  | C-N-CA   | 5.44  | 131.76      | 121.97   |
| 3   | N     | 639  | LEU  | CA-CB-CG | 5.44  | 135.34      | 116.30   |
| 3   | D     | 393  | ILE  | CB-CA-C  | -5.43 | 104.05      | 111.33   |
| 2   | M     | 114  | PHE  | CA-C-O   | 5.43  | 126.39      | 120.58   |
| 2   | M     | 655  | LEU  | N-CA-C   | -5.43 | 106.79      | 113.41   |
| 3   | N     | 1242 | HIS  | CB-CA-C  | 5.43  | 120.37      | 111.41   |
| 2   | C     | 7    | GLY  | CA-C-N   | -5.43 | 113.91      | 122.76   |
| 2   | C     | 7    | GLY  | C-N-CA   | -5.43 | 113.91      | 122.76   |
| 3   | N     | 829  | VAL  | CA-C-N   | -5.43 | 113.43      | 121.24   |
| 3   | N     | 829  | VAL  | C-N-CA   | -5.43 | 113.43      | 121.24   |
| 3   | N     | 98   | PRO  | CA-C-N   | 5.42  | 130.77      | 121.87   |
| 3   | N     | 98   | PRO  | C-N-CA   | 5.42  | 130.77      | 121.87   |
| 3   | D     | 1389 | LEU  | CA-C-O   | -5.42 | 115.12      | 120.70   |
| 3   | N     | 1243 | THR  | N-CA-C   | 5.42  | 122.33      | 110.80   |
| 3   | N     | 1267 | ARG  | CA-C-N   | -5.41 | 114.20      | 119.78   |
| 3   | N     | 1267 | ARG  | C-N-CA   | -5.41 | 114.20      | 119.78   |
| 3   | D     | 217  | LYS  | CA-C-O   | -5.41 | 112.77      | 120.51   |
| 2   | C     | 417  | GLY  | N-CA-C   | -5.40 | 105.77      | 113.86   |
| 2   | C     | 18   | LEU  | CA-CB-CG | -5.38 | 97.46       | 116.30   |
| 2   | C     | 282  | GLY  | CA-C-N   | -5.37 | 117.13      | 122.77   |
| 2   | C     | 282  | GLY  | C-N-CA   | -5.37 | 117.13      | 122.77   |
| 1   | K     | 226  | SER  | N-CA-C   | 5.37  | 119.53      | 111.96   |
| 1   | B     | 30   | ARG  | N-CA-C   | 5.37  | 118.35      | 110.30   |
| 3   | D     | 232  | GLU  | CA-C-N   | 5.36  | 131.78      | 121.54   |
| 3   | D     | 232  | GLU  | C-N-CA   | 5.36  | 131.78      | 121.54   |
| 5   | F     | 203  | THR  | N-CA-C   | 5.35  | 116.92      | 111.14   |
| 2   | M     | 506  | ASN  | N-CA-C   | -5.35 | 106.60      | 113.23   |
| 2   | M     | 1117 | SER  | CA-C-O   | -5.35 | 115.67      | 121.87   |
| 3   | N     | 199  | LEU  | CA-C-O   | -5.34 | 112.65      | 120.13   |
| 2   | C     | 16   | PRO  | CA-C-N   | -5.33 | 113.67      | 120.23   |
| 2   | C     | 16   | PRO  | C-N-CA   | -5.33 | 113.67      | 120.23   |
| 2   | M     | 249  | LYS  | N-CA-C   | 5.32  | 119.36      | 109.56   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | L     | 105  | GLY  | CA-C-N   | 5.32  | 126.49      | 119.84   |
| 1   | L     | 105  | GLY  | C-N-CA   | 5.32  | 126.49      | 119.84   |
| 3   | D     | 372  | ASP  | O-C-N    | -5.32 | 116.41      | 121.20   |
| 3   | N     | 1125 | PRO  | N-CA-C   | 5.32  | 123.43      | 112.47   |
| 1   | A     | 3    | ASP  | N-CA-C   | 5.31  | 122.11      | 110.80   |
| 2   | C     | 178  | PRO  | CA-C-N   | -5.31 | 111.11      | 120.99   |
| 2   | C     | 178  | PRO  | C-N-CA   | -5.31 | 111.11      | 120.99   |
| 1   | L     | 159  | LYS  | N-CA-C   | 5.31  | 117.24      | 108.49   |
| 1   | K     | 3    | ASP  | N-CA-C   | 5.30  | 122.10      | 110.80   |
| 2   | C     | 187  | ASN  | CA-C-N   | -5.30 | 112.29      | 120.88   |
| 2   | C     | 187  | ASN  | C-N-CA   | -5.30 | 112.29      | 120.88   |
| 3   | D     | 448  | GLU  | CA-C-N   | -5.30 | 113.50      | 122.67   |
| 3   | D     | 448  | GLU  | C-N-CA   | -5.30 | 113.50      | 122.67   |
| 5   | P     | 285  | GLU  | CA-C-N   | 5.30  | 126.47      | 119.84   |
| 5   | P     | 285  | GLU  | C-N-CA   | 5.30  | 126.47      | 119.84   |
| 1   | B     | 159  | LYS  | N-CA-C   | 5.30  | 117.23      | 108.49   |
| 3   | D     | 376  | GLU  | CA-C-N   | 5.30  | 130.01      | 123.12   |
| 3   | D     | 376  | GLU  | C-N-CA   | 5.30  | 130.01      | 123.12   |
| 1   | B     | 105  | GLY  | CA-C-N   | 5.29  | 126.45      | 119.84   |
| 1   | B     | 105  | GLY  | C-N-CA   | 5.29  | 126.45      | 119.84   |
| 1   | B     | 227  | ASN  | CA-C-N   | 5.28  | 126.44      | 119.84   |
| 1   | B     | 227  | ASN  | C-N-CA   | 5.28  | 126.44      | 119.84   |
| 3   | D     | 1043 | GLY  | CA-C-N   | -5.27 | 114.18      | 122.76   |
| 3   | D     | 1043 | GLY  | C-N-CA   | -5.27 | 114.18      | 122.76   |
| 3   | D     | 80   | VAL  | N-CA-C   | 5.26  | 120.29      | 109.34   |
| 1   | A     | 118  | ALA  | N-CA-C   | 5.26  | 117.44      | 111.02   |
| 2   | C     | 440  | PRO  | CA-C-N   | 5.26  | 128.97      | 120.55   |
| 2   | C     | 440  | PRO  | C-N-CA   | 5.26  | 128.97      | 120.55   |
| 5   | F     | 361  | LEU  | CA-C-N   | -5.26 | 113.17      | 122.74   |
| 5   | F     | 361  | LEU  | C-N-CA   | -5.26 | 113.17      | 122.74   |
| 2   | M     | 57   | GLU  | CA-C-N   | -5.26 | 113.06      | 121.58   |
| 2   | M     | 57   | GLU  | C-N-CA   | -5.26 | 113.06      | 121.58   |
| 3   | N     | 373  | PRO  | O-C-N    | -5.26 | 115.54      | 122.64   |
| 3   | N     | 211  | VAL  | N-CA-C   | 5.25  | 116.29      | 108.46   |
| 1   | A     | 159  | LYS  | N-CA-C   | 5.25  | 117.16      | 108.49   |
| 2   | C     | 269  | LEU  | CA-CB-CG | 5.25  | 134.66      | 116.30   |
| 3   | D     | 904  | VAL  | CB-CA-C  | -5.24 | 101.82      | 111.36   |
| 1   | K     | 159  | LYS  | N-CA-C   | 5.24  | 117.14      | 108.49   |
| 5   | P     | 393  | THR  | CA-C-N   | 5.24  | 128.08      | 120.79   |
| 5   | P     | 393  | THR  | C-N-CA   | 5.24  | 128.08      | 120.79   |
| 2   | M     | 879  | ARG  | CA-C-N   | -5.24 | 115.22      | 123.13   |
| 2   | M     | 879  | ARG  | C-N-CA   | -5.24 | 115.22      | 123.13   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5   | P     | 395  | GLU  | CA-C-O  | -5.24 | 114.18      | 120.10   |
| 2   | C     | 249  | LYS  | N-CA-C  | 5.23  | 119.19      | 109.56   |
| 5   | F     | 337  | HIS  | CB-CA-C | -5.23 | 99.70       | 110.38   |
| 2   | M     | 1110 | ASP  | N-CA-C  | 5.23  | 117.18      | 108.02   |
| 3   | N     | 810  | GLU  | N-CA-C  | -5.23 | 106.40      | 112.89   |
| 3   | D     | 810  | GLU  | N-CA-C  | -5.22 | 106.41      | 112.89   |
| 3   | D     | 1410 | GLU  | N-CA-C  | 5.22  | 118.05      | 110.17   |
| 1   | B     | 8    | ALA  | CA-C-N  | 5.21  | 126.36      | 119.84   |
| 1   | B     | 8    | ALA  | C-N-CA  | 5.21  | 126.36      | 119.84   |
| 1   | B     | 226  | SER  | N-CA-C  | 5.21  | 119.61      | 112.68   |
| 5   | F     | 213  | ILE  | CB-CA-C | -5.21 | 105.11      | 112.14   |
| 2   | C     | 319  | GLY  | CA-C-N  | -5.21 | 115.76      | 123.05   |
| 2   | C     | 319  | GLY  | C-N-CA  | -5.21 | 115.76      | 123.05   |
| 3   | D     | 213  | VAL  | CA-C-N  | -5.21 | 116.24      | 122.44   |
| 3   | D     | 213  | VAL  | C-N-CA  | -5.21 | 116.24      | 122.44   |
| 4   | E     | 45   | ARG  | CA-C-N  | 5.20  | 126.34      | 119.84   |
| 4   | E     | 45   | ARG  | C-N-CA  | 5.20  | 126.34      | 119.84   |
| 1   | A     | 30   | ARG  | N-CA-C  | 5.20  | 118.10      | 110.30   |
| 2   | C     | 611  | ILE  | CB-CA-C | -5.20 | 105.98      | 111.23   |
| 2   | M     | 441  | VAL  | N-CA-CB | -5.20 | 103.92      | 110.57   |
| 2   | C     | 73   | LEU  | CA-C-N  | -5.19 | 111.23      | 121.41   |
| 2   | C     | 73   | LEU  | C-N-CA  | -5.19 | 111.23      | 121.41   |
| 2   | C     | 421  | GLU  | N-CA-C  | 5.18  | 119.60      | 113.28   |
| 3   | D     | 218  | LYS  | CA-C-O  | -5.18 | 113.24      | 121.94   |
| 2   | C     | 246  | ASP  | CA-C-N  | 5.18  | 125.71      | 120.38   |
| 2   | C     | 246  | ASP  | C-N-CA  | 5.18  | 125.71      | 120.38   |
| 2   | C     | 793  | PRO  | CA-C-N  | -5.15 | 114.47      | 119.78   |
| 2   | C     | 793  | PRO  | C-N-CA  | -5.15 | 114.47      | 119.78   |
| 3   | D     | 79   | GLU  | CA-C-N  | -5.15 | 112.70      | 121.97   |
| 3   | D     | 79   | GLU  | C-N-CA  | -5.15 | 112.70      | 121.97   |
| 2   | M     | 39   | ARG  | N-CA-C  | 5.15  | 119.28      | 112.89   |
| 3   | D     | 562  | ALA  | N-CA-C  | 5.15  | 119.86      | 108.73   |
| 2   | M     | 730  | SER  | N-CA-C  | 5.15  | 116.90      | 109.07   |
| 3   | D     | 666  | ILE  | N-CA-C  | 5.15  | 116.49      | 110.62   |
| 3   | D     | 1411 | GLY  | N-CA-C  | -5.14 | 101.00      | 113.18   |
| 3   | N     | 9    | ARG  | N-CA-C  | 5.14  | 116.78      | 108.26   |
| 3   | D     | 1418 | LYS  | CA-C-N  | -5.13 | 114.47      | 119.76   |
| 3   | D     | 1418 | LYS  | C-N-CA  | -5.13 | 114.47      | 119.76   |
| 3   | N     | 588  | GLY  | CA-C-O  | -5.13 | 116.14      | 122.15   |
| 2   | M     | 697  | ARG  | CA-C-N  | -5.12 | 114.06      | 122.26   |
| 2   | M     | 697  | ARG  | C-N-CA  | -5.12 | 114.06      | 122.26   |
| 2   | M     | 165  | LEU  | C-N-CD  | -5.12 | 109.34      | 120.60   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | N     | 567  | ILE  | CB-CA-C | -5.12 | 105.31      | 112.02   |
| 2   | M     | 169  | GLY  | CA-C-N  | 5.12  | 126.23      | 119.84   |
| 2   | M     | 169  | GLY  | C-N-CA  | 5.12  | 126.23      | 119.84   |
| 5   | P     | 283  | GLY  | CA-C-O  | 5.12  | 125.37      | 119.13   |
| 3   | N     | 619  | LEU  | N-CA-C  | -5.11 | 106.55      | 112.89   |
| 3   | N     | 414  | ARG  | N-CA-C  | -5.11 | 102.90      | 110.46   |
| 3   | D     | 98   | PRO  | CA-C-N  | 5.11  | 130.25      | 121.87   |
| 3   | D     | 98   | PRO  | C-N-CA  | 5.11  | 130.25      | 121.87   |
| 3   | N     | 1410 | GLU  | N-CA-C  | 5.11  | 117.88      | 110.17   |
| 3   | D     | 380  | GLU  | CA-C-N  | -5.09 | 111.82      | 121.54   |
| 3   | D     | 380  | GLU  | C-N-CA  | -5.09 | 111.82      | 121.54   |
| 3   | D     | 73   | CYS  | N-CA-C  | 5.08  | 117.84      | 109.76   |
| 2   | M     | 181  | VAL  | N-CA-C  | 5.07  | 116.00      | 108.65   |
| 5   | P     | 412  | GLU  | CA-C-N  | 5.07  | 127.49      | 120.29   |
| 5   | P     | 412  | GLU  | C-N-CA  | 5.07  | 127.49      | 120.29   |
| 3   | D     | 564  | GLU  | N-CA-C  | 5.07  | 116.49      | 111.07   |
| 1   | B     | 3    | ASP  | N-CA-C  | 5.07  | 121.59      | 110.80   |
| 3   | D     | 107  | ASP  | CA-C-O  | -5.07 | 116.04      | 121.56   |
| 2   | C     | 1110 | ASP  | N-CA-C  | 5.06  | 116.88      | 108.02   |
| 5   | P     | 337  | HIS  | CB-CA-C | -5.06 | 100.06      | 110.38   |
| 2   | M     | 1104 | GLU  | N-CA-C  | -5.05 | 104.86      | 111.02   |
| 3   | N     | 107  | ASP  | CA-C-O  | -5.05 | 116.05      | 121.56   |
| 3   | D     | 1281 | VAL  | N-CA-C  | 5.05  | 116.80      | 108.97   |
| 2   | C     | 39   | ARG  | N-CA-C  | 5.05  | 119.15      | 112.89   |
| 1   | L     | 118  | ALA  | N-CA-C  | 5.05  | 117.17      | 111.11   |
| 3   | N     | 1165 | TYR  | CA-C-N  | -5.05 | 115.71      | 122.42   |
| 3   | N     | 1165 | TYR  | C-N-CA  | -5.05 | 115.71      | 122.42   |
| 5   | P     | 176  | ILE  | CB-CA-C | -5.04 | 105.44      | 112.04   |
| 3   | D     | 199  | LEU  | CA-C-O  | -5.04 | 113.08      | 120.13   |
| 1   | L     | 7    | LYS  | N-CA-C  | -5.04 | 107.16      | 113.15   |
| 3   | D     | 9    | ARG  | N-CA-C  | 5.03  | 116.78      | 108.13   |
| 5   | F     | 421  | PHE  | CA-C-N  | -5.03 | 111.89      | 121.94   |
| 5   | F     | 421  | PHE  | C-N-CA  | -5.03 | 111.89      | 121.94   |
| 5   | F     | 422  | LEU  | O-C-N   | 5.02  | 129.82      | 122.39   |
| 3   | D     | 829  | VAL  | CA-C-N  | -5.02 | 114.01      | 121.24   |
| 3   | D     | 829  | VAL  | C-N-CA  | -5.02 | 114.01      | 121.24   |
| 2   | C     | 114  | PHE  | CA-C-O  | 5.01  | 125.94      | 120.58   |
| 1   | A     | 226  | SER  | N-CA-C  | 5.01  | 119.34      | 112.68   |
| 5   | F     | 362  | SER  | CA-C-N  | 5.01  | 126.96      | 120.44   |
| 5   | F     | 362  | SER  | C-N-CA  | 5.01  | 126.96      | 120.44   |
| 2   | C     | 506  | ASN  | N-CA-C  | -5.01 | 107.17      | 113.28   |
| 3   | N     | 246  | PRO  | O-C-N   | -5.01 | 115.88      | 122.64   |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | D     | 132 | TYR  | Sidechain |
| 3   | D     | 379 | ALA  | Peptide   |
| 3   | D     | 380 | GLU  | Mainchain |
| 5   | F     | 421 | PHE  | Sidechain |
| 3   | N     | 132 | TYR  | Sidechain |
| 3   | N     | 379 | ALA  | Peptide   |
| 3   | N     | 380 | GLU  | Mainchain |

## 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     | 1806  | 0        | 1861     | 255     | 0            |
| 1   | B     | 1806  | 0        | 1861     | 218     | 0            |
| 1   | K     | 1806  | 0        | 1861     | 215     | 0            |
| 1   | L     | 1806  | 0        | 1861     | 213     | 0            |
| 2   | C     | 8829  | 0        | 8933     | 1337    | 0            |
| 2   | M     | 8829  | 0        | 8933     | 1310    | 0            |
| 3   | D     | 10801 | 0        | 10888    | 1589    | 0            |
| 3   | N     | 10801 | 0        | 10885    | 1588    | 0            |
| 4   | E     | 769   | 0        | 775      | 102     | 0            |
| 4   | O     | 769   | 0        | 775      | 111     | 0            |
| 5   | F     | 2771  | 0        | 2843     | 408     | 0            |
| 5   | P     | 2771  | 0        | 2844     | 435     | 0            |
| 6   | A     | 18    | 0        | 0        | 0       | 0            |
| 6   | B     | 24    | 0        | 0        | 0       | 0            |
| 6   | C     | 63    | 0        | 0        | 0       | 0            |
| 6   | D     | 118   | 0        | 0        | 1       | 0            |
| 6   | E     | 6     | 0        | 0        | 0       | 0            |
| 6   | F     | 31    | 0        | 0        | 0       | 0            |
| 6   | K     | 20    | 0        | 0        | 0       | 0            |
| 6   | L     | 19    | 0        | 0        | 0       | 0            |
| 6   | M     | 64    | 0        | 0        | 0       | 0            |
| 6   | N     | 92    | 0        | 0        | 0       | 0            |
| 6   | O     | 8     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | P     | 22    | 0        | 0        | 0       | 0            |
| 7   | D     | 2     | 0        | 0        | 0       | 0            |
| 7   | N     | 2     | 0        | 0        | 0       | 0            |
| 8   | A     | 194   | 0        | 0        | 46      | 0            |
| 8   | B     | 193   | 0        | 0        | 51      | 0            |
| 8   | C     | 869   | 0        | 0        | 256     | 0            |
| 8   | D     | 1163  | 0        | 0        | 330     | 0            |
| 8   | E     | 114   | 0        | 0        | 30      | 0            |
| 8   | F     | 381   | 0        | 0        | 67      | 0            |
| 8   | K     | 161   | 0        | 0        | 49      | 0            |
| 8   | L     | 157   | 0        | 0        | 53      | 0            |
| 8   | M     | 822   | 0        | 0        | 269     | 0            |
| 8   | N     | 983   | 0        | 0        | 293     | 0            |
| 8   | O     | 114   | 0        | 0        | 32      | 0            |
| 8   | P     | 325   | 0        | 0        | 75      | 0            |
| All | All   | 59529 | 0        | 54320    | 7258    | 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 67.

All (7258) 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) |
|-------------------|------------------|--------------------------|-------------------|
| 5:F:419:ARG:CB    | 5:F:419:ARG:CG   | 1.76                     | 1.60              |
| 5:P:401:GLU:CG    | 5:P:401:GLU:CB   | 1.76                     | 1.56              |
| 5:F:401:GLU:CB    | 5:F:401:GLU:CG   | 1.77                     | 1.55              |
| 3:N:218:LYS:CB    | 8:N:9902:HOH:O   | 1.85                     | 1.18              |
| 1:A:94:LEU:HD21   | 1:A:119:ASP:HB2  | 1.26                     | 1.16              |
| 5:F:358:LEU:HD11  | 5:F:370:LYS:HD2  | 1.28                     | 1.15              |
| 5:F:361:LEU:HD12  | 5:F:366:ALA:HB2  | 1.24                     | 1.15              |
| 1:B:94:LEU:HD21   | 1:B:119:ASP:HB2  | 1.29                     | 1.14              |
| 3:N:218:LYS:CB    | 3:N:372:ASP:O    | 1.94                     | 1.14              |
| 1:L:94:LEU:HD21   | 1:L:119:ASP:HB3  | 1.16                     | 1.11              |
| 1:L:1:MET:O       | 1:L:6:LEU:HB2    | 1.51                     | 1.10              |
| 2:M:1101:THR:HB   | 3:N:5:VAL:HG13   | 1.34                     | 1.08              |
| 2:M:328:LEU:HD13  | 2:M:433:THR:HB   | 1.36                     | 1.08              |
| 3:N:1045:MET:HG2  | 3:N:1073:SER:HA  | 1.32                     | 1.08              |
| 3:D:972:LEU:HG    | 3:D:976:GLN:NE2  | 1.69                     | 1.07              |
| 3:D:972:LEU:HG    | 3:D:976:GLN:HE22 | 0.94                     | 1.07              |
| 3:N:1258:ARG:HH21 | 3:N:1351:GLU:HG2 | 1.13                     | 1.06              |
| 1:B:1:MET:O       | 1:B:6:LEU:HB2    | 1.55                     | 1.06              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:1:MET:O       | 1:K:6:LEU:HB2    | 1.56                     | 1.06              |
| 3:N:616:GLN:HB2   | 5:P:326:ASP:HB2  | 1.36                     | 1.06              |
| 2:M:139:GLN:HE22  | 2:M:414:GLY:HA3  | 1.21                     | 1.05              |
| 5:P:76:SER:O      | 5:P:80:PRO:HD2   | 1.58                     | 1.04              |
| 3:N:137:PRO:HD2   | 3:N:453:ASP:HB3  | 1.38                     | 1.03              |
| 2:C:939:ARG:HB3   | 2:C:982:PRO:HG3  | 1.39                     | 1.03              |
| 5:P:402:ASN:O     | 5:P:406:ARG:HD2  | 1.58                     | 1.03              |
| 3:N:475:LYS:HA    | 3:N:478:LEU:HD12 | 1.41                     | 1.03              |
| 1:A:1:MET:O       | 1:A:6:LEU:HB2    | 1.60                     | 1.02              |
| 2:C:368:THR:HB    | 2:C:369:PRO:HD3  | 1.41                     | 1.02              |
| 3:N:87:ARG:O      | 3:N:521:PRO:HB3  | 1.59                     | 1.02              |
| 3:N:208:PRO:HB2   | 3:N:395:VAL:HG13 | 1.41                     | 1.02              |
| 3:D:370:ALA:HB1   | 6:D:9039:MG:MG   | 0.80                     | 1.01              |
| 3:D:87:ARG:O      | 3:D:521:PRO:HB3  | 1.60                     | 1.01              |
| 3:N:131:LYS:HG2   | 3:N:568:ARG:HG2  | 1.40                     | 1.01              |
| 5:P:394:ARG:H     | 5:P:394:ARG:HD2  | 1.22                     | 1.00              |
| 3:D:26:VAL:HG11   | 3:D:44:LEU:HD23  | 1.44                     | 1.00              |
| 3:N:434:ARG:HB2   | 3:N:447:VAL:HG22 | 1.44                     | 1.00              |
| 2:M:1055:LEU:HA   | 8:M:9570:HOH:O   | 1.62                     | 0.99              |
| 5:P:411:HIS:HA    | 5:P:414:ARG:HG3  | 1.41                     | 0.99              |
| 2:C:207:LEU:HD13  | 2:C:221:LEU:HD11 | 1.45                     | 0.99              |
| 1:B:50:GLY:HA3    | 1:B:171:PHE:O    | 1.62                     | 0.99              |
| 3:N:119:SER:HB2   | 3:N:123:LEU:HB2  | 1.42                     | 0.99              |
| 2:C:145:GLY:H     | 2:C:163:ILE:HG23 | 1.28                     | 0.99              |
| 5:P:416:ARG:HD3   | 5:P:419:ARG:HG3  | 1.44                     | 0.98              |
| 3:N:136:ASP:HB3   | 3:N:137:PRO:HD3  | 1.44                     | 0.98              |
| 3:D:148:GLU:HB3   | 3:D:151:GLN:HB2  | 1.45                     | 0.98              |
| 3:D:1033:GLN:HE21 | 3:D:1036:ARG:NH1 | 1.61                     | 0.98              |
| 2:M:516:ARG:HH11  | 2:M:521:PRO:HB3  | 1.28                     | 0.98              |
| 2:M:110:GLU:HG2   | 2:M:369:PRO:HG3  | 1.46                     | 0.97              |
| 2:M:1054:THR:HG21 | 2:M:1079:PRO:HB3 | 1.45                     | 0.97              |
| 1:A:180:GLN:NE2   | 2:C:934:PHE:HB2  | 1.78                     | 0.97              |
| 3:D:136:ASP:HB3   | 3:D:137:PRO:HD3  | 1.41                     | 0.97              |
| 3:D:197:SER:HB3   | 3:D:203:ALA:HB3  | 1.47                     | 0.97              |
| 3:D:972:LEU:CG    | 3:D:976:GLN:HE22 | 1.78                     | 0.97              |
| 1:K:35:THR:HB     | 8:K:1009:HOH:O   | 1.64                     | 0.97              |
| 1:K:54:THR:HG23   | 1:K:158:ILE:HG13 | 1.46                     | 0.97              |
| 5:F:420:ASP:O     | 5:F:422:LEU:HD23 | 1.63                     | 0.96              |
| 2:C:987:ILE:HG23  | 3:D:948:THR:HG21 | 1.44                     | 0.96              |
| 2:C:631:SER:HB3   | 2:C:637:LEU:HD21 | 1.48                     | 0.96              |
| 1:K:176:ARG:HD3   | 2:M:864:GLY:HA3  | 1.48                     | 0.96              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:181:VAL:O     | 2:C:937:ASP:HA    | 1.65                     | 0.96              |
| 2:C:770:GLU:HG2   | 3:D:65:ARG:HH22   | 1.26                     | 0.96              |
| 3:N:646:LYS:HA    | 3:N:720:LEU:HD22  | 1.45                     | 0.96              |
| 2:M:51:THR:HB     | 2:M:348:LEU:HD23  | 1.48                     | 0.95              |
| 3:D:1033:GLN:HE21 | 3:D:1036:ARG:HH11 | 0.99                     | 0.95              |
| 4:E:39:VAL:HB     | 4:E:72:ARG:HD2    | 1.44                     | 0.95              |
| 3:D:1310:ARG:HE   | 3:D:1327:ARG:HB3  | 1.29                     | 0.95              |
| 3:D:861:GLN:H     | 3:D:861:GLN:HE21  | 1.13                     | 0.95              |
| 3:N:197:SER:HB3   | 3:N:203:ALA:HB3   | 1.45                     | 0.95              |
| 5:P:94:LEU:HD13   | 5:P:96:LEU:H      | 1.28                     | 0.95              |
| 2:C:49:ARG:NH1    | 2:C:49:ARG:HB2    | 1.81                     | 0.95              |
| 3:D:699:VAL:H     | 3:D:756:GLN:HE22  | 0.98                     | 0.94              |
| 2:C:34:VAL:HB     | 2:C:38:LYS:HG3    | 1.47                     | 0.94              |
| 1:B:54:THR:HG23   | 1:B:158:ILE:HG13  | 1.47                     | 0.94              |
| 3:D:186:VAL:HG21  | 3:D:213:VAL:HB    | 1.48                     | 0.94              |
| 2:M:987:ILE:HG23  | 3:N:948:THR:HG21  | 1.50                     | 0.94              |
| 3:N:137:PRO:HD2   | 3:N:453:ASP:CB    | 1.98                     | 0.94              |
| 3:D:191:LEU:HB3   | 3:D:195:VAL:HG21  | 1.47                     | 0.94              |
| 3:N:1209:LEU:HD13 | 3:N:1216:SER:H    | 1.32                     | 0.94              |
| 3:N:1213:ARG:HB2  | 3:N:1214:PRO:HD2  | 1.49                     | 0.94              |
| 3:N:1389:LEU:H    | 3:N:1389:LEU:HD23 | 1.33                     | 0.94              |
| 3:N:425:GLY:HA3   | 5:P:135:ILE:HD13  | 1.49                     | 0.94              |
| 2:C:640:ARG:HH11  | 2:C:642:ARG:HH12  | 1.03                     | 0.93              |
| 2:C:461:VAL:HG13  | 2:C:465:GLY:HA2   | 1.48                     | 0.93              |
| 3:D:208:PRO:HB2   | 3:D:395:VAL:HG13  | 1.48                     | 0.93              |
| 3:D:126:VAL:HG13  | 3:D:132:TYR:HB2   | 1.51                     | 0.93              |
| 2:M:269:LEU:HA    | 2:M:288:ARG:HE    | 1.31                     | 0.93              |
| 2:M:274:ARG:HB2   | 2:M:288:ARG:HH12  | 1.32                     | 0.93              |
| 3:D:861:GLN:H     | 3:D:861:GLN:NE2   | 1.66                     | 0.93              |
| 2:M:461:VAL:HG13  | 2:M:465:GLY:HA2   | 1.50                     | 0.93              |
| 3:D:1232:PRO:HB3  | 3:D:1361:VAL:HG21 | 1.50                     | 0.93              |
| 3:D:424:GLY:HA2   | 3:D:436:GLU:HA    | 1.51                     | 0.92              |
| 2:M:572:ILE:HD11  | 2:M:701:THR:HB    | 1.51                     | 0.92              |
| 3:N:465:LEU:HD23  | 3:N:468:LEU:HD11  | 1.49                     | 0.92              |
| 3:D:65:ARG:HB2    | 5:F:375:LEU:HA    | 1.49                     | 0.92              |
| 3:D:145:VAL:HG22  | 3:D:146:PRO:HD2   | 1.49                     | 0.92              |
| 2:M:73:LEU:HB3    | 2:M:93:PRO:O      | 1.68                     | 0.92              |
| 5:P:358:LEU:HD21  | 5:P:370:LYS:HZ3   | 1.33                     | 0.92              |
| 5:P:369:LEU:HD11  | 5:P:401:GLU:HG3   | 1.50                     | 0.92              |
| 2:C:751:PRO:HB2   | 3:D:680:GLN:HG3   | 1.50                     | 0.92              |
| 2:M:100:LEU:HD23  | 2:M:372:LEU:HD11  | 1.49                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:161:LEU:O     | 3:N:449:SER:HB2   | 1.70                     | 0.92              |
| 2:M:1005:MET:HB3  | 8:N:9578:HOH:O    | 1.67                     | 0.92              |
| 3:N:861:GLN:HE21  | 3:N:861:GLN:H     | 0.94                     | 0.92              |
| 3:N:520:LEU:HD12  | 3:N:521:PRO:HD2   | 1.51                     | 0.92              |
| 2:C:1115:LEU:H    | 2:C:1115:LEU:HD12 | 1.35                     | 0.92              |
| 3:D:890:VAL:HG12  | 3:D:926:LYS:HG2   | 1.52                     | 0.92              |
| 3:N:1304:LYS:H    | 3:N:1304:LYS:HD3  | 1.35                     | 0.92              |
| 2:C:478:VAL:HG13  | 2:C:506:ASN:HB3   | 1.51                     | 0.92              |
| 3:N:784:ASP:HA    | 8:N:2330:HOH:O    | 1.69                     | 0.92              |
| 2:M:939:ARG:HB3   | 2:M:982:PRO:HG3   | 1.50                     | 0.91              |
| 3:N:138:LYS:H     | 3:N:138:LYS:HD2   | 1.35                     | 0.91              |
| 3:N:1090:ASP:HB3  | 3:N:1093:TYR:HB2  | 1.50                     | 0.91              |
| 3:D:1481:VAL:HG11 | 4:E:18:ARG:HA     | 1.49                     | 0.91              |
| 3:D:98:PRO:HG2    | 3:D:462:GLN:HE22  | 1.34                     | 0.91              |
| 3:D:101:HIS:CD2   | 3:D:582:LEU:HD13  | 2.05                     | 0.91              |
| 3:N:207:PHE:HB3   | 3:N:208:PRO:HD2   | 1.52                     | 0.91              |
| 1:L:12:THR:HG23   | 1:L:24:VAL:HB     | 1.49                     | 0.91              |
| 8:M:2268:HOH:O    | 5:P:342:VAL:HA    | 1.71                     | 0.91              |
| 5:P:413:SER:HA    | 5:P:419:ARG:HE    | 1.35                     | 0.91              |
| 2:M:328:LEU:H     | 2:M:433:THR:HG21  | 1.36                     | 0.91              |
| 2:M:130:ASN:HA    | 8:M:9667:HOH:O    | 1.70                     | 0.91              |
| 3:N:18:ILE:HG23   | 3:N:518:PRO:HG3   | 1.51                     | 0.91              |
| 3:N:422:ALA:H     | 3:N:427:VAL:HG11  | 1.36                     | 0.91              |
| 3:D:1304:LYS:H    | 3:D:1304:LYS:HD3  | 1.36                     | 0.91              |
| 3:N:422:ALA:HB1   | 5:P:178:ARG:HH12  | 1.34                     | 0.91              |
| 2:M:857:ASP:HB2   | 2:M:978:ARG:HG2   | 1.49                     | 0.91              |
| 5:P:416:ARG:HH11  | 5:P:419:ARG:HD2   | 1.34                     | 0.90              |
| 2:C:1095:LEU:HA   | 3:D:582:LEU:CD2   | 2.01                     | 0.90              |
| 2:M:145:GLY:H     | 2:M:163:ILE:HG23  | 1.36                     | 0.90              |
| 2:M:606:VAL:HG22  | 2:M:645:VAL:HG13  | 1.51                     | 0.90              |
| 2:C:436:GLY:HA2   | 2:C:538:GLN:O     | 1.71                     | 0.90              |
| 3:N:699:VAL:H     | 3:N:756:GLN:HE22  | 1.19                     | 0.90              |
| 3:N:1087:ARG:NH2  | 3:N:1256:LEU:HD22 | 1.85                     | 0.90              |
| 3:N:1376:MET:HE3  | 3:N:1421:LEU:HD13 | 1.54                     | 0.90              |
| 3:D:132:TYR:HA    | 8:D:9952:HOH:O    | 1.72                     | 0.90              |
| 5:F:76:SER:O      | 5:F:80:PRO:HD2    | 1.69                     | 0.90              |
| 2:M:108:ILE:HB    | 2:M:368:THR:OG1   | 1.70                     | 0.90              |
| 3:N:868:TYR:HD1   | 3:N:869:MET:H     | 1.16                     | 0.90              |
| 3:N:481:MET:HE3   | 3:N:493:ARG:HH21  | 1.36                     | 0.90              |
| 2:M:420:ARG:HD2   | 2:M:420:ARG:H     | 1.37                     | 0.90              |
| 2:M:66:LEU:HD22   | 2:M:372:LEU:HD13  | 1.54                     | 0.89              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1342:GLU:H    | 3:N:1342:GLU:CD  | 1.80                     | 0.89              |
| 1:L:108:GLU:HB3   | 1:L:128:HIS:HE1  | 1.36                     | 0.89              |
| 4:E:40:LEU:HB2    | 4:E:45:ARG:HD2   | 1.53                     | 0.89              |
| 3:N:424:GLY:HA2   | 3:N:436:GLU:HA   | 1.52                     | 0.89              |
| 5:P:135:ILE:HD11  | 5:P:178:ARG:HB3  | 1.52                     | 0.89              |
| 2:M:1015:LEU:HA   | 5:P:335:ASP:HB3  | 1.55                     | 0.89              |
| 2:C:585:GLU:HB3   | 8:C:9492:HOH:O   | 1.72                     | 0.89              |
| 2:M:478:VAL:HG13  | 2:M:506:ASN:HB3  | 1.55                     | 0.89              |
| 2:C:1005:MET:HE1  | 3:D:645:PRO:HG2  | 1.53                     | 0.88              |
| 2:C:140:ILE:HG23  | 2:C:333:ILE:HD12 | 1.53                     | 0.88              |
| 5:F:278:LEU:HD13  | 5:F:290:GLU:HB3  | 1.50                     | 0.88              |
| 3:D:1045:MET:HG2  | 3:D:1073:SER:HA  | 1.55                     | 0.88              |
| 3:D:136:ASP:HB3   | 3:D:137:PRO:CD   | 2.02                     | 0.88              |
| 2:M:73:LEU:HD23   | 2:M:94:LEU:HB2   | 1.55                     | 0.88              |
| 4:O:51:LEU:HG     | 4:O:53:GLY:H     | 1.38                     | 0.88              |
| 3:N:799:LYS:HA    | 8:N:2140:HOH:O   | 1.71                     | 0.88              |
| 2:C:1111:ILE:HG13 | 2:C:1112:PHE:H   | 1.38                     | 0.88              |
| 3:N:565:ILE:H     | 3:N:565:ILE:HD12 | 1.36                     | 0.88              |
| 3:N:984:THR:HG22  | 3:N:987:GLU:HG3  | 1.52                     | 0.88              |
| 3:D:462:GLN:HG3   | 3:D:513:ILE:HD13 | 1.56                     | 0.88              |
| 3:N:1481:VAL:HG11 | 4:O:18:ARG:HA    | 1.53                     | 0.88              |
| 2:C:15:LEU:HD22   | 2:C:15:LEU:H     | 1.39                     | 0.88              |
| 2:C:100:LEU:HG    | 2:C:368:THR:HG23 | 1.56                     | 0.88              |
| 1:K:86:VAL:HG12   | 1:K:124:ASN:HD22 | 1.38                     | 0.88              |
| 3:D:569:ASN:HD21  | 5:F:210:LEU:HD22 | 1.38                     | 0.87              |
| 3:N:556:LYS:HA    | 8:N:9490:HOH:O   | 1.72                     | 0.87              |
| 1:B:133:GLU:HG3   | 1:B:134:GLU:H    | 1.38                     | 0.87              |
| 3:D:118:LEU:HB3   | 3:D:123:LEU:HD22 | 1.56                     | 0.87              |
| 3:D:119:SER:HB2   | 3:D:123:LEU:H    | 1.37                     | 0.87              |
| 3:N:39:PRO:HB3    | 3:N:45:PHE:O     | 1.75                     | 0.87              |
| 3:N:126:VAL:HG13  | 3:N:132:TYR:HB2  | 1.57                     | 0.87              |
| 3:N:197:SER:HB2   | 3:N:205:TYR:CE1  | 2.08                     | 0.87              |
| 3:N:704:ARG:HG3   | 8:N:9496:HOH:O   | 1.74                     | 0.87              |
| 3:N:1385:GLY:HA2  | 8:N:9997:HOH:O   | 1.73                     | 0.87              |
| 2:C:586:ARG:HD3   | 2:C:590:ASP:OD2  | 1.75                     | 0.87              |
| 3:D:1394:VAL:HB   | 3:D:1397:LYS:HG3 | 1.56                     | 0.87              |
| 3:N:481:MET:SD    | 3:N:1388:ARG:HG2 | 2.14                     | 0.87              |
| 3:N:616:GLN:O     | 3:N:619:LEU:HB3  | 1.75                     | 0.87              |
| 2:C:413:LEU:H     | 2:C:413:LEU:HD12 | 1.40                     | 0.87              |
| 2:M:432:ARG:HH12  | 3:N:1047:LYS:HE2 | 1.35                     | 0.87              |
| 2:C:650:ARG:H     | 2:C:650:ARG:HD3  | 1.39                     | 0.87              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:1052:MET:HE3  | 3:D:623:VAL:HG21 | 1.56                     | 0.87              |
| 3:N:430:ASP:HB2   | 3:N:432:TYR:CE2  | 2.09                     | 0.87              |
| 3:N:483:HIS:HB2   | 3:N:484:PRO:HD3  | 1.56                     | 0.87              |
| 1:B:132:LEU:HD21  | 1:B:138:LEU:HD22 | 1.57                     | 0.87              |
| 2:M:577:PRO:HA    | 2:M:671:ASN:HD21 | 1.39                     | 0.87              |
| 1:K:143:ARG:HH11  | 1:K:143:ARG:HG3  | 1.40                     | 0.87              |
| 1:A:5:LYS:HA      | 1:A:5:LYS:HE3    | 1.56                     | 0.86              |
| 3:D:422:ALA:HB3   | 3:D:427:VAL:HG22 | 1.54                     | 0.86              |
| 3:N:994:GLN:HG3   | 8:N:2307:HOH:O   | 1.73                     | 0.86              |
| 3:D:101:HIS:HD2   | 3:D:582:LEU:HD13 | 1.41                     | 0.86              |
| 3:D:141:ILE:HD13  | 3:D:449:SER:HA   | 1.57                     | 0.86              |
| 2:M:430:VAL:HG23  | 3:N:1078:ARG:CZ  | 2.05                     | 0.86              |
| 3:N:1045:MET:CG   | 3:N:1073:SER:HA  | 2.05                     | 0.86              |
| 4:O:40:LEU:HD21   | 4:O:67:GLU:HA    | 1.57                     | 0.86              |
| 2:C:1102:LEU:HD13 | 3:D:9:ARG:HB3    | 1.55                     | 0.86              |
| 3:D:547:LEU:HD22  | 3:D:581:LEU:HD21 | 1.56                     | 0.86              |
| 3:N:148:GLU:HB3   | 3:N:151:GLN:HB2  | 1.58                     | 0.86              |
| 5:P:420:ASP:O     | 5:P:422:LEU:HD23 | 1.74                     | 0.86              |
| 2:C:36:PRO:HG2    | 2:C:70:GLU:HB3   | 1.56                     | 0.86              |
| 3:N:191:LEU:HB3   | 3:N:195:VAL:HG21 | 1.56                     | 0.86              |
| 2:C:487:THR:HG22  | 2:C:489:THR:H    | 1.38                     | 0.86              |
| 3:D:39:PRO:HB3    | 3:D:45:PHE:O     | 1.75                     | 0.86              |
| 3:N:1109:GLU:HG2  | 3:N:1202:GLN:H   | 1.39                     | 0.86              |
| 1:B:86:VAL:HG12   | 1:B:124:ASN:HD22 | 1.38                     | 0.86              |
| 3:D:1194:CYS:HB3  | 3:D:1373:ARG:NH2 | 1.90                     | 0.86              |
| 1:L:101:LEU:HD22  | 1:L:140:MET:HE1  | 1.57                     | 0.86              |
| 2:M:81:ASP:HA     | 8:M:9757:HOH:O   | 1.74                     | 0.86              |
| 2:C:420:ARG:H     | 2:C:420:ARG:HD2  | 1.40                     | 0.86              |
| 3:D:1026:SER:HA   | 8:D:2030:HOH:O   | 1.76                     | 0.86              |
| 2:C:383:ARG:HB2   | 2:C:383:ARG:HH11 | 1.40                     | 0.85              |
| 1:L:54:THR:HG23   | 1:L:158:ILE:HG13 | 1.57                     | 0.85              |
| 2:M:20:GLU:HG3    | 8:M:9519:HOH:O   | 1.76                     | 0.85              |
| 2:M:260:LEU:HA    | 2:M:291:ALA:CB   | 2.06                     | 0.85              |
| 1:A:180:GLN:HE22  | 2:C:934:PHE:HB2  | 1.39                     | 0.85              |
| 2:C:263:ASP:HB2   | 2:C:264:PRO:HD3  | 1.56                     | 0.85              |
| 2:C:517:ARG:HH21  | 2:C:524:VAL:HG23 | 1.39                     | 0.85              |
| 2:C:734:LEU:HD13  | 2:C:737:LEU:HD13 | 1.58                     | 0.85              |
| 3:N:52:PRO:HG2    | 8:N:9939:HOH:O   | 1.76                     | 0.85              |
| 3:N:422:ALA:HB1   | 5:P:178:ARG:NH1  | 1.90                     | 0.85              |
| 2:C:492:ASP:HA    | 2:C:518:LYS:HB3  | 1.57                     | 0.85              |
| 2:C:516:ARG:HD3   | 2:C:521:PRO:HA   | 1.58                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:94:LEU:HD13   | 5:F:96:LEU:H      | 1.39                     | 0.85              |
| 2:C:210:GLU:HG3   | 8:C:9693:HOH:O    | 1.75                     | 0.85              |
| 2:C:260:LEU:HA    | 2:C:291:ALA:CB    | 2.06                     | 0.85              |
| 5:P:408:LEU:O     | 5:P:412:GLU:HG2   | 1.75                     | 0.85              |
| 2:C:941:VAL:HA    | 2:C:944:LEU:HD12  | 1.55                     | 0.85              |
| 2:M:170:PRO:HD2   | 2:M:263:ASP:HB3   | 1.55                     | 0.85              |
| 4:O:39:VAL:HB     | 4:O:72:ARG:HD2    | 1.55                     | 0.85              |
| 2:C:519:GLY:HA3   | 8:C:9911:HOH:O    | 1.77                     | 0.85              |
| 3:D:64:LYS:HG2    | 8:D:9558:HOH:O    | 1.76                     | 0.85              |
| 3:D:139:GLY:HA3   | 3:D:452:ILE:HD12  | 1.58                     | 0.85              |
| 3:D:543:LEU:HD22  | 3:D:580:ALA:HB1   | 1.57                     | 0.85              |
| 5:F:408:LEU:O     | 5:F:412:GLU:HG2   | 1.76                     | 0.85              |
| 3:N:197:SER:HB2   | 3:N:205:TYR:HE1   | 1.40                     | 0.85              |
| 3:N:422:ALA:HB3   | 3:N:427:VAL:HG22  | 1.59                     | 0.85              |
| 3:N:890:VAL:HG12  | 3:N:926:LYS:HG2   | 1.57                     | 0.85              |
| 3:D:1033:GLN:NE2  | 3:D:1036:ARG:HH11 | 1.74                     | 0.85              |
| 4:E:51:LEU:HG     | 4:E:53:GLY:H      | 1.40                     | 0.85              |
| 1:K:193:ASP:HA    | 2:M:938:LYS:HZ3   | 1.42                     | 0.85              |
| 3:D:834:THR:HG22  | 3:D:838:ARG:HE    | 1.39                     | 0.84              |
| 2:M:396:ASP:HA    | 2:M:633:GLN:HE22  | 1.42                     | 0.84              |
| 3:N:32:ILE:HD12   | 3:N:527:MET:HG2   | 1.56                     | 0.84              |
| 2:C:100:LEU:HD21  | 2:C:368:THR:HA    | 1.57                     | 0.84              |
| 3:D:1389:LEU:HD23 | 3:D:1389:LEU:H    | 1.43                     | 0.84              |
| 5:P:416:ARG:NH1   | 5:P:419:ARG:HD2   | 1.92                     | 0.84              |
| 2:C:537:LYS:HA    | 2:C:545:ASN:HD21  | 1.40                     | 0.84              |
| 5:F:291:ILE:HG23  | 5:F:304:VAL:HG21  | 1.59                     | 0.84              |
| 2:M:140:ILE:HG13  | 8:M:2237:HOH:O    | 1.77                     | 0.84              |
| 2:M:1095:LEU:HA   | 8:M:9921:HOH:O    | 1.77                     | 0.84              |
| 3:N:171:LEU:HB3   | 3:N:390:PRO:HA    | 1.59                     | 0.84              |
| 2:C:1115:LEU:HB3  | 3:D:85:VAL:HG12   | 1.59                     | 0.84              |
| 3:D:865:THR:HG22  | 8:D:2489:HOH:O    | 1.75                     | 0.84              |
| 5:F:148:LYS:O     | 5:F:148:LYS:HD2   | 1.78                     | 0.84              |
| 2:M:34:VAL:HB     | 2:M:38:LYS:HG3    | 1.59                     | 0.84              |
| 5:P:166:LEU:HB3   | 5:P:170:HIS:HB2   | 1.58                     | 0.84              |
| 2:C:904:PRO:HB2   | 2:C:907:ASP:O     | 1.78                     | 0.84              |
| 3:D:808:THR:HB    | 3:D:809:PRO:HD3   | 1.58                     | 0.84              |
| 1:K:222:LEU:HD12  | 1:L:215:VAL:HB    | 1.57                     | 0.84              |
| 3:N:1389:LEU:H    | 3:N:1389:LEU:CD2  | 1.91                     | 0.84              |
| 2:C:857:ASP:HB2   | 2:C:978:ARG:HG2   | 1.58                     | 0.84              |
| 3:D:1097:LYS:O    | 3:D:1101:VAL:HG23 | 1.78                     | 0.84              |
| 5:P:141:VAL:O     | 5:P:145:PRO:HD2   | 1.76                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:219:ARG:HH12  | 1:B:219:ARG:HD2   | 1.40                     | 0.83              |
| 3:N:783:ARG:HB2   | 8:N:9557:HOH:O    | 1.78                     | 0.83              |
| 3:N:836:VAL:HA    | 3:N:839:LEU:HD12  | 1.60                     | 0.83              |
| 2:C:206:THR:HA    | 8:C:9693:HOH:O    | 1.78                     | 0.83              |
| 3:D:219:GLU:O     | 3:D:370:ALA:CB    | 2.26                     | 0.83              |
| 2:M:442:GLU:HG2   | 2:M:454:SER:HB2   | 1.59                     | 0.83              |
| 3:N:810:GLU:O     | 3:N:813:LEU:HG    | 1.78                     | 0.83              |
| 1:B:46:SER:O      | 1:B:148:VAL:HB    | 1.78                     | 0.83              |
| 3:D:836:VAL:HA    | 3:D:839:LEU:HD12  | 1.60                     | 0.83              |
| 2:M:64:LEU:HB2    | 2:M:359:MET:HE3   | 1.61                     | 0.83              |
| 5:F:407:LYS:HB3   | 8:F:9529:HOH:O    | 1.78                     | 0.83              |
| 2:M:1115:LEU:HB3  | 3:N:85:VAL:HG12   | 1.57                     | 0.83              |
| 4:O:23:VAL:HG22   | 8:O:3627:HOH:O    | 1.78                     | 0.83              |
| 2:C:710:ILE:HB    | 2:C:790:LEU:HD22  | 1.60                     | 0.83              |
| 1:L:86:VAL:HG12   | 1:L:124:ASN:HD22  | 1.42                     | 0.83              |
| 2:M:41:ASN:HA     | 8:M:9520:HOH:O    | 1.77                     | 0.83              |
| 1:B:153:ALA:HA    | 1:B:156:HIS:NE2   | 1.94                     | 0.83              |
| 2:C:64:LEU:HD13   | 2:C:359:MET:HE3   | 1.61                     | 0.83              |
| 2:C:620:LEU:HA    | 8:C:9571:HOH:O    | 1.77                     | 0.83              |
| 3:D:561:GLY:HA3   | 5:F:184:ARG:NH2   | 1.94                     | 0.83              |
| 5:P:411:HIS:HA    | 5:P:414:ARG:CG    | 2.09                     | 0.83              |
| 1:A:138:LEU:HD11  | 1:A:140:MET:HE2   | 1.61                     | 0.83              |
| 2:C:536:PRO:HB3   | 2:C:906:PHE:HD1   | 1.41                     | 0.83              |
| 2:C:710:ILE:HD12  | 2:C:790:LEU:HB2   | 1.61                     | 0.83              |
| 2:M:1092:LEU:HD23 | 2:M:1099:VAL:HG11 | 1.59                     | 0.83              |
| 3:N:149:LYS:HD3   | 3:N:149:LYS:H     | 1.43                     | 0.83              |
| 2:C:52:PHE:HB3    | 8:C:9488:HOH:O    | 1.78                     | 0.83              |
| 5:F:93:LEU:HD22   | 5:F:98:GLU:HB3    | 1.59                     | 0.83              |
| 2:M:95:TYR:CD2    | 2:M:114:PHE:HB3   | 2.12                     | 0.83              |
| 2:M:462:ASP:CG    | 2:M:463:GLU:H     | 1.87                     | 0.83              |
| 3:N:1348:LEU:HG   | 3:N:1375:MET:HE1  | 1.61                     | 0.83              |
| 5:P:392:VAL:HG22  | 8:P:9742:HOH:O    | 1.78                     | 0.83              |
| 2:C:443:THR:HG21  | 2:C:450:GLY:H     | 1.41                     | 0.83              |
| 2:C:690:ILE:HB    | 2:C:852:ILE:HD13  | 1.60                     | 0.83              |
| 3:N:170:PRO:O     | 3:N:391:ALA:HB3   | 1.79                     | 0.83              |
| 3:N:583:ASP:OD1   | 3:N:604:THR:HB    | 1.78                     | 0.83              |
| 5:P:369:LEU:CD1   | 5:P:401:GLU:HG3   | 2.09                     | 0.83              |
| 2:C:89:THR:HA     | 2:C:129:ILE:O     | 1.79                     | 0.82              |
| 3:N:45:PHE:HD1    | 3:N:86:ARG:HH22   | 1.26                     | 0.82              |
| 1:A:86:VAL:HG12   | 1:A:124:ASN:HD22  | 1.43                     | 0.82              |
| 3:D:36:THR:HB     | 8:D:9731:HOH:O    | 1.79                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1075:HIS:HA   | 8:N:9591:HOH:O    | 1.79                     | 0.82              |
| 1:A:30:ARG:HH12   | 1:B:155:LYS:HZ1   | 1.25                     | 0.82              |
| 2:C:170:PRO:HB3   | 2:C:186:VAL:HG12  | 1.60                     | 0.82              |
| 2:C:1107:ASN:HB3  | 8:C:2039:HOH:O    | 1.78                     | 0.82              |
| 1:K:18:ARG:O      | 1:K:207:PRO:HD3   | 1.79                     | 0.82              |
| 2:C:139:GLN:HB3   | 2:C:334:ARG:HG3   | 1.61                     | 0.82              |
| 2:C:288:ARG:HB3   | 8:C:2156:HOH:O    | 1.80                     | 0.82              |
| 3:N:391:ALA:HB1   | 8:N:2275:HOH:O    | 1.80                     | 0.82              |
| 3:D:1146:GLY:HA3  | 3:D:1207:TYR:HB2  | 1.60                     | 0.82              |
| 5:F:369:LEU:HD11  | 5:F:401:GLU:HG3   | 1.61                     | 0.82              |
| 2:M:711:GLU:HG2   | 2:M:822:VAL:HG12  | 1.59                     | 0.82              |
| 3:D:18:ILE:HG23   | 3:D:518:PRO:HG3   | 1.61                     | 0.82              |
| 3:D:210:ARG:HD2   | 3:D:398:ALA:HB3   | 1.59                     | 0.82              |
| 2:C:56:GLU:HB2    | 2:C:64:LEU:HD23   | 1.59                     | 0.82              |
| 2:C:458:TYR:HB3   | 2:C:470:PRO:HG2   | 1.62                     | 0.82              |
| 3:D:561:GLY:HA3   | 5:F:184:ARG:HH22  | 1.43                     | 0.82              |
| 3:N:988:ARG:NH1   | 3:N:992:ILE:HD11  | 1.95                     | 0.82              |
| 1:B:190:THR:HA    | 8:B:9553:HOH:O    | 1.78                     | 0.82              |
| 2:C:1076:VAL:HG22 | 3:D:752:SER:HB3   | 1.59                     | 0.82              |
| 3:D:131:LYS:HA    | 3:D:456:MET:HG3   | 1.62                     | 0.82              |
| 2:M:715:THR:HG22  | 2:M:717:LEU:H     | 1.42                     | 0.82              |
| 3:N:387:LEU:CB    | 5:P:94:LEU:HD11   | 2.09                     | 0.82              |
| 3:D:1168:MET:HE3  | 3:D:1171:VAL:HB   | 1.61                     | 0.82              |
| 5:F:364:ARG:O     | 5:F:368:VAL:HG23  | 1.79                     | 0.82              |
| 2:C:274:ARG:H     | 2:C:288:ARG:HH12  | 1.29                     | 0.81              |
| 2:C:412:ALA:HB3   | 8:C:9584:HOH:O    | 1.80                     | 0.81              |
| 3:D:772:PRO:HB3   | 3:D:1224:VAL:HG13 | 1.61                     | 0.81              |
| 5:F:394:ARG:HA    | 5:F:397:ILE:HD12  | 1.60                     | 0.81              |
| 3:N:539:ASP:HB2   | 5:P:318:GLU:CD    | 2.04                     | 0.81              |
| 5:P:132:ARG:O     | 5:P:136:LEU:HG    | 1.80                     | 0.81              |
| 3:D:202:VAL:O     | 3:D:204:LEU:HG    | 1.80                     | 0.81              |
| 2:M:368:THR:HB    | 2:M:369:PRO:HD3   | 1.61                     | 0.81              |
| 2:M:478:VAL:HA    | 2:M:506:ASN:O     | 1.81                     | 0.81              |
| 3:N:479:GLU:HG2   | 8:N:2227:HOH:O    | 1.80                     | 0.81              |
| 1:B:169:ALA:HA    | 8:B:9642:HOH:O    | 1.78                     | 0.81              |
| 2:C:169:GLY:HA2   | 2:C:263:ASP:HB3   | 1.60                     | 0.81              |
| 3:D:1495:ILE:HD11 | 4:E:84:ARG:HG2    | 1.62                     | 0.81              |
| 5:F:125:ASP:HA    | 8:F:9482:HOH:O    | 1.80                     | 0.81              |
| 2:M:728:HIS:CE1   | 5:P:423:ASP:O     | 2.33                     | 0.81              |
| 5:P:305:GLU:HG2   | 5:P:309:LYS:HE3   | 1.62                     | 0.81              |
| 5:P:395:GLU:O     | 5:P:399:GLN:HG2   | 1.80                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:562:ALA:HB1   | 3:N:567:ILE:HD11  | 1.60                     | 0.81              |
| 4:O:14:ASP:HA     | 8:O:2164:HOH:O    | 1.80                     | 0.81              |
| 5:F:166:LEU:HB3   | 5:F:170:HIS:HB2   | 1.62                     | 0.81              |
| 5:F:320:PRO:HA    | 8:F:9526:HOH:O    | 1.79                     | 0.81              |
| 2:M:93:PRO:HG3    | 2:M:117:HIS:HE1   | 1.45                     | 0.81              |
| 3:N:208:PRO:HB2   | 3:N:395:VAL:CG1   | 2.09                     | 0.81              |
| 3:N:1146:GLY:HA3  | 3:N:1207:TYR:HB2  | 1.62                     | 0.81              |
| 2:C:57:GLU:HG2    | 2:C:58:ASP:OD2    | 1.81                     | 0.81              |
| 2:M:44:ILE:HD12   | 8:M:9899:HOH:O    | 1.80                     | 0.81              |
| 2:M:462:ASP:HB3   | 2:M:468:ARG:HD2   | 1.62                     | 0.81              |
| 3:N:782:SER:O     | 3:N:786:ILE:HD12  | 1.80                     | 0.81              |
| 2:C:150:PRO:HA    | 2:C:158:TYR:HB3   | 1.61                     | 0.81              |
| 2:C:264:PRO:HB3   | 2:C:289:THR:HG21  | 1.61                     | 0.81              |
| 2:C:478:VAL:HA    | 2:C:506:ASN:O     | 1.80                     | 0.81              |
| 3:D:699:VAL:N     | 3:D:756:GLN:HE22  | 1.78                     | 0.81              |
| 3:N:139:GLY:HA3   | 3:N:452:ILE:HD12  | 1.61                     | 0.81              |
| 1:A:123:MET:HE3   | 1:A:203:GLY:O     | 1.81                     | 0.81              |
| 2:C:1091:GLU:HG2  | 3:D:606:ILE:HB    | 1.61                     | 0.81              |
| 3:D:422:ALA:H     | 3:D:427:VAL:HG11  | 1.45                     | 0.81              |
| 5:F:77:THR:O      | 5:F:81:VAL:HG23   | 1.81                     | 0.81              |
| 2:M:778:PHE:CZ    | 5:P:419:ARG:HD3   | 2.15                     | 0.81              |
| 5:P:88:ILE:HD13   | 5:P:193:ARG:HB2   | 1.59                     | 0.81              |
| 1:A:42:ARG:HG2    | 1:A:42:ARG:HH11   | 1.46                     | 0.81              |
| 2:C:345:ARG:HB2   | 8:C:2085:HOH:O    | 1.81                     | 0.81              |
| 2:M:207:LEU:HD13  | 2:M:221:LEU:HD11  | 1.63                     | 0.81              |
| 2:M:874:LEU:HD11  | 8:N:2330:HOH:O    | 1.81                     | 0.81              |
| 3:N:44:LEU:HB3    | 3:N:525:ARG:HH21  | 1.44                     | 0.81              |
| 5:P:364:ARG:O     | 5:P:368:VAL:HG23  | 1.81                     | 0.81              |
| 5:P:394:ARG:HA    | 5:P:397:ILE:HD12  | 1.60                     | 0.81              |
| 3:D:219:GLU:O     | 3:D:370:ALA:HB2   | 1.80                     | 0.81              |
| 3:D:1442:ASN:HB3  | 8:D:9715:HOH:O    | 1.80                     | 0.81              |
| 2:M:300:ASP:HA    | 8:M:9575:HOH:O    | 1.78                     | 0.81              |
| 3:N:1112:CYS:HA   | 8:N:9585:HOH:O    | 1.81                     | 0.81              |
| 2:M:1089:VAL:HG13 | 2:M:1099:VAL:HG23 | 1.60                     | 0.80              |
| 3:N:214:GLU:HB3   | 3:N:390:PRO:HD2   | 1.64                     | 0.80              |
| 3:N:507:ASN:HB2   | 8:N:9529:HOH:O    | 1.81                     | 0.80              |
| 3:N:899:LEU:HD23  | 3:N:917:GLN:HB3   | 1.61                     | 0.80              |
| 5:P:277:GLN:O     | 5:P:280:GLN:HB3   | 1.81                     | 0.80              |
| 3:D:826:PRO:HD2   | 3:D:829:VAL:HG22  | 1.63                     | 0.80              |
| 3:N:172:PRO:HB3   | 3:N:178:LEU:HB3   | 1.62                     | 0.80              |
| 3:D:207:PHE:HB3   | 3:D:208:PRO:HD2   | 1.62                     | 0.80              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:427:VAL:HA   | 8:M:9593:HOH:O    | 1.81                     | 0.80              |
| 3:N:861:GLN:H    | 3:N:861:GLN:NE2   | 1.78                     | 0.80              |
| 2:C:204:GLN:HG2  | 8:C:9564:HOH:O    | 1.80                     | 0.80              |
| 2:M:89:THR:HG23  | 2:M:129:ILE:HA    | 1.64                     | 0.80              |
| 2:M:244:PRO:HD2  | 2:M:245:GLY:H     | 1.43                     | 0.80              |
| 2:M:435:TYR:O    | 2:M:437:ARG:HG2   | 1.81                     | 0.80              |
| 5:P:266:GLU:HB3  | 8:P:9668:HOH:O    | 1.80                     | 0.80              |
| 1:A:222:LEU:HD12 | 1:B:215:VAL:HB    | 1.63                     | 0.80              |
| 2:M:107:LEU:HG   | 8:M:9718:HOH:O    | 1.82                     | 0.80              |
| 5:P:152:ASP:HB2  | 5:P:153:PRO:HD3   | 1.64                     | 0.80              |
| 3:D:834:THR:HG22 | 3:D:838:ARG:NE    | 1.97                     | 0.80              |
| 3:D:890:VAL:HG11 | 3:D:922:LEU:HD13  | 1.60                     | 0.80              |
| 3:N:1271:LYS:CE  | 3:N:1334:GLN:HE22 | 1.93                     | 0.80              |
| 5:P:163:LEU:HD22 | 5:P:174:LEU:HG    | 1.62                     | 0.80              |
| 4:E:30:LEU:O     | 4:E:35:PHE:HA     | 1.81                     | 0.80              |
| 3:N:119:SER:HB3  | 8:N:9542:HOH:O    | 1.82                     | 0.80              |
| 8:A:9594:HOH:O   | 1:B:39:PRO:HB3    | 1.82                     | 0.80              |
| 2:C:676:ILE:HG23 | 3:D:948:THR:HB    | 1.63                     | 0.80              |
| 2:C:979:THR:HG23 | 2:C:981:GLU:H     | 1.47                     | 0.80              |
| 3:D:12:LEU:HD23  | 3:D:13:ALA:H      | 1.47                     | 0.80              |
| 3:D:148:GLU:HG3  | 8:D:9742:HOH:O    | 1.81                     | 0.80              |
| 1:K:104:GLU:HG3  | 8:K:1171:HOH:O    | 1.81                     | 0.80              |
| 3:N:132:TYR:HB3  | 8:N:2215:HOH:O    | 1.81                     | 0.80              |
| 3:D:374:GLU:HA   | 8:D:9620:HOH:O    | 1.83                     | 0.79              |
| 3:D:1231:GLU:HB3 | 3:D:1232:PRO:HD3  | 1.64                     | 0.79              |
| 5:P:364:ARG:HB2  | 5:P:365:GLU:OE1   | 1.81                     | 0.79              |
| 2:C:767:PRO:HB2  | 8:C:9776:HOH:O    | 1.83                     | 0.79              |
| 3:N:616:GLN:HB2  | 5:P:326:ASP:CB    | 2.11                     | 0.79              |
| 2:C:810:ASP:HB3  | 2:C:813:VAL:HG22  | 1.64                     | 0.79              |
| 3:D:1103:HIS:HD2 | 3:D:1462:LEU:H    | 1.27                     | 0.79              |
| 5:P:214:GLN:HA   | 5:P:217:ASN:HD22  | 1.46                     | 0.79              |
| 2:C:238:LEU:HA   | 2:C:241:LEU:HD12  | 1.64                     | 0.79              |
| 3:D:1077:ALA:HB2 | 8:D:9889:HOH:O    | 1.82                     | 0.79              |
| 1:K:193:ASP:HA   | 2:M:938:LYS:NZ    | 1.97                     | 0.79              |
| 2:M:260:LEU:HA   | 2:M:291:ALA:HB1   | 1.63                     | 0.79              |
| 2:M:323:ASP:HB2  | 8:M:2151:HOH:O    | 1.82                     | 0.79              |
| 2:M:862:PRO:HA   | 2:M:975:TYR:HE1   | 1.45                     | 0.79              |
| 4:O:30:LEU:O     | 4:O:35:PHE:HA     | 1.83                     | 0.79              |
| 5:P:129:GLU:HB3  | 5:P:142:ARG:HH22  | 1.48                     | 0.79              |
| 1:B:22:GLU:HB3   | 8:B:9505:HOH:O    | 1.81                     | 0.79              |
| 3:D:957:PRO:HG2  | 3:D:1007:VAL:HG12 | 1.64                     | 0.79              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:962:GLN:HA    | 8:D:9754:HOH:O   | 1.82                     | 0.79              |
| 2:M:721:ARG:HE    | 2:M:783:ARG:NH2  | 1.80                     | 0.79              |
| 1:A:182:GLU:CD    | 2:C:934:PHE:HB3  | 2.07                     | 0.79              |
| 2:M:274:ARG:HD2   | 8:M:9866:HOH:O   | 1.81                     | 0.79              |
| 3:N:170:PRO:HB2   | 8:N:9760:HOH:O   | 1.83                     | 0.79              |
| 1:K:42:ARG:HG2    | 1:K:42:ARG:HH11  | 1.46                     | 0.79              |
| 2:M:64:LEU:HD22   | 2:M:359:MET:HG3  | 1.63                     | 0.79              |
| 1:A:218:LEU:HD23  | 1:B:222:LEU:HD11 | 1.65                     | 0.79              |
| 2:C:198:ARG:HH21  | 2:C:203:ASP:HB3  | 1.44                     | 0.79              |
| 8:N:9748:HOH:O    | 4:O:17:TYR:HB3   | 1.83                     | 0.79              |
| 3:N:639:LEU:HB2   | 8:N:9609:HOH:O   | 1.83                     | 0.79              |
| 2:C:71:TYR:H      | 2:C:71:TYR:HD2   | 1.31                     | 0.79              |
| 2:C:338:GLU:HB2   | 8:C:9884:HOH:O   | 1.81                     | 0.79              |
| 2:C:511:GLU:O     | 2:C:526:PRO:HD3  | 1.82                     | 0.79              |
| 2:C:1054:THR:HG21 | 2:C:1079:PRO:HB3 | 1.65                     | 0.79              |
| 3:D:542:ASP:O     | 3:D:546:ARG:HG2  | 1.83                     | 0.79              |
| 2:C:136:ILE:HG21  | 2:C:336:VAL:HG13 | 1.62                     | 0.78              |
| 2:C:627:ARG:HG3   | 2:C:628:PHE:H    | 1.48                     | 0.78              |
| 5:F:277:GLN:HA    | 8:F:9625:HOH:O   | 1.82                     | 0.78              |
| 2:C:110:GLU:HG2   | 2:C:369:PRO:HG3  | 1.65                     | 0.78              |
| 2:C:139:GLN:HE22  | 2:C:415:PRO:HD2  | 1.48                     | 0.78              |
| 5:F:200:LYS:HA    | 5:F:209:PHE:HE1  | 1.48                     | 0.78              |
| 2:C:411:SER:HB2   | 2:C:452:ILE:HG23 | 1.63                     | 0.78              |
| 5:P:278:LEU:HD13  | 5:P:290:GLU:HB3  | 1.64                     | 0.78              |
| 2:C:19:THR:HG22   | 2:C:23:VAL:HG23  | 1.66                     | 0.78              |
| 2:C:694:LEU:HD11  | 2:C:868:ASP:HB3  | 1.66                     | 0.78              |
| 3:D:44:LEU:HB3    | 3:D:525:ARG:HH21 | 1.49                     | 0.78              |
| 3:D:160:GLU:HG2   | 3:D:165:LYS:HD3  | 1.66                     | 0.78              |
| 3:D:170:PRO:O     | 3:D:391:ALA:HB3  | 1.83                     | 0.78              |
| 2:M:1059:ASP:HB3  | 8:M:9570:HOH:O   | 1.82                     | 0.78              |
| 3:N:732:VAL:HA    | 8:N:9711:HOH:O   | 1.82                     | 0.78              |
| 1:B:94:LEU:HD21   | 1:B:119:ASP:CB   | 2.11                     | 0.78              |
| 3:D:899:LEU:HD23  | 3:D:917:GLN:HB3  | 1.63                     | 0.78              |
| 1:L:175:ARG:HA    | 8:L:4017:HOH:O   | 1.81                     | 0.78              |
| 2:M:36:PRO:HG2    | 2:M:70:GLU:HB3   | 1.65                     | 0.78              |
| 3:N:36:THR:HG22   | 3:N:38:LYS:HG3   | 1.65                     | 0.78              |
| 3:D:130:SER:HB3   | 3:D:132:TYR:CE1  | 2.18                     | 0.78              |
| 5:F:363:GLU:OE2   | 5:F:364:ARG:HG2  | 1.83                     | 0.78              |
| 2:M:110:GLU:CG    | 2:M:369:PRO:HG3  | 2.13                     | 0.78              |
| 2:M:433:THR:HA    | 8:M:9545:HOH:O   | 1.83                     | 0.78              |
| 2:M:775:ARG:HD2   | 8:M:2224:HOH:O   | 1.82                     | 0.78              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:91:ASN:CG    | 1:A:92:PRO:HD2    | 2.08                     | 0.78              |
| 2:C:774:LEU:HD11 | 5:F:421:PHE:HE2   | 1.48                     | 0.78              |
| 2:M:660:ALA:O    | 2:M:667:ALA:HB3   | 1.84                     | 0.78              |
| 3:N:141:ILE:HD13 | 3:N:450:TYR:H     | 1.49                     | 0.78              |
| 2:C:74:GLY:HA2   | 8:C:9794:HOH:O    | 1.82                     | 0.78              |
| 2:C:603:VAL:HG21 | 2:C:643:VAL:HG11  | 1.63                     | 0.78              |
| 1:L:42:ARG:HG2   | 1:L:42:ARG:HH11   | 1.49                     | 0.78              |
| 3:N:396:VAL:HG13 | 3:N:447:VAL:HA    | 1.66                     | 0.78              |
| 3:N:426:LYS:HB3  | 5:P:134:LYS:O     | 1.82                     | 0.78              |
| 3:N:705:ALA:HB3  | 3:N:706:PRO:HD3   | 1.66                     | 0.78              |
| 3:N:1157:GLY:HA3 | 8:N:9681:HOH:O    | 1.84                     | 0.78              |
| 5:P:402:ASN:HB3  | 5:P:406:ARG:NH2   | 1.99                     | 0.78              |
| 2:C:470:PRO:HG3  | 2:C:485:TYR:CE2   | 2.19                     | 0.78              |
| 2:C:1094:ALA:HB1 | 3:D:603:LEU:HD13  | 1.66                     | 0.78              |
| 3:D:85:VAL:HG23  | 8:D:9655:HOH:O    | 1.84                     | 0.78              |
| 3:D:144:GLY:HA3  | 8:D:9577:HOH:O    | 1.84                     | 0.78              |
| 3:D:608:SER:HB2  | 8:D:2144:HOH:O    | 1.81                     | 0.78              |
| 5:F:92:PRO:HB3   | 8:F:9549:HOH:O    | 1.82                     | 0.78              |
| 2:M:139:GLN:NE2  | 2:M:414:GLY:HA3   | 1.98                     | 0.78              |
| 3:N:471:GLU:HB2  | 8:N:9762:HOH:O    | 1.84                     | 0.78              |
| 4:O:40:LEU:HB2   | 4:O:45:ARG:HD2    | 1.66                     | 0.78              |
| 5:P:416:ARG:HD3  | 5:P:419:ARG:CG    | 2.14                     | 0.78              |
| 2:C:1058:ASP:OD2 | 2:C:1083:GLU:HB2  | 1.84                     | 0.78              |
| 2:M:492:ASP:HB3  | 2:M:518:LYS:HD3   | 1.64                     | 0.78              |
| 2:C:1092:LEU:HA  | 2:C:1095:LEU:HD12 | 1.65                     | 0.77              |
| 3:D:710:ARG:HG3  | 3:D:711:LEU:HD23  | 1.66                     | 0.77              |
| 3:N:24:GLY:HA3   | 3:N:49:ILE:HG12   | 1.66                     | 0.77              |
| 3:D:502:PHE:CD2  | 3:D:509:PRO:HD3   | 2.19                     | 0.77              |
| 3:D:562:ALA:HB3  | 8:D:2463:HOH:O    | 1.84                     | 0.77              |
| 3:D:1472:ILE:O   | 3:D:1477:GLY:HA3  | 1.84                     | 0.77              |
| 5:F:361:LEU:HD12 | 5:F:366:ALA:CB    | 2.09                     | 0.77              |
| 2:M:492:ASP:HA   | 2:M:518:LYS:HB3   | 1.66                     | 0.77              |
| 3:N:192:ALA:O    | 3:N:195:VAL:HG23  | 1.83                     | 0.77              |
| 3:N:616:GLN:CB   | 5:P:326:ASP:HB2   | 2.14                     | 0.77              |
| 5:F:141:VAL:O    | 5:F:145:PRO:HD2   | 1.84                     | 0.77              |
| 1:L:132:LEU:HD21 | 1:L:138:LEU:HD22  | 1.66                     | 0.77              |
| 2:M:376:ARG:HB3  | 2:M:377:PRO:HD3   | 1.67                     | 0.77              |
| 3:N:1356:TYR:CD1 | 3:N:1363:LEU:HD21 | 2.19                     | 0.77              |
| 3:D:1082:ALA:O   | 3:D:1086:LEU:HD13 | 1.83                     | 0.77              |
| 3:D:1198:TYR:HA  | 8:D:2227:HOH:O    | 1.85                     | 0.77              |
| 5:F:128:ARG:HD3  | 8:F:9477:HOH:O    | 1.82                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:132:LEU:HD11  | 1:L:138:LEU:HD13  | 1.66                     | 0.77              |
| 1:B:42:ARG:HG2    | 1:B:42:ARG:HH11   | 1.47                     | 0.77              |
| 3:D:1362:LYS:HE3  | 8:D:9659:HOH:O    | 1.84                     | 0.77              |
| 3:N:1116:ASN:H    | 3:N:1116:ASN:HD22 | 1.32                     | 0.77              |
| 3:N:1372:VAL:HA   | 3:N:1375:MET:SD   | 2.23                     | 0.77              |
| 2:C:49:ARG:HB2    | 2:C:49:ARG:HH11   | 1.47                     | 0.77              |
| 5:F:419:ARG:C     | 5:F:419:ARG:HG3   | 2.09                     | 0.77              |
| 2:M:89:THR:HA     | 2:M:129:ILE:O     | 1.83                     | 0.77              |
| 3:N:561:GLY:HA2   | 8:N:9520:HOH:O    | 1.83                     | 0.77              |
| 3:N:1116:ASN:H    | 3:N:1116:ASN:ND2  | 1.83                     | 0.77              |
| 3:N:1173:LEU:HA   | 8:N:9906:HOH:O    | 1.83                     | 0.77              |
| 3:D:483:HIS:HB2   | 3:D:484:PRO:HD3   | 1.66                     | 0.77              |
| 3:N:1362:LYS:HG3  | 8:N:9772:HOH:O    | 1.83                     | 0.77              |
| 5:P:402:ASN:HB3   | 5:P:406:ARG:CZ    | 2.15                     | 0.77              |
| 3:N:1472:ILE:O    | 3:N:1477:GLY:HA3  | 1.83                     | 0.77              |
| 3:D:171:LEU:HD11  | 8:D:2193:HOH:O    | 1.83                     | 0.77              |
| 3:D:994:GLN:HB2   | 8:D:9576:HOH:O    | 1.85                     | 0.77              |
| 3:D:1057:VAL:HG21 | 8:D:9564:HOH:O    | 1.84                     | 0.77              |
| 3:D:1273:VAL:HG22 | 3:D:1326:THR:OG1  | 1.84                     | 0.77              |
| 2:M:9:ILE:HG21    | 2:M:499:ALA:HB1   | 1.67                     | 0.77              |
| 2:M:101:ILE:HG23  | 2:M:107:LEU:HD22  | 1.66                     | 0.77              |
| 2:M:909:ALA:HB1   | 2:M:914:ILE:HD11  | 1.67                     | 0.77              |
| 3:N:940:THR:HG21  | 8:N:9579:HOH:O    | 1.84                     | 0.77              |
| 3:N:1397:LYS:NZ   | 3:N:1432:LYS:HB3  | 1.99                     | 0.77              |
| 3:D:1314:LYS:NZ   | 3:D:1317:ASP:HB2  | 2.00                     | 0.76              |
| 3:D:1376:MET:HE3  | 3:D:1421:LEU:HD13 | 1.65                     | 0.76              |
| 2:M:220:GLY:HA3   | 8:M:2108:HOH:O    | 1.86                     | 0.76              |
| 2:M:336:VAL:HA    | 2:M:339:LEU:HD12  | 1.67                     | 0.76              |
| 3:N:205:TYR:HD2   | 3:N:393:ILE:HG12  | 1.49                     | 0.76              |
| 3:N:540:LEU:HA    | 3:N:543:LEU:HD12  | 1.67                     | 0.76              |
| 3:N:806:PHE:CE1   | 3:N:813:LEU:HB3   | 2.20                     | 0.76              |
| 1:A:229:GLN:HB3   | 8:A:9609:HOH:O    | 1.85                     | 0.76              |
| 1:B:182:GLU:HA    | 8:B:9564:HOH:O    | 1.86                     | 0.76              |
| 3:D:1243:THR:HB   | 3:D:1253:THR:HB   | 1.66                     | 0.76              |
| 3:D:1433:SER:HB2  | 3:D:1457:ASP:OD2  | 1.84                     | 0.76              |
| 4:O:41:GLU:CA     | 4:O:45:ARG:HG3    | 2.16                     | 0.76              |
| 2:C:1057:SER:HB2  | 3:D:622:ARG:O     | 1.84                     | 0.76              |
| 3:D:383:GLY:HA2   | 8:D:9900:HOH:O    | 1.84                     | 0.76              |
| 3:D:868:TYR:HD1   | 3:D:869:MET:H     | 1.33                     | 0.76              |
| 2:C:197:LEU:HD22  | 2:C:202:TYR:HD2   | 1.48                     | 0.76              |
| 2:C:516:ARG:NE    | 3:D:1068:LEU:HD13 | 2.00                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:208:PRO:HB2   | 3:D:395:VAL:CG1   | 2.14                     | 0.76              |
| 2:M:1018:GLN:NE2  | 2:M:1063:ARG:HH22 | 1.84                     | 0.76              |
| 3:D:163:TYR:HB2   | 8:D:9658:HOH:O    | 1.86                     | 0.76              |
| 2:C:568:ALA:HB1   | 2:C:668:LEU:HB3   | 1.66                     | 0.76              |
| 3:D:131:LYS:HG2   | 3:D:568:ARG:HG2   | 1.68                     | 0.76              |
| 3:D:537:THR:HG23  | 8:D:2538:HOH:O    | 1.86                     | 0.76              |
| 3:D:793:THR:HA    | 8:D:9489:HOH:O    | 1.84                     | 0.76              |
| 2:M:12:VAL:HG12   | 2:M:534:VAL:HG13  | 1.67                     | 0.76              |
| 2:M:573:ARG:HG3   | 2:M:698:ASP:O     | 1.85                     | 0.76              |
| 2:M:710:ILE:HG22  | 2:M:823:VAL:HB    | 1.68                     | 0.76              |
| 3:N:1166:LEU:HD11 | 8:N:2033:HOH:O    | 1.84                     | 0.76              |
| 1:A:189:ARG:NH2   | 1:B:155:LYS:HG2   | 2.01                     | 0.76              |
| 2:C:260:LEU:HA    | 2:C:291:ALA:HB1   | 1.66                     | 0.76              |
| 2:M:1001:VAL:HA   | 8:M:9560:HOH:O    | 1.86                     | 0.76              |
| 5:P:76:SER:HB2    | 8:P:9639:HOH:O    | 1.85                     | 0.76              |
| 2:C:269:LEU:HD23  | 2:C:288:ARG:HB2   | 1.68                     | 0.76              |
| 2:C:660:ALA:O     | 2:C:667:ALA:HB3   | 1.85                     | 0.76              |
| 8:C:9676:HOH:O    | 3:D:656:PHE:HA    | 1.84                     | 0.76              |
| 3:D:1299:PHE:HB3  | 8:D:2129:HOH:O    | 1.86                     | 0.76              |
| 2:M:1082:PRO:HG2  | 3:N:1469:GLY:HA3  | 1.67                     | 0.76              |
| 3:N:1388:ARG:HG3  | 3:N:1389:LEU:CD2  | 2.16                     | 0.76              |
| 3:D:953:ASP:HA    | 8:D:9507:HOH:O    | 1.85                     | 0.75              |
| 3:D:1412:LYS:O    | 3:D:1414:PRO:HD3  | 1.85                     | 0.75              |
| 2:M:204:GLN:CD    | 2:M:222:MET:HB3   | 2.11                     | 0.75              |
| 1:A:226:SER:O     | 1:A:228:PRO:HD3   | 1.86                     | 0.75              |
| 2:C:64:LEU:HD22   | 2:C:359:MET:HG3   | 1.68                     | 0.75              |
| 3:D:133:ILE:HG21  | 3:D:454:ALA:HB1   | 1.67                     | 0.75              |
| 1:K:226:SER:O     | 1:K:228:PRO:HD3   | 1.86                     | 0.75              |
| 2:M:600:ASP:HB3   | 8:M:2091:HOH:O    | 1.84                     | 0.75              |
| 3:N:1087:ARG:CZ   | 3:N:1238:MET:HG3  | 2.16                     | 0.75              |
| 2:C:957:LYS:HD3   | 2:C:961:GLU:HB3   | 1.69                     | 0.75              |
| 3:D:527:MET:HE2   | 3:D:535:PHE:HB3   | 1.68                     | 0.75              |
| 2:M:290:LEU:HD22  | 2:M:302:VAL:HG11  | 1.67                     | 0.75              |
| 2:M:710:ILE:HD12  | 2:M:790:LEU:HB2   | 1.66                     | 0.75              |
| 3:N:219:GLU:O     | 3:N:370:ALA:CB    | 2.34                     | 0.75              |
| 3:N:908:LYS:HB3   | 3:N:1027:GLY:HA3  | 1.67                     | 0.75              |
| 3:N:1314:LYS:HA   | 8:N:2212:HOH:O    | 1.85                     | 0.75              |
| 2:C:101:ILE:HG23  | 2:C:107:LEU:HD22  | 1.67                     | 0.75              |
| 2:C:343:GLN:HG2   | 2:C:385:PHE:HB2   | 1.68                     | 0.75              |
| 3:D:633:VAL:HG22  | 3:D:635:PRO:HD3   | 1.68                     | 0.75              |
| 1:L:156:HIS:HD2   | 1:L:157:GLY:H     | 1.35                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:183:SER:HB3   | 2:M:190:LYS:NZ    | 2.01                     | 0.75              |
| 2:M:274:ARG:HB2   | 2:M:288:ARG:NH1   | 2.02                     | 0.75              |
| 2:M:411:SER:HB3   | 8:M:2133:HOH:O    | 1.86                     | 0.75              |
| 3:N:994:GLN:HE21  | 3:N:998:GLU:HG3   | 1.52                     | 0.75              |
| 2:C:672:VAL:HG23  | 2:C:868:ASP:HB2   | 1.67                     | 0.75              |
| 3:D:1101:VAL:HG21 | 3:D:1424:VAL:HG22 | 1.68                     | 0.75              |
| 5:F:210:LEU:HA    | 5:F:213:ILE:HD12  | 1.68                     | 0.75              |
| 5:F:277:GLN:O     | 5:F:280:GLN:HB3   | 1.87                     | 0.75              |
| 5:F:376:ILE:HG22  | 5:F:377:ASP:HB2   | 1.68                     | 0.75              |
| 2:M:778:PHE:CE2   | 5:P:419:ARG:HD3   | 2.21                     | 0.75              |
| 2:C:841:ASN:HD22  | 2:C:843:HIS:H     | 1.34                     | 0.75              |
| 3:D:812:ALA:HA    | 8:D:9496:HOH:O    | 1.85                     | 0.75              |
| 4:E:54:LEU:HG     | 4:E:58:PRO:HD2    | 1.68                     | 0.75              |
| 2:M:65:VAL:HG23   | 2:M:101:ILE:HB    | 1.68                     | 0.75              |
| 2:M:603:VAL:HG21  | 2:M:643:VAL:HG11  | 1.67                     | 0.75              |
| 3:N:44:LEU:HB3    | 3:N:525:ARG:NH2   | 2.01                     | 0.75              |
| 3:N:119:SER:HB2   | 3:N:123:LEU:CB    | 2.16                     | 0.75              |
| 3:D:411:THR:HG23  | 3:D:429:SER:HB3   | 1.69                     | 0.75              |
| 3:D:646:LYS:HA    | 3:D:720:LEU:HD23  | 1.66                     | 0.75              |
| 3:D:1279:GLY:O    | 3:D:1318:TYR:HA   | 1.87                     | 0.75              |
| 5:F:108:GLU:HG3   | 5:F:176:ILE:HG21  | 1.66                     | 0.75              |
| 2:M:528:GLU:HB3   | 8:M:9589:HOH:O    | 1.85                     | 0.75              |
| 2:M:897:LEU:HB3   | 2:M:899:GLN:HE21  | 1.50                     | 0.75              |
| 2:C:173:ASP:HB2   | 8:C:2311:HOH:O    | 1.87                     | 0.75              |
| 2:C:640:ARG:NH1   | 2:C:642:ARG:HH12  | 1.82                     | 0.75              |
| 2:C:911:GLU:O     | 2:C:915:LYS:HG2   | 1.86                     | 0.75              |
| 3:D:30:GLU:HG3    | 3:D:41:ARG:HG2    | 1.69                     | 0.75              |
| 3:D:126:VAL:CG1   | 3:D:132:TYR:HB2   | 2.17                     | 0.75              |
| 3:D:131:LYS:HD2   | 5:F:83:GLN:OE1    | 1.86                     | 0.75              |
| 4:E:25:LYS:HA     | 4:E:28:GLN:CD     | 2.10                     | 0.75              |
| 2:M:52:PHE:CZ     | 2:M:98:LEU:HD21   | 2.21                     | 0.75              |
| 2:M:341:THR:HG21  | 8:M:9646:HOH:O    | 1.86                     | 0.75              |
| 2:M:418:LEU:HB3   | 8:M:9802:HOH:O    | 1.85                     | 0.75              |
| 2:M:423:ALA:HA    | 8:M:2231:HOH:O    | 1.86                     | 0.75              |
| 2:M:1051:GLU:OE2  | 3:N:752:SER:HB3   | 1.86                     | 0.75              |
| 3:N:1273:VAL:HG22 | 3:N:1326:THR:OG1  | 1.86                     | 0.75              |
| 2:C:725:ASP:O     | 2:C:727:PRO:HD3   | 1.87                     | 0.75              |
| 3:D:800:LYS:HE2   | 3:D:830:ALA:HB3   | 1.68                     | 0.75              |
| 2:M:148:PHE:HZ    | 2:M:281:LEU:HD22  | 1.52                     | 0.75              |
| 2:M:511:GLU:O     | 2:M:526:PRO:HD3   | 1.84                     | 0.75              |
| 3:N:1412:LYS:O    | 3:N:1414:PRO:HD3  | 1.86                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:289:THR:HG22 | 2:C:290:LEU:HD23 | 1.66                     | 0.74              |
| 1:L:220:GLU:O    | 1:L:223:THR:HG22 | 1.87                     | 0.74              |
| 3:N:133:ILE:HD13 | 8:N:9573:HOH:O   | 1.86                     | 0.74              |
| 3:D:699:VAL:H    | 3:D:756:GLN:NE2  | 1.81                     | 0.74              |
| 3:N:123:LEU:HD21 | 3:N:152:LEU:HD22 | 1.68                     | 0.74              |
| 3:N:1258:ARG:NH2 | 3:N:1351:GLU:HG2 | 1.96                     | 0.74              |
| 2:C:546:LEU:HD12 | 2:C:565:GLN:HE22 | 1.51                     | 0.74              |
| 2:C:774:LEU:HD11 | 5:F:421:PHE:CE2  | 2.21                     | 0.74              |
| 3:D:429:SER:HB2  | 8:D:9724:HOH:O   | 1.85                     | 0.74              |
| 2:M:723:THR:HG23 | 2:M:725:ASP:H    | 1.50                     | 0.74              |
| 3:N:128:TYR:HE1  | 3:N:461:ILE:HG13 | 1.53                     | 0.74              |
| 3:N:800:LYS:HA   | 8:N:2379:HOH:O   | 1.87                     | 0.74              |
| 2:C:838:LYS:HD2  | 2:C:997:LEU:HD12 | 1.69                     | 0.74              |
| 1:B:70:GLY:HA2   | 8:B:9650:HOH:O   | 1.87                     | 0.74              |
| 2:C:195:LEU:HA   | 8:C:9981:HOH:O   | 1.88                     | 0.74              |
| 2:C:356:ARG:HA   | 8:C:9554:HOH:O   | 1.86                     | 0.74              |
| 3:D:657:LEU:HD22 | 3:D:691:LEU:HD13 | 1.69                     | 0.74              |
| 2:M:147:TYR:HA   | 8:M:2202:HOH:O   | 1.87                     | 0.74              |
| 2:M:728:HIS:O    | 2:M:729:LEU:HD22 | 1.87                     | 0.74              |
| 4:O:74:VAL:HG12  | 4:O:79:LEU:HD21  | 1.66                     | 0.74              |
| 1:A:97:VAL:HG23  | 8:A:9431:HOH:O   | 1.87                     | 0.74              |
| 2:C:729:LEU:HD11 | 5:F:419:ARG:NH2  | 2.01                     | 0.74              |
| 5:F:369:LEU:CD1  | 5:F:401:GLU:HG3  | 2.17                     | 0.74              |
| 2:M:675:ALA:HB2  | 2:M:867:VAL:HG11 | 1.69                     | 0.74              |
| 3:N:86:ARG:O     | 3:N:522:PRO:HD2  | 1.87                     | 0.74              |
| 5:P:163:LEU:HB3  | 5:P:174:LEU:HG   | 1.70                     | 0.74              |
| 2:C:211:LEU:HD11 | 8:C:9607:HOH:O   | 1.87                     | 0.74              |
| 2:C:889:HIS:CE1  | 3:D:951:ILE:H    | 2.06                     | 0.74              |
| 3:D:984:THR:HG23 | 3:D:987:GLU:H    | 1.52                     | 0.74              |
| 3:N:776:GLU:HG3  | 8:N:9518:HOH:O   | 1.88                     | 0.74              |
| 3:N:875:THR:HG21 | 3:N:902:LEU:HD13 | 1.69                     | 0.74              |
| 2:C:480:THR:HG22 | 2:C:482:GLU:H    | 1.52                     | 0.74              |
| 3:D:192:ALA:O    | 3:D:195:VAL:HG23 | 1.88                     | 0.74              |
| 2:M:1101:THR:HB  | 3:N:5:VAL:CG1    | 2.15                     | 0.74              |
| 3:N:112:ILE:HG22 | 3:N:512:MET:SD   | 2.28                     | 0.74              |
| 3:N:469:ASP:HB3  | 8:N:9534:HOH:O   | 1.87                     | 0.74              |
| 5:P:297:PRO:HB2  | 8:P:9575:HOH:O   | 1.87                     | 0.74              |
| 2:C:313:LEU:HD13 | 2:C:321:GLU:HB2  | 1.68                     | 0.74              |
| 3:D:172:PRO:HB3  | 3:D:178:LEU:HB3  | 1.69                     | 0.74              |
| 3:D:1101:VAL:CG1 | 3:D:1427:SER:HB3 | 2.17                     | 0.74              |
| 5:F:416:ARG:NH1  | 5:F:419:ARG:HB2  | 2.02                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:130:ASN:HB3   | 8:M:9869:HOH:O    | 1.88                     | 0.74              |
| 2:M:580:MET:HB3   | 2:M:584:GLU:CD    | 2.13                     | 0.74              |
| 3:N:434:ARG:HB2   | 3:N:447:VAL:CG2   | 2.16                     | 0.74              |
| 5:P:169:GLU:H     | 5:P:169:GLU:CD    | 1.96                     | 0.74              |
| 5:P:260:ILE:HG12  | 5:P:264:MET:HB2   | 1.67                     | 0.74              |
| 2:C:629:TYR:HB2   | 8:C:9559:HOH:O    | 1.86                     | 0.74              |
| 5:F:371:LEU:HD11  | 8:F:9822:HOH:O    | 1.87                     | 0.74              |
| 2:M:1025:ALA:HA   | 8:M:9816:HOH:O    | 1.87                     | 0.74              |
| 3:N:131:LYS:CG    | 3:N:568:ARG:HG2   | 2.17                     | 0.74              |
| 3:N:136:ASP:HB3   | 3:N:137:PRO:CD    | 2.16                     | 0.74              |
| 3:N:1396:GLU:HA   | 3:N:1399:ASP:OD2  | 1.87                     | 0.74              |
| 5:P:361:LEU:HD13  | 5:P:404:ALA:HB1   | 1.70                     | 0.74              |
| 5:F:270:LYS:HD3   | 5:F:295:MET:HE1   | 1.70                     | 0.73              |
| 1:L:185:ARG:HD2   | 8:L:3631:HOH:O    | 1.88                     | 0.73              |
| 2:M:874:LEU:HD23  | 3:N:1023:MET:SD   | 2.28                     | 0.73              |
| 3:N:698:LYS:HA    | 3:N:756:GLN:NE2   | 2.03                     | 0.73              |
| 5:P:395:GLU:HA    | 8:P:9476:HOH:O    | 1.87                     | 0.73              |
| 2:C:1074:GLU:HB3  | 8:C:2223:HOH:O    | 1.87                     | 0.73              |
| 2:M:56:GLU:HB2    | 2:M:64:LEU:HD23   | 1.69                     | 0.73              |
| 2:M:536:PRO:HB3   | 2:M:906:PHE:HB2   | 1.70                     | 0.73              |
| 2:M:795:GLY:O     | 2:M:796:GLU:HG2   | 1.86                     | 0.73              |
| 5:P:130:VAL:HG21  | 5:P:159:ILE:HG21  | 1.70                     | 0.73              |
| 5:P:410:TYR:HA    | 5:P:413:SER:OG    | 1.88                     | 0.73              |
| 2:C:762:LYS:HZ3   | 2:C:762:LYS:HB2   | 1.53                     | 0.73              |
| 2:C:853:LEU:HD23  | 2:C:858:MET:HE2   | 1.70                     | 0.73              |
| 2:C:881:ASN:HD22  | 2:C:881:ASN:N     | 1.84                     | 0.73              |
| 3:D:32:ILE:O      | 5:F:258:ILE:HG23  | 1.89                     | 0.73              |
| 3:D:396:VAL:HG13  | 3:D:447:VAL:HA    | 1.70                     | 0.73              |
| 3:D:427:VAL:HB    | 3:D:435:VAL:HB    | 1.71                     | 0.73              |
| 3:D:1209:LEU:HD13 | 3:D:1216:SER:H    | 1.54                     | 0.73              |
| 2:M:578:VAL:HG23  | 2:M:579:VAL:HG12  | 1.70                     | 0.73              |
| 3:N:219:GLU:O     | 3:N:370:ALA:HB2   | 1.88                     | 0.73              |
| 2:C:811:PRO:HD3   | 8:C:2192:HOH:O    | 1.87                     | 0.73              |
| 3:D:544:TYR:CE1   | 3:D:581:LEU:HD13  | 2.23                     | 0.73              |
| 3:D:1398:TRP:CZ3  | 3:D:1415:VAL:HG11 | 2.23                     | 0.73              |
| 1:K:39:PRO:HG2    | 1:L:39:PRO:HG2    | 1.70                     | 0.73              |
| 1:L:190:THR:HG21  | 8:L:5177:HOH:O    | 1.87                     | 0.73              |
| 2:M:66:LEU:HD13   | 2:M:100:LEU:HB3   | 1.70                     | 0.73              |
| 2:M:148:PHE:HB2   | 8:M:9596:HOH:O    | 1.88                     | 0.73              |
| 3:N:101:HIS:HD2   | 3:N:582:LEU:HD13  | 1.53                     | 0.73              |
| 3:N:563:PRO:HG2   | 5:P:188:ILE:HG21  | 1.69                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:291:ILE:HG23  | 5:P:304:VAL:HG21  | 1.69                     | 0.73              |
| 1:K:94:LEU:HD21   | 1:K:119:ASP:HB2   | 1.71                     | 0.73              |
| 3:N:177:ALA:HB1   | 3:N:199:LEU:HD22  | 1.70                     | 0.73              |
| 3:N:216:VAL:HG13  | 8:N:9883:HOH:O    | 1.87                     | 0.73              |
| 3:N:728:LEU:HD13  | 3:N:745:MET:HE1   | 1.70                     | 0.73              |
| 3:N:1353:GLN:HE21 | 3:N:1357:ARG:NE   | 1.86                     | 0.73              |
| 5:P:119:ILE:HG13  | 8:P:9609:HOH:O    | 1.86                     | 0.73              |
| 1:A:198:ARG:HH22  | 2:C:932:GLU:HB3   | 1.54                     | 0.73              |
| 2:C:110:GLU:CG    | 2:C:369:PRO:HG3   | 2.18                     | 0.73              |
| 2:C:762:LYS:HB2   | 2:C:762:LYS:NZ    | 2.01                     | 0.73              |
| 2:C:1030:GLN:HE22 | 3:D:628:ARG:HE    | 1.35                     | 0.73              |
| 3:D:789:LEU:HD12  | 3:D:911:LEU:HD21  | 1.69                     | 0.73              |
| 3:D:1380:GLU:OE2  | 3:D:1390:LEU:HD22 | 1.88                     | 0.73              |
| 1:L:27:PRO:HB3    | 1:L:192:LEU:HD13  | 1.70                     | 0.73              |
| 1:L:101:LEU:HB3   | 1:L:140:MET:SD    | 2.28                     | 0.73              |
| 2:M:418:LEU:HB2   | 8:M:9616:HOH:O    | 1.88                     | 0.73              |
| 3:N:101:HIS:CD2   | 3:N:582:LEU:HD13  | 2.23                     | 0.73              |
| 3:N:897:TRP:CZ2   | 3:N:902:LEU:HD21  | 2.23                     | 0.73              |
| 5:P:82:ARG:O      | 5:P:86:HIS:HB2    | 1.88                     | 0.73              |
| 1:A:67:THR:HG21   | 2:C:609:ASN:ND2   | 2.04                     | 0.73              |
| 1:A:88:ARG:HG3    | 1:A:204:SER:O     | 1.88                     | 0.73              |
| 2:M:660:ALA:HB1   | 2:M:667:ALA:O     | 1.89                     | 0.73              |
| 2:M:880:MET:HE1   | 3:N:1037:GLN:NE2  | 2.02                     | 0.73              |
| 2:M:1053:LEU:HA   | 8:M:9509:HOH:O    | 1.87                     | 0.73              |
| 3:N:573:MET:SD    | 5:P:210:LEU:HB3   | 2.29                     | 0.73              |
| 2:C:250:ARG:NE    | 2:C:253:ALA:HB1   | 2.04                     | 0.73              |
| 2:C:748:GLU:HA    | 2:C:799:ILE:HG22  | 1.70                     | 0.73              |
| 2:C:1111:ILE:HG13 | 2:C:1112:PHE:N    | 2.01                     | 0.73              |
| 3:D:705:ALA:HB3   | 3:D:706:PRO:HD3   | 1.69                     | 0.73              |
| 5:F:357:ALA:HB2   | 5:F:412:GLU:OE2   | 1.88                     | 0.73              |
| 2:M:250:ARG:HG3   | 8:M:2200:HOH:O    | 1.87                     | 0.73              |
| 2:M:405:ARG:NH2   | 2:M:409:ARG:HH21  | 1.86                     | 0.73              |
| 3:N:177:ALA:HB1   | 3:N:199:LEU:HD13  | 1.70                     | 0.73              |
| 1:A:206:THR:HG22  | 1:A:209:GLU:H     | 1.54                     | 0.73              |
| 2:C:500:ASN:HB3   | 8:C:9512:HOH:O    | 1.89                     | 0.73              |
| 2:C:943:VAL:HG22  | 2:C:985:GLY:H     | 1.53                     | 0.73              |
| 2:C:1040:LEU:HD21 | 2:C:1048:THR:HG22 | 1.71                     | 0.73              |
| 3:D:1003:VAL:O    | 3:D:1007:VAL:HG13 | 1.89                     | 0.73              |
| 4:E:82:GLU:H      | 4:E:82:GLU:CD     | 1.95                     | 0.73              |
| 1:K:86:VAL:HG12   | 1:K:124:ASN:ND2   | 2.04                     | 0.73              |
| 1:A:54:THR:HG23   | 1:A:158:ILE:HG13  | 1.70                     | 0.73              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:1028:GLY:HA2  | 8:C:2253:HOH:O   | 1.88                     | 0.73              |
| 8:C:2215:HOH:O    | 3:D:1047:LYS:HE2 | 1.89                     | 0.73              |
| 5:F:140:ARG:HG3   | 5:F:141:VAL:H    | 1.53                     | 0.73              |
| 5:F:205:ARG:HD2   | 5:F:251:ILE:HG21 | 1.71                     | 0.73              |
| 1:L:95:GLN:HG3    | 8:L:1866:HOH:O   | 1.89                     | 0.73              |
| 2:M:84:ARG:HD2    | 8:M:9757:HOH:O   | 1.89                     | 0.73              |
| 3:N:1383:ASP:HB2  | 3:N:1416:ALA:HB3 | 1.70                     | 0.73              |
| 3:N:496:LEU:HB3   | 8:N:9704:HOH:O   | 1.89                     | 0.72              |
| 5:P:401:GLU:O     | 5:P:405:LEU:HB2  | 1.89                     | 0.72              |
| 2:C:266:ARG:HH11  | 2:C:266:ARG:HG3  | 1.54                     | 0.72              |
| 3:D:68:PHE:HB2    | 8:D:9549:HOH:O   | 1.90                     | 0.72              |
| 5:F:292:ALA:HB2   | 8:F:9565:HOH:O   | 1.89                     | 0.72              |
| 5:F:408:LEU:HD23  | 5:F:409:LYS:N    | 2.04                     | 0.72              |
| 2:M:470:PRO:HG3   | 2:M:485:TYR:CZ   | 2.24                     | 0.72              |
| 5:P:358:LEU:HD21  | 5:P:370:LYS:NZ   | 2.03                     | 0.72              |
| 2:C:241:LEU:HD11  | 8:C:9948:HOH:O   | 1.89                     | 0.72              |
| 5:F:200:LYS:HA    | 5:F:209:PHE:CE1  | 2.24                     | 0.72              |
| 2:M:262:ALA:HB2   | 8:M:2129:HOH:O   | 1.90                     | 0.72              |
| 3:N:800:LYS:HE2   | 3:N:830:ALA:HB3  | 1.71                     | 0.72              |
| 3:N:1144:LEU:HB3  | 8:N:2033:HOH:O   | 1.89                     | 0.72              |
| 1:B:123:MET:C     | 1:B:125:PRO:HD3  | 2.14                     | 0.72              |
| 2:C:710:ILE:HD11  | 2:C:758:ARG:HE   | 1.55                     | 0.72              |
| 2:C:953:VAL:HG13  | 2:C:966:LEU:HD13 | 1.72                     | 0.72              |
| 3:D:996:TRP:CD2   | 3:D:1056:PRO:HG2 | 2.24                     | 0.72              |
| 8:K:2135:HOH:O    | 1:L:10:VAL:HG13  | 1.89                     | 0.72              |
| 2:M:170:PRO:HB3   | 2:M:186:VAL:HG12 | 1.70                     | 0.72              |
| 3:N:826:PRO:HD2   | 3:N:829:VAL:HG22 | 1.70                     | 0.72              |
| 3:D:860:LEU:HA    | 3:D:877:PRO:HB2  | 1.72                     | 0.72              |
| 5:F:361:LEU:HD13  | 5:F:404:ALA:HB1  | 1.69                     | 0.72              |
| 2:M:314:THR:HG23  | 8:M:9735:HOH:O   | 1.90                     | 0.72              |
| 3:N:126:VAL:HG11  | 3:N:152:LEU:CD1  | 2.20                     | 0.72              |
| 3:N:1326:THR:HG22 | 3:N:1327:ARG:H   | 1.53                     | 0.72              |
| 5:P:416:ARG:HH11  | 5:P:419:ARG:CD   | 2.03                     | 0.72              |
| 3:D:471:GLU:HB3   | 8:D:9613:HOH:O   | 1.90                     | 0.72              |
| 3:D:796:ARG:HD3   | 3:D:862:ASP:OD2  | 1.89                     | 0.72              |
| 3:D:810:GLU:O     | 3:D:813:LEU:HG   | 1.89                     | 0.72              |
| 2:M:205:GLU:O     | 2:M:209:ARG:HD2  | 1.89                     | 0.72              |
| 5:P:84:TYR:O      | 5:P:88:ILE:HD12  | 1.90                     | 0.72              |
| 2:C:368:THR:HB    | 2:C:369:PRO:CD   | 2.18                     | 0.72              |
| 2:C:660:ALA:HB1   | 2:C:667:ALA:O    | 1.90                     | 0.72              |
| 3:D:172:PRO:HD2   | 3:D:389:GLU:O    | 1.90                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:683:ILE:HG22  | 3:D:687:VAL:HG21  | 1.72                     | 0.72              |
| 3:D:798:GLU:HG2   | 3:D:799:LYS:H     | 1.55                     | 0.72              |
| 2:M:269:LEU:HA    | 2:M:288:ARG:NE    | 2.02                     | 0.72              |
| 1:A:27:PRO:HG2    | 1:A:186:LEU:HD22  | 1.72                     | 0.72              |
| 1:B:23:PHE:HE1    | 1:B:208:LEU:HD13  | 1.53                     | 0.72              |
| 3:D:430:ASP:HB2   | 3:D:432:TYR:CE2   | 2.25                     | 0.72              |
| 5:F:82:ARG:O      | 5:F:86:HIS:HB2    | 1.89                     | 0.72              |
| 3:N:1269:LYS:HE2  | 3:N:1269:LYS:HA   | 1.71                     | 0.72              |
| 1:A:94:LEU:HD21   | 1:A:119:ASP:CB    | 2.14                     | 0.72              |
| 5:F:419:ARG:CG    | 5:F:419:ARG:C     | 2.62                     | 0.72              |
| 2:M:10:ARG:HD2    | 8:M:9719:HOH:O    | 1.88                     | 0.72              |
| 2:M:145:GLY:HA3   | 2:M:276:LYS:HD2   | 1.70                     | 0.72              |
| 2:M:250:ARG:NH2   | 2:M:253:ALA:HB1   | 2.05                     | 0.72              |
| 2:M:266:ARG:HD2   | 8:M:9502:HOH:O    | 1.90                     | 0.72              |
| 2:M:490:GLU:HA    | 2:M:493:ARG:HD2   | 1.71                     | 0.72              |
| 2:M:1110:ASP:HA   | 8:M:9592:HOH:O    | 1.90                     | 0.72              |
| 2:C:690:ILE:HG21  | 2:C:833:LEU:HD21  | 1.72                     | 0.71              |
| 3:D:218:LYS:CB    | 3:D:373:PRO:HA    | 2.20                     | 0.71              |
| 2:M:727:PRO:HG2   | 2:M:785:VAL:HG12  | 1.70                     | 0.71              |
| 2:C:829:GLN:NE2   | 2:C:831:ARG:HD3   | 2.04                     | 0.71              |
| 2:C:1054:THR:HG23 | 2:C:1059:ASP:HB2  | 1.71                     | 0.71              |
| 4:E:40:LEU:HB2    | 4:E:45:ARG:CD     | 2.20                     | 0.71              |
| 1:K:206:THR:HG22  | 1:K:209:GLU:HG3   | 1.72                     | 0.71              |
| 3:N:133:ILE:HG21  | 3:N:454:ALA:HB1   | 1.72                     | 0.71              |
| 3:N:654:LYS:HB3   | 3:N:655:PRO:HD3   | 1.72                     | 0.71              |
| 3:N:808:THR:HB    | 3:N:809:PRO:HD3   | 1.70                     | 0.71              |
| 3:N:1438:ALA:O    | 3:N:1443:THR:HG22 | 1.89                     | 0.71              |
| 5:P:350:LEU:CD1   | 5:P:422:LEU:HB3   | 2.19                     | 0.71              |
| 5:P:368:VAL:O     | 5:P:372:ARG:HB2   | 1.90                     | 0.71              |
| 2:C:386:PHE:HA    | 8:C:9659:HOH:O    | 1.89                     | 0.71              |
| 1:K:110:LYS:HD3   | 8:K:2970:HOH:O    | 1.90                     | 0.71              |
| 2:M:264:PRO:HB3   | 2:M:289:THR:HG21  | 1.70                     | 0.71              |
| 2:M:943:VAL:HG13  | 2:M:985:GLY:H     | 1.56                     | 0.71              |
| 3:N:1279:GLY:O    | 3:N:1318:TYR:HA   | 1.91                     | 0.71              |
| 5:P:94:LEU:HD13   | 5:P:96:LEU:N      | 2.05                     | 0.71              |
| 1:A:123:MET:C     | 1:A:125:PRO:HD3   | 2.14                     | 0.71              |
| 1:B:38:ASN:HB3    | 1:B:39:PRO:HD3    | 1.71                     | 0.71              |
| 2:C:971:LYS:HA    | 2:C:988:VAL:HA    | 1.72                     | 0.71              |
| 3:N:1440:PHE:HB2  | 3:N:1442:ASN:HD21 | 1.56                     | 0.71              |
| 2:C:442:GLU:HB3   | 8:C:9551:HOH:O    | 1.88                     | 0.71              |
| 2:C:477:GLY:HA3   | 8:C:9519:HOH:O    | 1.90                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:14:PRO:HA     | 8:M:9924:HOH:O    | 1.89                     | 0.71              |
| 3:N:1459:LEU:HD11 | 3:N:1468:LEU:HD13 | 1.73                     | 0.71              |
| 2:C:53:PRO:HB3    | 8:C:2065:HOH:O    | 1.91                     | 0.71              |
| 2:C:328:LEU:HD13  | 2:C:433:THR:HB    | 1.71                     | 0.71              |
| 3:D:1262:LEU:HD21 | 3:D:1351:GLU:HG3  | 1.72                     | 0.71              |
| 5:F:393:THR:HG22  | 5:F:394:ARG:N     | 2.06                     | 0.71              |
| 1:K:34:VAL:HG22   | 1:K:181:VAL:HG21  | 1.73                     | 0.71              |
| 3:N:1258:ARG:HH21 | 3:N:1351:GLU:CG   | 1.99                     | 0.71              |
| 1:A:65:PHE:HE1    | 2:C:799:ILE:HD11  | 1.55                     | 0.71              |
| 2:C:1109:VAL:HG11 | 3:D:5:VAL:HG13    | 1.72                     | 0.71              |
| 3:D:119:SER:HB2   | 3:D:123:LEU:N     | 2.05                     | 0.71              |
| 3:D:1398:TRP:CH2  | 3:D:1415:VAL:HG11 | 2.26                     | 0.71              |
| 5:F:347:GLN:HB3   | 8:F:9613:HOH:O    | 1.90                     | 0.71              |
| 3:N:1109:GLU:HG2  | 3:N:1202:GLN:N    | 2.06                     | 0.71              |
| 2:C:383:ARG:HB2   | 2:C:383:ARG:NH1   | 2.06                     | 0.71              |
| 2:C:876:VAL:H     | 2:C:877:PRO:HD2   | 1.54                     | 0.71              |
| 1:K:123:MET:C     | 1:K:125:PRO:HD3   | 2.16                     | 0.71              |
| 1:K:143:ARG:HH11  | 1:K:143:ARG:CG    | 2.02                     | 0.71              |
| 1:L:123:MET:C     | 1:L:125:PRO:HD3   | 2.16                     | 0.71              |
| 2:M:21:ILE:HG22   | 8:M:9955:HOH:O    | 1.90                     | 0.71              |
| 3:N:902:LEU:HA    | 8:N:9832:HOH:O    | 1.90                     | 0.71              |
| 5:P:161:GLN:HG2   | 8:P:9608:HOH:O    | 1.89                     | 0.71              |
| 5:P:205:ARG:HG3   | 5:P:251:ILE:HD13  | 1.72                     | 0.71              |
| 5:P:413:SER:CB    | 5:P:419:ARG:HH21  | 2.02                     | 0.71              |
| 3:D:152:LEU:HD23  | 3:D:152:LEU:H     | 1.56                     | 0.71              |
| 4:E:40:LEU:HD21   | 4:E:67:GLU:HA     | 1.73                     | 0.71              |
| 5:F:164:LYS:HA    | 5:F:171:LYS:NZ    | 2.06                     | 0.71              |
| 2:M:1:MET:HE1     | 8:M:2194:HOH:O    | 1.91                     | 0.71              |
| 2:M:260:LEU:CA    | 2:M:291:ALA:HB1   | 2.19                     | 0.71              |
| 3:N:145:VAL:HG13  | 3:N:146:PRO:HD2   | 1.72                     | 0.71              |
| 1:A:39:PRO:HG2    | 1:B:39:PRO:HG2    | 1.73                     | 0.70              |
| 3:D:676:MET:HG3   | 8:D:9511:HOH:O    | 1.89                     | 0.70              |
| 3:D:742:GLY:HA3   | 8:D:2298:HOH:O    | 1.90                     | 0.70              |
| 5:F:358:LEU:HD11  | 5:F:370:LYS:CD    | 2.16                     | 0.70              |
| 3:N:1320:GLU:HB3  | 8:N:9773:HOH:O    | 1.91                     | 0.70              |
| 5:P:129:GLU:HB3   | 5:P:142:ARG:NH2   | 2.06                     | 0.70              |
| 2:C:198:ARG:NH2   | 2:C:203:ASP:HB3   | 2.05                     | 0.70              |
| 2:C:929:ARG:HG3   | 8:C:9628:HOH:O    | 1.91                     | 0.70              |
| 3:D:1262:LEU:HD23 | 3:D:1352:ILE:HG13 | 1.73                     | 0.70              |
| 3:N:806:PHE:HA    | 8:N:9498:HOH:O    | 1.91                     | 0.70              |
| 1:B:86:VAL:HG12   | 1:B:124:ASN:ND2   | 2.05                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:683:ASN:HA   | 2:C:687:ALA:HB3  | 1.72                     | 0.70              |
| 3:D:879:ARG:HG2  | 8:D:9489:HOH:O   | 1.89                     | 0.70              |
| 3:D:924:MET:HG2  | 8:D:9757:HOH:O   | 1.90                     | 0.70              |
| 1:L:221:HIS:HA   | 1:L:224:TYR:CD2  | 2.26                     | 0.70              |
| 3:N:728:LEU:HD22 | 3:N:745:MET:SD   | 2.31                     | 0.70              |
| 3:N:955:VAL:O    | 3:N:1039:CYS:HB3 | 1.90                     | 0.70              |
| 3:N:1465:ASN:ND2 | 3:N:1473:PRO:HG3 | 2.06                     | 0.70              |
| 5:P:291:ILE:HG21 | 5:P:304:VAL:HG11 | 1.72                     | 0.70              |
| 1:K:127:LEU:HD12 | 1:K:128:HIS:N    | 2.07                     | 0.70              |
| 2:M:1056:LYS:O   | 3:N:624:ASP:HB2  | 1.92                     | 0.70              |
| 1:B:78:ILE:HA    | 8:B:9519:HOH:O   | 1.91                     | 0.70              |
| 3:D:102:ILE:HD12 | 3:D:579:ASP:HB3  | 1.73                     | 0.70              |
| 2:M:874:LEU:HD21 | 3:N:787:LEU:HD22 | 1.72                     | 0.70              |
| 3:N:1209:LEU:CD1 | 3:N:1216:SER:H   | 2.03                     | 0.70              |
| 1:A:14:ARG:HB3   | 8:A:9617:HOH:O   | 1.92                     | 0.70              |
| 2:C:139:GLN:O    | 2:C:333:ILE:HA   | 1.90                     | 0.70              |
| 2:C:475:VAL:HA   | 8:C:2211:HOH:O   | 1.91                     | 0.70              |
| 2:C:1018:GLN:HG3 | 2:C:1083:GLU:HG3 | 1.74                     | 0.70              |
| 3:D:30:GLU:HB3   | 3:D:40:GLU:HB3   | 1.72                     | 0.70              |
| 3:D:474:GLU:HA   | 8:D:9706:HOH:O   | 1.91                     | 0.70              |
| 5:F:92:PRO:HG2   | 8:F:9678:HOH:O   | 1.91                     | 0.70              |
| 3:N:491:LYS:HE3  | 8:N:2434:HOH:O   | 1.91                     | 0.70              |
| 5:P:408:LEU:HD23 | 5:P:409:LYS:N    | 2.07                     | 0.70              |
| 3:D:18:ILE:HD12  | 3:D:518:PRO:HG3  | 1.72                     | 0.70              |
| 1:K:67:THR:HG22  | 8:K:913:HOH:O    | 1.91                     | 0.70              |
| 2:M:123:GLU:HA   | 8:M:9669:HOH:O   | 1.91                     | 0.70              |
| 3:N:508:ARG:HG2  | 3:N:509:PRO:HD2  | 1.73                     | 0.70              |
| 3:N:777:PRO:HG2  | 3:N:915:VAL:HB   | 1.72                     | 0.70              |
| 3:N:1490:LYS:NZ  | 4:O:39:VAL:HA    | 2.05                     | 0.70              |
| 2:C:254:VAL:O    | 2:C:257:VAL:HG23 | 1.91                     | 0.70              |
| 1:L:80:LEU:HB3   | 8:N:9812:HOH:O   | 1.91                     | 0.70              |
| 1:L:87:VAL:HG21  | 1:L:144:VAL:HG11 | 1.74                     | 0.70              |
| 2:M:904:PRO:HB2  | 2:M:907:ASP:O    | 1.91                     | 0.70              |
| 3:N:1213:ARG:HB2 | 3:N:1214:PRO:CD  | 2.22                     | 0.70              |
| 2:C:588:VAL:HB   | 8:C:9533:HOH:O   | 1.92                     | 0.70              |
| 2:C:1005:MET:HE1 | 3:D:645:PRO:CG   | 2.21                     | 0.70              |
| 3:D:379:ALA:HB3  | 8:D:2234:HOH:O   | 1.91                     | 0.70              |
| 3:D:1046:GLN:HA  | 3:D:1052:THR:HA  | 1.73                     | 0.70              |
| 5:F:137:GLY:HA3  | 5:F:140:ARG:HH12 | 1.56                     | 0.70              |
| 5:F:207:LEU:HB3  | 5:F:212:LEU:HG   | 1.73                     | 0.70              |
| 1:L:137:ARG:HG2  | 1:L:137:ARG:HH11 | 1.57                     | 0.70              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:P:371:LEU:HD22  | 5:P:375:LEU:CD1  | 2.22                     | 0.70              |
| 2:C:11:GLU:HG2    | 2:C:537:LYS:NZ   | 2.07                     | 0.70              |
| 2:C:73:LEU:HB3    | 2:C:93:PRO:O     | 1.91                     | 0.70              |
| 2:C:91:GLN:OE1    | 2:C:117:HIS:HB3  | 1.92                     | 0.70              |
| 2:C:391:LEU:HA    | 8:C:9691:HOH:O   | 1.92                     | 0.70              |
| 2:C:881:ASN:HD22  | 2:C:881:ASN:H    | 1.38                     | 0.70              |
| 2:M:1014:SER:HB3  | 2:M:1017:THR:O   | 1.92                     | 0.70              |
| 3:N:30:GLU:HG3    | 3:N:41:ARG:HE    | 1.57                     | 0.70              |
| 3:N:477:LEU:HD22  | 3:N:492:ALA:HB1  | 1.72                     | 0.70              |
| 3:N:490:ALA:HA    | 8:N:9506:HOH:O   | 1.92                     | 0.70              |
| 3:N:675:ARG:O     | 3:N:678:GLU:HG2  | 1.92                     | 0.70              |
| 1:A:221:HIS:HA    | 1:A:224:TYR:CD2  | 2.27                     | 0.69              |
| 2:C:34:VAL:HG12   | 8:C:9992:HOH:O   | 1.92                     | 0.69              |
| 2:C:328:LEU:HD11  | 2:C:434:HIS:CD2  | 2.27                     | 0.69              |
| 2:C:428:ARG:HH21  | 2:C:451:LEU:HD11 | 1.56                     | 0.69              |
| 3:D:1299:PHE:HB2  | 8:D:2268:HOH:O   | 1.92                     | 0.69              |
| 1:K:34:VAL:HG21   | 2:M:939:ARG:NH2  | 2.07                     | 0.69              |
| 2:M:563:ASN:HB3   | 8:M:2167:HOH:O   | 1.90                     | 0.69              |
| 2:M:729:LEU:HD11  | 8:P:9571:HOH:O   | 1.92                     | 0.69              |
| 2:M:829:GLN:HB2   | 8:M:9535:HOH:O   | 1.90                     | 0.69              |
| 2:M:1043:TYR:CE2  | 3:N:763:MET:HA   | 2.27                     | 0.69              |
| 5:P:162:LYS:HG3   | 8:P:9778:HOH:O   | 1.92                     | 0.69              |
| 5:P:366:ALA:O     | 5:P:370:LYS:HB3  | 1.92                     | 0.69              |
| 2:C:260:LEU:CA    | 2:C:291:ALA:HB1  | 2.22                     | 0.69              |
| 2:C:266:ARG:H     | 2:C:266:ARG:HD2  | 1.57                     | 0.69              |
| 2:C:454:SER:HB3   | 8:C:9803:HOH:O   | 1.91                     | 0.69              |
| 3:D:171:LEU:HB3   | 3:D:390:PRO:HA   | 1.72                     | 0.69              |
| 3:D:196:VAL:HG13  | 3:D:202:VAL:HG11 | 1.72                     | 0.69              |
| 3:D:1109:GLU:HG2  | 3:D:1202:GLN:H   | 1.55                     | 0.69              |
| 2:M:580:MET:O     | 2:M:903:SER:N    | 2.25                     | 0.69              |
| 2:M:832:LYS:HB2   | 8:M:2063:HOH:O   | 1.92                     | 0.69              |
| 2:M:1111:ILE:HG13 | 2:M:1112:PHE:H   | 1.54                     | 0.69              |
| 3:N:136:ASP:CB    | 3:N:137:PRO:HD3  | 2.21                     | 0.69              |
| 3:N:168:THR:C     | 3:N:170:PRO:HD3  | 2.17                     | 0.69              |
| 3:N:1061:PHE:HA   | 8:N:9640:HOH:O   | 1.90                     | 0.69              |
| 5:P:348:SER:HA    | 8:P:9549:HOH:O   | 1.91                     | 0.69              |
| 2:C:1101:THR:HG22 | 3:D:8:VAL:HG22   | 1.74                     | 0.69              |
| 2:C:1115:LEU:HD23 | 3:D:85:VAL:HA    | 1.74                     | 0.69              |
| 3:D:168:THR:HB    | 3:D:393:ILE:HG13 | 1.75                     | 0.69              |
| 3:D:564:GLU:HA    | 3:D:567:ILE:HD12 | 1.74                     | 0.69              |
| 2:M:343:GLN:HG2   | 2:M:385:PHE:HB2  | 1.73                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:768:THR:HB    | 2:M:771:GLU:HB3   | 1.75                     | 0.69              |
| 3:N:55:ASP:HB3    | 3:N:82:LYS:HE2    | 1.74                     | 0.69              |
| 3:D:35:ARG:HD2    | 8:D:9736:HOH:O    | 1.92                     | 0.69              |
| 5:F:371:LEU:HD22  | 5:F:375:LEU:CD1   | 2.22                     | 0.69              |
| 1:K:38:ASN:HB3    | 1:K:39:PRO:HD3    | 1.74                     | 0.69              |
| 1:L:86:VAL:HG12   | 1:L:124:ASN:ND2   | 2.07                     | 0.69              |
| 2:M:461:VAL:CG1   | 2:M:465:GLY:HA2   | 2.22                     | 0.69              |
| 3:N:18:ILE:HG21   | 3:N:516:ALA:O     | 1.92                     | 0.69              |
| 5:P:87:GLU:O      | 5:P:91:VAL:HG23   | 1.92                     | 0.69              |
| 2:C:341:THR:HG23  | 2:C:345:ARG:NH2   | 2.08                     | 0.69              |
| 2:C:557:ARG:NH1   | 2:C:879:ARG:HG2   | 2.07                     | 0.69              |
| 2:C:675:ALA:HB2   | 2:C:867:VAL:HG11  | 1.73                     | 0.69              |
| 3:D:434:ARG:HB2   | 3:D:447:VAL:HG22  | 1.72                     | 0.69              |
| 3:D:459:GLU:HB3   | 8:D:2363:HOH:O    | 1.92                     | 0.69              |
| 3:D:1410:GLU:HG3  | 8:D:2074:HOH:O    | 1.92                     | 0.69              |
| 1:K:91:ASN:CG     | 1:K:92:PRO:HD2    | 2.18                     | 0.69              |
| 2:M:44:ILE:HD11   | 2:M:340:MET:HE1   | 1.75                     | 0.69              |
| 2:M:848:VAL:HB    | 3:N:740:PHE:O     | 1.91                     | 0.69              |
| 3:N:177:ALA:CB    | 3:N:199:LEU:HD22  | 2.21                     | 0.69              |
| 3:N:624:ASP:N     | 8:N:2406:HOH:O    | 2.25                     | 0.69              |
| 2:C:42:VAL:HG12   | 2:C:43:GLY:H      | 1.58                     | 0.69              |
| 3:D:1047:LYS:HB3  | 3:D:1048:PRO:CD   | 2.22                     | 0.69              |
| 3:D:1307:LYS:HE3  | 8:D:2368:HOH:O    | 1.91                     | 0.69              |
| 1:L:22:GLU:HG2    | 1:L:198:ARG:HG2   | 1.74                     | 0.69              |
| 3:N:50:PHE:HB3    | 3:N:522:PRO:HG2   | 1.75                     | 0.69              |
| 3:N:1262:LEU:HD23 | 3:N:1352:ILE:HG13 | 1.74                     | 0.69              |
| 4:O:94:PRO:HA     | 8:O:893:HOH:O     | 1.93                     | 0.69              |
| 1:B:23:PHE:CE1    | 1:B:208:LEU:HD13  | 2.27                     | 0.69              |
| 2:C:162:ILE:HD12  | 2:C:172:ILE:HB    | 1.74                     | 0.69              |
| 2:C:676:ILE:CG2   | 2:C:988:VAL:HG13  | 2.23                     | 0.69              |
| 1:K:94:LEU:HD21   | 1:K:119:ASP:CB    | 2.23                     | 0.69              |
| 8:K:4458:HOH:O    | 1:L:11:PHE:HB2    | 1.93                     | 0.69              |
| 2:M:52:PHE:CD2    | 2:M:68:PHE:HB2    | 2.28                     | 0.69              |
| 3:N:661:MET:HE3   | 3:N:673:ALA:HB1   | 1.75                     | 0.69              |
| 1:A:87:VAL:HG21   | 1:A:144:VAL:HG11  | 1.74                     | 0.69              |
| 2:C:149:THR:HB    | 8:C:9648:HOH:O    | 1.91                     | 0.69              |
| 2:C:1054:THR:HG21 | 2:C:1079:PRO:CB   | 2.22                     | 0.69              |
| 3:D:148:GLU:HB3   | 3:D:151:GLN:CB    | 2.20                     | 0.69              |
| 3:D:524:LEU:C     | 3:D:526:PRO:HD3   | 2.18                     | 0.69              |
| 3:D:897:TRP:CZ2   | 3:D:902:LEU:HD21  | 2.28                     | 0.69              |
| 5:F:330:GLY:HA2   | 5:F:333:ILE:HD12  | 1.75                     | 0.69              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:59:GLU:HG3    | 1:K:60:ASP:H     | 1.57                     | 0.69              |
| 1:K:87:VAL:HG21   | 1:K:144:VAL:HG11 | 1.75                     | 0.69              |
| 1:L:59:GLU:HG3    | 1:L:60:ASP:H     | 1.57                     | 0.69              |
| 2:M:570:PRO:HA    | 8:M:9977:HOH:O   | 1.91                     | 0.69              |
| 2:M:930:LYS:HA    | 8:M:2157:HOH:O   | 1.91                     | 0.69              |
| 3:N:128:TYR:CE1   | 3:N:461:ILE:HG13 | 2.27                     | 0.69              |
| 3:N:984:THR:HG23  | 3:N:987:GLU:H    | 1.58                     | 0.69              |
| 3:N:997:THR:HG23  | 8:N:9593:HOH:O   | 1.93                     | 0.69              |
| 2:C:283:ILE:HG22  | 2:C:284:ARG:HG3  | 1.75                     | 0.69              |
| 3:D:474:GLU:O     | 3:D:478:LEU:HG   | 1.92                     | 0.69              |
| 5:F:209:PHE:O     | 5:F:213:ILE:HG13 | 1.93                     | 0.69              |
| 2:M:1105:LYS:HD2  | 8:M:9576:HOH:O   | 1.92                     | 0.69              |
| 3:N:52:PRO:HG3    | 3:N:80:VAL:HG23  | 1.75                     | 0.69              |
| 3:N:125:GLN:HG2   | 8:N:9888:HOH:O   | 1.93                     | 0.69              |
| 3:N:171:LEU:HD23  | 3:N:390:PRO:HG3  | 1.75                     | 0.69              |
| 3:N:404:GLU:OE1   | 3:N:414:ARG:HD3  | 1.92                     | 0.69              |
| 3:N:422:ALA:HB3   | 3:N:427:VAL:CG2  | 2.23                     | 0.69              |
| 3:N:1264:GLU:O    | 3:N:1266:ARG:HG3 | 1.92                     | 0.69              |
| 3:N:1327:ARG:HB3  | 8:N:9839:HOH:O   | 1.93                     | 0.69              |
| 5:P:351:SER:O     | 5:P:355:GLU:HB2  | 1.92                     | 0.69              |
| 1:A:67:THR:HG21   | 2:C:609:ASN:HD21 | 1.57                     | 0.69              |
| 1:B:176:ARG:HH22  | 3:D:884:ARG:NE   | 1.90                     | 0.69              |
| 2:C:575:GLN:H     | 2:C:667:ALA:HB1  | 1.58                     | 0.69              |
| 2:C:841:ASN:HD22  | 2:C:841:ASN:C    | 2.01                     | 0.69              |
| 2:C:1094:ALA:HB3  | 3:D:603:LEU:HD22 | 1.75                     | 0.69              |
| 3:D:432:TYR:HD2   | 8:D:9724:HOH:O   | 1.76                     | 0.69              |
| 5:F:273:ARG:HA    | 5:F:276:ARG:HG3  | 1.76                     | 0.69              |
| 2:M:553:ASP:HA    | 2:M:881:ASN:HA   | 1.74                     | 0.69              |
| 2:M:1045:ALA:HA   | 3:N:758:GLU:CD   | 2.17                     | 0.69              |
| 3:N:96:ALA:HB1    | 3:N:554:LEU:HD12 | 1.73                     | 0.69              |
| 3:N:149:LYS:H     | 3:N:149:LYS:CD   | 2.01                     | 0.69              |
| 3:N:218:LYS:CB    | 3:N:373:PRO:HA   | 2.23                     | 0.69              |
| 3:N:496:LEU:HD23  | 3:N:500:ARG:HG3  | 1.75                     | 0.69              |
| 3:N:1311:LEU:HD23 | 3:N:1311:LEU:H   | 1.58                     | 0.69              |
| 2:C:260:LEU:HA    | 2:C:291:ALA:HB2  | 1.74                     | 0.68              |
| 2:C:490:GLU:HB3   | 8:C:9678:HOH:O   | 1.92                     | 0.68              |
| 2:C:730:SER:O     | 2:C:734:LEU:HD23 | 1.92                     | 0.68              |
| 8:C:9511:HOH:O    | 3:D:13:ALA:HA    | 1.92                     | 0.68              |
| 3:D:223:LEU:HA    | 8:D:9492:HOH:O   | 1.93                     | 0.68              |
| 3:D:702:LEU:HD23  | 3:D:745:MET:CE   | 2.22                     | 0.68              |
| 5:F:93:LEU:HG     | 5:F:190:ALA:CB   | 2.22                     | 0.68              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:95:GLN:HG3    | 8:K:802:HOH:O    | 1.92                     | 0.68              |
| 2:M:432:ARG:HH22  | 3:N:1047:LYS:HD3 | 1.58                     | 0.68              |
| 2:M:783:ARG:O     | 2:M:785:VAL:N    | 2.26                     | 0.68              |
| 5:P:316:SER:OG    | 5:P:318:GLU:HG3  | 1.93                     | 0.68              |
| 1:A:9:PRO:HD2     | 1:B:224:TYR:CE1  | 2.27                     | 0.68              |
| 1:B:5:LYS:O       | 1:B:8:ALA:HB2    | 1.92                     | 0.68              |
| 1:B:59:GLU:HG3    | 1:B:60:ASP:H     | 1.58                     | 0.68              |
| 2:C:283:ILE:HG21  | 8:C:9739:HOH:O   | 1.93                     | 0.68              |
| 2:C:292:ARG:NH1   | 2:C:299:LYS:HD3  | 2.09                     | 0.68              |
| 3:D:1009:LYS:O    | 3:D:1013:GLU:HG2 | 1.93                     | 0.68              |
| 3:D:1162:GLU:HB2  | 8:D:9602:HOH:O   | 1.92                     | 0.68              |
| 3:D:1218:GLY:HA2  | 8:D:9761:HOH:O   | 1.93                     | 0.68              |
| 1:K:5:LYS:O       | 1:K:8:ALA:HB2    | 1.93                     | 0.68              |
| 3:N:1036:ARG:HH21 | 3:N:1042:ARG:HA  | 1.58                     | 0.68              |
| 4:O:41:GLU:HB3    | 8:O:3641:HOH:O   | 1.94                     | 0.68              |
| 5:P:232:ARG:HG2   | 8:P:9663:HOH:O   | 1.93                     | 0.68              |
| 5:P:413:SER:HA    | 5:P:419:ARG:NE   | 2.07                     | 0.68              |
| 1:B:90:LEU:HD12   | 8:B:9478:HOH:O   | 1.94                     | 0.68              |
| 1:B:191:ASP:HB2   | 8:B:9576:HOH:O   | 1.93                     | 0.68              |
| 2:C:69:LEU:HD12   | 2:C:97:ARG:HB3   | 1.76                     | 0.68              |
| 2:C:760:SER:O     | 2:C:785:VAL:HG22 | 1.93                     | 0.68              |
| 2:C:876:VAL:HG22  | 2:C:884:GLN:NE2  | 2.08                     | 0.68              |
| 3:D:55:ASP:HA     | 3:D:82:LYS:HG2   | 1.74                     | 0.68              |
| 3:D:1209:LEU:HD23 | 3:D:1211:MET:HE2 | 1.74                     | 0.68              |
| 3:D:1314:LYS:HZ1  | 3:D:1317:ASP:HB2 | 1.57                     | 0.68              |
| 5:F:118:GLU:HB3   | 8:F:9490:HOH:O   | 1.92                     | 0.68              |
| 1:K:139:ASN:HB2   | 8:K:845:HOH:O    | 1.92                     | 0.68              |
| 2:M:725:ASP:O     | 2:M:727:PRO:HD3  | 1.92                     | 0.68              |
| 2:C:728:HIS:O     | 2:C:729:LEU:HD22 | 1.93                     | 0.68              |
| 1:L:38:ASN:HB3    | 1:L:39:PRO:HD3   | 1.74                     | 0.68              |
| 1:L:106:PRO:HB2   | 8:L:1100:HOH:O   | 1.92                     | 0.68              |
| 2:M:231:PRO:HA    | 8:M:9534:HOH:O   | 1.93                     | 0.68              |
| 3:N:135:LEU:HD11  | 3:N:452:ILE:HD11 | 1.75                     | 0.68              |
| 3:N:660:LYS:HD3   | 8:N:9491:HOH:O   | 1.91                     | 0.68              |
| 2:C:31:GLN:OE1    | 2:C:40:GLU:HB2   | 1.93                     | 0.68              |
| 3:D:443:VAL:HG21  | 8:D:9877:HOH:O   | 1.93                     | 0.68              |
| 3:D:550:ARG:HD3   | 8:D:9518:HOH:O   | 1.93                     | 0.68              |
| 3:D:863:VAL:HG23  | 8:D:9469:HOH:O   | 1.93                     | 0.68              |
| 3:D:1312:LEU:HD12 | 3:D:1326:THR:O   | 1.93                     | 0.68              |
| 3:D:1327:ARG:HD2  | 8:D:9883:HOH:O   | 1.91                     | 0.68              |
| 3:D:1412:LYS:HD2  | 3:D:1414:PRO:HG3 | 1.74                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:130:VAL:HG21  | 5:F:159:ILE:HG21  | 1.76                     | 0.68              |
| 2:M:250:ARG:HB3   | 2:M:253:ALA:CB    | 2.24                     | 0.68              |
| 3:N:824:ASN:HB2   | 8:N:9847:HOH:O    | 1.93                     | 0.68              |
| 3:N:861:GLN:HE21  | 3:N:861:GLN:N     | 1.79                     | 0.68              |
| 3:N:1232:PRO:HB3  | 3:N:1361:VAL:HG21 | 1.75                     | 0.68              |
| 1:A:86:VAL:HG12   | 1:A:124:ASN:ND2   | 2.08                     | 0.68              |
| 2:C:580:MET:HB3   | 2:C:584:GLU:CD    | 2.18                     | 0.68              |
| 2:C:906:PHE:CD1   | 3:D:1067:VAL:HG22 | 2.29                     | 0.68              |
| 3:D:235:ALA:HA    | 8:D:9481:HOH:O    | 1.93                     | 0.68              |
| 3:D:970:LYS:HD2   | 3:D:995:LEU:HD13  | 1.74                     | 0.68              |
| 5:F:401:GLU:O     | 5:F:405:LEU:HB2   | 1.92                     | 0.68              |
| 1:L:34:VAL:HG22   | 1:L:181:VAL:HG21  | 1.74                     | 0.68              |
| 2:C:12:VAL:HG12   | 8:C:2224:HOH:O    | 1.94                     | 0.68              |
| 3:D:149:LYS:H     | 3:D:149:LYS:CD    | 2.06                     | 0.68              |
| 3:D:1336:LEU:HD22 | 3:D:1421:LEU:HB2  | 1.76                     | 0.68              |
| 4:E:74:VAL:HG12   | 4:E:79:LEU:HD21   | 1.75                     | 0.68              |
| 1:K:227:ASN:HD22  | 1:K:227:ASN:H     | 1.39                     | 0.68              |
| 1:L:94:LEU:HD21   | 1:L:119:ASP:CB    | 2.09                     | 0.68              |
| 1:L:137:ARG:HH12  | 1:L:139:ASN:CB    | 2.07                     | 0.68              |
| 3:N:1468:LEU:HD22 | 3:N:1470:ARG:HB2  | 1.76                     | 0.68              |
| 5:P:367:MET:HE2   | 5:P:371:LEU:HD11  | 1.76                     | 0.68              |
| 2:C:264:PRO:HB3   | 2:C:289:THR:CG2   | 2.24                     | 0.68              |
| 2:C:326:ASP:HB2   | 8:C:9825:HOH:O    | 1.92                     | 0.68              |
| 2:C:432:ARG:HG3   | 8:C:9911:HOH:O    | 1.93                     | 0.68              |
| 2:C:589:ARG:HD3   | 2:C:596:TYR:CE1   | 2.29                     | 0.68              |
| 2:C:694:LEU:HD23  | 2:C:697:ARG:HH21  | 1.58                     | 0.68              |
| 2:M:73:LEU:CD2    | 2:M:94:LEU:HB2    | 2.24                     | 0.68              |
| 3:N:1422:MET:CE   | 3:N:1427:SER:HA   | 2.23                     | 0.68              |
| 5:P:148:LYS:HD2   | 8:P:9482:HOH:O    | 1.92                     | 0.68              |
| 2:C:65:VAL:O      | 2:C:101:ILE:HG12  | 1.93                     | 0.68              |
| 2:C:352:ALA:HA    | 2:C:355:VAL:HG12  | 1.76                     | 0.68              |
| 2:C:952:LEU:HD12  | 2:C:969:GLN:HE22  | 1.58                     | 0.68              |
| 3:D:33:ASN:HB2    | 3:D:40:GLU:OE1    | 1.93                     | 0.68              |
| 3:D:422:ALA:HB1   | 5:F:178:ARG:HH12  | 1.59                     | 0.68              |
| 1:L:151:VAL:HB    | 1:L:169:ALA:HB3   | 1.74                     | 0.68              |
| 1:L:206:THR:HG22  | 1:L:209:GLU:H     | 1.57                     | 0.68              |
| 3:N:386:HIS:O     | 5:P:96:LEU:HD12   | 1.94                     | 0.68              |
| 3:N:795:VAL:HG23  | 3:N:879:ARG:NH2   | 2.09                     | 0.68              |
| 3:N:1046:GLN:HA   | 3:N:1052:THR:HA   | 1.76                     | 0.68              |
| 2:C:889:HIS:HE1   | 3:D:951:ILE:H     | 1.38                     | 0.68              |
| 3:D:417:PRO:HB2   | 8:D:9534:HOH:O    | 1.92                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:98:THR:HG21   | 8:K:2063:HOH:O    | 1.93                     | 0.68              |
| 3:N:908:LYS:HG2   | 8:N:9858:HOH:O    | 1.94                     | 0.68              |
| 3:N:957:PRO:HG2   | 3:N:1007:VAL:HG12 | 1.76                     | 0.68              |
| 2:C:691:SER:HB2   | 2:C:858:MET:SD    | 2.34                     | 0.67              |
| 2:C:734:LEU:HA    | 2:C:737:LEU:HD12  | 1.76                     | 0.67              |
| 4:E:23:VAL:HG21   | 4:E:65:MET:HG2    | 1.76                     | 0.67              |
| 2:M:135:VAL:HB    | 2:M:406:HIS:CE1   | 2.29                     | 0.67              |
| 2:M:198:ARG:HG2   | 8:M:9515:HOH:O    | 1.93                     | 0.67              |
| 2:M:950:LEU:HB3   | 2:M:952:LEU:HD23  | 1.77                     | 0.67              |
| 3:N:131:LYS:HB3   | 3:N:456:MET:HE3   | 1.74                     | 0.67              |
| 3:N:1083:ASP:O    | 3:N:1087:ARG:HG2  | 1.93                     | 0.67              |
| 5:P:234:LYS:HE3   | 5:P:236:SER:HB2   | 1.74                     | 0.67              |
| 1:B:11:PHE:HD1    | 1:B:25:LEU:HD12   | 1.58                     | 0.67              |
| 1:B:195:LEU:HD12  | 1:B:196:THR:N     | 2.08                     | 0.67              |
| 2:C:342:ASP:HA    | 2:C:345:ARG:HE    | 1.59                     | 0.67              |
| 2:C:1005:MET:SD   | 3:D:648:MET:HB2   | 2.34                     | 0.67              |
| 2:C:1081:VAL:HB   | 2:C:1086:ARG:HH21 | 1.59                     | 0.67              |
| 2:C:1095:LEU:HA   | 3:D:582:LEU:HD22  | 1.73                     | 0.67              |
| 3:D:133:ILE:HD12  | 8:D:2265:HOH:O    | 1.94                     | 0.67              |
| 3:D:1162:GLU:HB3  | 8:D:2357:HOH:O    | 1.93                     | 0.67              |
| 2:M:484:VAL:HG22  | 8:M:9670:HOH:O    | 1.94                     | 0.67              |
| 2:M:1046:ALA:CB   | 3:N:1476:THR:HB   | 2.24                     | 0.67              |
| 3:N:558:LEU:HB3   | 5:P:145:PRO:HB3   | 1.75                     | 0.67              |
| 3:N:617:ASN:C     | 3:N:619:LEU:H     | 2.01                     | 0.67              |
| 3:N:861:GLN:HA    | 8:N:9914:HOH:O    | 1.94                     | 0.67              |
| 3:N:1192:LEU:HD22 | 3:N:1345:GLU:CD   | 2.18                     | 0.67              |
| 3:N:1397:LYS:HZ1  | 3:N:1432:LYS:HB3  | 1.56                     | 0.67              |
| 4:O:51:LEU:HD12   | 4:O:52:GLU:H      | 1.57                     | 0.67              |
| 3:D:775:GLY:HA3   | 3:D:1145:TYR:CE1  | 2.29                     | 0.67              |
| 3:D:818:ARG:HA    | 8:D:2054:HOH:O    | 1.94                     | 0.67              |
| 2:M:1018:GLN:HG3  | 2:M:1060:ILE:HD11 | 1.75                     | 0.67              |
| 1:A:93:SER:HB3    | 8:A:9454:HOH:O    | 1.95                     | 0.67              |
| 1:B:39:PRO:O      | 1:B:43:ILE:HG12   | 1.94                     | 0.67              |
| 2:C:64:LEU:HD11   | 8:C:9904:HOH:O    | 1.94                     | 0.67              |
| 2:C:221:LEU:HG    | 8:C:9564:HOH:O    | 1.94                     | 0.67              |
| 2:C:571:LEU:HD23  | 2:C:700:TYR:HA    | 1.75                     | 0.67              |
| 3:D:149:LYS:H     | 3:D:149:LYS:HE2   | 1.59                     | 0.67              |
| 3:D:177:ALA:HB1   | 3:D:199:LEU:HD22  | 1.76                     | 0.67              |
| 3:D:1452:ILE:HD12 | 8:D:9532:HOH:O    | 1.94                     | 0.67              |
| 5:F:356:LYS:HG2   | 8:F:9639:HOH:O    | 1.95                     | 0.67              |
| 1:K:11:PHE:HB3    | 8:L:679:HOH:O     | 1.95                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:568:ALA:HB3   | 2:M:668:LEU:HD22  | 1.75                     | 0.67              |
| 1:A:227:ASN:H     | 1:A:227:ASN:HD22  | 1.40                     | 0.67              |
| 2:C:601:GLY:HA2   | 2:C:616:GLU:HG2   | 1.76                     | 0.67              |
| 3:D:127:LEU:HD11  | 3:D:461:ILE:HD11  | 1.76                     | 0.67              |
| 3:D:154:THR:HG22  | 3:D:156:GLU:H     | 1.60                     | 0.67              |
| 1:L:73:GLU:OE1    | 1:L:130:ALA:HA    | 1.95                     | 0.67              |
| 2:M:655:LEU:HD11  | 8:M:9608:HOH:O    | 1.94                     | 0.67              |
| 2:M:676:ILE:CG2   | 2:M:988:VAL:HG13  | 2.25                     | 0.67              |
| 3:N:1422:MET:HE3  | 3:N:1427:SER:HA   | 1.76                     | 0.67              |
| 1:A:110:LYS:HE2   | 8:A:9467:HOH:O    | 1.93                     | 0.67              |
| 1:B:176:ARG:HH22  | 3:D:884:ARG:HD3   | 1.60                     | 0.67              |
| 2:C:185:LYS:HD2   | 8:C:9927:HOH:O    | 1.93                     | 0.67              |
| 2:C:328:LEU:HD11  | 2:C:434:HIS:HD2   | 1.60                     | 0.67              |
| 2:C:1021:LEU:HG   | 2:C:1022:GLY:N    | 2.07                     | 0.67              |
| 2:C:1074:GLU:HG2  | 2:C:1075:ASP:N    | 2.10                     | 0.67              |
| 3:D:93:ILE:HG12   | 3:D:548:ILE:HD11  | 1.77                     | 0.67              |
| 3:D:422:ALA:HB3   | 3:D:427:VAL:CG2   | 2.24                     | 0.67              |
| 3:D:756:GLN:O     | 3:D:760:ARG:HG2   | 1.95                     | 0.67              |
| 2:M:148:PHE:CZ    | 2:M:281:LEU:HD22  | 2.29                     | 0.67              |
| 2:M:1004:LYS:HE2  | 2:M:1027:PHE:CZ   | 2.29                     | 0.67              |
| 5:P:291:ILE:CG2   | 5:P:304:VAL:HG21  | 2.24                     | 0.67              |
| 1:A:59:GLU:HG3    | 1:A:60:ASP:H      | 1.59                     | 0.67              |
| 1:B:172:SER:HB2   | 8:B:9529:HOH:O    | 1.94                     | 0.67              |
| 1:B:176:ARG:HH22  | 3:D:884:ARG:CD    | 2.08                     | 0.67              |
| 3:D:1459:LEU:HB3  | 3:D:1465:ASN:HD22 | 1.59                     | 0.67              |
| 2:M:1054:THR:HG21 | 2:M:1079:PRO:CB   | 2.23                     | 0.67              |
| 3:N:785:ILE:HG22  | 3:N:789:LEU:HD12  | 1.76                     | 0.67              |
| 3:N:1295:GLU:HB3  | 3:N:1300:SER:OG   | 1.94                     | 0.67              |
| 3:N:1389:LEU:HD23 | 3:N:1389:LEU:N    | 2.06                     | 0.67              |
| 5:P:214:GLN:HA    | 5:P:217:ASN:ND2   | 2.09                     | 0.67              |
| 1:B:133:GLU:HG3   | 1:B:134:GLU:N     | 2.09                     | 0.67              |
| 2:C:66:LEU:HD13   | 2:C:100:LEU:HB3   | 1.76                     | 0.67              |
| 2:C:256:TYR:HE1   | 2:C:293:PHE:HB2   | 1.59                     | 0.67              |
| 2:M:135:VAL:HB    | 2:M:406:HIS:HE1   | 1.60                     | 0.67              |
| 2:M:136:ILE:HD13  | 2:M:392:SER:HB2   | 1.76                     | 0.67              |
| 2:M:810:ASP:HB3   | 2:M:813:VAL:HG22  | 1.77                     | 0.67              |
| 3:N:1489:GLN:HE22 | 3:N:1492:LEU:HG   | 1.60                     | 0.67              |
| 3:D:550:ARG:HA    | 8:D:9518:HOH:O    | 1.94                     | 0.67              |
| 5:F:88:ILE:HD13   | 5:F:193:ARG:HB2   | 1.75                     | 0.67              |
| 5:F:366:ALA:O     | 5:F:370:LYS:HB3   | 1.94                     | 0.67              |
| 2:M:352:ALA:HA    | 2:M:355:VAL:HG12  | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:445:GLU:HG2   | 8:M:9829:HOH:O    | 1.94                     | 0.67              |
| 3:N:777:PRO:HD2   | 3:N:912:LYS:HG2   | 1.75                     | 0.67              |
| 5:P:257:THR:HB    | 5:P:314:PRO:HG2   | 1.75                     | 0.67              |
| 1:A:18:ARG:NH1    | 1:A:88:ARG:HE     | 1.93                     | 0.67              |
| 1:A:191:ASP:HB2   | 8:C:9606:HOH:O    | 1.95                     | 0.67              |
| 1:B:32:PHE:HB3    | 8:B:9655:HOH:O    | 1.94                     | 0.67              |
| 1:B:87:VAL:HG21   | 1:B:144:VAL:HG11  | 1.77                     | 0.67              |
| 2:C:944:LEU:HD21  | 2:C:963:LEU:HD23  | 1.77                     | 0.67              |
| 3:D:817:GLU:O     | 3:D:821:VAL:HG23  | 1.95                     | 0.67              |
| 3:D:1211:MET:HE1  | 4:E:16:LYS:HE3    | 1.77                     | 0.67              |
| 2:M:185:LYS:HD2   | 8:M:9773:HOH:O    | 1.95                     | 0.67              |
| 2:M:841:ASN:HD21  | 2:M:843:HIS:CD2   | 2.13                     | 0.67              |
| 2:M:966:LEU:HD11  | 2:M:986:PRO:HG2   | 1.76                     | 0.67              |
| 3:N:233:LYS:HA    | 8:N:2413:HOH:O    | 1.95                     | 0.67              |
| 3:N:675:ARG:HD3   | 8:N:9600:HOH:O    | 1.94                     | 0.67              |
| 3:N:699:VAL:N     | 3:N:756:GLN:HE22  | 1.92                     | 0.67              |
| 1:B:34:VAL:HG22   | 1:B:181:VAL:HG21  | 1.76                     | 0.66              |
| 2:C:163:ILE:O     | 2:C:163:ILE:HG12  | 1.95                     | 0.66              |
| 2:C:961:GLU:HG2   | 8:C:9994:HOH:O    | 1.94                     | 0.66              |
| 3:D:449:SER:HB3   | 8:D:9476:HOH:O    | 1.94                     | 0.66              |
| 3:D:908:LYS:HB3   | 3:D:1027:GLY:HA3  | 1.76                     | 0.66              |
| 3:D:1307:LYS:HA   | 8:D:9947:HOH:O    | 1.95                     | 0.66              |
| 3:D:1383:ASP:HB2  | 3:D:1416:ALA:HB3  | 1.77                     | 0.66              |
| 5:F:115:LYS:HD2   | 8:F:9528:HOH:O    | 1.95                     | 0.66              |
| 5:F:291:ILE:CG2   | 5:F:304:VAL:HG21  | 2.23                     | 0.66              |
| 5:F:346:THR:HG23  | 5:F:422:LEU:HB3   | 1.78                     | 0.66              |
| 2:M:730:SER:O     | 2:M:734:LEU:HD23  | 1.94                     | 0.66              |
| 3:N:785:ILE:H     | 3:N:785:ILE:HD12  | 1.59                     | 0.66              |
| 3:N:1277:ILE:HD12 | 3:N:1301:LYS:HB2  | 1.77                     | 0.66              |
| 1:A:5:LYS:O       | 1:A:8:ALA:HB2     | 1.93                     | 0.66              |
| 2:C:288:ARG:NE    | 2:C:288:ARG:HA    | 2.10                     | 0.66              |
| 2:C:758:ARG:HB3   | 2:C:788:THR:O     | 1.95                     | 0.66              |
| 3:D:1203:LYS:HG3  | 8:D:2468:HOH:O    | 1.92                     | 0.66              |
| 3:D:1341:PRO:HA   | 3:D:1344:VAL:HG23 | 1.78                     | 0.66              |
| 1:K:42:ARG:HH12   | 2:M:857:ASP:HB3   | 1.59                     | 0.66              |
| 1:L:94:LEU:CD2    | 1:L:119:ASP:HB3   | 2.09                     | 0.66              |
| 1:A:38:ASN:HB3    | 1:A:39:PRO:HD3    | 1.75                     | 0.66              |
| 2:C:172:ILE:H     | 2:C:172:ILE:HD12  | 1.60                     | 0.66              |
| 2:C:715:THR:HG22  | 2:C:717:LEU:H     | 1.60                     | 0.66              |
| 3:D:705:ALA:HB2   | 8:D:9759:HOH:O    | 1.94                     | 0.66              |
| 3:D:1472:ILE:HG22 | 3:D:1474:ALA:H    | 1.59                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:F:209:PHE:CD2  | 5:F:213:ILE:HD11 | 2.29                     | 0.66              |
| 2:M:247:PRO:HG3  | 8:M:9717:HOH:O   | 1.94                     | 0.66              |
| 2:M:251:ASP:HB3  | 2:M:252:LYS:HD2  | 1.76                     | 0.66              |
| 2:M:289:THR:HG23 | 8:M:9502:HOH:O   | 1.95                     | 0.66              |
| 5:P:102:LEU:O    | 5:P:106:VAL:HG23 | 1.95                     | 0.66              |
| 5:P:167:PRO:HB2  | 5:P:169:GLU:OE1  | 1.95                     | 0.66              |
| 1:A:6:LEU:C      | 1:A:8:ALA:H      | 2.02                     | 0.66              |
| 1:A:18:ARG:O     | 1:A:207:PRO:HD3  | 1.96                     | 0.66              |
| 1:B:123:MET:HE1  | 8:B:9499:HOH:O   | 1.93                     | 0.66              |
| 3:D:108:VAL:HB   | 3:D:109:PRO:HD3  | 1.77                     | 0.66              |
| 3:D:190:GLU:CD   | 3:D:190:GLU:H    | 2.03                     | 0.66              |
| 3:D:1126:ASP:OD1 | 3:D:1129:THR:HA  | 1.95                     | 0.66              |
| 3:N:864:VAL:HG12 | 3:N:865:THR:H    | 1.60                     | 0.66              |
| 5:P:200:LYS:HG3  | 5:P:209:PHE:CZ   | 2.30                     | 0.66              |
| 2:C:433:THR:HG21 | 2:C:488:ALA:HB1  | 1.77                     | 0.66              |
| 2:C:453:THR:HG21 | 8:C:9979:HOH:O   | 1.95                     | 0.66              |
| 3:D:161:LEU:O    | 3:D:449:SER:HB2  | 1.96                     | 0.66              |
| 3:D:584:ASN:ND2  | 3:D:590:PRO:HD2  | 2.10                     | 0.66              |
| 3:D:979:GLU:HG3  | 8:D:9614:HOH:O   | 1.95                     | 0.66              |
| 3:D:1269:LYS:HA  | 3:D:1269:LYS:HE2 | 1.77                     | 0.66              |
| 5:F:260:ILE:HG12 | 5:F:264:MET:HB2  | 1.78                     | 0.66              |
| 1:L:89:PHE:CB    | 1:L:94:LEU:HD22  | 2.25                     | 0.66              |
| 1:L:162:ILE:HG23 | 8:L:4097:HOH:O   | 1.93                     | 0.66              |
| 2:M:579:VAL:HG11 | 2:M:887:GLU:HG3  | 1.78                     | 0.66              |
| 2:M:693:GLU:HG2  | 8:M:9913:HOH:O   | 1.96                     | 0.66              |
| 3:N:119:SER:H    | 3:N:123:LEU:CD1  | 2.08                     | 0.66              |
| 3:N:133:ILE:HG22 | 3:N:455:ARG:N    | 2.10                     | 0.66              |
| 3:N:393:ILE:HG21 | 8:N:2370:HOH:O   | 1.95                     | 0.66              |
| 3:N:984:THR:CG2  | 3:N:987:GLU:H    | 2.09                     | 0.66              |
| 5:P:415:THR:O    | 5:P:417:LYS:HG3  | 1.95                     | 0.66              |
| 1:B:89:PHE:CB    | 1:B:94:LEU:HD22  | 2.26                     | 0.66              |
| 2:C:626:ARG:HB3  | 8:C:9559:HOH:O   | 1.96                     | 0.66              |
| 3:D:148:GLU:CB   | 3:D:151:GLN:HB2  | 2.25                     | 0.66              |
| 2:M:798:GLY:H    | 2:M:827:VAL:HG11 | 1.59                     | 0.66              |
| 3:N:786:ILE:HD13 | 3:N:908:LYS:HB3  | 1.77                     | 0.66              |
| 5:P:110:MET:HE1  | 8:P:9585:HOH:O   | 1.94                     | 0.66              |
| 2:C:63:GLY:O     | 2:C:103:LYS:HE2  | 1.95                     | 0.66              |
| 2:C:577:PRO:HA   | 2:C:671:ASN:HD21 | 1.60                     | 0.66              |
| 3:D:63:TYR:HB3   | 3:D:68:PHE:HD1   | 1.60                     | 0.66              |
| 5:F:199:ALA:HA   | 8:F:9547:HOH:O   | 1.95                     | 0.66              |
| 5:F:262:VAL:HG23 | 8:F:9481:HOH:O   | 1.95                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:162:ILE:HG21  | 8:L:5120:HOH:O    | 1.95                     | 0.66              |
| 2:M:360:LEU:HD21  | 8:M:2232:HOH:O    | 1.95                     | 0.66              |
| 3:N:543:LEU:HD21  | 3:N:600:LEU:HB2   | 1.77                     | 0.66              |
| 3:N:1497:GLU:O    | 3:N:1501:GLU:HG3  | 1.96                     | 0.66              |
| 1:B:7:LYS:HZ2     | 1:B:186:LEU:HD13  | 1.60                     | 0.66              |
| 1:B:27:PRO:HG2    | 1:B:186:LEU:HD12  | 1.77                     | 0.66              |
| 2:C:128:ILE:HG22  | 8:C:9592:HOH:O    | 1.94                     | 0.66              |
| 2:C:368:THR:HG22  | 8:C:9664:HOH:O    | 1.95                     | 0.66              |
| 3:D:422:ALA:H     | 3:D:427:VAL:CG1   | 2.09                     | 0.66              |
| 3:D:456:MET:HG2   | 3:D:568:ARG:NH1   | 2.11                     | 0.66              |
| 3:D:1326:THR:HG22 | 3:D:1327:ARG:H    | 1.58                     | 0.66              |
| 1:K:6:LEU:C       | 1:K:8:ALA:H       | 2.02                     | 0.66              |
| 1:L:23:PHE:HE1    | 1:L:208:LEU:HD13  | 1.60                     | 0.66              |
| 1:L:77:GLU:HB2    | 3:N:872:ARG:HH21  | 1.60                     | 0.66              |
| 2:M:36:PRO:CG     | 2:M:70:GLU:HB3    | 2.25                     | 0.66              |
| 2:M:353:ARG:HG2   | 8:M:9875:HOH:O    | 1.95                     | 0.66              |
| 2:M:1003:ASP:HB3  | 8:M:2181:HOH:O    | 1.95                     | 0.66              |
| 3:N:210:ARG:HG3   | 3:N:398:ALA:H     | 1.60                     | 0.66              |
| 3:N:1312:LEU:HA   | 8:N:2142:HOH:O    | 1.96                     | 0.66              |
| 8:N:2375:HOH:O    | 5:P:374:GLY:HA3   | 1.95                     | 0.66              |
| 2:C:301:GLU:HB2   | 8:C:9986:HOH:O    | 1.95                     | 0.66              |
| 3:D:1459:LEU:HD12 | 3:D:1470:ARG:HH11 | 1.61                     | 0.66              |
| 2:M:420:ARG:HD2   | 2:M:420:ARG:N     | 2.11                     | 0.66              |
| 2:M:516:ARG:NH1   | 2:M:521:PRO:HB3   | 2.07                     | 0.66              |
| 5:P:222:ARG:HA    | 8:P:9484:HOH:O    | 1.96                     | 0.66              |
| 1:A:27:PRO:HB2    | 8:A:9548:HOH:O    | 1.95                     | 0.66              |
| 2:C:51:THR:HB     | 2:C:348:LEU:HD23  | 1.76                     | 0.66              |
| 2:C:97:ARG:HH21   | 2:C:109:LYS:HD2   | 1.61                     | 0.66              |
| 2:C:729:LEU:HD11  | 5:F:419:ARG:HH22  | 1.59                     | 0.66              |
| 3:D:149:LYS:HB3   | 8:D:2307:HOH:O    | 1.95                     | 0.66              |
| 3:D:510:GLU:O     | 3:D:513:ILE:HD12  | 1.95                     | 0.66              |
| 3:D:526:PRO:O     | 3:D:537:THR:HA    | 1.95                     | 0.66              |
| 3:D:1197:ARG:HD3  | 3:D:1396:GLU:HB2  | 1.77                     | 0.66              |
| 5:F:406:ARG:O     | 5:F:409:LYS:HG2   | 1.96                     | 0.66              |
| 2:M:599:GLU:HB3   | 8:M:2119:HOH:O    | 1.95                     | 0.66              |
| 1:A:58:ILE:HB     | 1:A:61:VAL:HB     | 1.79                     | 0.65              |
| 2:C:650:ARG:HD3   | 2:C:650:ARG:N     | 2.11                     | 0.65              |
| 2:C:1081:VAL:HB   | 2:C:1086:ARG:HE   | 1.60                     | 0.65              |
| 5:F:92:PRO:HB2    | 8:F:9823:HOH:O    | 1.95                     | 0.65              |
| 2:M:194:VAL:HG13  | 2:M:221:LEU:HD12  | 1.77                     | 0.65              |
| 3:N:1398:TRP:CE3  | 3:N:1415:VAL:HG11 | 2.31                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:350:LEU:HD12  | 5:P:422:LEU:HD12  | 1.77                     | 0.65              |
| 3:D:481:MET:HG2   | 3:D:493:ARG:NH2   | 2.11                     | 0.65              |
| 3:D:805:GLU:HB2   | 8:D:2175:HOH:O    | 1.95                     | 0.65              |
| 3:D:842:VAL:HG23  | 8:D:2600:HOH:O    | 1.95                     | 0.65              |
| 3:D:873:LEU:HD21  | 8:D:9775:HOH:O    | 1.97                     | 0.65              |
| 3:D:1359:GLN:HG2  | 8:D:9842:HOH:O    | 1.96                     | 0.65              |
| 1:K:97:VAL:HG23   | 8:K:1185:HOH:O    | 1.95                     | 0.65              |
| 2:M:1005:MET:HE1  | 3:N:645:PRO:HB2   | 1.78                     | 0.65              |
| 3:N:1025:GLN:OE1  | 3:N:1025:GLN:HA   | 1.94                     | 0.65              |
| 3:N:1435:LEU:HD23 | 3:N:1464:GLU:HB2  | 1.78                     | 0.65              |
| 4:O:41:GLU:HA     | 4:O:45:ARG:HG3    | 1.79                     | 0.65              |
| 2:C:408:ARG:NH1   | 2:C:542:VAL:HG23  | 2.11                     | 0.65              |
| 2:C:612:VAL:HG22  | 2:C:622:GLU:HA    | 1.78                     | 0.65              |
| 3:D:87:ARG:HG3    | 3:D:88:TYR:N      | 2.12                     | 0.65              |
| 3:D:1400:VAL:HG12 | 8:D:9583:HOH:O    | 1.95                     | 0.65              |
| 1:K:42:ARG:NH1    | 2:M:857:ASP:HB3   | 2.11                     | 0.65              |
| 2:M:172:ILE:HA    | 2:M:185:LYS:O     | 1.96                     | 0.65              |
| 2:M:176:VAL:C     | 2:M:178:PRO:HD3   | 2.21                     | 0.65              |
| 2:M:411:SER:OG    | 2:M:452:ILE:HG23  | 1.96                     | 0.65              |
| 3:N:87:ARG:HB2    | 3:N:523:ASP:HB2   | 1.78                     | 0.65              |
| 3:N:525:ARG:HE    | 3:N:541:ASN:HD21  | 1.43                     | 0.65              |
| 2:C:120:LEU:HD13  | 8:C:2036:HOH:O    | 1.95                     | 0.65              |
| 3:D:613:ARG:HG3   | 3:D:613:ARG:HH11  | 1.61                     | 0.65              |
| 3:D:1132:LEU:HD23 | 8:D:9601:HOH:O    | 1.95                     | 0.65              |
| 3:D:1481:VAL:HG22 | 8:E:9450:HOH:O    | 1.97                     | 0.65              |
| 5:F:138:SER:O     | 5:F:141:VAL:HG12  | 1.97                     | 0.65              |
| 3:N:28:LYS:CD     | 3:N:41:ARG:HD2    | 2.26                     | 0.65              |
| 3:N:1271:LYS:NZ   | 3:N:1334:GLN:HE22 | 1.93                     | 0.65              |
| 5:P:367:MET:CE    | 5:P:371:LEU:HD11  | 2.26                     | 0.65              |
| 1:A:90:LEU:HD21   | 8:A:9506:HOH:O    | 1.96                     | 0.65              |
| 2:C:399:ASN:ND2   | 2:C:568:ALA:HB3   | 2.12                     | 0.65              |
| 2:C:874:LEU:HD21  | 3:D:787:LEU:CD2   | 2.27                     | 0.65              |
| 3:D:814:ALA:O     | 3:D:818:ARG:HG3   | 1.97                     | 0.65              |
| 5:F:234:LYS:HD2   | 5:F:236:SER:H     | 1.61                     | 0.65              |
| 2:M:805:ARG:HD3   | 8:M:2083:HOH:O    | 1.96                     | 0.65              |
| 2:M:1087:VAL:HA   | 8:M:9750:HOH:O    | 1.95                     | 0.65              |
| 3:N:693:GLU:HG2   | 4:O:48:MET:SD     | 2.37                     | 0.65              |
| 5:P:406:ARG:HA    | 5:P:409:LYS:CG    | 2.26                     | 0.65              |
| 1:A:65:PHE:CE1    | 2:C:799:ILE:HD11  | 2.31                     | 0.65              |
| 2:C:1033:GLY:O    | 2:C:1037:VAL:HG23 | 1.95                     | 0.65              |
| 3:D:119:SER:HB2   | 3:D:123:LEU:HB2   | 1.77                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:O:40:LEU:HD12  | 4:O:40:LEU:O      | 1.97                     | 0.65              |
| 4:O:54:LEU:HG    | 4:O:58:PRO:HD2    | 1.79                     | 0.65              |
| 2:C:22:GLN:NE2   | 2:C:336:VAL:HG21  | 2.12                     | 0.65              |
| 2:C:464:LEU:HD12 | 2:C:465:GLY:N     | 2.11                     | 0.65              |
| 3:D:1489:GLN:O   | 3:D:1493:LYS:HG2  | 1.97                     | 0.65              |
| 5:F:371:LEU:HD22 | 5:F:375:LEU:HD13  | 1.78                     | 0.65              |
| 5:F:403:LYS:HB3  | 8:F:9814:HOH:O    | 1.95                     | 0.65              |
| 2:M:43:GLY:HA2   | 2:M:341:THR:CG2   | 2.27                     | 0.65              |
| 2:M:107:LEU:HD11 | 8:M:9696:HOH:O    | 1.96                     | 0.65              |
| 2:M:804:VAL:HB   | 2:M:824:ARG:HB2   | 1.79                     | 0.65              |
| 3:N:181:ASP:CG   | 3:N:198:ARG:HB2   | 2.21                     | 0.65              |
| 3:N:481:MET:HE3  | 3:N:493:ARG:NH2   | 2.10                     | 0.65              |
| 3:N:601:ARG:HH11 | 3:N:613:ARG:HH21  | 1.44                     | 0.65              |
| 3:N:786:ILE:CD1  | 3:N:908:LYS:HB3   | 2.26                     | 0.65              |
| 3:N:1271:LYS:HE3 | 3:N:1334:GLN:HE22 | 1.62                     | 0.65              |
| 1:B:151:VAL:HB   | 1:B:169:ALA:HB3   | 1.78                     | 0.65              |
| 1:B:226:SER:O    | 1:B:228:PRO:HD3   | 1.96                     | 0.65              |
| 2:C:100:LEU:HD13 | 8:C:9627:HOH:O    | 1.96                     | 0.65              |
| 2:C:244:PRO:HG2  | 2:C:246:ASP:OD2   | 1.97                     | 0.65              |
| 2:C:383:ARG:HD2  | 8:C:2220:HOH:O    | 1.95                     | 0.65              |
| 2:C:420:ARG:HD2  | 2:C:420:ARG:N     | 2.09                     | 0.65              |
| 3:D:98:PRO:HG2   | 3:D:462:GLN:NE2   | 2.10                     | 0.65              |
| 1:L:152:PRO:HD2  | 1:L:155:LYS:HB2   | 1.79                     | 0.65              |
| 3:N:414:ARG:HG3  | 3:N:418:GLY:O     | 1.97                     | 0.65              |
| 2:C:112:GLU:HG2  | 8:C:2042:HOH:O    | 1.97                     | 0.65              |
| 2:C:274:ARG:H    | 2:C:288:ARG:NH1   | 1.94                     | 0.65              |
| 2:C:290:LEU:HD23 | 2:C:290:LEU:H     | 1.62                     | 0.65              |
| 2:C:721:ARG:HE   | 2:C:783:ARG:HH21  | 1.44                     | 0.65              |
| 2:C:909:ALA:HB1  | 2:C:914:ILE:HD11  | 1.79                     | 0.65              |
| 3:D:434:ARG:HB2  | 3:D:447:VAL:HG13  | 1.79                     | 0.65              |
| 2:M:17:PRO:HD2   | 8:M:9519:HOH:O    | 1.96                     | 0.65              |
| 2:M:504:GLU:HB2  | 2:M:507:ARG:HD2   | 1.77                     | 0.65              |
| 2:M:593:ALA:HA   | 8:M:9732:HOH:O    | 1.96                     | 0.65              |
| 2:M:820:ARG:HA   | 8:M:9511:HOH:O    | 1.95                     | 0.65              |
| 3:N:54:LYS:HD3   | 3:N:57:GLU:HB2    | 1.79                     | 0.65              |
| 3:N:119:SER:CB   | 3:N:123:LEU:HB2   | 2.21                     | 0.65              |
| 3:N:864:VAL:HG12 | 3:N:865:THR:N     | 2.12                     | 0.65              |
| 1:A:184:THR:O    | 1:A:192:LEU:HD12  | 1.97                     | 0.65              |
| 2:C:554:ASP:OD2  | 2:C:556:ASN:HB3   | 1.97                     | 0.65              |
| 3:D:534:ARG:HG2  | 5:F:312:GLN:NE2   | 2.12                     | 0.65              |
| 2:M:260:LEU:HA   | 2:M:291:ALA:HB2   | 1.77                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:34:VAL:HG22   | 1:A:181:VAL:HG21  | 1.78                     | 0.64              |
| 1:A:56:VAL:HG22   | 1:A:142:VAL:HG12  | 1.78                     | 0.64              |
| 3:D:396:VAL:HG22  | 3:D:447:VAL:HB    | 1.79                     | 0.64              |
| 3:D:1432:LYS:HZ3  | 3:D:1460:ILE:HB   | 1.62                     | 0.64              |
| 3:N:441:ARG:HB3   | 3:N:443:VAL:HG23  | 1.79                     | 0.64              |
| 3:N:1378:TYR:O    | 3:N:1420:LEU:HB3  | 1.97                     | 0.64              |
| 1:B:6:LEU:C       | 1:B:8:ALA:H       | 2.03                     | 0.64              |
| 2:C:172:ILE:HA    | 2:C:185:LYS:O     | 1.97                     | 0.64              |
| 2:C:227:PHE:HB2   | 8:C:2150:HOH:O    | 1.96                     | 0.64              |
| 2:C:810:ASP:HA    | 8:C:2192:HOH:O    | 1.97                     | 0.64              |
| 3:D:212:ARG:HD2   | 3:D:445:ARG:HH12  | 1.62                     | 0.64              |
| 3:D:657:LEU:O     | 3:D:661:MET:HG2   | 1.97                     | 0.64              |
| 3:D:1422:MET:HE2  | 3:D:1427:SER:HA   | 1.79                     | 0.64              |
| 2:M:263:ASP:HB2   | 2:M:264:PRO:HD3   | 1.78                     | 0.64              |
| 2:M:412:ALA:HA    | 8:M:9833:HOH:O    | 1.96                     | 0.64              |
| 2:M:601:GLY:O     | 2:M:648:ARG:HA    | 1.97                     | 0.64              |
| 2:M:798:GLY:H     | 2:M:827:VAL:CG1   | 2.10                     | 0.64              |
| 2:M:1085:PHE:CZ   | 3:N:1468:LEU:HG   | 2.31                     | 0.64              |
| 3:N:553:ARG:HH21  | 5:P:215:GLU:HG2   | 1.61                     | 0.64              |
| 3:N:1127:GLU:HB3  | 8:N:2461:HOH:O    | 1.95                     | 0.64              |
| 3:N:1271:LYS:NZ   | 3:N:1273:VAL:HA   | 2.12                     | 0.64              |
| 3:N:1454:GLY:HA3  | 8:N:9670:HOH:O    | 1.97                     | 0.64              |
| 1:B:20:TYR:HB3    | 8:B:9497:HOH:O    | 1.96                     | 0.64              |
| 2:C:34:VAL:HG23   | 8:C:2231:HOH:O    | 1.98                     | 0.64              |
| 2:C:462:ASP:CG    | 2:C:463:GLU:H     | 2.05                     | 0.64              |
| 2:C:1088:LEU:HD12 | 8:D:2415:HOH:O    | 1.96                     | 0.64              |
| 3:D:415:VAL:HG11  | 8:D:2050:HOH:O    | 1.96                     | 0.64              |
| 3:D:425:GLY:HA3   | 5:F:135:ILE:HD13  | 1.79                     | 0.64              |
| 3:D:1364:HIS:CE1  | 3:D:1366:LYS:HG3  | 2.32                     | 0.64              |
| 3:D:1487:VAL:HG11 | 3:D:1492:LEU:HD23 | 1.79                     | 0.64              |
| 1:K:102:LYS:HG2   | 8:K:1171:HOH:O    | 1.97                     | 0.64              |
| 2:M:290:LEU:HD22  | 2:M:302:VAL:CG1   | 2.27                     | 0.64              |
| 3:N:73:CYS:HB3    | 3:N:76:CYS:O      | 1.96                     | 0.64              |
| 3:N:423:ASP:OD1   | 5:P:175:HIS:HA    | 1.98                     | 0.64              |
| 4:O:95:GLY:HA3    | 8:O:830:HOH:O     | 1.97                     | 0.64              |
| 5:P:409:LYS:HB3   | 8:P:9577:HOH:O    | 1.98                     | 0.64              |
| 2:C:976:ASP:HB3   | 2:C:979:THR:HG22  | 1.78                     | 0.64              |
| 2:C:1095:LEU:HG   | 3:D:603:LEU:HB3   | 1.79                     | 0.64              |
| 3:D:566:ILE:HD13  | 5:F:217:ASN:HB3   | 1.78                     | 0.64              |
| 3:D:1412:LYS:HE3  | 8:D:2116:HOH:O    | 1.96                     | 0.64              |
| 5:F:361:LEU:HD22  | 5:F:404:ALA:HB1   | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:670:GLN:HB3   | 2:M:699:PHE:CE2   | 2.32                     | 0.64              |
| 2:M:767:PRO:HG2   | 8:M:2141:HOH:O    | 1.98                     | 0.64              |
| 2:M:1005:MET:HE1  | 3:N:648:MET:HB2   | 1.80                     | 0.64              |
| 3:N:60:CYS:HB2    | 8:N:9509:HOH:O    | 1.98                     | 0.64              |
| 3:N:817:GLU:O     | 3:N:821:VAL:HG23  | 1.98                     | 0.64              |
| 2:C:66:LEU:HB2    | 8:C:9904:HOH:O    | 1.97                     | 0.64              |
| 2:C:1032:PHE:HZ   | 2:C:1040:LEU:HD22 | 1.62                     | 0.64              |
| 3:D:988:ARG:O     | 3:D:992:ILE:HG13  | 1.98                     | 0.64              |
| 3:D:1304:LYS:H    | 3:D:1304:LYS:CD   | 2.07                     | 0.64              |
| 5:F:289:GLU:HA    | 8:F:9486:HOH:O    | 1.96                     | 0.64              |
| 2:M:110:GLU:CB    | 2:M:369:PRO:HG3   | 2.27                     | 0.64              |
| 2:M:1089:VAL:HG13 | 2:M:1099:VAL:CG2  | 2.26                     | 0.64              |
| 3:N:185:VAL:HG11  | 8:N:2341:HOH:O    | 1.97                     | 0.64              |
| 3:N:486:ARG:HH21  | 3:N:489:ARG:CZ    | 2.09                     | 0.64              |
| 3:N:558:LEU:HD13  | 5:P:145:PRO:HB3   | 1.78                     | 0.64              |
| 5:P:220:LEU:HD12  | 5:P:243:ILE:HD11  | 1.79                     | 0.64              |
| 5:P:279:GLN:HG3   | 8:P:9541:HOH:O    | 1.98                     | 0.64              |
| 1:A:73:GLU:OE1    | 1:A:130:ALA:HA    | 1.97                     | 0.64              |
| 1:A:198:ARG:NH2   | 2:C:932:GLU:HB3   | 2.13                     | 0.64              |
| 1:B:189:ARG:HD2   | 8:B:9558:HOH:O    | 1.98                     | 0.64              |
| 2:C:5:ARG:HB3     | 2:C:902:ILE:HB    | 1.80                     | 0.64              |
| 2:C:247:PRO:HD2   | 8:C:9536:HOH:O    | 1.97                     | 0.64              |
| 2:C:961:GLU:HG3   | 8:C:9735:HOH:O    | 1.96                     | 0.64              |
| 2:C:1031:ARG:HD3  | 3:D:619:LEU:HD21  | 1.79                     | 0.64              |
| 2:C:1095:LEU:HD21 | 3:D:604:THR:N     | 2.12                     | 0.64              |
| 3:D:813:LEU:HD11  | 8:D:9968:HOH:O    | 1.98                     | 0.64              |
| 5:F:270:LYS:HA    | 8:F:9592:HOH:O    | 1.96                     | 0.64              |
| 1:K:171:PHE:O     | 1:K:173:PRO:HD3   | 1.98                     | 0.64              |
| 1:L:90:LEU:HD13   | 8:L:1194:HOH:O    | 1.96                     | 0.64              |
| 2:M:158:TYR:HB2   | 2:M:313:LEU:HD21  | 1.79                     | 0.64              |
| 2:M:744:ARG:HG3   | 2:M:747:ALA:HB2   | 1.80                     | 0.64              |
| 2:M:1090:LYS:HE3  | 3:N:88:TYR:O      | 1.98                     | 0.64              |
| 3:N:1243:THR:HB   | 3:N:1253:THR:HB   | 1.79                     | 0.64              |
| 2:C:599:GLU:HG3   | 2:C:600:ASP:N     | 2.13                     | 0.64              |
| 3:D:658:LEU:HD13  | 3:D:670:VAL:HG13  | 1.78                     | 0.64              |
| 5:F:205:ARG:HG3   | 5:F:251:ILE:HD13  | 1.79                     | 0.64              |
| 2:M:139:GLN:HB3   | 2:M:334:ARG:HD2   | 1.79                     | 0.64              |
| 2:M:269:LEU:HD23  | 2:M:269:LEU:H     | 1.62                     | 0.64              |
| 2:M:630:ARG:HD3   | 2:M:705:ILE:HG22  | 1.79                     | 0.64              |
| 3:N:28:LYS:HD3    | 3:N:41:ARG:HD2    | 1.79                     | 0.64              |
| 3:N:694:VAL:HG13  | 8:N:9768:HOH:O    | 1.96                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:882:PHE:CE1   | 3:N:906:GLN:HG3   | 2.32                     | 0.64              |
| 2:C:141:HIS:HB2   | 2:C:418:LEU:HD12  | 1.79                     | 0.64              |
| 2:C:200:LEU:HD13  | 2:C:300:ASP:CG    | 2.22                     | 0.64              |
| 3:D:972:LEU:HD23  | 3:D:973:GLN:N     | 2.11                     | 0.64              |
| 3:D:1264:GLU:OE2  | 3:D:1424:VAL:HG12 | 1.98                     | 0.64              |
| 3:D:1312:LEU:HD21 | 8:D:2130:HOH:O    | 1.98                     | 0.64              |
| 3:D:1438:ALA:O    | 3:D:1443:THR:HG22 | 1.98                     | 0.64              |
| 1:K:58:ILE:HB     | 1:K:61:VAL:HB     | 1.80                     | 0.64              |
| 2:M:129:ILE:HG22  | 2:M:130:ASN:N     | 2.13                     | 0.64              |
| 2:M:332:ARG:NE    | 2:M:464:LEU:HD21  | 2.13                     | 0.64              |
| 3:N:369:ALA:O     | 3:N:370:ALA:HB2   | 1.98                     | 0.64              |
| 3:N:422:ALA:HB1   | 5:P:178:ARG:CZ    | 2.28                     | 0.64              |
| 3:N:598:ARG:HG2   | 8:N:9783:HOH:O    | 1.97                     | 0.64              |
| 3:N:1388:ARG:HG3  | 3:N:1389:LEU:HD23 | 1.80                     | 0.64              |
| 5:P:160:ASP:O     | 5:P:164:LYS:HG3   | 1.97                     | 0.64              |
| 1:A:194:LYS:HG2   | 8:A:9445:HOH:O    | 1.98                     | 0.64              |
| 1:B:103:ALA:HB2   | 8:B:9640:HOH:O    | 1.96                     | 0.64              |
| 1:B:130:ALA:HB2   | 8:B:9503:HOH:O    | 1.98                     | 0.64              |
| 3:D:369:ALA:O     | 3:D:370:ALA:HB2   | 1.98                     | 0.64              |
| 3:D:422:ALA:HB2   | 8:F:9563:HOH:O    | 1.98                     | 0.64              |
| 3:D:584:ASN:HD21  | 3:D:590:PRO:HB2   | 1.61                     | 0.64              |
| 5:F:393:THR:HG22  | 5:F:394:ARG:H     | 1.63                     | 0.64              |
| 1:L:5:LYS:O       | 1:L:8:ALA:HB2     | 1.98                     | 0.64              |
| 1:L:175:ARG:HD2   | 8:N:2419:HOH:O    | 1.97                     | 0.64              |
| 2:M:150:PRO:HA    | 2:M:158:TYR:HB3   | 1.79                     | 0.64              |
| 2:M:432:ARG:HH22  | 3:N:1047:LYS:CD   | 2.11                     | 0.64              |
| 2:M:707:ARG:HD2   | 2:M:824:ARG:HH11  | 1.63                     | 0.64              |
| 3:N:116:LEU:CD2   | 3:N:468:LEU:HD21  | 2.28                     | 0.64              |
| 1:A:89:PHE:HB3    | 1:A:94:LEU:HD22   | 1.80                     | 0.64              |
| 2:C:14:PRO:HA     | 8:C:9630:HOH:O    | 1.98                     | 0.64              |
| 2:C:244:PRO:HD2   | 2:C:245:GLY:H     | 1.62                     | 0.64              |
| 2:C:442:GLU:HG3   | 8:C:2023:HOH:O    | 1.97                     | 0.64              |
| 2:C:650:ARG:H     | 2:C:650:ARG:CD    | 2.00                     | 0.64              |
| 2:C:834:GLN:HG2   | 8:C:9652:HOH:O    | 1.97                     | 0.64              |
| 2:C:866:PRO:HD2   | 8:C:9576:HOH:O    | 1.98                     | 0.64              |
| 3:D:63:TYR:HB3    | 3:D:68:PHE:CD1    | 2.33                     | 0.64              |
| 3:D:462:GLN:HA    | 3:D:513:ILE:CD1   | 2.29                     | 0.64              |
| 3:D:696:HIS:HA    | 8:D:2155:HOH:O    | 1.98                     | 0.64              |
| 3:N:440:VAL:HG13  | 8:N:9706:HOH:O    | 1.97                     | 0.64              |
| 3:N:787:LEU:HD21  | 3:N:947:ILE:HD11  | 1.80                     | 0.64              |
| 3:N:1101:VAL:HG11 | 3:N:1424:VAL:CG2  | 2.28                     | 0.64              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1314:LYS:HD3  | 3:N:1314:LYS:N   | 2.13                     | 0.64              |
| 4:O:50:THR:HG22   | 8:O:4507:HOH:O   | 1.98                     | 0.64              |
| 1:B:10:VAL:HG12   | 1:B:12:THR:HG22  | 1.81                     | 0.63              |
| 2:C:73:LEU:HG     | 2:C:94:LEU:HD13  | 1.80                     | 0.63              |
| 3:D:404:GLU:HB3   | 3:D:414:ARG:NE   | 2.13                     | 0.63              |
| 2:M:571:LEU:CD2   | 2:M:700:TYR:HA   | 2.28                     | 0.63              |
| 2:M:672:VAL:HG23  | 2:M:868:ASP:HB2  | 1.80                     | 0.63              |
| 3:N:1434:TRP:CZ3  | 3:N:1457:ASP:HB2 | 2.33                     | 0.63              |
| 5:P:358:LEU:O     | 5:P:358:LEU:HD23 | 1.97                     | 0.63              |
| 1:A:34:VAL:HG23   | 8:A:9440:HOH:O   | 1.97                     | 0.63              |
| 2:C:36:PRO:CG     | 2:C:70:GLU:HB3   | 2.26                     | 0.63              |
| 3:D:820:GLU:HB2   | 3:D:836:VAL:HG11 | 1.79                     | 0.63              |
| 4:E:47:LYS:HE3    | 8:E:9392:HOH:O   | 1.97                     | 0.63              |
| 1:K:73:GLU:OE1    | 1:K:130:ALA:HA   | 1.98                     | 0.63              |
| 1:L:58:ILE:HB     | 1:L:61:VAL:HB    | 1.80                     | 0.63              |
| 3:N:227:LEU:HA    | 8:N:9599:HOH:O   | 1.97                     | 0.63              |
| 3:N:427:VAL:CG2   | 3:N:435:VAL:HB   | 2.28                     | 0.63              |
| 1:A:224:TYR:HB3   | 1:B:9:PRO:HB2    | 1.79                     | 0.63              |
| 2:C:441:VAL:O     | 2:C:559:LEU:HD13 | 1.99                     | 0.63              |
| 2:C:536:PRO:HB3   | 2:C:906:PHE:CD1  | 2.30                     | 0.63              |
| 2:C:607:ASP:HB3   | 2:C:609:ASN:H    | 1.63                     | 0.63              |
| 3:D:54:LYS:HG2    | 3:D:55:ASP:H     | 1.63                     | 0.63              |
| 3:D:185:VAL:HG11  | 8:D:9744:HOH:O   | 1.99                     | 0.63              |
| 3:D:1407:LEU:HA   | 8:D:2362:HOH:O   | 1.98                     | 0.63              |
| 1:K:66:SER:HA     | 8:K:913:HOH:O    | 1.99                     | 0.63              |
| 2:M:670:GLN:HB3   | 2:M:699:PHE:HE2  | 1.62                     | 0.63              |
| 2:M:712:ALA:O     | 2:M:820:ARG:N    | 2.30                     | 0.63              |
| 3:N:421:LEU:HD23  | 3:N:421:LEU:O    | 1.99                     | 0.63              |
| 3:N:829:VAL:HA    | 8:N:9503:HOH:O   | 1.99                     | 0.63              |
| 3:N:1046:GLN:NE2  | 3:N:1050:GLY:HA2 | 2.13                     | 0.63              |
| 3:N:1055:VAL:HG12 | 8:N:9865:HOH:O   | 1.97                     | 0.63              |
| 2:C:9:ILE:HG13    | 2:C:9:ILE:O      | 1.97                     | 0.63              |
| 3:D:177:ALA:HB1   | 3:D:199:LEU:HD13 | 1.81                     | 0.63              |
| 3:D:179:VAL:HG11  | 8:D:9501:HOH:O   | 1.97                     | 0.63              |
| 3:D:658:LEU:HD11  | 3:D:674:ARG:HH11 | 1.63                     | 0.63              |
| 3:D:683:ILE:HB    | 8:D:2010:HOH:O   | 1.97                     | 0.63              |
| 3:D:1232:PRO:HB3  | 3:D:1361:VAL:CG2 | 2.26                     | 0.63              |
| 1:L:6:LEU:C       | 1:L:8:ALA:H      | 2.05                     | 0.63              |
| 2:M:502:PRO:HB2   | 2:M:509:ALA:HB3  | 1.81                     | 0.63              |
| 3:N:646:LYS:HA    | 3:N:720:LEU:CD2  | 2.25                     | 0.63              |
| 3:N:833:GLU:HB3   | 8:N:2025:HOH:O   | 1.99                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1100:ASP:HB2  | 8:N:9612:HOH:O    | 1.97                     | 0.63              |
| 3:N:1191:PRO:HB3  | 3:N:1370:ILE:HD13 | 1.79                     | 0.63              |
| 2:C:204:GLN:HE21  | 2:C:228:ALA:CB    | 2.12                     | 0.63              |
| 2:C:591:SER:HB2   | 8:C:9725:HOH:O    | 1.98                     | 0.63              |
| 2:C:605:LYS:CB    | 2:C:610:ARG:HH12  | 2.12                     | 0.63              |
| 2:C:952:LEU:HD12  | 2:C:969:GLN:NE2   | 2.13                     | 0.63              |
| 3:D:893:GLU:HG2   | 8:D:9710:HOH:O    | 1.98                     | 0.63              |
| 3:D:1208:ASP:HB2  | 8:D:9803:HOH:O    | 1.99                     | 0.63              |
| 4:E:46:PRO:HD2    | 8:E:9375:HOH:O    | 1.99                     | 0.63              |
| 1:K:127:LEU:HD12  | 1:K:128:HIS:H     | 1.61                     | 0.63              |
| 1:L:171:PHE:HB2   | 8:L:5023:HOH:O    | 1.98                     | 0.63              |
| 2:M:252:LYS:NZ    | 2:M:296:GLY:HA3   | 2.13                     | 0.63              |
| 2:M:347:GLY:HA2   | 2:M:350:ARG:HD2   | 1.80                     | 0.63              |
| 2:M:1035:MET:HA   | 2:M:1038:TRP:CE3  | 2.34                     | 0.63              |
| 3:N:148:GLU:HB3   | 3:N:151:GLN:CB    | 2.27                     | 0.63              |
| 3:N:420:VAL:HG13  | 8:P:9538:HOH:O    | 1.98                     | 0.63              |
| 3:N:1110:ALA:HB1  | 8:N:9775:HOH:O    | 1.98                     | 0.63              |
| 3:N:1462:LEU:HD23 | 3:N:1473:PRO:HD2  | 1.80                     | 0.63              |
| 5:P:406:ARG:HA    | 5:P:409:LYS:HG2   | 1.79                     | 0.63              |
| 1:B:58:ILE:HB     | 1:B:61:VAL:HB     | 1.80                     | 0.63              |
| 2:C:1056:LYS:HB3  | 3:D:624:ASP:H     | 1.64                     | 0.63              |
| 3:D:73:CYS:HB2    | 3:D:76:CYS:O      | 1.98                     | 0.63              |
| 5:F:276:ARG:HG3   | 5:F:276:ARG:HH11  | 1.63                     | 0.63              |
| 1:K:223:THR:HG22  | 8:K:1154:HOH:O    | 1.98                     | 0.63              |
| 2:M:290:LEU:HB3   | 8:M:9575:HOH:O    | 1.98                     | 0.63              |
| 2:M:1061:GLU:HG2  | 8:M:2175:HOH:O    | 1.98                     | 0.63              |
| 3:N:422:ALA:CB    | 5:P:178:ARG:HH12  | 2.07                     | 0.63              |
| 3:N:957:PRO:HG3   | 3:N:1007:VAL:HA   | 1.80                     | 0.63              |
| 3:N:1440:PHE:HA   | 8:N:9784:HOH:O    | 1.97                     | 0.63              |
| 1:B:201:THR:HG22  | 1:B:203:GLY:H     | 1.64                     | 0.63              |
| 2:C:1095:LEU:HA   | 3:D:582:LEU:HD23  | 1.80                     | 0.63              |
| 3:D:131:LYS:HG2   | 3:D:568:ARG:HD3   | 1.81                     | 0.63              |
| 3:D:1277:ILE:HD12 | 3:D:1301:LYS:HB2  | 1.81                     | 0.63              |
| 3:D:1503:VAL:HG22 | 8:D:2106:HOH:O    | 1.99                     | 0.63              |
| 4:E:48:MET:CB     | 4:E:54:LEU:HB2    | 2.29                     | 0.63              |
| 4:E:60:ALA:O      | 4:E:63:TRP:HB2    | 1.98                     | 0.63              |
| 1:K:206:THR:HG22  | 1:K:209:GLU:H     | 1.62                     | 0.63              |
| 1:L:39:PRO:O      | 1:L:43:ILE:HG12   | 1.98                     | 0.63              |
| 2:M:368:THR:HB    | 2:M:369:PRO:CD    | 2.29                     | 0.63              |
| 2:M:462:ASP:CG    | 2:M:463:GLU:N     | 2.57                     | 0.63              |
| 3:N:10:ILE:HG22   | 3:N:1451:ALA:HA   | 1.79                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:423:ASP:OD2   | 5:P:178:ARG:HG3   | 1.99                     | 0.63              |
| 3:N:493:ARG:NE    | 3:N:1389:LEU:HD21 | 2.14                     | 0.63              |
| 3:N:659:LYS:HE2   | 3:N:663:GLU:HG2   | 1.80                     | 0.63              |
| 5:P:131:VAL:HG13  | 5:P:178:ARG:HG2   | 1.80                     | 0.63              |
| 5:P:393:THR:HG23  | 5:P:394:ARG:HD2   | 1.79                     | 0.63              |
| 1:A:108:GLU:HB3   | 8:A:9467:HOH:O    | 1.98                     | 0.63              |
| 1:A:150:TYR:CE1   | 2:C:696:LYS:HA    | 2.34                     | 0.63              |
| 1:A:229:GLN:O     | 8:A:9443:HOH:O    | 2.15                     | 0.63              |
| 2:C:299:LYS:HG3   | 8:C:2020:HOH:O    | 1.98                     | 0.63              |
| 2:C:573:ARG:HD2   | 8:C:9990:HOH:O    | 1.97                     | 0.63              |
| 2:C:606:VAL:CG2   | 2:C:645:VAL:HG22  | 2.29                     | 0.63              |
| 3:D:1095:THR:OG1  | 3:D:1230:GLY:HA3  | 1.99                     | 0.63              |
| 3:D:1112:CYS:HA   | 8:D:9721:HOH:O    | 1.99                     | 0.63              |
| 5:F:365:GLU:HB2   | 5:F:400:ILE:CG2   | 2.29                     | 0.63              |
| 1:K:212:ASN:O     | 1:K:215:VAL:HG22  | 1.98                     | 0.63              |
| 2:M:332:ARG:HB2   | 2:M:466:PHE:CE1   | 2.34                     | 0.63              |
| 3:N:545:ARG:NH1   | 3:N:545:ARG:HB3   | 2.14                     | 0.63              |
| 3:D:149:LYS:H     | 3:D:149:LYS:CE    | 2.12                     | 0.63              |
| 3:D:162:ARG:HG2   | 8:D:9658:HOH:O    | 1.99                     | 0.63              |
| 3:D:495:ARG:HB2   | 8:D:2090:HOH:O    | 1.98                     | 0.63              |
| 3:D:1432:LYS:HD3  | 3:D:1460:ILE:HD12 | 1.81                     | 0.63              |
| 1:K:115:LEU:HD12  | 1:K:115:LEU:O     | 1.99                     | 0.63              |
| 8:K:5027:HOH:O    | 1:L:215:VAL:HG21  | 1.97                     | 0.63              |
| 1:L:186:LEU:HB2   | 1:L:192:LEU:CD1   | 2.29                     | 0.63              |
| 3:N:996:TRP:CD2   | 3:N:1056:PRO:HG2  | 2.34                     | 0.63              |
| 3:N:1116:ASN:HD22 | 3:N:1116:ASN:N    | 1.94                     | 0.63              |
| 5:P:226:LYS:HG3   | 5:P:242:TRP:CZ2   | 2.34                     | 0.63              |
| 2:C:911:GLU:HB2   | 8:C:9947:HOH:O    | 1.99                     | 0.62              |
| 3:D:168:THR:C     | 3:D:170:PRO:HD3   | 2.23                     | 0.62              |
| 3:D:795:VAL:HG11  | 3:D:863:VAL:HG13  | 1.81                     | 0.62              |
| 3:D:812:ALA:HB1   | 8:D:9956:HOH:O    | 1.98                     | 0.62              |
| 3:D:1405:GLU:HA   | 8:D:9486:HOH:O    | 1.98                     | 0.62              |
| 1:L:30:ARG:HE     | 2:M:854:PRO:HG3   | 1.63                     | 0.62              |
| 2:M:23:VAL:HG12   | 8:M:9500:HOH:O    | 1.98                     | 0.62              |
| 3:N:694:VAL:HA    | 8:N:9485:HOH:O    | 1.98                     | 0.62              |
| 3:N:956:ILE:HD13  | 8:N:9750:HOH:O    | 1.99                     | 0.62              |
| 3:N:1161:GLU:HG2  | 3:N:1164:ARG:HB2  | 1.79                     | 0.62              |
| 1:A:89:PHE:CB     | 1:A:94:LEU:HD22   | 2.30                     | 0.62              |
| 2:C:468:ARG:HG2   | 2:C:487:THR:HA    | 1.82                     | 0.62              |
| 2:C:601:GLY:O     | 2:C:648:ARG:HA    | 2.00                     | 0.62              |
| 3:D:486:ARG:O     | 3:D:489:ARG:HG2   | 2.00                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:806:PHE:CE1   | 3:D:813:LEU:HB3   | 2.34                     | 0.62              |
| 2:M:195:LEU:HD21  | 2:M:238:LEU:HG    | 1.80                     | 0.62              |
| 2:M:250:ARG:HB3   | 2:M:253:ALA:HB3   | 1.81                     | 0.62              |
| 2:M:1071:ILE:HG23 | 3:N:670:VAL:HG21  | 1.80                     | 0.62              |
| 3:N:126:VAL:HG11  | 3:N:152:LEU:HD13  | 1.81                     | 0.62              |
| 3:N:1052:THR:HG22 | 8:N:9487:HOH:O    | 1.99                     | 0.62              |
| 3:N:1242:HIS:C    | 3:N:1269:LYS:HD2  | 2.24                     | 0.62              |
| 3:N:1271:LYS:HZ1  | 3:N:1273:VAL:HA   | 1.63                     | 0.62              |
| 1:B:81:ASN:HA     | 8:B:9514:HOH:O    | 1.99                     | 0.62              |
| 2:C:1106:ASP:CG   | 3:D:1456:LYS:HD3  | 2.24                     | 0.62              |
| 3:D:152:LEU:HD23  | 3:D:152:LEU:N     | 2.13                     | 0.62              |
| 3:D:957:PRO:CG    | 3:D:1007:VAL:HG12 | 2.30                     | 0.62              |
| 3:D:1489:GLN:O    | 3:D:1493:LYS:HE2  | 2.00                     | 0.62              |
| 4:E:48:MET:HB3    | 4:E:54:LEU:HB2    | 1.82                     | 0.62              |
| 5:F:81:VAL:O      | 5:F:85:LEU:HG     | 1.99                     | 0.62              |
| 5:F:344:ALA:HA    | 8:F:9487:HOH:O    | 1.98                     | 0.62              |
| 2:M:472:ARG:HD2   | 2:M:480:THR:O     | 1.99                     | 0.62              |
| 2:M:971:LYS:HA    | 2:M:988:VAL:HA    | 1.80                     | 0.62              |
| 3:N:556:LYS:HE2   | 5:P:218:GLN:HE22  | 1.64                     | 0.62              |
| 2:C:197:LEU:HB3   | 2:C:202:TYR:HB2   | 1.81                     | 0.62              |
| 2:C:338:GLU:HA    | 2:C:341:THR:HG22  | 1.81                     | 0.62              |
| 2:C:512:ARG:CD    | 2:C:523:ILE:HD11  | 2.29                     | 0.62              |
| 3:D:199:LEU:O     | 3:D:199:LEU:HD23  | 1.98                     | 0.62              |
| 3:D:972:LEU:HD23  | 3:D:972:LEU:C     | 2.24                     | 0.62              |
| 5:F:93:LEU:HD11   | 5:F:102:LEU:HD12  | 1.81                     | 0.62              |
| 1:L:54:THR:CG2    | 1:L:158:ILE:HG13  | 2.29                     | 0.62              |
| 3:N:58:CYS:SG     | 3:N:59:ALA:N      | 2.71                     | 0.62              |
| 3:N:127:LEU:HD12  | 3:N:457:GLY:H     | 1.62                     | 0.62              |
| 3:N:655:PRO:HA    | 3:N:658:LEU:HD12  | 1.81                     | 0.62              |
| 3:N:1472:ILE:HG22 | 3:N:1475:GLY:H    | 1.63                     | 0.62              |
| 5:P:402:ASN:O     | 5:P:406:ARG:CD    | 2.43                     | 0.62              |
| 1:A:167:VAL:HA    | 8:A:9446:HOH:O    | 1.99                     | 0.62              |
| 1:B:91:ASN:OD1    | 1:B:93:SER:HB2    | 1.99                     | 0.62              |
| 2:C:443:THR:HG23  | 2:C:444:PRO:HD2   | 1.80                     | 0.62              |
| 3:D:572:ARG:NE    | 5:F:80:PRO:HG3    | 2.14                     | 0.62              |
| 3:D:862:ASP:O     | 3:D:877:PRO:HD2   | 2.00                     | 0.62              |
| 3:D:1346:ARG:HA   | 3:D:1346:ARG:HH11 | 1.65                     | 0.62              |
| 3:D:1493:LYS:O    | 3:D:1497:GLU:HG2  | 1.98                     | 0.62              |
| 5:F:405:LEU:O     | 5:F:408:LEU:HD22  | 1.98                     | 0.62              |
| 1:K:27:PRO:HB2    | 8:K:1253:HOH:O    | 1.97                     | 0.62              |
| 1:L:137:ARG:HH12  | 1:L:139:ASN:HB3   | 1.65                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:598:GLU:O    | 2:M:651:LYS:HG3   | 2.00                     | 0.62              |
| 2:M:1049:LEU:O   | 2:M:1053:LEU:HD23 | 1.98                     | 0.62              |
| 3:N:179:VAL:HG13 | 8:N:9757:HOH:O    | 1.99                     | 0.62              |
| 3:N:440:VAL:HA   | 8:N:2151:HOH:O    | 1.99                     | 0.62              |
| 4:O:40:LEU:HB2   | 4:O:45:ARG:CD     | 2.30                     | 0.62              |
| 4:O:51:LEU:HD21  | 8:O:709:HOH:O     | 2.00                     | 0.62              |
| 5:P:350:LEU:HD12 | 5:P:422:LEU:HB3   | 1.81                     | 0.62              |
| 5:P:395:GLU:O    | 5:P:399:GLN:CG    | 2.45                     | 0.62              |
| 1:A:72:LYS:HZ1   | 2:C:644:VAL:HA    | 1.65                     | 0.62              |
| 1:B:107:LYS:HB3  | 8:B:9534:HOH:O    | 1.98                     | 0.62              |
| 2:C:197:LEU:HD22 | 2:C:202:TYR:CD2   | 2.34                     | 0.62              |
| 3:D:774:SER:HB3  | 3:D:1362:LYS:O    | 2.00                     | 0.62              |
| 3:D:843:PHE:CE1  | 3:D:864:VAL:HG11  | 2.34                     | 0.62              |
| 4:E:4:PRO:HD2    | 8:E:9453:HOH:O    | 1.98                     | 0.62              |
| 4:E:23:VAL:CG2   | 4:E:65:MET:HG2    | 2.30                     | 0.62              |
| 5:F:367:MET:HE2  | 5:F:367:MET:N     | 2.14                     | 0.62              |
| 1:K:23:PHE:O     | 1:K:196:THR:HA    | 1.98                     | 0.62              |
| 1:K:27:PRO:HG2   | 1:K:186:LEU:HD22  | 1.82                     | 0.62              |
| 1:K:47:SER:HB2   | 1:K:217:ILE:HD13  | 1.81                     | 0.62              |
| 2:M:537:LYS:HA   | 2:M:905:ILE:HD11  | 1.81                     | 0.62              |
| 2:M:1013:TYR:HE2 | 5:P:341:PRO:HD2   | 1.65                     | 0.62              |
| 2:M:1101:THR:CB  | 3:N:5:VAL:HG13    | 2.21                     | 0.62              |
| 3:N:656:PHE:CE2  | 3:N:698:LYS:HE3   | 2.34                     | 0.62              |
| 3:N:1418:LYS:HB3 | 8:N:9558:HOH:O    | 1.99                     | 0.62              |
| 5:P:416:ARG:HH11 | 5:P:419:ARG:HB3   | 1.63                     | 0.62              |
| 1:B:159:LYS:HB2  | 8:B:9544:HOH:O    | 1.98                     | 0.62              |
| 2:C:176:VAL:C    | 2:C:178:PRO:HD3   | 2.24                     | 0.62              |
| 3:D:131:LYS:HB3  | 3:D:456:MET:CE    | 2.30                     | 0.62              |
| 3:D:670:VAL:O    | 3:D:674:ARG:HG3   | 2.00                     | 0.62              |
| 2:M:91:GLN:OE1   | 2:M:117:HIS:HB3   | 2.00                     | 0.62              |
| 2:M:396:ASP:HA   | 2:M:633:GLN:NE2   | 2.13                     | 0.62              |
| 2:M:1044:GLY:N   | 3:N:762:GLN:OE1   | 2.31                     | 0.62              |
| 3:N:404:GLU:HB3  | 8:N:2350:HOH:O    | 2.00                     | 0.62              |
| 3:N:558:LEU:HD22 | 5:P:145:PRO:HG3   | 1.80                     | 0.62              |
| 3:N:1030:GLY:HA3 | 8:N:9601:HOH:O    | 1.98                     | 0.62              |
| 5:P:376:ILE:HD12 | 8:P:9528:HOH:O    | 2.00                     | 0.62              |
| 2:C:254:VAL:HG13 | 2:C:258:TYR:HE1   | 1.65                     | 0.62              |
| 2:C:957:LYS:CD   | 2:C:961:GLU:HB3   | 2.30                     | 0.62              |
| 3:D:984:THR:HG22 | 3:D:987:GLU:CD    | 2.24                     | 0.62              |
| 2:M:25:SER:OG    | 2:M:336:VAL:HB    | 2.00                     | 0.62              |
| 2:M:332:ARG:HB2  | 2:M:466:PHE:HE1   | 1.64                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:926:PHE:HE1  | 2:M:929:ARG:NH2   | 1.97                     | 0.62              |
| 2:M:931:GLY:HA3  | 8:M:9835:HOH:O    | 1.99                     | 0.62              |
| 3:N:195:VAL:HG13 | 8:N:9862:HOH:O    | 1.98                     | 0.62              |
| 3:N:484:PRO:O    | 3:N:489:ARG:HD2   | 1.99                     | 0.62              |
| 3:N:486:ARG:HA   | 3:N:489:ARG:HD3   | 1.82                     | 0.62              |
| 3:N:543:LEU:O    | 3:N:546:ARG:HB2   | 2.00                     | 0.62              |
| 3:N:961:LYS:HA   | 8:N:2262:HOH:O    | 2.00                     | 0.62              |
| 5:P:304:VAL:O    | 5:P:308:LEU:HG    | 2.00                     | 0.62              |
| 2:C:443:THR:HG21 | 2:C:450:GLY:N     | 2.14                     | 0.62              |
| 3:D:111:LYS:HE2  | 3:D:1452:ILE:HG12 | 1.81                     | 0.62              |
| 3:D:906:GLN:HB3  | 3:D:911:LEU:CD1   | 2.30                     | 0.62              |
| 1:L:77:GLU:CB    | 3:N:872:ARG:HH21  | 2.11                     | 0.62              |
| 2:M:341:THR:HG23 | 8:M:9899:HOH:O    | 1.99                     | 0.62              |
| 2:M:536:PRO:HD2  | 8:M:9912:HOH:O    | 2.00                     | 0.62              |
| 3:N:699:VAL:HG21 | 3:N:760:ARG:HB3   | 1.82                     | 0.62              |
| 3:N:781:PRO:HG2  | 3:N:934:LEU:HD22  | 1.81                     | 0.62              |
| 3:N:1344:VAL:HB  | 3:N:1376:MET:HE1  | 1.81                     | 0.62              |
| 2:C:881:ASN:N    | 2:C:881:ASN:ND2   | 2.47                     | 0.62              |
| 2:C:886:LEU:HA   | 8:C:9674:HOH:O    | 1.98                     | 0.62              |
| 3:D:32:ILE:HG22  | 5:F:258:ILE:HD13  | 1.81                     | 0.62              |
| 3:D:83:SER:HB2   | 8:D:9611:HOH:O    | 2.00                     | 0.62              |
| 3:D:949:ILE:HD11 | 3:D:1023:MET:HE1  | 1.82                     | 0.62              |
| 3:D:986:ARG:HG3  | 3:D:990:ASP:OD1   | 2.00                     | 0.62              |
| 3:D:1412:LYS:O   | 3:D:1412:LYS:HG3  | 1.99                     | 0.62              |
| 2:M:92:ALA:HB2   | 2:M:120:LEU:HD21  | 1.79                     | 0.62              |
| 2:M:279:GLU:HG3  | 2:M:280:LYS:HG3   | 1.81                     | 0.62              |
| 2:M:841:ASN:ND2  | 2:M:843:HIS:CD2   | 2.68                     | 0.62              |
| 8:M:9750:HOH:O   | 3:N:524:LEU:HD11  | 2.00                     | 0.62              |
| 3:N:1314:LYS:HD3 | 3:N:1314:LYS:H    | 1.64                     | 0.62              |
| 1:A:162:ILE:HG13 | 1:A:163:ASN:ND2   | 2.15                     | 0.61              |
| 1:B:175:ARG:O    | 3:D:851:LEU:HD21  | 2.00                     | 0.61              |
| 2:C:444:PRO:HG2  | 2:C:452:ILE:HD12  | 1.82                     | 0.61              |
| 2:C:759:THR:HG21 | 2:C:783:ARG:NH1   | 2.15                     | 0.61              |
| 3:D:58:CYS:SG    | 3:D:78:VAL:HB     | 2.40                     | 0.61              |
| 3:D:565:ILE:HD13 | 5:F:192:LEU:CD1   | 2.30                     | 0.61              |
| 3:D:630:VAL:HA   | 3:D:744:GLN:HG2   | 1.82                     | 0.61              |
| 3:D:809:PRO:HB2  | 3:D:812:ALA:HB2   | 1.82                     | 0.61              |
| 2:M:101:ILE:HG22 | 2:M:102:HIS:H     | 1.65                     | 0.61              |
| 2:M:181:VAL:HG23 | 8:M:9655:HOH:O    | 2.00                     | 0.61              |
| 2:M:987:ILE:HD12 | 3:N:948:THR:CG2   | 2.30                     | 0.61              |
| 2:M:1097:LEU:HB3 | 3:N:10:ILE:HG23   | 1.81                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:11:ALA:HB1   | 3:N:507:ASN:OD1   | 2.00                     | 0.61              |
| 3:N:434:ARG:CB   | 3:N:447:VAL:HG22  | 2.27                     | 0.61              |
| 3:N:868:TYR:CD1  | 3:N:869:MET:HG3   | 2.34                     | 0.61              |
| 5:P:94:LEU:HD12  | 5:P:97:GLU:N      | 2.15                     | 0.61              |
| 1:A:198:ARG:HB2  | 1:A:200:TRP:CZ3   | 2.35                     | 0.61              |
| 1:B:74:ASP:O     | 1:B:78:ILE:HG13   | 2.00                     | 0.61              |
| 3:D:66:GLN:HB2   | 8:D:2184:HOH:O    | 2.00                     | 0.61              |
| 3:D:438:ASP:OD2  | 3:D:440:VAL:HB    | 2.00                     | 0.61              |
| 3:D:470:LEU:HD23 | 8:D:9988:HOH:O    | 1.99                     | 0.61              |
| 3:D:546:ARG:O    | 3:D:550:ARG:HG2   | 2.00                     | 0.61              |
| 1:A:14:ARG:HH22  | 1:A:24:VAL:CG2    | 2.13                     | 0.61              |
| 1:A:185:ARG:HD2  | 8:A:9484:HOH:O    | 2.00                     | 0.61              |
| 2:C:645:VAL:HG23 | 8:C:9746:HOH:O    | 2.00                     | 0.61              |
| 2:C:893:ALA:O    | 2:C:897:LEU:HB2   | 1.99                     | 0.61              |
| 3:D:770:LEU:HB2  | 3:D:1210:SER:O    | 2.00                     | 0.61              |
| 5:F:295:MET:HE2  | 5:F:295:MET:O     | 2.00                     | 0.61              |
| 1:K:150:TYR:HE2  | 1:K:152:PRO:HG3   | 1.65                     | 0.61              |
| 1:K:176:ARG:HG3  | 1:K:200:TRP:CE3   | 2.35                     | 0.61              |
| 2:M:30:LEU:O     | 2:M:30:LEU:HD12   | 2.00                     | 0.61              |
| 2:M:480:THR:HG22 | 2:M:482:GLU:H     | 1.64                     | 0.61              |
| 2:M:722:ILE:HG21 | 2:M:821:GLU:OE1   | 2.00                     | 0.61              |
| 2:M:1101:THR:C   | 2:M:1102:LEU:HD12 | 2.25                     | 0.61              |
| 3:N:87:ARG:HG3   | 3:N:88:TYR:N      | 2.14                     | 0.61              |
| 3:N:1045:MET:HE3 | 8:N:9780:HOH:O    | 2.01                     | 0.61              |
| 5:P:365:GLU:HB2  | 5:P:400:ILE:CG2   | 2.30                     | 0.61              |
| 5:P:369:LEU:O    | 5:P:373:LYS:HD3   | 2.00                     | 0.61              |
| 1:A:154:GLU:HA   | 8:C:9698:HOH:O    | 1.99                     | 0.61              |
| 1:B:89:PHE:HB3   | 1:B:94:LEU:HD22   | 1.81                     | 0.61              |
| 2:C:110:GLU:HG2  | 2:C:369:PRO:CG    | 2.30                     | 0.61              |
| 2:C:624:PRO:O    | 2:C:625:LEU:HD23  | 2.00                     | 0.61              |
| 2:C:722:ILE:O    | 2:C:722:ILE:HD13  | 2.00                     | 0.61              |
| 2:C:1090:LYS:HG3 | 3:D:521:PRO:HG2   | 1.82                     | 0.61              |
| 2:C:1109:VAL:HA  | 8:C:2004:HOH:O    | 2.00                     | 0.61              |
| 3:D:572:ARG:CZ   | 5:F:80:PRO:HD3    | 2.30                     | 0.61              |
| 3:D:581:LEU:O    | 3:D:603:LEU:HD12  | 2.00                     | 0.61              |
| 3:D:770:LEU:HD23 | 3:D:777:PRO:HA    | 1.82                     | 0.61              |
| 3:D:1377:LYS:HE2 | 3:D:1378:TYR:OH   | 2.00                     | 0.61              |
| 4:E:41:GLU:N     | 4:E:45:ARG:HG3    | 2.14                     | 0.61              |
| 1:K:46:SER:HB3   | 2:M:856:GLU:CD    | 2.25                     | 0.61              |
| 1:L:125:PRO:HD2  | 8:L:2988:HOH:O    | 2.00                     | 0.61              |
| 2:M:30:LEU:HD22  | 2:M:118:ILE:HD11  | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:474:VAL:HG13  | 2:M:530:GLU:C     | 2.26                     | 0.61              |
| 2:M:1019:GLN:HE22 | 3:N:621:LYS:HE3   | 1.65                     | 0.61              |
| 3:N:703:ASN:ND2   | 3:N:713:ILE:HG12  | 2.15                     | 0.61              |
| 3:N:789:LEU:HD13  | 3:N:934:LEU:HD23  | 1.81                     | 0.61              |
| 3:N:806:PHE:HE1   | 3:N:813:LEU:HB3   | 1.65                     | 0.61              |
| 5:P:393:THR:CG2   | 5:P:394:ARG:HD2   | 2.30                     | 0.61              |
| 1:B:73:GLU:OE1    | 1:B:130:ALA:HA    | 2.00                     | 0.61              |
| 2:C:333:ILE:HD13  | 2:C:467:ILE:HD11  | 1.80                     | 0.61              |
| 2:C:859:PRO:O     | 2:C:867:VAL:HG22  | 2.01                     | 0.61              |
| 2:C:1094:ALA:CB   | 3:D:603:LEU:HD13  | 2.31                     | 0.61              |
| 3:D:9:ARG:NH1     | 3:D:11:ALA:HB2    | 2.15                     | 0.61              |
| 3:D:52:PRO:HG3    | 3:D:78:VAL:HG13   | 1.81                     | 0.61              |
| 3:D:1243:THR:CB   | 3:D:1253:THR:HB   | 2.31                     | 0.61              |
| 4:E:47:LYS:N      | 4:E:54:LEU:HD22   | 2.14                     | 0.61              |
| 3:N:568:ARG:CZ    | 8:N:2401:HOH:O    | 2.47                     | 0.61              |
| 3:N:769:LEU:HG    | 3:N:931:LEU:HD11  | 1.83                     | 0.61              |
| 4:O:87:LYS:HA     | 8:O:728:HOH:O     | 2.00                     | 0.61              |
| 5:P:371:LEU:HD22  | 5:P:375:LEU:HD13  | 1.82                     | 0.61              |
| 2:C:431:HIS:CE1   | 2:C:432:ARG:HG2   | 2.36                     | 0.61              |
| 3:D:462:GLN:HA    | 3:D:513:ILE:HD13  | 1.82                     | 0.61              |
| 3:D:576:GLU:HA    | 3:D:579:ASP:OD2   | 2.01                     | 0.61              |
| 3:D:1264:GLU:HG2  | 3:D:1266:ARG:CZ   | 2.31                     | 0.61              |
| 2:M:164:PRO:HG2   | 8:M:9585:HOH:O    | 2.00                     | 0.61              |
| 3:N:436:GLU:HB2   | 3:N:445:ARG:HB3   | 1.81                     | 0.61              |
| 3:N:1332:PRO:HB3  | 3:N:1421:LEU:HD21 | 1.83                     | 0.61              |
| 3:N:1342:GLU:CD   | 3:N:1342:GLU:N    | 2.57                     | 0.61              |
| 3:N:1409:ALA:HB3  | 8:N:9829:HOH:O    | 2.01                     | 0.61              |
| 5:P:289:GLU:HA    | 8:P:9504:HOH:O    | 2.00                     | 0.61              |
| 1:A:101:LEU:HD23  | 1:A:102:LYS:N     | 2.16                     | 0.61              |
| 8:C:9889:HOH:O    | 3:D:659:LYS:HG2   | 2.00                     | 0.61              |
| 3:D:551:ASN:O     | 3:D:554:LEU:HB3   | 2.00                     | 0.61              |
| 3:D:984:THR:HG22  | 3:D:987:GLU:CG    | 2.31                     | 0.61              |
| 3:D:1377:LYS:HE2  | 3:D:1378:TYR:CZ   | 2.36                     | 0.61              |
| 5:F:291:ILE:HG21  | 5:F:304:VAL:HG11  | 1.82                     | 0.61              |
| 5:F:350:LEU:CD1   | 5:F:422:LEU:HB2   | 2.30                     | 0.61              |
| 5:F:361:LEU:CD1   | 5:F:366:ALA:HB2   | 2.16                     | 0.61              |
| 1:L:186:LEU:HB2   | 1:L:192:LEU:HD11  | 1.83                     | 0.61              |
| 2:M:380:ALA:O     | 2:M:384:GLU:HB2   | 2.00                     | 0.61              |
| 2:M:510:ALA:HB3   | 2:M:513:VAL:CG2   | 2.31                     | 0.61              |
| 2:M:916:GLU:O     | 2:M:919:ALA:HB3   | 2.01                     | 0.61              |
| 3:N:39:PRO:HB3    | 3:N:45:PHE:C      | 2.25                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1267:ARG:NH1  | 3:N:1271:LYS:HG3  | 2.16                     | 0.61              |
| 4:O:57:ASP:HB3    | 8:O:5269:HOH:O    | 1.99                     | 0.61              |
| 5:P:377:ASP:HB3   | 8:P:9661:HOH:O    | 2.00                     | 0.61              |
| 1:B:156:HIS:HD2   | 1:B:157:GLY:H     | 1.49                     | 0.61              |
| 1:B:212:ASN:O     | 1:B:215:VAL:HG22  | 2.01                     | 0.61              |
| 2:C:723:THR:HG21  | 2:C:783:ARG:HH22  | 1.66                     | 0.61              |
| 2:C:816:LYS:HB2   | 2:C:819:VAL:HG21  | 1.82                     | 0.61              |
| 3:D:675:ARG:O     | 3:D:678:GLU:HG2   | 2.01                     | 0.61              |
| 3:D:925:GLU:OE1   | 4:E:6:ILE:HG22    | 2.00                     | 0.61              |
| 3:D:1286:THR:HG22 | 3:D:1287:GLU:H    | 1.66                     | 0.61              |
| 3:D:1432:LYS:HD2  | 3:D:1433:SER:H    | 1.66                     | 0.61              |
| 5:F:135:ILE:HD11  | 5:F:178:ARG:HB3   | 1.82                     | 0.61              |
| 1:K:219:ARG:HG3   | 8:L:961:HOH:O     | 2.00                     | 0.61              |
| 1:L:101:LEU:HD23  | 1:L:102:LYS:N     | 2.15                     | 0.61              |
| 1:L:212:ASN:O     | 1:L:215:VAL:HG22  | 2.00                     | 0.61              |
| 2:M:264:PRO:HB2   | 2:M:289:THR:OG1   | 2.00                     | 0.61              |
| 2:M:762:LYS:HZ3   | 2:M:784:ASP:C     | 2.09                     | 0.61              |
| 3:N:191:LEU:CB    | 3:N:195:VAL:HG21  | 2.30                     | 0.61              |
| 5:P:340:SER:O     | 5:P:342:VAL:N     | 2.33                     | 0.61              |
| 1:B:101:LEU:HD23  | 1:B:102:LYS:N     | 2.15                     | 0.61              |
| 2:C:15:LEU:H      | 2:C:15:LEU:CD2    | 2.11                     | 0.61              |
| 2:C:18:LEU:HD23   | 2:C:542:VAL:HG21  | 1.83                     | 0.61              |
| 2:C:1038:TRP:CZ2  | 3:D:1096:ARG:HD2  | 2.36                     | 0.61              |
| 3:D:583:ASP:OD2   | 3:D:604:THR:HB    | 2.01                     | 0.61              |
| 3:D:654:LYS:HB3   | 3:D:655:PRO:HD3   | 1.83                     | 0.61              |
| 3:D:1122:LEU:HD11 | 3:D:1186:VAL:HG23 | 1.83                     | 0.61              |
| 2:M:683:ASN:HA    | 2:M:687:ALA:HB3   | 1.83                     | 0.61              |
| 2:M:976:ASP:HB3   | 2:M:979:THR:HG22  | 1.81                     | 0.61              |
| 3:N:65:ARG:HG3    | 3:N:66:GLN:H      | 1.65                     | 0.61              |
| 3:N:422:ALA:HB1   | 5:P:178:ARG:NH2   | 2.15                     | 0.61              |
| 3:N:539:ASP:HB2   | 5:P:318:GLU:OE2   | 1.99                     | 0.61              |
| 3:N:560:GLN:HE21  | 3:N:560:GLN:HA    | 1.66                     | 0.61              |
| 3:N:804:LEU:HD11  | 8:N:9675:HOH:O    | 1.99                     | 0.61              |
| 3:N:1450:ALA:HA   | 3:N:1455:LYS:HG3  | 1.83                     | 0.61              |
| 5:P:324:GLU:HG3   | 8:P:9622:HOH:O    | 2.00                     | 0.61              |
| 1:A:23:PHE:O      | 1:A:196:THR:HA    | 2.00                     | 0.61              |
| 1:B:86:VAL:HG23   | 8:B:9484:HOH:O    | 2.00                     | 0.61              |
| 2:C:676:ILE:HG23  | 2:C:676:ILE:O     | 2.00                     | 0.61              |
| 3:D:1426:LYS:HB2  | 3:D:1426:LYS:NZ   | 2.16                     | 0.61              |
| 2:M:266:ARG:HB3   | 8:M:9764:HOH:O    | 2.00                     | 0.61              |
| 3:N:527:MET:HE3   | 3:N:527:MET:HA    | 1.83                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:860:LEU:HA   | 3:N:877:PRO:HB2   | 1.83                     | 0.61              |
| 1:B:67:THR:HB    | 8:B:9510:HOH:O    | 2.01                     | 0.60              |
| 2:C:89:THR:O     | 2:C:91:GLN:HG3    | 2.01                     | 0.60              |
| 2:C:129:ILE:HB   | 8:C:2312:HOH:O    | 2.00                     | 0.60              |
| 2:C:1020:PRO:O   | 3:D:622:ARG:HD2   | 2.01                     | 0.60              |
| 3:D:13:ALA:HB1   | 3:D:18:ILE:HD11   | 1.82                     | 0.60              |
| 3:D:50:PHE:HB3   | 3:D:522:PRO:HG2   | 1.82                     | 0.60              |
| 3:D:466:LYS:HE2  | 8:D:9933:HOH:O    | 2.00                     | 0.60              |
| 3:D:543:LEU:HA   | 3:D:546:ARG:HG3   | 1.82                     | 0.60              |
| 3:D:636:GLN:HB2  | 8:D:2028:HOH:O    | 2.01                     | 0.60              |
| 3:D:970:LYS:HG2  | 8:D:2147:HOH:O    | 2.00                     | 0.60              |
| 3:D:1309:ALA:HB1 | 3:D:1326:THR:HG23 | 1.82                     | 0.60              |
| 1:L:74:ASP:O     | 1:L:78:ILE:HG13   | 2.01                     | 0.60              |
| 2:M:69:LEU:C     | 2:M:70:GLU:HG3    | 2.26                     | 0.60              |
| 2:M:195:LEU:O    | 2:M:199:VAL:HG23  | 2.00                     | 0.60              |
| 2:M:762:LYS:HB2  | 2:M:762:LYS:NZ    | 2.16                     | 0.60              |
| 2:M:1018:GLN:NE2 | 2:M:1063:ARG:NH2  | 2.49                     | 0.60              |
| 3:N:639:LEU:HD11 | 3:N:931:LEU:HD12  | 1.82                     | 0.60              |
| 3:N:729:HIS:CE1  | 3:N:731:LEU:HG    | 2.36                     | 0.60              |
| 3:N:814:ALA:HB2  | 8:N:9621:HOH:O    | 2.01                     | 0.60              |
| 3:N:1095:THR:OG1 | 3:N:1230:GLY:HA3  | 2.01                     | 0.60              |
| 3:N:1147:ARG:H   | 3:N:1166:LEU:HD23 | 1.66                     | 0.60              |
| 3:N:1309:ALA:HB1 | 3:N:1326:THR:HG23 | 1.82                     | 0.60              |
| 5:P:118:GLU:HB3  | 8:P:9609:HOH:O    | 2.01                     | 0.60              |
| 5:P:160:ASP:HA   | 5:P:163:LEU:HD12  | 1.82                     | 0.60              |
| 1:A:182:GLU:OE1  | 2:C:934:PHE:HB3   | 2.00                     | 0.60              |
| 2:C:49:ARG:HD3   | 8:C:2304:HOH:O    | 2.00                     | 0.60              |
| 2:C:528:GLU:O    | 2:C:530:GLU:HG3   | 2.01                     | 0.60              |
| 2:C:1090:LYS:HB3 | 3:D:521:PRO:HD2   | 1.83                     | 0.60              |
| 3:D:547:LEU:CD2  | 3:D:581:LEU:HD21  | 2.31                     | 0.60              |
| 3:D:556:LYS:HD2  | 8:D:2572:HOH:O    | 2.01                     | 0.60              |
| 3:D:710:ARG:HG3  | 3:D:711:LEU:N     | 2.15                     | 0.60              |
| 3:D:1031:ASN:HB3 | 3:D:1034:GLN:CD   | 2.25                     | 0.60              |
| 3:D:1459:LEU:HB3 | 3:D:1465:ASN:ND2  | 2.16                     | 0.60              |
| 5:F:346:THR:HG21 | 5:F:422:LEU:O     | 2.01                     | 0.60              |
| 1:L:108:GLU:HB3  | 1:L:128:HIS:CE1   | 2.27                     | 0.60              |
| 2:M:288:ARG:HD2  | 8:M:2222:HOH:O    | 2.01                     | 0.60              |
| 3:N:127:LEU:HD21 | 3:N:461:ILE:HD11  | 1.82                     | 0.60              |
| 3:N:422:ALA:H    | 3:N:427:VAL:CG1   | 2.13                     | 0.60              |
| 3:N:834:THR:HB   | 3:N:838:ARG:HB2   | 1.83                     | 0.60              |
| 1:A:54:THR:CG2   | 1:A:158:ILE:HG13  | 2.31                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:73:LEU:HD23  | 2:C:94:LEU:HB2   | 1.83                     | 0.60              |
| 2:C:205:GLU:HB2  | 8:C:9906:HOH:O   | 2.00                     | 0.60              |
| 2:C:876:VAL:HG22 | 2:C:884:GLN:HE21 | 1.65                     | 0.60              |
| 2:C:1096:ALA:HB3 | 3:D:101:HIS:ND1  | 2.16                     | 0.60              |
| 8:C:2084:HOH:O   | 3:D:3:LYS:HG3    | 2.01                     | 0.60              |
| 3:D:119:SER:CB   | 3:D:123:LEU:HB2  | 2.32                     | 0.60              |
| 3:D:583:ASP:CG   | 3:D:604:THR:HB   | 2.26                     | 0.60              |
| 3:D:1491:THR:HB  | 4:E:89:MET:HE1   | 1.81                     | 0.60              |
| 5:F:140:ARG:HG3  | 5:F:141:VAL:N    | 2.15                     | 0.60              |
| 5:F:350:LEU:HD13 | 5:F:422:LEU:HB2  | 1.82                     | 0.60              |
| 1:K:39:PRO:O     | 1:K:43:ILE:HG12  | 2.02                     | 0.60              |
| 2:M:254:VAL:O    | 2:M:257:VAL:HG23 | 2.00                     | 0.60              |
| 2:M:846:LYS:NZ   | 3:N:741:ASP:O    | 2.34                     | 0.60              |
| 2:M:1103:ASP:CG  | 2:M:1104:GLU:H   | 2.07                     | 0.60              |
| 3:N:960:LYS:HG2  | 3:N:964:LEU:HD12 | 1.83                     | 0.60              |
| 2:C:379:GLU:O    | 2:C:383:ARG:HB3  | 2.01                     | 0.60              |
| 2:C:498:GLN:HB3  | 8:C:9751:HOH:O   | 2.02                     | 0.60              |
| 2:C:584:GLU:CD   | 2:C:584:GLU:H    | 2.08                     | 0.60              |
| 2:C:1009:SER:HB2 | 3:D:651:GLU:O    | 2.02                     | 0.60              |
| 3:D:10:ILE:HG13  | 3:D:1434:TRP:CZ2 | 2.36                     | 0.60              |
| 3:D:127:LEU:HD21 | 3:D:461:ILE:HD11 | 1.83                     | 0.60              |
| 3:D:148:GLU:HA   | 3:D:149:LYS:HE2  | 1.83                     | 0.60              |
| 3:D:512:MET:HB3  | 8:D:2085:HOH:O   | 1.99                     | 0.60              |
| 3:D:572:ARG:HH22 | 5:F:83:GLN:NE2   | 2.00                     | 0.60              |
| 3:D:584:ASN:HB2  | 3:D:602:SER:OG   | 2.02                     | 0.60              |
| 3:D:772:PRO:O    | 3:D:1367:HIS:NE2 | 2.34                     | 0.60              |
| 3:D:894:LYS:HG2  | 8:D:9710:HOH:O   | 2.01                     | 0.60              |
| 3:D:1357:ARG:HG3 | 8:D:2490:HOH:O   | 2.01                     | 0.60              |
| 4:E:41:GLU:HB3   | 4:E:42:PRO:HD3   | 1.84                     | 0.60              |
| 5:F:114:LYS:HE3  | 8:F:9811:HOH:O   | 2.01                     | 0.60              |
| 5:F:160:ASP:O    | 5:F:164:LYS:HG3  | 2.01                     | 0.60              |
| 1:K:12:THR:HG23  | 1:K:24:VAL:HB    | 1.84                     | 0.60              |
| 1:L:216:GLU:HG3  | 1:L:220:GLU:OE1  | 2.01                     | 0.60              |
| 2:M:110:GLU:H    | 2:M:368:THR:HG21 | 1.66                     | 0.60              |
| 2:M:313:LEU:HD13 | 2:M:321:GLU:O    | 2.02                     | 0.60              |
| 2:M:405:ARG:HH21 | 2:M:409:ARG:HH21 | 1.47                     | 0.60              |
| 3:N:535:PHE:O    | 5:P:314:PRO:HA   | 2.01                     | 0.60              |
| 3:N:798:GLU:HG2  | 3:N:799:LYS:H    | 1.65                     | 0.60              |
| 3:N:868:TYR:HD1  | 3:N:869:MET:HG3  | 1.66                     | 0.60              |
| 3:N:1033:GLN:HG2 | 8:N:2106:HOH:O   | 2.00                     | 0.60              |
| 4:O:60:ALA:O     | 4:O:63:TRP:HB2   | 2.01                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:4:LYS:HD3     | 8:C:2222:HOH:O    | 2.00                     | 0.60              |
| 2:C:49:ARG:HB2    | 2:C:49:ARG:CZ     | 2.31                     | 0.60              |
| 3:D:957:PRO:HG3   | 3:D:1007:VAL:HA   | 1.83                     | 0.60              |
| 1:L:89:PHE:HB3    | 1:L:120:VAL:HG22  | 1.82                     | 0.60              |
| 2:M:398:THR:HG23  | 2:M:635:THR:HG21  | 1.82                     | 0.60              |
| 2:M:432:ARG:NH1   | 3:N:1047:LYS:HE2  | 2.12                     | 0.60              |
| 2:M:905:ILE:HG12  | 8:M:9571:HOH:O    | 2.00                     | 0.60              |
| 2:M:1096:ALA:O    | 3:N:13:ALA:HB2    | 2.01                     | 0.60              |
| 3:N:1092:GLY:O    | 3:N:1096:ARG:HB2  | 2.01                     | 0.60              |
| 3:N:1161:GLU:CG   | 3:N:1164:ARG:HB2  | 2.32                     | 0.60              |
| 1:A:115:LEU:HD12  | 1:A:115:LEU:O     | 2.00                     | 0.60              |
| 2:C:170:PRO:HG2   | 2:C:258:TYR:CD2   | 2.37                     | 0.60              |
| 2:C:176:VAL:HG12  | 2:C:182:VAL:CG1   | 2.31                     | 0.60              |
| 2:C:244:PRO:HA    | 8:C:2250:HOH:O    | 2.01                     | 0.60              |
| 2:C:462:ASP:HB2   | 8:C:9962:HOH:O    | 2.02                     | 0.60              |
| 2:C:776:SER:HA    | 2:C:780:GLU:HB3   | 1.83                     | 0.60              |
| 2:C:1115:LEU:HG   | 8:C:9518:HOH:O    | 2.01                     | 0.60              |
| 4:E:44:GLU:N      | 8:E:9370:HOH:O    | 2.33                     | 0.60              |
| 4:E:74:VAL:CG1    | 4:E:79:LEU:HD21   | 2.31                     | 0.60              |
| 2:M:42:VAL:HG12   | 2:M:43:GLY:H      | 1.65                     | 0.60              |
| 2:M:93:PRO:HG3    | 2:M:117:HIS:CE1   | 2.32                     | 0.60              |
| 2:M:206:THR:HB    | 8:M:9850:HOH:O    | 2.00                     | 0.60              |
| 2:M:208:ALA:HB1   | 2:M:218:VAL:HG11  | 1.82                     | 0.60              |
| 2:M:1019:GLN:HE22 | 3:N:621:LYS:CE    | 2.14                     | 0.60              |
| 3:N:462:GLN:HA    | 3:N:513:ILE:CD1   | 2.30                     | 0.60              |
| 3:N:786:ILE:HG21  | 3:N:1027:GLY:N    | 2.16                     | 0.60              |
| 5:P:225:GLU:HB3   | 5:P:226:LYS:HZ2   | 1.66                     | 0.60              |
| 1:B:185:ARG:HA    | 8:B:9553:HOH:O    | 2.01                     | 0.60              |
| 1:B:206:THR:HG22  | 1:B:209:GLU:CG    | 2.32                     | 0.60              |
| 1:B:206:THR:HG22  | 1:B:209:GLU:HG3   | 1.83                     | 0.60              |
| 3:D:380:GLU:O     | 3:D:382:GLU:N     | 2.34                     | 0.60              |
| 3:D:486:ARG:HA    | 3:D:489:ARG:HD3   | 1.83                     | 0.60              |
| 3:D:1258:ARG:NH2  | 3:D:1262:LEU:HD11 | 2.17                     | 0.60              |
| 4:E:46:PRO:HB3    | 4:E:54:LEU:HD21   | 1.84                     | 0.60              |
| 5:F:156:VAL:HG13  | 8:F:9476:HOH:O    | 2.02                     | 0.60              |
| 1:K:29:GLU:N      | 8:K:1204:HOH:O    | 2.34                     | 0.60              |
| 2:M:686:ASP:O     | 3:N:740:PHE:HB2   | 2.02                     | 0.60              |
| 3:N:843:PHE:CE1   | 3:N:864:VAL:HG11  | 2.36                     | 0.60              |
| 3:N:1346:ARG:O    | 3:N:1350:GLU:HG3  | 2.01                     | 0.60              |
| 3:N:1388:ARG:O    | 3:N:1391:GLU:HG2  | 2.00                     | 0.60              |
| 1:A:218:LEU:CD2   | 1:B:222:LEU:HD11  | 2.31                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:18:ARG:O     | 1:B:207:PRO:HD3  | 2.02                     | 0.60              |
| 1:B:215:VAL:HG23 | 8:B:9526:HOH:O   | 2.01                     | 0.60              |
| 2:C:1050:GLN:HB2 | 8:D:2065:HOH:O   | 2.02                     | 0.60              |
| 3:D:477:LEU:HD21 | 3:D:495:ARG:NH1  | 2.17                     | 0.60              |
| 3:D:560:GLN:O    | 5:F:184:ARG:NH2  | 2.35                     | 0.60              |
| 4:E:9:LEU:HB3    | 4:E:19:LEU:HD21  | 1.84                     | 0.60              |
| 5:F:277:GLN:HG3  | 8:F:9724:HOH:O   | 2.00                     | 0.60              |
| 1:K:96:THR:OG1   | 1:K:143:ARG:NH1  | 2.35                     | 0.60              |
| 1:K:123:MET:HE3  | 1:K:203:GLY:O    | 2.02                     | 0.60              |
| 1:K:197:LEU:HD23 | 1:K:197:LEU:H    | 1.66                     | 0.60              |
| 1:L:18:ARG:O     | 1:L:207:PRO:HD3  | 2.01                     | 0.60              |
| 1:L:226:SER:HA   | 8:L:3072:HOH:O   | 2.02                     | 0.60              |
| 2:M:397:GLU:HG3  | 2:M:631:SER:HB2  | 1.83                     | 0.60              |
| 2:M:803:THR:HG22 | 2:M:825:VAL:HG22 | 1.82                     | 0.60              |
| 8:M:9822:HOH:O   | 3:N:651:GLU:HB3  | 2.01                     | 0.60              |
| 3:N:90:MET:HE3   | 3:N:521:PRO:HD3  | 1.82                     | 0.60              |
| 3:N:1441:GLN:HB2 | 8:N:9617:HOH:O   | 2.01                     | 0.60              |
| 4:O:48:MET:HB3   | 4:O:54:LEU:HB2   | 1.83                     | 0.60              |
| 5:P:406:ARG:HA   | 5:P:409:LYS:HD3  | 1.83                     | 0.60              |
| 1:A:212:ASN:O    | 1:A:215:VAL:HG22 | 2.02                     | 0.60              |
| 2:C:774:LEU:HD13 | 2:C:774:LEU:C    | 2.27                     | 0.60              |
| 3:D:18:ILE:HG21  | 3:D:516:ALA:O    | 2.02                     | 0.60              |
| 1:K:1:MET:O      | 1:K:6:LEU:HD22   | 2.01                     | 0.60              |
| 1:L:86:VAL:HA    | 8:L:1948:HOH:O   | 2.01                     | 0.60              |
| 1:L:162:ILE:HD13 | 8:L:5120:HOH:O   | 2.01                     | 0.60              |
| 2:M:535:SER:HB2  | 8:M:9912:HOH:O   | 2.02                     | 0.60              |
| 3:N:785:ILE:HD12 | 3:N:785:ILE:N    | 2.16                     | 0.60              |
| 3:N:1397:LYS:HG2 | 8:N:2381:HOH:O   | 2.01                     | 0.60              |
| 2:C:841:ASN:ND2  | 2:C:843:HIS:H    | 2.00                     | 0.60              |
| 4:E:50:THR:HG22  | 8:E:9360:HOH:O   | 2.01                     | 0.60              |
| 5:F:94:LEU:HD13  | 5:F:96:LEU:N     | 2.15                     | 0.60              |
| 5:F:358:LEU:HD21 | 5:F:367:MET:HE1  | 1.83                     | 0.60              |
| 5:F:419:ARG:O    | 5:F:421:PHE:N    | 2.35                     | 0.60              |
| 1:K:108:GLU:O    | 1:K:110:LYS:HG3  | 2.01                     | 0.60              |
| 1:L:185:ARG:HH12 | 3:N:692:GLU:HG3  | 1.67                     | 0.60              |
| 2:M:200:LEU:HD13 | 2:M:300:ASP:CG   | 2.27                     | 0.60              |
| 2:M:443:THR:HG22 | 2:M:452:ILE:O    | 2.02                     | 0.60              |
| 2:M:878:SER:HA   | 3:N:1034:GLN:OE1 | 2.02                     | 0.60              |
| 3:N:52:PRO:HB3   | 3:N:80:VAL:HB    | 1.83                     | 0.60              |
| 3:N:538:SER:N    | 5:P:317:LEU:HD12 | 2.16                     | 0.60              |
| 5:P:376:ILE:HG22 | 5:P:377:ASP:CB   | 2.31                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:7:LYS:CE      | 1:B:186:LEU:HD13  | 2.31                     | 0.59              |
| 2:C:41:ASN:O      | 2:C:46:ALA:HB2    | 2.02                     | 0.59              |
| 2:C:288:ARG:HA    | 2:C:288:ARG:HE    | 1.66                     | 0.59              |
| 2:C:530:GLU:C     | 2:C:531:PHE:HD1   | 2.09                     | 0.59              |
| 3:D:601:ARG:HD3   | 3:D:613:ARG:HH21  | 1.67                     | 0.59              |
| 1:L:76:VAL:HA     | 1:L:79:ILE:HG12   | 1.82                     | 0.59              |
| 2:M:49:ARG:NH2    | 8:M:9564:HOH:O    | 2.35                     | 0.59              |
| 3:N:380:GLU:O     | 3:N:382:GLU:N     | 2.35                     | 0.59              |
| 3:N:984:THR:HG22  | 3:N:987:GLU:CG    | 2.29                     | 0.59              |
| 3:N:1046:GLN:HB3  | 8:N:9803:HOH:O    | 2.01                     | 0.59              |
| 3:N:1122:LEU:HD23 | 3:N:1178:ALA:HB2  | 1.84                     | 0.59              |
| 2:C:1001:VAL:HG12 | 8:C:2021:HOH:O    | 2.02                     | 0.59              |
| 3:D:594:PRO:HB2   | 8:D:2420:HOH:O    | 2.02                     | 0.59              |
| 3:D:1213:ARG:HB2  | 3:D:1214:PRO:CD   | 2.31                     | 0.59              |
| 1:K:101:LEU:HD23  | 1:K:102:LYS:N     | 2.17                     | 0.59              |
| 1:L:108:GLU:O     | 1:L:110:LYS:HG3   | 2.02                     | 0.59              |
| 2:M:1009:SER:HB2  | 3:N:651:GLU:OE1   | 2.02                     | 0.59              |
| 3:N:47:GLU:HB2    | 3:N:78:VAL:HG22   | 1.84                     | 0.59              |
| 5:P:166:LEU:O     | 5:P:171:LYS:HB2   | 2.02                     | 0.59              |
| 1:B:7:LYS:NZ      | 1:B:186:LEU:HD13  | 2.18                     | 0.59              |
| 1:B:38:ASN:HB2    | 8:C:2221:HOH:O    | 2.00                     | 0.59              |
| 2:C:42:VAL:HG11   | 8:C:9546:HOH:O    | 2.01                     | 0.59              |
| 2:C:162:ILE:HB    | 2:C:172:ILE:HD13  | 1.83                     | 0.59              |
| 2:C:208:ALA:HB1   | 2:C:218:VAL:HG11  | 1.85                     | 0.59              |
| 2:C:1042:ALA:O    | 3:D:1220:ALA:HB3  | 2.01                     | 0.59              |
| 3:D:4:GLU:HB2     | 8:D:9671:HOH:O    | 2.02                     | 0.59              |
| 3:D:407:VAL:HA    | 8:D:9600:HOH:O    | 2.01                     | 0.59              |
| 3:D:525:ARG:HA    | 3:D:538:SER:OG    | 2.01                     | 0.59              |
| 3:D:546:ARG:NH2   | 3:D:550:ARG:HH22  | 2.00                     | 0.59              |
| 5:F:184:ARG:O     | 5:F:188:ILE:HG13  | 2.02                     | 0.59              |
| 2:M:376:ARG:HH12  | 5:P:285:GLU:HG2   | 1.66                     | 0.59              |
| 2:M:1083:GLU:O    | 2:M:1087:VAL:HG23 | 2.02                     | 0.59              |
| 3:N:111:LYS:HE2   | 3:N:111:LYS:HA    | 1.85                     | 0.59              |
| 3:N:177:ALA:HB1   | 3:N:199:LEU:CG    | 2.32                     | 0.59              |
| 3:N:555:LYS:HA    | 3:N:558:LEU:HD12  | 1.84                     | 0.59              |
| 3:N:1489:GLN:HA   | 3:N:1489:GLN:NE2  | 2.16                     | 0.59              |
| 2:C:101:ILE:HG22  | 2:C:102:HIS:H     | 1.67                     | 0.59              |
| 3:D:488:ARG:HD3   | 8:D:2340:HOH:O    | 2.01                     | 0.59              |
| 3:D:1022:VAL:HG21 | 8:D:9500:HOH:O    | 2.02                     | 0.59              |
| 3:D:1109:GLU:HG2  | 3:D:1202:GLN:N    | 2.16                     | 0.59              |
| 3:D:1109:GLU:CG   | 3:D:1202:GLN:H    | 2.15                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1295:GLU:HB3  | 3:D:1300:SER:CB   | 2.32                     | 0.59              |
| 2:M:250:ARG:CZ    | 2:M:253:ALA:HB1   | 2.31                     | 0.59              |
| 2:M:297:GLU:HB2   | 8:M:9925:HOH:O    | 2.03                     | 0.59              |
| 2:M:674:VAL:HG11  | 2:M:992:MET:HE3   | 1.82                     | 0.59              |
| 3:N:58:CYS:SG     | 3:N:78:VAL:HB     | 2.43                     | 0.59              |
| 3:N:558:LEU:HD13  | 5:P:145:PRO:CB    | 2.32                     | 0.59              |
| 3:N:1336:LEU:HD22 | 3:N:1421:LEU:HB2  | 1.83                     | 0.59              |
| 5:P:359:SER:HB3   | 8:P:9756:HOH:O    | 2.00                     | 0.59              |
| 2:C:34:VAL:HB     | 2:C:38:LYS:CG     | 2.29                     | 0.59              |
| 2:C:751:PRO:HB2   | 3:D:680:GLN:CG    | 2.30                     | 0.59              |
| 3:D:452:ILE:HG23  | 3:D:452:ILE:O     | 2.01                     | 0.59              |
| 3:D:702:LEU:HB3   | 3:D:745:MET:HE3   | 1.85                     | 0.59              |
| 3:D:783:ARG:HH21  | 3:D:1029:ARG:HG2  | 1.68                     | 0.59              |
| 3:D:1263:PHE:CZ   | 3:D:1352:ILE:HD13 | 2.37                     | 0.59              |
| 3:D:1264:GLU:HB3  | 3:D:1266:ARG:HD2  | 1.84                     | 0.59              |
| 3:D:1390:LEU:HG   | 8:D:9868:HOH:O    | 2.02                     | 0.59              |
| 3:D:1399:ASP:O    | 3:D:1403:LEU:HB2  | 2.02                     | 0.59              |
| 1:K:53:VAL:HG12   | 1:K:167:VAL:HG21  | 1.83                     | 0.59              |
| 1:K:89:PHE:HB3    | 1:K:120:VAL:HG22  | 1.84                     | 0.59              |
| 2:M:176:VAL:HG12  | 2:M:182:VAL:HG13  | 1.84                     | 0.59              |
| 2:M:514:VAL:HG11  | 2:M:516:ARG:CZ    | 2.32                     | 0.59              |
| 2:M:571:LEU:HD22  | 2:M:670:GLN:OE1   | 2.02                     | 0.59              |
| 2:M:862:PRO:HA    | 2:M:975:TYR:CE1   | 2.34                     | 0.59              |
| 3:N:75:ARG:HH11   | 3:N:75:ARG:HG3    | 1.67                     | 0.59              |
| 3:N:146:PRO:HA    | 8:N:9562:HOH:O    | 2.03                     | 0.59              |
| 3:N:756:GLN:O     | 3:N:760:ARG:HG2   | 2.02                     | 0.59              |
| 5:P:200:LYS:HA    | 5:P:209:PHE:HE1   | 1.67                     | 0.59              |
| 1:B:102:LYS:HB3   | 8:B:9575:HOH:O    | 2.02                     | 0.59              |
| 1:B:206:THR:HG22  | 1:B:209:GLU:H     | 1.68                     | 0.59              |
| 2:C:42:VAL:HG12   | 2:C:43:GLY:N      | 2.18                     | 0.59              |
| 2:C:57:GLU:O      | 2:C:62:GLY:HA3    | 2.02                     | 0.59              |
| 2:C:120:LEU:HB2   | 8:C:2229:HOH:O    | 2.01                     | 0.59              |
| 3:D:23:TYR:O      | 3:D:49:ILE:HG23   | 2.02                     | 0.59              |
| 3:D:65:ARG:HB2    | 5:F:375:LEU:CA    | 2.28                     | 0.59              |
| 3:D:126:VAL:HG13  | 3:D:132:TYR:CB    | 2.31                     | 0.59              |
| 3:D:423:ASP:O     | 3:D:425:GLY:N     | 2.30                     | 0.59              |
| 3:D:481:MET:HG2   | 3:D:493:ARG:HH21  | 1.65                     | 0.59              |
| 3:D:829:VAL:HG13  | 8:D:2203:HOH:O    | 2.03                     | 0.59              |
| 3:D:1310:ARG:NE   | 3:D:1327:ARG:HB3  | 2.11                     | 0.59              |
| 2:M:8:ARG:HG2     | 8:M:9832:HOH:O    | 2.02                     | 0.59              |
| 2:M:143:SER:CB    | 2:M:276:LYS:HZ3   | 2.15                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:250:ARG:HH21  | 2:M:253:ALA:HB1   | 1.67                     | 0.59              |
| 2:M:266:ARG:HD3   | 2:M:273:GLY:HA3   | 1.85                     | 0.59              |
| 2:M:676:ILE:O     | 2:M:676:ILE:HG23  | 2.02                     | 0.59              |
| 3:N:116:LEU:HD23  | 3:N:468:LEU:HD21  | 1.84                     | 0.59              |
| 3:N:470:LEU:HD22  | 3:N:499:VAL:HG22  | 1.84                     | 0.59              |
| 3:N:499:VAL:O     | 3:N:503:LEU:HB2   | 2.02                     | 0.59              |
| 3:N:787:LEU:HD21  | 3:N:947:ILE:CD1   | 2.32                     | 0.59              |
| 3:N:845:ASN:H     | 3:N:848:GLU:HG3   | 1.68                     | 0.59              |
| 4:O:41:GLU:HB3    | 4:O:42:PRO:HD3    | 1.83                     | 0.59              |
| 1:A:227:ASN:H     | 1:A:227:ASN:ND2   | 2.00                     | 0.59              |
| 1:B:176:ARG:NH2   | 3:D:884:ARG:CZ    | 2.66                     | 0.59              |
| 2:C:188:LYS:HE2   | 2:C:188:LYS:O     | 2.01                     | 0.59              |
| 2:C:225:SER:HB2   | 2:C:229:MET:HE1   | 1.83                     | 0.59              |
| 2:C:437:ARG:NH2   | 2:C:488:ALA:HA    | 2.16                     | 0.59              |
| 3:D:730:PRO:HA    | 3:D:733:CYS:SG    | 2.42                     | 0.59              |
| 3:D:897:TRP:HZ3   | 8:D:2492:HOH:O    | 1.85                     | 0.59              |
| 5:F:195:VAL:HG11  | 5:F:217:ASN:OD1   | 2.01                     | 0.59              |
| 1:K:96:THR:CB     | 1:K:143:ARG:HH12  | 2.15                     | 0.59              |
| 2:M:41:ASN:O      | 2:M:46:ALA:HB2    | 2.02                     | 0.59              |
| 2:M:501:THR:HG22  | 2:M:513:VAL:CG1   | 2.33                     | 0.59              |
| 2:M:603:VAL:HG21  | 2:M:643:VAL:CG1   | 2.31                     | 0.59              |
| 3:N:601:ARG:HH11  | 3:N:613:ARG:NH2   | 1.99                     | 0.59              |
| 1:A:197:LEU:N     | 1:A:197:LEU:HD23  | 2.17                     | 0.59              |
| 1:A:227:ASN:HD22  | 1:A:227:ASN:N     | 1.97                     | 0.59              |
| 1:B:91:ASN:HB3    | 8:B:9492:HOH:O    | 2.02                     | 0.59              |
| 8:C:9694:HOH:O    | 3:D:1068:LEU:HD21 | 2.03                     | 0.59              |
| 3:D:456:MET:HG2   | 3:D:568:ARG:HH11  | 1.68                     | 0.59              |
| 3:D:1101:VAL:HG11 | 3:D:1427:SER:HB3  | 1.85                     | 0.59              |
| 5:F:163:LEU:HD13  | 5:F:174:LEU:HG    | 1.85                     | 0.59              |
| 2:M:238:LEU:O     | 2:M:242:LEU:HD22  | 2.03                     | 0.59              |
| 2:M:431:HIS:HD2   | 2:M:433:THR:OG1   | 1.85                     | 0.59              |
| 2:M:545:ASN:O     | 2:M:581:THR:HG21  | 2.03                     | 0.59              |
| 2:M:707:ARG:HG3   | 2:M:826:TYR:CE2   | 2.38                     | 0.59              |
| 2:M:846:LYS:O     | 3:N:741:ASP:HB3   | 2.02                     | 0.59              |
| 2:M:1020:PRO:O    | 3:N:622:ARG:HD2   | 2.03                     | 0.59              |
| 3:N:422:ALA:HB1   | 5:P:178:ARG:HH22  | 1.68                     | 0.59              |
| 3:N:498:VAL:HG11  | 8:N:9878:HOH:O    | 2.02                     | 0.59              |
| 3:N:820:GLU:HG2   | 3:N:825:ALA:O     | 2.03                     | 0.59              |
| 5:P:94:LEU:H      | 5:P:98:GLU:HB2    | 1.67                     | 0.59              |
| 1:A:143:ARG:HD3   | 1:A:160:ASP:OD2   | 2.03                     | 0.59              |
| 2:C:194:VAL:HG21  | 2:C:221:LEU:O     | 2.02                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:371:LYS:O     | 2:C:372:LEU:HD12  | 2.02                     | 0.59              |
| 2:C:858:MET:HB2   | 2:C:859:PRO:HD2   | 1.84                     | 0.59              |
| 2:C:938:LYS:HE3   | 8:C:9606:HOH:O    | 2.03                     | 0.59              |
| 3:D:13:ALA:O      | 3:D:511:TRP:HB3   | 2.03                     | 0.59              |
| 3:D:166:GLN:HG2   | 3:D:207:PHE:HB2   | 1.85                     | 0.59              |
| 3:D:379:ALA:HB1   | 8:D:2450:HOH:O    | 2.02                     | 0.59              |
| 3:D:1489:GLN:HE21 | 3:D:1493:LYS:NZ   | 2.01                     | 0.59              |
| 8:D:9617:HOH:O    | 5:F:141:VAL:HG21  | 2.02                     | 0.59              |
| 4:E:40:LEU:HD12   | 4:E:40:LEU:O      | 2.03                     | 0.59              |
| 5:F:132:ARG:HG2   | 5:F:181:GLU:OE1   | 2.03                     | 0.59              |
| 5:F:267:THR:HA    | 8:F:9561:HOH:O    | 2.02                     | 0.59              |
| 2:M:183:SER:HB3   | 2:M:190:LYS:HZ1   | 1.66                     | 0.59              |
| 2:M:567:GLN:HB2   | 2:M:997:LEU:HD22  | 1.85                     | 0.59              |
| 2:M:1097:LEU:HD21 | 3:N:103:TRP:HZ3   | 1.68                     | 0.59              |
| 3:N:477:LEU:HB3   | 3:N:496:LEU:HD12  | 1.84                     | 0.59              |
| 2:C:162:ILE:HG12  | 2:C:306:THR:HG21  | 1.84                     | 0.59              |
| 2:C:220:GLY:HA3   | 8:C:9517:HOH:O    | 2.01                     | 0.59              |
| 2:C:254:VAL:HG13  | 2:C:258:TYR:CE1   | 2.38                     | 0.59              |
| 2:C:474:VAL:HG13  | 2:C:530:GLU:C     | 2.27                     | 0.59              |
| 2:C:537:LYS:CA    | 2:C:545:ASN:HD21  | 2.15                     | 0.59              |
| 2:C:583:LEU:O     | 2:C:587:VAL:HG23  | 2.03                     | 0.59              |
| 2:C:767:PRO:HG3   | 8:C:2016:HOH:O    | 2.02                     | 0.59              |
| 2:C:798:GLY:H     | 2:C:827:VAL:CG1   | 2.16                     | 0.59              |
| 2:C:1032:PHE:CZ   | 2:C:1040:LEU:HD22 | 2.38                     | 0.59              |
| 2:C:1081:VAL:HB   | 2:C:1086:ARG:NH2  | 2.18                     | 0.59              |
| 3:D:56:TYR:HB2    | 8:D:9482:HOH:O    | 2.02                     | 0.59              |
| 3:D:583:ASP:HA    | 3:D:602:SER:HB2   | 1.83                     | 0.59              |
| 3:D:759:ALA:HA    | 3:D:763:MET:HE2   | 1.85                     | 0.59              |
| 3:D:785:ILE:HG12  | 3:D:935:LYS:HA    | 1.85                     | 0.59              |
| 3:D:826:PRO:HD3   | 8:D:9587:HOH:O    | 2.01                     | 0.59              |
| 1:K:50:GLY:O      | 1:K:146:ARG:HA    | 2.03                     | 0.59              |
| 2:M:242:LEU:HA    | 8:M:9620:HOH:O    | 2.02                     | 0.59              |
| 2:M:393:GLN:HE21  | 2:M:409:ARG:NH1   | 2.00                     | 0.59              |
| 3:N:646:LYS:CA    | 3:N:720:LEU:HD22  | 2.27                     | 0.59              |
| 5:P:398:ARG:HD2   | 8:P:9476:HOH:O    | 2.02                     | 0.59              |
| 1:A:42:ARG:NH1    | 2:C:857:ASP:HB3   | 2.18                     | 0.58              |
| 1:A:189:ARG:HH22  | 1:B:155:LYS:HG2   | 1.67                     | 0.58              |
| 1:B:77:GLU:HB2    | 3:D:872:ARG:NH2   | 2.18                     | 0.58              |
| 2:C:19:THR:HG21   | 2:C:124:ASP:O     | 2.03                     | 0.58              |
| 2:C:266:ARG:HG3   | 2:C:266:ARG:NH1   | 2.16                     | 0.58              |
| 2:C:442:GLU:HG2   | 2:C:454:SER:HB2   | 1.84                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:447:ALA:HA    | 3:D:1085:ALA:HB1  | 1.84                     | 0.58              |
| 2:C:679:PHE:N     | 8:C:9687:HOH:O    | 2.36                     | 0.58              |
| 2:C:900:ARG:HD2   | 8:C:9612:HOH:O    | 2.02                     | 0.58              |
| 2:C:902:ILE:HG22  | 2:C:904:PRO:HD3   | 1.84                     | 0.58              |
| 3:D:416:ALA:H     | 3:D:417:PRO:CD    | 2.15                     | 0.58              |
| 3:D:502:PHE:CZ    | 3:D:1452:ILE:HG13 | 2.38                     | 0.58              |
| 3:D:1066:THR:HG23 | 3:D:1069:GLU:OE1  | 2.03                     | 0.58              |
| 3:D:1460:ILE:HA   | 8:D:9474:HOH:O    | 2.03                     | 0.58              |
| 1:L:89:PHE:HB3    | 1:L:94:LEU:HD22   | 1.85                     | 0.58              |
| 2:M:139:GLN:HB3   | 2:M:334:ARG:CD    | 2.33                     | 0.58              |
| 2:M:610:ARG:HH11  | 2:M:610:ARG:HG3   | 1.68                     | 0.58              |
| 2:M:613:VAL:HG21  | 8:M:9608:HOH:O    | 2.02                     | 0.58              |
| 2:M:727:PRO:HB3   | 8:M:9890:HOH:O    | 2.03                     | 0.58              |
| 2:M:955:PRO:HD3   | 8:M:9758:HOH:O    | 2.02                     | 0.58              |
| 3:N:699:VAL:H     | 3:N:756:GLN:NE2   | 1.97                     | 0.58              |
| 1:B:41:ARG:HG3    | 1:B:41:ARG:HH11   | 1.68                     | 0.58              |
| 2:C:292:ARG:HH11  | 2:C:299:LYS:HD3   | 1.68                     | 0.58              |
| 2:C:347:GLY:HA2   | 2:C:350:ARG:HD2   | 1.85                     | 0.58              |
| 2:C:524:VAL:HB    | 8:C:2063:HOH:O    | 2.02                     | 0.58              |
| 2:C:1010:THR:HG21 | 5:F:341:PRO:HB2   | 1.84                     | 0.58              |
| 2:C:1056:LYS:HD3  | 3:D:623:VAL:HG22  | 1.85                     | 0.58              |
| 3:D:65:ARG:CB     | 5:F:375:LEU:HA    | 2.29                     | 0.58              |
| 3:D:396:VAL:CG2   | 3:D:447:VAL:HB    | 2.32                     | 0.58              |
| 3:D:697:GLY:HA3   | 4:E:59:ASN:OD1    | 2.01                     | 0.58              |
| 3:D:1464:GLU:HA   | 3:D:1467:ILE:HD12 | 1.84                     | 0.58              |
| 2:M:256:TYR:HB3   | 8:M:2097:HOH:O    | 2.01                     | 0.58              |
| 2:M:445:GLU:OE2   | 2:M:560:MET:HG2   | 2.02                     | 0.58              |
| 2:M:909:ALA:HB1   | 2:M:914:ILE:CD1   | 2.31                     | 0.58              |
| 2:M:1031:ARG:HD3  | 3:N:620:GLY:O     | 2.03                     | 0.58              |
| 2:C:95:TYR:CD2    | 2:C:114:PHE:HB3   | 2.38                     | 0.58              |
| 2:C:673:LEU:HD23  | 2:C:867:VAL:HG12  | 1.84                     | 0.58              |
| 3:D:609:GLY:CA    | 3:D:613:ARG:HB3   | 2.33                     | 0.58              |
| 3:D:659:LYS:C     | 3:D:659:LYS:HD3   | 2.28                     | 0.58              |
| 5:F:272:SER:O     | 5:F:276:ARG:HG2   | 2.02                     | 0.58              |
| 1:L:132:LEU:HD22  | 8:L:960:HOH:O     | 2.02                     | 0.58              |
| 2:M:244:PRO:CD    | 2:M:245:GLY:H     | 2.16                     | 0.58              |
| 2:M:354:GLY:HA3   | 8:M:2246:HOH:O    | 2.03                     | 0.58              |
| 2:M:545:ASN:OD1   | 2:M:905:ILE:HD13  | 2.03                     | 0.58              |
| 2:M:858:MET:HE2   | 2:M:867:VAL:O     | 2.03                     | 0.58              |
| 3:N:186:VAL:HG11  | 3:N:213:VAL:HB    | 1.85                     | 0.58              |
| 3:N:524:LEU:C     | 3:N:526:PRO:HD3   | 2.28                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:777:PRO:CG    | 3:N:915:VAL:HB    | 2.33                     | 0.58              |
| 3:N:813:LEU:HD12  | 3:N:814:ALA:N     | 2.18                     | 0.58              |
| 3:N:1236:LEU:HD11 | 3:N:1356:TYR:CE2  | 2.38                     | 0.58              |
| 1:B:78:ILE:HG12   | 8:B:9503:HOH:O    | 2.02                     | 0.58              |
| 2:C:129:ILE:HG22  | 2:C:130:ASN:N     | 2.18                     | 0.58              |
| 2:C:174:LEU:HD22  | 2:C:193:LEU:HD23  | 1.85                     | 0.58              |
| 2:C:218:VAL:O     | 2:C:221:LEU:HB3   | 2.02                     | 0.58              |
| 2:C:382:ILE:HA    | 8:C:9515:HOH:O    | 2.03                     | 0.58              |
| 3:D:12:LEU:CD2    | 3:D:13:ALA:H      | 2.16                     | 0.58              |
| 3:D:131:LYS:HD2   | 5:F:83:GLN:CD     | 2.28                     | 0.58              |
| 3:D:1020:LEU:HA   | 3:D:1023:MET:HE2  | 1.85                     | 0.58              |
| 3:D:1339:LYS:HD2  | 8:D:2350:HOH:O    | 2.02                     | 0.58              |
| 5:F:310:ILE:HA    | 8:F:9654:HOH:O    | 2.03                     | 0.58              |
| 5:F:340:SER:O     | 5:F:342:VAL:N     | 2.36                     | 0.58              |
| 5:F:415:THR:HG21  | 5:F:417:LYS:NZ    | 2.18                     | 0.58              |
| 1:K:51:THR:HA     | 1:K:145:ASP:O     | 2.03                     | 0.58              |
| 1:K:89:PHE:HB3    | 1:K:94:LEU:HD22   | 1.86                     | 0.58              |
| 1:L:89:PHE:HB2    | 1:L:94:LEU:HD22   | 1.86                     | 0.58              |
| 2:M:226:VAL:HA    | 8:M:9817:HOH:O    | 2.03                     | 0.58              |
| 2:M:675:ALA:HA    | 2:M:989:VAL:HG12  | 1.84                     | 0.58              |
| 3:N:196:VAL:HG13  | 3:N:202:VAL:HG11  | 1.84                     | 0.58              |
| 3:N:558:LEU:HD13  | 5:P:145:PRO:HA    | 1.84                     | 0.58              |
| 3:N:1148:VAL:HB   | 3:N:1203:LYS:O    | 2.04                     | 0.58              |
| 3:N:1458:GLU:O    | 3:N:1460:ILE:HG13 | 2.03                     | 0.58              |
| 4:O:40:LEU:HG     | 4:O:67:GLU:HG2    | 1.83                     | 0.58              |
| 1:B:206:THR:CG2   | 1:B:209:GLU:H     | 2.16                     | 0.58              |
| 2:C:15:LEU:HD22   | 2:C:15:LEU:N      | 2.14                     | 0.58              |
| 2:C:102:HIS:HB2   | 2:C:106:GLY:O     | 2.04                     | 0.58              |
| 2:C:165:LEU:HD12  | 2:C:166:PRO:N     | 2.18                     | 0.58              |
| 2:C:279:GLU:OE2   | 2:C:489:THR:HG21  | 2.03                     | 0.58              |
| 2:C:1101:THR:C    | 2:C:1102:LEU:HD12 | 2.28                     | 0.58              |
| 3:D:195:VAL:HB    | 3:D:205:TYR:HB2   | 1.85                     | 0.58              |
| 3:D:379:ALA:HA    | 8:D:9674:HOH:O    | 2.02                     | 0.58              |
| 3:D:507:ASN:HA    | 8:D:9897:HOH:O    | 2.03                     | 0.58              |
| 3:D:583:ASP:OD1   | 3:D:604:THR:HB    | 2.04                     | 0.58              |
| 5:F:85:LEU:HA     | 5:F:88:ILE:HD12   | 1.84                     | 0.58              |
| 5:F:352:GLU:HG2   | 8:F:9501:HOH:O    | 2.03                     | 0.58              |
| 1:K:224:TYR:CD1   | 1:L:9:PRO:HD2     | 2.39                     | 0.58              |
| 3:N:1043:GLY:O    | 3:N:1056:PRO:HB3  | 2.04                     | 0.58              |
| 5:P:411:HIS:CB    | 5:P:414:ARG:HE    | 2.16                     | 0.58              |
| 1:A:39:PRO:O      | 1:A:43:ILE:HG12   | 2.04                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:178:ALA:CB    | 2:C:864:GLY:H     | 2.16                     | 0.58              |
| 1:A:196:THR:HG21  | 2:C:934:PHE:CD2   | 2.39                     | 0.58              |
| 2:C:309:TYR:HA    | 2:C:312:ALA:HB3   | 1.86                     | 0.58              |
| 2:C:637:LEU:HA    | 2:C:659:PRO:HG3   | 1.85                     | 0.58              |
| 2:C:916:GLU:O     | 2:C:919:ALA:HB3   | 2.04                     | 0.58              |
| 3:D:112:ILE:HG22  | 3:D:512:MET:SD    | 2.43                     | 0.58              |
| 3:D:181:ASP:CG    | 3:D:198:ARG:HB2   | 2.27                     | 0.58              |
| 3:D:897:TRP:CE2   | 3:D:902:LEU:HD21  | 2.38                     | 0.58              |
| 1:K:224:TYR:CE1   | 1:L:9:PRO:HD2     | 2.39                     | 0.58              |
| 1:L:76:VAL:O      | 1:L:80:LEU:HB2    | 2.04                     | 0.58              |
| 2:M:39:ARG:HG3    | 2:M:39:ARG:O      | 2.04                     | 0.58              |
| 2:M:73:LEU:HD23   | 2:M:94:LEU:CB     | 2.31                     | 0.58              |
| 2:M:588:VAL:HG21  | 2:M:664:GLY:O     | 2.02                     | 0.58              |
| 2:M:720:GLU:HG2   | 2:M:760:SER:HB3   | 1.86                     | 0.58              |
| 3:N:87:ARG:CB     | 3:N:523:ASP:HB2   | 2.33                     | 0.58              |
| 3:N:99:ALA:HA     | 3:N:575:GLN:NE2   | 2.18                     | 0.58              |
| 3:N:212:ARG:HA    | 8:N:9712:HOH:O    | 2.04                     | 0.58              |
| 5:P:172:ARG:O     | 5:P:176:ILE:HG13  | 2.03                     | 0.58              |
| 1:B:7:LYS:HE3     | 1:B:186:LEU:HD13  | 1.86                     | 0.58              |
| 1:B:89:PHE:HB3    | 1:B:120:VAL:HG22  | 1.86                     | 0.58              |
| 2:C:512:ARG:HD2   | 2:C:523:ILE:HD11  | 1.85                     | 0.58              |
| 2:C:516:ARG:NH1   | 3:D:1068:LEU:HD22 | 2.19                     | 0.58              |
| 2:C:742:VAL:HB    | 8:C:9959:HOH:O    | 2.03                     | 0.58              |
| 2:C:1013:TYR:HE1  | 2:C:1020:PRO:HG3  | 1.68                     | 0.58              |
| 3:D:761:ILE:CD1   | 4:E:23:VAL:HG11   | 2.32                     | 0.58              |
| 2:M:354:GLY:HA2   | 8:M:9663:HOH:O    | 2.02                     | 0.58              |
| 2:M:734:LEU:HA    | 2:M:737:LEU:HD12  | 1.85                     | 0.58              |
| 2:M:744:ARG:HG3   | 2:M:744:ARG:O     | 2.02                     | 0.58              |
| 3:N:181:ASP:O     | 3:N:185:VAL:HG23  | 2.03                     | 0.58              |
| 3:N:564:GLU:H     | 3:N:564:GLU:CD    | 2.12                     | 0.58              |
| 3:N:1065:LEU:HD12 | 3:N:1069:GLU:OE2  | 2.04                     | 0.58              |
| 1:A:35:THR:HG22   | 8:A:9594:HOH:O    | 2.02                     | 0.58              |
| 1:B:26:GLU:HB3    | 1:B:194:LYS:HG3   | 1.86                     | 0.58              |
| 1:B:156:HIS:CD2   | 1:B:157:GLY:H     | 2.22                     | 0.58              |
| 2:C:49:ARG:HH11   | 2:C:49:ARG:CB     | 2.15                     | 0.58              |
| 2:C:195:LEU:O     | 2:C:199:VAL:HG23  | 2.04                     | 0.58              |
| 2:C:358:ARG:HH22  | 2:C:374:ASN:HB3   | 1.69                     | 0.58              |
| 2:C:710:ILE:HB    | 2:C:790:LEU:CD2   | 2.32                     | 0.58              |
| 2:C:1005:MET:HE2  | 3:D:648:MET:HE3   | 1.85                     | 0.58              |
| 3:D:1065:LEU:HD12 | 3:D:1069:GLU:HB3  | 1.86                     | 0.58              |
| 3:D:1388:ARG:O    | 3:D:1391:GLU:HG2  | 2.04                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:162:ILE:HD11  | 2:M:306:THR:HG21  | 1.86                     | 0.58              |
| 2:M:352:ALA:O     | 2:M:355:VAL:HG12  | 2.04                     | 0.58              |
| 2:M:906:PHE:CG    | 3:N:1067:VAL:HG22 | 2.38                     | 0.58              |
| 3:N:28:LYS:O      | 3:N:43:GLY:HA2    | 2.04                     | 0.58              |
| 3:N:651:GLU:HG2   | 8:N:2376:HOH:O    | 2.04                     | 0.58              |
| 3:N:701:LEU:HD21  | 3:N:763:MET:HE3   | 1.86                     | 0.58              |
| 3:N:978:TYR:HE1   | 3:N:985:ASP:HA    | 1.69                     | 0.58              |
| 3:N:1274:ILE:HD11 | 3:N:1334:GLN:NE2  | 2.18                     | 0.58              |
| 1:A:108:GLU:O     | 1:A:110:LYS:HG3   | 2.04                     | 0.58              |
| 2:C:35:PRO:HD3    | 8:C:9992:HOH:O    | 2.04                     | 0.58              |
| 2:C:331:ARG:HG2   | 8:C:2153:HOH:O    | 2.03                     | 0.58              |
| 2:C:443:THR:CG2   | 2:C:449:ILE:HA    | 2.33                     | 0.58              |
| 2:C:720:GLU:CD    | 2:C:758:ARG:HH11  | 2.11                     | 0.58              |
| 2:C:896:PHE:CD2   | 2:C:925:TYR:HB2   | 2.39                     | 0.58              |
| 3:D:135:LEU:HD13  | 3:D:147:VAL:HG12  | 1.85                     | 0.58              |
| 3:D:828:LYS:HD3   | 3:D:828:LYS:N     | 2.19                     | 0.58              |
| 3:D:1038:LEU:O    | 3:D:1060:SER:HB2  | 2.04                     | 0.58              |
| 3:D:1043:GLY:O    | 3:D:1056:PRO:HB3  | 2.04                     | 0.58              |
| 2:M:607:ASP:HB2   | 2:M:610:ARG:H     | 1.69                     | 0.58              |
| 2:M:1047:HIS:O    | 2:M:1051:GLU:HG3  | 2.03                     | 0.58              |
| 3:N:25:GLU:O      | 3:N:27:GLU:HG2    | 2.03                     | 0.58              |
| 3:N:486:ARG:HH21  | 3:N:489:ARG:NE    | 2.02                     | 0.58              |
| 5:P:405:LEU:O     | 5:P:408:LEU:HD22  | 2.04                     | 0.58              |
| 2:C:18:LEU:HD12   | 2:C:18:LEU:N      | 2.18                     | 0.58              |
| 2:C:549:PHE:CZ    | 2:C:886:LEU:HB3   | 2.39                     | 0.58              |
| 2:C:647:GLN:HA    | 8:C:9499:HOH:O    | 2.04                     | 0.58              |
| 3:D:86:ARG:O      | 3:D:522:PRO:HD2   | 2.04                     | 0.58              |
| 3:D:422:ALA:N     | 3:D:427:VAL:HG11  | 2.17                     | 0.58              |
| 2:M:332:ARG:CZ    | 2:M:464:LEU:HD21  | 2.34                     | 0.58              |
| 2:M:583:LEU:O     | 2:M:587:VAL:HG23  | 2.04                     | 0.58              |
| 2:M:872:ASN:HB3   | 8:M:9634:HOH:O    | 2.04                     | 0.58              |
| 2:M:913:GLU:O     | 2:M:916:GLU:HB3   | 2.03                     | 0.58              |
| 3:N:462:GLN:HA    | 3:N:513:ILE:HD13  | 1.85                     | 0.58              |
| 3:N:466:LYS:HG3   | 3:N:510:GLU:HG2   | 1.85                     | 0.58              |
| 3:N:554:LEU:O     | 3:N:558:LEU:HG    | 2.03                     | 0.58              |
| 3:N:662:GLU:HB2   | 8:N:9492:HOH:O    | 2.04                     | 0.58              |
| 3:N:704:ARG:NE    | 3:N:705:ALA:H     | 2.02                     | 0.58              |
| 3:N:888:GLU:HG2   | 8:N:2229:HOH:O    | 2.04                     | 0.58              |
| 2:C:52:PHE:CD2    | 2:C:68:PHE:HB2    | 2.39                     | 0.57              |
| 2:C:333:ILE:HG12  | 2:C:410:ILE:HD13  | 1.86                     | 0.57              |
| 2:C:430:VAL:CG1   | 3:D:1075:HIS:HA   | 2.34                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:825:ALA:HA    | 8:D:9587:HOH:O    | 2.03                     | 0.57              |
| 2:M:54:ILE:O      | 2:M:54:ILE:HG23   | 2.03                     | 0.57              |
| 2:M:69:LEU:HD13   | 2:M:97:ARG:CZ     | 2.34                     | 0.57              |
| 2:M:257:VAL:HG12  | 2:M:263:ASP:CG    | 2.29                     | 0.57              |
| 2:M:367:LEU:O     | 2:M:371:LYS:HB3   | 2.04                     | 0.57              |
| 2:M:1107:ASN:HB3  | 8:M:9586:HOH:O    | 2.02                     | 0.57              |
| 8:M:2233:HOH:O    | 3:N:532:GLY:HA3   | 2.02                     | 0.57              |
| 3:N:12:LEU:HB2    | 8:N:9529:HOH:O    | 2.02                     | 0.57              |
| 3:N:502:PHE:CE2   | 3:N:1452:ILE:HG13 | 2.39                     | 0.57              |
| 3:N:609:GLY:CA    | 3:N:613:ARG:HB3   | 2.34                     | 0.57              |
| 3:N:704:ARG:CD    | 3:N:705:ALA:H     | 2.17                     | 0.57              |
| 3:N:1159:ARG:O    | 3:N:1159:ARG:HG3  | 2.04                     | 0.57              |
| 3:N:1243:THR:CB   | 3:N:1253:THR:HB   | 2.34                     | 0.57              |
| 3:N:1286:THR:HG22 | 3:N:1287:GLU:N    | 2.17                     | 0.57              |
| 1:B:208:LEU:HB2   | 8:B:9488:HOH:O    | 2.04                     | 0.57              |
| 2:C:19:THR:HG22   | 2:C:19:THR:O      | 2.02                     | 0.57              |
| 2:C:605:LYS:HB2   | 2:C:610:ARG:HH12  | 1.68                     | 0.57              |
| 3:D:68:PHE:CZ     | 5:F:375:LEU:HD23  | 2.39                     | 0.57              |
| 3:D:196:VAL:HG13  | 3:D:202:VAL:CG1   | 2.34                     | 0.57              |
| 3:D:223:LEU:CB    | 8:D:9844:HOH:O    | 2.51                     | 0.57              |
| 3:D:1478:SER:HB2  | 8:D:9761:HOH:O    | 2.03                     | 0.57              |
| 2:M:290:LEU:HD23  | 2:M:290:LEU:H     | 1.69                     | 0.57              |
| 2:M:1085:PHE:HE1  | 2:M:1111:ILE:HG21 | 1.69                     | 0.57              |
| 3:N:153:LEU:HD12  | 3:N:158:TYR:HB2   | 1.86                     | 0.57              |
| 3:N:177:ALA:HB1   | 3:N:199:LEU:CD1   | 2.34                     | 0.57              |
| 3:N:473:LEU:HD11  | 8:N:9502:HOH:O    | 2.02                     | 0.57              |
| 3:N:1155:VAL:CG1  | 3:N:1183:ILE:HD11 | 2.35                     | 0.57              |
| 3:N:1197:ARG:CD   | 3:N:1396:GLU:HB2  | 2.33                     | 0.57              |
| 3:N:1267:ARG:NH2  | 3:N:1271:LYS:HD2  | 2.18                     | 0.57              |
| 3:N:1354:LYS:HE3  | 8:N:9859:HOH:O    | 2.04                     | 0.57              |
| 5:P:136:LEU:HD12  | 5:P:137:GLY:N     | 2.19                     | 0.57              |
| 5:P:371:LEU:HD12  | 8:P:9520:HOH:O    | 2.04                     | 0.57              |
| 1:B:74:ASP:HB2    | 8:B:9510:HOH:O    | 2.04                     | 0.57              |
| 1:B:115:LEU:HD12  | 1:B:115:LEU:O     | 2.03                     | 0.57              |
| 2:C:285:LEU:HD11  | 2:C:290:LEU:HA    | 1.86                     | 0.57              |
| 2:C:342:ASP:O     | 2:C:346:VAL:HG23  | 2.04                     | 0.57              |
| 2:C:913:GLU:HA    | 8:C:9822:HOH:O    | 2.04                     | 0.57              |
| 3:D:18:ILE:HD12   | 3:D:518:PRO:CG    | 2.33                     | 0.57              |
| 3:D:95:LEU:HA     | 3:D:551:ASN:HD21  | 1.68                     | 0.57              |
| 3:D:817:GLU:HG3   | 3:D:839:LEU:HD13  | 1.85                     | 0.57              |
| 5:F:373:LYS:HB3   | 8:F:9489:HOH:O    | 2.03                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:9:PRO:HB2     | 1:L:224:TYR:HB3   | 1.86                     | 0.57              |
| 2:M:627:ARG:HD2   | 8:M:2249:HOH:O    | 2.03                     | 0.57              |
| 3:N:150:ARG:NH1   | 3:N:464:LEU:HD22  | 2.20                     | 0.57              |
| 3:N:508:ARG:CG    | 3:N:509:PRO:HD2   | 2.34                     | 0.57              |
| 3:N:609:GLY:HA2   | 3:N:613:ARG:HB3   | 1.86                     | 0.57              |
| 3:N:895:VAL:HG23  | 8:N:2399:HOH:O    | 2.05                     | 0.57              |
| 5:P:310:ILE:HA    | 8:P:9658:HOH:O    | 2.04                     | 0.57              |
| 1:A:18:ARG:HH12   | 1:A:88:ARG:NH2    | 2.02                     | 0.57              |
| 1:A:26:GLU:HB3    | 1:A:194:LYS:HG3   | 1.85                     | 0.57              |
| 2:C:359:MET:HB2   | 8:C:9554:HOH:O    | 2.03                     | 0.57              |
| 2:C:370:ALA:HB3   | 8:C:9960:HOH:O    | 2.02                     | 0.57              |
| 3:D:50:PHE:CB     | 3:D:522:PRO:HG2   | 2.34                     | 0.57              |
| 3:D:864:VAL:HG12  | 3:D:865:THR:H     | 1.69                     | 0.57              |
| 3:D:1379:VAL:HG11 | 3:D:1395:LEU:HD23 | 1.87                     | 0.57              |
| 5:F:415:THR:HG21  | 5:F:417:LYS:HZ1   | 1.69                     | 0.57              |
| 1:K:89:PHE:CB     | 1:K:94:LEU:HD22   | 2.33                     | 0.57              |
| 2:M:101:ILE:HG22  | 2:M:102:HIS:N     | 2.19                     | 0.57              |
| 3:N:29:PRO:HB3    | 3:N:545:ARG:HG2   | 1.86                     | 0.57              |
| 3:N:486:ARG:O     | 3:N:489:ARG:HG2   | 2.04                     | 0.57              |
| 3:N:1437:ALA:HB3  | 3:N:1446:VAL:HG11 | 1.86                     | 0.57              |
| 1:A:178:ALA:HB2   | 2:C:864:GLY:H     | 1.69                     | 0.57              |
| 1:B:121:GLU:HB2   | 8:B:9495:HOH:O    | 2.05                     | 0.57              |
| 2:C:431:HIS:H     | 2:C:434:HIS:CE1   | 2.22                     | 0.57              |
| 2:C:589:ARG:HB2   | 2:C:589:ARG:HH11  | 1.69                     | 0.57              |
| 3:D:136:ASP:CB    | 3:D:137:PRO:HD3   | 2.27                     | 0.57              |
| 3:D:171:LEU:HD22  | 3:D:390:PRO:HG3   | 1.86                     | 0.57              |
| 3:D:477:LEU:HD22  | 3:D:492:ALA:HB1   | 1.85                     | 0.57              |
| 3:D:861:GLN:HE21  | 3:D:861:GLN:N     | 1.92                     | 0.57              |
| 3:D:1092:GLY:O    | 3:D:1096:ARG:HB2  | 2.03                     | 0.57              |
| 3:D:1095:THR:O    | 3:D:1099:VAL:HG23 | 2.05                     | 0.57              |
| 3:D:1148:VAL:HG21 | 3:D:1203:LYS:HA   | 1.85                     | 0.57              |
| 4:E:34:GLY:HA3    | 8:E:9401:HOH:O    | 2.03                     | 0.57              |
| 5:F:94:LEU:HD12   | 5:F:97:GLU:N      | 2.20                     | 0.57              |
| 5:F:351:SER:HA    | 8:F:9585:HOH:O    | 2.04                     | 0.57              |
| 1:K:104:GLU:HG2   | 1:K:137:ARG:HD2   | 1.86                     | 0.57              |
| 1:K:132:LEU:HD11  | 1:K:138:LEU:HD22  | 1.86                     | 0.57              |
| 2:M:36:PRO:HA     | 8:M:9498:HOH:O    | 2.03                     | 0.57              |
| 2:M:193:LEU:O     | 2:M:193:LEU:HD13  | 2.05                     | 0.57              |
| 2:M:580:MET:SD    | 2:M:584:GLU:HG3   | 2.45                     | 0.57              |
| 2:M:1008:ARG:NH2  | 2:M:1020:PRO:HB3  | 2.20                     | 0.57              |
| 3:N:75:ARG:HG2    | 8:N:2006:HOH:O    | 2.05                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:1242:HIS:NE2 | 3:N:1266:ARG:HD2  | 2.19                     | 0.57              |
| 2:C:183:SER:HB3  | 2:C:190:LYS:HD3   | 1.87                     | 0.57              |
| 2:C:1007:ALA:HB1 | 3:D:652:LEU:HD13  | 1.85                     | 0.57              |
| 3:D:52:PRO:HG2   | 3:D:80:VAL:HB     | 1.86                     | 0.57              |
| 3:D:171:LEU:CB   | 3:D:390:PRO:HA    | 2.33                     | 0.57              |
| 3:D:573:MET:HE1  | 5:F:214:GLN:HG3   | 1.85                     | 0.57              |
| 3:D:584:ASN:CG   | 3:D:590:PRO:HD2   | 2.30                     | 0.57              |
| 3:D:705:ALA:CB   | 3:D:706:PRO:HD3   | 2.34                     | 0.57              |
| 3:D:1373:ARG:HG2 | 3:D:1374:GLN:HE21 | 1.68                     | 0.57              |
| 5:F:367:MET:SD   | 5:F:370:LYS:HD3   | 2.44                     | 0.57              |
| 1:K:27:PRO:HG3   | 1:K:186:LEU:HD13  | 1.85                     | 0.57              |
| 1:L:52:ALA:HB2   | 1:L:170:VAL:O     | 2.04                     | 0.57              |
| 2:M:364:GLU:HA   | 8:M:9849:HOH:O    | 2.03                     | 0.57              |
| 2:M:553:ASP:OD2  | 2:M:881:ASN:HB2   | 2.04                     | 0.57              |
| 3:N:112:ILE:HD13 | 3:N:461:ILE:HG21  | 1.86                     | 0.57              |
| 3:N:135:LEU:HD21 | 3:N:452:ILE:CD1   | 2.35                     | 0.57              |
| 3:N:185:VAL:HB   | 8:N:2354:HOH:O    | 2.03                     | 0.57              |
| 3:N:534:ARG:HG2  | 8:N:9604:HOH:O    | 2.04                     | 0.57              |
| 3:N:822:ALA:HB1  | 8:N:9817:HOH:O    | 2.04                     | 0.57              |
| 3:N:1041:LEU:O   | 3:N:1041:LEU:HD23 | 2.05                     | 0.57              |
| 3:N:1173:LEU:HG  | 8:N:9906:HOH:O    | 2.04                     | 0.57              |
| 3:N:1440:PHE:HB2 | 3:N:1442:ASN:ND2  | 2.19                     | 0.57              |
| 1:B:77:GLU:HB2   | 3:D:872:ARG:HH21  | 1.70                     | 0.57              |
| 1:B:176:ARG:NH2  | 3:D:884:ARG:NE    | 2.53                     | 0.57              |
| 2:C:260:LEU:HG   | 2:C:261:ILE:HG12  | 1.86                     | 0.57              |
| 2:C:905:ILE:HG22 | 2:C:906:PHE:N     | 2.20                     | 0.57              |
| 3:D:440:VAL:HA   | 8:D:2292:HOH:O    | 2.04                     | 0.57              |
| 4:E:59:ASN:HB2   | 8:E:9410:HOH:O    | 2.04                     | 0.57              |
| 5:F:266:GLU:HA   | 5:F:269:ASN:HD22  | 1.69                     | 0.57              |
| 1:K:119:ASP:HB3  | 8:K:742:HOH:O     | 2.05                     | 0.57              |
| 3:N:112:ILE:HD11 | 3:N:124:GLU:OE1   | 2.04                     | 0.57              |
| 3:N:550:ARG:NE   | 3:N:573:MET:HB3   | 2.20                     | 0.57              |
| 3:N:1266:ARG:O   | 3:N:1268:PRO:HD3  | 2.05                     | 0.57              |
| 3:N:1320:GLU:O   | 3:N:1323:GLN:HB2  | 2.04                     | 0.57              |
| 2:C:328:LEU:CD1  | 2:C:433:THR:HB    | 2.35                     | 0.57              |
| 2:C:605:LYS:HD3  | 2:C:610:ARG:HH22  | 1.69                     | 0.57              |
| 2:C:672:VAL:CG2  | 2:C:868:ASP:HB2   | 2.34                     | 0.57              |
| 2:C:770:GLU:HG2  | 3:D:65:ARG:NH2    | 2.09                     | 0.57              |
| 3:D:904:VAL:HG12 | 3:D:905:PRO:HD2   | 1.85                     | 0.57              |
| 3:D:1489:GLN:HG3 | 8:D:2185:HOH:O    | 2.04                     | 0.57              |
| 3:D:1498:ALA:HB1 | 8:E:9390:HOH:O    | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:74:LYS:HB2    | 8:F:9509:HOH:O    | 2.04                     | 0.57              |
| 1:K:116:PRO:HD2   | 8:K:5139:HOH:O    | 2.03                     | 0.57              |
| 1:K:162:ILE:HG13  | 1:K:163:ASN:N     | 2.19                     | 0.57              |
| 2:M:183:SER:HB3   | 2:M:190:LYS:HZ3   | 1.70                     | 0.57              |
| 2:M:270:GLY:H     | 2:M:288:ARG:NH2   | 2.03                     | 0.57              |
| 2:M:555:ALA:HA    | 3:N:1070:TYR:OH   | 2.05                     | 0.57              |
| 2:M:585:GLU:HG3   | 2:M:665:PHE:CE2   | 2.39                     | 0.57              |
| 2:M:740:GLU:HB3   | 8:M:9868:HOH:O    | 2.05                     | 0.57              |
| 3:N:177:ALA:HB1   | 3:N:199:LEU:CD2   | 2.33                     | 0.57              |
| 3:N:441:ARG:O     | 3:N:443:VAL:N     | 2.38                     | 0.57              |
| 3:N:1149:LEU:HD12 | 3:N:1161:GLU:O    | 2.05                     | 0.57              |
| 3:N:1205:TYR:O    | 3:N:1366:LYS:HD3  | 2.04                     | 0.57              |
| 2:C:571:LEU:CD2   | 2:C:700:TYR:HA    | 2.35                     | 0.57              |
| 3:D:7:LYS:HD3     | 3:D:1458:GLU:OE1  | 2.05                     | 0.57              |
| 3:D:658:LEU:HD11  | 3:D:674:ARG:NH1   | 2.19                     | 0.57              |
| 3:D:1197:ARG:CD   | 3:D:1396:GLU:HB2  | 2.35                     | 0.57              |
| 3:D:1500:LYS:O    | 3:D:1503:VAL:HG23 | 2.05                     | 0.57              |
| 5:F:166:LEU:O     | 5:F:171:LYS:HB2   | 2.05                     | 0.57              |
| 1:L:23:PHE:O      | 1:L:196:THR:HA    | 2.05                     | 0.57              |
| 2:M:436:GLY:HA2   | 2:M:538:GLN:O     | 2.05                     | 0.57              |
| 2:M:448:ASN:CG    | 2:M:452:ILE:HD11  | 2.29                     | 0.57              |
| 2:M:710:ILE:HB    | 2:M:790:LEU:HD23  | 1.85                     | 0.57              |
| 3:N:75:ARG:HG3    | 3:N:75:ARG:NH1    | 2.20                     | 0.57              |
| 3:N:205:TYR:HB3   | 3:N:393:ILE:HD13  | 1.85                     | 0.57              |
| 3:N:1045:MET:SD   | 3:N:1073:SER:HA   | 2.44                     | 0.57              |
| 5:P:331:ASP:HB2   | 8:P:9474:HOH:O    | 2.05                     | 0.57              |
| 1:A:88:ARG:HA     | 8:A:9600:HOH:O    | 2.05                     | 0.57              |
| 1:B:22:GLU:HG2    | 1:B:198:ARG:HG2   | 1.87                     | 0.57              |
| 1:B:127:LEU:HD12  | 1:B:128:HIS:N     | 2.20                     | 0.57              |
| 2:C:430:VAL:HG11  | 8:D:9725:HOH:O    | 2.05                     | 0.57              |
| 2:C:495:THR:HG21  | 2:C:524:VAL:HG21  | 1.87                     | 0.57              |
| 3:D:616:GLN:HA    | 3:D:619:LEU:HB3   | 1.87                     | 0.57              |
| 3:D:1262:LEU:HD23 | 3:D:1352:ILE:CG1  | 2.34                     | 0.57              |
| 3:D:1377:LYS:HG2  | 3:D:1378:TYR:CE1  | 2.39                     | 0.57              |
| 3:D:1471:LEU:HA   | 8:D:2065:HOH:O    | 2.04                     | 0.57              |
| 2:M:100:LEU:HD23  | 2:M:372:LEU:CD1   | 2.28                     | 0.57              |
| 5:P:110:MET:HE2   | 5:P:111:GLU:HG3   | 1.87                     | 0.57              |
| 5:P:113:ILE:HG23  | 5:P:127:ILE:CG2   | 2.35                     | 0.57              |
| 5:P:140:ARG:HG3   | 5:P:141:VAL:H     | 1.69                     | 0.57              |
| 2:C:69:LEU:C      | 2:C:70:GLU:HG3    | 2.30                     | 0.56              |
| 2:C:176:VAL:HB    | 8:C:9957:HOH:O    | 2.04                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:216:GLU:HG2   | 2:C:217:LEU:HD23 | 1.87                     | 0.56              |
| 2:C:352:ALA:O     | 2:C:356:ARG:HG3  | 2.05                     | 0.56              |
| 2:C:1016:ILE:HG21 | 5:F:317:LEU:HD21 | 1.87                     | 0.56              |
| 3:D:1500:LYS:HB3  | 8:D:2094:HOH:O   | 2.05                     | 0.56              |
| 1:K:29:GLU:C      | 8:K:1204:HOH:O   | 2.48                     | 0.56              |
| 1:K:186:LEU:HB2   | 1:K:192:LEU:CD1  | 2.35                     | 0.56              |
| 1:K:201:THR:HG22  | 1:K:203:GLY:H    | 1.69                     | 0.56              |
| 2:M:20:GLU:HG3    | 2:M:460:ARG:HH21 | 1.69                     | 0.56              |
| 2:M:710:ILE:HB    | 2:M:790:LEU:CD2  | 2.35                     | 0.56              |
| 2:M:717:LEU:HB3   | 2:M:761:PHE:HB2  | 1.87                     | 0.56              |
| 2:M:893:ALA:O     | 2:M:897:LEU:HB2  | 2.05                     | 0.56              |
| 3:N:574:LEU:O     | 3:N:578:VAL:HG23 | 2.05                     | 0.56              |
| 3:N:704:ARG:HH21  | 3:N:706:PRO:HD3  | 1.69                     | 0.56              |
| 3:N:1083:ASP:OD1  | 3:N:1238:MET:HB3 | 2.05                     | 0.56              |
| 5:P:94:LEU:HD22   | 5:P:95:THR:H     | 1.69                     | 0.56              |
| 5:P:393:THR:HG22  | 5:P:394:ARG:N    | 2.19                     | 0.56              |
| 1:A:49:PRO:HA     | 1:A:148:VAL:HG22 | 1.88                     | 0.56              |
| 1:A:177:VAL:O     | 2:C:864:GLY:HA3  | 2.04                     | 0.56              |
| 2:C:256:TYR:CE1   | 2:C:293:PHE:HB2  | 2.38                     | 0.56              |
| 2:C:273:GLY:HA2   | 2:C:276:LYS:HD3  | 1.87                     | 0.56              |
| 2:C:573:ARG:NH1   | 8:C:2347:HOH:O   | 2.38                     | 0.56              |
| 3:D:127:LEU:CD1   | 3:D:457:GLY:H    | 2.17                     | 0.56              |
| 3:D:658:LEU:HA    | 3:D:661:MET:HG3  | 1.86                     | 0.56              |
| 3:D:1324:PRO:HB3  | 8:D:2070:HOH:O   | 2.04                     | 0.56              |
| 3:D:1372:VAL:HA   | 3:D:1375:MET:HE3 | 1.87                     | 0.56              |
| 5:F:88:ILE:HD13   | 5:F:193:ARG:CB   | 2.35                     | 0.56              |
| 5:F:185:GLN:O     | 5:F:189:GLU:HG3  | 2.05                     | 0.56              |
| 5:F:287:THR:HG23  | 5:F:289:GLU:HB2  | 1.88                     | 0.56              |
| 5:F:367:MET:HE2   | 5:F:367:MET:CA   | 2.35                     | 0.56              |
| 1:K:150:TYR:CD1   | 2:M:696:LYS:HG2  | 2.40                     | 0.56              |
| 1:L:50:GLY:HA3    | 1:L:171:PHE:O    | 2.05                     | 0.56              |
| 2:M:108:ILE:HB    | 2:M:368:THR:HG1  | 1.66                     | 0.56              |
| 2:M:918:LEU:HB3   | 2:M:968:LEU:HD23 | 1.87                     | 0.56              |
| 2:M:1043:TYR:CD2  | 3:N:763:MET:HA   | 2.39                     | 0.56              |
| 3:N:19:ARG:HH21   | 3:N:94:GLU:CD    | 2.13                     | 0.56              |
| 3:N:41:ARG:O      | 8:N:9493:HOH:O   | 2.18                     | 0.56              |
| 3:N:617:ASN:O     | 3:N:619:LEU:N    | 2.38                     | 0.56              |
| 3:N:683:ILE:HG22  | 3:N:687:VAL:HG21 | 1.86                     | 0.56              |
| 3:N:890:VAL:HG12  | 3:N:926:LYS:CG   | 2.33                     | 0.56              |
| 5:P:358:LEU:HD11  | 5:P:370:LYS:HD2  | 1.87                     | 0.56              |
| 5:P:411:HIS:HB2   | 5:P:414:ARG:HE   | 1.70                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:65:PHE:HB2   | 8:B:9631:HOH:O    | 2.04                     | 0.56              |
| 1:B:108:GLU:O    | 1:B:110:LYS:HG3   | 2.04                     | 0.56              |
| 2:C:250:ARG:HH22 | 2:C:254:VAL:HG23  | 1.70                     | 0.56              |
| 2:C:435:TYR:C    | 2:C:437:ARG:H     | 2.11                     | 0.56              |
| 2:C:675:ALA:HA   | 2:C:989:VAL:HG12  | 1.86                     | 0.56              |
| 2:C:958:THR:HB   | 8:C:2248:HOH:O    | 2.05                     | 0.56              |
| 2:C:1015:LEU:HB3 | 2:C:1016:ILE:HD13 | 1.87                     | 0.56              |
| 2:C:1115:LEU:CD2 | 3:D:85:VAL:HA     | 2.35                     | 0.56              |
| 3:D:58:CYS:SG    | 3:D:59:ALA:N      | 2.78                     | 0.56              |
| 3:D:502:PHE:CE2  | 3:D:1452:ILE:HG13 | 2.40                     | 0.56              |
| 3:D:609:GLY:HA2  | 3:D:613:ARG:HB3   | 1.87                     | 0.56              |
| 3:D:897:TRP:CZ2  | 3:D:902:LEU:HD11  | 2.40                     | 0.56              |
| 3:D:957:PRO:HG3  | 8:D:9477:HOH:O    | 2.04                     | 0.56              |
| 3:D:1416:ALA:HA  | 8:D:9707:HOH:O    | 2.05                     | 0.56              |
| 4:E:90:GLU:HG2   | 8:E:9383:HOH:O    | 2.04                     | 0.56              |
| 5:F:113:ILE:HG23 | 5:F:127:ILE:CG2   | 2.35                     | 0.56              |
| 5:F:282:LEU:HB3  | 5:F:284:ARG:HB2   | 1.87                     | 0.56              |
| 5:F:393:THR:CG2  | 5:F:394:ARG:H     | 2.18                     | 0.56              |
| 5:F:394:ARG:NH1  | 8:F:9729:HOH:O    | 2.37                     | 0.56              |
| 1:K:29:GLU:CA    | 8:K:1204:HOH:O    | 2.53                     | 0.56              |
| 2:M:401:LEU:HD13 | 2:M:587:VAL:HG11  | 1.87                     | 0.56              |
| 2:M:841:ASN:ND2  | 2:M:843:HIS:H     | 2.03                     | 0.56              |
| 2:M:1050:GLN:HG2 | 2:M:1079:PRO:HG2  | 1.88                     | 0.56              |
| 2:M:1056:LYS:HE2 | 3:N:623:VAL:HG13  | 1.87                     | 0.56              |
| 3:N:46:ASP:N     | 8:N:9483:HOH:O    | 2.37                     | 0.56              |
| 3:N:770:LEU:HD11 | 3:N:919:PHE:CG    | 2.40                     | 0.56              |
| 3:N:829:VAL:HG13 | 8:N:9503:HOH:O    | 2.06                     | 0.56              |
| 3:N:879:ARG:HD2  | 3:N:902:LEU:O     | 2.05                     | 0.56              |
| 3:N:1320:GLU:HG2 | 8:N:9694:HOH:O    | 2.05                     | 0.56              |
| 4:O:51:LEU:HD12  | 4:O:52:GLU:N      | 2.19                     | 0.56              |
| 5:P:354:LEU:HG   | 8:P:9633:HOH:O    | 2.06                     | 0.56              |
| 5:P:413:SER:OG   | 5:P:419:ARG:NH2   | 2.32                     | 0.56              |
| 1:A:123:MET:O    | 1:A:125:PRO:HD3   | 2.05                     | 0.56              |
| 2:C:141:HIS:CE1  | 2:C:332:ARG:HD3   | 2.41                     | 0.56              |
| 2:C:918:LEU:HD23 | 2:C:967:PHE:O     | 2.05                     | 0.56              |
| 2:C:1081:VAL:HB  | 2:C:1086:ARG:NE   | 2.20                     | 0.56              |
| 3:D:87:ARG:CB    | 3:D:523:ASP:HB2   | 2.35                     | 0.56              |
| 3:D:162:ARG:HA   | 8:D:9476:HOH:O    | 2.05                     | 0.56              |
| 3:D:214:GLU:CB   | 3:D:390:PRO:HD2   | 2.35                     | 0.56              |
| 3:D:400:VAL:HG22 | 3:D:441:ARG:HG2   | 1.87                     | 0.56              |
| 3:D:1076:GLY:O   | 3:D:1079:LYS:HG2  | 2.06                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1101:VAL:HG13 | 3:D:1427:SER:HB3  | 1.85                     | 0.56              |
| 2:M:1071:ILE:CG2  | 3:N:670:VAL:HG21  | 2.35                     | 0.56              |
| 3:N:162:ARG:HE    | 3:N:434:ARG:HH21  | 1.52                     | 0.56              |
| 3:N:1133:ARG:HG2  | 3:N:1134:LEU:O    | 2.05                     | 0.56              |
| 5:P:81:VAL:HG13   | 8:P:9754:HOH:O    | 2.05                     | 0.56              |
| 5:P:124:PRO:HB3   | 8:P:9525:HOH:O    | 2.04                     | 0.56              |
| 2:C:1:MET:SD      | 2:C:900:ARG:HD3   | 2.44                     | 0.56              |
| 2:C:139:GLN:HA    | 2:C:411:SER:O     | 2.05                     | 0.56              |
| 3:D:1109:GLU:HG2  | 3:D:1201:CYS:HA   | 1.86                     | 0.56              |
| 3:D:1267:ARG:HH21 | 3:D:1271:LYS:HD2  | 1.70                     | 0.56              |
| 3:D:1396:GLU:O    | 3:D:1400:VAL:HG23 | 2.05                     | 0.56              |
| 4:E:41:GLU:CA     | 4:E:45:ARG:HG3    | 2.35                     | 0.56              |
| 5:F:101:GLU:O     | 5:F:105:LYS:HG3   | 2.06                     | 0.56              |
| 5:F:368:VAL:O     | 5:F:372:ARG:HB2   | 2.05                     | 0.56              |
| 1:L:156:HIS:CD2   | 1:L:157:GLY:H     | 2.19                     | 0.56              |
| 2:M:441:VAL:HG22  | 2:M:559:LEU:HA    | 1.87                     | 0.56              |
| 2:M:723:THR:HG23  | 2:M:725:ASP:HB2   | 1.86                     | 0.56              |
| 3:N:89:ARG:NE     | 8:N:9574:HOH:O    | 2.38                     | 0.56              |
| 3:N:172:PRO:HD3   | 8:N:9638:HOH:O    | 2.05                     | 0.56              |
| 3:N:186:VAL:HG21  | 3:N:213:VAL:HB    | 1.87                     | 0.56              |
| 3:N:613:ARG:HA    | 8:P:9750:HOH:O    | 2.06                     | 0.56              |
| 3:N:853:VAL:HG13  | 3:N:858:VAL:O     | 2.06                     | 0.56              |
| 3:N:1041:LEU:HD12 | 3:N:1058:ARG:HA   | 1.87                     | 0.56              |
| 4:O:48:MET:CB     | 4:O:54:LEU:HB2    | 2.36                     | 0.56              |
| 5:P:270:LYS:NZ    | 8:P:9668:HOH:O    | 2.37                     | 0.56              |
| 2:C:182:VAL:HG22  | 8:C:9517:HOH:O    | 2.05                     | 0.56              |
| 2:C:710:ILE:CD1   | 2:C:758:ARG:HE    | 2.19                     | 0.56              |
| 3:D:629:SER:HB3   | 3:D:726:ILE:HD11  | 1.88                     | 0.56              |
| 3:D:650:LEU:HD12  | 3:D:657:LEU:CD2   | 2.35                     | 0.56              |
| 3:D:708:LEU:HD12  | 3:D:1231:GLU:HG2  | 1.87                     | 0.56              |
| 3:D:871:LYS:HB3   | 3:D:873:LEU:HG    | 1.87                     | 0.56              |
| 3:D:916:TYR:HE2   | 3:D:920:LEU:HD13  | 1.70                     | 0.56              |
| 1:L:92:PRO:HD3    | 8:L:879:HOH:O     | 2.04                     | 0.56              |
| 2:M:571:LEU:HD23  | 2:M:700:TYR:HA    | 1.86                     | 0.56              |
| 2:M:685:GLU:N     | 8:M:9693:HOH:O    | 2.38                     | 0.56              |
| 2:M:719:PRO:HB3   | 2:M:820:ARG:NE    | 2.21                     | 0.56              |
| 3:N:631:ILE:HG21  | 3:N:745:MET:SD    | 2.46                     | 0.56              |
| 3:N:706:PRO:HG2   | 8:N:2226:HOH:O    | 2.04                     | 0.56              |
| 3:N:709:HIS:CD2   | 3:N:711:LEU:HB2   | 2.41                     | 0.56              |
| 3:N:715:ALA:HB3   | 3:N:764:LEU:HA    | 1.88                     | 0.56              |
| 3:N:1264:GLU:OE2  | 3:N:1424:VAL:HG12 | 2.06                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1432:LYS:HD2  | 3:N:1433:SER:H    | 1.70                     | 0.56              |
| 5:P:376:ILE:HG22  | 5:P:377:ASP:HB2   | 1.87                     | 0.56              |
| 1:A:209:GLU:HA    | 8:A:9590:HOH:O    | 2.05                     | 0.56              |
| 1:A:219:ARG:HH12  | 1:B:219:ARG:CD    | 2.14                     | 0.56              |
| 2:C:72:ARG:NH1    | 2:C:95:TYR:HE1    | 2.03                     | 0.56              |
| 3:D:12:LEU:HD11   | 3:D:104:PHE:HE1   | 1.71                     | 0.56              |
| 3:D:1195:GLN:HA   | 8:D:9914:HOH:O    | 2.05                     | 0.56              |
| 3:D:1372:VAL:O    | 3:D:1375:MET:HB2  | 2.06                     | 0.56              |
| 3:D:1442:ASN:HA   | 8:D:9499:HOH:O    | 2.04                     | 0.56              |
| 5:F:364:ARG:HB2   | 5:F:365:GLU:OE1   | 2.06                     | 0.56              |
| 1:L:98:THR:HB     | 8:L:1011:HOH:O    | 2.04                     | 0.56              |
| 2:M:503:LEU:HD13  | 2:M:507:ARG:O     | 2.06                     | 0.56              |
| 2:M:833:LEU:HD13  | 2:M:996:LYS:HD2   | 1.86                     | 0.56              |
| 2:M:979:THR:HG23  | 2:M:981:GLU:H     | 1.71                     | 0.56              |
| 2:M:1004:LYS:HE2  | 2:M:1027:PHE:CE1  | 2.40                     | 0.56              |
| 3:N:12:LEU:HD21   | 3:N:104:PHE:CZ    | 2.40                     | 0.56              |
| 3:N:42:ASP:O      | 3:N:46:ASP:HB2    | 2.06                     | 0.56              |
| 3:N:775:GLY:HA2   | 8:N:9633:HOH:O    | 2.04                     | 0.56              |
| 5:P:398:ARG:HD3   | 5:P:399:GLN:N     | 2.20                     | 0.56              |
| 1:A:1:MET:O       | 1:A:6:LEU:HD22    | 2.05                     | 0.56              |
| 1:B:23:PHE:O      | 1:B:196:THR:HA    | 2.06                     | 0.56              |
| 1:B:101:LEU:HD21  | 8:B:9640:HOH:O    | 2.05                     | 0.56              |
| 3:D:684:LYS:HG3   | 8:D:9823:HOH:O    | 2.06                     | 0.56              |
| 3:D:1266:ARG:HA   | 8:D:2318:HOH:O    | 2.06                     | 0.56              |
| 3:D:1412:LYS:HB3  | 8:D:9962:HOH:O    | 2.05                     | 0.56              |
| 1:L:91:ASN:HB2    | 1:L:92:PRO:HD2    | 1.86                     | 0.56              |
| 1:L:115:LEU:HD12  | 1:L:115:LEU:O     | 2.04                     | 0.56              |
| 1:L:166:PRO:HB2   | 8:L:705:HOH:O     | 2.04                     | 0.56              |
| 2:M:159:ILE:HG21  | 2:M:175:GLU:OE1   | 2.05                     | 0.56              |
| 3:N:483:HIS:HB2   | 3:N:484:PRO:CD    | 2.34                     | 0.56              |
| 3:N:565:ILE:H     | 3:N:565:ILE:CD1   | 2.11                     | 0.56              |
| 3:N:1115:THR:HG22 | 3:N:1151:ARG:HH21 | 1.71                     | 0.56              |
| 2:C:14:PRO:HG3    | 8:C:9667:HOH:O    | 2.06                     | 0.56              |
| 2:C:31:GLN:HB2    | 8:C:9887:HOH:O    | 2.05                     | 0.56              |
| 2:C:141:HIS:O     | 2:C:331:ARG:HA    | 2.05                     | 0.56              |
| 2:C:435:TYR:C     | 2:C:437:ARG:N     | 2.64                     | 0.56              |
| 2:C:677:MET:HB3   | 2:C:987:ILE:HD13  | 1.88                     | 0.56              |
| 2:C:874:LEU:HD21  | 3:D:787:LEU:HD22  | 1.87                     | 0.56              |
| 2:C:897:LEU:HB3   | 2:C:899:GLN:NE2   | 2.20                     | 0.56              |
| 3:D:138:LYS:H     | 3:D:138:LYS:HD2   | 1.70                     | 0.56              |
| 5:F:225:GLU:HG2   | 5:F:226:LYS:HZ2   | 1.71                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:413:SER:O     | 5:F:416:ARG:HG2   | 2.06                     | 0.56              |
| 1:L:211:LEU:O     | 1:L:215:VAL:HG13  | 2.06                     | 0.56              |
| 2:M:43:GLY:HA2    | 2:M:341:THR:HG21  | 1.87                     | 0.56              |
| 2:M:97:ARG:HH21   | 2:M:109:LYS:HD2   | 1.71                     | 0.56              |
| 2:M:102:HIS:HB2   | 2:M:106:GLY:O     | 2.05                     | 0.56              |
| 2:M:250:ARG:NE    | 2:M:253:ALA:HB1   | 2.21                     | 0.56              |
| 2:M:265:ARG:HE    | 2:M:267:TYR:HA    | 1.69                     | 0.56              |
| 2:M:585:GLU:O     | 2:M:588:VAL:HG22  | 2.06                     | 0.56              |
| 3:N:863:VAL:HG12  | 8:N:9933:HOH:O    | 2.06                     | 0.56              |
| 3:N:1049:SER:HB2  | 8:N:2290:HOH:O    | 2.06                     | 0.56              |
| 3:N:1258:ARG:NH2  | 3:N:1262:LEU:HD11 | 2.21                     | 0.56              |
| 4:O:51:LEU:HG     | 4:O:53:GLY:N      | 2.16                     | 0.56              |
| 5:P:420:ASP:OD2   | 5:P:420:ASP:N     | 2.35                     | 0.56              |
| 1:B:178:ALA:HB3   | 1:B:198:ARG:HB2   | 1.87                     | 0.56              |
| 2:C:516:ARG:NH1   | 2:C:521:PRO:HB3   | 2.21                     | 0.56              |
| 2:C:1060:ILE:HG12 | 2:C:1063:ARG:NH2  | 2.20                     | 0.56              |
| 2:C:1067:TYR:CB   | 5:F:341:PRO:HB3   | 2.36                     | 0.56              |
| 3:D:43:GLY:N      | 8:D:2541:HOH:O    | 2.39                     | 0.56              |
| 3:D:168:THR:HG22  | 3:D:170:PRO:HD3   | 1.87                     | 0.56              |
| 3:D:214:GLU:HB2   | 3:D:390:PRO:HD2   | 1.87                     | 0.56              |
| 3:D:1042:ARG:HH11 | 3:D:1065:LEU:HD22 | 1.71                     | 0.56              |
| 3:D:1149:LEU:HG   | 3:D:1166:LEU:HD22 | 1.88                     | 0.56              |
| 3:D:1374:GLN:HA   | 8:D:2457:HOH:O    | 2.05                     | 0.56              |
| 3:D:1440:PHE:HB2  | 3:D:1442:ASN:HD21 | 1.70                     | 0.56              |
| 4:E:68:LEU:HD13   | 4:E:73:LEU:HD12   | 1.87                     | 0.56              |
| 5:F:220:LEU:HB2   | 5:F:243:ILE:HD11  | 1.88                     | 0.56              |
| 5:F:419:ARG:HG3   | 5:F:420:ASP:N     | 2.20                     | 0.56              |
| 1:K:123:MET:HB3   | 8:K:4466:HOH:O    | 2.05                     | 0.56              |
| 1:K:206:THR:CG2   | 1:K:209:GLU:HG3   | 2.35                     | 0.56              |
| 2:M:69:LEU:HD12   | 2:M:97:ARG:HB3    | 1.87                     | 0.56              |
| 2:M:283:ILE:HG22  | 2:M:284:ARG:CG    | 2.35                     | 0.56              |
| 2:M:448:ASN:HB2   | 8:M:9510:HOH:O    | 2.05                     | 0.56              |
| 2:M:516:ARG:HD2   | 3:N:1068:LEU:HD22 | 1.88                     | 0.56              |
| 3:N:131:LYS:O     | 3:N:133:ILE:HG12  | 2.05                     | 0.56              |
| 3:N:182:GLY:O     | 3:N:186:VAL:HB    | 2.06                     | 0.56              |
| 3:N:642:CYS:HB3   | 3:N:716:PHE:CD2   | 2.40                     | 0.56              |
| 3:N:1003:VAL:O    | 3:N:1007:VAL:HG13 | 2.05                     | 0.56              |
| 3:N:1098:LEU:O    | 3:N:1102:THR:HB   | 2.06                     | 0.56              |
| 3:N:1283:ILE:C    | 3:N:1284:GLU:HG2  | 2.31                     | 0.56              |
| 4:O:84:ARG:HG2    | 8:O:1862:HOH:O    | 2.04                     | 0.56              |
| 5:P:376:ILE:HG22  | 5:P:377:ASP:N     | 2.20                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1:MET:O       | 1:A:6:LEU:CB      | 2.45                     | 0.55              |
| 1:B:123:MET:O     | 1:B:125:PRO:HD3   | 2.06                     | 0.55              |
| 2:C:89:THR:HG23   | 2:C:129:ILE:HA    | 1.86                     | 0.55              |
| 2:C:133:ASP:N     | 2:C:632:ASN:HD21  | 2.04                     | 0.55              |
| 2:C:250:ARG:HB3   | 2:C:253:ALA:HB3   | 1.87                     | 0.55              |
| 2:C:396:ASP:OD1   | 2:C:402:SER:HB3   | 2.06                     | 0.55              |
| 2:C:704:HIS:CD2   | 2:C:831:ARG:HH22  | 2.23                     | 0.55              |
| 2:C:1118:LYS:HZ3  | 3:D:20:SER:HA     | 1.70                     | 0.55              |
| 3:D:36:THR:C      | 3:D:38:LYS:H      | 2.13                     | 0.55              |
| 3:D:633:VAL:C     | 3:D:635:PRO:HD3   | 2.31                     | 0.55              |
| 4:E:54:LEU:HD12   | 4:E:58:PRO:HB2    | 1.88                     | 0.55              |
| 5:F:195:VAL:HG22  | 5:F:243:ILE:HD11  | 1.88                     | 0.55              |
| 2:M:218:VAL:O     | 2:M:221:LEU:HB3   | 2.05                     | 0.55              |
| 2:M:612:VAL:HG22  | 2:M:622:GLU:HA    | 1.87                     | 0.55              |
| 2:M:700:TYR:N     | 8:M:2053:HOH:O    | 2.38                     | 0.55              |
| 2:M:1052:MET:SD   | 2:M:1056:LYS:HD3  | 2.46                     | 0.55              |
| 3:N:111:LYS:HE2   | 8:N:9878:HOH:O    | 2.06                     | 0.55              |
| 3:N:1209:LEU:HD13 | 3:N:1216:SER:N    | 2.14                     | 0.55              |
| 3:N:1258:ARG:CZ   | 3:N:1262:LEU:HD11 | 2.36                     | 0.55              |
| 5:P:137:GLY:HA2   | 5:P:140:ARG:NH2   | 2.21                     | 0.55              |
| 1:A:128:HIS:HB2   | 8:A:9598:HOH:O    | 2.06                     | 0.55              |
| 2:C:188:LYS:HE2   | 2:C:188:LYS:C     | 2.31                     | 0.55              |
| 2:C:193:LEU:HD13  | 2:C:193:LEU:O     | 2.06                     | 0.55              |
| 2:C:643:VAL:HG13  | 2:C:647:GLN:CD    | 2.31                     | 0.55              |
| 2:C:958:THR:HG23  | 2:C:961:GLU:HB2   | 1.87                     | 0.55              |
| 2:C:1004:LYS:HE3  | 2:C:1027:PHE:HE1  | 1.69                     | 0.55              |
| 3:D:25:GLU:O      | 3:D:27:GLU:HG2    | 2.06                     | 0.55              |
| 3:D:28:LYS:N      | 8:D:2541:HOH:O    | 2.39                     | 0.55              |
| 3:D:951:ILE:HG23  | 3:D:1062:ARG:HH21 | 1.71                     | 0.55              |
| 3:D:1146:GLY:HA3  | 3:D:1207:TYR:CB   | 2.34                     | 0.55              |
| 4:E:17:TYR:O      | 4:E:21:VAL:HG23   | 2.05                     | 0.55              |
| 1:K:42:ARG:HG2    | 1:K:42:ARG:NH1    | 2.17                     | 0.55              |
| 1:K:96:THR:HB     | 1:K:143:ARG:HH12  | 1.70                     | 0.55              |
| 1:L:102:LYS:HB2   | 1:L:139:ASN:OD1   | 2.06                     | 0.55              |
| 2:M:280:LYS:HB3   | 8:M:9645:HOH:O    | 2.05                     | 0.55              |
| 2:M:567:GLN:CB    | 2:M:997:LEU:HD22  | 2.36                     | 0.55              |
| 3:N:32:ILE:HD12   | 3:N:527:MET:CG    | 2.34                     | 0.55              |
| 3:N:416:ALA:H     | 3:N:417:PRO:CD    | 2.19                     | 0.55              |
| 3:N:562:ALA:CB    | 3:N:567:ILE:HD11  | 2.32                     | 0.55              |
| 3:N:912:LYS:HB3   | 3:N:912:LYS:NZ    | 2.21                     | 0.55              |
| 3:N:1236:LEU:HD21 | 3:N:1356:TYR:CD2  | 2.40                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:P:138:SER:H     | 5:P:140:ARG:CZ   | 2.19                     | 0.55              |
| 1:A:50:GLY:O      | 1:A:146:ARG:HA   | 2.07                     | 0.55              |
| 1:A:195:LEU:HD11  | 1:A:197:LEU:HD22 | 1.87                     | 0.55              |
| 1:A:206:THR:HG22  | 1:A:209:GLU:HG3  | 1.87                     | 0.55              |
| 2:C:1016:ILE:HD12 | 5:F:317:LEU:HD11 | 1.88                     | 0.55              |
| 3:D:667:ALA:HB2   | 8:D:9511:HOH:O   | 2.05                     | 0.55              |
| 3:D:803:GLY:HA2   | 8:D:9895:HOH:O   | 2.06                     | 0.55              |
| 5:F:94:LEU:H      | 5:F:98:GLU:HB2   | 1.71                     | 0.55              |
| 5:F:376:ILE:HG22  | 5:F:377:ASP:N    | 2.20                     | 0.55              |
| 2:M:672:VAL:HG23  | 2:M:868:ASP:OD2  | 2.06                     | 0.55              |
| 2:M:719:PRO:HB3   | 2:M:820:ARG:HE   | 1.70                     | 0.55              |
| 2:M:815:LEU:HD21  | 2:M:821:GLU:HA   | 1.88                     | 0.55              |
| 8:M:9602:HOH:O    | 3:N:618:LEU:HB2  | 2.06                     | 0.55              |
| 3:N:191:LEU:HD13  | 3:N:195:VAL:HG11 | 1.87                     | 0.55              |
| 3:N:196:VAL:HG13  | 3:N:202:VAL:CG1  | 2.36                     | 0.55              |
| 8:N:2195:HOH:O    | 5:P:90:GLN:HG2   | 2.05                     | 0.55              |
| 5:P:339:PRO:HB3   | 5:P:343:ASP:HB2  | 1.87                     | 0.55              |
| 1:A:137:ARG:HD3   | 8:A:9486:HOH:O   | 2.06                     | 0.55              |
| 2:C:16:PRO:O      | 2:C:18:LEU:HD12  | 2.07                     | 0.55              |
| 2:C:759:THR:HB    | 2:C:785:VAL:HG11 | 1.89                     | 0.55              |
| 2:C:858:MET:HB2   | 2:C:859:PRO:CD   | 2.36                     | 0.55              |
| 2:C:1090:LYS:NZ   | 3:D:90:MET:HG3   | 2.21                     | 0.55              |
| 3:D:114:THR:O     | 3:D:495:ARG:HG3  | 2.06                     | 0.55              |
| 3:D:679:ARG:HH12  | 3:D:681:ARG:HD2  | 1.70                     | 0.55              |
| 3:D:1258:ARG:HH21 | 3:D:1351:GLU:HG2 | 1.71                     | 0.55              |
| 4:E:86:GLN:HB3    | 8:E:9362:HOH:O   | 2.06                     | 0.55              |
| 5:F:160:ASP:OD2   | 5:F:178:ARG:NH2  | 2.39                     | 0.55              |
| 1:K:41:ARG:HH11   | 1:K:41:ARG:HG3   | 1.70                     | 0.55              |
| 1:L:149:GLY:N     | 8:L:5023:HOH:O   | 2.40                     | 0.55              |
| 2:M:16:PRO:O      | 2:M:18:LEU:HD12  | 2.06                     | 0.55              |
| 2:M:229:MET:HA    | 8:M:2154:HOH:O   | 2.07                     | 0.55              |
| 3:N:99:ALA:HB1    | 3:N:575:GLN:OE1  | 2.06                     | 0.55              |
| 3:N:221:ALA:HA    | 8:N:9545:HOH:O   | 2.05                     | 0.55              |
| 3:N:567:ILE:HG22  | 3:N:571:LYS:NZ   | 2.22                     | 0.55              |
| 3:N:858:VAL:HG12  | 3:N:859:ASP:O    | 2.06                     | 0.55              |
| 3:N:1353:GLN:NE2  | 3:N:1357:ARG:HE  | 2.03                     | 0.55              |
| 3:N:1472:ILE:CG2  | 3:N:1475:GLY:H   | 2.19                     | 0.55              |
| 3:N:1490:LYS:HZ1  | 4:O:39:VAL:HA    | 1.70                     | 0.55              |
| 5:P:282:LEU:HD12  | 5:P:284:ARG:CD   | 2.36                     | 0.55              |
| 5:P:361:LEU:HD12  | 5:P:366:ALA:HB2  | 1.88                     | 0.55              |
| 2:C:304:LEU:HB3   | 2:C:305:PRO:HD3  | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:326:ASP:HA    | 2:C:331:ARG:HD3   | 1.88                     | 0.55              |
| 2:C:889:HIS:HB2   | 8:C:9674:HOH:O    | 2.07                     | 0.55              |
| 3:D:527:MET:HA    | 3:D:527:MET:HE3   | 1.88                     | 0.55              |
| 3:D:793:THR:HG22  | 3:D:879:ARG:HA    | 1.88                     | 0.55              |
| 3:D:1153:VAL:HG12 | 3:D:1155:VAL:HG23 | 1.88                     | 0.55              |
| 4:E:45:ARG:HG2    | 8:E:9370:HOH:O    | 2.07                     | 0.55              |
| 5:F:78:SER:HB2    | 5:F:82:ARG:NH2    | 2.21                     | 0.55              |
| 5:F:128:ARG:HD2   | 8:F:9482:HOH:O    | 2.06                     | 0.55              |
| 5:F:361:LEU:CD1   | 5:F:404:ALA:HB1   | 2.37                     | 0.55              |
| 2:M:127:PHE:O     | 2:M:133:ASP:HA    | 2.07                     | 0.55              |
| 2:M:721:ARG:HD2   | 8:M:9788:HOH:O    | 2.06                     | 0.55              |
| 2:M:722:ILE:O     | 2:M:722:ILE:HD13  | 2.06                     | 0.55              |
| 3:N:29:PRO:HG2    | 3:N:549:ASN:ND2   | 2.20                     | 0.55              |
| 3:N:133:ILE:HG23  | 3:N:456:MET:SD    | 2.46                     | 0.55              |
| 3:N:148:GLU:CB    | 3:N:151:GLN:HB2   | 2.33                     | 0.55              |
| 3:N:554:LEU:HD12  | 3:N:558:LEU:HD11  | 1.89                     | 0.55              |
| 3:N:649:ALA:CB    | 3:N:720:LEU:HD21  | 2.36                     | 0.55              |
| 3:N:1267:ARG:HH12 | 3:N:1271:LYS:HE3  | 1.71                     | 0.55              |
| 5:P:161:GLN:HG3   | 5:P:164:LYS:HZ2   | 1.72                     | 0.55              |
| 1:A:41:ARG:HH11   | 1:A:41:ARG:HG3    | 1.70                     | 0.55              |
| 1:B:132:LEU:HD11  | 1:B:138:LEU:HD13  | 1.88                     | 0.55              |
| 2:C:217:LEU:HB2   | 2:C:311:PHE:CZ    | 2.42                     | 0.55              |
| 2:C:510:ALA:HB3   | 2:C:513:VAL:CG2   | 2.37                     | 0.55              |
| 3:D:715:ALA:HB3   | 3:D:764:LEU:HA    | 1.88                     | 0.55              |
| 3:D:1109:GLU:CD   | 3:D:1202:GLN:H    | 2.14                     | 0.55              |
| 3:D:1154:GLU:OE2  | 3:D:1159:ARG:HG2  | 2.06                     | 0.55              |
| 2:M:18:LEU:HD12   | 2:M:18:LEU:N      | 2.22                     | 0.55              |
| 2:M:721:ARG:HE    | 2:M:783:ARG:HH22  | 1.54                     | 0.55              |
| 3:N:584:ASN:CG    | 3:N:590:PRO:HD2   | 2.31                     | 0.55              |
| 3:N:691:LEU:HG    | 3:N:720:LEU:HD11  | 1.88                     | 0.55              |
| 1:A:46:SER:HB3    | 8:A:9595:HOH:O    | 2.06                     | 0.55              |
| 2:C:433:THR:CG2   | 2:C:488:ALA:HB1   | 2.36                     | 0.55              |
| 2:C:476:GLY:HA2   | 8:C:9625:HOH:O    | 2.06                     | 0.55              |
| 2:C:1018:GLN:HE21 | 2:C:1063:ARG:HH22 | 1.53                     | 0.55              |
| 3:D:28:LYS:O      | 3:D:43:GLY:HA2    | 2.07                     | 0.55              |
| 3:D:39:PRO:HB3    | 3:D:45:PHE:C      | 2.31                     | 0.55              |
| 3:D:131:LYS:HG2   | 3:D:568:ARG:CG    | 2.37                     | 0.55              |
| 3:D:500:ARG:HH22  | 3:D:1388:ARG:HH11 | 1.55                     | 0.55              |
| 3:D:1286:THR:HG22 | 3:D:1287:GLU:N    | 2.21                     | 0.55              |
| 3:D:1365:ASP:O    | 3:D:1369:GLU:HG3  | 2.06                     | 0.55              |
| 3:D:1495:ILE:CD1  | 4:E:84:ARG:HG2    | 2.36                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:F:282:LEU:HD12  | 5:F:284:ARG:HD2  | 1.88                     | 0.55              |
| 1:L:170:VAL:O     | 1:L:170:VAL:HG23 | 2.07                     | 0.55              |
| 2:M:352:ALA:HA    | 2:M:355:VAL:CG1  | 2.37                     | 0.55              |
| 2:M:899:GLN:HG3   | 2:M:901:TYR:CZ   | 2.42                     | 0.55              |
| 4:O:41:GLU:N      | 4:O:45:ARG:HG3   | 2.22                     | 0.55              |
| 2:C:799:ILE:O     | 2:C:799:ILE:HG12 | 2.07                     | 0.55              |
| 3:D:135:LEU:HD11  | 3:D:452:ILE:HD11 | 1.88                     | 0.55              |
| 3:D:213:VAL:HG23  | 3:D:391:ALA:HA   | 1.89                     | 0.55              |
| 3:D:563:PRO:HG3   | 5:F:188:ILE:HG21 | 1.88                     | 0.55              |
| 3:D:711:LEU:HD11  | 8:D:2469:HOH:O   | 2.06                     | 0.55              |
| 3:D:806:PHE:CG    | 3:D:806:PHE:O    | 2.60                     | 0.55              |
| 3:D:1311:LEU:HD23 | 3:D:1311:LEU:H   | 1.70                     | 0.55              |
| 5:F:225:GLU:HG2   | 5:F:226:LYS:NZ   | 2.22                     | 0.55              |
| 5:F:316:SER:C     | 5:F:318:GLU:H    | 2.13                     | 0.55              |
| 5:F:369:LEU:HD11  | 8:F:9847:HOH:O   | 2.06                     | 0.55              |
| 2:M:77:PRO:HD2    | 2:M:91:GLN:O     | 2.06                     | 0.55              |
| 2:M:100:LEU:HD12  | 2:M:100:LEU:O    | 2.06                     | 0.55              |
| 2:M:228:ALA:HB3   | 8:M:9807:HOH:O   | 2.06                     | 0.55              |
| 2:M:385:PHE:O     | 2:M:389:SER:HB3  | 2.07                     | 0.55              |
| 2:M:432:ARG:NE    | 3:N:1048:PRO:HD2 | 2.21                     | 0.55              |
| 2:M:514:VAL:HB    | 8:M:9879:HOH:O   | 2.06                     | 0.55              |
| 2:M:738:ASP:HB3   | 8:M:9801:HOH:O   | 2.07                     | 0.55              |
| 2:M:967:PHE:HD1   | 2:M:972:VAL:HG12 | 1.72                     | 0.55              |
| 3:N:199:LEU:HD23  | 3:N:199:LEU:O    | 2.07                     | 0.55              |
| 3:N:1084:THR:HA   | 3:N:1087:ARG:HG2 | 1.89                     | 0.55              |
| 3:N:1209:LEU:CD2  | 4:O:16:LYS:HD2   | 2.37                     | 0.55              |
| 3:N:1476:THR:HA   | 8:N:9748:HOH:O   | 2.07                     | 0.55              |
| 1:A:9:PRO:HB2     | 1:B:224:TYR:HB3  | 1.89                     | 0.55              |
| 2:C:47:ALA:HB1    | 8:C:2085:HOH:O   | 2.07                     | 0.55              |
| 2:C:250:ARG:NH2   | 2:C:254:VAL:HG23 | 2.22                     | 0.55              |
| 2:C:328:LEU:HD12  | 2:C:328:LEU:N    | 2.21                     | 0.55              |
| 2:C:568:ALA:CB    | 2:C:668:LEU:HB3  | 2.36                     | 0.55              |
| 2:C:630:ARG:NE    | 2:C:705:ILE:O    | 2.40                     | 0.55              |
| 2:C:643:VAL:HG13  | 2:C:647:GLN:NE2  | 2.21                     | 0.55              |
| 2:C:725:ASP:HB2   | 2:C:783:ARG:HH12 | 1.72                     | 0.55              |
| 3:D:98:PRO:HD3    | 8:D:9851:HOH:O   | 2.07                     | 0.55              |
| 3:D:555:LYS:HE2   | 8:D:2118:HOH:O   | 2.06                     | 0.55              |
| 3:D:584:ASN:H     | 3:D:602:SER:CB   | 2.20                     | 0.55              |
| 3:D:618:LEU:HD23  | 8:D:2051:HOH:O   | 2.06                     | 0.55              |
| 3:D:1049:SER:OG   | 3:D:1051:GLU:HG2 | 2.07                     | 0.55              |
| 5:F:128:ARG:HG2   | 8:F:9604:HOH:O   | 2.07                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:181:GLU:O    | 5:F:184:ARG:HB3   | 2.06                     | 0.55              |
| 5:F:276:ARG:HG3  | 5:F:276:ARG:NH1   | 2.22                     | 0.55              |
| 1:L:101:LEU:HD22 | 1:L:140:MET:CE    | 2.34                     | 0.55              |
| 1:L:169:ALA:HB1  | 1:L:171:PHE:CE1   | 2.42                     | 0.55              |
| 2:M:34:VAL:HB    | 2:M:38:LYS:CG     | 2.35                     | 0.55              |
| 2:M:752:GLY:O    | 2:M:791:ARG:HD2   | 2.06                     | 0.55              |
| 3:N:1437:ALA:O   | 3:N:1446:VAL:HG21 | 2.07                     | 0.55              |
| 1:A:89:PHE:HB3   | 1:A:120:VAL:HG22  | 1.88                     | 0.55              |
| 1:B:52:ALA:HB2   | 1:B:170:VAL:O     | 2.06                     | 0.55              |
| 2:C:135:VAL:HB   | 2:C:406:HIS:CE1   | 2.42                     | 0.55              |
| 2:C:233:GLU:HG2  | 8:C:9873:HOH:O    | 2.07                     | 0.55              |
| 2:C:275:TYR:OH   | 2:C:487:THR:HG21  | 2.07                     | 0.55              |
| 2:C:418:LEU:HD12 | 8:C:9500:HOH:O    | 2.06                     | 0.55              |
| 2:C:598:GLU:O    | 2:C:651:LYS:HG3   | 2.06                     | 0.55              |
| 2:C:949:LYS:HD2  | 3:D:859:ASP:OD2   | 2.07                     | 0.55              |
| 3:D:645:PRO:HB3  | 3:D:723:GLY:O     | 2.07                     | 0.55              |
| 3:D:804:LEU:HD12 | 3:D:804:LEU:O     | 2.07                     | 0.55              |
| 4:E:3:GLU:HB3    | 8:E:9453:HOH:O    | 2.06                     | 0.55              |
| 1:L:176:ARG:HB2  | 8:L:2002:HOH:O    | 2.06                     | 0.55              |
| 2:M:164:PRO:CB   | 8:M:9843:HOH:O    | 2.55                     | 0.55              |
| 2:M:537:LYS:CA   | 2:M:905:ILE:HD11  | 2.36                     | 0.55              |
| 2:M:1016:ILE:H   | 2:M:1016:ILE:HD13 | 1.71                     | 0.55              |
| 3:N:625:TYR:O    | 3:N:749:VAL:HG23  | 2.06                     | 0.55              |
| 3:N:897:TRP:CH2  | 3:N:902:LEU:HD21  | 2.41                     | 0.55              |
| 5:P:124:PRO:HG2  | 8:P:9646:HOH:O    | 2.07                     | 0.55              |
| 1:A:27:PRO:CG    | 1:A:186:LEU:HD22  | 2.37                     | 0.54              |
| 1:A:47:SER:HB2   | 1:A:217:ILE:HD13  | 1.88                     | 0.54              |
| 2:C:31:GLN:NE2   | 8:C:2231:HOH:O    | 2.40                     | 0.54              |
| 2:C:653:ASP:OD1  | 2:C:654:LEU:HD23  | 2.07                     | 0.54              |
| 3:D:55:ASP:CA    | 3:D:82:LYS:HG2    | 2.37                     | 0.54              |
| 3:D:179:VAL:HG22 | 8:D:9925:HOH:O    | 2.07                     | 0.54              |
| 3:D:181:ASP:O    | 3:D:185:VAL:HG23  | 2.07                     | 0.54              |
| 3:D:569:ASN:C    | 3:D:569:ASN:HD22  | 2.15                     | 0.54              |
| 3:D:1379:VAL:O   | 3:D:1392:GLY:HA2  | 2.07                     | 0.54              |
| 3:D:1437:ALA:O   | 3:D:1446:VAL:HG21 | 2.07                     | 0.54              |
| 4:E:91:ARG:HG2   | 8:E:9368:HOH:O    | 2.06                     | 0.54              |
| 1:L:41:ARG:HH11  | 1:L:41:ARG:HG3    | 1.71                     | 0.54              |
| 2:M:17:PRO:O     | 2:M:20:GLU:HB2    | 2.07                     | 0.54              |
| 2:M:113:VAL:HG13 | 8:M:9704:HOH:O    | 2.06                     | 0.54              |
| 2:M:264:PRO:HB3  | 2:M:289:THR:CG2   | 2.37                     | 0.54              |
| 2:M:442:GLU:O    | 2:M:442:GLU:HG3   | 2.06                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:497:ALA:HA   | 2:M:515:ALA:HA   | 1.88                     | 0.54              |
| 2:M:726:ILE:HD11 | 2:M:737:LEU:HD11 | 1.89                     | 0.54              |
| 8:M:9821:HOH:O   | 3:N:3:LYS:HB3    | 2.07                     | 0.54              |
| 3:N:87:ARG:O     | 3:N:521:PRO:CB   | 2.46                     | 0.54              |
| 3:N:162:ARG:NE   | 3:N:434:ARG:HH21 | 2.03                     | 0.54              |
| 3:N:1265:ALA:HB1 | 3:N:1332:PRO:HB2 | 1.87                     | 0.54              |
| 3:N:1377:LYS:HG2 | 3:N:1378:TYR:CD1 | 2.42                     | 0.54              |
| 1:A:131:THR:HG21 | 8:A:9522:HOH:O   | 2.07                     | 0.54              |
| 1:B:89:PHE:HB2   | 1:B:94:LEU:HD22  | 1.89                     | 0.54              |
| 2:C:108:ILE:HD11 | 2:C:365:ASP:OD1  | 2.07                     | 0.54              |
| 2:C:172:ILE:HD12 | 2:C:172:ILE:N    | 2.21                     | 0.54              |
| 2:C:274:ARG:N    | 2:C:288:ARG:HH12 | 2.01                     | 0.54              |
| 2:C:679:PHE:CE2  | 2:C:853:LEU:HD21 | 2.42                     | 0.54              |
| 2:C:999:HIS:HE1  | 8:C:9820:HOH:O   | 1.89                     | 0.54              |
| 3:D:118:LEU:HA   | 3:D:123:LEU:HD13 | 1.88                     | 0.54              |
| 3:D:743:ASP:HA   | 8:D:9498:HOH:O   | 2.08                     | 0.54              |
| 1:L:50:GLY:O     | 1:L:146:ARG:HA   | 2.07                     | 0.54              |
| 2:M:284:ARG:O    | 2:M:301:GLU:HB3  | 2.08                     | 0.54              |
| 2:M:333:ILE:O    | 2:M:465:GLY:HA3  | 2.06                     | 0.54              |
| 2:M:480:THR:HG22 | 2:M:481:ASP:N    | 2.23                     | 0.54              |
| 2:M:789:SER:O    | 2:M:791:ARG:HG2  | 2.08                     | 0.54              |
| 3:N:149:LYS:HD3  | 3:N:149:LYS:N    | 2.19                     | 0.54              |
| 3:N:154:THR:HG22 | 3:N:155:ASP:N    | 2.22                     | 0.54              |
| 3:N:195:VAL:O    | 3:N:205:TYR:HD1  | 1.90                     | 0.54              |
| 3:N:381:ALA:HB1  | 8:N:9952:HOH:O   | 2.08                     | 0.54              |
| 3:N:645:PRO:HB3  | 3:N:723:GLY:O    | 2.08                     | 0.54              |
| 3:N:827:ILE:HG22 | 3:N:837:GLY:HA2  | 1.87                     | 0.54              |
| 3:N:1036:ARG:NH2 | 3:N:1042:ARG:HA  | 2.21                     | 0.54              |
| 5:P:413:SER:O    | 5:P:416:ARG:HG2  | 2.07                     | 0.54              |
| 1:A:18:ARG:HH12  | 1:A:88:ARG:HH21  | 1.54                     | 0.54              |
| 2:C:4:LYS:HG3    | 8:C:9575:HOH:O   | 2.07                     | 0.54              |
| 2:C:11:GLU:HA    | 8:C:2224:HOH:O   | 2.07                     | 0.54              |
| 2:C:101:ILE:HG22 | 2:C:102:HIS:N    | 2.21                     | 0.54              |
| 2:C:983:ILE:HG21 | 2:C:987:ILE:CD1  | 2.38                     | 0.54              |
| 2:C:1090:LYS:HE2 | 2:C:1112:PHE:CZ  | 2.43                     | 0.54              |
| 3:D:423:ASP:OD2  | 5:F:174:LEU:HD22 | 2.07                     | 0.54              |
| 3:D:1409:ALA:HB2 | 8:D:9593:HOH:O   | 2.07                     | 0.54              |
| 5:F:164:LYS:HA   | 5:F:171:LYS:HZ2  | 1.72                     | 0.54              |
| 5:F:167:PRO:HB2  | 5:F:169:GLU:OE1  | 2.07                     | 0.54              |
| 5:F:300:ASP:CG   | 5:F:301:ALA:N    | 2.65                     | 0.54              |
| 5:F:358:LEU:CD2  | 5:F:367:MET:HE1  | 2.38                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:18:ARG:HH22   | 1:K:88:ARG:HH21   | 1.54                     | 0.54              |
| 1:L:169:ALA:HB1   | 1:L:171:PHE:CZ    | 2.42                     | 0.54              |
| 2:M:51:THR:O      | 2:M:51:THR:HG22   | 2.07                     | 0.54              |
| 2:M:164:PRO:HB2   | 8:M:9843:HOH:O    | 2.08                     | 0.54              |
| 2:M:510:ALA:O     | 2:M:513:VAL:HG23  | 2.08                     | 0.54              |
| 2:M:587:VAL:O     | 2:M:591:SER:HB3   | 2.07                     | 0.54              |
| 2:M:953:VAL:HG13  | 2:M:966:LEU:HD13  | 1.88                     | 0.54              |
| 3:N:80:VAL:HG12   | 8:N:2191:HOH:O    | 2.07                     | 0.54              |
| 3:N:139:GLY:CA    | 3:N:452:ILE:HD12  | 2.36                     | 0.54              |
| 3:N:660:LYS:HA    | 3:N:663:GLU:HG3   | 1.88                     | 0.54              |
| 3:N:660:LYS:HD2   | 3:N:663:GLU:OE2   | 2.07                     | 0.54              |
| 3:N:703:ASN:HD22  | 3:N:713:ILE:HG12  | 1.72                     | 0.54              |
| 3:N:1437:ALA:HB3  | 3:N:1446:VAL:CG1  | 2.36                     | 0.54              |
| 1:B:24:VAL:HG23   | 8:B:9505:HOH:O    | 2.06                     | 0.54              |
| 2:C:44:ILE:H      | 2:C:44:ILE:HD12   | 1.73                     | 0.54              |
| 2:C:231:PRO:HB2   | 8:C:9804:HOH:O    | 2.08                     | 0.54              |
| 3:D:169:TYR:CG    | 3:D:169:TYR:O     | 2.60                     | 0.54              |
| 3:D:628:ARG:HG2   | 3:D:629:SER:N     | 2.22                     | 0.54              |
| 3:D:647:ARG:HD2   | 3:D:680:GLN:NE2   | 2.22                     | 0.54              |
| 3:D:710:ARG:HH21  | 3:D:1224:VAL:HG21 | 1.71                     | 0.54              |
| 3:D:799:LYS:HD2   | 8:D:2525:HOH:O    | 2.07                     | 0.54              |
| 3:D:996:TRP:CG    | 3:D:1056:PRO:HG2  | 2.41                     | 0.54              |
| 4:E:40:LEU:C      | 4:E:45:ARG:HG3    | 2.33                     | 0.54              |
| 5:F:163:LEU:HB3   | 5:F:174:LEU:HG    | 1.89                     | 0.54              |
| 5:F:290:GLU:HB2   | 8:F:9483:HOH:O    | 2.07                     | 0.54              |
| 5:F:369:LEU:HG    | 8:F:9532:HOH:O    | 2.07                     | 0.54              |
| 1:K:65:PHE:CE2    | 2:M:830:LYS:HG3   | 2.42                     | 0.54              |
| 2:M:415:PRO:HA    | 8:M:9730:HOH:O    | 2.07                     | 0.54              |
| 2:M:897:LEU:HD23  | 2:M:899:GLN:NE2   | 2.22                     | 0.54              |
| 3:N:434:ARG:NH1   | 8:N:2094:HOH:O    | 2.41                     | 0.54              |
| 3:N:562:ALA:HB1   | 3:N:567:ILE:CD1   | 2.35                     | 0.54              |
| 3:N:1047:LYS:HG2  | 3:N:1053:PHE:CZ   | 2.43                     | 0.54              |
| 3:N:1101:VAL:HG11 | 3:N:1424:VAL:HG23 | 1.90                     | 0.54              |
| 3:N:1332:PRO:CB   | 3:N:1421:LEU:HD21 | 2.38                     | 0.54              |
| 3:N:1498:ALA:HB2  | 4:O:88:GLU:OE1    | 2.07                     | 0.54              |
| 5:P:288:TYR:CD1   | 5:P:288:TYR:N     | 2.74                     | 0.54              |
| 1:A:9:PRO:HD2     | 1:B:224:TYR:CD1   | 2.41                     | 0.54              |
| 2:C:129:ILE:HD11  | 2:C:386:PHE:HD2   | 1.72                     | 0.54              |
| 2:C:207:LEU:HB3   | 2:C:221:LEU:HD21  | 1.88                     | 0.54              |
| 2:C:604:ALA:HB3   | 2:C:612:VAL:O     | 2.07                     | 0.54              |
| 2:C:722:ILE:HG23  | 2:C:805:ARG:HH21  | 1.73                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:869:VAL:HG22  | 2:C:871:LEU:HD13 | 1.89                     | 0.54              |
| 3:D:54:LYS:HG2    | 3:D:55:ASP:OD1   | 2.08                     | 0.54              |
| 3:D:763:MET:HA    | 8:D:9596:HOH:O   | 2.08                     | 0.54              |
| 3:D:919:PHE:HD2   | 3:D:919:PHE:C    | 2.15                     | 0.54              |
| 5:F:399:GLN:HG3   | 8:F:9828:HOH:O   | 2.08                     | 0.54              |
| 2:M:507:ARG:HG3   | 8:M:9565:HOH:O   | 2.06                     | 0.54              |
| 2:M:820:ARG:HG3   | 8:M:9511:HOH:O   | 2.08                     | 0.54              |
| 2:M:1008:ARG:HH12 | 3:N:624:ASP:CG   | 2.15                     | 0.54              |
| 2:M:1052:MET:HE1  | 3:N:748:HIS:HB3  | 1.90                     | 0.54              |
| 2:M:1111:ILE:HG13 | 2:M:1112:PHE:N   | 2.22                     | 0.54              |
| 3:N:738:ALA:HB2   | 8:N:9496:HOH:O   | 2.08                     | 0.54              |
| 3:N:1320:GLU:HA   | 8:N:9629:HOH:O   | 2.07                     | 0.54              |
| 4:O:87:LYS:HB2    | 8:O:724:HOH:O    | 2.08                     | 0.54              |
| 5:P:207:LEU:HB3   | 5:P:212:LEU:HG   | 1.90                     | 0.54              |
| 5:P:267:THR:HG23  | 5:P:299:TRP:HH2  | 1.73                     | 0.54              |
| 5:P:325:LYS:HD3   | 8:P:9772:HOH:O   | 2.07                     | 0.54              |
| 1:A:187:GLY:HA2   | 8:A:9473:HOH:O   | 2.07                     | 0.54              |
| 2:C:93:PRO:HA     | 8:C:9502:HOH:O   | 2.08                     | 0.54              |
| 2:C:163:ILE:HG13  | 2:C:171:TRP:HZ3  | 1.71                     | 0.54              |
| 2:C:328:LEU:HD22  | 2:C:437:ARG:HD3  | 1.89                     | 0.54              |
| 2:C:443:THR:CG2   | 2:C:450:GLY:H    | 2.15                     | 0.54              |
| 2:C:549:PHE:CE2   | 2:C:886:LEU:HB3  | 2.42                     | 0.54              |
| 2:C:889:HIS:NE2   | 2:C:970:GLY:HA3  | 2.23                     | 0.54              |
| 2:C:1039:ALA:HB2  | 3:D:707:THR:CG2  | 2.37                     | 0.54              |
| 3:D:11:ALA:HB1    | 3:D:507:ASN:OD1  | 2.07                     | 0.54              |
| 3:D:638:LYS:HE3   | 8:D:2552:HOH:O   | 2.06                     | 0.54              |
| 3:D:1395:LEU:HG   | 8:D:2279:HOH:O   | 2.07                     | 0.54              |
| 3:D:1487:VAL:HG12 | 3:D:1488:ASP:N   | 2.23                     | 0.54              |
| 5:F:192:LEU:O     | 5:F:196:VAL:HG23 | 2.08                     | 0.54              |
| 5:F:412:GLU:HG3   | 5:F:418:LEU:HD13 | 1.89                     | 0.54              |
| 1:L:91:ASN:HA     | 8:L:879:HOH:O    | 2.07                     | 0.54              |
| 1:L:156:HIS:HD2   | 1:L:157:GLY:N    | 2.04                     | 0.54              |
| 1:L:156:HIS:CD2   | 1:L:157:GLY:N    | 2.75                     | 0.54              |
| 2:M:723:THR:CG2   | 2:M:725:ASP:HB2  | 2.38                     | 0.54              |
| 2:M:1062:GLY:HA3  | 8:M:9570:HOH:O   | 2.06                     | 0.54              |
| 2:M:1090:LYS:HE2  | 2:M:1112:PHE:CE2 | 2.43                     | 0.54              |
| 3:N:36:THR:C      | 3:N:38:LYS:H     | 2.16                     | 0.54              |
| 3:N:55:ASP:HA     | 3:N:82:LYS:HG2   | 1.90                     | 0.54              |
| 3:N:972:LEU:HD12  | 8:N:2464:HOH:O   | 2.08                     | 0.54              |
| 3:N:1020:LEU:HD21 | 3:N:1038:LEU:CD2 | 2.37                     | 0.54              |
| 3:N:1116:ASN:CG   | 3:N:1193:THR:HB  | 2.32                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1455:LYS:HD2  | 8:N:2323:HOH:O    | 2.08                     | 0.54              |
| 5:P:130:VAL:HG13  | 5:P:156:VAL:HG23  | 1.90                     | 0.54              |
| 1:A:42:ARG:HG2    | 1:A:42:ARG:NH1    | 2.18                     | 0.54              |
| 2:C:15:LEU:HD22   | 8:C:9630:HOH:O    | 2.08                     | 0.54              |
| 2:C:22:GLN:HE22   | 2:C:336:VAL:HG21  | 1.71                     | 0.54              |
| 2:C:270:GLY:H     | 2:C:288:ARG:NH2   | 2.05                     | 0.54              |
| 2:C:358:ARG:NH2   | 2:C:374:ASN:HB3   | 2.23                     | 0.54              |
| 2:C:738:ASP:HB2   | 2:C:744:ARG:HB3   | 1.90                     | 0.54              |
| 2:C:1021:LEU:HD22 | 5:F:332:PHE:HA    | 1.89                     | 0.54              |
| 2:C:1049:LEU:HD23 | 3:D:1472:ILE:HD11 | 1.87                     | 0.54              |
| 3:D:77:GLY:O      | 3:D:78:VAL:HG23   | 2.07                     | 0.54              |
| 3:D:195:VAL:HG13  | 8:D:9592:HOH:O    | 2.07                     | 0.54              |
| 3:D:441:ARG:O     | 3:D:443:VAL:N     | 2.41                     | 0.54              |
| 3:D:510:GLU:HG2   | 8:D:2069:HOH:O    | 2.07                     | 0.54              |
| 3:D:797:LYS:HG2   | 8:D:2474:HOH:O    | 2.07                     | 0.54              |
| 3:D:1079:LYS:HG3  | 3:D:1080:GLY:N    | 2.22                     | 0.54              |
| 3:D:1339:LYS:HG2  | 3:D:1343:ALA:HB2  | 1.88                     | 0.54              |
| 5:F:130:VAL:HG21  | 5:F:159:ILE:CG2   | 2.37                     | 0.54              |
| 5:F:172:ARG:O     | 5:F:176:ILE:HG13  | 2.07                     | 0.54              |
| 1:L:133:GLU:HG3   | 1:L:134:GLU:H     | 1.73                     | 0.54              |
| 1:L:196:THR:HG21  | 8:L:3509:HOH:O    | 2.07                     | 0.54              |
| 2:M:283:ILE:HG22  | 2:M:284:ARG:HG3   | 1.90                     | 0.54              |
| 2:M:470:PRO:HB2   | 2:M:534:VAL:HG21  | 1.90                     | 0.54              |
| 2:M:843:HIS:CD2   | 2:M:884:GLN:HA    | 2.41                     | 0.54              |
| 3:N:55:ASP:CA     | 3:N:82:LYS:HG2    | 2.37                     | 0.54              |
| 3:N:496:LEU:CD2   | 3:N:500:ARG:HG3   | 2.38                     | 0.54              |
| 3:N:584:ASN:ND2   | 3:N:590:PRO:HD2   | 2.23                     | 0.54              |
| 3:N:704:ARG:HD2   | 3:N:705:ALA:H     | 1.72                     | 0.54              |
| 4:O:40:LEU:CD2    | 4:O:67:GLU:HA     | 2.34                     | 0.54              |
| 2:C:73:LEU:HD23   | 2:C:93:PRO:O      | 2.08                     | 0.54              |
| 3:D:80:VAL:HG23   | 3:D:81:THR:O      | 2.08                     | 0.54              |
| 3:D:402:PRO:HB3   | 8:D:2109:HOH:O    | 2.07                     | 0.54              |
| 3:D:950:GLY:N     | 3:D:953:ASP:OD1   | 2.35                     | 0.54              |
| 1:K:34:VAL:HG21   | 2:M:939:ARG:CZ    | 2.38                     | 0.54              |
| 2:M:69:LEU:HB2    | 2:M:97:ARG:HB2    | 1.89                     | 0.54              |
| 2:M:211:LEU:HD12  | 2:M:308:ARG:HD3   | 1.89                     | 0.54              |
| 2:M:383:ARG:NH2   | 8:M:9873:HOH:O    | 2.38                     | 0.54              |
| 2:M:503:LEU:HB3   | 8:M:9597:HOH:O    | 2.08                     | 0.54              |
| 2:M:739:GLU:HG2   | 8:M:9580:HOH:O    | 2.08                     | 0.54              |
| 2:M:808:ARG:HH21  | 2:M:820:ARG:NH2   | 2.06                     | 0.54              |
| 3:N:444:VAL:O     | 3:N:444:VAL:HG22  | 2.07                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:477:LEU:O     | 3:N:481:MET:HB2  | 2.08                     | 0.54              |
| 3:N:626:SER:C     | 3:N:652:LEU:HD11 | 2.32                     | 0.54              |
| 3:N:806:PHE:CG    | 3:N:806:PHE:O    | 2.61                     | 0.54              |
| 3:N:1020:LEU:HA   | 3:N:1023:MET:HE3 | 1.90                     | 0.54              |
| 3:N:1114:THR:HB   | 3:N:1195:GLN:HB2 | 1.90                     | 0.54              |
| 3:N:1243:THR:O    | 3:N:1269:LYS:HD3 | 2.08                     | 0.54              |
| 3:N:1420:LEU:HD12 | 8:N:9548:HOH:O   | 2.07                     | 0.54              |
| 5:P:398:ARG:HB3   | 8:P:9476:HOH:O   | 2.07                     | 0.54              |
| 1:A:51:THR:HA     | 1:A:145:ASP:O    | 2.07                     | 0.54              |
| 1:B:58:ILE:HG21   | 1:B:68:ILE:HD11  | 1.90                     | 0.54              |
| 1:B:101:LEU:HB2   | 1:B:114:PHE:CD2  | 2.43                     | 0.54              |
| 2:C:195:LEU:HG    | 2:C:238:LEU:HD12 | 1.90                     | 0.54              |
| 2:C:625:LEU:CD1   | 2:C:641:PRO:HG3  | 2.38                     | 0.54              |
| 2:C:1096:ALA:HB3  | 3:D:101:HIS:CE1  | 2.43                     | 0.54              |
| 3:D:843:PHE:CD1   | 3:D:849:ALA:HA   | 2.43                     | 0.54              |
| 3:D:1439:SER:HB3  | 8:D:2132:HOH:O   | 2.07                     | 0.54              |
| 1:K:150:TYR:CE1   | 2:M:696:LYS:HA   | 2.42                     | 0.54              |
| 1:L:94:LEU:HD11   | 1:L:119:ASP:OD2  | 2.07                     | 0.54              |
| 2:M:19:THR:HG21   | 2:M:124:ASP:O    | 2.07                     | 0.54              |
| 2:M:63:GLY:O      | 2:M:103:LYS:HE2  | 2.08                     | 0.54              |
| 2:M:162:ILE:O     | 2:M:164:PRO:HD2  | 2.08                     | 0.54              |
| 2:M:203:ASP:HB2   | 8:M:9850:HOH:O   | 2.08                     | 0.54              |
| 2:M:435:TYR:C     | 2:M:437:ARG:H    | 2.15                     | 0.54              |
| 2:M:448:ASN:HA    | 2:M:451:LEU:HD12 | 1.89                     | 0.54              |
| 2:M:501:THR:O     | 2:M:503:LEU:HD23 | 2.08                     | 0.54              |
| 2:M:778:PHE:HZ    | 5:P:419:ARG:HD3  | 1.68                     | 0.54              |
| 2:M:1089:VAL:O    | 2:M:1093:GLN:HG3 | 2.08                     | 0.54              |
| 3:N:770:LEU:HD11  | 3:N:919:PHE:CD2  | 2.42                     | 0.54              |
| 3:N:950:GLY:O     | 3:N:953:ASP:N    | 2.36                     | 0.54              |
| 3:N:1498:ALA:HB1  | 8:N:2333:HOH:O   | 2.07                     | 0.54              |
| 5:P:181:GLU:OE2   | 5:P:184:ARG:HD3  | 2.07                     | 0.54              |
| 2:C:95:TYR:HD2    | 2:C:114:PHE:HB3  | 1.73                     | 0.54              |
| 2:C:139:GLN:HE22  | 2:C:415:PRO:CD   | 2.18                     | 0.54              |
| 2:C:679:PHE:HB2   | 8:C:9687:HOH:O   | 2.08                     | 0.54              |
| 2:C:738:ASP:O     | 2:C:739:GLU:C    | 2.50                     | 0.54              |
| 2:C:749:VAL:HA    | 8:C:2219:HOH:O   | 2.07                     | 0.54              |
| 3:D:434:ARG:HB2   | 3:D:447:VAL:CG2  | 2.37                     | 0.54              |
| 3:D:806:PHE:O     | 3:D:808:THR:N    | 2.40                     | 0.54              |
| 1:K:32:PHE:HB2    | 8:K:1204:HOH:O   | 2.08                     | 0.54              |
| 2:M:204:GLN:HG3   | 8:M:2184:HOH:O   | 2.08                     | 0.54              |
| 2:M:325:ILE:HA    | 8:M:2182:HOH:O   | 2.08                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:554:ASP:HB2   | 2:M:880:MET:HB2  | 1.90                     | 0.54              |
| 3:N:102:ILE:HD12  | 3:N:579:ASP:CG   | 2.33                     | 0.54              |
| 3:N:166:GLN:HG2   | 3:N:207:PHE:HB2  | 1.90                     | 0.54              |
| 3:N:558:LEU:HD13  | 5:P:145:PRO:CA   | 2.37                     | 0.54              |
| 3:N:711:LEU:HD12  | 3:N:778:LEU:HD23 | 1.88                     | 0.54              |
| 3:N:781:PRO:O     | 3:N:786:ILE:HG13 | 2.08                     | 0.54              |
| 3:N:988:ARG:HG2   | 3:N:988:ARG:HH11 | 1.72                     | 0.54              |
| 3:N:1377:LYS:HE2  | 3:N:1378:TYR:CZ  | 2.43                     | 0.54              |
| 5:P:134:LYS:HE3   | 5:P:134:LYS:HA   | 1.90                     | 0.54              |
| 5:P:361:LEU:HD21  | 5:P:408:LEU:HB2  | 1.90                     | 0.54              |
| 1:A:196:THR:HG22  | 8:A:9445:HOH:O   | 2.08                     | 0.53              |
| 2:C:328:LEU:HD13  | 2:C:433:THR:CB   | 2.38                     | 0.53              |
| 2:C:474:VAL:HG13  | 2:C:530:GLU:O    | 2.09                     | 0.53              |
| 2:C:534:VAL:N     | 2:C:538:GLN:HE22 | 2.05                     | 0.53              |
| 2:C:572:ILE:HD11  | 2:C:698:ASP:HB3  | 1.90                     | 0.53              |
| 2:C:1013:TYR:HB2  | 5:F:335:ASP:OD2  | 2.07                     | 0.53              |
| 3:D:865:THR:HG23  | 3:D:874:GLU:HG2  | 1.89                     | 0.53              |
| 3:D:1103:HIS:HD2  | 3:D:1462:LEU:N   | 2.01                     | 0.53              |
| 5:F:376:ILE:HG22  | 5:F:377:ASP:CB   | 2.35                     | 0.53              |
| 2:M:127:PHE:HB3   | 2:M:129:ILE:HD13 | 1.90                     | 0.53              |
| 2:M:432:ARG:HB3   | 8:M:9836:HOH:O   | 2.08                     | 0.53              |
| 3:N:33:ASN:CG     | 3:N:40:GLU:HG2   | 2.33                     | 0.53              |
| 3:N:1130:ARG:HB2  | 8:N:2015:HOH:O   | 2.07                     | 0.53              |
| 2:C:352:ALA:HA    | 2:C:355:VAL:CG1  | 2.37                     | 0.53              |
| 2:C:876:VAL:O     | 2:C:879:ARG:O    | 2.26                     | 0.53              |
| 3:D:116:LEU:HB3   | 3:D:118:LEU:HD13 | 1.90                     | 0.53              |
| 3:D:160:GLU:HG2   | 3:D:165:LYS:CD   | 2.37                     | 0.53              |
| 3:D:175:VAL:HG21  | 8:D:2442:HOH:O   | 2.08                     | 0.53              |
| 3:D:421:LEU:HD23  | 3:D:421:LEU:O    | 2.09                     | 0.53              |
| 3:D:774:SER:HB2   | 3:D:776:GLU:HG2  | 1.91                     | 0.53              |
| 3:D:776:GLU:HG3   | 8:D:9714:HOH:O   | 2.09                     | 0.53              |
| 3:D:1114:THR:HG23 | 3:D:1114:THR:O   | 2.07                     | 0.53              |
| 3:D:1489:GLN:HE21 | 3:D:1493:LYS:HZ1 | 1.57                     | 0.53              |
| 5:F:361:LEU:HD13  | 5:F:404:ALA:CB   | 2.37                     | 0.53              |
| 1:K:58:ILE:HG21   | 1:K:68:ILE:HD11  | 1.91                     | 0.53              |
| 2:M:405:ARG:HD2   | 2:M:442:GLU:OE1  | 2.09                     | 0.53              |
| 2:M:441:VAL:HA    | 8:M:9785:HOH:O   | 2.08                     | 0.53              |
| 2:M:554:ASP:N     | 2:M:880:MET:O    | 2.28                     | 0.53              |
| 2:M:566:THR:HG21  | 8:M:2185:HOH:O   | 2.07                     | 0.53              |
| 2:M:610:ARG:HG3   | 2:M:610:ARG:NH1  | 2.21                     | 0.53              |
| 2:M:840:ALA:O     | 2:M:995:MET:HE3  | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:841:ASN:HD21  | 2:M:843:HIS:CG    | 2.25                     | 0.53              |
| 2:M:910:LYS:HG3   | 8:M:9715:HOH:O    | 2.07                     | 0.53              |
| 2:M:1039:ALA:HB3  | 3:N:713:ILE:HD12  | 1.89                     | 0.53              |
| 3:N:421:LEU:HG    | 3:N:422:ALA:O     | 2.08                     | 0.53              |
| 3:N:452:ILE:HG23  | 3:N:452:ILE:O     | 2.07                     | 0.53              |
| 3:N:761:ILE:HD13  | 4:O:19:LEU:HD23   | 1.90                     | 0.53              |
| 3:N:820:GLU:HB2   | 3:N:836:VAL:HG11  | 1.90                     | 0.53              |
| 3:N:827:ILE:HG13  | 8:N:9926:HOH:O    | 2.07                     | 0.53              |
| 3:N:1031:ASN:OD1  | 3:N:1033:GLN:N    | 2.41                     | 0.53              |
| 3:N:1281:VAL:HG21 | 3:N:1313:VAL:HG21 | 1.90                     | 0.53              |
| 5:P:83:GLN:O      | 5:P:87:GLU:HG3    | 2.08                     | 0.53              |
| 5:P:99:GLU:OE1    | 5:P:234:LYS:HB2   | 2.07                     | 0.53              |
| 5:P:392:VAL:CG1   | 5:P:396:ARG:HB2   | 2.38                     | 0.53              |
| 2:C:43:GLY:HA2    | 8:C:9879:HOH:O    | 2.08                     | 0.53              |
| 2:C:158:TYR:CE1   | 2:C:313:LEU:HG    | 2.43                     | 0.53              |
| 2:C:237:ARG:O     | 2:C:240:THR:HB    | 2.09                     | 0.53              |
| 2:C:843:HIS:CD2   | 2:C:884:GLN:HA    | 2.43                     | 0.53              |
| 2:C:843:HIS:HD2   | 2:C:884:GLN:CB    | 2.21                     | 0.53              |
| 3:D:112:ILE:O     | 3:D:112:ILE:HD12  | 2.08                     | 0.53              |
| 3:D:1033:GLN:NE2  | 3:D:1036:ARG:NH1  | 2.44                     | 0.53              |
| 5:F:202:TYR:HB2   | 8:F:9547:HOH:O    | 2.08                     | 0.53              |
| 1:L:176:ARG:NH2   | 3:N:884:ARG:NE    | 2.56                     | 0.53              |
| 2:M:153:ALA:O     | 2:M:155:PRO:HD3   | 2.08                     | 0.53              |
| 2:M:263:ASP:HB2   | 2:M:264:PRO:CD    | 2.39                     | 0.53              |
| 2:M:412:ALA:HA    | 8:M:2237:HOH:O    | 2.09                     | 0.53              |
| 2:M:501:THR:HG22  | 2:M:513:VAL:HG11  | 1.88                     | 0.53              |
| 2:M:770:GLU:HB3   | 8:M:9573:HOH:O    | 2.08                     | 0.53              |
| 3:N:42:ASP:O      | 3:N:43:GLY:O      | 2.26                     | 0.53              |
| 3:N:528:VAL:HG22  | 8:P:9581:HOH:O    | 2.07                     | 0.53              |
| 3:N:1065:LEU:HD23 | 3:N:1070:TYR:HD2  | 1.73                     | 0.53              |
| 3:N:1090:ASP:C    | 3:N:1092:GLY:N    | 2.62                     | 0.53              |
| 5:P:164:LYS:HE2   | 8:P:9648:HOH:O    | 2.08                     | 0.53              |
| 5:P:406:ARG:HB3   | 8:P:9621:HOH:O    | 2.08                     | 0.53              |
| 2:C:194:VAL:HG13  | 2:C:221:LEU:HD12  | 1.90                     | 0.53              |
| 2:C:497:ALA:HA    | 2:C:515:ALA:HA    | 1.90                     | 0.53              |
| 8:C:9763:HOH:O    | 5:F:373:LYS:HD2   | 2.09                     | 0.53              |
| 3:D:19:ARG:HH21   | 3:D:94:GLU:CD     | 2.16                     | 0.53              |
| 3:D:209:ARG:CZ    | 3:D:397:LYS:HB2   | 2.38                     | 0.53              |
| 3:D:209:ARG:NH2   | 3:D:397:LYS:HB2   | 2.23                     | 0.53              |
| 3:D:1104:GLU:HG3  | 3:D:1105:ILE:HD13 | 1.91                     | 0.53              |
| 5:F:142:ARG:HD3   | 8:F:9733:HOH:O    | 2.08                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:292:ALA:HB1  | 5:F:299:TRP:O     | 2.08                     | 0.53              |
| 5:F:393:THR:CG2  | 5:F:394:ARG:N     | 2.69                     | 0.53              |
| 1:K:28:LEU:HA    | 8:K:2870:HOH:O    | 2.08                     | 0.53              |
| 1:L:51:THR:HA    | 1:L:145:ASP:O     | 2.07                     | 0.53              |
| 1:L:77:GLU:HB2   | 3:N:872:ARG:NH2   | 2.24                     | 0.53              |
| 2:M:264:PRO:CB   | 2:M:289:THR:HG21  | 2.37                     | 0.53              |
| 2:M:677:MET:HE1  | 2:M:983:ILE:HD12  | 1.91                     | 0.53              |
| 2:M:751:PRO:HA   | 2:M:792:VAL:CG1   | 2.39                     | 0.53              |
| 2:M:944:LEU:HB3  | 8:M:9761:HOH:O    | 2.09                     | 0.53              |
| 3:N:148:GLU:HB3  | 3:N:151:GLN:CG    | 2.38                     | 0.53              |
| 3:N:432:TYR:HA   | 3:N:448:GLU:O     | 2.09                     | 0.53              |
| 3:N:484:PRO:HB3  | 8:N:9566:HOH:O    | 2.09                     | 0.53              |
| 3:N:601:ARG:NE   | 3:N:605:ASP:HB3   | 2.23                     | 0.53              |
| 3:N:1232:PRO:HB3 | 3:N:1361:VAL:HG11 | 1.89                     | 0.53              |
| 3:N:1461:GLY:O   | 3:N:1473:PRO:HG2  | 2.08                     | 0.53              |
| 8:N:2187:HOH:O   | 5:P:90:GLN:HG3    | 2.07                     | 0.53              |
| 5:P:134:LYS:HB3  | 5:P:178:ARG:CZ    | 2.38                     | 0.53              |
| 2:C:195:LEU:O    | 2:C:195:LEU:HD12  | 2.08                     | 0.53              |
| 2:C:257:VAL:C    | 2:C:259:GLY:H     | 2.17                     | 0.53              |
| 2:C:399:ASN:HB3  | 2:C:568:ALA:O     | 2.09                     | 0.53              |
| 2:C:438:ILE:HG21 | 8:C:9979:HOH:O    | 2.07                     | 0.53              |
| 2:C:569:VAL:HG12 | 2:C:996:LYS:O     | 2.09                     | 0.53              |
| 2:C:850:ALA:HA   | 3:D:632:VAL:HG11  | 1.90                     | 0.53              |
| 2:C:949:LYS:CB   | 3:D:796:ARG:HH21  | 2.22                     | 0.53              |
| 3:D:142:LEU:HA   | 8:D:9493:HOH:O    | 2.08                     | 0.53              |
| 3:D:541:ASN:O    | 3:D:545:ARG:HG3   | 2.08                     | 0.53              |
| 3:D:968:ASP:O    | 3:D:971:LEU:HB3   | 2.09                     | 0.53              |
| 3:D:1011:PHE:HE1 | 3:D:1018:ASN:ND2  | 2.05                     | 0.53              |
| 3:D:1133:ARG:HB2 | 8:D:2100:HOH:O    | 2.08                     | 0.53              |
| 1:K:182:GLU:O    | 1:K:194:LYS:HB3   | 2.09                     | 0.53              |
| 1:L:206:THR:HB   | 1:L:209:GLU:OE2   | 2.09                     | 0.53              |
| 2:M:384:GLU:CD   | 2:M:388:ARG:HH21  | 2.16                     | 0.53              |
| 2:M:1104:GLU:HG2 | 8:M:9503:HOH:O    | 2.08                     | 0.53              |
| 3:N:535:PHE:HA   | 8:N:9957:HOH:O    | 2.08                     | 0.53              |
| 3:N:560:GLN:HE21 | 3:N:560:GLN:CA    | 2.22                     | 0.53              |
| 3:N:633:VAL:HG22 | 3:N:635:PRO:HD3   | 1.89                     | 0.53              |
| 3:N:1017:PHE:HA  | 3:N:1022:VAL:CG2  | 2.38                     | 0.53              |
| 1:B:50:GLY:O     | 1:B:146:ARG:HA    | 2.08                     | 0.53              |
| 2:C:144:PRO:HG2  | 2:C:165:LEU:HD23  | 1.91                     | 0.53              |
| 2:C:266:ARG:HD3  | 2:C:273:GLY:HA3   | 1.88                     | 0.53              |
| 2:C:286:SER:HB3  | 2:C:299:LYS:NZ    | 2.23                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:290:LEU:HD12  | 8:C:9781:HOH:O    | 2.08                     | 0.53              |
| 2:C:484:VAL:HG12  | 2:C:486:MET:HG3   | 1.89                     | 0.53              |
| 2:C:674:VAL:HG23  | 2:C:869:VAL:O     | 2.08                     | 0.53              |
| 2:C:679:PHE:O     | 2:C:681:GLY:N     | 2.41                     | 0.53              |
| 2:C:704:HIS:CD2   | 2:C:831:ARG:HH12  | 2.27                     | 0.53              |
| 2:C:768:THR:HB    | 2:C:771:GLU:HB3   | 1.89                     | 0.53              |
| 2:C:911:GLU:HG2   | 2:C:915:LYS:HE3   | 1.91                     | 0.53              |
| 3:D:653:PHE:CD1   | 3:D:695:ILE:HD11  | 2.43                     | 0.53              |
| 5:F:326:ASP:HA    | 8:F:9543:HOH:O    | 2.08                     | 0.53              |
| 1:K:181:VAL:O     | 2:M:938:LYS:HD2   | 2.08                     | 0.53              |
| 2:M:516:ARG:HG3   | 3:N:1068:LEU:HD13 | 1.90                     | 0.53              |
| 2:M:672:VAL:CG2   | 2:M:868:ASP:HB2   | 2.38                     | 0.53              |
| 2:M:1008:ARG:CZ   | 2:M:1020:PRO:HB3  | 2.38                     | 0.53              |
| 3:N:379:ALA:HB2   | 8:N:9770:HOH:O    | 2.09                     | 0.53              |
| 3:N:482:LYS:HG2   | 8:N:9980:HOH:O    | 2.08                     | 0.53              |
| 4:O:74:VAL:CG1    | 4:O:79:LEU:HD21   | 2.35                     | 0.53              |
| 1:A:58:ILE:HG21   | 1:A:68:ILE:HD11   | 1.90                     | 0.53              |
| 2:C:862:PRO:HG3   | 2:C:975:TYR:HE1   | 1.74                     | 0.53              |
| 3:D:74:GLU:HB2    | 3:D:75:ARG:HD2    | 1.91                     | 0.53              |
| 3:D:115:LEU:HD11  | 3:D:468:LEU:HD13  | 1.90                     | 0.53              |
| 3:D:484:PRO:O     | 3:D:489:ARG:HD2   | 2.09                     | 0.53              |
| 3:D:633:VAL:HG22  | 3:D:635:PRO:CD    | 2.39                     | 0.53              |
| 3:D:895:VAL:O     | 3:D:899:LEU:HD12  | 2.08                     | 0.53              |
| 3:D:955:VAL:HG11  | 3:D:1015:TYR:HE2  | 1.74                     | 0.53              |
| 3:D:1403:LEU:HD22 | 8:D:9569:HOH:O    | 2.08                     | 0.53              |
| 1:K:220:GLU:HG2   | 8:K:1270:HOH:O    | 2.08                     | 0.53              |
| 1:L:47:SER:HB2    | 1:L:217:ILE:HD13  | 1.91                     | 0.53              |
| 2:M:71:TYR:H      | 2:M:71:TYR:HD2    | 1.51                     | 0.53              |
| 2:M:74:GLY:HA2    | 8:M:9521:HOH:O    | 2.09                     | 0.53              |
| 2:M:435:TYR:C     | 2:M:437:ARG:N     | 2.67                     | 0.53              |
| 2:M:890:LEU:HD12  | 2:M:890:LEU:O     | 2.09                     | 0.53              |
| 2:M:1017:THR:OG1  | 2:M:1019:GLN:HG2  | 2.09                     | 0.53              |
| 3:N:40:GLU:OE1    | 3:N:40:GLU:HA     | 2.08                     | 0.53              |
| 3:N:119:SER:H     | 3:N:123:LEU:HD12  | 1.73                     | 0.53              |
| 3:N:658:LEU:HD11  | 3:N:674:ARG:NH1   | 2.24                     | 0.53              |
| 2:C:480:THR:HG22  | 2:C:481:ASP:N     | 2.24                     | 0.53              |
| 2:C:763:GLY:HA3   | 8:C:2108:HOH:O    | 2.09                     | 0.53              |
| 2:C:837:ASP:OD2   | 2:C:838:LYS:N     | 2.41                     | 0.53              |
| 2:C:1083:GLU:HG2  | 8:C:9782:HOH:O    | 2.09                     | 0.53              |
| 3:D:131:LYS:HB3   | 3:D:456:MET:HE3   | 1.90                     | 0.53              |
| 3:D:480:GLU:O     | 3:D:484:PRO:HD2   | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:219:ARG:HH12  | 1:K:220:GLU:HG3   | 1.74                     | 0.53              |
| 1:L:57:TYR:HE1    | 1:L:163:ASN:HB2   | 1.74                     | 0.53              |
| 2:M:317:VAL:HG22  | 2:M:320:HIS:CE1   | 2.43                     | 0.53              |
| 2:M:520:GLU:O     | 2:M:522:VAL:HG23  | 2.08                     | 0.53              |
| 2:M:537:LYS:N     | 2:M:905:ILE:HD11  | 2.24                     | 0.53              |
| 2:M:1054:THR:CG2  | 2:M:1079:PRO:HB3  | 2.30                     | 0.53              |
| 3:N:141:ILE:HD12  | 3:N:141:ILE:N     | 2.24                     | 0.53              |
| 3:N:396:VAL:HG22  | 3:N:447:VAL:HB    | 1.90                     | 0.53              |
| 3:N:598:ARG:NH2   | 5:P:318:GLU:O     | 2.42                     | 0.53              |
| 3:N:1485:GLN:HB3  | 8:N:2188:HOH:O    | 2.08                     | 0.53              |
| 1:A:39:PRO:CG     | 1:B:39:PRO:HG2    | 2.39                     | 0.53              |
| 1:B:211:LEU:O     | 1:B:215:VAL:HG13  | 2.09                     | 0.53              |
| 2:C:252:LYS:HE2   | 2:C:296:GLY:HA3   | 1.89                     | 0.53              |
| 2:C:290:LEU:HD13  | 8:C:9742:HOH:O    | 2.08                     | 0.53              |
| 2:C:322:VAL:HA    | 8:C:9963:HOH:O    | 2.08                     | 0.53              |
| 2:C:720:GLU:OE2   | 2:C:760:SER:HB3   | 2.08                     | 0.53              |
| 2:C:1001:VAL:HA   | 8:C:9545:HOH:O    | 2.09                     | 0.53              |
| 2:C:1039:ALA:HB2  | 3:D:707:THR:HG21  | 1.91                     | 0.53              |
| 3:D:42:ASP:O      | 3:D:43:GLY:O      | 2.27                     | 0.53              |
| 3:D:1462:LEU:HD22 | 3:D:1472:ILE:HG23 | 1.91                     | 0.53              |
| 5:F:122:LEU:HD23  | 5:F:126:LEU:HB3   | 1.91                     | 0.53              |
| 1:K:205:VAL:HG23  | 1:K:206:THR:N     | 2.23                     | 0.53              |
| 1:L:185:ARG:NH1   | 3:N:692:GLU:HG3   | 2.24                     | 0.53              |
| 2:M:247:PRO:HG2   | 8:M:2139:HOH:O    | 2.09                     | 0.53              |
| 2:M:432:ARG:NH2   | 3:N:1047:LYS:HB3  | 2.24                     | 0.53              |
| 2:M:448:ASN:ND2   | 2:M:452:ILE:HD11  | 2.24                     | 0.53              |
| 2:M:455:LEU:HD13  | 2:M:456:ALA:O     | 2.09                     | 0.53              |
| 2:M:971:LYS:NZ    | 3:N:950:GLY:HA3   | 2.23                     | 0.53              |
| 3:N:774:SER:HB2   | 3:N:776:GLU:HG2   | 1.91                     | 0.53              |
| 3:N:820:GLU:CB    | 3:N:836:VAL:HG21  | 2.38                     | 0.53              |
| 4:O:70:THR:HG22   | 4:O:71:GLY:H      | 1.73                     | 0.53              |
| 5:P:300:ASP:CG    | 5:P:301:ALA:N     | 2.66                     | 0.53              |
| 1:A:212:ASN:HA    | 8:A:9434:HOH:O    | 2.09                     | 0.53              |
| 1:A:212:ASN:HB2   | 8:A:9590:HOH:O    | 2.09                     | 0.53              |
| 1:B:65:PHE:HB2    | 8:B:9547:HOH:O    | 2.08                     | 0.53              |
| 2:C:263:ASP:HB2   | 2:C:264:PRO:CD    | 2.34                     | 0.53              |
| 3:D:24:GLY:HA3    | 3:D:49:ILE:HG12   | 1.91                     | 0.53              |
| 3:D:30:GLU:HB3    | 3:D:40:GLU:CB     | 2.39                     | 0.53              |
| 3:D:820:GLU:HB3   | 3:D:836:VAL:HG21  | 1.91                     | 0.53              |
| 3:D:1150:ALA:C    | 3:D:1151:ARG:HG2  | 2.31                     | 0.53              |
| 5:F:287:THR:C     | 5:F:289:GLU:H     | 2.17                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:918:LEU:HD23  | 2:M:968:LEU:HA   | 1.91                     | 0.53              |
| 2:M:1035:MET:HB2  | 2:M:1036:GLU:OE1 | 2.09                     | 0.53              |
| 3:N:80:VAL:HG23   | 3:N:81:THR:O     | 2.09                     | 0.53              |
| 3:N:138:LYS:HD2   | 3:N:138:LYS:N    | 2.15                     | 0.53              |
| 3:N:190:GLU:CD    | 3:N:190:GLU:H    | 2.17                     | 0.53              |
| 3:N:792:ILE:HG23  | 3:N:793:THR:HG23 | 1.91                     | 0.53              |
| 3:N:885:ILE:HG23  | 3:N:937:TYR:CE1  | 2.44                     | 0.53              |
| 3:N:930:LEU:O     | 3:N:934:LEU:HD12 | 2.09                     | 0.53              |
| 3:N:1399:ASP:O    | 3:N:1403:LEU:HB2 | 2.08                     | 0.53              |
| 1:B:132:LEU:CD2   | 1:B:138:LEU:HD22 | 2.34                     | 0.52              |
| 2:C:501:THR:HG22  | 2:C:513:VAL:CG1  | 2.39                     | 0.52              |
| 2:C:909:ALA:HB1   | 2:C:914:ILE:CD1  | 2.39                     | 0.52              |
| 2:C:1007:ALA:HB2  | 3:D:648:MET:HG3  | 1.90                     | 0.52              |
| 2:C:1034:GLU:HG3  | 2:C:1035:MET:N   | 2.24                     | 0.52              |
| 3:D:84:ILE:HA     | 8:D:2066:HOH:O   | 2.09                     | 0.52              |
| 3:D:529:GLN:HB2   | 8:D:2263:HOH:O   | 2.07                     | 0.52              |
| 3:D:775:GLY:HA3   | 3:D:1145:TYR:HE1 | 1.74                     | 0.52              |
| 3:D:919:PHE:C     | 3:D:919:PHE:CD2  | 2.86                     | 0.52              |
| 3:D:1047:LYS:HG2  | 3:D:1053:PHE:CZ  | 2.44                     | 0.52              |
| 3:D:1106:VAL:HG21 | 3:D:1474:ALA:HB2 | 1.91                     | 0.52              |
| 3:D:1283:ILE:C    | 3:D:1284:GLU:HG2 | 2.33                     | 0.52              |
| 4:E:4:PRO:HB2     | 8:E:9361:HOH:O   | 2.08                     | 0.52              |
| 5:F:85:LEU:HD22   | 5:F:193:ARG:HG3  | 1.90                     | 0.52              |
| 5:F:153:PRO:HB2   | 8:F:9637:HOH:O   | 2.09                     | 0.52              |
| 5:F:289:GLU:O     | 5:F:293:GLU:HG3  | 2.09                     | 0.52              |
| 5:F:412:GLU:CG    | 5:F:418:LEU:HD13 | 2.40                     | 0.52              |
| 2:M:358:ARG:HB3   | 2:M:371:LYS:O    | 2.09                     | 0.52              |
| 3:N:104:PHE:HA    | 8:N:9484:HOH:O   | 2.09                     | 0.52              |
| 3:N:399:ARG:HD3   | 3:N:402:PRO:HG3  | 1.91                     | 0.52              |
| 3:N:422:ALA:N     | 3:N:427:VAL:HG11 | 2.15                     | 0.52              |
| 3:N:496:LEU:HD21  | 3:N:500:ARG:NE   | 2.25                     | 0.52              |
| 3:N:908:LYS:O     | 3:N:912:LYS:HB2  | 2.09                     | 0.52              |
| 3:N:992:ILE:O     | 3:N:995:LEU:HB3  | 2.08                     | 0.52              |
| 3:N:1105:ILE:HD11 | 3:N:1374:GLN:NE2 | 2.24                     | 0.52              |
| 4:O:18:ARG:NH1    | 8:O:4048:HOH:O   | 2.43                     | 0.52              |
| 5:P:292:ALA:HB1   | 5:P:299:TRP:O    | 2.09                     | 0.52              |
| 8:A:9609:HOH:O    | 1:B:12:THR:HG22  | 2.10                     | 0.52              |
| 2:C:428:ARG:HH21  | 2:C:451:LEU:CD1  | 2.22                     | 0.52              |
| 2:C:1005:MET:O    | 2:C:1005:MET:HG2 | 2.07                     | 0.52              |
| 2:C:1115:LEU:O    | 3:D:89:ARG:HG2   | 2.09                     | 0.52              |
| 3:D:10:ILE:HG13   | 3:D:1434:TRP:CE2 | 2.43                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:444:VAL:HG22 | 3:D:444:VAL:O     | 2.09                     | 0.52              |
| 3:D:470:LEU:HD12 | 3:D:508:ARG:NH1   | 2.24                     | 0.52              |
| 4:E:8:LYS:O      | 4:E:12:MET:HG3    | 2.08                     | 0.52              |
| 2:M:100:LEU:HD21 | 2:M:367:LEU:HG    | 1.91                     | 0.52              |
| 2:M:146:VAL:HG12 | 2:M:162:ILE:HA    | 1.91                     | 0.52              |
| 2:M:181:VAL:HG12 | 2:M:182:VAL:H     | 1.74                     | 0.52              |
| 2:M:241:LEU:HB3  | 8:M:9936:HOH:O    | 2.09                     | 0.52              |
| 2:M:617:ASP:HB3  | 8:M:9992:HOH:O    | 2.08                     | 0.52              |
| 2:M:1085:PHE:CE1 | 2:M:1111:ILE:HG21 | 2.44                     | 0.52              |
| 3:N:558:LEU:CB   | 5:P:145:PRO:HB3   | 2.39                     | 0.52              |
| 3:N:680:GLN:O    | 3:N:683:ILE:HG13  | 2.09                     | 0.52              |
| 3:N:806:PHE:O    | 3:N:808:THR:N     | 2.42                     | 0.52              |
| 3:N:827:ILE:HD12 | 3:N:828:LYS:NZ    | 2.24                     | 0.52              |
| 5:P:282:LEU:HD12 | 5:P:284:ARG:HD2   | 1.90                     | 0.52              |
| 1:B:90:LEU:HD11  | 8:B:9549:HOH:O    | 2.08                     | 0.52              |
| 2:C:281:LEU:CD1  | 2:C:306:THR:HA    | 2.39                     | 0.52              |
| 2:C:985:GLY:HA3  | 8:D:9822:HOH:O    | 2.09                     | 0.52              |
| 2:C:1118:LYS:NZ  | 3:D:20:SER:HA     | 2.24                     | 0.52              |
| 3:D:708:LEU:O    | 3:D:1227:GLN:HG2  | 2.08                     | 0.52              |
| 3:D:1432:LYS:NZ  | 3:D:1460:ILE:HB   | 2.23                     | 0.52              |
| 3:D:1493:LYS:HG3 | 8:D:9515:HOH:O    | 2.09                     | 0.52              |
| 5:F:286:PRO:HB3  | 5:F:290:GLU:HB2   | 1.91                     | 0.52              |
| 1:K:146:ARG:NH2  | 1:K:147:GLY:HA2   | 2.23                     | 0.52              |
| 2:M:42:VAL:HG12  | 2:M:43:GLY:N      | 2.23                     | 0.52              |
| 2:M:52:PHE:HD2   | 2:M:68:PHE:HB2    | 1.71                     | 0.52              |
| 2:M:339:LEU:HD21 | 8:M:9656:HOH:O    | 2.09                     | 0.52              |
| 2:M:686:ASP:HB2  | 8:N:2331:HOH:O    | 2.09                     | 0.52              |
| 2:M:722:ILE:O    | 2:M:722:ILE:HG23  | 2.08                     | 0.52              |
| 2:M:1014:SER:HB2 | 8:M:9765:HOH:O    | 2.09                     | 0.52              |
| 2:M:1019:GLN:NE2 | 3:N:621:LYS:HB3   | 2.25                     | 0.52              |
| 2:M:1065:ALA:HB1 | 2:M:1077:PRO:HG2  | 1.91                     | 0.52              |
| 3:N:128:TYR:HB3  | 3:N:129:PHE:CD1   | 2.44                     | 0.52              |
| 3:N:584:ASN:H    | 3:N:602:SER:CB    | 2.22                     | 0.52              |
| 3:N:847:ASP:HB2  | 8:N:2224:HOH:O    | 2.09                     | 0.52              |
| 3:N:1462:LEU:CD2 | 3:N:1473:PRO:HD2  | 2.39                     | 0.52              |
| 5:P:261:PRO:O    | 5:P:265:VAL:HG23  | 2.10                     | 0.52              |
| 5:P:405:LEU:O    | 5:P:408:LEU:CD2   | 2.58                     | 0.52              |
| 5:P:406:ARG:HA   | 5:P:409:LYS:CD    | 2.39                     | 0.52              |
| 1:A:124:ASN:HB3  | 1:A:127:LEU:HD23  | 1.92                     | 0.52              |
| 2:C:26:TYR:OH    | 2:C:340:MET:HE2   | 2.10                     | 0.52              |
| 2:C:139:GLN:HB3  | 2:C:334:ARG:CG    | 2.38                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:151:ASP:CG    | 2:C:152:PRO:HD2  | 2.35                     | 0.52              |
| 2:C:344:PHE:HD2   | 2:C:382:ILE:HD11 | 1.74                     | 0.52              |
| 2:C:987:ILE:HD11  | 3:D:946:GLY:HA2  | 1.91                     | 0.52              |
| 3:D:17:LYS:HG3    | 8:D:9805:HOH:O   | 2.08                     | 0.52              |
| 3:D:736:PHE:HA    | 8:D:9665:HOH:O   | 2.08                     | 0.52              |
| 3:D:907:GLU:HA    | 8:D:2030:HOH:O   | 2.10                     | 0.52              |
| 3:D:1045:MET:HA   | 3:D:1045:MET:HE3 | 1.91                     | 0.52              |
| 1:L:12:THR:CG2    | 1:L:24:VAL:HB    | 2.31                     | 0.52              |
| 1:L:124:ASN:HA    | 8:L:932:HOH:O    | 2.09                     | 0.52              |
| 2:M:65:VAL:O      | 2:M:101:ILE:HG12 | 2.08                     | 0.52              |
| 2:M:462:ASP:HB2   | 8:M:9695:HOH:O   | 2.09                     | 0.52              |
| 2:M:568:ALA:HB1   | 2:M:668:LEU:HB3  | 1.91                     | 0.52              |
| 2:M:728:HIS:NE2   | 5:P:423:ASP:OD1  | 2.43                     | 0.52              |
| 2:M:854:PRO:C     | 2:M:856:GLU:N    | 2.67                     | 0.52              |
| 3:N:66:GLN:O      | 3:N:67:ARG:C     | 2.52                     | 0.52              |
| 3:N:114:THR:O     | 3:N:495:ARG:HG3  | 2.09                     | 0.52              |
| 3:N:1096:ARG:HH11 | 3:N:1096:ARG:CG  | 2.21                     | 0.52              |
| 3:N:1103:HIS:CE1  | 3:N:1463:LYS:HE2 | 2.45                     | 0.52              |
| 3:N:1397:LYS:HZ2  | 3:N:1432:LYS:HB3 | 1.73                     | 0.52              |
| 5:P:88:ILE:CD1    | 5:P:193:ARG:HB2  | 2.33                     | 0.52              |
| 1:A:35:THR:HG21   | 1:B:43:ILE:HD11  | 1.92                     | 0.52              |
| 2:C:290:LEU:HG    | 8:C:9714:HOH:O   | 2.09                     | 0.52              |
| 2:C:683:ASN:HB2   | 2:C:687:ALA:O    | 2.09                     | 0.52              |
| 3:D:131:LYS:HB3   | 3:D:456:MET:HE2  | 1.91                     | 0.52              |
| 3:D:404:GLU:HB3   | 3:D:414:ARG:CD   | 2.39                     | 0.52              |
| 3:D:1062:ARG:HH11 | 3:D:1062:ARG:HG3 | 1.74                     | 0.52              |
| 3:D:1364:HIS:ND1  | 3:D:1366:LYS:HG3 | 2.23                     | 0.52              |
| 5:F:163:LEU:HD22  | 5:F:174:LEU:HG   | 1.92                     | 0.52              |
| 2:M:266:ARG:HH11  | 2:M:266:ARG:HG3  | 1.75                     | 0.52              |
| 2:M:807:ARG:HG2   | 8:M:9793:HOH:O   | 2.08                     | 0.52              |
| 3:N:119:SER:N     | 3:N:123:LEU:HB2  | 2.23                     | 0.52              |
| 3:N:131:LYS:HG2   | 3:N:568:ARG:CG   | 2.28                     | 0.52              |
| 3:N:471:GLU:HG2   | 8:N:9534:HOH:O   | 2.09                     | 0.52              |
| 3:N:633:VAL:C     | 3:N:635:PRO:HD3  | 2.34                     | 0.52              |
| 3:N:633:VAL:O     | 3:N:635:PRO:HD3  | 2.09                     | 0.52              |
| 3:N:1286:THR:CG2  | 3:N:1287:GLU:N   | 2.71                     | 0.52              |
| 3:N:1500:LYS:HA   | 8:N:9894:HOH:O   | 2.09                     | 0.52              |
| 5:P:144:ILE:HB    | 5:P:145:PRO:HD3  | 1.91                     | 0.52              |
| 5:P:169:GLU:HA    | 5:P:172:ARG:NH2  | 2.25                     | 0.52              |
| 5:P:256:ARG:HD2   | 8:P:9506:HOH:O   | 2.10                     | 0.52              |
| 5:P:377:ASP:O     | 5:P:378:GLY:C    | 2.52                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:33:GLY:O     | 1:A:195:LEU:HD22 | 2.10                     | 0.52              |
| 2:C:837:ASP:HA   | 8:C:9820:HOH:O   | 2.09                     | 0.52              |
| 2:C:964:LYS:HD2  | 8:C:9496:HOH:O   | 2.10                     | 0.52              |
| 3:D:64:LYS:HD3   | 5:F:376:ILE:O    | 2.09                     | 0.52              |
| 3:D:112:ILE:HD13 | 3:D:461:ILE:HG21 | 1.91                     | 0.52              |
| 3:D:166:GLN:HG3  | 3:D:168:THR:OG1  | 2.10                     | 0.52              |
| 3:D:177:ALA:CB   | 3:D:199:LEU:HD13 | 2.40                     | 0.52              |
| 3:D:418:GLY:HA2  | 8:D:9642:HOH:O   | 2.09                     | 0.52              |
| 3:D:553:ARG:HH12 | 5:F:211:ASP:HA   | 1.75                     | 0.52              |
| 3:D:566:ILE:HG23 | 5:F:217:ASN:HD22 | 1.75                     | 0.52              |
| 3:D:660:LYS:HA   | 3:D:663:GLU:HG3  | 1.91                     | 0.52              |
| 3:D:1062:ARG:C   | 3:D:1062:ARG:HD3 | 2.34                     | 0.52              |
| 2:M:492:ASP:CA   | 2:M:518:LYS:HB3  | 2.39                     | 0.52              |
| 2:M:516:ARG:HG3  | 3:N:1068:LEU:CD1 | 2.40                     | 0.52              |
| 2:M:610:ARG:HD3  | 2:M:622:GLU:OE1  | 2.09                     | 0.52              |
| 2:M:816:LYS:HB2  | 2:M:819:VAL:HG21 | 1.92                     | 0.52              |
| 2:M:841:ASN:HD21 | 2:M:843:HIS:CB   | 2.23                     | 0.52              |
| 2:M:1103:ASP:CG  | 2:M:1104:GLU:N   | 2.67                     | 0.52              |
| 3:N:428:LYS:HB3  | 3:N:450:TYR:CE1  | 2.45                     | 0.52              |
| 3:N:777:PRO:HG2  | 3:N:912:LYS:O    | 2.08                     | 0.52              |
| 3:N:1133:ARG:HG3 | 8:N:9895:HOH:O   | 2.08                     | 0.52              |
| 5:P:137:GLY:HA2  | 5:P:140:ARG:HH22 | 1.74                     | 0.52              |
| 5:P:337:HIS:HB2  | 8:P:9745:HOH:O   | 2.09                     | 0.52              |
| 2:C:139:GLN:NE2  | 2:C:415:PRO:HD2  | 2.22                     | 0.52              |
| 2:C:468:ARG:HD3  | 2:C:485:TYR:O    | 2.10                     | 0.52              |
| 2:C:577:PRO:HG3  | 2:C:993:PHE:CE1  | 2.44                     | 0.52              |
| 2:C:671:ASN:N    | 2:C:671:ASN:HD22 | 2.08                     | 0.52              |
| 3:D:9:ARG:HB2    | 3:D:1456:LYS:HA  | 1.92                     | 0.52              |
| 3:D:55:ASP:HB3   | 3:D:82:LYS:HE2   | 1.92                     | 0.52              |
| 3:D:820:GLU:CB   | 3:D:836:VAL:HG21 | 2.40                     | 0.52              |
| 3:D:864:VAL:HG23 | 3:D:877:PRO:HD3  | 1.92                     | 0.52              |
| 5:F:191:ASN:HB3  | 5:F:220:LEU:HD11 | 1.91                     | 0.52              |
| 5:F:331:ASP:N    | 8:F:9658:HOH:O   | 2.42                     | 0.52              |
| 1:K:206:THR:HG21 | 8:K:1068:HOH:O   | 2.10                     | 0.52              |
| 2:M:352:ALA:C    | 2:M:355:VAL:HG12 | 2.34                     | 0.52              |
| 2:M:564:MET:HG2  | 2:M:840:ALA:HB3  | 1.92                     | 0.52              |
| 3:N:213:VAL:HG23 | 3:N:391:ALA:HA   | 1.92                     | 0.52              |
| 5:P:257:THR:O    | 5:P:258:ILE:HD13 | 2.09                     | 0.52              |
| 1:B:51:THR:HA    | 1:B:145:ASP:O    | 2.09                     | 0.52              |
| 2:C:64:LEU:HB2   | 8:C:9487:HOH:O   | 2.10                     | 0.52              |
| 2:C:352:ALA:O    | 2:C:355:VAL:HG12 | 2.10                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:546:LEU:CD1   | 2:C:565:GLN:HE22 | 2.22                     | 0.52              |
| 3:D:415:VAL:HG12  | 3:D:416:ALA:N    | 2.25                     | 0.52              |
| 3:D:1087:ARG:C    | 3:D:1089:ALA:H   | 2.17                     | 0.52              |
| 3:D:1281:VAL:HG23 | 3:D:1317:ASP:O   | 2.10                     | 0.52              |
| 8:D:2217:HOH:O    | 4:E:92:ILE:HD13  | 2.10                     | 0.52              |
| 5:F:138:SER:OG    | 5:F:140:ARG:HG2  | 2.09                     | 0.52              |
| 5:F:416:ARG:NH1   | 5:F:419:ARG:CB   | 2.72                     | 0.52              |
| 1:K:150:TYR:HD1   | 1:K:170:VAL:HG13 | 1.74                     | 0.52              |
| 2:M:473:ARG:HB3   | 8:M:9483:HOH:O   | 2.08                     | 0.52              |
| 2:M:838:LYS:HD3   | 2:M:846:LYS:NZ   | 2.25                     | 0.52              |
| 3:N:23:TYR:HB2    | 3:N:49:ILE:O     | 2.10                     | 0.52              |
| 3:N:169:TYR:N     | 3:N:170:PRO:HD3  | 2.23                     | 0.52              |
| 3:N:426:LYS:HE2   | 3:N:428:LYS:HE3  | 1.92                     | 0.52              |
| 3:N:478:LEU:HD23  | 3:N:1388:ARG:NH1 | 2.24                     | 0.52              |
| 3:N:675:ARG:HA    | 3:N:678:GLU:OE2  | 2.09                     | 0.52              |
| 3:N:1093:TYR:CE1  | 3:N:1097:LYS:HE2 | 2.45                     | 0.52              |
| 3:N:1133:ARG:NH1  | 8:N:2461:HOH:O   | 2.42                     | 0.52              |
| 5:P:286:PRO:HB3   | 5:P:290:GLU:HB2  | 1.92                     | 0.52              |
| 1:A:30:ARG:NH1    | 1:B:155:LYS:HZ1  | 2.03                     | 0.52              |
| 1:A:72:LYS:O      | 2:C:608:GLY:HA2  | 2.10                     | 0.52              |
| 2:C:158:TYR:CD1   | 2:C:313:LEU:HG   | 2.45                     | 0.52              |
| 2:C:676:ILE:O     | 3:D:948:THR:HG22 | 2.09                     | 0.52              |
| 3:D:172:PRO:HG3   | 3:D:178:LEU:HD22 | 1.91                     | 0.52              |
| 3:D:187:LYS:HE2   | 3:D:213:VAL:HG12 | 1.92                     | 0.52              |
| 3:D:781:PRO:HB3   | 3:D:785:ILE:CG2  | 2.40                     | 0.52              |
| 3:D:838:ARG:HG3   | 3:D:838:ARG:HH11 | 1.75                     | 0.52              |
| 3:D:920:LEU:HD21  | 8:D:9484:HOH:O   | 2.10                     | 0.52              |
| 3:D:1304:LYS:HD3  | 3:D:1304:LYS:N   | 2.16                     | 0.52              |
| 5:F:392:VAL:CG1   | 5:F:396:ARG:HB2  | 2.40                     | 0.52              |
| 2:M:839:LEU:HD12  | 2:M:994:ILE:HG21 | 1.92                     | 0.52              |
| 2:M:862:PRO:HG2   | 2:M:925:TYR:OH   | 2.10                     | 0.52              |
| 2:M:892:LEU:HD21  | 2:M:967:PHE:CE1  | 2.45                     | 0.52              |
| 2:M:976:ASP:HB3   | 2:M:979:THR:CG2  | 2.39                     | 0.52              |
| 3:N:187:LYS:HE2   | 8:N:2337:HOH:O   | 2.08                     | 0.52              |
| 3:N:423:ASP:O     | 3:N:425:GLY:N    | 2.34                     | 0.52              |
| 3:N:760:ARG:NE    | 4:O:3:GLU:OE1    | 2.43                     | 0.52              |
| 5:P:123:ASP:HB3   | 5:P:125:ASP:OD1  | 2.10                     | 0.52              |
| 2:C:682:TYR:HA    | 3:D:635:PRO:HG2  | 1.92                     | 0.52              |
| 2:C:770:GLU:CG    | 3:D:65:ARG:HH22  | 2.11                     | 0.52              |
| 2:C:896:PHE:CE2   | 2:C:925:TYR:HB2  | 2.44                     | 0.52              |
| 2:C:1032:PHE:CD1  | 2:C:1052:MET:HG2 | 2.44                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:C:9560:HOH:O    | 5:F:405:LEU:HD22  | 2.09                     | 0.52              |
| 3:D:416:ALA:HB3   | 8:D:2272:HOH:O    | 2.10                     | 0.52              |
| 3:D:1381:VAL:O    | 3:D:1389:LEU:O    | 2.28                     | 0.52              |
| 8:D:9635:HOH:O    | 5:F:101:GLU:HG3   | 2.10                     | 0.52              |
| 5:F:144:ILE:HB    | 5:F:145:PRO:HD3   | 1.92                     | 0.52              |
| 1:K:6:LEU:C       | 1:K:8:ALA:N       | 2.68                     | 0.52              |
| 1:K:187:GLY:HA2   | 8:K:2920:HOH:O    | 2.10                     | 0.52              |
| 1:L:101:LEU:HB2   | 1:L:114:PHE:CD2   | 2.45                     | 0.52              |
| 2:M:270:GLY:H     | 2:M:288:ARG:CZ    | 2.22                     | 0.52              |
| 2:M:512:ARG:HD3   | 2:M:523:ILE:HD11  | 1.92                     | 0.52              |
| 2:M:554:ASP:OD2   | 2:M:556:ASN:HB2   | 2.10                     | 0.52              |
| 2:M:572:ILE:CD1   | 2:M:701:THR:HB    | 2.34                     | 0.52              |
| 2:M:714:ASP:N     | 2:M:818:GLY:O     | 2.41                     | 0.52              |
| 2:M:861:LEU:HD23  | 2:M:862:PRO:HD2   | 1.93                     | 0.52              |
| 3:N:55:ASP:O      | 3:N:82:LYS:HA     | 2.10                     | 0.52              |
| 3:N:75:ARG:HB2    | 8:N:2407:HOH:O    | 2.10                     | 0.52              |
| 3:N:481:MET:HE1   | 3:N:1388:ARG:NE   | 2.25                     | 0.52              |
| 3:N:496:LEU:HD21  | 3:N:500:ARG:HE    | 1.73                     | 0.52              |
| 3:N:638:LYS:HD3   | 8:N:9823:HOH:O    | 2.10                     | 0.52              |
| 3:N:850:LEU:CD2   | 3:N:881:LEU:HD13  | 2.40                     | 0.52              |
| 3:N:888:GLU:HB3   | 8:N:9679:HOH:O    | 2.09                     | 0.52              |
| 3:N:1459:LEU:HD12 | 3:N:1470:ARG:HH11 | 1.75                     | 0.52              |
| 5:P:147:LEU:HD12  | 8:P:9554:HOH:O    | 2.10                     | 0.52              |
| 1:A:91:ASN:HB3    | 8:A:9436:HOH:O    | 2.09                     | 0.51              |
| 2:C:257:VAL:HG12  | 2:C:263:ASP:CG    | 2.35                     | 0.51              |
| 2:C:528:GLU:HB3   | 8:C:2302:HOH:O    | 2.09                     | 0.51              |
| 2:C:1016:ILE:HG23 | 3:D:526:PRO:HG2   | 1.92                     | 0.51              |
| 3:D:528:VAL:O     | 3:D:535:PHE:HA    | 2.10                     | 0.51              |
| 3:D:591:VAL:CG1   | 3:D:597:ASP:HA    | 2.40                     | 0.51              |
| 3:D:637:LEU:HD11  | 3:D:642:CYS:HA    | 1.91                     | 0.51              |
| 3:D:1087:ARG:C    | 3:D:1089:ALA:N    | 2.64                     | 0.51              |
| 3:D:1192:LEU:HD22 | 3:D:1345:GLU:OE2  | 2.10                     | 0.51              |
| 3:D:1341:PRO:HA   | 3:D:1376:MET:HE1  | 1.91                     | 0.51              |
| 1:L:42:ARG:HG2    | 1:L:42:ARG:NH1    | 2.19                     | 0.51              |
| 1:L:178:ALA:HB3   | 1:L:198:ARG:HB2   | 1.90                     | 0.51              |
| 2:M:536:PRO:CB    | 2:M:906:PHE:HB2   | 2.38                     | 0.51              |
| 2:M:596:TYR:HD1   | 8:M:2274:HOH:O    | 1.92                     | 0.51              |
| 3:N:12:LEU:HD21   | 3:N:104:PHE:CE1   | 2.45                     | 0.51              |
| 3:N:163:TYR:OH    | 3:N:394:LEU:HD21  | 2.10                     | 0.51              |
| 3:N:1286:THR:HB   | 8:N:2263:HOH:O    | 2.08                     | 0.51              |
| 3:N:1393:GLN:CB   | 3:N:1398:TRP:HE1  | 2.23                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:P:94:LEU:HD22  | 5:P:95:THR:N      | 2.25                     | 0.51              |
| 5:P:218:GLN:HA   | 5:P:221:ILE:HD12  | 1.91                     | 0.51              |
| 2:C:263:ASP:CB   | 2:C:264:PRO:HD3   | 2.35                     | 0.51              |
| 2:C:1084:SER:HA  | 8:C:2139:HOH:O    | 2.09                     | 0.51              |
| 3:D:118:LEU:CA   | 3:D:123:LEU:HD13  | 2.40                     | 0.51              |
| 3:D:411:THR:HG22 | 8:D:9544:HOH:O    | 2.10                     | 0.51              |
| 3:D:669:ASN:HD22 | 3:D:672:ALA:H     | 1.56                     | 0.51              |
| 3:D:844:ALA:O    | 3:D:867:ARG:HB3   | 2.10                     | 0.51              |
| 3:D:1270:ALA:HB3 | 8:D:9570:HOH:O    | 2.10                     | 0.51              |
| 3:D:1304:LYS:HB2 | 8:D:9970:HOH:O    | 2.09                     | 0.51              |
| 1:L:91:ASN:H     | 1:L:94:LEU:HD13   | 1.76                     | 0.51              |
| 2:M:516:ARG:NE   | 3:N:1068:LEU:HD13 | 2.25                     | 0.51              |
| 3:N:477:LEU:HD21 | 3:N:495:ARG:HD3   | 1.91                     | 0.51              |
| 3:N:711:LEU:HD21 | 8:N:2357:HOH:O    | 2.09                     | 0.51              |
| 3:N:953:ASP:OD2  | 3:N:1019:PRO:HD2  | 2.09                     | 0.51              |
| 3:N:1042:ARG:O   | 3:N:1057:VAL:HB   | 2.10                     | 0.51              |
| 3:N:1353:GLN:NE2 | 3:N:1357:ARG:NE   | 2.55                     | 0.51              |
| 5:P:163:LEU:HD13 | 5:P:174:LEU:CD2   | 2.40                     | 0.51              |
| 5:P:337:HIS:HA   | 8:P:9567:HOH:O    | 2.09                     | 0.51              |
| 1:A:6:LEU:C      | 1:A:8:ALA:N       | 2.68                     | 0.51              |
| 1:A:156:HIS:CD2  | 1:A:158:ILE:HG12  | 2.46                     | 0.51              |
| 2:C:225:SER:HB2  | 2:C:229:MET:CE    | 2.41                     | 0.51              |
| 2:C:358:ARG:HB3  | 2:C:371:LYS:O     | 2.10                     | 0.51              |
| 2:C:816:LYS:HB2  | 2:C:819:VAL:CG2   | 2.40                     | 0.51              |
| 2:C:860:HIS:NE2  | 2:C:975:TYR:HB2   | 2.25                     | 0.51              |
| 2:C:1004:LYS:HE3 | 2:C:1027:PHE:CE1  | 2.45                     | 0.51              |
| 2:C:1051:GLU:HB3 | 8:C:9565:HOH:O    | 2.10                     | 0.51              |
| 3:D:434:ARG:HB3  | 8:D:9567:HOH:O    | 2.09                     | 0.51              |
| 3:D:826:PRO:O    | 3:D:836:VAL:HG13  | 2.10                     | 0.51              |
| 3:D:1241:PHE:O   | 3:D:1243:THR:N    | 2.44                     | 0.51              |
| 5:F:276:ARG:HB3  | 8:F:9780:HOH:O    | 2.10                     | 0.51              |
| 5:F:363:GLU:O    | 5:F:367:MET:HG2   | 2.10                     | 0.51              |
| 2:M:177:GLU:N    | 2:M:178:PRO:HD3   | 2.26                     | 0.51              |
| 2:M:379:GLU:O    | 2:M:383:ARG:HB3   | 2.11                     | 0.51              |
| 3:N:1191:PRO:O   | 3:N:1373:ARG:HD2  | 2.10                     | 0.51              |
| 3:N:1493:LYS:O   | 3:N:1497:GLU:HG2  | 2.10                     | 0.51              |
| 2:C:11:GLU:HG2   | 2:C:537:LYS:HZ1   | 1.75                     | 0.51              |
| 2:C:78:PHE:HB3   | 2:C:79:PRO:CD     | 2.41                     | 0.51              |
| 3:D:164:GLY:HA2  | 8:D:9590:HOH:O    | 2.09                     | 0.51              |
| 3:D:820:GLU:HG2  | 3:D:825:ALA:O     | 2.10                     | 0.51              |
| 3:D:838:ARG:HD3  | 3:D:874:GLU:HB3   | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:983:LEU:HA    | 3:D:987:GLU:OE2   | 2.09                     | 0.51              |
| 5:F:194:LEU:HD23  | 8:F:9810:HOH:O    | 2.10                     | 0.51              |
| 5:F:287:THR:O     | 5:F:289:GLU:N     | 2.44                     | 0.51              |
| 5:F:392:VAL:HG22  | 8:F:9801:HOH:O    | 2.10                     | 0.51              |
| 1:K:109:VAL:HG23  | 1:K:132:LEU:HD13  | 1.93                     | 0.51              |
| 2:M:25:SER:HB2    | 2:M:335:THR:OG1   | 2.10                     | 0.51              |
| 2:M:266:ARG:HG3   | 2:M:266:ARG:NH1   | 2.24                     | 0.51              |
| 2:M:1029:GLY:HA2  | 8:M:2100:HOH:O    | 2.10                     | 0.51              |
| 3:N:12:LEU:HD11   | 3:N:104:PHE:CE1   | 2.46                     | 0.51              |
| 3:N:1068:LEU:HD23 | 3:N:1072:ILE:HD13 | 1.92                     | 0.51              |
| 3:N:1129:THR:HG23 | 3:N:1130:ARG:H    | 1.74                     | 0.51              |
| 3:N:1209:LEU:HB3  | 3:N:1211:MET:HB2  | 1.93                     | 0.51              |
| 3:N:1231:GLU:HB3  | 3:N:1232:PRO:HD3  | 1.93                     | 0.51              |
| 3:N:1357:ARG:HG2  | 8:N:2014:HOH:O    | 2.09                     | 0.51              |
| 3:N:1381:VAL:O    | 3:N:1389:LEU:O    | 2.29                     | 0.51              |
| 3:N:1441:GLN:O    | 3:N:1441:GLN:HG3  | 2.11                     | 0.51              |
| 5:P:135:ILE:HG12  | 5:P:178:ARG:HD3   | 1.92                     | 0.51              |
| 5:P:402:ASN:HB2   | 8:P:9753:HOH:O    | 2.09                     | 0.51              |
| 2:C:2:GLU:HB2     | 8:C:2326:HOH:O    | 2.09                     | 0.51              |
| 2:C:610:ARG:HB2   | 8:C:9839:HOH:O    | 2.10                     | 0.51              |
| 2:C:620:LEU:HD23  | 8:C:2191:HOH:O    | 2.09                     | 0.51              |
| 2:C:817:PRO:C     | 2:C:819:VAL:H     | 2.19                     | 0.51              |
| 2:C:939:ARG:HE    | 2:C:939:ARG:N     | 2.08                     | 0.51              |
| 2:C:1030:GLN:OE1  | 3:D:628:ARG:HB2   | 2.10                     | 0.51              |
| 3:D:781:PRO:HB2   | 3:D:911:LEU:HD23  | 1.91                     | 0.51              |
| 3:D:894:LYS:O     | 3:D:898:GLU:HG3   | 2.09                     | 0.51              |
| 3:D:1350:GLU:O    | 3:D:1354:LYS:HG2  | 2.11                     | 0.51              |
| 3:D:1429:LEU:HD11 | 8:D:9681:HOH:O    | 2.10                     | 0.51              |
| 4:E:63:TRP:O      | 4:E:67:GLU:HG3    | 2.10                     | 0.51              |
| 5:F:137:GLY:HA2   | 5:F:140:ARG:HH22  | 1.75                     | 0.51              |
| 1:L:184:THR:O     | 1:L:192:LEU:HB2   | 2.11                     | 0.51              |
| 2:M:418:LEU:HD21  | 8:M:2225:HOH:O    | 2.10                     | 0.51              |
| 2:M:612:VAL:HG21  | 8:M:9617:HOH:O    | 2.10                     | 0.51              |
| 2:M:616:GLU:OE1   | 2:M:616:GLU:HA    | 2.11                     | 0.51              |
| 2:M:686:ASP:N     | 8:N:2331:HOH:O    | 2.43                     | 0.51              |
| 8:M:9948:HOH:O    | 5:P:354:LEU:HD11  | 2.10                     | 0.51              |
| 3:N:36:THR:CG2    | 3:N:38:LYS:HG3    | 2.38                     | 0.51              |
| 3:N:154:THR:HG22  | 3:N:156:GLU:HG2   | 1.92                     | 0.51              |
| 3:N:779:ALA:O     | 3:N:931:LEU:HD22  | 2.11                     | 0.51              |
| 3:N:965:GLU:HA    | 3:N:968:ASP:HB2   | 1.93                     | 0.51              |
| 3:N:970:LYS:HD2   | 3:N:995:LEU:HD13  | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1042:ARG:NH2  | 3:N:1045:MET:HE1  | 2.26                     | 0.51              |
| 3:N:1074:SER:O    | 3:N:1077:ALA:HB3  | 2.11                     | 0.51              |
| 3:N:1459:LEU:HD12 | 3:N:1470:ARG:NH1  | 2.24                     | 0.51              |
| 3:N:1463:LYS:HG2  | 8:N:9565:HOH:O    | 2.09                     | 0.51              |
| 3:N:1498:ALA:HA   | 3:N:1501:GLU:OE2  | 2.11                     | 0.51              |
| 5:P:133:ALA:O     | 5:P:137:GLY:O     | 2.27                     | 0.51              |
| 5:P:161:GLN:HA    | 5:P:164:LYS:HD2   | 1.91                     | 0.51              |
| 5:P:372:ARG:O     | 5:P:377:ASP:O     | 2.29                     | 0.51              |
| 1:A:143:ARG:HH21  | 1:A:158:ILE:HD12  | 1.76                     | 0.51              |
| 1:B:127:LEU:HD12  | 1:B:128:HIS:H     | 1.75                     | 0.51              |
| 2:C:78:PHE:HB3    | 2:C:79:PRO:HD2    | 1.92                     | 0.51              |
| 2:C:191:PHE:CE1   | 2:C:238:LEU:HD21  | 2.46                     | 0.51              |
| 2:C:480:THR:HG22  | 2:C:482:GLU:N     | 2.23                     | 0.51              |
| 2:C:579:VAL:HG11  | 2:C:887:GLU:HG3   | 1.91                     | 0.51              |
| 2:C:674:VAL:HB    | 2:C:869:VAL:HG13  | 1.91                     | 0.51              |
| 2:C:1054:THR:HG23 | 2:C:1059:ASP:CB   | 2.41                     | 0.51              |
| 3:D:173:PRO:HG2   | 3:D:200:ASP:OD2   | 2.11                     | 0.51              |
| 3:D:496:LEU:HD12  | 8:D:9706:HOH:O    | 2.11                     | 0.51              |
| 3:D:590:PRO:HD2   | 8:D:9687:HOH:O    | 2.11                     | 0.51              |
| 3:D:875:THR:HG22  | 3:D:879:ARG:HB2   | 1.90                     | 0.51              |
| 5:F:368:VAL:HG13  | 5:F:388:ALA:O     | 2.11                     | 0.51              |
| 1:K:17:GLY:HA3    | 8:K:1202:HOH:O    | 2.09                     | 0.51              |
| 1:L:120:VAL:HG23  | 8:L:4092:HOH:O    | 2.10                     | 0.51              |
| 2:M:341:THR:HB    | 2:M:345:ARG:NH2   | 2.26                     | 0.51              |
| 2:M:396:ASP:OD1   | 2:M:402:SER:HB2   | 2.10                     | 0.51              |
| 2:M:480:THR:HA    | 8:M:9505:HOH:O    | 2.10                     | 0.51              |
| 3:N:12:LEU:HD11   | 3:N:104:PHE:HE1   | 1.75                     | 0.51              |
| 3:N:14:SER:HB3    | 3:N:511:TRP:CE2   | 2.45                     | 0.51              |
| 3:N:22:SER:OG     | 3:N:91:GLY:HA2    | 2.10                     | 0.51              |
| 3:N:162:ARG:HA    | 3:N:449:SER:HB3   | 1.92                     | 0.51              |
| 3:N:814:ALA:O     | 3:N:818:ARG:HG3   | 2.11                     | 0.51              |
| 3:N:1379:VAL:HG11 | 3:N:1395:LEU:HD23 | 1.92                     | 0.51              |
| 5:P:367:MET:HA    | 5:P:370:LYS:HD3   | 1.93                     | 0.51              |
| 2:C:108:ILE:HD13  | 8:C:9686:HOH:O    | 2.09                     | 0.51              |
| 2:C:127:PHE:O     | 2:C:133:ASP:HA    | 2.11                     | 0.51              |
| 2:C:197:LEU:CD1   | 2:C:207:LEU:HD21  | 2.41                     | 0.51              |
| 2:C:250:ARG:NE    | 2:C:253:ALA:CB    | 2.73                     | 0.51              |
| 2:C:332:ARG:HE    | 2:C:464:LEU:HD11  | 1.76                     | 0.51              |
| 2:C:648:ARG:HB2   | 8:C:9859:HOH:O    | 2.09                     | 0.51              |
| 2:C:1067:TYR:CG   | 5:F:341:PRO:HB3   | 2.46                     | 0.51              |
| 3:D:36:THR:HG22   | 3:D:38:LYS:HG3    | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:152:LEU:HD21  | 8:D:2093:HOH:O    | 2.11                     | 0.51              |
| 3:D:432:TYR:HA    | 3:D:448:GLU:O     | 2.11                     | 0.51              |
| 3:D:1215:VAL:HB   | 8:D:9589:HOH:O    | 2.09                     | 0.51              |
| 5:F:372:ARG:O     | 5:F:377:ASP:O     | 2.29                     | 0.51              |
| 8:L:4017:HOH:O    | 3:N:851:LEU:HD11  | 2.11                     | 0.51              |
| 2:M:178:PRO:HB3   | 8:M:9974:HOH:O    | 2.10                     | 0.51              |
| 2:M:244:PRO:HD2   | 2:M:245:GLY:N     | 2.18                     | 0.51              |
| 2:M:707:ARG:CZ    | 2:M:824:ARG:HH12  | 2.24                     | 0.51              |
| 3:N:95:LEU:HD11   | 3:N:517:VAL:HG23  | 1.92                     | 0.51              |
| 3:N:96:ALA:H      | 3:N:551:ASN:ND2   | 2.09                     | 0.51              |
| 3:N:96:ALA:N      | 3:N:551:ASN:ND2   | 2.59                     | 0.51              |
| 3:N:510:GLU:O     | 3:N:513:ILE:HD12  | 2.11                     | 0.51              |
| 3:N:550:ARG:HD3   | 3:N:573:MET:HE3   | 1.92                     | 0.51              |
| 3:N:1144:LEU:HD22 | 8:N:2033:HOH:O    | 2.10                     | 0.51              |
| 5:P:306:GLU:O     | 5:P:310:ILE:HG13  | 2.10                     | 0.51              |
| 5:P:372:ARG:NH2   | 8:P:9689:HOH:O    | 2.44                     | 0.51              |
| 1:B:19:GLU:HG3    | 1:B:201:THR:O     | 2.11                     | 0.51              |
| 1:B:108:GLU:HB3   | 1:B:128:HIS:HE1   | 1.76                     | 0.51              |
| 2:C:110:GLU:H     | 2:C:368:THR:HG21  | 1.76                     | 0.51              |
| 2:C:686:ASP:O     | 3:D:740:PHE:HB2   | 2.11                     | 0.51              |
| 2:C:689:VAL:HB    | 2:C:870:ILE:HD12  | 1.93                     | 0.51              |
| 2:C:848:VAL:HB    | 3:D:740:PHE:O     | 2.10                     | 0.51              |
| 2:C:1083:GLU:O    | 2:C:1087:VAL:HG23 | 2.10                     | 0.51              |
| 3:D:601:ARG:HH22  | 3:D:611:GLN:HB2   | 1.75                     | 0.51              |
| 2:M:252:LYS:HG2   | 2:M:296:GLY:HA2   | 1.93                     | 0.51              |
| 2:M:266:ARG:HA    | 8:M:9486:HOH:O    | 2.10                     | 0.51              |
| 2:M:552:HIS:CE1   | 2:M:886:LEU:HD13  | 2.45                     | 0.51              |
| 2:M:599:GLU:HG3   | 2:M:600:ASP:OD2   | 2.11                     | 0.51              |
| 2:M:604:ALA:HB3   | 2:M:612:VAL:O     | 2.10                     | 0.51              |
| 2:M:643:VAL:HG13  | 2:M:647:GLN:CD    | 2.36                     | 0.51              |
| 2:M:707:ARG:CD    | 2:M:824:ARG:HH11  | 2.24                     | 0.51              |
| 2:M:787:ASP:HA    | 8:M:2208:HOH:O    | 2.10                     | 0.51              |
| 3:N:47:GLU:HA     | 3:N:51:GLY:O      | 2.10                     | 0.51              |
| 3:N:107:ASP:HB2   | 8:N:9484:HOH:O    | 2.09                     | 0.51              |
| 3:N:404:GLU:HB2   | 3:N:414:ARG:NH2   | 2.26                     | 0.51              |
| 3:N:459:GLU:HB2   | 8:N:9942:HOH:O    | 2.11                     | 0.51              |
| 3:N:1242:HIS:CE1  | 3:N:1266:ARG:HD2  | 2.45                     | 0.51              |
| 3:N:1274:ILE:CG1  | 3:N:1334:GLN:HE21 | 2.22                     | 0.51              |
| 4:O:54:LEU:O      | 4:O:54:LEU:HD23   | 2.10                     | 0.51              |
| 5:P:82:ARG:HB3    | 8:P:9558:HOH:O    | 2.09                     | 0.51              |
| 2:C:4:LYS:HA      | 8:C:9926:HOH:O    | 2.11                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:290:LEU:HB2   | 8:C:9836:HOH:O    | 2.10                     | 0.51              |
| 2:C:476:GLY:C     | 2:C:478:VAL:H     | 2.19                     | 0.51              |
| 2:C:832:LYS:HD2   | 8:C:2228:HOH:O    | 2.11                     | 0.51              |
| 3:D:66:GLN:O      | 3:D:67:ARG:C      | 2.53                     | 0.51              |
| 3:D:402:PRO:HG2   | 3:D:444:VAL:HG11  | 1.93                     | 0.51              |
| 3:D:416:ALA:HB2   | 8:D:9825:HOH:O    | 2.10                     | 0.51              |
| 3:D:650:LEU:HD12  | 3:D:657:LEU:HD23  | 1.93                     | 0.51              |
| 3:D:1127:GLU:HB2  | 8:D:2519:HOH:O    | 2.11                     | 0.51              |
| 3:D:1459:LEU:HD11 | 3:D:1468:LEU:HD12 | 1.91                     | 0.51              |
| 5:F:254:GLN:HB3   | 8:F:9518:HOH:O    | 2.09                     | 0.51              |
| 1:K:30:ARG:HA     | 8:K:1905:HOH:O    | 2.10                     | 0.51              |
| 2:M:383:ARG:CZ    | 8:M:9872:HOH:O    | 2.58                     | 0.51              |
| 2:M:640:ARG:HB3   | 2:M:640:ARG:HH11  | 1.74                     | 0.51              |
| 2:M:751:PRO:HA    | 2:M:792:VAL:HG12  | 1.93                     | 0.51              |
| 3:N:77:GLY:O      | 3:N:78:VAL:HG23   | 2.11                     | 0.51              |
| 3:N:466:LYS:CG    | 3:N:510:GLU:HG2   | 2.41                     | 0.51              |
| 3:N:754:PHE:HA    | 4:O:24:ALA:HB1    | 1.93                     | 0.51              |
| 3:N:850:LEU:HD22  | 3:N:884:ARG:HH22  | 1.75                     | 0.51              |
| 5:P:148:LYS:O     | 5:P:148:LYS:HG2   | 2.11                     | 0.51              |
| 1:A:127:LEU:HD12  | 1:A:128:HIS:N     | 2.26                     | 0.51              |
| 1:A:177:VAL:HG12  | 8:A:9451:HOH:O    | 2.09                     | 0.51              |
| 1:A:222:LEU:HD21  | 1:B:218:LEU:HD23  | 1.93                     | 0.51              |
| 2:C:461:VAL:CG1   | 2:C:465:GLY:HA2   | 2.31                     | 0.51              |
| 3:D:434:ARG:HB2   | 3:D:447:VAL:CG1   | 2.41                     | 0.51              |
| 3:D:907:GLU:HG3   | 8:D:2030:HOH:O    | 2.10                     | 0.51              |
| 3:D:1104:GLU:HA   | 3:D:1461:GLY:HA2  | 1.92                     | 0.51              |
| 3:D:1364:HIS:NE2  | 3:D:1366:LYS:HE3  | 2.26                     | 0.51              |
| 1:K:173:PRO:O     | 1:K:201:THR:HG23  | 2.11                     | 0.51              |
| 2:M:34:VAL:HG22   | 8:M:2159:HOH:O    | 2.10                     | 0.51              |
| 2:M:263:ASP:CB    | 2:M:264:PRO:HD3   | 2.39                     | 0.51              |
| 2:M:285:LEU:HD13  | 2:M:302:VAL:HG23  | 1.93                     | 0.51              |
| 2:M:906:PHE:CB    | 3:N:1067:VAL:HG22 | 2.41                     | 0.51              |
| 3:N:17:LYS:HG2    | 8:N:9686:HOH:O    | 2.10                     | 0.51              |
| 3:N:81:THR:HB     | 3:N:85:VAL:HG22   | 1.93                     | 0.51              |
| 3:N:519:VAL:HG13  | 3:N:544:TYR:CZ    | 2.46                     | 0.51              |
| 3:N:768:ASN:HB3   | 8:N:2357:HOH:O    | 2.10                     | 0.51              |
| 3:N:850:LEU:HD22  | 3:N:884:ARG:NH2   | 2.26                     | 0.51              |
| 3:N:873:LEU:HD11  | 8:N:2008:HOH:O    | 2.10                     | 0.51              |
| 1:A:77:GLU:HG3    | 8:A:9496:HOH:O    | 2.10                     | 0.50              |
| 1:A:154:GLU:H     | 1:A:154:GLU:CD    | 2.20                     | 0.50              |
| 2:C:70:GLU:OE1    | 2:C:97:ARG:HD3    | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:170:PRO:HG2   | 2:C:258:TYR:HD2   | 1.76                     | 0.50              |
| 2:C:419:THR:HG22  | 8:C:2202:HOH:O    | 2.11                     | 0.50              |
| 2:C:471:TYR:CE2   | 2:C:496:ILE:HG21  | 2.46                     | 0.50              |
| 2:C:897:LEU:HB3   | 2:C:899:GLN:CD    | 2.36                     | 0.50              |
| 2:C:1013:TYR:CE1  | 2:C:1020:PRO:HG3  | 2.45                     | 0.50              |
| 2:C:1115:LEU:HD12 | 2:C:1115:LEU:N    | 2.17                     | 0.50              |
| 2:C:1115:LEU:HD23 | 3:D:85:VAL:CG1    | 2.40                     | 0.50              |
| 3:D:34:TYR:CD1    | 3:D:35:ARG:N      | 2.79                     | 0.50              |
| 3:D:659:LYS:HD3   | 3:D:659:LYS:O     | 2.11                     | 0.50              |
| 3:D:868:TYR:HE1   | 3:D:869:MET:SD    | 2.33                     | 0.50              |
| 4:E:48:MET:HG2    | 8:E:9382:HOH:O    | 2.11                     | 0.50              |
| 5:F:163:LEU:HB3   | 5:F:174:LEU:CD1   | 2.41                     | 0.50              |
| 2:M:164:PRO:HA    | 2:M:266:ARG:HH12  | 1.76                     | 0.50              |
| 2:M:264:PRO:HG3   | 8:M:9995:HOH:O    | 2.10                     | 0.50              |
| 2:M:304:LEU:HB3   | 2:M:305:PRO:HD3   | 1.93                     | 0.50              |
| 2:M:334:ARG:HD3   | 2:M:339:LEU:HD21  | 1.94                     | 0.50              |
| 2:M:1040:LEU:CD2  | 2:M:1048:THR:HG22 | 2.41                     | 0.50              |
| 2:M:1092:LEU:HD23 | 2:M:1099:VAL:CG1  | 2.37                     | 0.50              |
| 3:N:181:ASP:HB2   | 8:N:2389:HOH:O    | 2.11                     | 0.50              |
| 3:N:820:GLU:HB3   | 3:N:836:VAL:HG21  | 1.93                     | 0.50              |
| 4:O:42:PRO:HD3    | 8:O:3641:HOH:O    | 2.11                     | 0.50              |
| 5:P:278:LEU:CB    | 5:P:286:PRO:HG2   | 2.41                     | 0.50              |
| 1:B:57:TYR:HE1    | 1:B:163:ASN:HB2   | 1.76                     | 0.50              |
| 2:C:98:LEU:O      | 2:C:109:LYS:HG3   | 2.11                     | 0.50              |
| 2:C:232:GLU:HG3   | 8:C:9807:HOH:O    | 2.10                     | 0.50              |
| 2:C:798:GLY:H     | 2:C:827:VAL:HG11  | 1.75                     | 0.50              |
| 5:F:377:ASP:O     | 5:F:378:GLY:C     | 2.53                     | 0.50              |
| 1:K:72:LYS:HA     | 8:M:9524:HOH:O    | 2.11                     | 0.50              |
| 1:L:132:LEU:CD2   | 1:L:138:LEU:HD22  | 2.40                     | 0.50              |
| 1:L:180:GLN:OE1   | 1:L:198:ARG:NH2   | 2.33                     | 0.50              |
| 2:M:254:VAL:HG22  | 8:M:2121:HOH:O    | 2.10                     | 0.50              |
| 2:M:355:VAL:HG13  | 2:M:356:ARG:N     | 2.26                     | 0.50              |
| 2:M:946:ARG:HD2   | 2:M:984:GLU:HB2   | 1.94                     | 0.50              |
| 2:M:986:PRO:C     | 2:M:987:ILE:HD13  | 2.35                     | 0.50              |
| 3:N:937:TYR:HA    | 3:N:940:THR:OG1   | 2.12                     | 0.50              |
| 3:N:1074:SER:HA   | 8:N:9822:HOH:O    | 2.10                     | 0.50              |
| 3:N:1118:ILE:HD12 | 3:N:1346:ARG:HE   | 1.76                     | 0.50              |
| 3:N:1249:ALA:HB3  | 8:N:2022:HOH:O    | 2.10                     | 0.50              |
| 3:N:1304:LYS:HD3  | 3:N:1304:LYS:N    | 2.16                     | 0.50              |
| 3:N:1491:THR:HG21 | 4:O:89:MET:SD     | 2.51                     | 0.50              |
| 5:P:358:LEU:HD23  | 5:P:358:LEU:C     | 2.35                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:412:GLU:OE1   | 5:P:412:GLU:HA    | 2.10                     | 0.50              |
| 2:C:134:ARG:HH12  | 2:C:392:SER:C     | 2.20                     | 0.50              |
| 2:C:162:ILE:O     | 2:C:164:PRO:HD2   | 2.11                     | 0.50              |
| 2:C:615:TYR:HB2   | 2:C:617:ASP:OD1   | 2.11                     | 0.50              |
| 3:D:671:LYS:HG2   | 8:F:9767:HOH:O    | 2.12                     | 0.50              |
| 3:D:711:LEU:CD1   | 3:D:778:LEU:HD23  | 2.42                     | 0.50              |
| 3:D:1422:MET:CE   | 3:D:1427:SER:HA   | 2.41                     | 0.50              |
| 5:F:88:ILE:HG21   | 5:F:193:ARG:HD3   | 1.94                     | 0.50              |
| 5:F:339:PRO:HB3   | 5:F:343:ASP:HB2   | 1.93                     | 0.50              |
| 2:M:10:ARG:NH1    | 8:M:9832:HOH:O    | 2.43                     | 0.50              |
| 2:M:472:ARG:NH2   | 8:M:9697:HOH:O    | 2.43                     | 0.50              |
| 2:M:516:ARG:CZ    | 3:N:1068:LEU:HD22 | 2.41                     | 0.50              |
| 2:M:1003:ASP:O    | 2:M:1005:MET:N    | 2.44                     | 0.50              |
| 3:N:85:VAL:HG12   | 8:N:9574:HOH:O    | 2.12                     | 0.50              |
| 3:N:125:GLN:CD    | 3:N:587:ARG:HH21  | 2.19                     | 0.50              |
| 3:N:127:LEU:CD1   | 3:N:457:GLY:H     | 2.24                     | 0.50              |
| 3:N:737:ASN:C     | 8:N:9496:HOH:O    | 2.53                     | 0.50              |
| 3:N:1148:VAL:HG12 | 3:N:1189:ARG:HG3  | 1.92                     | 0.50              |
| 5:P:372:ARG:NH2   | 8:P:9523:HOH:O    | 2.44                     | 0.50              |
| 1:B:101:LEU:HD23  | 1:B:101:LEU:C     | 2.37                     | 0.50              |
| 2:C:158:TYR:O     | 2:C:310:LEU:HD11  | 2.12                     | 0.50              |
| 2:C:194:VAL:HG22  | 2:C:221:LEU:HD12  | 1.93                     | 0.50              |
| 2:C:578:VAL:HG23  | 2:C:579:VAL:HG12  | 1.93                     | 0.50              |
| 2:C:582:GLY:N     | 2:C:584:GLU:OE2   | 2.44                     | 0.50              |
| 3:D:55:ASP:O      | 3:D:82:LYS:HA     | 2.11                     | 0.50              |
| 3:D:113:GLY:HA3   | 3:D:124:GLU:OE2   | 2.11                     | 0.50              |
| 3:D:513:ILE:HG13  | 8:D:9594:HOH:O    | 2.11                     | 0.50              |
| 3:D:566:ILE:HG22  | 5:F:214:GLN:HE22  | 1.77                     | 0.50              |
| 3:D:704:ARG:HD2   | 3:D:705:ALA:H     | 1.76                     | 0.50              |
| 3:D:864:VAL:HG12  | 3:D:865:THR:N     | 2.26                     | 0.50              |
| 5:F:133:ALA:O     | 5:F:137:GLY:O     | 2.29                     | 0.50              |
| 5:F:262:VAL:O     | 5:F:266:GLU:HG3   | 2.12                     | 0.50              |
| 1:K:2:LEU:HD22    | 8:K:3063:HOH:O    | 2.12                     | 0.50              |
| 2:M:257:VAL:HG22  | 8:M:9999:HOH:O    | 2.10                     | 0.50              |
| 2:M:393:GLN:NE2   | 2:M:409:ARG:NH1   | 2.60                     | 0.50              |
| 2:M:474:VAL:HG13  | 2:M:530:GLU:O     | 2.11                     | 0.50              |
| 2:M:738:ASP:O     | 2:M:739:GLU:C     | 2.52                     | 0.50              |
| 2:M:817:PRO:C     | 2:M:819:VAL:H     | 2.20                     | 0.50              |
| 3:N:30:GLU:HB3    | 3:N:40:GLU:HB3    | 1.93                     | 0.50              |
| 3:N:214:GLU:HG2   | 3:N:215:TYR:CE1   | 2.46                     | 0.50              |
| 3:N:729:HIS:HE1   | 3:N:731:LEU:HG    | 1.75                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1381:VAL:HG23 | 3:N:1391:GLU:HB2  | 1.92                     | 0.50              |
| 1:A:70:GLY:H      | 2:C:607:ASP:CG    | 2.19                     | 0.50              |
| 2:C:59:LYS:HE3    | 8:C:9798:HOH:O    | 2.09                     | 0.50              |
| 2:C:678:PRO:HB2   | 3:D:942:SER:OG    | 2.11                     | 0.50              |
| 2:C:1015:LEU:N    | 5:F:333:ILE:O     | 2.44                     | 0.50              |
| 2:C:1067:TYR:HE2  | 5:F:345:ALA:HB2   | 1.77                     | 0.50              |
| 3:D:36:THR:O      | 3:D:38:LYS:N      | 2.44                     | 0.50              |
| 3:D:119:SER:HB2   | 3:D:123:LEU:CB    | 2.41                     | 0.50              |
| 3:D:404:GLU:HB3   | 3:D:414:ARG:HD3   | 1.92                     | 0.50              |
| 3:D:788:GLY:O     | 3:D:792:ILE:HG22  | 2.11                     | 0.50              |
| 3:D:902:LEU:HD23  | 8:D:2567:HOH:O    | 2.10                     | 0.50              |
| 3:D:1161:GLU:HG2  | 3:D:1164:ARG:HB2  | 1.93                     | 0.50              |
| 3:D:1242:HIS:CE1  | 3:D:1266:ARG:HD3  | 2.47                     | 0.50              |
| 3:D:1379:VAL:HG13 | 3:D:1395:LEU:HB2  | 1.93                     | 0.50              |
| 1:L:58:ILE:HG21   | 1:L:68:ILE:HD11   | 1.92                     | 0.50              |
| 1:L:108:GLU:HB2   | 8:L:2022:HOH:O    | 2.10                     | 0.50              |
| 2:M:242:LEU:HD12  | 8:M:9620:HOH:O    | 2.11                     | 0.50              |
| 2:M:398:THR:HA    | 2:M:633:GLN:HG3   | 1.93                     | 0.50              |
| 2:M:503:LEU:HD21  | 2:M:508:ILE:HD13  | 1.94                     | 0.50              |
| 2:M:717:LEU:HD11  | 2:M:763:GLY:O     | 2.10                     | 0.50              |
| 3:N:28:LYS:HD2    | 3:N:41:ARG:HD2    | 1.94                     | 0.50              |
| 3:N:804:LEU:C     | 3:N:804:LEU:HD12  | 2.37                     | 0.50              |
| 3:N:1232:PRO:HB3  | 3:N:1361:VAL:CG2  | 2.41                     | 0.50              |
| 5:P:282:LEU:HB3   | 5:P:284:ARG:HB2   | 1.94                     | 0.50              |
| 5:P:356:LYS:HD3   | 8:P:9751:HOH:O    | 2.10                     | 0.50              |
| 1:A:47:SER:CB     | 1:A:217:ILE:HD13  | 2.42                     | 0.50              |
| 1:A:156:HIS:CD2   | 1:A:157:GLY:N     | 2.79                     | 0.50              |
| 1:B:76:VAL:HA     | 1:B:79:ILE:HG12   | 1.92                     | 0.50              |
| 1:B:132:LEU:HB3   | 8:B:9645:HOH:O    | 2.10                     | 0.50              |
| 1:B:133:GLU:CG    | 1:B:134:GLU:H     | 2.18                     | 0.50              |
| 2:C:288:ARG:NE    | 2:C:288:ARG:CA    | 2.75                     | 0.50              |
| 2:C:516:ARG:HD2   | 3:D:1068:LEU:HD22 | 1.94                     | 0.50              |
| 2:C:854:PRO:C     | 2:C:856:GLU:N     | 2.69                     | 0.50              |
| 3:D:47:GLU:OE1    | 3:D:59:ALA:HB2    | 2.11                     | 0.50              |
| 3:D:68:PHE:CD2    | 3:D:68:PHE:N      | 2.80                     | 0.50              |
| 3:D:477:LEU:HD21  | 3:D:495:ARG:HH11  | 1.77                     | 0.50              |
| 3:D:488:ARG:HB3   | 8:D:2340:HOH:O    | 2.10                     | 0.50              |
| 3:D:724:GLN:NE2   | 8:D:9936:HOH:O    | 2.44                     | 0.50              |
| 3:D:858:VAL:HG11  | 3:D:864:VAL:HG21  | 1.93                     | 0.50              |
| 5:F:151:LEU:HB2   | 5:F:155:THR:HB    | 1.93                     | 0.50              |
| 5:F:373:LYS:HE2   | 8:F:9560:HOH:O    | 2.12                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:443:THR:HG21  | 2:M:450:GLY:H    | 1.76                     | 0.50              |
| 2:M:493:ARG:HD3   | 8:M:9690:HOH:O   | 2.11                     | 0.50              |
| 2:M:897:LEU:HB3   | 2:M:899:GLN:HG2  | 1.94                     | 0.50              |
| 3:N:45:PHE:HD1    | 3:N:86:ARG:NH2   | 2.03                     | 0.50              |
| 3:N:169:TYR:CG    | 3:N:169:TYR:O    | 2.65                     | 0.50              |
| 3:N:425:GLY:HA3   | 5:P:135:ILE:CD1  | 2.31                     | 0.50              |
| 3:N:456:MET:C     | 8:N:9942:HOH:O   | 2.55                     | 0.50              |
| 3:N:495:ARG:O     | 3:N:495:ARG:HG2  | 2.11                     | 0.50              |
| 3:N:1353:GLN:HE21 | 3:N:1357:ARG:HE  | 1.54                     | 0.50              |
| 5:P:271:LEU:HD23  | 5:P:295:MET:HG3  | 1.93                     | 0.50              |
| 1:B:6:LEU:C       | 1:B:8:ALA:N      | 2.70                     | 0.50              |
| 1:B:17:GLY:HA2    | 8:B:9562:HOH:O   | 2.11                     | 0.50              |
| 2:C:184:MET:SD    | 2:C:196:LEU:HD13 | 2.52                     | 0.50              |
| 2:C:374:ASN:O     | 2:C:377:PRO:HD2  | 2.12                     | 0.50              |
| 2:C:432:ARG:HD3   | 2:C:432:ARG:H    | 1.76                     | 0.50              |
| 2:C:1004:LYS:O    | 2:C:1006:HIS:ND1 | 2.45                     | 0.50              |
| 3:D:410:SER:CB    | 3:D:414:ARG:HH21 | 2.25                     | 0.50              |
| 3:D:704:ARG:CD    | 3:D:705:ALA:H    | 2.25                     | 0.50              |
| 3:D:1105:ILE:HD11 | 3:D:1374:GLN:OE1 | 2.11                     | 0.50              |
| 5:F:141:VAL:HG13  | 5:F:142:ARG:N    | 2.25                     | 0.50              |
| 1:K:101:LEU:HB2   | 1:K:114:PHE:CD2  | 2.46                     | 0.50              |
| 1:L:27:PRO:HG2    | 1:L:186:LEU:HD12 | 1.94                     | 0.50              |
| 1:L:206:THR:HB    | 1:L:209:GLU:CD   | 2.36                     | 0.50              |
| 3:N:166:GLN:HG3   | 3:N:168:THR:OG1  | 2.12                     | 0.50              |
| 3:N:826:PRO:O     | 3:N:836:VAL:HG13 | 2.12                     | 0.50              |
| 3:N:1145:TYR:CD2  | 3:N:1168:MET:HE3 | 2.46                     | 0.50              |
| 5:P:129:GLU:CB    | 5:P:142:ARG:HH22 | 2.22                     | 0.50              |
| 5:P:287:THR:C     | 5:P:289:GLU:H    | 2.20                     | 0.50              |
| 2:C:53:PRO:HG2    | 8:C:9708:HOH:O   | 2.10                     | 0.50              |
| 2:C:181:VAL:HG12  | 2:C:182:VAL:N    | 2.26                     | 0.50              |
| 3:D:139:GLY:CA    | 3:D:452:ILE:HD12 | 2.38                     | 0.50              |
| 3:D:813:LEU:HD12  | 3:D:814:ALA:N    | 2.27                     | 0.50              |
| 3:D:920:LEU:HD11  | 8:D:9608:HOH:O   | 2.12                     | 0.50              |
| 8:D:9740:HOH:O    | 5:F:136:LEU:HD21 | 2.12                     | 0.50              |
| 4:E:54:LEU:HA     | 4:E:58:PRO:HG2   | 1.93                     | 0.50              |
| 5:F:346:THR:CG2   | 5:F:422:LEU:HB3  | 2.40                     | 0.50              |
| 1:K:224:TYR:CD2   | 1:L:9:PRO:HG2    | 2.46                     | 0.50              |
| 2:M:95:TYR:HD2    | 2:M:114:PHE:HB3  | 1.72                     | 0.50              |
| 2:M:98:LEU:O      | 2:M:109:LYS:HG3  | 2.12                     | 0.50              |
| 2:M:674:VAL:HB    | 2:M:869:VAL:HG13 | 1.93                     | 0.50              |
| 2:M:839:LEU:HD21  | 2:M:849:VAL:HG22 | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:1008:ARG:HD2  | 2:M:1027:PHE:O    | 2.12                     | 0.50              |
| 3:N:54:LYS:HD3    | 3:N:57:GLU:CB     | 2.40                     | 0.50              |
| 3:N:75:ARG:HD3    | 8:N:9538:HOH:O    | 2.11                     | 0.50              |
| 3:N:207:PHE:HB2   | 8:N:9756:HOH:O    | 2.11                     | 0.50              |
| 3:N:452:ILE:HG21  | 8:N:9771:HOH:O    | 2.12                     | 0.50              |
| 3:N:502:PHE:CZ    | 3:N:1452:ILE:HG13 | 2.45                     | 0.50              |
| 3:N:617:ASN:C     | 3:N:619:LEU:N     | 2.67                     | 0.50              |
| 3:N:1209:LEU:O    | 3:N:1210:SER:C    | 2.52                     | 0.50              |
| 4:O:64:ALA:C      | 8:O:3627:HOH:O    | 2.53                     | 0.50              |
| 5:P:74:LYS:HD3    | 8:P:9694:HOH:O    | 2.12                     | 0.50              |
| 1:A:195:LEU:HD12  | 1:A:196:THR:H     | 1.76                     | 0.50              |
| 2:C:178:PRO:HA    | 8:C:9721:HOH:O    | 2.12                     | 0.50              |
| 2:C:397:GLU:H     | 2:C:633:GLN:CD    | 2.19                     | 0.50              |
| 2:C:444:PRO:HB2   | 2:C:448:ASN:O     | 2.12                     | 0.50              |
| 2:C:472:ARG:HD2   | 2:C:480:THR:O     | 2.11                     | 0.50              |
| 2:C:988:VAL:HG12  | 3:D:948:THR:OG1   | 2.12                     | 0.50              |
| 2:C:1021:LEU:HD22 | 5:F:331:ASP:O     | 2.12                     | 0.50              |
| 2:C:1043:TYR:CE2  | 3:D:710:ARG:HD3   | 2.47                     | 0.50              |
| 3:D:169:TYR:N     | 3:D:170:PRO:HD3   | 2.26                     | 0.50              |
| 3:D:376:GLU:HA    | 3:D:384:VAL:HA    | 1.94                     | 0.50              |
| 3:D:728:LEU:HD12  | 3:D:729:HIS:H     | 1.77                     | 0.50              |
| 3:D:986:ARG:NH1   | 8:D:2314:HOH:O    | 2.44                     | 0.50              |
| 3:D:1211:MET:HG2  | 3:D:1213:ARG:HD2  | 1.94                     | 0.50              |
| 3:D:1472:ILE:HA   | 8:D:9619:HOH:O    | 2.10                     | 0.50              |
| 3:D:1478:SER:OG   | 3:D:1480:PHE:HB3  | 2.12                     | 0.50              |
| 5:F:129:GLU:HB3   | 5:F:142:ARG:NH2   | 2.27                     | 0.50              |
| 1:L:112:ARG:HB2   | 8:L:5359:HOH:O    | 2.10                     | 0.50              |
| 1:L:116:PRO:HG3   | 8:L:726:HOH:O     | 2.10                     | 0.50              |
| 1:L:146:ARG:HD2   | 8:L:1866:HOH:O    | 2.11                     | 0.50              |
| 2:M:404:LEU:O     | 2:M:408:ARG:HG2   | 2.11                     | 0.50              |
| 2:M:599:GLU:HG3   | 2:M:600:ASP:H     | 1.77                     | 0.50              |
| 2:M:889:HIS:CD2   | 2:M:970:GLY:HA3   | 2.47                     | 0.50              |
| 3:N:118:LEU:O     | 3:N:120:ALA:N     | 2.44                     | 0.50              |
| 3:N:601:ARG:HE    | 3:N:605:ASP:HB3   | 1.77                     | 0.50              |
| 3:N:819:GLY:HA3   | 8:N:9847:HOH:O    | 2.11                     | 0.50              |
| 3:N:1031:ASN:HB3  | 3:N:1034:GLN:HB2  | 1.92                     | 0.50              |
| 3:N:1107:VAL:HG22 | 3:N:1200:VAL:HG12 | 1.93                     | 0.50              |
| 3:N:1236:LEU:HD22 | 3:N:1355:VAL:HG12 | 1.93                     | 0.50              |
| 3:N:1239:ARG:NH1  | 8:N:9974:HOH:O    | 2.41                     | 0.50              |
| 3:N:1304:LYS:H    | 3:N:1304:LYS:CD   | 2.16                     | 0.50              |
| 3:N:1350:GLU:HB3  | 8:N:9495:HOH:O    | 2.11                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:P:223:ALA:HB2   | 5:P:242:TRP:HB2  | 1.94                     | 0.50              |
| 5:P:295:MET:HB3   | 5:P:299:TRP:CD1  | 2.47                     | 0.50              |
| 1:A:101:LEU:HB2   | 1:A:114:PHE:CD2  | 2.47                     | 0.49              |
| 1:B:42:ARG:HG2    | 1:B:42:ARG:NH1   | 2.20                     | 0.49              |
| 2:C:502:PRO:HB2   | 2:C:509:ALA:HB3  | 1.94                     | 0.49              |
| 2:C:739:GLU:HA    | 8:C:2058:HOH:O   | 2.11                     | 0.49              |
| 2:C:971:LYS:HE3   | 8:C:9513:HOH:O   | 2.11                     | 0.49              |
| 2:C:1035:MET:HG3  | 2:C:1038:TRP:CZ3 | 2.47                     | 0.49              |
| 2:C:1038:TRP:HZ2  | 3:D:1096:ARG:HD2 | 1.76                     | 0.49              |
| 3:D:47:GLU:HA     | 3:D:51:GLY:O     | 2.11                     | 0.49              |
| 3:D:191:LEU:CB    | 3:D:195:VAL:HG21 | 2.29                     | 0.49              |
| 3:D:194:GLY:H     | 3:D:206:ARG:HA   | 1.77                     | 0.49              |
| 3:D:470:LEU:HB2   | 3:D:503:LEU:HD11 | 1.93                     | 0.49              |
| 3:D:710:ARG:CG    | 3:D:711:LEU:HD23 | 2.37                     | 0.49              |
| 3:D:1207:TYR:O    | 3:D:1213:ARG:O   | 2.30                     | 0.49              |
| 3:D:1327:ARG:NH2  | 8:D:2130:HOH:O   | 2.45                     | 0.49              |
| 3:D:1459:LEU:HD11 | 3:D:1468:LEU:CD1 | 2.41                     | 0.49              |
| 5:F:79:ASP:HB3    | 5:F:80:PRO:CD    | 2.42                     | 0.49              |
| 5:F:94:LEU:HD12   | 5:F:97:GLU:HB2   | 1.94                     | 0.49              |
| 5:F:316:SER:C     | 5:F:318:GLU:N    | 2.64                     | 0.49              |
| 1:K:86:VAL:HG11   | 8:K:5289:HOH:O   | 2.11                     | 0.49              |
| 1:L:123:MET:O     | 1:L:125:PRO:HD3  | 2.11                     | 0.49              |
| 1:L:196:THR:HG23  | 1:L:196:THR:O    | 2.11                     | 0.49              |
| 2:M:504:GLU:CB    | 2:M:507:ARG:HD2  | 2.41                     | 0.49              |
| 3:N:123:LEU:CD2   | 3:N:152:LEU:HD22 | 2.37                     | 0.49              |
| 3:N:465:LEU:CD2   | 3:N:468:LEU:HD11 | 2.34                     | 0.49              |
| 3:N:1201:CYS:SG   | 3:N:1202:GLN:N   | 2.85                     | 0.49              |
| 3:N:1236:LEU:HD21 | 3:N:1356:TYR:HD2 | 1.76                     | 0.49              |
| 3:N:1377:LYS:HE2  | 3:N:1378:TYR:CE1 | 2.47                     | 0.49              |
| 5:P:82:ARG:HD2    | 8:P:9475:HOH:O   | 2.12                     | 0.49              |
| 5:P:163:LEU:HD13  | 5:P:174:LEU:HD21 | 1.93                     | 0.49              |
| 5:P:205:ARG:CG    | 5:P:251:ILE:HD13 | 2.41                     | 0.49              |
| 5:P:214:GLN:O     | 5:P:217:ASN:HB2  | 2.11                     | 0.49              |
| 5:P:316:SER:C     | 5:P:318:GLU:H    | 2.19                     | 0.49              |
| 5:P:396:ARG:O     | 5:P:399:GLN:HB2  | 2.12                     | 0.49              |
| 1:B:196:THR:HG23  | 1:B:196:THR:O    | 2.12                     | 0.49              |
| 2:C:41:ASN:HD22   | 2:C:41:ASN:H     | 1.59                     | 0.49              |
| 2:C:723:THR:C     | 2:C:725:ASP:H    | 2.20                     | 0.49              |
| 2:C:757:GLY:HA2   | 2:C:789:SER:HB3  | 1.94                     | 0.49              |
| 2:C:780:GLU:HG3   | 2:C:781:LYS:H    | 1.77                     | 0.49              |
| 2:C:885:ILE:HG23  | 3:D:949:ILE:O    | 2.10                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:107:ASP:O     | 3:D:108:VAL:C     | 2.55                     | 0.49              |
| 3:D:141:ILE:CD1   | 3:D:449:SER:HA    | 2.38                     | 0.49              |
| 3:D:153:LEU:HD12  | 3:D:158:TYR:HB2   | 1.94                     | 0.49              |
| 3:D:989:TYR:CZ    | 3:D:993:LEU:HD11  | 2.46                     | 0.49              |
| 3:D:1272:ALA:HA   | 3:D:1326:THR:HB   | 1.94                     | 0.49              |
| 5:F:94:LEU:CD1    | 5:F:96:LEU:H      | 2.19                     | 0.49              |
| 5:F:158:GLU:HA    | 5:F:161:GLN:CD    | 2.37                     | 0.49              |
| 5:F:278:LEU:CB    | 5:F:286:PRO:HG2   | 2.42                     | 0.49              |
| 5:F:303:ARG:HA    | 8:F:9545:HOH:O    | 2.12                     | 0.49              |
| 1:L:91:ASN:OD1    | 1:L:93:SER:HB2    | 2.13                     | 0.49              |
| 2:M:697:ARG:O     | 2:M:699:PHE:N     | 2.44                     | 0.49              |
| 2:M:782:ALA:HB2   | 8:M:2224:HOH:O    | 2.11                     | 0.49              |
| 2:M:1031:ARG:HG2  | 3:N:621:LYS:O     | 2.12                     | 0.49              |
| 3:N:8:VAL:O       | 3:N:1434:TRP:HH2  | 1.95                     | 0.49              |
| 3:N:107:ASP:HA    | 8:N:2416:HOH:O    | 2.11                     | 0.49              |
| 3:N:140:ALA:HA    | 8:N:9588:HOH:O    | 2.12                     | 0.49              |
| 3:N:890:VAL:O     | 3:N:890:VAL:HG23  | 2.12                     | 0.49              |
| 3:N:1280:VAL:HG13 | 3:N:1316:GLY:O    | 2.11                     | 0.49              |
| 3:N:1372:VAL:HG13 | 3:N:1375:MET:HE2  | 1.94                     | 0.49              |
| 5:P:120:THR:HG22  | 5:P:122:LEU:HD13  | 1.94                     | 0.49              |
| 5:P:163:LEU:CD2   | 5:P:174:LEU:HG    | 2.36                     | 0.49              |
| 5:P:416:ARG:NH1   | 5:P:419:ARG:HB3   | 2.27                     | 0.49              |
| 2:C:136:ILE:HG22  | 2:C:336:VAL:HG22  | 1.93                     | 0.49              |
| 2:C:625:LEU:HB3   | 2:C:639:GLN:HB2   | 1.92                     | 0.49              |
| 2:C:704:HIS:HB3   | 2:C:831:ARG:NH1   | 2.27                     | 0.49              |
| 2:C:710:ILE:CD1   | 2:C:790:LEU:HB2   | 2.36                     | 0.49              |
| 2:C:1042:ALA:HB2  | 3:D:1223:ILE:HG22 | 1.94                     | 0.49              |
| 3:D:565:ILE:H     | 3:D:565:ILE:HD12  | 1.76                     | 0.49              |
| 3:D:671:LYS:HE3   | 5:F:421:PHE:O     | 2.12                     | 0.49              |
| 3:D:683:ILE:HG22  | 3:D:687:VAL:CG2   | 2.39                     | 0.49              |
| 3:D:728:LEU:HD22  | 3:D:745:MET:HE1   | 1.93                     | 0.49              |
| 3:D:1092:GLY:O    | 3:D:1096:ARG:HD3  | 2.11                     | 0.49              |
| 1:L:137:ARG:HH12  | 1:L:139:ASN:HB2   | 1.75                     | 0.49              |
| 2:M:64:LEU:HD22   | 2:M:359:MET:CG    | 2.37                     | 0.49              |
| 2:M:197:LEU:HA    | 2:M:200:LEU:HD12  | 1.94                     | 0.49              |
| 2:M:283:ILE:HA    | 8:M:9830:HOH:O    | 2.12                     | 0.49              |
| 2:M:352:ALA:CA    | 2:M:355:VAL:HG12  | 2.40                     | 0.49              |
| 2:M:496:ILE:O     | 2:M:515:ALA:HB1   | 2.12                     | 0.49              |
| 2:M:564:MET:SD    | 2:M:846:LYS:HD2   | 2.53                     | 0.49              |
| 2:M:683:ASN:ND2   | 2:M:872:ASN:HB2   | 2.27                     | 0.49              |
| 3:N:97:THR:CG2    | 3:N:571:LYS:HD3   | 2.42                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:107:ASP:O     | 3:N:108:VAL:C     | 2.55                     | 0.49              |
| 3:N:547:LEU:HD11  | 3:N:578:VAL:HG22  | 1.93                     | 0.49              |
| 3:N:1286:THR:CG2  | 3:N:1287:GLU:H    | 2.24                     | 0.49              |
| 3:N:1396:GLU:O    | 3:N:1400:VAL:HG23 | 2.13                     | 0.49              |
| 5:P:276:ARG:HH11  | 5:P:276:ARG:HG3   | 1.78                     | 0.49              |
| 1:B:91:ASN:HB2    | 1:B:92:PRO:HD2    | 1.94                     | 0.49              |
| 2:C:833:LEU:HD11  | 2:C:849:VAL:HG21  | 1.95                     | 0.49              |
| 2:C:1007:ALA:O    | 2:C:1027:PHE:HD2  | 1.96                     | 0.49              |
| 2:C:1058:ASP:HB2  | 3:D:621:LYS:HE3   | 1.94                     | 0.49              |
| 3:D:28:LYS:HD3    | 3:D:41:ARG:HD2    | 1.93                     | 0.49              |
| 3:D:65:ARG:HD3    | 5:F:374:GLY:O     | 2.12                     | 0.49              |
| 3:D:418:GLY:HA3   | 8:D:9466:HOH:O    | 2.12                     | 0.49              |
| 3:D:495:ARG:HD2   | 8:D:2090:HOH:O    | 2.12                     | 0.49              |
| 3:D:571:LYS:HB2   | 3:D:571:LYS:NZ    | 2.26                     | 0.49              |
| 3:D:806:PHE:O     | 3:D:806:PHE:CD1   | 2.65                     | 0.49              |
| 3:D:829:VAL:H     | 3:D:835:SER:HB2   | 1.78                     | 0.49              |
| 3:D:939:PHE:O     | 3:D:942:SER:HB3   | 2.12                     | 0.49              |
| 3:D:1164:ARG:NH2  | 3:D:1170:ASP:OD1  | 2.45                     | 0.49              |
| 3:D:1284:GLU:HB3  | 8:D:2537:HOH:O    | 2.10                     | 0.49              |
| 3:D:1389:LEU:H    | 3:D:1389:LEU:CD2  | 2.12                     | 0.49              |
| 3:D:1476:THR:HG23 | 4:E:21:VAL:HG22   | 1.93                     | 0.49              |
| 1:K:169:ALA:HB1   | 1:K:171:PHE:CZ    | 2.47                     | 0.49              |
| 2:M:290:LEU:H     | 2:M:290:LEU:CD2   | 2.13                     | 0.49              |
| 2:M:375:SER:H     | 5:P:279:GLN:HE22  | 1.61                     | 0.49              |
| 2:M:523:ILE:HD13  | 8:M:2099:HOH:O    | 2.12                     | 0.49              |
| 2:M:650:ARG:HB2   | 8:M:9572:HOH:O    | 2.12                     | 0.49              |
| 2:M:728:HIS:CE1   | 2:M:775:ARG:NH1   | 2.81                     | 0.49              |
| 2:M:897:LEU:CB    | 2:M:899:GLN:HE21  | 2.21                     | 0.49              |
| 2:M:1066:ALA:O    | 2:M:1070:ILE:HG13 | 2.11                     | 0.49              |
| 3:N:421:LEU:HD12  | 3:N:435:VAL:CG1   | 2.42                     | 0.49              |
| 3:N:559:ALA:HB3   | 8:N:9490:HOH:O    | 2.12                     | 0.49              |
| 3:N:1357:ARG:HD2  | 8:N:9692:HOH:O    | 2.12                     | 0.49              |
| 3:N:1403:LEU:O    | 3:N:1407:LEU:HB2  | 2.11                     | 0.49              |
| 4:O:51:LEU:CG     | 4:O:53:GLY:H      | 2.17                     | 0.49              |
| 5:P:156:VAL:HG12  | 8:P:9471:HOH:O    | 2.11                     | 0.49              |
| 1:A:30:ARG:HH12   | 1:B:155:LYS:NZ    | 2.02                     | 0.49              |
| 2:C:352:ALA:C     | 2:C:355:VAL:HG12  | 2.37                     | 0.49              |
| 2:C:501:THR:O     | 2:C:503:LEU:HD23  | 2.13                     | 0.49              |
| 2:C:944:LEU:HD22  | 2:C:962:GLN:OE1   | 2.13                     | 0.49              |
| 3:D:165:LYS:HD2   | 8:D:2157:HOH:O    | 2.12                     | 0.49              |
| 3:D:168:THR:HB    | 3:D:393:ILE:CG1   | 2.42                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:572:ARG:HE    | 5:F:80:PRO:HG3   | 1.77                     | 0.49              |
| 3:D:573:MET:SD    | 5:F:210:LEU:HB3  | 2.52                     | 0.49              |
| 3:D:1089:ALA:HA   | 8:D:2088:HOH:O   | 2.11                     | 0.49              |
| 3:D:1280:VAL:HG13 | 3:D:1316:GLY:O   | 2.13                     | 0.49              |
| 5:F:361:LEU:CD2   | 5:F:404:ALA:HB1  | 2.43                     | 0.49              |
| 1:K:33:GLY:O      | 1:K:195:LEU:HD22 | 2.13                     | 0.49              |
| 1:K:61:VAL:HG11   | 1:K:75:VAL:HG21  | 1.93                     | 0.49              |
| 1:K:183:ASP:OD1   | 2:M:938:LYS:HE3  | 2.13                     | 0.49              |
| 2:M:41:ASN:C      | 2:M:41:ASN:HD22  | 2.21                     | 0.49              |
| 2:M:204:GLN:OE1   | 2:M:222:MET:HB3  | 2.12                     | 0.49              |
| 3:N:438:ASP:OD2   | 3:N:440:VAL:HB   | 2.12                     | 0.49              |
| 3:N:921:ARG:HG2   | 8:N:9891:HOH:O   | 2.11                     | 0.49              |
| 3:N:1457:ASP:C    | 3:N:1457:ASP:OD1 | 2.55                     | 0.49              |
| 3:N:1462:LEU:HD21 | 3:N:1474:ALA:HB2 | 1.93                     | 0.49              |
| 5:P:288:TYR:C     | 5:P:291:ILE:HG22 | 2.37                     | 0.49              |
| 2:C:73:LEU:CD2    | 2:C:94:LEU:HB2   | 2.42                     | 0.49              |
| 2:C:109:LYS:HE3   | 8:C:9787:HOH:O   | 2.12                     | 0.49              |
| 2:C:141:HIS:O     | 2:C:332:ARG:N    | 2.44                     | 0.49              |
| 2:C:276:LYS:O     | 2:C:280:LYS:HG3  | 2.12                     | 0.49              |
| 2:C:1045:ALA:HB1  | 2:C:1048:THR:HB  | 1.93                     | 0.49              |
| 3:D:445:ARG:HG2   | 3:D:445:ARG:HH11 | 1.77                     | 0.49              |
| 3:D:473:LEU:HD11  | 3:D:495:ARG:NH2  | 2.27                     | 0.49              |
| 3:D:669:ASN:O     | 3:D:672:ALA:HB3  | 2.12                     | 0.49              |
| 3:D:1194:CYS:HB3  | 3:D:1373:ARG:CZ  | 2.42                     | 0.49              |
| 3:D:1389:LEU:HG   | 8:D:9868:HOH:O   | 2.12                     | 0.49              |
| 3:D:1432:LYS:HD2  | 3:D:1433:SER:N   | 2.27                     | 0.49              |
| 5:F:148:LYS:HA    | 8:F:9536:HOH:O   | 2.11                     | 0.49              |
| 1:L:139:ASN:HB3   | 8:L:1052:HOH:O   | 2.11                     | 0.49              |
| 1:L:176:ARG:HH22  | 3:N:884:ARG:NE   | 2.10                     | 0.49              |
| 2:M:413:LEU:H     | 2:M:413:LEU:HD12 | 1.77                     | 0.49              |
| 2:M:775:ARG:O     | 2:M:779:GLY:C    | 2.55                     | 0.49              |
| 3:N:177:ALA:CB    | 3:N:199:LEU:HD13 | 2.41                     | 0.49              |
| 3:N:212:ARG:HD3   | 3:N:394:LEU:HD13 | 1.95                     | 0.49              |
| 3:N:764:LEU:HD23  | 3:N:767:HIS:CD2  | 2.47                     | 0.49              |
| 3:N:1031:ASN:HB3  | 3:N:1034:GLN:CG  | 2.43                     | 0.49              |
| 5:P:94:LEU:HB3    | 5:P:98:GLU:HG3   | 1.95                     | 0.49              |
| 1:A:176:ARG:HG3   | 1:A:200:TRP:CE3  | 2.48                     | 0.49              |
| 1:A:187:GLY:HA2   | 8:A:9484:HOH:O   | 2.13                     | 0.49              |
| 2:C:139:GLN:HG3   | 2:C:411:SER:O    | 2.11                     | 0.49              |
| 2:C:209:ARG:HB3   | 8:C:9869:HOH:O   | 2.12                     | 0.49              |
| 2:C:462:ASP:CG    | 2:C:463:GLU:N    | 2.71                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:496:ILE:O     | 2:C:515:ALA:HB1   | 2.13                     | 0.49              |
| 2:C:671:ASN:N     | 2:C:671:ASN:ND2   | 2.60                     | 0.49              |
| 2:C:721:ARG:HE    | 2:C:783:ARG:NH2   | 2.10                     | 0.49              |
| 2:C:826:TYR:CD1   | 2:C:826:TYR:N     | 2.81                     | 0.49              |
| 2:C:945:ARG:HB3   | 8:D:2414:HOH:O    | 2.12                     | 0.49              |
| 2:C:1083:GLU:OE2  | 3:D:87:ARG:HD2    | 2.13                     | 0.49              |
| 3:D:543:LEU:O     | 3:D:546:ARG:HB2   | 2.12                     | 0.49              |
| 3:D:964:LEU:HD22  | 3:D:1058:ARG:HH11 | 1.77                     | 0.49              |
| 3:D:1103:HIS:CD2  | 3:D:1463:LYS:H    | 2.30                     | 0.49              |
| 3:D:1209:LEU:O    | 3:D:1210:SER:C    | 2.53                     | 0.49              |
| 3:D:1434:TRP:CZ3  | 3:D:1457:ASP:HB2  | 2.48                     | 0.49              |
| 3:D:1443:THR:HG23 | 8:D:2144:HOH:O    | 2.13                     | 0.49              |
| 1:K:159:LYS:HD3   | 8:K:4474:HOH:O    | 2.13                     | 0.49              |
| 1:L:26:GLU:HB3    | 1:L:194:LYS:HG3   | 1.94                     | 0.49              |
| 2:M:102:HIS:NE2   | 2:M:365:ASP:OD2   | 2.45                     | 0.49              |
| 2:M:288:ARG:HB3   | 8:M:9987:HOH:O    | 2.12                     | 0.49              |
| 2:M:585:GLU:HG3   | 2:M:665:PHE:HE2   | 1.77                     | 0.49              |
| 2:M:719:PRO:HB3   | 2:M:820:ARG:CD    | 2.43                     | 0.49              |
| 2:M:724:ARG:O     | 2:M:734:LEU:HD11  | 2.13                     | 0.49              |
| 2:M:734:LEU:HD13  | 2:M:737:LEU:HD13  | 1.94                     | 0.49              |
| 2:M:759:THR:HB    | 2:M:785:VAL:HG11  | 1.93                     | 0.49              |
| 2:M:767:PRO:HA    | 8:M:9989:HOH:O    | 2.11                     | 0.49              |
| 2:M:774:LEU:HD13  | 2:M:775:ARG:N     | 2.27                     | 0.49              |
| 2:M:1102:LEU:HD22 | 3:N:7:LYS:HD2     | 1.95                     | 0.49              |
| 3:N:99:ALA:HA     | 3:N:575:GLN:HE22  | 1.77                     | 0.49              |
| 3:N:162:ARG:HB2   | 8:N:9771:HOH:O    | 2.11                     | 0.49              |
| 3:N:1109:GLU:CG   | 3:N:1202:GLN:H    | 2.20                     | 0.49              |
| 3:N:1118:ILE:HD12 | 3:N:1346:ARG:NE   | 2.28                     | 0.49              |
| 3:N:1456:LYS:HD3  | 8:N:9815:HOH:O    | 2.13                     | 0.49              |
| 4:O:43:GLU:HG2    | 8:O:5067:HOH:O    | 2.11                     | 0.49              |
| 4:O:54:LEU:HD21   | 4:O:63:TRP:HE1    | 1.77                     | 0.49              |
| 1:B:184:THR:O     | 1:B:192:LEU:HB2   | 2.13                     | 0.49              |
| 2:C:154:ARG:O     | 2:C:156:GLY:N     | 2.46                     | 0.49              |
| 2:C:247:PRO:HB2   | 8:C:9690:HOH:O    | 2.12                     | 0.49              |
| 2:C:250:ARG:HE    | 2:C:253:ALA:CB    | 2.26                     | 0.49              |
| 2:C:260:LEU:CB    | 2:C:291:ALA:HB1   | 2.42                     | 0.49              |
| 2:C:876:VAL:N     | 2:C:877:PRO:HD2   | 2.27                     | 0.49              |
| 3:D:40:GLU:N      | 8:D:9464:HOH:O    | 2.45                     | 0.49              |
| 3:D:44:LEU:HB3    | 3:D:525:ARG:NH2   | 2.23                     | 0.49              |
| 3:D:131:LYS:HG2   | 3:D:568:ARG:CD    | 2.43                     | 0.49              |
| 3:D:893:GLU:O     | 3:D:896:ALA:HB3   | 2.12                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:1033:GLN:HG3  | 3:D:1036:ARG:NH1 | 2.28                     | 0.49              |
| 3:D:1149:LEU:HG   | 3:D:1166:LEU:CD2 | 2.42                     | 0.49              |
| 5:F:134:LYS:HG3   | 5:F:178:ARG:NH2  | 2.28                     | 0.49              |
| 5:F:137:GLY:HA3   | 5:F:140:ARG:NH1  | 2.25                     | 0.49              |
| 5:F:162:LYS:NZ    | 8:F:9643:HOH:O   | 2.46                     | 0.49              |
| 5:F:196:VAL:HG22  | 5:F:213:ILE:HG21 | 1.94                     | 0.49              |
| 5:F:325:LYS:NZ    | 8:F:9539:HOH:O   | 2.46                     | 0.49              |
| 5:F:370:LYS:HG2   | 5:F:371:LEU:N    | 2.28                     | 0.49              |
| 2:M:16:PRO:HB3    | 2:M:460:ARG:HD2  | 1.93                     | 0.49              |
| 2:M:479:VAL:HG21  | 2:M:503:LEU:HD11 | 1.95                     | 0.49              |
| 2:M:607:ASP:HB3   | 2:M:609:ASN:H    | 1.78                     | 0.49              |
| 2:M:737:LEU:HA    | 2:M:743:VAL:HA   | 1.94                     | 0.49              |
| 2:M:1032:PHE:CE2  | 2:M:1052:MET:HG2 | 2.48                     | 0.49              |
| 2:M:1063:ARG:O    | 2:M:1066:ALA:HB3 | 2.12                     | 0.49              |
| 3:N:36:THR:O      | 3:N:38:LYS:N     | 2.46                     | 0.49              |
| 3:N:477:LEU:CB    | 3:N:496:LEU:HD12 | 2.42                     | 0.49              |
| 3:N:601:ARG:CD    | 3:N:613:ARG:HH21 | 2.26                     | 0.49              |
| 3:N:676:MET:HE1   | 3:N:684:LYS:H    | 1.78                     | 0.49              |
| 3:N:785:ILE:HG23  | 3:N:938:GLY:HA3  | 1.95                     | 0.49              |
| 3:N:996:TRP:CE2   | 3:N:1056:PRO:HG2 | 2.48                     | 0.49              |
| 3:N:1042:ARG:NH1  | 3:N:1045:MET:SD  | 2.81                     | 0.49              |
| 3:N:1448:THR:HG21 | 8:N:9484:HOH:O   | 2.12                     | 0.49              |
| 1:A:57:TYR:HE1    | 1:A:163:ASN:HB2  | 1.77                     | 0.49              |
| 1:A:86:VAL:HG21   | 1:A:202:ASP:O    | 2.13                     | 0.49              |
| 1:B:47:SER:HB2    | 1:B:217:ILE:HD13 | 1.95                     | 0.49              |
| 2:C:604:ALA:HB2   | 8:C:9615:HOH:O   | 2.13                     | 0.49              |
| 2:C:683:ASN:ND2   | 2:C:872:ASN:HB2  | 2.28                     | 0.49              |
| 2:C:952:LEU:HD11  | 8:C:9620:HOH:O   | 2.13                     | 0.49              |
| 3:D:701:LEU:HD21  | 3:D:763:MET:CE   | 2.43                     | 0.49              |
| 3:D:1236:LEU:HA   | 3:D:1359:GLN:OE1 | 2.13                     | 0.49              |
| 3:D:1390:LEU:N    | 8:D:9868:HOH:O   | 2.45                     | 0.49              |
| 1:K:132:LEU:HD11  | 1:K:138:LEU:CD2  | 2.43                     | 0.49              |
| 1:L:7:LYS:HA      | 8:L:2136:HOH:O   | 2.12                     | 0.49              |
| 2:M:110:GLU:HG2   | 2:M:369:PRO:CG   | 2.32                     | 0.49              |
| 2:M:252:LYS:HZ3   | 2:M:296:GLY:HA3  | 1.77                     | 0.49              |
| 2:M:437:ARG:HA    | 2:M:467:ILE:HG21 | 1.94                     | 0.49              |
| 2:M:929:ARG:HG3   | 2:M:929:ARG:HH11 | 1.77                     | 0.49              |
| 2:M:1037:VAL:HG12 | 2:M:1041:GLU:CD  | 2.36                     | 0.49              |
| 3:N:11:ALA:HB1    | 3:N:507:ASN:CG   | 2.38                     | 0.49              |
| 3:N:550:ARG:HH11  | 3:N:550:ARG:HG3  | 1.78                     | 0.49              |
| 3:N:569:ASN:O     | 3:N:573:MET:HG3  | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:698:LYS:HA    | 3:N:756:GLN:HE21  | 1.77                     | 0.49              |
| 3:N:849:ALA:HB2   | 8:N:9489:HOH:O    | 2.12                     | 0.49              |
| 3:N:1020:LEU:HD21 | 3:N:1038:LEU:HD22 | 1.95                     | 0.49              |
| 3:N:1487:VAL:HG12 | 3:N:1488:ASP:N    | 2.28                     | 0.49              |
| 1:A:154:GLU:N     | 1:A:154:GLU:OE2   | 2.46                     | 0.49              |
| 2:C:333:ILE:HD11  | 2:C:410:ILE:HG21  | 1.95                     | 0.49              |
| 2:C:442:GLU:HG2   | 2:C:454:SER:CB    | 2.42                     | 0.49              |
| 2:C:492:ASP:CA    | 2:C:518:LYS:HB3   | 2.36                     | 0.49              |
| 2:C:1029:GLY:O    | 3:D:622:ARG:HD3   | 2.13                     | 0.49              |
| 2:C:1090:LYS:HB3  | 3:D:520:LEU:HD12  | 1.95                     | 0.49              |
| 3:D:205:TYR:HB3   | 3:D:393:ILE:HD13  | 1.94                     | 0.49              |
| 3:D:563:PRO:O     | 3:D:567:ILE:HG13  | 2.13                     | 0.49              |
| 3:D:806:PHE:O     | 3:D:807:ALA:C     | 2.55                     | 0.49              |
| 3:D:1047:LYS:HB3  | 3:D:1048:PRO:HD3  | 1.94                     | 0.49              |
| 3:D:1134:LEU:HD11 | 3:D:1179:GLU:HG2  | 1.95                     | 0.49              |
| 4:E:23:VAL:HG12   | 4:E:24:ALA:N      | 2.28                     | 0.49              |
| 2:M:184:MET:CE    | 2:M:186:VAL:HG22  | 2.43                     | 0.49              |
| 2:M:269:LEU:HD23  | 2:M:269:LEU:N     | 2.28                     | 0.49              |
| 2:M:290:LEU:HD22  | 2:M:302:VAL:CB    | 2.43                     | 0.49              |
| 2:M:554:ASP:HB3   | 2:M:880:MET:O     | 2.13                     | 0.49              |
| 2:M:929:ARG:HG3   | 2:M:929:ARG:NH1   | 2.28                     | 0.49              |
| 2:M:987:ILE:HD12  | 3:N:948:THR:HG21  | 1.95                     | 0.49              |
| 2:M:1038:TRP:NE1  | 3:N:1099:VAL:HG11 | 2.28                     | 0.49              |
| 2:M:1050:GLN:CG   | 2:M:1079:PRO:HG2  | 2.42                     | 0.49              |
| 2:M:1056:LYS:HB3  | 3:N:624:ASP:H     | 1.77                     | 0.49              |
| 2:M:1090:LYS:NZ   | 8:M:9629:HOH:O    | 2.46                     | 0.49              |
| 2:M:1109:VAL:HG22 | 3:N:3:LYS:CB      | 2.43                     | 0.49              |
| 3:N:55:ASP:HB3    | 3:N:82:LYS:HG2    | 1.95                     | 0.49              |
| 3:N:1209:LEU:HD21 | 4:O:16:LYS:HD2    | 1.95                     | 0.49              |
| 3:N:1243:THR:O    | 3:N:1269:LYS:CD   | 2.61                     | 0.49              |
| 5:P:160:ASP:O     | 5:P:163:LEU:HB2   | 2.12                     | 0.49              |
| 5:P:337:HIS:CE1   | 8:P:9510:HOH:O    | 2.65                     | 0.49              |
| 1:A:224:TYR:HB3   | 1:B:9:PRO:CB      | 2.43                     | 0.48              |
| 2:C:28:ARG:HG2    | 2:C:40:GLU:OE1    | 2.13                     | 0.48              |
| 2:C:63:GLY:HA3    | 2:C:103:LYS:CG    | 2.43                     | 0.48              |
| 2:C:176:VAL:HG12  | 2:C:182:VAL:HG12  | 1.94                     | 0.48              |
| 2:C:603:VAL:HG21  | 2:C:643:VAL:CG1   | 2.36                     | 0.48              |
| 2:C:679:PHE:CE1   | 2:C:870:ILE:HD13  | 2.48                     | 0.48              |
| 3:D:426:LYS:HE3   | 8:D:2232:HOH:O    | 2.13                     | 0.48              |
| 3:D:661:MET:HE1   | 3:D:677:LEU:HD21  | 1.95                     | 0.48              |
| 3:D:703:ASN:O     | 3:D:745:MET:HG2   | 2.12                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1066:THR:O    | 3:D:1070:TYR:HB2  | 2.13                     | 0.48              |
| 3:D:1166:LEU:N    | 3:D:1166:LEU:HD23 | 2.28                     | 0.48              |
| 4:E:74:VAL:HG13   | 8:E:9364:HOH:O    | 2.12                     | 0.48              |
| 5:F:288:TYR:HE2   | 5:F:305:GLU:HG3   | 1.78                     | 0.48              |
| 1:L:24:VAL:CG1    | 1:L:194:LYS:HE3   | 2.43                     | 0.48              |
| 2:M:418:LEU:HD22  | 2:M:418:LEU:N     | 2.28                     | 0.48              |
| 2:M:430:VAL:HG23  | 3:N:1078:ARG:NH2  | 2.28                     | 0.48              |
| 2:M:728:HIS:NE2   | 5:P:423:ASP:O     | 2.46                     | 0.48              |
| 2:M:782:ALA:O     | 2:M:784:ASP:N     | 2.45                     | 0.48              |
| 2:M:906:PHE:CE1   | 3:N:1067:VAL:HA   | 2.47                     | 0.48              |
| 2:M:939:ARG:HD3   | 2:M:982:PRO:HD3   | 1.95                     | 0.48              |
| 2:M:971:LYS:HD2   | 8:M:2221:HOH:O    | 2.13                     | 0.48              |
| 2:M:1087:VAL:HG22 | 8:M:9750:HOH:O    | 2.13                     | 0.48              |
| 3:N:715:ALA:O     | 3:N:764:LEU:HD12  | 2.12                     | 0.48              |
| 3:N:806:PHE:O     | 3:N:807:ALA:C     | 2.56                     | 0.48              |
| 5:P:95:THR:C      | 5:P:96:LEU:HD23   | 2.38                     | 0.48              |
| 5:P:142:ARG:HG3   | 8:P:9619:HOH:O    | 2.13                     | 0.48              |
| 5:P:274:THR:O     | 5:P:278:LEU:HG    | 2.13                     | 0.48              |
| 5:P:394:ARG:HG2   | 5:P:394:ARG:HH11  | 1.78                     | 0.48              |
| 1:A:151:VAL:HB    | 1:A:169:ALA:HB3   | 1.96                     | 0.48              |
| 2:C:257:VAL:C     | 2:C:259:GLY:N     | 2.69                     | 0.48              |
| 2:C:300:ASP:CG    | 2:C:300:ASP:O     | 2.55                     | 0.48              |
| 2:C:775:ARG:O     | 2:C:779:GLY:C     | 2.56                     | 0.48              |
| 2:C:1017:THR:OG1  | 2:C:1019:GLN:HG2  | 2.13                     | 0.48              |
| 2:C:1098:ASP:C    | 2:C:1098:ASP:OD1  | 2.56                     | 0.48              |
| 8:C:2291:HOH:O    | 3:D:859:ASP:HA    | 2.13                     | 0.48              |
| 3:D:1203:LYS:HE3  | 8:D:2355:HOH:O    | 2.12                     | 0.48              |
| 3:D:1264:GLU:HG2  | 3:D:1266:ARG:NH2  | 2.27                     | 0.48              |
| 1:K:123:MET:O     | 1:K:125:PRO:HD3   | 2.12                     | 0.48              |
| 1:L:19:GLU:HG3    | 1:L:201:THR:O     | 2.13                     | 0.48              |
| 2:M:257:VAL:C     | 2:M:259:GLY:H     | 2.20                     | 0.48              |
| 2:M:277:ALA:O     | 2:M:281:LEU:O     | 2.31                     | 0.48              |
| 2:M:309:TYR:O     | 2:M:313:LEU:N     | 2.40                     | 0.48              |
| 2:M:442:GLU:HG2   | 2:M:454:SER:CB    | 2.37                     | 0.48              |
| 2:M:754:ILE:HD13  | 2:M:791:ARG:HD3   | 1.96                     | 0.48              |
| 2:M:879:ARG:HD2   | 2:M:879:ARG:H     | 1.78                     | 0.48              |
| 3:N:9:ARG:HA      | 3:N:1434:TRP:CH2  | 2.48                     | 0.48              |
| 3:N:172:PRO:HB3   | 3:N:178:LEU:HD13  | 1.95                     | 0.48              |
| 3:N:769:LEU:CG    | 3:N:931:LEU:HD11  | 2.42                     | 0.48              |
| 3:N:871:LYS:HE2   | 8:N:2008:HOH:O    | 2.13                     | 0.48              |
| 3:N:1241:PHE:O    | 3:N:1257:PRO:HB3  | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:1302:GLU:HG3 | 8:N:9623:HOH:O   | 2.13                     | 0.48              |
| 3:N:1379:VAL:O   | 3:N:1392:GLY:HA2 | 2.12                     | 0.48              |
| 5:P:152:ASP:HB2  | 5:P:153:PRO:CD   | 2.37                     | 0.48              |
| 5:P:350:LEU:HD12 | 5:P:422:LEU:CB   | 2.42                     | 0.48              |
| 1:A:32:PHE:HZ    | 1:B:47:SER:HG    | 1.61                     | 0.48              |
| 1:A:191:ASP:O    | 1:A:192:LEU:HD23 | 2.13                     | 0.48              |
| 2:C:54:ILE:O     | 2:C:54:ILE:HG13  | 2.13                     | 0.48              |
| 2:C:88:LEU:N     | 2:C:88:LEU:HD23  | 2.29                     | 0.48              |
| 2:C:98:LEU:HA    | 8:C:9557:HOH:O   | 2.13                     | 0.48              |
| 2:C:193:LEU:CD1  | 2:C:307:LEU:HD22 | 2.43                     | 0.48              |
| 2:C:256:TYR:HD1  | 8:C:9480:HOH:O   | 1.96                     | 0.48              |
| 2:C:328:LEU:H    | 2:C:433:THR:HG21 | 1.76                     | 0.48              |
| 2:C:356:ARG:HD2  | 8:C:9550:HOH:O   | 2.12                     | 0.48              |
| 2:C:574:ALA:HB3  | 8:C:9508:HOH:O   | 2.13                     | 0.48              |
| 2:C:725:ASP:HB2  | 2:C:783:ARG:NH1  | 2.29                     | 0.48              |
| 2:C:939:ARG:CB   | 2:C:982:PRO:HG3  | 2.29                     | 0.48              |
| 2:C:1035:MET:HE1 | 8:C:2133:HOH:O   | 2.13                     | 0.48              |
| 3:D:65:ARG:CB    | 5:F:375:LEU:HG   | 2.44                     | 0.48              |
| 3:D:87:ARG:O     | 3:D:521:PRO:CB   | 2.48                     | 0.48              |
| 3:D:99:ALA:HA    | 3:D:575:GLN:HE22 | 1.78                     | 0.48              |
| 3:D:179:VAL:HG22 | 3:D:389:GLU:HG3  | 1.95                     | 0.48              |
| 3:D:653:PHE:CG   | 3:D:695:ILE:HD11 | 2.48                     | 0.48              |
| 3:D:772:PRO:HB3  | 3:D:1224:VAL:CG1 | 2.39                     | 0.48              |
| 3:D:786:ILE:HD11 | 3:D:908:LYS:CB   | 2.43                     | 0.48              |
| 3:D:808:THR:HB   | 3:D:809:PRO:CD   | 2.39                     | 0.48              |
| 3:D:826:PRO:CD   | 3:D:829:VAL:HG22 | 2.36                     | 0.48              |
| 3:D:1031:ASN:HB3 | 3:D:1034:GLN:HB2 | 1.95                     | 0.48              |
| 3:D:1047:LYS:HA  | 3:D:1053:PHE:CE1 | 2.47                     | 0.48              |
| 8:D:2111:HOH:O   | 4:E:11:GLY:HA2   | 2.14                     | 0.48              |
| 5:F:358:LEU:HG   | 5:F:367:MET:HE1  | 1.95                     | 0.48              |
| 1:K:198:ARG:HB2  | 1:K:200:TRP:CZ3  | 2.48                     | 0.48              |
| 2:M:719:PRO:HB3  | 2:M:820:ARG:HD2  | 1.95                     | 0.48              |
| 3:N:34:TYR:O     | 3:N:35:ARG:C     | 2.55                     | 0.48              |
| 3:N:421:LEU:HD11 | 3:N:437:VAL:HG22 | 1.94                     | 0.48              |
| 3:N:483:HIS:ND1  | 3:N:483:HIS:N    | 2.59                     | 0.48              |
| 3:N:807:ALA:HB3  | 8:N:2405:HOH:O   | 2.13                     | 0.48              |
| 3:N:939:PHE:O    | 3:N:942:SER:HB3  | 2.13                     | 0.48              |
| 3:N:1026:SER:C   | 3:N:1028:ALA:H   | 2.21                     | 0.48              |
| 5:P:79:ASP:HB3   | 5:P:80:PRO:CD    | 2.43                     | 0.48              |
| 1:A:169:ALA:HB1  | 1:A:171:PHE:CZ   | 2.48                     | 0.48              |
| 1:A:191:ASP:O    | 1:A:191:ASP:CG   | 2.57                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:96:ALA:HB2    | 8:C:9663:HOH:O   | 2.12                     | 0.48              |
| 2:C:773:LEU:O     | 2:C:777:ILE:HG13 | 2.14                     | 0.48              |
| 3:D:550:ARG:HH11  | 3:D:550:ARG:HG3  | 1.77                     | 0.48              |
| 3:D:781:PRO:O     | 3:D:786:ILE:HG13 | 2.13                     | 0.48              |
| 3:D:967:ALA:O     | 3:D:995:LEU:HD21 | 2.14                     | 0.48              |
| 3:D:1107:VAL:HA   | 3:D:1200:VAL:O   | 2.13                     | 0.48              |
| 3:D:1152:GLU:N    | 8:D:9602:HOH:O   | 2.46                     | 0.48              |
| 3:D:1460:ILE:HG12 | 8:D:9667:HOH:O   | 2.12                     | 0.48              |
| 1:K:67:THR:N      | 8:K:913:HOH:O    | 2.46                     | 0.48              |
| 1:L:7:LYS:O       | 1:L:7:LYS:HG2    | 2.14                     | 0.48              |
| 1:L:143:ARG:HH11  | 1:L:143:ARG:HG3  | 1.78                     | 0.48              |
| 1:L:216:GLU:OE2   | 1:L:219:ARG:CZ   | 2.61                     | 0.48              |
| 2:M:260:LEU:CB    | 2:M:291:ALA:HB1  | 2.43                     | 0.48              |
| 2:M:276:LYS:HG3   | 8:M:9622:HOH:O   | 2.13                     | 0.48              |
| 2:M:287:GLY:O     | 2:M:288:ARG:C    | 2.56                     | 0.48              |
| 2:M:328:LEU:HB2   | 2:M:433:THR:HG21 | 1.96                     | 0.48              |
| 2:M:595:LEU:HD21  | 2:M:623:TYR:HB3  | 1.95                     | 0.48              |
| 3:N:101:HIS:HD2   | 3:N:582:LEU:CD1  | 2.24                     | 0.48              |
| 3:N:1150:ALA:O    | 3:N:1151:ARG:HD3 | 2.12                     | 0.48              |
| 3:N:1354:LYS:HB3  | 8:N:2203:HOH:O   | 2.14                     | 0.48              |
| 2:C:191:PHE:CZ    | 2:C:238:LEU:HD21 | 2.49                     | 0.48              |
| 2:C:577:PRO:HG3   | 2:C:993:PHE:CZ   | 2.49                     | 0.48              |
| 2:C:993:PHE:HB3   | 8:C:2157:HOH:O   | 2.13                     | 0.48              |
| 3:D:543:LEU:HB3   | 8:D:2488:HOH:O   | 2.13                     | 0.48              |
| 3:D:906:GLN:HB3   | 3:D:911:LEU:HD11 | 1.94                     | 0.48              |
| 3:D:1109:GLU:HA   | 8:D:9566:HOH:O   | 2.13                     | 0.48              |
| 3:D:1243:THR:HG22 | 3:D:1244:GLY:H   | 1.79                     | 0.48              |
| 3:D:1278:ASP:N    | 3:D:1278:ASP:OD1 | 2.46                     | 0.48              |
| 3:D:1354:LYS:HE2  | 8:D:2197:HOH:O   | 2.13                     | 0.48              |
| 5:F:274:THR:O     | 5:F:278:LEU:HG   | 2.13                     | 0.48              |
| 5:F:369:LEU:O     | 5:F:373:LYS:CG   | 2.61                     | 0.48              |
| 1:K:189:ARG:NH2   | 1:L:155:LYS:HD3  | 2.28                     | 0.48              |
| 1:L:59:GLU:OE1    | 1:L:137:ARG:NH1  | 2.46                     | 0.48              |
| 2:M:194:VAL:HG21  | 2:M:221:LEU:O    | 2.13                     | 0.48              |
| 2:M:578:VAL:HA    | 2:M:900:ARG:HD2  | 1.95                     | 0.48              |
| 2:M:705:ILE:HG22  | 2:M:705:ILE:O    | 2.12                     | 0.48              |
| 2:M:774:LEU:O     | 2:M:774:LEU:HD22 | 2.13                     | 0.48              |
| 3:N:138:LYS:H     | 3:N:138:LYS:CD   | 2.07                     | 0.48              |
| 3:N:142:LEU:HG    | 8:N:9766:HOH:O   | 2.13                     | 0.48              |
| 3:N:194:GLY:H     | 3:N:206:ARG:HA   | 1.77                     | 0.48              |
| 4:O:48:MET:HB2    | 4:O:48:MET:HE3   | 1.74                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:94:LEU:HB2    | 8:P:9522:HOH:O    | 2.14                     | 0.48              |
| 5:P:282:LEU:O     | 5:P:282:LEU:HD13  | 2.13                     | 0.48              |
| 5:P:384:GLU:O     | 5:P:388:ALA:N     | 2.46                     | 0.48              |
| 1:A:60:ASP:HB3    | 8:A:9497:HOH:O    | 2.14                     | 0.48              |
| 2:C:428:ARG:HA    | 2:C:450:GLY:HA3   | 1.94                     | 0.48              |
| 2:C:1100:GLN:HE21 | 2:C:1100:GLN:HB2  | 1.49                     | 0.48              |
| 3:D:481:MET:SD    | 3:D:1388:ARG:HG3  | 2.53                     | 0.48              |
| 3:D:500:ARG:NH2   | 3:D:1388:ARG:HD3  | 2.29                     | 0.48              |
| 3:D:543:LEU:HA    | 3:D:546:ARG:CG    | 2.44                     | 0.48              |
| 3:D:651:GLU:OE1   | 3:D:651:GLU:HA    | 2.12                     | 0.48              |
| 4:E:47:LYS:HG3    | 8:E:9443:HOH:O    | 2.12                     | 0.48              |
| 5:F:331:ASP:HB2   | 8:F:9658:HOH:O    | 2.12                     | 0.48              |
| 2:M:200:LEU:HD13  | 2:M:300:ASP:OD2   | 2.14                     | 0.48              |
| 2:M:233:GLU:OE2   | 2:M:237:ARG:HD3   | 2.13                     | 0.48              |
| 2:M:247:PRO:HB2   | 8:M:2200:HOH:O    | 2.13                     | 0.48              |
| 2:M:336:VAL:CA    | 2:M:339:LEU:HD12  | 2.42                     | 0.48              |
| 2:M:377:PRO:HG3   | 8:M:9526:HOH:O    | 2.13                     | 0.48              |
| 2:M:568:ALA:CB    | 2:M:668:LEU:HB3   | 2.43                     | 0.48              |
| 2:M:880:MET:HE2   | 3:N:1034:GLN:HG2  | 1.94                     | 0.48              |
| 3:N:14:SER:HB3    | 3:N:511:TRP:CZ2   | 2.49                     | 0.48              |
| 3:N:819:GLY:O     | 3:N:822:ALA:HB3   | 2.13                     | 0.48              |
| 4:O:16:LYS:HD3    | 4:O:17:TYR:CE1    | 2.49                     | 0.48              |
| 4:O:52:GLU:OE2    | 4:O:52:GLU:HA     | 2.14                     | 0.48              |
| 4:O:73:LEU:N      | 8:O:690:HOH:O     | 2.46                     | 0.48              |
| 5:P:266:GLU:HG2   | 8:P:9618:HOH:O    | 2.14                     | 0.48              |
| 1:A:14:ARG:HH22   | 1:A:24:VAL:HG23   | 1.78                     | 0.48              |
| 1:A:107:LYS:HG2   | 1:A:108:GLU:N     | 2.28                     | 0.48              |
| 1:A:198:ARG:HH22  | 2:C:932:GLU:CB    | 2.21                     | 0.48              |
| 2:C:100:LEU:CD2   | 2:C:368:THR:HA    | 2.38                     | 0.48              |
| 2:C:198:ARG:HD2   | 8:C:9779:HOH:O    | 2.13                     | 0.48              |
| 2:C:760:SER:O     | 2:C:786:LYS:N     | 2.35                     | 0.48              |
| 3:D:191:LEU:HD22  | 3:D:195:VAL:CG1   | 2.44                     | 0.48              |
| 3:D:669:ASN:ND2   | 3:D:672:ALA:HB2   | 2.28                     | 0.48              |
| 1:K:18:ARG:HH12   | 1:K:88:ARG:HE     | 1.62                     | 0.48              |
| 2:M:44:ILE:O      | 2:M:48:PHE:HB2    | 2.14                     | 0.48              |
| 2:M:357:GLU:HA    | 8:M:2296:HOH:O    | 2.13                     | 0.48              |
| 2:M:445:GLU:CD    | 2:M:560:MET:HE3   | 2.39                     | 0.48              |
| 2:M:731:GLU:HB3   | 8:M:9529:HOH:O    | 2.13                     | 0.48              |
| 2:M:840:ALA:HB2   | 2:M:846:LYS:HA    | 1.95                     | 0.48              |
| 2:M:875:GLY:HA2   | 2:M:879:ARG:HH11  | 1.77                     | 0.48              |
| 2:M:1054:THR:HG22 | 2:M:1055:LEU:HD23 | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:79:GLU:HG2    | 3:N:80:VAL:N      | 2.28                     | 0.48              |
| 3:N:477:LEU:HD11  | 3:N:495:ARG:HD3   | 1.95                     | 0.48              |
| 3:N:1171:VAL:O    | 3:N:1171:VAL:HG12 | 2.12                     | 0.48              |
| 3:N:1243:THR:HG22 | 8:N:9796:HOH:O    | 2.14                     | 0.48              |
| 3:N:1286:THR:N    | 8:N:2263:HOH:O    | 2.46                     | 0.48              |
| 3:N:1339:LYS:HG2  | 3:N:1343:ALA:HB2  | 1.96                     | 0.48              |
| 5:P:76:SER:O      | 5:P:77:THR:C      | 2.56                     | 0.48              |
| 5:P:163:LEU:HB3   | 5:P:174:LEU:CG    | 2.40                     | 0.48              |
| 1:A:22:GLU:OE1    | 2:C:934:PHE:HZ    | 1.96                     | 0.48              |
| 2:C:274:ARG:NH2   | 2:C:284:ARG:HG2   | 2.28                     | 0.48              |
| 2:C:734:LEU:HA    | 2:C:737:LEU:CD1   | 2.42                     | 0.48              |
| 3:D:154:THR:HG22  | 3:D:155:ASP:N     | 2.28                     | 0.48              |
| 3:D:191:LEU:HD22  | 3:D:195:VAL:HG11  | 1.96                     | 0.48              |
| 3:D:510:GLU:HB2   | 3:D:511:TRP:CZ3   | 2.49                     | 0.48              |
| 3:D:526:PRO:HB2   | 5:F:317:LEU:CD1   | 2.43                     | 0.48              |
| 3:D:1026:SER:C    | 3:D:1028:ALA:H    | 2.22                     | 0.48              |
| 3:D:1202:GLN:HA   | 3:D:1215:VAL:CG1  | 2.44                     | 0.48              |
| 4:E:51:LEU:HG     | 4:E:53:GLY:N      | 2.19                     | 0.48              |
| 1:K:90:LEU:N      | 8:K:742:HOH:O     | 2.46                     | 0.48              |
| 1:L:126:ASP:HB2   | 8:L:919:HOH:O     | 2.13                     | 0.48              |
| 1:L:127:LEU:HD12  | 1:L:128:HIS:H     | 1.79                     | 0.48              |
| 1:L:206:THR:HG23  | 1:L:207:PRO:HD2   | 1.94                     | 0.48              |
| 2:M:43:GLY:HA2    | 2:M:341:THR:HG23  | 1.95                     | 0.48              |
| 2:M:76:PRO:HG2    | 8:M:2023:HOH:O    | 2.13                     | 0.48              |
| 2:M:89:THR:O      | 2:M:91:GLN:HG3    | 2.13                     | 0.48              |
| 2:M:203:ASP:O     | 2:M:207:LEU:HB2   | 2.13                     | 0.48              |
| 2:M:444:PRO:HB2   | 8:M:9543:HOH:O    | 2.12                     | 0.48              |
| 2:M:603:VAL:HG23  | 2:M:647:GLN:O     | 2.14                     | 0.48              |
| 2:M:726:ILE:HD11  | 2:M:737:LEU:CD1   | 2.43                     | 0.48              |
| 2:M:790:LEU:C     | 2:M:790:LEU:HD12  | 2.39                     | 0.48              |
| 2:M:860:HIS:NE2   | 2:M:975:TYR:HB2   | 2.29                     | 0.48              |
| 2:M:881:ASN:HD22  | 2:M:881:ASN:H     | 1.61                     | 0.48              |
| 2:M:1109:VAL:HG11 | 3:N:5:VAL:HG22    | 1.95                     | 0.48              |
| 3:N:98:PRO:HG3    | 3:N:515:GLU:HB3   | 1.94                     | 0.48              |
| 3:N:108:VAL:HB    | 3:N:109:PRO:HD3   | 1.95                     | 0.48              |
| 3:N:527:MET:HE1   | 3:N:537:THR:HB    | 1.94                     | 0.48              |
| 3:N:695:ILE:O     | 3:N:696:HIS:C     | 2.57                     | 0.48              |
| 3:N:785:ILE:H     | 3:N:785:ILE:CD1   | 2.27                     | 0.48              |
| 3:N:1096:ARG:HH11 | 3:N:1096:ARG:CB   | 2.26                     | 0.48              |
| 3:N:1489:GLN:O    | 3:N:1493:LYS:HG2  | 2.13                     | 0.48              |
| 3:N:1499:ARG:HD3  | 8:N:9594:HOH:O    | 2.13                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:P:371:LEU:HD22  | 5:P:375:LEU:HD12 | 1.95                     | 0.48              |
| 1:B:20:TYR:HE1    | 8:B:9522:HOH:O   | 1.97                     | 0.48              |
| 2:C:159:ILE:HG22  | 2:C:175:GLU:HG3  | 1.95                     | 0.48              |
| 2:C:282:GLY:HA2   | 2:C:308:ARG:HH21 | 1.79                     | 0.48              |
| 2:C:313:LEU:HD12  | 2:C:313:LEU:O    | 2.13                     | 0.48              |
| 2:C:451:LEU:HB3   | 8:C:9584:HOH:O   | 2.12                     | 0.48              |
| 2:C:493:ARG:HA    | 8:C:2274:HOH:O   | 2.14                     | 0.48              |
| 2:C:708:TYR:N     | 2:C:708:TYR:CD1  | 2.82                     | 0.48              |
| 2:C:911:GLU:HB3   | 2:C:912:PRO:HD3  | 1.96                     | 0.48              |
| 2:C:1087:VAL:HG12 | 2:C:1091:GLU:OE1 | 2.14                     | 0.48              |
| 3:D:119:SER:H     | 3:D:123:LEU:HD13 | 1.79                     | 0.48              |
| 3:D:212:ARG:HB2   | 3:D:445:ARG:HH22 | 1.77                     | 0.48              |
| 3:D:397:LYS:CE    | 3:D:399:ARG:HE   | 2.27                     | 0.48              |
| 3:D:809:PRO:HB2   | 3:D:812:ALA:CB   | 2.44                     | 0.48              |
| 3:D:901:GLN:HG3   | 8:D:9734:HOH:O   | 2.14                     | 0.48              |
| 3:D:1092:GLY:O    | 3:D:1096:ARG:N   | 2.47                     | 0.48              |
| 3:D:1198:TYR:OH   | 3:D:1397:LYS:HE3 | 2.13                     | 0.48              |
| 3:D:1225:ALA:HA   | 3:D:1367:HIS:ND1 | 2.29                     | 0.48              |
| 4:E:24:ALA:O      | 4:E:28:GLN:HG3   | 2.14                     | 0.48              |
| 5:F:102:LEU:O     | 5:F:106:VAL:HG23 | 2.13                     | 0.48              |
| 5:F:325:LYS:HB2   | 8:F:9479:HOH:O   | 2.14                     | 0.48              |
| 5:F:363:GLU:HG2   | 5:F:364:ARG:N    | 2.28                     | 0.48              |
| 5:F:367:MET:HA    | 5:F:370:LYS:HD3  | 1.95                     | 0.48              |
| 1:L:214:ALA:HA    | 1:L:217:ILE:HD12 | 1.96                     | 0.48              |
| 2:M:26:TYR:CE2    | 2:M:30:LEU:HD21  | 2.49                     | 0.48              |
| 3:N:41:ARG:O      | 3:N:42:ASP:C     | 2.57                     | 0.48              |
| 3:N:116:LEU:C     | 3:N:118:LEU:HD13 | 2.39                     | 0.48              |
| 3:N:470:LEU:HB2   | 8:N:9989:HOH:O   | 2.13                     | 0.48              |
| 3:N:553:ARG:NH1   | 3:N:573:MET:HE1  | 2.29                     | 0.48              |
| 3:N:567:ILE:HG22  | 3:N:571:LYS:HZ2  | 1.79                     | 0.48              |
| 3:N:699:VAL:CG2   | 3:N:760:ARG:HB3  | 2.43                     | 0.48              |
| 3:N:780:LYS:HD3   | 3:N:912:LYS:HG3  | 1.95                     | 0.48              |
| 3:N:809:PRO:HB2   | 3:N:812:ALA:HB2  | 1.95                     | 0.48              |
| 3:N:1046:GLN:N    | 8:N:9803:HOH:O   | 2.46                     | 0.48              |
| 3:N:1057:VAL:HG13 | 3:N:1069:GLU:HB3 | 1.96                     | 0.48              |
| 3:N:1281:VAL:HG23 | 3:N:1317:ASP:O   | 2.14                     | 0.48              |
| 4:O:50:THR:HG23   | 8:O:1851:HOH:O   | 2.14                     | 0.48              |
| 5:P:408:LEU:HD23  | 5:P:408:LEU:C    | 2.39                     | 0.48              |
| 1:A:206:THR:CG2   | 1:A:209:GLU:H    | 2.23                     | 0.48              |
| 1:B:109:VAL:HG23  | 1:B:132:LEU:HD13 | 1.96                     | 0.48              |
| 1:B:182:GLU:O     | 1:B:194:LYS:HB3  | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:21:ILE:H     | 2:C:21:ILE:HD12  | 1.79                     | 0.48              |
| 2:C:79:PRO:O     | 2:C:83:CYS:SG    | 2.69                     | 0.48              |
| 2:C:195:LEU:HD12 | 2:C:234:ALA:HB1  | 1.96                     | 0.48              |
| 2:C:355:VAL:HG13 | 2:C:356:ARG:N    | 2.28                     | 0.48              |
| 2:C:605:LYS:HB3  | 2:C:610:ARG:HH12 | 1.79                     | 0.48              |
| 2:C:716:LYS:HD3  | 2:C:716:LYS:HA   | 1.70                     | 0.48              |
| 3:D:23:TYR:HB2   | 3:D:49:ILE:O     | 2.13                     | 0.48              |
| 3:D:31:THR:HG23  | 3:D:45:PHE:CE2   | 2.49                     | 0.48              |
| 3:D:87:ARG:HB2   | 3:D:523:ASP:HB2  | 1.94                     | 0.48              |
| 3:D:175:VAL:N    | 8:D:2366:HOH:O   | 2.44                     | 0.48              |
| 3:D:400:VAL:HG12 | 3:D:401:TYR:HD1  | 1.78                     | 0.48              |
| 3:D:549:ASN:ND2  | 5:F:254:GLN:NE2  | 2.62                     | 0.48              |
| 3:D:638:LYS:C    | 3:D:729:HIS:HD2  | 2.22                     | 0.48              |
| 3:D:705:ALA:HB3  | 3:D:706:PRO:CD   | 2.43                     | 0.48              |
| 3:D:891:GLU:O    | 3:D:893:GLU:N    | 2.46                     | 0.48              |
| 3:D:1087:ARG:NH1 | 3:D:1234:THR:O   | 2.46                     | 0.48              |
| 5:F:112:ALA:O    | 5:F:116:LEU:HG   | 2.13                     | 0.48              |
| 5:F:123:ASP:HB3  | 5:F:125:ASP:OD1  | 2.14                     | 0.48              |
| 1:K:9:PRO:CB     | 1:L:224:TYR:HB3  | 2.43                     | 0.48              |
| 2:M:11:GLU:HG2   | 2:M:537:LYS:HZ1  | 1.78                     | 0.48              |
| 2:M:114:PHE:CE1  | 5:P:283:GLY:HA3  | 2.48                     | 0.48              |
| 2:M:177:GLU:HG3  | 8:M:9679:HOH:O   | 2.13                     | 0.48              |
| 2:M:358:ARG:HH22 | 2:M:374:ASN:CG   | 2.21                     | 0.48              |
| 2:M:433:THR:O    | 2:M:435:TYR:N    | 2.47                     | 0.48              |
| 2:M:724:ARG:HG2  | 2:M:734:LEU:HD12 | 1.95                     | 0.48              |
| 3:N:827:ILE:HG22 | 3:N:837:GLY:CA   | 2.44                     | 0.48              |
| 3:N:1047:LYS:HG2 | 3:N:1053:PHE:CE2 | 2.49                     | 0.48              |
| 4:O:45:ARG:NH1   | 4:O:72:ARG:HH21  | 2.12                     | 0.48              |
| 5:P:252:ALA:HB1  | 5:P:265:VAL:HG21 | 1.96                     | 0.48              |
| 5:P:333:ILE:HA   | 5:P:334:PRO:HD3  | 1.77                     | 0.48              |
| 1:A:72:LYS:HE2   | 2:C:643:VAL:O    | 2.13                     | 0.47              |
| 2:C:35:PRO:HD2   | 2:C:38:LYS:HG2   | 1.95                     | 0.47              |
| 2:C:113:VAL:HB   | 2:C:115:LEU:HD23 | 1.95                     | 0.47              |
| 2:C:195:LEU:CD1  | 2:C:234:ALA:HB1  | 2.44                     | 0.47              |
| 2:C:403:SER:HB2  | 2:C:407:LYS:NZ   | 2.29                     | 0.47              |
| 2:C:443:THR:O    | 2:C:559:LEU:HD11 | 2.14                     | 0.47              |
| 2:C:458:TYR:CB   | 2:C:470:PRO:HG2  | 2.38                     | 0.47              |
| 2:C:780:GLU:HG3  | 2:C:781:LYS:N    | 2.29                     | 0.47              |
| 2:C:1014:SER:HB3 | 2:C:1017:THR:O   | 2.14                     | 0.47              |
| 3:D:416:ALA:HB1  | 8:D:2533:HOH:O   | 2.13                     | 0.47              |
| 3:D:520:LEU:HD12 | 3:D:521:PRO:HD2  | 1.94                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:955:VAL:HG21  | 3:D:1015:TYR:CD2  | 2.49                     | 0.47              |
| 3:D:969:ARG:HG3   | 3:D:970:LYS:N     | 2.29                     | 0.47              |
| 3:D:1264:GLU:OE2  | 3:D:1425:THR:N    | 2.44                     | 0.47              |
| 5:F:171:LYS:HG3   | 5:F:175:HIS:CD2   | 2.48                     | 0.47              |
| 5:F:216:GLY:O     | 5:F:243:ILE:HG12  | 2.13                     | 0.47              |
| 5:F:288:TYR:C     | 5:F:291:ILE:HG22  | 2.39                     | 0.47              |
| 1:K:176:ARG:NE    | 8:K:1966:HOH:O    | 2.45                     | 0.47              |
| 2:M:154:ARG:O     | 2:M:156:GLY:N     | 2.47                     | 0.47              |
| 2:M:431:HIS:CD2   | 2:M:433:THR:OG1   | 2.67                     | 0.47              |
| 2:M:444:PRO:HB3   | 8:M:9878:HOH:O    | 2.14                     | 0.47              |
| 2:M:575:GLN:HA    | 2:M:662:GLU:HG3   | 1.96                     | 0.47              |
| 2:M:650:ARG:CG    | 2:M:653:ASP:HB2   | 2.44                     | 0.47              |
| 2:M:681:GLY:HA2   | 8:M:2103:HOH:O    | 2.14                     | 0.47              |
| 2:M:773:LEU:HD23  | 5:P:354:LEU:HD13  | 1.96                     | 0.47              |
| 3:N:104:PHE:CD1   | 3:N:512:MET:HG2   | 2.49                     | 0.47              |
| 3:N:145:VAL:HG13  | 3:N:146:PRO:CD    | 2.43                     | 0.47              |
| 3:N:669:ASN:O     | 3:N:672:ALA:HB3   | 2.13                     | 0.47              |
| 3:N:792:ILE:HG23  | 3:N:793:THR:N     | 2.29                     | 0.47              |
| 3:N:865:THR:HG23  | 3:N:874:GLU:HG2   | 1.96                     | 0.47              |
| 3:N:970:LYS:HD2   | 3:N:995:LEU:CD1   | 2.44                     | 0.47              |
| 3:N:1042:ARG:HH22 | 3:N:1045:MET:HE1  | 1.78                     | 0.47              |
| 3:N:1045:MET:HG2  | 3:N:1073:SER:CA   | 2.24                     | 0.47              |
| 3:N:1109:GLU:HG2  | 3:N:1201:CYS:HA   | 1.96                     | 0.47              |
| 3:N:1145:TYR:HA   | 3:N:1171:VAL:HG21 | 1.95                     | 0.47              |
| 8:N:9520:HOH:O    | 5:P:136:LEU:HD21  | 2.14                     | 0.47              |
| 4:O:25:LYS:O      | 4:O:28:GLN:HB2    | 2.14                     | 0.47              |
| 4:O:37:ASN:C      | 8:O:691:HOH:O     | 2.57                     | 0.47              |
| 4:O:54:LEU:HG     | 4:O:58:PRO:CD     | 2.43                     | 0.47              |
| 5:P:167:PRO:HB2   | 5:P:169:GLU:CD    | 2.39                     | 0.47              |
| 5:P:395:GLU:HA    | 5:P:398:ARG:HD2   | 1.95                     | 0.47              |
| 1:A:10:VAL:HG13   | 1:B:229:GLN:NE2   | 2.28                     | 0.47              |
| 1:A:19:GLU:HG3    | 1:A:201:THR:O     | 2.14                     | 0.47              |
| 1:A:133:GLU:HG2   | 1:A:134:GLU:N     | 2.28                     | 0.47              |
| 1:A:170:VAL:CG1   | 2:C:696:LYS:HD3   | 2.44                     | 0.47              |
| 2:C:142:ARG:NH1   | 2:C:325:ILE:HG12  | 2.30                     | 0.47              |
| 2:C:164:PRO:HG2   | 8:C:2104:HOH:O    | 2.13                     | 0.47              |
| 2:C:292:ARG:HD2   | 2:C:299:LYS:HG2   | 1.95                     | 0.47              |
| 2:C:512:ARG:HD3   | 2:C:523:ILE:HD11  | 1.97                     | 0.47              |
| 2:C:539:VAL:HG21  | 3:D:1067:VAL:CG1  | 2.43                     | 0.47              |
| 2:C:841:ASN:HD21  | 2:C:845:ASN:H     | 1.63                     | 0.47              |
| 2:C:861:LEU:HD23  | 2:C:862:PRO:HD2   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:446:VAL:HG11  | 8:D:2498:HOH:O    | 2.13                     | 0.47              |
| 3:D:636:GLN:HB3   | 8:D:2240:HOH:O    | 2.13                     | 0.47              |
| 3:D:932:ASP:HA    | 3:D:935:LYS:HB3   | 1.97                     | 0.47              |
| 3:D:1155:VAL:HG12 | 3:D:1156:LEU:N    | 2.28                     | 0.47              |
| 3:D:1495:ILE:HG12 | 4:E:80:VAL:HG13   | 1.95                     | 0.47              |
| 4:E:3:GLU:OE2     | 4:E:65:MET:HE1    | 2.13                     | 0.47              |
| 5:F:136:LEU:HD12  | 5:F:137:GLY:N     | 2.29                     | 0.47              |
| 1:K:101:LEU:HD23  | 1:K:101:LEU:C     | 2.39                     | 0.47              |
| 2:M:84:ARG:HB3    | 8:M:9692:HOH:O    | 2.14                     | 0.47              |
| 2:M:442:GLU:HB3   | 8:M:9508:HOH:O    | 2.13                     | 0.47              |
| 2:M:476:GLY:C     | 2:M:478:VAL:H     | 2.22                     | 0.47              |
| 2:M:857:ASP:HB2   | 2:M:978:ARG:CG    | 2.33                     | 0.47              |
| 3:N:205:TYR:HB3   | 3:N:393:ILE:CD1   | 2.44                     | 0.47              |
| 3:N:440:VAL:HG21  | 8:N:2202:HOH:O    | 2.14                     | 0.47              |
| 3:N:700:VAL:HG22  | 3:N:718:PRO:HG3   | 1.96                     | 0.47              |
| 3:N:895:VAL:O     | 3:N:899:LEU:HD12  | 2.14                     | 0.47              |
| 3:N:1111:ASP:HB3  | 3:N:1203:LYS:HG3  | 1.97                     | 0.47              |
| 3:N:1274:ILE:HG13 | 3:N:1334:GLN:HE21 | 1.79                     | 0.47              |
| 3:N:1363:LEU:HD11 | 3:N:1368:ILE:HD11 | 1.96                     | 0.47              |
| 5:P:413:SER:CB    | 5:P:419:ARG:NH2   | 2.74                     | 0.47              |
| 1:A:165:ILE:O     | 1:A:165:ILE:HG13  | 2.13                     | 0.47              |
| 1:B:76:VAL:O      | 1:B:80:LEU:HB2    | 2.14                     | 0.47              |
| 2:C:136:ILE:CG2   | 2:C:336:VAL:HG13  | 2.40                     | 0.47              |
| 2:C:177:GLU:N     | 2:C:178:PRO:HD3   | 2.29                     | 0.47              |
| 2:C:455:LEU:HD13  | 2:C:456:ALA:O     | 2.15                     | 0.47              |
| 2:C:572:ILE:HG12  | 2:C:701:THR:O     | 2.14                     | 0.47              |
| 2:C:679:PHE:HE1   | 2:C:859:PRO:HD3   | 1.79                     | 0.47              |
| 2:C:889:HIS:CD2   | 2:C:970:GLY:HA3   | 2.50                     | 0.47              |
| 2:C:1016:ILE:HD13 | 2:C:1016:ILE:N    | 2.29                     | 0.47              |
| 2:C:1092:LEU:HG   | 3:D:607:LEU:HD11  | 1.95                     | 0.47              |
| 3:D:22:SER:OG     | 3:D:91:GLY:HA2    | 2.14                     | 0.47              |
| 3:D:191:LEU:HD13  | 3:D:195:VAL:HG11  | 1.96                     | 0.47              |
| 3:D:249:TYR:CB    | 8:D:9465:HOH:O    | 2.61                     | 0.47              |
| 3:D:843:PHE:HB2   | 3:D:866:VAL:HG22  | 1.95                     | 0.47              |
| 3:D:1005:GLN:HG2  | 8:D:9660:HOH:O    | 2.15                     | 0.47              |
| 3:D:1263:PHE:O    | 3:D:1424:VAL:HB   | 2.13                     | 0.47              |
| 5:F:84:TYR:HE1    | 5:F:196:VAL:CG2   | 2.26                     | 0.47              |
| 1:L:106:PRO:HG2   | 1:L:134:GLU:OE1   | 2.15                     | 0.47              |
| 1:L:201:THR:HG22  | 1:L:203:GLY:H     | 1.79                     | 0.47              |
| 2:M:35:PRO:HD2    | 2:M:38:LYS:HG2    | 1.96                     | 0.47              |
| 2:M:419:THR:HG23  | 8:M:9802:HOH:O    | 2.13                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:430:VAL:O     | 2:M:430:VAL:HG12  | 2.14                     | 0.47              |
| 2:M:881:ASN:HD22  | 2:M:881:ASN:N     | 2.11                     | 0.47              |
| 2:M:921:ALA:HB3   | 2:M:967:PHE:HE2   | 1.78                     | 0.47              |
| 2:M:934:PHE:N     | 2:M:934:PHE:CD1   | 2.82                     | 0.47              |
| 2:M:1000:MET:HB3  | 2:M:1002:GLU:HG2  | 1.96                     | 0.47              |
| 3:N:129:PHE:O     | 3:N:572:ARG:HG3   | 2.14                     | 0.47              |
| 3:N:168:THR:HG23  | 8:N:2247:HOH:O    | 2.14                     | 0.47              |
| 3:N:550:ARG:NH1   | 3:N:577:ALA:HB2   | 2.29                     | 0.47              |
| 3:N:871:LYS:HB3   | 3:N:873:LEU:HG    | 1.96                     | 0.47              |
| 3:N:1087:ARG:NH1  | 3:N:1238:MET:HG3  | 2.29                     | 0.47              |
| 3:N:1262:LEU:HD23 | 3:N:1352:ILE:CG1  | 2.41                     | 0.47              |
| 5:P:148:LYS:O     | 5:P:148:LYS:CG    | 2.62                     | 0.47              |
| 5:P:305:GLU:O     | 5:P:309:LYS:HG3   | 2.14                     | 0.47              |
| 1:A:25:LEU:HD13   | 1:B:225:PHE:CE2   | 2.50                     | 0.47              |
| 1:A:101:LEU:HD23  | 1:A:101:LEU:C     | 2.40                     | 0.47              |
| 2:C:176:VAL:O     | 2:C:176:VAL:HG23  | 2.14                     | 0.47              |
| 2:C:352:ALA:CA    | 2:C:355:VAL:HG12  | 2.42                     | 0.47              |
| 2:C:435:TYR:O     | 2:C:437:ARG:HG3   | 2.14                     | 0.47              |
| 2:C:626:ARG:H     | 2:C:639:GLN:HE21  | 1.63                     | 0.47              |
| 2:C:850:ALA:HA    | 3:D:632:VAL:CG1   | 2.43                     | 0.47              |
| 3:D:166:GLN:HB3   | 3:D:395:VAL:CG2   | 2.44                     | 0.47              |
| 3:D:181:ASP:OD2   | 3:D:199:LEU:HD12  | 2.13                     | 0.47              |
| 3:D:441:ARG:HG3   | 8:D:2480:HOH:O    | 2.14                     | 0.47              |
| 3:D:481:MET:SD    | 3:D:1388:ARG:CG   | 3.02                     | 0.47              |
| 3:D:523:ASP:O     | 3:D:526:PRO:HG3   | 2.14                     | 0.47              |
| 3:D:1166:LEU:HD23 | 3:D:1166:LEU:H    | 1.79                     | 0.47              |
| 3:D:1258:ARG:CZ   | 3:D:1262:LEU:HD11 | 2.44                     | 0.47              |
| 3:D:1465:ASN:HB3  | 8:D:9619:HOH:O    | 2.15                     | 0.47              |
| 5:F:395:GLU:O     | 5:F:399:GLN:HB2   | 2.14                     | 0.47              |
| 2:M:264:PRO:HB2   | 2:M:289:THR:CB    | 2.43                     | 0.47              |
| 2:M:393:GLN:OE1   | 2:M:393:GLN:N     | 2.47                     | 0.47              |
| 2:M:460:ARG:NH2   | 8:M:9491:HOH:O    | 2.46                     | 0.47              |
| 2:M:752:GLY:H     | 2:M:792:VAL:HB    | 1.78                     | 0.47              |
| 3:N:133:ILE:HG21  | 8:N:9573:HOH:O    | 2.14                     | 0.47              |
| 3:N:496:LEU:HD23  | 3:N:496:LEU:O     | 2.14                     | 0.47              |
| 3:N:565:ILE:HD12  | 3:N:565:ILE:N     | 2.17                     | 0.47              |
| 3:N:1110:ALA:O    | 3:N:1111:ASP:C    | 2.54                     | 0.47              |
| 3:N:1124:GLN:HE21 | 3:N:1133:ARG:HD2  | 1.80                     | 0.47              |
| 8:N:9520:HOH:O    | 5:P:132:ARG:HD3   | 2.13                     | 0.47              |
| 4:O:36:LYS:HE2    | 8:O:2142:HOH:O    | 2.14                     | 0.47              |
| 5:P:200:LYS:HG3   | 5:P:209:PHE:CE1   | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:14:ARG:HH12   | 1:A:24:VAL:HG21   | 1.80                     | 0.47              |
| 1:A:18:ARG:HH22   | 1:A:88:ARG:HH21   | 1.62                     | 0.47              |
| 2:C:227:PHE:HB3   | 8:C:9481:HOH:O    | 2.15                     | 0.47              |
| 2:C:282:GLY:HA2   | 2:C:308:ARG:NH2   | 2.28                     | 0.47              |
| 2:C:643:VAL:HG22  | 2:C:647:GLN:HE22  | 1.79                     | 0.47              |
| 2:C:739:GLU:O     | 2:C:741:GLY:N     | 2.47                     | 0.47              |
| 2:C:1065:ALA:CB   | 2:C:1077:PRO:HG2  | 2.44                     | 0.47              |
| 3:D:41:ARG:O      | 3:D:42:ASP:C      | 2.57                     | 0.47              |
| 3:D:154:THR:CG2   | 3:D:155:ASP:N     | 2.78                     | 0.47              |
| 3:D:661:MET:CE    | 3:D:673:ALA:HB1   | 2.44                     | 0.47              |
| 3:D:701:LEU:C     | 3:D:702:LEU:HD12  | 2.40                     | 0.47              |
| 3:D:890:VAL:CG1   | 3:D:926:LYS:HG2   | 2.34                     | 0.47              |
| 3:D:899:LEU:HD23  | 3:D:917:GLN:CB    | 2.41                     | 0.47              |
| 3:D:1429:LEU:HD23 | 3:D:1429:LEU:O    | 2.14                     | 0.47              |
| 5:F:273:ARG:HD3   | 8:F:9778:HOH:O    | 2.13                     | 0.47              |
| 5:F:288:TYR:N     | 5:F:288:TYR:CD1   | 2.82                     | 0.47              |
| 1:L:206:THR:HG21  | 8:L:5234:HOH:O    | 2.15                     | 0.47              |
| 2:M:169:GLY:HA3   | 2:M:263:ASP:O     | 2.14                     | 0.47              |
| 2:M:342:ASP:O     | 2:M:346:VAL:HG23  | 2.14                     | 0.47              |
| 2:M:442:GLU:HG3   | 8:M:9552:HOH:O    | 2.13                     | 0.47              |
| 2:M:601:GLY:HA3   | 2:M:615:TYR:HA    | 1.97                     | 0.47              |
| 2:M:728:HIS:CE1   | 2:M:775:ARG:HH12  | 2.33                     | 0.47              |
| 2:M:848:VAL:HG11  | 3:N:632:VAL:HG22  | 1.95                     | 0.47              |
| 2:M:1040:LEU:HD23 | 2:M:1048:THR:HG22 | 1.96                     | 0.47              |
| 2:M:1087:VAL:HG12 | 2:M:1091:GLU:OE2  | 2.13                     | 0.47              |
| 3:N:30:GLU:HG3    | 3:N:41:ARG:NE     | 2.25                     | 0.47              |
| 3:N:114:THR:HB    | 8:N:9878:HOH:O    | 2.13                     | 0.47              |
| 3:N:475:LYS:O     | 3:N:478:LEU:HB2   | 2.15                     | 0.47              |
| 3:N:558:LEU:HD22  | 5:P:145:PRO:CG    | 2.43                     | 0.47              |
| 3:N:598:ARG:HD2   | 8:N:2171:HOH:O    | 2.14                     | 0.47              |
| 3:N:729:HIS:HB3   | 3:N:732:VAL:HG22  | 1.96                     | 0.47              |
| 3:N:899:LEU:HD13  | 3:N:900:ILE:HG23  | 1.96                     | 0.47              |
| 3:N:1295:GLU:HB3  | 3:N:1300:SER:CB   | 2.44                     | 0.47              |
| 4:O:54:LEU:HA     | 4:O:58:PRO:HG2    | 1.97                     | 0.47              |
| 5:P:368:VAL:HG13  | 5:P:388:ALA:O     | 2.14                     | 0.47              |
| 1:A:109:VAL:HG23  | 1:A:132:LEU:HD13  | 1.96                     | 0.47              |
| 1:A:171:PHE:O     | 1:A:173:PRO:HD3   | 2.14                     | 0.47              |
| 1:B:45:LEU:HD21   | 1:B:177:VAL:HG23  | 1.96                     | 0.47              |
| 2:C:108:ILE:HB    | 2:C:368:THR:OG1   | 2.14                     | 0.47              |
| 2:C:910:LYS:HB3   | 2:C:912:PRO:HD2   | 1.96                     | 0.47              |
| 3:D:74:GLU:H      | 3:D:74:GLU:HG3    | 1.33                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:695:ILE:O    | 3:D:696:HIS:C    | 2.56                     | 0.47              |
| 3:D:711:LEU:HD12 | 3:D:778:LEU:HD23 | 1.96                     | 0.47              |
| 3:D:955:VAL:HG21 | 3:D:1015:TYR:CE2 | 2.49                     | 0.47              |
| 3:D:964:LEU:HD22 | 3:D:1058:ARG:NH1 | 2.29                     | 0.47              |
| 5:F:110:MET:HG3  | 8:F:9811:HOH:O   | 2.13                     | 0.47              |
| 5:F:119:ILE:HD13 | 5:F:170:HIS:CG   | 2.49                     | 0.47              |
| 5:F:140:ARG:NH1  | 8:F:9661:HOH:O   | 2.47                     | 0.47              |
| 1:K:211:LEU:O    | 1:K:215:VAL:HG13 | 2.14                     | 0.47              |
| 1:L:161:ARG:HG2  | 8:L:4097:HOH:O   | 2.14                     | 0.47              |
| 1:L:216:GLU:HA   | 8:L:1203:HOH:O   | 2.14                     | 0.47              |
| 2:M:577:PRO:HG2  | 2:M:842:ARG:NH1  | 2.30                     | 0.47              |
| 2:M:589:ARG:HD3  | 2:M:596:TYR:CZ   | 2.50                     | 0.47              |
| 3:N:205:TYR:CD2  | 3:N:393:ILE:HG12 | 2.39                     | 0.47              |
| 3:N:601:ARG:HD2  | 3:N:613:ARG:HH21 | 1.79                     | 0.47              |
| 3:N:701:LEU:CD1  | 3:N:750:PRO:HD3  | 2.45                     | 0.47              |
| 3:N:843:PHE:CD1  | 3:N:864:VAL:HG11 | 2.49                     | 0.47              |
| 3:N:971:LEU:O    | 3:N:975:GLU:HG2  | 2.15                     | 0.47              |
| 3:N:1107:VAL:HA  | 3:N:1200:VAL:O   | 2.14                     | 0.47              |
| 3:N:1314:LYS:NZ  | 3:N:1317:ASP:HB2 | 2.29                     | 0.47              |
| 4:O:8:LYS:O      | 4:O:12:MET:HG3   | 2.15                     | 0.47              |
| 4:O:26:ARG:HH21  | 4:O:67:GLU:CD    | 2.22                     | 0.47              |
| 5:P:94:LEU:N     | 5:P:98:GLU:HB2   | 2.29                     | 0.47              |
| 1:A:19:GLU:O     | 1:A:207:PRO:HG3  | 2.15                     | 0.47              |
| 1:A:156:HIS:HD2  | 1:A:157:GLY:N    | 2.12                     | 0.47              |
| 2:C:30:LEU:HD12  | 2:C:30:LEU:O     | 2.14                     | 0.47              |
| 2:C:34:VAL:CB    | 2:C:38:LYS:HG3   | 2.33                     | 0.47              |
| 2:C:100:LEU:HD22 | 2:C:367:LEU:HD12 | 1.96                     | 0.47              |
| 2:C:155:PRO:HB3  | 8:C:2281:HOH:O   | 2.14                     | 0.47              |
| 2:C:167:LYS:HE2  | 2:C:167:LYS:O    | 2.15                     | 0.47              |
| 2:C:218:VAL:HG23 | 2:C:311:PHE:HE1  | 1.78                     | 0.47              |
| 2:C:370:ALA:HB1  | 8:C:2217:HOH:O   | 2.14                     | 0.47              |
| 2:C:525:SER:O    | 2:C:529:VAL:HG23 | 2.15                     | 0.47              |
| 2:C:636:ALA:HB2  | 2:C:703:ILE:HG22 | 1.96                     | 0.47              |
| 2:C:675:ALA:O    | 2:C:870:ILE:HA   | 2.14                     | 0.47              |
| 2:C:683:ASN:HD22 | 2:C:872:ASN:N    | 2.12                     | 0.47              |
| 2:C:816:LYS:O    | 2:C:819:VAL:HB   | 2.15                     | 0.47              |
| 2:C:879:ARG:HB3  | 8:C:9530:HOH:O   | 2.15                     | 0.47              |
| 2:C:1021:LEU:C   | 8:C:2253:HOH:O   | 2.56                     | 0.47              |
| 3:D:30:GLU:HG3   | 3:D:41:ARG:CG    | 2.40                     | 0.47              |
| 3:D:34:TYR:O     | 3:D:35:ARG:C     | 2.55                     | 0.47              |
| 3:D:85:VAL:HB    | 3:D:89:ARG:HE    | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:100:ALA:N     | 8:D:9989:HOH:O    | 2.42                     | 0.47              |
| 3:D:118:LEU:O     | 3:D:120:ALA:N     | 2.48                     | 0.47              |
| 3:D:127:LEU:HD13  | 3:D:457:GLY:H     | 1.77                     | 0.47              |
| 3:D:131:LYS:CA    | 3:D:456:MET:HG3   | 2.40                     | 0.47              |
| 3:D:145:VAL:CG2   | 3:D:146:PRO:HD2   | 2.31                     | 0.47              |
| 3:D:186:VAL:HG13  | 3:D:187:LYS:N     | 2.29                     | 0.47              |
| 3:D:211:VAL:HG13  | 3:D:393:ILE:HG23  | 1.97                     | 0.47              |
| 3:D:427:VAL:CB    | 3:D:435:VAL:HB    | 2.43                     | 0.47              |
| 3:D:428:LYS:HB2   | 8:D:2076:HOH:O    | 2.15                     | 0.47              |
| 3:D:526:PRO:HD2   | 3:D:538:SER:OG    | 2.15                     | 0.47              |
| 3:D:563:PRO:HG3   | 5:F:188:ILE:CG2   | 2.45                     | 0.47              |
| 3:D:646:LYS:HA    | 3:D:720:LEU:CD2   | 2.41                     | 0.47              |
| 3:D:761:ILE:HD11  | 4:E:23:VAL:HG11   | 1.96                     | 0.47              |
| 3:D:826:PRO:HD2   | 3:D:829:VAL:CG2   | 2.41                     | 0.47              |
| 3:D:1066:THR:HA   | 8:D:9463:HOH:O    | 2.13                     | 0.47              |
| 8:D:2493:HOH:O    | 5:F:264:MET:HE2   | 2.14                     | 0.47              |
| 5:F:384:GLU:O     | 5:F:385:GLU:C     | 2.57                     | 0.47              |
| 1:K:172:SER:N     | 8:K:5034:HOH:O    | 2.48                     | 0.47              |
| 1:L:42:ARG:CZ     | 8:L:4157:HOH:O    | 2.62                     | 0.47              |
| 1:L:111:ALA:HB3   | 1:L:124:ASN:O     | 2.15                     | 0.47              |
| 1:L:180:GLN:CD    | 1:L:198:ARG:HH22  | 2.19                     | 0.47              |
| 1:L:182:GLU:O     | 1:L:194:LYS:HB3   | 2.15                     | 0.47              |
| 2:M:78:PHE:HB3    | 2:M:79:PRO:HD2    | 1.96                     | 0.47              |
| 2:M:88:LEU:HD23   | 2:M:814:GLU:HG2   | 1.97                     | 0.47              |
| 2:M:301:GLU:O     | 2:M:305:PRO:HG2   | 2.15                     | 0.47              |
| 2:M:304:LEU:HD23  | 2:M:305:PRO:N     | 2.30                     | 0.47              |
| 2:M:328:LEU:HB2   | 2:M:433:THR:CG2   | 2.44                     | 0.47              |
| 2:M:332:ARG:HE    | 2:M:464:LEU:HD11  | 1.78                     | 0.47              |
| 2:M:346:VAL:HG12  | 2:M:350:ARG:HE    | 1.80                     | 0.47              |
| 2:M:369:PRO:HD2   | 8:M:2250:HOH:O    | 2.15                     | 0.47              |
| 2:M:474:VAL:HG23  | 2:M:478:VAL:O     | 2.15                     | 0.47              |
| 2:M:479:VAL:CG2   | 2:M:503:LEU:HD11  | 2.44                     | 0.47              |
| 2:M:569:VAL:HG23  | 2:M:635:THR:HG22  | 1.97                     | 0.47              |
| 2:M:580:MET:O     | 2:M:902:ILE:HA    | 2.14                     | 0.47              |
| 2:M:580:MET:HE1   | 2:M:665:PHE:CE2   | 2.50                     | 0.47              |
| 2:M:1033:GLY:O    | 2:M:1037:VAL:HG23 | 2.15                     | 0.47              |
| 2:M:1097:LEU:HD21 | 3:N:103:TRP:CZ3   | 2.49                     | 0.47              |
| 2:M:1115:LEU:HD22 | 3:N:85:VAL:HG13   | 1.96                     | 0.47              |
| 3:N:96:ALA:H      | 3:N:551:ASN:HD22  | 1.62                     | 0.47              |
| 3:N:119:SER:CB    | 3:N:123:LEU:H     | 2.28                     | 0.47              |
| 3:N:556:LYS:CE    | 5:P:218:GLN:HE22  | 2.27                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:572:ARG:HB2   | 8:N:2401:HOH:O    | 2.13                     | 0.47              |
| 3:N:958:GLU:OE2   | 3:N:958:GLU:HA    | 2.14                     | 0.47              |
| 3:N:1155:VAL:HG11 | 3:N:1183:ILE:HD11 | 1.94                     | 0.47              |
| 3:N:1277:ILE:CD1  | 3:N:1301:LYS:HB2  | 2.41                     | 0.47              |
| 5:P:384:GLU:O     | 5:P:385:GLU:C     | 2.57                     | 0.47              |
| 1:A:137:ARG:C     | 8:A:9482:HOH:O    | 2.57                     | 0.47              |
| 1:A:186:LEU:H     | 1:A:192:LEU:HD12  | 1.79                     | 0.47              |
| 1:A:197:LEU:HD23  | 1:A:197:LEU:H     | 1.79                     | 0.47              |
| 1:B:221:HIS:HA    | 1:B:224:TYR:CD2   | 2.50                     | 0.47              |
| 2:C:159:ILE:HG21  | 2:C:175:GLU:OE1   | 2.14                     | 0.47              |
| 2:C:173:ASP:O     | 2:C:184:MET:HA    | 2.14                     | 0.47              |
| 2:C:287:GLY:O     | 2:C:288:ARG:C     | 2.58                     | 0.47              |
| 2:C:523:ILE:O     | 2:C:523:ILE:HG12  | 2.14                     | 0.47              |
| 2:C:627:ARG:HG3   | 2:C:628:PHE:N     | 2.25                     | 0.47              |
| 2:C:693:GLU:OE1   | 2:C:696:LYS:HD2   | 2.15                     | 0.47              |
| 2:C:695:LEU:HD21  | 2:C:833:LEU:O     | 2.15                     | 0.47              |
| 3:D:191:LEU:HD12  | 3:D:211:VAL:HG21  | 1.96                     | 0.47              |
| 3:D:427:VAL:CG2   | 3:D:435:VAL:HB    | 2.44                     | 0.47              |
| 3:D:440:VAL:HG12  | 3:D:441:ARG:N     | 2.29                     | 0.47              |
| 3:D:444:VAL:HG22  | 3:D:446:VAL:HG23  | 1.97                     | 0.47              |
| 3:D:445:ARG:HG2   | 3:D:445:ARG:NH1   | 2.30                     | 0.47              |
| 3:D:462:GLN:CG    | 3:D:513:ILE:HD13  | 2.38                     | 0.47              |
| 3:D:586:ARG:NH1   | 3:D:1444:THR:HG21 | 2.29                     | 0.47              |
| 3:D:728:LEU:HD22  | 3:D:745:MET:SD    | 2.55                     | 0.47              |
| 3:D:1357:ARG:HB3  | 8:D:2102:HOH:O    | 2.14                     | 0.47              |
| 5:F:411:HIS:HA    | 5:F:414:ARG:HG3   | 1.96                     | 0.47              |
| 1:K:54:THR:CG2    | 1:K:158:ILE:HG13  | 2.31                     | 0.47              |
| 1:K:88:ARG:HG3    | 1:K:204:SER:O     | 2.14                     | 0.47              |
| 2:M:193:LEU:HD12  | 2:M:307:LEU:HD22  | 1.95                     | 0.47              |
| 2:M:721:ARG:HH11  | 2:M:721:ARG:HG3   | 1.79                     | 0.47              |
| 2:M:841:ASN:HD21  | 2:M:843:HIS:HB2   | 1.80                     | 0.47              |
| 2:M:1046:ALA:HB2  | 3:N:1476:THR:H    | 1.79                     | 0.47              |
| 3:N:828:LYS:N     | 3:N:828:LYS:HD3   | 2.29                     | 0.47              |
| 3:N:1314:LYS:HZ3  | 3:N:1317:ASP:HB2  | 1.80                     | 0.47              |
| 4:O:45:ARG:HH12   | 4:O:72:ARG:NH2    | 2.12                     | 0.47              |
| 4:O:70:THR:HG22   | 4:O:71:GLY:N      | 2.29                     | 0.47              |
| 1:A:182:GLU:O     | 1:A:194:LYS:HB3   | 2.15                     | 0.47              |
| 2:C:443:THR:HG23  | 2:C:444:PRO:CD    | 2.45                     | 0.47              |
| 2:C:537:LYS:HD3   | 2:C:537:LYS:H     | 1.80                     | 0.47              |
| 2:C:547:ILE:HA    | 2:C:548:PRO:HD3   | 1.78                     | 0.47              |
| 2:C:789:SER:O     | 2:C:791:ARG:HG2   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1063:ARG:O    | 2:C:1066:ALA:HB3  | 2.15                     | 0.47              |
| 2:C:1067:TYR:CE1  | 2:C:1071:ILE:HD11 | 2.50                     | 0.47              |
| 3:D:54:LYS:HD3    | 3:D:57:GLU:HB2    | 1.97                     | 0.47              |
| 3:D:441:ARG:HB3   | 3:D:443:VAL:CG2   | 2.45                     | 0.47              |
| 3:D:838:ARG:HG3   | 3:D:838:ARG:NH1   | 2.30                     | 0.47              |
| 3:D:999:THR:O     | 3:D:1002:LYS:HB2  | 2.15                     | 0.47              |
| 3:D:1058:ARG:HH11 | 3:D:1058:ARG:HG3  | 1.80                     | 0.47              |
| 3:D:1403:LEU:O    | 3:D:1407:LEU:HB2  | 2.15                     | 0.47              |
| 5:F:367:MET:HE2   | 5:F:367:MET:HA    | 1.96                     | 0.47              |
| 5:F:384:GLU:N     | 8:F:9689:HOH:O    | 2.47                     | 0.47              |
| 1:L:227:ASN:C     | 8:L:679:HOH:O     | 2.57                     | 0.47              |
| 2:M:288:ARG:NE    | 2:M:288:ARG:HA    | 2.28                     | 0.47              |
| 2:M:512:ARG:HD2   | 8:M:9619:HOH:O    | 2.13                     | 0.47              |
| 2:M:672:VAL:HG23  | 2:M:868:ASP:CB    | 2.43                     | 0.47              |
| 3:N:507:ASN:H     | 3:N:507:ASN:ND2   | 2.12                     | 0.47              |
| 3:N:679:ARG:HD3   | 8:N:2378:HOH:O    | 2.15                     | 0.47              |
| 3:N:822:ALA:HA    | 8:N:9525:HOH:O    | 2.15                     | 0.47              |
| 3:N:899:LEU:HD21  | 3:N:914:LEU:HD23  | 1.97                     | 0.47              |
| 3:N:935:LYS:HG2   | 3:N:939:PHE:CE1   | 2.50                     | 0.47              |
| 3:N:958:GLU:N     | 8:N:2345:HOH:O    | 2.48                     | 0.47              |
| 3:N:960:LYS:HE2   | 3:N:964:LEU:HD11  | 1.97                     | 0.47              |
| 4:O:93:TYR:HA     | 4:O:94:PRO:HD3    | 1.62                     | 0.47              |
| 1:A:104:GLU:HG2   | 1:A:137:ARG:HD2   | 1.97                     | 0.47              |
| 1:B:73:GLU:HB3    | 8:B:9545:HOH:O    | 2.15                     | 0.47              |
| 3:D:724:GLN:HA    | 8:D:9554:HOH:O    | 2.15                     | 0.47              |
| 3:D:1377:LYS:HB3  | 8:D:2457:HOH:O    | 2.14                     | 0.47              |
| 1:K:184:THR:O     | 1:K:192:LEU:HD12  | 2.15                     | 0.47              |
| 1:L:227:ASN:N     | 8:L:679:HOH:O     | 2.48                     | 0.47              |
| 2:M:181:VAL:HG11  | 8:M:9805:HOH:O    | 2.14                     | 0.47              |
| 2:M:266:ARG:HD2   | 2:M:266:ARG:H     | 1.80                     | 0.47              |
| 2:M:340:MET:HE3   | 2:M:340:MET:HB3   | 1.68                     | 0.47              |
| 2:M:1109:VAL:HG22 | 3:N:3:LYS:HB2     | 1.97                     | 0.47              |
| 3:N:198:ARG:HG2   | 8:N:9544:HOH:O    | 2.14                     | 0.47              |
| 3:N:447:VAL:HG11  | 8:N:2391:HOH:O    | 2.14                     | 0.47              |
| 3:N:553:ARG:NH2   | 5:P:215:GLU:HG2   | 2.26                     | 0.47              |
| 3:N:623:VAL:HA    | 8:N:2406:HOH:O    | 2.14                     | 0.47              |
| 3:N:1258:ARG:HG3  | 3:N:1258:ARG:HH11 | 1.80                     | 0.47              |
| 5:P:86:HIS:HB3    | 8:P:9560:HOH:O    | 2.14                     | 0.47              |
| 5:P:130:VAL:HG21  | 5:P:159:ILE:CG2   | 2.42                     | 0.47              |
| 2:C:342:ASP:HA    | 2:C:345:ARG:NE    | 2.27                     | 0.46              |
| 2:C:769:PRO:HD2   | 8:D:9888:HOH:O    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1054:THR:HG21 | 2:C:1079:PRO:CA   | 2.45                     | 0.46              |
| 3:D:3:LYS:HD3     | 3:D:3:LYS:N       | 2.30                     | 0.46              |
| 3:D:175:VAL:HG11  | 8:D:2442:HOH:O    | 2.14                     | 0.46              |
| 3:D:177:ALA:HB1   | 3:D:199:LEU:CG    | 2.45                     | 0.46              |
| 3:D:177:ALA:CA    | 3:D:199:LEU:HD13  | 2.46                     | 0.46              |
| 3:D:603:LEU:HD23  | 3:D:606:ILE:HD12  | 1.97                     | 0.46              |
| 3:D:786:ILE:CD1   | 3:D:908:LYS:HB3   | 2.45                     | 0.46              |
| 3:D:1066:THR:O    | 3:D:1070:TYR:N    | 2.45                     | 0.46              |
| 5:F:280:GLN:HG2   | 5:F:280:GLN:O     | 2.15                     | 0.46              |
| 5:F:316:SER:HB3   | 5:F:318:GLU:O     | 2.16                     | 0.46              |
| 5:F:356:LYS:HE3   | 8:F:9501:HOH:O    | 2.14                     | 0.46              |
| 5:F:401:GLU:CG    | 5:F:402:ASN:OD1   | 2.62                     | 0.46              |
| 5:F:412:GLU:HA    | 5:F:412:GLU:OE1   | 2.15                     | 0.46              |
| 1:L:219:ARG:HG3   | 8:L:3455:HOH:O    | 2.15                     | 0.46              |
| 2:M:173:ASP:O     | 2:M:184:MET:HA    | 2.15                     | 0.46              |
| 2:M:260:LEU:HD12  | 2:M:260:LEU:O     | 2.14                     | 0.46              |
| 2:M:537:LYS:HA    | 2:M:905:ILE:CD1   | 2.45                     | 0.46              |
| 2:M:573:ARG:HB2   | 2:M:670:GLN:HE22  | 1.80                     | 0.46              |
| 2:M:691:SER:HB2   | 2:M:858:MET:CE    | 2.45                     | 0.46              |
| 2:M:739:GLU:O     | 2:M:740:GLU:C     | 2.58                     | 0.46              |
| 3:N:83:SER:HA     | 8:N:9939:HOH:O    | 2.13                     | 0.46              |
| 3:N:450:TYR:O     | 3:N:452:ILE:N     | 2.48                     | 0.46              |
| 3:N:476:GLU:HG2   | 8:N:9610:HOH:O    | 2.15                     | 0.46              |
| 3:N:1001:GLU:HG2  | 8:N:2177:HOH:O    | 2.15                     | 0.46              |
| 3:N:1186:VAL:HG11 | 8:N:2033:HOH:O    | 2.15                     | 0.46              |
| 5:P:135:ILE:HD11  | 5:P:178:ARG:CB    | 2.36                     | 0.46              |
| 5:P:285:GLU:HG2   | 8:P:9682:HOH:O    | 2.15                     | 0.46              |
| 1:B:44:LEU:HD23   | 1:B:48:ILE:CD1    | 2.46                     | 0.46              |
| 2:C:464:LEU:HD22  | 8:C:9598:HOH:O    | 2.15                     | 0.46              |
| 2:C:697:ARG:O     | 2:C:699:PHE:N     | 2.46                     | 0.46              |
| 2:C:704:HIS:CG    | 2:C:831:ARG:HH22  | 2.33                     | 0.46              |
| 2:C:1066:ALA:O    | 2:C:1070:ILE:HG13 | 2.15                     | 0.46              |
| 2:C:1096:ALA:HB2  | 3:D:514:LEU:HD11  | 1.97                     | 0.46              |
| 3:D:177:ALA:HB1   | 3:D:199:LEU:CB    | 2.45                     | 0.46              |
| 3:D:1441:GLN:HA   | 8:D:2144:HOH:O    | 2.15                     | 0.46              |
| 1:K:2:LEU:HD11    | 8:K:5314:HOH:O    | 2.15                     | 0.46              |
| 1:L:62:LEU:HD12   | 1:L:62:LEU:H      | 1.81                     | 0.46              |
| 1:L:107:LYS:HG2   | 1:L:108:GLU:N     | 2.30                     | 0.46              |
| 1:L:229:GLN:HG3   | 8:L:2218:HOH:O    | 2.13                     | 0.46              |
| 2:M:36:PRO:HD2    | 8:M:9886:HOH:O    | 2.15                     | 0.46              |
| 2:M:61:LYS:HD2    | 8:M:9710:HOH:O    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:191:PHE:HE2   | 2:M:196:LEU:HD12  | 1.81                     | 0.46              |
| 2:M:286:SER:O     | 2:M:299:LYS:HE3   | 2.15                     | 0.46              |
| 2:M:757:GLY:HA2   | 2:M:789:SER:OG    | 2.16                     | 0.46              |
| 3:N:396:VAL:CG2   | 3:N:447:VAL:HB    | 2.46                     | 0.46              |
| 3:N:538:SER:HA    | 5:P:317:LEU:HB2   | 1.97                     | 0.46              |
| 3:N:1232:PRO:CB   | 3:N:1361:VAL:HG11 | 2.44                     | 0.46              |
| 3:N:1441:GLN:HB3  | 8:N:9662:HOH:O    | 2.14                     | 0.46              |
| 4:O:46:PRO:HB3    | 4:O:54:LEU:CD2    | 2.45                     | 0.46              |
| 5:P:181:GLU:O     | 5:P:184:ARG:HB3   | 2.16                     | 0.46              |
| 1:A:161:ARG:HH11  | 1:A:161:ARG:HG3   | 1.79                     | 0.46              |
| 1:B:191:ASP:O     | 1:B:191:ASP:CG    | 2.57                     | 0.46              |
| 2:C:11:GLU:HG2    | 2:C:537:LYS:HZ2   | 1.77                     | 0.46              |
| 2:C:31:GLN:HE21   | 2:C:31:GLN:HB3    | 1.42                     | 0.46              |
| 2:C:304:LEU:HD23  | 2:C:305:PRO:N     | 2.31                     | 0.46              |
| 2:C:484:VAL:CG1   | 2:C:486:MET:HG3   | 2.46                     | 0.46              |
| 2:C:564:MET:HA    | 2:C:564:MET:HE3   | 1.96                     | 0.46              |
| 2:C:815:LEU:HD23  | 2:C:819:VAL:O     | 2.14                     | 0.46              |
| 3:D:567:ILE:C     | 3:D:571:LYS:HZ2   | 2.24                     | 0.46              |
| 3:D:781:PRO:HG2   | 3:D:911:LEU:HD23  | 1.98                     | 0.46              |
| 3:D:787:LEU:HD21  | 3:D:947:ILE:HD13  | 1.97                     | 0.46              |
| 3:D:1047:LYS:HG2  | 3:D:1053:PHE:CE1  | 2.49                     | 0.46              |
| 3:D:1104:GLU:O    | 3:D:1106:VAL:HG23 | 2.14                     | 0.46              |
| 1:K:14:ARG:HA     | 8:K:2767:HOH:O    | 2.14                     | 0.46              |
| 1:K:43:ILE:HD12   | 1:L:32:PHE:CZ     | 2.50                     | 0.46              |
| 1:K:90:LEU:HD11   | 8:K:2043:HOH:O    | 2.15                     | 0.46              |
| 1:L:42:ARG:NE     | 8:L:4157:HOH:O    | 2.49                     | 0.46              |
| 1:L:80:LEU:HD23   | 8:N:9812:HOH:O    | 2.14                     | 0.46              |
| 2:M:163:ILE:HG13  | 2:M:171:TRP:HZ3   | 1.80                     | 0.46              |
| 2:M:689:VAL:HG23  | 2:M:870:ILE:HB    | 1.97                     | 0.46              |
| 2:M:944:LEU:HD22  | 2:M:962:GLN:HG2   | 1.96                     | 0.46              |
| 2:M:1019:GLN:NE2  | 3:N:621:LYS:HE3   | 2.31                     | 0.46              |
| 2:M:1071:ILE:O    | 3:N:659:LYS:HD3   | 2.16                     | 0.46              |
| 3:N:55:ASP:CB     | 3:N:82:LYS:HG2    | 2.46                     | 0.46              |
| 3:N:1272:ALA:HA   | 3:N:1326:THR:HB   | 1.97                     | 0.46              |
| 3:N:1495:ILE:HD13 | 4:O:88:GLU:HG3    | 1.96                     | 0.46              |
| 4:O:48:MET:HG2    | 4:O:54:LEU:HB2    | 1.97                     | 0.46              |
| 2:C:142:ARG:HB2   | 8:C:9877:HOH:O    | 2.15                     | 0.46              |
| 2:C:260:LEU:HD12  | 2:C:260:LEU:O     | 2.14                     | 0.46              |
| 2:C:433:THR:O     | 2:C:435:TYR:N     | 2.49                     | 0.46              |
| 2:C:853:LEU:HD23  | 2:C:858:MET:HB3   | 1.97                     | 0.46              |
| 2:C:905:ILE:CG2   | 2:C:906:PHE:N     | 2.78                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:171:LEU:CD2   | 3:D:390:PRO:HG3   | 2.45                     | 0.46              |
| 3:D:820:GLU:HA    | 3:D:825:ALA:O     | 2.14                     | 0.46              |
| 3:D:1211:MET:HE1  | 4:E:16:LYS:CE     | 2.45                     | 0.46              |
| 3:D:1324:PRO:HG3  | 3:D:1330:ILE:HD11 | 1.98                     | 0.46              |
| 5:F:94:LEU:N      | 5:F:98:GLU:HB2    | 2.30                     | 0.46              |
| 5:F:282:LEU:HD12  | 5:F:284:ARG:HB2   | 1.97                     | 0.46              |
| 5:F:358:LEU:CG    | 5:F:367:MET:HE1   | 2.46                     | 0.46              |
| 1:K:111:ALA:HB3   | 1:K:124:ASN:O     | 2.16                     | 0.46              |
| 1:L:101:LEU:HD23  | 1:L:101:LEU:C     | 2.41                     | 0.46              |
| 2:M:78:PHE:HB3    | 2:M:79:PRO:CD     | 2.45                     | 0.46              |
| 2:M:157:ARG:HB2   | 8:M:9963:HOH:O    | 2.15                     | 0.46              |
| 2:M:252:LYS:HZ2   | 2:M:296:GLY:HA3   | 1.78                     | 0.46              |
| 2:M:270:GLY:N     | 2:M:288:ARG:NH2   | 2.63                     | 0.46              |
| 2:M:345:ARG:HG2   | 8:M:9798:HOH:O    | 2.15                     | 0.46              |
| 2:M:408:ARG:NH1   | 2:M:542:VAL:HG23  | 2.30                     | 0.46              |
| 2:M:816:LYS:O     | 2:M:819:VAL:HB    | 2.16                     | 0.46              |
| 2:M:1031:ARG:HA   | 3:N:621:LYS:O     | 2.15                     | 0.46              |
| 2:M:1096:ALA:HB1  | 3:N:13:ALA:HB3    | 1.98                     | 0.46              |
| 3:N:153:LEU:HD23  | 3:N:153:LEU:H     | 1.78                     | 0.46              |
| 3:N:166:GLN:HG2   | 3:N:207:PHE:CG    | 2.49                     | 0.46              |
| 3:N:195:VAL:HB    | 3:N:205:TYR:HB2   | 1.98                     | 0.46              |
| 3:N:205:TYR:HD2   | 3:N:393:ILE:CG1   | 2.26                     | 0.46              |
| 3:N:412:GLY:O     | 3:N:421:LEU:HB3   | 2.16                     | 0.46              |
| 3:N:684:LYS:HE2   | 8:N:2408:HOH:O    | 2.16                     | 0.46              |
| 3:N:1106:VAL:HG21 | 3:N:1474:ALA:HB2  | 1.96                     | 0.46              |
| 3:N:1115:THR:O    | 3:N:1151:ARG:NH2  | 2.48                     | 0.46              |
| 5:P:393:THR:HG23  | 5:P:394:ARG:CD    | 2.44                     | 0.46              |
| 5:P:402:ASN:OD1   | 5:P:402:ASN:N     | 2.48                     | 0.46              |
| 5:P:405:LEU:HA    | 5:P:408:LEU:HD22  | 1.98                     | 0.46              |
| 1:A:202:ASP:HA    | 8:A:9549:HOH:O    | 2.15                     | 0.46              |
| 1:B:111:ALA:HB3   | 1:B:124:ASN:O     | 2.15                     | 0.46              |
| 1:B:156:HIS:HD2   | 1:B:157:GLY:N     | 2.14                     | 0.46              |
| 2:C:52:PHE:CE1    | 2:C:98:LEU:HD21   | 2.51                     | 0.46              |
| 2:C:341:THR:HG23  | 2:C:345:ARG:HH22  | 1.81                     | 0.46              |
| 2:C:620:LEU:HD23  | 2:C:620:LEU:O     | 2.15                     | 0.46              |
| 2:C:810:ASP:HA    | 2:C:811:PRO:HD3   | 1.57                     | 0.46              |
| 2:C:880:MET:N     | 8:C:9530:HOH:O    | 2.47                     | 0.46              |
| 3:D:72:VAL:HG22   | 3:D:78:VAL:H      | 1.81                     | 0.46              |
| 3:D:426:LYS:HB3   | 5:F:134:LYS:O     | 2.15                     | 0.46              |
| 3:D:621:LYS:N     | 8:D:9762:HOH:O    | 2.48                     | 0.46              |
| 3:D:872:ARG:C     | 8:D:2489:HOH:O    | 2.59                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:899:LEU:HB2  | 3:D:917:GLN:HG2  | 1.97                     | 0.46              |
| 5:F:88:ILE:HD13  | 5:F:193:ARG:CG   | 2.45                     | 0.46              |
| 5:F:347:GLN:O    | 5:F:351:SER:HB2  | 2.16                     | 0.46              |
| 1:K:48:ILE:HG22  | 1:K:173:PRO:HD2  | 1.98                     | 0.46              |
| 2:M:15:LEU:HD12  | 2:M:15:LEU:N     | 2.30                     | 0.46              |
| 2:M:63:GLY:CA    | 2:M:103:LYS:HE2  | 2.46                     | 0.46              |
| 2:M:89:THR:N     | 8:M:9667:HOH:O   | 2.49                     | 0.46              |
| 2:M:129:ILE:HD11 | 2:M:386:PHE:CD2  | 2.51                     | 0.46              |
| 2:M:217:LEU:HA   | 8:M:9626:HOH:O   | 2.16                     | 0.46              |
| 2:M:398:THR:N    | 2:M:633:GLN:OE1  | 2.48                     | 0.46              |
| 3:N:22:SER:HA    | 3:N:90:MET:O     | 2.16                     | 0.46              |
| 3:N:145:VAL:HG12 | 8:N:2383:HOH:O   | 2.15                     | 0.46              |
| 3:N:523:ASP:O    | 3:N:526:PRO:HG3  | 2.15                     | 0.46              |
| 3:N:546:ARG:NH1  | 3:N:550:ARG:HH22 | 2.14                     | 0.46              |
| 3:N:959:GLU:HG3  | 3:N:1006:ALA:HB1 | 1.97                     | 0.46              |
| 5:P:188:ILE:HD11 | 5:P:221:ILE:HA   | 1.97                     | 0.46              |
| 5:P:287:THR:O    | 5:P:289:GLU:N    | 2.49                     | 0.46              |
| 1:A:88:ARG:NE    | 8:A:9503:HOH:O   | 2.49                     | 0.46              |
| 1:A:222:LEU:CD1  | 1:B:215:VAL:HB   | 2.42                     | 0.46              |
| 1:B:103:ALA:HB1  | 8:B:9534:HOH:O   | 2.16                     | 0.46              |
| 2:C:69:LEU:HG    | 8:C:9557:HOH:O   | 2.15                     | 0.46              |
| 2:C:650:ARG:HG2  | 2:C:653:ASP:HB2  | 1.97                     | 0.46              |
| 2:C:670:GLN:O    | 2:C:672:VAL:HG12 | 2.13                     | 0.46              |
| 2:C:744:ARG:HD2  | 8:C:9769:HOH:O   | 2.16                     | 0.46              |
| 2:C:886:LEU:HD23 | 8:C:9674:HOH:O   | 2.15                     | 0.46              |
| 2:C:953:VAL:CG1  | 2:C:966:LEU:HD13 | 2.44                     | 0.46              |
| 3:D:106:LYS:HE2  | 3:D:125:GLN:OE1  | 2.16                     | 0.46              |
| 3:D:149:LYS:HE2  | 3:D:149:LYS:N    | 2.27                     | 0.46              |
| 3:D:177:ALA:HB1  | 3:D:199:LEU:CD2  | 2.43                     | 0.46              |
| 3:D:1111:ASP:O   | 3:D:1112:CYS:C   | 2.58                     | 0.46              |
| 3:D:1132:LEU:N   | 8:D:9601:HOH:O   | 2.48                     | 0.46              |
| 3:D:1405:GLU:HG2 | 8:D:9486:HOH:O   | 2.15                     | 0.46              |
| 5:F:384:GLU:O    | 5:F:388:ALA:N    | 2.48                     | 0.46              |
| 1:L:81:ASN:CG    | 8:L:1941:HOH:O   | 2.58                     | 0.46              |
| 1:L:172:SER:N    | 8:L:5023:HOH:O   | 2.46                     | 0.46              |
| 2:M:56:GLU:HB3   | 8:M:2105:HOH:O   | 2.15                     | 0.46              |
| 2:M:99:GLN:HG3   | 2:M:99:GLN:O     | 2.15                     | 0.46              |
| 2:M:333:ILE:HD11 | 2:M:410:ILE:HG21 | 1.98                     | 0.46              |
| 2:M:707:ARG:CZ   | 2:M:824:ARG:NH1  | 2.79                     | 0.46              |
| 2:M:734:LEU:O    | 2:M:735:ARG:C    | 2.58                     | 0.46              |
| 2:M:762:LYS:HZ3  | 2:M:784:ASP:HB3  | 1.81                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:901:TYR:CD1   | 2:M:901:TYR:N    | 2.82                     | 0.46              |
| 2:M:939:ARG:CB    | 2:M:982:PRO:HG3  | 2.33                     | 0.46              |
| 2:M:950:LEU:HB3   | 2:M:952:LEU:CD2  | 2.44                     | 0.46              |
| 3:N:41:ARG:HG3    | 3:N:42:ASP:N     | 2.31                     | 0.46              |
| 3:N:97:THR:HG21   | 3:N:571:LYS:HD3  | 1.98                     | 0.46              |
| 3:N:116:LEU:HA    | 8:N:9831:HOH:O   | 2.15                     | 0.46              |
| 3:N:132:TYR:CD1   | 3:N:132:TYR:N    | 2.79                     | 0.46              |
| 3:N:154:THR:CG2   | 3:N:156:GLU:HG2  | 2.45                     | 0.46              |
| 3:N:428:LYS:HD3   | 3:N:451:ASP:OD1  | 2.16                     | 0.46              |
| 3:N:1092:GLY:O    | 3:N:1096:ARG:N   | 2.48                     | 0.46              |
| 3:N:1102:THR:HG22 | 3:N:1222:GLY:CA  | 2.45                     | 0.46              |
| 4:O:47:LYS:HA     | 4:O:54:LEU:HB3   | 1.97                     | 0.46              |
| 5:P:151:LEU:HB2   | 5:P:155:THR:HB   | 1.98                     | 0.46              |
| 5:P:316:SER:C     | 5:P:318:GLU:N    | 2.71                     | 0.46              |
| 5:P:409:LYS:HG3   | 8:P:9621:HOH:O   | 2.16                     | 0.46              |
| 5:P:415:THR:HG22  | 5:P:417:LYS:CG   | 2.46                     | 0.46              |
| 1:A:72:LYS:HZ1    | 2:C:644:VAL:CA   | 2.28                     | 0.46              |
| 2:C:274:ARG:HD2   | 8:C:9567:HOH:O   | 2.15                     | 0.46              |
| 2:C:480:THR:HG23  | 8:C:9749:HOH:O   | 2.14                     | 0.46              |
| 2:C:500:ASN:HA    | 8:C:9900:HOH:O   | 2.16                     | 0.46              |
| 3:D:240:GLU:O     | 3:D:242:LEU:N    | 2.49                     | 0.46              |
| 3:D:525:ARG:HA    | 3:D:538:SER:CB   | 2.46                     | 0.46              |
| 3:D:632:VAL:O     | 3:D:727:GLN:HA   | 2.15                     | 0.46              |
| 3:D:701:LEU:O     | 3:D:747:VAL:HA   | 2.16                     | 0.46              |
| 3:D:1376:MET:HE3  | 3:D:1421:LEU:CD1 | 2.41                     | 0.46              |
| 3:D:1385:GLY:HA2  | 8:D:9913:HOH:O   | 2.15                     | 0.46              |
| 1:K:44:LEU:HD23   | 1:K:48:ILE:CD1   | 2.46                     | 0.46              |
| 1:K:94:LEU:HD21   | 1:K:119:ASP:HB3  | 1.97                     | 0.46              |
| 1:L:62:LEU:HD13   | 1:L:63:HIS:ND1   | 2.30                     | 0.46              |
| 1:L:74:ASP:HB2    | 8:L:5263:HOH:O   | 2.14                     | 0.46              |
| 2:M:278:GLU:HB2   | 8:M:2038:HOH:O   | 2.15                     | 0.46              |
| 2:M:338:GLU:HA    | 2:M:341:THR:OG1  | 2.16                     | 0.46              |
| 2:M:428:ARG:O     | 3:N:1078:ARG:NH1 | 2.48                     | 0.46              |
| 2:M:471:TYR:CE2   | 2:M:496:ILE:HG21 | 2.50                     | 0.46              |
| 2:M:541:SER:HB2   | 8:M:9853:HOH:O   | 2.14                     | 0.46              |
| 2:M:739:GLU:O     | 2:M:741:GLY:N    | 2.49                     | 0.46              |
| 2:M:816:LYS:HE3   | 8:M:9538:HOH:O   | 2.14                     | 0.46              |
| 2:M:876:VAL:O     | 2:M:879:ARG:O    | 2.34                     | 0.46              |
| 3:N:139:GLY:N     | 3:N:147:VAL:HG11 | 2.30                     | 0.46              |
| 3:N:465:LEU:HD11  | 3:N:512:MET:HE3  | 1.98                     | 0.46              |
| 3:N:546:ARG:NH2   | 3:N:576:GLU:OE1  | 2.48                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:590:PRO:HB3   | 8:N:2178:HOH:O    | 2.16                     | 0.46              |
| 3:N:678:GLU:HG3   | 3:N:679:ARG:HG3   | 1.98                     | 0.46              |
| 3:N:804:LEU:HD12  | 3:N:804:LEU:O     | 2.15                     | 0.46              |
| 3:N:1209:LEU:C    | 3:N:1211:MET:N    | 2.69                     | 0.46              |
| 4:O:12:MET:O      | 4:O:75:PHE:HZ     | 1.98                     | 0.46              |
| 5:P:225:GLU:HB3   | 5:P:226:LYS:NZ    | 2.29                     | 0.46              |
| 1:A:42:ARG:HH12   | 2:C:856:GLU:C     | 2.24                     | 0.46              |
| 1:A:89:PHE:HB2    | 1:A:94:LEU:HD22   | 1.98                     | 0.46              |
| 1:A:183:ASP:HB3   | 8:A:9448:HOH:O    | 2.15                     | 0.46              |
| 2:C:615:TYR:N     | 8:C:9571:HOH:O    | 2.40                     | 0.46              |
| 2:C:626:ARG:HD3   | 8:C:9724:HOH:O    | 2.16                     | 0.46              |
| 2:C:1115:LEU:CB   | 3:D:85:VAL:HG12   | 2.38                     | 0.46              |
| 3:D:389:GLU:HG3   | 8:D:9925:HOH:O    | 2.16                     | 0.46              |
| 3:D:675:ARG:NH2   | 5:F:420:ASP:OD2   | 2.48                     | 0.46              |
| 3:D:1118:ILE:CD1  | 3:D:1192:LEU:HD12 | 2.45                     | 0.46              |
| 3:D:1118:ILE:HG13 | 8:D:9509:HOH:O    | 2.15                     | 0.46              |
| 3:D:1281:VAL:HG21 | 3:D:1313:VAL:HG21 | 1.96                     | 0.46              |
| 4:E:32:ARG:CZ     | 4:E:32:ARG:HB2    | 2.46                     | 0.46              |
| 5:F:96:LEU:O      | 5:F:100:VAL:HG23  | 2.15                     | 0.46              |
| 5:F:151:LEU:HG    | 5:F:155:THR:OG1   | 2.16                     | 0.46              |
| 5:F:265:VAL:HG12  | 8:F:9687:HOH:O    | 2.16                     | 0.46              |
| 1:K:7:LYS:HG2     | 1:K:7:LYS:O       | 2.16                     | 0.46              |
| 1:K:19:GLU:HG3    | 1:K:201:THR:O     | 2.16                     | 0.46              |
| 1:K:171:PHE:HZ    | 8:K:972:HOH:O     | 1.97                     | 0.46              |
| 2:M:211:LEU:O     | 2:M:211:LEU:HG    | 2.11                     | 0.46              |
| 2:M:226:VAL:HG13  | 2:M:227:PHE:CD1   | 2.50                     | 0.46              |
| 2:M:773:LEU:HD23  | 8:M:9948:HOH:O    | 2.16                     | 0.46              |
| 2:M:909:ALA:HA    | 2:M:913:GLU:OE1   | 2.16                     | 0.46              |
| 2:M:1064:ASN:HD21 | 5:P:344:ALA:CB    | 2.28                     | 0.46              |
| 2:M:1106:ASP:CA   | 3:N:7:LYS:HE3     | 2.46                     | 0.46              |
| 3:N:12:LEU:HD23   | 3:N:12:LEU:HA     | 1.74                     | 0.46              |
| 3:N:191:LEU:HD12  | 3:N:211:VAL:HG21  | 1.97                     | 0.46              |
| 3:N:960:LYS:HE2   | 3:N:964:LEU:CD1   | 2.46                     | 0.46              |
| 3:N:1024:ALA:HB2  | 8:N:9601:HOH:O    | 2.14                     | 0.46              |
| 3:N:1336:LEU:HB2  | 3:N:1344:VAL:HG21 | 1.97                     | 0.46              |
| 5:P:140:ARG:NH1   | 5:P:141:VAL:HG23  | 2.31                     | 0.46              |
| 5:P:358:LEU:HD11  | 5:P:370:LYS:CE    | 2.45                     | 0.46              |
| 5:P:358:LEU:HD11  | 5:P:370:LYS:CD    | 2.44                     | 0.46              |
| 1:A:173:PRO:O     | 1:A:201:THR:HG23  | 2.16                     | 0.46              |
| 1:A:192:LEU:HA    | 8:A:9591:HOH:O    | 2.15                     | 0.46              |
| 2:C:127:PHE:CE1   | 2:C:386:PHE:HE2   | 2.34                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:298:PHE:N     | 2:C:298:PHE:CD1  | 2.84                     | 0.46              |
| 2:C:726:ILE:HG13  | 2:C:734:LEU:HD21 | 1.96                     | 0.46              |
| 2:C:730:SER:N     | 8:C:9532:HOH:O   | 2.49                     | 0.46              |
| 3:D:8:VAL:HG12    | 3:D:1434:TRP:CH2 | 2.50                     | 0.46              |
| 3:D:81:THR:HG22   | 3:D:82:LYS:N     | 2.29                     | 0.46              |
| 3:D:100:ALA:HB3   | 8:D:9989:HOH:O   | 2.15                     | 0.46              |
| 3:D:204:LEU:HD12  | 8:D:2181:HOH:O   | 2.16                     | 0.46              |
| 3:D:562:ALA:HB1   | 3:D:567:ILE:HD11 | 1.98                     | 0.46              |
| 3:D:639:LEU:N     | 3:D:729:HIS:CD2  | 2.84                     | 0.46              |
| 3:D:702:LEU:HD23  | 3:D:745:MET:HE2  | 1.98                     | 0.46              |
| 3:D:710:ARG:HH21  | 3:D:1224:VAL:CG2 | 2.28                     | 0.46              |
| 3:D:782:SER:O     | 3:D:786:ILE:HD12 | 2.15                     | 0.46              |
| 3:D:794:GLN:O     | 3:D:861:GLN:HB3  | 2.16                     | 0.46              |
| 3:D:850:LEU:HD13  | 3:D:884:ARG:NH2  | 2.31                     | 0.46              |
| 3:D:906:GLN:OE1   | 3:D:906:GLN:HA   | 2.16                     | 0.46              |
| 3:D:991:GLN:HG3   | 8:D:9597:HOH:O   | 2.16                     | 0.46              |
| 3:D:1130:ARG:HD2  | 8:D:9601:HOH:O   | 2.14                     | 0.46              |
| 4:E:30:LEU:HD21   | 4:E:63:TRP:HE3   | 1.80                     | 0.46              |
| 1:L:176:ARG:HH22  | 3:N:884:ARG:CD   | 2.28                     | 0.46              |
| 2:M:10:ARG:O      | 2:M:12:VAL:N     | 2.49                     | 0.46              |
| 2:M:44:ILE:CD1    | 2:M:340:MET:HE1  | 2.44                     | 0.46              |
| 2:M:247:PRO:HA    | 2:M:248:PRO:HD3  | 1.83                     | 0.46              |
| 2:M:261:ILE:H     | 2:M:261:ILE:HG13 | 1.63                     | 0.46              |
| 2:M:352:ALA:O     | 2:M:356:ARG:HG3  | 2.16                     | 0.46              |
| 2:M:432:ARG:CZ    | 3:N:1048:PRO:HD2 | 2.46                     | 0.46              |
| 2:M:501:THR:O     | 2:M:502:PRO:C    | 2.59                     | 0.46              |
| 2:M:773:LEU:O     | 2:M:777:ILE:HG13 | 2.16                     | 0.46              |
| 2:M:810:ASP:HA    | 2:M:811:PRO:HD3  | 1.56                     | 0.46              |
| 2:M:1046:ALA:HB3  | 3:N:1476:THR:HB  | 1.98                     | 0.46              |
| 3:N:98:PRO:C      | 3:N:458:ALA:HB3  | 2.41                     | 0.46              |
| 3:N:422:ALA:HB3   | 3:N:427:VAL:HG13 | 1.98                     | 0.46              |
| 3:N:676:MET:O     | 3:N:676:MET:SD   | 2.74                     | 0.46              |
| 3:N:806:PHE:O     | 3:N:806:PHE:CD1  | 2.68                     | 0.46              |
| 3:N:912:LYS:HB3   | 3:N:912:LYS:HZ2  | 1.81                     | 0.46              |
| 3:N:1057:VAL:HG12 | 3:N:1069:GLU:OE2 | 2.15                     | 0.46              |
| 1:A:118:ALA:HB2   | 8:A:9586:HOH:O   | 2.15                     | 0.46              |
| 1:A:138:LEU:CD1   | 1:A:140:MET:HE2  | 2.39                     | 0.46              |
| 2:C:31:GLN:HG3    | 8:C:9887:HOH:O   | 2.15                     | 0.46              |
| 2:C:118:ILE:HA    | 2:C:119:PRO:HD3  | 1.85                     | 0.46              |
| 2:C:264:PRO:HG2   | 8:C:9714:HOH:O   | 2.16                     | 0.46              |
| 2:C:338:GLU:HA    | 2:C:341:THR:CG2  | 2.43                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:426:ASP:HA    | 2:C:429:ASP:OD2   | 2.15                     | 0.46              |
| 2:C:571:LEU:HD21  | 2:C:700:TYR:HD2   | 1.80                     | 0.46              |
| 2:C:679:PHE:CZ    | 2:C:853:LEU:HD21  | 2.51                     | 0.46              |
| 2:C:987:ILE:CG2   | 3:D:948:THR:HG21  | 2.30                     | 0.46              |
| 2:C:1054:THR:HG22 | 2:C:1055:LEU:HD23 | 1.97                     | 0.46              |
| 2:C:1117:SER:O    | 3:D:23:TYR:OH     | 2.29                     | 0.46              |
| 3:D:53:ILE:C      | 8:D:9932:HOH:O    | 2.59                     | 0.46              |
| 3:D:182:GLY:O     | 3:D:186:VAL:HB    | 2.16                     | 0.46              |
| 3:D:859:ASP:HB3   | 3:D:861:GLN:HE22  | 1.81                     | 0.46              |
| 3:D:873:LEU:N     | 8:D:2489:HOH:O    | 2.48                     | 0.46              |
| 3:D:1346:ARG:HA   | 3:D:1346:ARG:NH1  | 2.31                     | 0.46              |
| 3:D:1393:GLN:NE2  | 8:D:2138:HOH:O    | 2.46                     | 0.46              |
| 3:D:1436:SER:OG   | 3:D:1463:LYS:HD2  | 2.16                     | 0.46              |
| 1:K:14:ARG:HH12   | 1:K:24:VAL:HG21   | 1.81                     | 0.46              |
| 1:K:62:LEU:H      | 1:K:62:LEU:HD12   | 1.81                     | 0.46              |
| 1:K:219:ARG:HH12  | 1:K:220:GLU:CG    | 2.28                     | 0.46              |
| 2:M:54:ILE:HG23   | 2:M:64:LEU:HD21   | 1.98                     | 0.46              |
| 2:M:54:ILE:HD13   | 8:M:9525:HOH:O    | 2.14                     | 0.46              |
| 2:M:63:GLY:HA3    | 2:M:103:LYS:CG    | 2.45                     | 0.46              |
| 2:M:73:LEU:HD23   | 2:M:94:LEU:HD13   | 1.98                     | 0.46              |
| 2:M:151:ASP:CG    | 2:M:152:PRO:HD2   | 2.41                     | 0.46              |
| 2:M:335:THR:HG22  | 2:M:461:VAL:HG11  | 1.98                     | 0.46              |
| 2:M:412:ALA:CA    | 8:M:2237:HOH:O    | 2.64                     | 0.46              |
| 2:M:441:VAL:O     | 2:M:559:LEU:HD13  | 2.16                     | 0.46              |
| 2:M:554:ASP:CB    | 2:M:880:MET:O     | 2.64                     | 0.46              |
| 2:M:683:ASN:HB2   | 2:M:687:ALA:O     | 2.16                     | 0.46              |
| 2:M:755:LEU:HD23  | 2:M:755:LEU:HA    | 1.76                     | 0.46              |
| 2:M:772:ARG:HG3   | 8:P:9568:HOH:O    | 2.16                     | 0.46              |
| 2:M:850:ALA:HA    | 3:N:632:VAL:HG11  | 1.98                     | 0.46              |
| 2:M:906:PHE:HB3   | 3:N:1067:VAL:HG22 | 1.95                     | 0.46              |
| 2:M:1050:GLN:CD   | 2:M:1079:PRO:HG2  | 2.40                     | 0.46              |
| 2:M:1056:LYS:C    | 8:N:2406:HOH:O    | 2.59                     | 0.46              |
| 3:N:472:ALA:N     | 8:N:9762:HOH:O    | 2.48                     | 0.46              |
| 3:N:640:HIS:HE1   | 3:N:717:GLN:CD    | 2.24                     | 0.46              |
| 3:N:794:GLN:O     | 3:N:861:GLN:HB3   | 2.15                     | 0.46              |
| 3:N:1408:ILE:HG21 | 8:N:9555:HOH:O    | 2.16                     | 0.46              |
| 3:N:1490:LYS:HZ2  | 4:O:39:VAL:HA     | 1.79                     | 0.46              |
| 5:P:94:LEU:HD12   | 5:P:97:GLU:HG2    | 1.98                     | 0.46              |
| 5:P:151:LEU:HB2   | 5:P:155:THR:CB    | 2.45                     | 0.46              |
| 1:B:32:PHE:C      | 8:B:9655:HOH:O    | 2.58                     | 0.45              |
| 2:C:449:ILE:N     | 8:C:9931:HOH:O    | 2.48                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:474:VAL:HG23  | 2:C:478:VAL:O    | 2.16                     | 0.45              |
| 2:C:647:GLN:NE2   | 2:C:650:ARG:NH2  | 2.64                     | 0.45              |
| 2:C:843:HIS:HD2   | 2:C:884:GLN:HB3  | 1.81                     | 0.45              |
| 2:C:949:LYS:HB3   | 3:D:796:ARG:HH21 | 1.79                     | 0.45              |
| 3:D:119:SER:H     | 3:D:123:LEU:CD1  | 2.29                     | 0.45              |
| 3:D:609:GLY:HA3   | 3:D:613:ARG:HB3  | 1.97                     | 0.45              |
| 3:D:613:ARG:HB2   | 8:D:9728:HOH:O   | 2.15                     | 0.45              |
| 3:D:1031:ASN:HB3  | 3:D:1034:GLN:CG  | 2.46                     | 0.45              |
| 3:D:1086:LEU:N    | 3:D:1086:LEU:CD1 | 2.79                     | 0.45              |
| 5:F:261:PRO:O     | 5:F:265:VAL:HG23 | 2.16                     | 0.45              |
| 1:K:64:GLU:O      | 1:K:64:GLU:HG2   | 2.16                     | 0.45              |
| 1:K:65:PHE:HE2    | 2:M:830:LYS:HG3  | 1.78                     | 0.45              |
| 1:K:149:GLY:N     | 8:K:5034:HOH:O   | 2.45                     | 0.45              |
| 2:M:63:GLY:HA3    | 2:M:103:LYS:HG2  | 1.97                     | 0.45              |
| 2:M:226:VAL:HG13  | 2:M:227:PHE:CE1  | 2.51                     | 0.45              |
| 2:M:237:ARG:O     | 2:M:240:THR:HB   | 2.17                     | 0.45              |
| 2:M:239:PHE:HE1   | 2:M:246:ASP:HB3  | 1.80                     | 0.45              |
| 2:M:589:ARG:HH11  | 2:M:589:ARG:HB2  | 1.81                     | 0.45              |
| 2:M:723:THR:C     | 2:M:725:ASP:H    | 2.23                     | 0.45              |
| 2:M:778:PHE:HA    | 8:M:9540:HOH:O   | 2.15                     | 0.45              |
| 2:M:1099:VAL:HG13 | 8:M:9533:HOH:O   | 2.15                     | 0.45              |
| 3:N:396:VAL:HG13  | 3:N:447:VAL:CA   | 2.42                     | 0.45              |
| 3:N:544:TYR:CZ    | 3:N:581:LEU:HD11 | 2.51                     | 0.45              |
| 3:N:956:ILE:HD11  | 3:N:1062:ARG:HB3 | 1.98                     | 0.45              |
| 3:N:1241:PHE:O    | 3:N:1243:THR:N   | 2.49                     | 0.45              |
| 4:O:46:PRO:HD2    | 8:O:707:HOH:O    | 2.15                     | 0.45              |
| 4:O:52:GLU:HB2    | 4:O:55:PHE:HE2   | 1.79                     | 0.45              |
| 5:P:170:HIS:HA    | 5:P:173:TYR:CD1  | 2.51                     | 0.45              |
| 5:P:318:GLU:HB2   | 5:P:328:PHE:HE2  | 1.81                     | 0.45              |
| 1:A:162:ILE:HG13  | 1:A:163:ASN:N    | 2.31                     | 0.45              |
| 2:C:54:ILE:HG12   | 8:C:9524:HOH:O   | 2.17                     | 0.45              |
| 2:C:277:ALA:O     | 2:C:281:LEU:O    | 2.33                     | 0.45              |
| 2:C:341:THR:HG23  | 2:C:345:ARG:HH21 | 1.81                     | 0.45              |
| 2:C:428:ARG:HE    | 2:C:451:LEU:HG   | 1.80                     | 0.45              |
| 2:C:516:ARG:HB2   | 8:C:9494:HOH:O   | 2.15                     | 0.45              |
| 2:C:516:ARG:HH11  | 2:C:521:PRO:HG3  | 1.81                     | 0.45              |
| 2:C:575:GLN:HA    | 2:C:662:GLU:OE2  | 2.17                     | 0.45              |
| 2:C:679:PHE:CD1   | 2:C:870:ILE:HD13 | 2.51                     | 0.45              |
| 2:C:1044:GLY:O    | 2:C:1046:ALA:N   | 2.49                     | 0.45              |
| 3:D:469:ASP:N     | 8:D:2520:HOH:O   | 2.48                     | 0.45              |
| 3:D:902:LEU:N     | 8:D:2567:HOH:O   | 2.48                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:916:TYR:C     | 3:D:916:TYR:CD2   | 2.94                     | 0.45              |
| 5:F:371:LEU:HD22  | 5:F:375:LEU:HD12  | 1.96                     | 0.45              |
| 1:K:191:ASP:O     | 1:K:192:LEU:HD23  | 2.16                     | 0.45              |
| 1:K:213:GLN:O     | 1:K:217:ILE:HG13  | 2.15                     | 0.45              |
| 1:K:224:TYR:HB3   | 1:L:9:PRO:HB2     | 1.99                     | 0.45              |
| 1:L:91:ASN:HB2    | 1:L:92:PRO:CD     | 2.46                     | 0.45              |
| 1:L:222:LEU:HB2   | 8:L:2116:HOH:O    | 2.15                     | 0.45              |
| 2:M:309:TYR:O     | 2:M:313:LEU:HB3   | 2.17                     | 0.45              |
| 2:M:691:SER:HB2   | 2:M:858:MET:SD    | 2.56                     | 0.45              |
| 3:N:101:HIS:CD2   | 3:N:582:LEU:CD1   | 2.96                     | 0.45              |
| 3:N:891:GLU:O     | 3:N:891:GLU:HG3   | 2.16                     | 0.45              |
| 3:N:1304:LYS:HA   | 8:N:9663:HOH:O    | 2.14                     | 0.45              |
| 3:N:1433:SER:HB2  | 3:N:1457:ASP:CG   | 2.41                     | 0.45              |
| 5:P:97:GLU:O      | 5:P:101:GLU:HB2   | 2.16                     | 0.45              |
| 5:P:163:LEU:HD22  | 5:P:174:LEU:CG    | 2.39                     | 0.45              |
| 5:P:410:TYR:O     | 5:P:414:ARG:HG2   | 2.16                     | 0.45              |
| 2:C:148:PHE:CE1   | 2:C:309:TYR:HB3   | 2.50                     | 0.45              |
| 2:C:474:VAL:HA    | 2:C:478:VAL:O     | 2.16                     | 0.45              |
| 2:C:734:LEU:O     | 2:C:735:ARG:C     | 2.59                     | 0.45              |
| 2:C:1031:ARG:HG2  | 2:C:1031:ARG:HH11 | 1.81                     | 0.45              |
| 3:D:65:ARG:CD     | 5:F:374:GLY:O     | 2.65                     | 0.45              |
| 3:D:116:LEU:C     | 3:D:118:LEU:HD13  | 2.41                     | 0.45              |
| 3:D:118:LEU:O     | 3:D:119:SER:C     | 2.59                     | 0.45              |
| 3:D:186:VAL:CG1   | 3:D:187:LYS:N     | 2.79                     | 0.45              |
| 3:D:549:ASN:ND2   | 8:D:9505:HOH:O    | 2.48                     | 0.45              |
| 3:D:678:GLU:HG3   | 3:D:679:ARG:HG3   | 1.98                     | 0.45              |
| 3:D:984:THR:CG2   | 3:D:987:GLU:H     | 2.25                     | 0.45              |
| 3:D:1073:SER:HB2  | 8:D:9564:HOH:O    | 2.15                     | 0.45              |
| 3:D:1207:TYR:H    | 3:D:1366:LYS:NZ   | 2.14                     | 0.45              |
| 3:D:1437:ALA:HB3  | 3:D:1446:VAL:CG1  | 2.47                     | 0.45              |
| 3:D:1503:VAL:HG11 | 8:D:2173:HOH:O    | 2.16                     | 0.45              |
| 1:K:44:LEU:HD23   | 1:K:48:ILE:HD12   | 1.99                     | 0.45              |
| 2:M:3:ILE:HD13    | 2:M:900:ARG:O     | 2.16                     | 0.45              |
| 2:M:77:PRO:HD3    | 2:M:93:PRO:HD3    | 1.97                     | 0.45              |
| 2:M:318:PRO:HB2   | 2:M:321:GLU:OE1   | 2.16                     | 0.45              |
| 2:M:473:ARG:HG3   | 2:M:474:VAL:N     | 2.30                     | 0.45              |
| 2:M:606:VAL:CG2   | 2:M:645:VAL:HG13  | 2.35                     | 0.45              |
| 2:M:1043:TYR:CZ   | 3:N:763:MET:HG3   | 2.51                     | 0.45              |
| 2:M:1097:LEU:HD13 | 2:M:1097:LEU:N    | 2.30                     | 0.45              |
| 3:N:379:ALA:HB2   | 8:N:9622:HOH:O    | 2.15                     | 0.45              |
| 3:N:550:ARG:CD    | 3:N:573:MET:HE3   | 2.47                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:576:GLU:O     | 3:N:579:ASP:HB2  | 2.16                     | 0.45              |
| 3:N:786:ILE:HD13  | 3:N:1027:GLY:HA3 | 1.99                     | 0.45              |
| 3:N:809:PRO:HD2   | 8:N:9498:HOH:O   | 2.14                     | 0.45              |
| 3:N:893:GLU:O     | 3:N:896:ALA:HB3  | 2.16                     | 0.45              |
| 3:N:1124:GLN:CD   | 3:N:1135:ARG:HA  | 2.41                     | 0.45              |
| 3:N:1159:ARG:CZ   | 3:N:1159:ARG:HB2 | 2.46                     | 0.45              |
| 2:C:10:ARG:O      | 2:C:12:VAL:N     | 2.49                     | 0.45              |
| 2:C:216:GLU:C     | 2:C:218:VAL:H    | 2.25                     | 0.45              |
| 2:C:309:TYR:O     | 2:C:313:LEU:N    | 2.37                     | 0.45              |
| 2:C:338:GLU:CA    | 2:C:341:THR:HG22 | 2.45                     | 0.45              |
| 2:C:413:LEU:HD11  | 2:C:451:LEU:HB3  | 1.99                     | 0.45              |
| 2:C:840:ALA:HB2   | 2:C:846:LYS:HA   | 1.98                     | 0.45              |
| 3:D:2:LYS:HD2     | 8:D:2092:HOH:O   | 2.17                     | 0.45              |
| 3:D:397:LYS:HG2   | 3:D:397:LYS:O    | 2.15                     | 0.45              |
| 3:D:567:ILE:HG22  | 3:D:571:LYS:HE3  | 1.99                     | 0.45              |
| 3:D:994:GLN:HG2   | 8:D:9597:HOH:O   | 2.16                     | 0.45              |
| 3:D:1111:ASP:O    | 3:D:1111:ASP:OD2 | 2.34                     | 0.45              |
| 3:D:1162:GLU:HG2  | 3:D:1163:GLY:N   | 2.32                     | 0.45              |
| 3:D:1491:THR:HG21 | 4:E:89:MET:SD    | 2.57                     | 0.45              |
| 5:F:141:VAL:CG1   | 5:F:142:ARG:N    | 2.79                     | 0.45              |
| 5:F:278:LEU:HB2   | 5:F:286:PRO:HG2  | 1.98                     | 0.45              |
| 5:F:365:GLU:HB2   | 5:F:400:ILE:HG21 | 1.97                     | 0.45              |
| 2:M:276:LYS:HG2   | 2:M:280:LYS:HE3  | 1.97                     | 0.45              |
| 2:M:626:ARG:NH2   | 8:M:2096:HOH:O   | 2.50                     | 0.45              |
| 2:M:711:GLU:HB2   | 8:M:9684:HOH:O   | 2.16                     | 0.45              |
| 2:M:888:THR:HG21  | 8:M:9676:HOH:O   | 2.16                     | 0.45              |
| 3:N:9:ARG:HA      | 3:N:1434:TRP:HH2 | 1.82                     | 0.45              |
| 3:N:414:ARG:HG2   | 8:N:2350:HOH:O   | 2.16                     | 0.45              |
| 3:N:471:GLU:CG    | 8:N:9534:HOH:O   | 2.64                     | 0.45              |
| 3:N:545:ARG:HB3   | 3:N:545:ARG:HH11 | 1.80                     | 0.45              |
| 3:N:865:THR:HG23  | 3:N:874:GLU:CG   | 2.45                     | 0.45              |
| 3:N:1436:SER:HA   | 8:N:2074:HOH:O   | 2.16                     | 0.45              |
| 1:A:13:VAL:HG12   | 1:A:15:THR:HG22  | 1.98                     | 0.45              |
| 1:A:62:LEU:HD12   | 1:A:62:LEU:H     | 1.81                     | 0.45              |
| 2:C:774:LEU:HD13  | 2:C:775:ARG:N    | 2.32                     | 0.45              |
| 2:C:957:LYS:CG    | 2:C:961:GLU:HB3  | 2.47                     | 0.45              |
| 3:D:161:LEU:O     | 3:D:449:SER:CB   | 2.63                     | 0.45              |
| 3:D:540:LEU:HD23  | 3:D:540:LEU:HA   | 1.84                     | 0.45              |
| 3:D:540:LEU:HD23  | 3:D:543:LEU:HD12 | 1.99                     | 0.45              |
| 3:D:914:LEU:HD23  | 3:D:914:LEU:O    | 2.17                     | 0.45              |
| 3:D:1164:ARG:HH11 | 3:D:1164:ARG:HG3 | 1.82                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:1312:LEU:HD11 | 3:D:1327:ARG:HG3 | 1.98                     | 0.45              |
| 1:K:18:ARG:N      | 8:K:1202:HOH:O   | 2.49                     | 0.45              |
| 2:M:637:LEU:N     | 2:M:637:LEU:HD23 | 2.32                     | 0.45              |
| 2:M:713:ARG:HB2   | 2:M:720:GLU:OE1  | 2.17                     | 0.45              |
| 2:M:873:PRO:HB3   | 3:N:949:ILE:HG13 | 1.98                     | 0.45              |
| 2:M:928:LYS:O     | 2:M:932:GLU:HG3  | 2.16                     | 0.45              |
| 3:N:27:GLU:C      | 3:N:28:LYS:HG3   | 2.42                     | 0.45              |
| 3:N:166:GLN:HB3   | 3:N:395:VAL:CG2  | 2.46                     | 0.45              |
| 3:N:423:ASP:OD1   | 5:P:175:HIS:ND1  | 2.49                     | 0.45              |
| 3:N:423:ASP:HB2   | 5:P:178:ARG:HB2  | 1.98                     | 0.45              |
| 3:N:525:ARG:NE    | 3:N:541:ASN:HD21 | 2.10                     | 0.45              |
| 3:N:581:LEU:O     | 3:N:603:LEU:HG   | 2.17                     | 0.45              |
| 3:N:754:PHE:HA    | 4:O:24:ALA:CB    | 2.47                     | 0.45              |
| 3:N:828:LYS:NZ    | 3:N:862:ASP:OD1  | 2.49                     | 0.45              |
| 3:N:843:PHE:HB3   | 8:N:9489:HOH:O   | 2.16                     | 0.45              |
| 3:N:1412:LYS:O    | 3:N:1412:LYS:HG3 | 2.16                     | 0.45              |
| 5:P:84:TYR:CE1    | 5:P:196:VAL:HG21 | 2.51                     | 0.45              |
| 5:P:263:HIS:NE2   | 5:P:264:MET:HE3  | 2.31                     | 0.45              |
| 1:A:5:LYS:HE3     | 1:A:5:LYS:CA     | 2.36                     | 0.45              |
| 1:A:49:PRO:O      | 1:A:173:PRO:CD   | 2.65                     | 0.45              |
| 1:A:53:VAL:HG12   | 1:A:167:VAL:HG21 | 1.99                     | 0.45              |
| 2:C:546:LEU:HD12  | 2:C:565:GLN:NE2  | 2.24                     | 0.45              |
| 2:C:774:LEU:HA    | 2:C:777:ILE:HD12 | 1.99                     | 0.45              |
| 2:C:957:LYS:HG2   | 2:C:961:GLU:CB   | 2.47                     | 0.45              |
| 2:C:1050:GLN:HG2  | 2:C:1079:PRO:HG2 | 1.97                     | 0.45              |
| 3:D:500:ARG:HH22  | 3:D:1388:ARG:HD3 | 1.80                     | 0.45              |
| 1:K:151:VAL:HB    | 1:K:169:ALA:HB3  | 1.98                     | 0.45              |
| 1:L:124:ASN:OD1   | 1:L:127:LEU:HB2  | 2.17                     | 0.45              |
| 2:M:17:PRO:HB2    | 8:M:9519:HOH:O   | 2.17                     | 0.45              |
| 2:M:44:ILE:HD12   | 2:M:44:ILE:H     | 1.82                     | 0.45              |
| 2:M:184:MET:HB2   | 2:M:193:LEU:HD23 | 1.98                     | 0.45              |
| 2:M:1047:HIS:CG   | 3:N:754:PHE:HB3  | 2.52                     | 0.45              |
| 2:M:1105:LYS:O    | 2:M:1107:ASN:N   | 2.50                     | 0.45              |
| 3:N:118:LEU:O     | 3:N:119:SER:C    | 2.60                     | 0.45              |
| 3:N:130:SER:HB2   | 3:N:132:TYR:HE1  | 1.82                     | 0.45              |
| 3:N:133:ILE:HA    | 3:N:455:ARG:O    | 2.16                     | 0.45              |
| 3:N:388:HIS:O     | 5:P:97:GLU:HG3   | 2.16                     | 0.45              |
| 3:N:539:ASP:HA    | 8:N:9616:HOH:O   | 2.16                     | 0.45              |
| 3:N:828:LYS:HD2   | 3:N:862:ASP:OD2  | 2.17                     | 0.45              |
| 3:N:1031:ASN:HB3  | 3:N:1034:GLN:CD  | 2.42                     | 0.45              |
| 3:N:1166:LEU:HB2  | 3:N:1170:ASP:HB2 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1336:LEU:HD12 | 3:N:1340:GLY:C    | 2.42                     | 0.45              |
| 4:O:40:LEU:HB2    | 4:O:45:ARG:NE     | 2.31                     | 0.45              |
| 4:O:72:ARG:HG2    | 4:O:72:ARG:HH11   | 1.81                     | 0.45              |
| 5:P:235:PHE:CE2   | 5:P:239:ALA:HB2   | 2.52                     | 0.45              |
| 1:A:45:LEU:HD21   | 1:A:177:VAL:HG23  | 1.98                     | 0.45              |
| 1:B:7:LYS:HZ2     | 1:B:186:LEU:HD22  | 1.82                     | 0.45              |
| 2:C:121:MET:HB2   | 2:C:127:PHE:HE2   | 1.82                     | 0.45              |
| 2:C:134:ARG:NH1   | 2:C:392:SER:OG    | 2.50                     | 0.45              |
| 2:C:216:GLU:O     | 2:C:218:VAL:N     | 2.49                     | 0.45              |
| 2:C:417:GLY:C     | 2:C:418:LEU:HD13  | 2.41                     | 0.45              |
| 2:C:501:THR:O     | 2:C:502:PRO:C     | 2.57                     | 0.45              |
| 2:C:730:SER:HB2   | 8:C:9654:HOH:O    | 2.16                     | 0.45              |
| 2:C:762:LYS:HA    | 2:C:786:LYS:HG3   | 1.98                     | 0.45              |
| 2:C:843:HIS:CD2   | 2:C:884:GLN:CA    | 3.00                     | 0.45              |
| 2:C:1102:LEU:HD23 | 2:C:1107:ASN:N    | 2.32                     | 0.45              |
| 3:D:580:ALA:HB3   | 8:D:2488:HOH:O    | 2.16                     | 0.45              |
| 3:D:633:VAL:O     | 3:D:635:PRO:HD3   | 2.16                     | 0.45              |
| 3:D:898:GLU:HA    | 8:D:2553:HOH:O    | 2.16                     | 0.45              |
| 3:D:1074:SER:O    | 3:D:1077:ALA:HB3  | 2.16                     | 0.45              |
| 3:D:1197:ARG:HG3  | 3:D:1198:TYR:CD1  | 2.51                     | 0.45              |
| 3:D:1401:GLU:HA   | 8:D:9583:HOH:O    | 2.16                     | 0.45              |
| 5:F:155:THR:HG22  | 5:F:156:VAL:N     | 2.31                     | 0.45              |
| 5:F:163:LEU:HB3   | 5:F:174:LEU:CG    | 2.46                     | 0.45              |
| 1:L:9:PRO:HG2     | 1:L:224:TYR:HB3   | 1.98                     | 0.45              |
| 1:L:161:ARG:HH11  | 1:L:161:ARG:HG3   | 1.81                     | 0.45              |
| 2:M:137:VAL:HG21  | 2:M:393:GLN:HE22  | 1.81                     | 0.45              |
| 2:M:188:LYS:HB2   | 8:M:9908:HOH:O    | 2.17                     | 0.45              |
| 2:M:292:ARG:HD2   | 2:M:299:LYS:HD3   | 1.99                     | 0.45              |
| 2:M:334:ARG:HB2   | 8:M:9656:HOH:O    | 2.17                     | 0.45              |
| 2:M:714:ASP:HB2   | 2:M:818:GLY:O     | 2.17                     | 0.45              |
| 2:M:1051:GLU:CD   | 3:N:752:SER:H     | 2.23                     | 0.45              |
| 3:N:126:VAL:HG11  | 3:N:152:LEU:HD12  | 1.97                     | 0.45              |
| 3:N:376:GLU:HA    | 3:N:384:VAL:HA    | 1.98                     | 0.45              |
| 3:N:521:PRO:HA    | 3:N:522:PRO:HD3   | 1.69                     | 0.45              |
| 3:N:591:VAL:CG1   | 3:N:597:ASP:HA    | 2.47                     | 0.45              |
| 3:N:711:LEU:HD12  | 3:N:778:LEU:CD2   | 2.47                     | 0.45              |
| 3:N:873:LEU:HD21  | 8:N:2008:HOH:O    | 2.17                     | 0.45              |
| 3:N:890:VAL:HG11  | 3:N:922:LEU:HD13  | 1.98                     | 0.45              |
| 3:N:1095:THR:O    | 3:N:1099:VAL:HG23 | 2.17                     | 0.45              |
| 3:N:1312:LEU:HD13 | 3:N:1326:THR:O    | 2.16                     | 0.45              |
| 4:O:32:ARG:NH2    | 8:O:1198:HOH:O    | 2.49                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:136:GLY:HA3   | 8:B:9645:HOH:O    | 2.17                     | 0.45              |
| 2:C:273:GLY:HA2   | 2:C:276:LYS:CD    | 2.45                     | 0.45              |
| 2:C:324:ASP:HB2   | 8:C:9878:HOH:O    | 2.15                     | 0.45              |
| 2:C:458:TYR:HB3   | 2:C:470:PRO:CG    | 2.40                     | 0.45              |
| 2:C:474:VAL:HG22  | 2:C:474:VAL:O     | 2.17                     | 0.45              |
| 2:C:666:LEU:HD11  | 2:C:668:LEU:HD21  | 1.99                     | 0.45              |
| 2:C:744:ARG:HG3   | 2:C:747:ALA:HB2   | 1.98                     | 0.45              |
| 2:C:752:GLY:H     | 2:C:792:VAL:HB    | 1.81                     | 0.45              |
| 2:C:1092:LEU:HA   | 2:C:1095:LEU:CD1  | 2.40                     | 0.45              |
| 3:D:481:MET:HE1   | 3:D:1388:ARG:HE   | 1.81                     | 0.45              |
| 3:D:546:ARG:NH2   | 3:D:550:ARG:NH2   | 2.65                     | 0.45              |
| 3:D:750:PRO:HG2   | 3:D:756:GLN:OE1   | 2.16                     | 0.45              |
| 3:D:1212:ALA:HB1  | 8:D:9608:HOH:O    | 2.17                     | 0.45              |
| 1:K:143:ARG:CG    | 1:K:143:ARG:NH1   | 2.70                     | 0.45              |
| 2:M:183:SER:HB2   | 2:M:190:LYS:HG2   | 1.98                     | 0.45              |
| 2:M:196:LEU:HD23  | 2:M:200:LEU:HD11  | 1.98                     | 0.45              |
| 2:M:263:ASP:CB    | 2:M:264:PRO:CD    | 2.95                     | 0.45              |
| 2:M:431:HIS:CG    | 2:M:432:ARG:N     | 2.85                     | 0.45              |
| 2:M:749:VAL:HG11  | 2:M:755:LEU:HD21  | 1.98                     | 0.45              |
| 3:N:67:ARG:HD3    | 8:N:2440:HOH:O    | 2.17                     | 0.45              |
| 3:N:126:VAL:HG12  | 3:N:127:LEU:N     | 2.32                     | 0.45              |
| 3:N:249:TYR:HA    | 8:N:2240:HOH:O    | 2.16                     | 0.45              |
| 3:N:899:LEU:HB2   | 3:N:917:GLN:HG2   | 1.98                     | 0.45              |
| 3:N:996:TRP:HB3   | 3:N:1044:LEU:HD11 | 1.99                     | 0.45              |
| 3:N:1041:LEU:HD12 | 3:N:1058:ARG:C    | 2.42                     | 0.45              |
| 3:N:1066:THR:OG1  | 3:N:1067:VAL:N    | 2.50                     | 0.45              |
| 3:N:1271:LYS:HE3  | 3:N:1334:GLN:NE2  | 2.31                     | 0.45              |
| 3:N:1485:GLN:HB2  | 8:N:2421:HOH:O    | 2.17                     | 0.45              |
| 5:P:321:ILE:HD11  | 5:P:329:TYR:HB2   | 1.98                     | 0.45              |
| 2:C:67:ASP:O      | 2:C:98:LEU:HD23   | 2.16                     | 0.45              |
| 2:C:148:PHE:HZ    | 2:C:281:LEU:HD13  | 1.81                     | 0.45              |
| 2:C:148:PHE:CZ    | 2:C:309:TYR:HB3   | 2.52                     | 0.45              |
| 2:C:243:ARG:HH11  | 2:C:243:ARG:HG2   | 1.82                     | 0.45              |
| 2:C:484:VAL:HG11  | 8:C:2006:HOH:O    | 2.17                     | 0.45              |
| 2:C:984:GLU:H     | 2:C:984:GLU:HG2   | 1.37                     | 0.45              |
| 2:C:1097:LEU:HD13 | 2:C:1097:LEU:HA   | 1.69                     | 0.45              |
| 2:C:1115:LEU:HD22 | 3:D:88:TYR:HD1    | 1.82                     | 0.45              |
| 3:D:9:ARG:CZ      | 3:D:11:ALA:HB2    | 2.47                     | 0.45              |
| 3:D:819:GLY:O     | 3:D:822:ALA:HB3   | 2.16                     | 0.45              |
| 3:D:879:ARG:NH1   | 3:D:904:VAL:C     | 2.74                     | 0.45              |
| 3:D:1129:THR:HG23 | 3:D:1130:ARG:H    | 1.82                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1213:ARG:HD3  | 8:D:9784:HOH:O    | 2.16                     | 0.45              |
| 3:D:1306:PRO:HG2  | 8:D:2005:HOH:O    | 2.17                     | 0.45              |
| 3:D:1460:ILE:HG23 | 8:D:9667:HOH:O    | 2.16                     | 0.45              |
| 4:E:41:GLU:HA     | 4:E:45:ARG:HG3    | 1.97                     | 0.45              |
| 5:F:271:LEU:HD23  | 5:F:295:MET:HG3   | 1.99                     | 0.45              |
| 1:K:89:PHE:HB2    | 1:K:94:LEU:HD22   | 1.99                     | 0.45              |
| 1:L:19:GLU:O      | 1:L:207:PRO:HG3   | 2.16                     | 0.45              |
| 1:L:24:VAL:HG22   | 1:L:196:THR:OG1   | 2.17                     | 0.45              |
| 1:L:109:VAL:HG23  | 1:L:132:LEU:HD13  | 1.99                     | 0.45              |
| 2:M:101:ILE:HD12  | 2:M:107:LEU:HD22  | 1.98                     | 0.45              |
| 2:M:460:ARG:NH2   | 8:M:9519:HOH:O    | 2.50                     | 0.45              |
| 2:M:625:LEU:CD1   | 2:M:641:PRO:HG3   | 2.47                     | 0.45              |
| 2:M:710:ILE:CG2   | 2:M:823:VAL:HB    | 2.43                     | 0.45              |
| 2:M:881:ASN:N     | 2:M:881:ASN:ND2   | 2.65                     | 0.45              |
| 2:M:939:ARG:NH1   | 2:M:981:GLU:HG2   | 2.32                     | 0.45              |
| 2:M:1071:ILE:O    | 3:N:659:LYS:HB2   | 2.17                     | 0.45              |
| 2:M:1095:LEU:HD13 | 3:N:103:TRP:CH2   | 2.52                     | 0.45              |
| 3:N:78:VAL:HG12   | 8:N:2191:HOH:O    | 2.17                     | 0.45              |
| 3:N:529:GLN:HA    | 8:N:9957:HOH:O    | 2.15                     | 0.45              |
| 3:N:600:LEU:HD23  | 8:N:9783:HOH:O    | 2.16                     | 0.45              |
| 3:N:975:GLU:CD    | 3:N:988:ARG:HH22  | 2.25                     | 0.45              |
| 3:N:1238:MET:HE3  | 3:N:1241:PHE:CE1  | 2.52                     | 0.45              |
| 3:N:1271:LYS:HZ3  | 3:N:1273:VAL:HG12 | 1.82                     | 0.45              |
| 3:N:1394:VAL:HB   | 3:N:1397:LYS:HD2  | 1.99                     | 0.45              |
| 5:P:114:LYS:HG3   | 8:P:9525:HOH:O    | 2.16                     | 0.45              |
| 5:P:142:ARG:HD3   | 5:P:150:THR:OG1   | 2.17                     | 0.45              |
| 5:P:222:ARG:HB3   | 5:P:242:TRP:CE3   | 2.52                     | 0.45              |
| 5:P:276:ARG:HG3   | 5:P:276:ARG:NH1   | 2.31                     | 0.45              |
| 5:P:278:LEU:HB2   | 5:P:286:PRO:HG2   | 1.99                     | 0.45              |
| 5:P:291:ILE:HG23  | 5:P:292:ALA:N     | 2.31                     | 0.45              |
| 1:A:48:ILE:HA     | 1:A:49:PRO:HD3    | 1.83                     | 0.45              |
| 1:A:50:GLY:HA3    | 1:A:171:PHE:O     | 2.17                     | 0.45              |
| 1:B:107:LYS:HG2   | 1:B:108:GLU:N     | 2.32                     | 0.45              |
| 2:C:525:SER:HA    | 8:C:9516:HOH:O    | 2.16                     | 0.45              |
| 2:C:551:GLU:H     | 2:C:551:GLU:HG3   | 1.38                     | 0.45              |
| 2:C:666:LEU:HD12  | 2:C:667:ALA:H     | 1.82                     | 0.45              |
| 2:C:983:ILE:HG21  | 2:C:987:ILE:HD11  | 1.99                     | 0.45              |
| 3:D:135:LEU:HD21  | 3:D:452:ILE:CD1   | 2.47                     | 0.45              |
| 3:D:166:GLN:HB3   | 3:D:395:VAL:HG21  | 1.99                     | 0.45              |
| 3:D:674:ARG:HH11  | 3:D:674:ARG:HG2   | 1.82                     | 0.45              |
| 3:D:1102:THR:O    | 3:D:1102:THR:HG22 | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1209:LEU:C    | 3:D:1211:MET:N    | 2.70                     | 0.45              |
| 4:E:27:ALA:HB2    | 4:E:61:GLU:HB3    | 1.99                     | 0.45              |
| 5:F:148:LYS:O     | 5:F:148:LYS:CD    | 2.58                     | 0.45              |
| 5:F:291:ILE:HG23  | 5:F:292:ALA:N     | 2.31                     | 0.45              |
| 1:K:39:PRO:CG     | 1:L:39:PRO:HG2    | 2.43                     | 0.45              |
| 2:M:265:ARG:HB3   | 8:M:9905:HOH:O    | 2.16                     | 0.45              |
| 2:M:375:SER:HA    | 8:M:9662:HOH:O    | 2.16                     | 0.45              |
| 2:M:393:GLN:HE21  | 2:M:409:ARG:HH12  | 1.63                     | 0.45              |
| 2:M:444:PRO:HD3   | 2:M:452:ILE:O     | 2.17                     | 0.45              |
| 2:M:1006:HIS:HA   | 2:M:1027:PHE:CZ   | 2.51                     | 0.45              |
| 3:N:240:GLU:O     | 3:N:242:LEU:N     | 2.50                     | 0.45              |
| 3:N:583:ASP:OD1   | 3:N:604:THR:CB    | 2.58                     | 0.45              |
| 3:N:778:LEU:HA    | 3:N:778:LEU:HD12  | 1.74                     | 0.45              |
| 3:N:914:LEU:HD22  | 3:N:930:LEU:HD21  | 1.99                     | 0.45              |
| 3:N:1126:ASP:OD1  | 3:N:1129:THR:O    | 2.35                     | 0.45              |
| 3:N:1148:VAL:HG23 | 3:N:1165:TYR:CD2  | 2.51                     | 0.45              |
| 4:O:94:PRO:HG3    | 8:O:4486:HOH:O    | 2.17                     | 0.45              |
| 5:P:209:PHE:CE2   | 5:P:213:ILE:HD11  | 2.52                     | 0.45              |
| 5:P:411:HIS:HB2   | 5:P:414:ARG:NE    | 2.31                     | 0.45              |
| 1:B:81:ASN:ND2    | 8:B:9514:HOH:O    | 2.50                     | 0.44              |
| 1:B:88:ARG:CB     | 1:B:123:MET:HE2   | 2.47                     | 0.44              |
| 2:C:136:ILE:HD11  | 8:C:9659:HOH:O    | 2.17                     | 0.44              |
| 2:C:230:ARG:HA    | 2:C:231:PRO:HD3   | 1.57                     | 0.44              |
| 2:C:486:MET:HG2   | 8:C:9678:HOH:O    | 2.16                     | 0.44              |
| 2:C:544:THR:HG22  | 2:C:547:ILE:HD12  | 1.99                     | 0.44              |
| 2:C:625:LEU:O     | 2:C:627:ARG:N     | 2.50                     | 0.44              |
| 2:C:774:LEU:CD1   | 5:F:421:PHE:HE2   | 2.24                     | 0.44              |
| 2:C:926:PHE:HD1   | 8:C:9628:HOH:O    | 2.00                     | 0.44              |
| 3:D:10:ILE:HD11   | 3:D:1434:TRP:NE1  | 2.31                     | 0.44              |
| 3:D:146:PRO:HB2   | 8:D:9853:HOH:O    | 2.17                     | 0.44              |
| 3:D:695:ILE:HG22  | 8:D:2155:HOH:O    | 2.17                     | 0.44              |
| 3:D:701:LEU:HD21  | 3:D:763:MET:HE3   | 1.99                     | 0.44              |
| 3:D:1336:LEU:HD13 | 3:D:1344:VAL:HG21 | 1.99                     | 0.44              |
| 3:D:1476:THR:CG2  | 4:E:21:VAL:HG22   | 2.47                     | 0.44              |
| 3:D:1491:THR:CB   | 4:E:89:MET:HE1    | 2.46                     | 0.44              |
| 5:F:76:SER:O      | 5:F:77:THR:C      | 2.58                     | 0.44              |
| 5:F:284:ARG:O     | 5:F:285:GLU:C     | 2.59                     | 0.44              |
| 1:L:27:PRO:HG2    | 1:L:186:LEU:CD1   | 2.46                     | 0.44              |
| 1:L:115:LEU:HB3   | 8:L:2300:HOH:O    | 2.16                     | 0.44              |
| 2:M:3:ILE:HD13    | 2:M:3:ILE:HA      | 1.81                     | 0.44              |
| 2:M:264:PRO:CB    | 2:M:289:THR:CB    | 2.94                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:266:ARG:CD    | 2:M:273:GLY:HA3  | 2.47                     | 0.44              |
| 2:M:597:ALA:HB2   | 2:M:655:LEU:HD21 | 1.98                     | 0.44              |
| 2:M:1018:GLN:NE2  | 5:P:338:LEU:HD13 | 2.32                     | 0.44              |
| 3:N:141:ILE:HD12  | 3:N:141:ILE:H    | 1.80                     | 0.44              |
| 3:N:433:GLY:HA3   | 8:N:2094:HOH:O   | 2.17                     | 0.44              |
| 3:N:486:ARG:CA    | 3:N:489:ARG:HD3  | 2.47                     | 0.44              |
| 3:N:683:ILE:CG2   | 3:N:687:VAL:HG21 | 2.47                     | 0.44              |
| 3:N:1209:LEU:HD21 | 3:N:1216:SER:HB2 | 1.99                     | 0.44              |
| 3:N:1341:PRO:HD2  | 3:N:1342:GLU:OE2 | 2.17                     | 0.44              |
| 4:O:3:GLU:HB3     | 8:O:1282:HOH:O   | 2.17                     | 0.44              |
| 5:P:393:THR:CG2   | 5:P:394:ARG:N    | 2.79                     | 0.44              |
| 1:A:156:HIS:CD2   | 1:A:157:GLY:H    | 2.35                     | 0.44              |
| 2:C:67:ASP:HA     | 8:C:9488:HOH:O   | 2.17                     | 0.44              |
| 2:C:89:THR:CA     | 2:C:129:ILE:O    | 2.61                     | 0.44              |
| 2:C:192:PRO:C     | 2:C:194:VAL:N    | 2.75                     | 0.44              |
| 2:C:772:ARG:NH2   | 8:C:2204:HOH:O   | 2.49                     | 0.44              |
| 2:C:843:HIS:NE2   | 2:C:887:GLU:OE2  | 2.50                     | 0.44              |
| 3:D:98:PRO:C      | 3:D:458:ALA:HB3  | 2.42                     | 0.44              |
| 3:D:447:VAL:HG23  | 3:D:448:GLU:N    | 2.32                     | 0.44              |
| 3:D:567:ILE:C     | 3:D:571:LYS:NZ   | 2.76                     | 0.44              |
| 3:D:637:LEU:HD11  | 3:D:642:CYS:CA   | 2.46                     | 0.44              |
| 3:D:693:GLU:HG3   | 4:E:48:MET:HE1   | 1.99                     | 0.44              |
| 3:D:729:HIS:ND1   | 3:D:730:PRO:N    | 2.66                     | 0.44              |
| 3:D:1097:LYS:H    | 3:D:1097:LYS:HG2 | 1.47                     | 0.44              |
| 4:E:51:LEU:CG     | 4:E:53:GLY:H     | 2.21                     | 0.44              |
| 5:F:358:LEU:O     | 5:F:358:LEU:HD23 | 2.17                     | 0.44              |
| 5:F:408:LEU:HA    | 5:F:411:HIS:CE1  | 2.52                     | 0.44              |
| 5:F:415:THR:CG2   | 5:F:417:LYS:NZ   | 2.80                     | 0.44              |
| 1:K:20:TYR:HE2    | 1:K:198:ARG:HB3  | 1.82                     | 0.44              |
| 2:M:136:ILE:CD1   | 2:M:392:SER:HB2  | 2.43                     | 0.44              |
| 2:M:190:LYS:HE2   | 8:M:2075:HOH:O   | 2.17                     | 0.44              |
| 2:M:433:THR:O     | 2:M:437:ARG:HG3  | 2.17                     | 0.44              |
| 2:M:557:ARG:NE    | 2:M:560:MET:SD   | 2.90                     | 0.44              |
| 2:M:589:ARG:HD3   | 2:M:596:TYR:CE2  | 2.52                     | 0.44              |
| 2:M:858:MET:HB2   | 2:M:859:PRO:HD2  | 1.98                     | 0.44              |
| 2:M:939:ARG:HH11  | 2:M:981:GLU:HG2  | 1.82                     | 0.44              |
| 3:N:75:ARG:HD3    | 8:N:2038:HOH:O   | 2.17                     | 0.44              |
| 3:N:207:PHE:CB    | 3:N:208:PRO:HD2  | 2.30                     | 0.44              |
| 3:N:436:GLU:HB2   | 3:N:445:ARG:CB   | 2.45                     | 0.44              |
| 3:N:704:ARG:HG3   | 3:N:736:PHE:HB3  | 1.99                     | 0.44              |
| 3:N:807:ALA:HB1   | 8:N:2335:HOH:O   | 2.17                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:826:PRO:CD    | 3:N:829:VAL:HG22 | 2.41                     | 0.44              |
| 3:N:830:ALA:HB2   | 8:N:9597:HOH:O   | 2.17                     | 0.44              |
| 3:N:1012:GLU:CD   | 8:N:2184:HOH:O   | 2.59                     | 0.44              |
| 3:N:1045:MET:SD   | 3:N:1073:SER:HB2 | 2.57                     | 0.44              |
| 3:N:1148:VAL:HG23 | 3:N:1165:TYR:CE2 | 2.52                     | 0.44              |
| 3:N:1487:VAL:HG21 | 4:O:79:LEU:HG    | 2.00                     | 0.44              |
| 1:A:9:PRO:HG2     | 1:B:224:TYR:CG   | 2.53                     | 0.44              |
| 1:A:83:LYS:NZ     | 2:C:698:ASP:OD2  | 2.50                     | 0.44              |
| 1:B:81:ASN:HB2    | 8:B:9519:HOH:O   | 2.18                     | 0.44              |
| 2:C:49:ARG:HB3    | 8:C:9834:HOH:O   | 2.18                     | 0.44              |
| 2:C:260:LEU:HB2   | 2:C:291:ALA:HB1  | 2.00                     | 0.44              |
| 2:C:627:ARG:HD2   | 8:C:2176:HOH:O   | 2.17                     | 0.44              |
| 2:C:722:ILE:HG21  | 2:C:821:GLU:OE1  | 2.18                     | 0.44              |
| 2:C:1024:LYS:HB2  | 2:C:1024:LYS:HE3 | 1.88                     | 0.44              |
| 3:D:79:GLU:HG2    | 3:D:80:VAL:N     | 2.31                     | 0.44              |
| 3:D:127:LEU:HD12  | 3:D:457:GLY:H    | 1.82                     | 0.44              |
| 3:D:207:PHE:HB3   | 3:D:208:PRO:CD   | 2.42                     | 0.44              |
| 3:D:642:CYS:SG    | 3:D:716:PHE:HB2  | 2.58                     | 0.44              |
| 3:D:804:LEU:HD12  | 3:D:831:GLY:HA3  | 1.99                     | 0.44              |
| 3:D:937:TYR:HA    | 3:D:940:THR:OG1  | 2.17                     | 0.44              |
| 3:D:964:LEU:O     | 3:D:968:ASP:HB2  | 2.17                     | 0.44              |
| 4:E:51:LEU:HB2    | 8:E:9429:HOH:O   | 2.17                     | 0.44              |
| 2:M:71:TYR:O      | 2:M:71:TYR:CG    | 2.70                     | 0.44              |
| 2:M:172:ILE:HG22  | 2:M:173:ASP:N    | 2.32                     | 0.44              |
| 2:M:411:SER:CB    | 2:M:452:ILE:HG23 | 2.47                     | 0.44              |
| 2:M:559:LEU:CD1   | 2:M:563:ASN:ND2  | 2.81                     | 0.44              |
| 2:M:588:VAL:HG23  | 2:M:589:ARG:N    | 2.31                     | 0.44              |
| 3:N:194:GLY:N     | 3:N:206:ARG:HD3  | 2.32                     | 0.44              |
| 3:N:710:ARG:NH1   | 3:N:1210:SER:OG  | 2.50                     | 0.44              |
| 3:N:796:ARG:H     | 3:N:796:ARG:HG2  | 1.59                     | 0.44              |
| 3:N:950:GLY:C     | 3:N:952:ASP:N    | 2.70                     | 0.44              |
| 3:N:1057:VAL:CG1  | 3:N:1069:GLU:HB3 | 2.47                     | 0.44              |
| 3:N:1062:ARG:HH11 | 3:N:1062:ARG:HG3 | 1.83                     | 0.44              |
| 3:N:1504:GLU:HB2  | 8:N:2110:HOH:O   | 2.16                     | 0.44              |
| 5:P:94:LEU:HD12   | 5:P:97:GLU:H     | 1.82                     | 0.44              |
| 5:P:278:LEU:HB3   | 5:P:286:PRO:HG2  | 2.00                     | 0.44              |
| 5:P:358:LEU:CD2   | 5:P:370:LYS:NZ   | 2.78                     | 0.44              |
| 5:P:416:ARG:HH11  | 5:P:419:ARG:CB   | 2.27                     | 0.44              |
| 1:A:81:ASN:ND2    | 1:A:128:HIS:O    | 2.51                     | 0.44              |
| 2:C:136:ILE:CG2   | 2:C:336:VAL:HG22 | 2.48                     | 0.44              |
| 2:C:175:GLU:HB3   | 2:C:183:SER:OG   | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:205:GLU:O     | 2:C:209:ARG:HD2   | 2.18                     | 0.44              |
| 2:C:486:MET:HE3   | 2:C:491:GLU:HA    | 1.99                     | 0.44              |
| 2:C:630:ARG:HH21  | 2:C:707:ARG:N     | 2.15                     | 0.44              |
| 2:C:1085:PHE:CE2  | 3:D:1468:LEU:HD23 | 2.53                     | 0.44              |
| 3:D:30:GLU:CB     | 3:D:40:GLU:HB3    | 2.43                     | 0.44              |
| 3:D:521:PRO:O     | 3:D:525:ARG:HG2   | 2.18                     | 0.44              |
| 3:D:565:ILE:HD13  | 5:F:192:LEU:HD13  | 2.00                     | 0.44              |
| 3:D:637:LEU:HD11  | 3:D:643:GLY:N     | 2.32                     | 0.44              |
| 3:D:680:GLN:O     | 3:D:683:ILE:HG13  | 2.18                     | 0.44              |
| 3:D:716:PHE:CE2   | 3:D:765:SER:HB3   | 2.53                     | 0.44              |
| 3:D:1101:VAL:O    | 3:D:1374:GLN:HG3  | 2.17                     | 0.44              |
| 3:D:1146:GLY:CA   | 3:D:1207:TYR:HB2  | 2.40                     | 0.44              |
| 3:D:1286:THR:CG2  | 3:D:1287:GLU:H    | 2.30                     | 0.44              |
| 5:F:328:PHE:HD2   | 5:F:328:PHE:HA    | 1.71                     | 0.44              |
| 5:F:406:ARG:HA    | 5:F:409:LYS:HG2   | 1.98                     | 0.44              |
| 1:L:143:ARG:HD3   | 1:L:158:ILE:HG21  | 1.99                     | 0.44              |
| 2:M:259:GLY:O     | 2:M:290:LEU:O     | 2.34                     | 0.44              |
| 2:M:326:ASP:HB3   | 2:M:431:HIS:CG    | 2.52                     | 0.44              |
| 2:M:610:ARG:CZ    | 8:M:2156:HOH:O    | 2.65                     | 0.44              |
| 2:M:1036:GLU:OE1  | 2:M:1036:GLU:N    | 2.49                     | 0.44              |
| 3:N:3:LYS:H       | 3:N:3:LYS:HG2     | 1.37                     | 0.44              |
| 3:N:153:LEU:HD23  | 3:N:153:LEU:N     | 2.33                     | 0.44              |
| 3:N:524:LEU:O     | 3:N:526:PRO:HD3   | 2.18                     | 0.44              |
| 3:N:1202:GLN:HE21 | 3:N:1202:GLN:HB2  | 1.62                     | 0.44              |
| 3:N:1393:GLN:HB2  | 3:N:1398:TRP:HE1  | 1.83                     | 0.44              |
| 4:O:28:GLN:HG2    | 8:O:1198:HOH:O    | 2.16                     | 0.44              |
| 5:P:89:GLY:HA3    | 8:P:9699:HOH:O    | 2.16                     | 0.44              |
| 5:P:122:LEU:HG    | 5:P:126:LEU:HD23  | 1.98                     | 0.44              |
| 1:A:158:ILE:HD13  | 1:A:158:ILE:HA    | 1.83                     | 0.44              |
| 2:C:106:GLY:O     | 2:C:107:LEU:HD23  | 2.17                     | 0.44              |
| 2:C:737:LEU:HA    | 2:C:743:VAL:HA    | 1.99                     | 0.44              |
| 2:C:737:LEU:O     | 2:C:738:ASP:C     | 2.61                     | 0.44              |
| 2:C:755:LEU:HD11  | 2:C:792:VAL:HG22  | 1.98                     | 0.44              |
| 2:C:843:HIS:HD2   | 2:C:884:GLN:CA    | 2.31                     | 0.44              |
| 2:C:950:LEU:HG    | 2:C:952:LEU:HD23  | 2.00                     | 0.44              |
| 3:D:8:VAL:HG12    | 3:D:1434:TRP:HH2  | 1.83                     | 0.44              |
| 3:D:699:VAL:HG12  | 3:D:717:GLN:HA    | 2.00                     | 0.44              |
| 3:D:1095:THR:HG23 | 3:D:1226:ALA:O    | 2.18                     | 0.44              |
| 3:D:1133:ARG:HB3  | 8:D:9645:HOH:O    | 2.17                     | 0.44              |
| 3:D:1241:PHE:CD2  | 3:D:1260:ILE:HG13 | 2.51                     | 0.44              |
| 3:D:1247:ALA:O    | 3:D:1248:GLY:C    | 2.61                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1311:LEU:C    | 8:D:9883:HOH:O    | 2.60                     | 0.44              |
| 3:D:1462:LEU:HD21 | 3:D:1474:ALA:HB2  | 1.99                     | 0.44              |
| 3:D:1464:GLU:HA   | 3:D:1467:ILE:CD1  | 2.47                     | 0.44              |
| 4:E:16:LYS:NZ     | 8:E:9422:HOH:O    | 2.50                     | 0.44              |
| 4:E:46:PRO:HB3    | 4:E:54:LEU:CD2    | 2.47                     | 0.44              |
| 5:F:88:ILE:HD13   | 5:F:193:ARG:HD3   | 1.98                     | 0.44              |
| 5:F:188:ILE:HD13  | 5:F:221:ILE:HG12  | 1.99                     | 0.44              |
| 5:F:260:ILE:CG1   | 5:F:264:MET:HB2   | 2.46                     | 0.44              |
| 5:F:270:LYS:HB3   | 5:F:295:MET:SD    | 2.57                     | 0.44              |
| 2:M:115:LEU:H     | 2:M:115:LEU:HG    | 1.53                     | 0.44              |
| 2:M:516:ARG:CD    | 3:N:1068:LEU:HD22 | 2.48                     | 0.44              |
| 2:M:572:ILE:HG12  | 2:M:701:THR:O     | 2.18                     | 0.44              |
| 2:M:679:PHE:O     | 2:M:681:GLY:N     | 2.43                     | 0.44              |
| 2:M:776:SER:HA    | 2:M:780:GLU:HB2   | 2.00                     | 0.44              |
| 2:M:841:ASN:ND2   | 2:M:843:HIS:N     | 2.65                     | 0.44              |
| 2:M:1019:GLN:HE22 | 3:N:621:LYS:CG    | 2.30                     | 0.44              |
| 2:M:1097:LEU:HD13 | 2:M:1097:LEU:H    | 1.83                     | 0.44              |
| 2:M:1109:VAL:HG13 | 3:N:3:LYS:O       | 2.18                     | 0.44              |
| 3:N:86:ARG:HD3    | 3:N:523:ASP:OD1   | 2.17                     | 0.44              |
| 3:N:137:PRO:HA    | 8:N:9761:HOH:O    | 2.17                     | 0.44              |
| 3:N:553:ARG:HH12  | 3:N:573:MET:HE1   | 1.82                     | 0.44              |
| 3:N:568:ARG:HB3   | 8:N:9947:HOH:O    | 2.17                     | 0.44              |
| 3:N:602:SER:O     | 3:N:605:ASP:HB2   | 2.17                     | 0.44              |
| 3:N:649:ALA:HB3   | 3:N:691:LEU:HD21  | 1.99                     | 0.44              |
| 3:N:955:VAL:HA    | 8:N:2329:HOH:O    | 2.17                     | 0.44              |
| 3:N:988:ARG:CZ    | 3:N:992:ILE:HD11  | 2.47                     | 0.44              |
| 3:N:1121:PRO:C    | 3:N:1122:LEU:HD12 | 2.43                     | 0.44              |
| 3:N:1364:HIS:CE1  | 3:N:1366:LYS:HG3  | 2.53                     | 0.44              |
| 3:N:1413:THR:O    | 3:N:1413:THR:HG22 | 2.17                     | 0.44              |
| 3:N:1475:GLY:HA2  | 8:N:9507:HOH:O    | 2.17                     | 0.44              |
| 3:N:1476:THR:O    | 3:N:1476:THR:HG22 | 2.17                     | 0.44              |
| 5:P:105:LYS:HD3   | 5:P:183:ALA:HB2   | 1.99                     | 0.44              |
| 5:P:347:GLN:O     | 5:P:351:SER:HB2   | 2.16                     | 0.44              |
| 5:P:419:ARG:O     | 5:P:421:PHE:N     | 2.51                     | 0.44              |
| 1:A:139:ASN:ND2   | 8:A:9489:HOH:O    | 2.50                     | 0.44              |
| 1:B:7:LYS:O       | 1:B:7:LYS:HG2     | 2.18                     | 0.44              |
| 1:B:119:ASP:OD1   | 1:B:119:ASP:N     | 2.49                     | 0.44              |
| 1:B:165:ILE:HA    | 1:B:166:PRO:HD3   | 1.88                     | 0.44              |
| 1:B:166:PRO:HB2   | 8:B:9542:HOH:O    | 2.17                     | 0.44              |
| 2:C:135:VAL:HB    | 2:C:406:HIS:HE1   | 1.81                     | 0.44              |
| 2:C:218:VAL:HG12  | 2:C:222:MET:HE2   | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:264:PRO:HB3   | 2:C:289:THR:CB    | 2.48                     | 0.44              |
| 2:C:515:ALA:C     | 2:C:516:ARG:HG2   | 2.42                     | 0.44              |
| 2:C:846:LYS:O     | 3:D:741:ASP:HB2   | 2.17                     | 0.44              |
| 3:D:179:VAL:HG12  | 3:D:183:GLU:OE2   | 2.18                     | 0.44              |
| 3:D:414:ARG:HA    | 8:D:9502:HOH:O    | 2.17                     | 0.44              |
| 3:D:589:ALA:HA    | 8:D:9687:HOH:O    | 2.17                     | 0.44              |
| 3:D:714:GLN:HE22  | 3:D:735:ALA:CB    | 2.30                     | 0.44              |
| 3:D:1000:THR:O    | 3:D:1003:VAL:HG22 | 2.17                     | 0.44              |
| 3:D:1007:VAL:CG2  | 3:D:1008:PHE:N    | 2.79                     | 0.44              |
| 3:D:1273:VAL:HG23 | 3:D:1273:VAL:O    | 2.16                     | 0.44              |
| 3:D:1359:GLN:HE21 | 3:D:1359:GLN:HB3  | 1.58                     | 0.44              |
| 5:F:301:ALA:N     | 8:F:9565:HOH:O    | 2.50                     | 0.44              |
| 1:K:5:LYS:O       | 1:K:8:ALA:CB      | 2.64                     | 0.44              |
| 1:K:9:PRO:CG      | 1:L:224:TYR:HB3   | 2.48                     | 0.44              |
| 2:M:12:VAL:HG13   | 2:M:13:ILE:HG12   | 1.99                     | 0.44              |
| 2:M:122:THR:HG22  | 2:M:123:GLU:N     | 2.32                     | 0.44              |
| 2:M:368:THR:CB    | 2:M:369:PRO:CD    | 2.96                     | 0.44              |
| 2:M:569:VAL:HG12  | 2:M:996:LYS:O     | 2.18                     | 0.44              |
| 2:M:625:LEU:O     | 2:M:627:ARG:N     | 2.51                     | 0.44              |
| 3:N:87:ARG:CG     | 3:N:88:TYR:N      | 2.79                     | 0.44              |
| 3:N:709:HIS:HD2   | 3:N:711:LEU:H     | 1.64                     | 0.44              |
| 3:N:786:ILE:HD13  | 3:N:1027:GLY:CA   | 2.48                     | 0.44              |
| 3:N:786:ILE:HD11  | 3:N:908:LYS:HB3   | 1.98                     | 0.44              |
| 3:N:825:ALA:HA    | 3:N:826:PRO:HD3   | 1.87                     | 0.44              |
| 3:N:965:GLU:OE1   | 3:N:968:ASP:HB3   | 2.18                     | 0.44              |
| 3:N:1118:ILE:HD13 | 3:N:1118:ILE:HA   | 1.80                     | 0.44              |
| 3:N:1273:VAL:HG23 | 3:N:1273:VAL:O    | 2.18                     | 0.44              |
| 3:N:1361:VAL:CG1  | 3:N:1363:LEU:HD23 | 2.48                     | 0.44              |
| 4:O:46:PRO:HG2    | 4:O:63:TRP:CD1    | 2.51                     | 0.44              |
| 5:P:385:GLU:O     | 5:P:397:ILE:HD13  | 2.18                     | 0.44              |
| 1:A:95:GLN:C      | 8:A:9431:HOH:O    | 2.61                     | 0.44              |
| 1:A:178:ALA:HB3   | 1:A:198:ARG:HG3   | 2.00                     | 0.44              |
| 1:A:180:GLN:HE21  | 2:C:934:PHE:HB2   | 1.76                     | 0.44              |
| 2:C:208:ALA:HA    | 2:C:218:VAL:CG2   | 2.48                     | 0.44              |
| 3:D:36:THR:C      | 3:D:38:LYS:N      | 2.76                     | 0.44              |
| 3:D:68:PHE:CZ     | 5:F:375:LEU:CD2   | 3.01                     | 0.44              |
| 3:D:83:SER:O      | 3:D:86:ARG:HB3    | 2.16                     | 0.44              |
| 3:D:88:TYR:HA     | 8:D:9471:HOH:O    | 2.17                     | 0.44              |
| 3:D:177:ALA:HB1   | 3:D:199:LEU:CD1   | 2.47                     | 0.44              |
| 3:D:539:ASP:HA    | 8:D:2538:HOH:O    | 2.17                     | 0.44              |
| 3:D:539:ASP:OD1   | 3:D:600:LEU:HD22  | 2.17                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:960:LYS:HG2   | 3:D:964:LEU:CD1  | 2.47                     | 0.44              |
| 3:D:1065:LEU:CD1  | 3:D:1069:GLU:HB3 | 2.46                     | 0.44              |
| 3:D:1320:GLU:H    | 3:D:1323:GLN:NE2 | 2.16                     | 0.44              |
| 5:F:95:THR:HG22   | 5:F:96:LEU:HD23  | 1.99                     | 0.44              |
| 1:K:11:PHE:HD2    | 8:L:679:HOH:O    | 2.00                     | 0.44              |
| 1:K:189:ARG:NH1   | 1:L:155:LYS:NZ   | 2.65                     | 0.44              |
| 2:M:202:TYR:O     | 2:M:207:LEU:HD12 | 2.18                     | 0.44              |
| 2:M:687:ALA:CB    | 8:M:9693:HOH:O   | 2.66                     | 0.44              |
| 2:M:762:LYS:NZ    | 2:M:784:ASP:C    | 2.74                     | 0.44              |
| 2:M:787:ASP:C     | 2:M:787:ASP:OD1  | 2.60                     | 0.44              |
| 2:M:1006:HIS:HA   | 2:M:1027:PHE:CE2 | 2.53                     | 0.44              |
| 2:M:1054:THR:CG2  | 2:M:1059:ASP:HB2 | 2.48                     | 0.44              |
| 3:N:395:VAL:O     | 3:N:395:VAL:HG12 | 2.17                     | 0.44              |
| 3:N:430:ASP:HB2   | 3:N:432:TYR:CZ   | 2.51                     | 0.44              |
| 3:N:566:ILE:HD11  | 5:P:192:LEU:HD21 | 2.00                     | 0.44              |
| 3:N:658:LEU:HD11  | 3:N:674:ARG:HH11 | 1.83                     | 0.44              |
| 3:N:660:LYS:HE3   | 3:N:693:GLU:OE1  | 2.18                     | 0.44              |
| 3:N:764:LEU:HG    | 3:N:765:SER:N    | 2.33                     | 0.44              |
| 3:N:1083:ASP:O    | 3:N:1087:ARG:CG  | 2.65                     | 0.44              |
| 3:N:1281:VAL:HG21 | 3:N:1313:VAL:CG2 | 2.48                     | 0.44              |
| 1:A:111:ALA:HB3   | 1:A:124:ASN:O    | 2.18                     | 0.44              |
| 2:C:203:ASP:OD1   | 2:C:206:THR:HB   | 2.18                     | 0.44              |
| 2:C:272:ALA:O     | 2:C:276:LYS:HD2  | 2.17                     | 0.44              |
| 2:C:301:GLU:O     | 2:C:305:PRO:HG2  | 2.17                     | 0.44              |
| 3:D:138:LYS:HA    | 8:D:2105:HOH:O   | 2.18                     | 0.44              |
| 3:D:202:VAL:HG22  | 8:D:2526:HOH:O   | 2.18                     | 0.44              |
| 3:D:210:ARG:CD    | 3:D:398:ALA:HB3  | 2.40                     | 0.44              |
| 3:D:240:GLU:O     | 3:D:241:ILE:C    | 2.61                     | 0.44              |
| 3:D:423:ASP:OD1   | 5:F:175:HIS:CE1  | 2.71                     | 0.44              |
| 3:D:936:TYR:C     | 3:D:936:TYR:CD2  | 2.95                     | 0.44              |
| 3:D:959:GLU:HG3   | 3:D:1006:ALA:HB1 | 1.99                     | 0.44              |
| 4:E:44:GLU:O      | 4:E:45:ARG:HD3   | 2.17                     | 0.44              |
| 5:F:93:LEU:HG     | 5:F:190:ALA:HB3  | 1.98                     | 0.44              |
| 5:F:394:ARG:HA    | 5:F:397:ILE:CD1  | 2.38                     | 0.44              |
| 1:K:19:GLU:O      | 1:K:207:PRO:HG3  | 2.18                     | 0.44              |
| 1:K:88:ARG:CB     | 1:K:123:MET:HE2  | 2.48                     | 0.44              |
| 1:L:66:SER:O      | 1:L:75:VAL:HG23  | 2.18                     | 0.44              |
| 2:M:18:LEU:HD13   | 2:M:590:ASP:CG   | 2.43                     | 0.44              |
| 2:M:428:ARG:HA    | 2:M:450:GLY:HA3  | 1.99                     | 0.44              |
| 2:M:474:VAL:HA    | 2:M:478:VAL:O    | 2.18                     | 0.44              |
| 2:M:685:GLU:CB    | 8:N:2331:HOH:O   | 2.66                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:859:PRO:HB3   | 2:M:974:LEU:HD23  | 1.99                     | 0.44              |
| 2:M:1008:ARG:HG2  | 2:M:1008:ARG:HH11 | 1.83                     | 0.44              |
| 2:M:1108:PRO:O    | 3:N:3:LYS:HG3     | 2.16                     | 0.44              |
| 2:M:1115:LEU:HB3  | 8:N:9574:HOH:O    | 2.17                     | 0.44              |
| 3:N:93:ILE:HD13   | 3:N:547:LEU:HD23  | 1.98                     | 0.44              |
| 3:N:178:LEU:HD22  | 8:N:9638:HOH:O    | 2.18                     | 0.44              |
| 3:N:528:VAL:HG12  | 3:N:529:GLN:N     | 2.33                     | 0.44              |
| 3:N:669:ASN:OD1   | 3:N:672:ALA:HB2   | 2.18                     | 0.44              |
| 3:N:1197:ARG:HB2  | 3:N:1396:GLU:CG   | 2.48                     | 0.44              |
| 5:P:411:HIS:HA    | 5:P:414:ARG:HE    | 1.82                     | 0.44              |
| 1:B:156:HIS:CD2   | 1:B:157:GLY:N     | 2.85                     | 0.44              |
| 1:B:165:ILE:HG13  | 1:B:165:ILE:O     | 2.18                     | 0.44              |
| 2:C:148:PHE:HB2   | 2:C:313:LEU:HD22  | 1.99                     | 0.44              |
| 2:C:158:TYR:HE1   | 2:C:313:LEU:O     | 2.01                     | 0.44              |
| 2:C:204:GLN:NE2   | 8:C:9840:HOH:O    | 2.51                     | 0.44              |
| 2:C:304:LEU:HD23  | 2:C:304:LEU:C     | 2.43                     | 0.44              |
| 2:C:367:LEU:HA    | 2:C:371:LYS:HB2   | 2.00                     | 0.44              |
| 2:C:603:VAL:HG22  | 2:C:613:VAL:HG12  | 1.99                     | 0.44              |
| 2:C:742:VAL:HG12  | 2:C:743:VAL:N     | 2.33                     | 0.44              |
| 2:C:775:ARG:CZ    | 2:C:782:ALA:CB    | 2.96                     | 0.44              |
| 2:C:1021:LEU:CD2  | 5:F:332:PHE:HA    | 2.48                     | 0.44              |
| 3:D:128:TYR:HB3   | 3:D:129:PHE:CD1   | 2.52                     | 0.44              |
| 3:D:395:VAL:O     | 3:D:395:VAL:HG12  | 2.16                     | 0.44              |
| 3:D:631:ILE:CG2   | 3:D:745:MET:HB2   | 2.48                     | 0.44              |
| 3:D:762:GLN:HE21  | 4:E:20:THR:HG21   | 1.83                     | 0.44              |
| 3:D:998:GLU:O     | 3:D:1002:LYS:HG3  | 2.18                     | 0.44              |
| 3:D:1120:VAL:HB   | 3:D:1144:LEU:HD21 | 2.00                     | 0.44              |
| 3:D:1389:LEU:HD12 | 8:D:2466:HOH:O    | 2.18                     | 0.44              |
| 5:F:181:GLU:OE2   | 5:F:184:ARG:HD3   | 2.18                     | 0.44              |
| 5:F:385:GLU:O     | 5:F:397:ILE:HD13  | 2.17                     | 0.44              |
| 1:K:47:SER:CB     | 1:K:217:ILE:HD13  | 2.47                     | 0.44              |
| 1:K:64:GLU:OE2    | 1:K:76:VAL:HG22   | 2.18                     | 0.44              |
| 1:K:151:VAL:HG22  | 8:K:3959:HOH:O    | 2.18                     | 0.44              |
| 2:M:168:ARG:NH1   | 8:M:9881:HOH:O    | 2.50                     | 0.44              |
| 2:M:198:ARG:NH2   | 2:M:203:ASP:HB3   | 2.33                     | 0.44              |
| 2:M:974:LEU:HD11  | 2:M:989:VAL:HG11  | 2.00                     | 0.44              |
| 2:M:1005:MET:CE   | 3:N:648:MET:HB2   | 2.47                     | 0.44              |
| 2:M:1054:THR:HG23 | 2:M:1059:ASP:HB2  | 1.99                     | 0.44              |
| 3:N:413:ASP:OD1   | 3:N:421:LEU:HD13  | 2.16                     | 0.44              |
| 3:N:704:ARG:HE    | 3:N:705:ALA:H     | 1.64                     | 0.44              |
| 3:N:750:PRO:HG2   | 3:N:756:GLN:OE1   | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1106:VAL:HG12 | 3:N:1107:VAL:N    | 2.33                     | 0.44              |
| 3:N:1223:ILE:O    | 3:N:1227:GLN:HG3  | 2.18                     | 0.44              |
| 4:O:71:GLY:C      | 8:O:690:HOH:O     | 2.60                     | 0.44              |
| 5:P:328:PHE:HD1   | 8:P:9750:HOH:O    | 2.00                     | 0.44              |
| 1:A:44:LEU:HD23   | 1:A:48:ILE:CD1    | 2.48                     | 0.43              |
| 1:A:83:LYS:HE3    | 1:A:167:VAL:HG12  | 2.00                     | 0.43              |
| 1:A:177:VAL:O     | 2:C:864:GLY:CA    | 2.65                     | 0.43              |
| 2:C:50:GLU:HG3    | 2:C:265:ARG:NH1   | 2.33                     | 0.43              |
| 2:C:94:LEU:CD1    | 8:C:9663:HOH:O    | 2.66                     | 0.43              |
| 2:C:133:ASP:CG    | 8:C:2286:HOH:O    | 2.62                     | 0.43              |
| 2:C:395:LYS:HE2   | 2:C:403:SER:HB2   | 1.99                     | 0.43              |
| 2:C:517:ARG:HD2   | 8:C:9983:HOH:O    | 2.17                     | 0.43              |
| 2:C:787:ASP:N     | 8:C:2178:HOH:O    | 2.45                     | 0.43              |
| 2:C:1005:MET:HE1  | 3:D:645:PRO:CB    | 2.48                     | 0.43              |
| 2:C:1035:MET:HE3  | 2:C:1035:MET:HB2  | 1.72                     | 0.43              |
| 2:C:1091:GLU:O    | 3:D:603:LEU:HD22  | 2.17                     | 0.43              |
| 3:D:786:ILE:HD11  | 3:D:908:LYS:HB2   | 2.00                     | 0.43              |
| 3:D:1114:THR:O    | 3:D:1114:THR:CG2  | 2.66                     | 0.43              |
| 3:D:1356:TYR:N    | 3:D:1356:TYR:CD1  | 2.86                     | 0.43              |
| 3:D:1394:VAL:HG23 | 8:D:2077:HOH:O    | 2.17                     | 0.43              |
| 3:D:1440:PHE:HB2  | 3:D:1442:ASN:ND2  | 2.32                     | 0.43              |
| 3:D:1487:VAL:HB   | 4:E:74:VAL:HB     | 1.99                     | 0.43              |
| 4:E:55:PHE:H      | 4:E:55:PHE:HD2    | 1.65                     | 0.43              |
| 5:F:405:LEU:O     | 5:F:408:LEU:CD2   | 2.65                     | 0.43              |
| 2:M:18:LEU:HD13   | 2:M:590:ASP:OD2   | 2.18                     | 0.43              |
| 2:M:24:GLU:HG2    | 8:M:9500:HOH:O    | 2.17                     | 0.43              |
| 2:M:118:ILE:O     | 2:M:118:ILE:HG12  | 2.17                     | 0.43              |
| 2:M:122:THR:HG22  | 2:M:124:ASP:H     | 1.83                     | 0.43              |
| 2:M:163:ILE:O     | 2:M:163:ILE:HG12  | 2.17                     | 0.43              |
| 2:M:368:THR:CB    | 2:M:369:PRO:HD3   | 2.39                     | 0.43              |
| 2:M:630:ARG:HH11  | 2:M:630:ARG:HG3   | 1.83                     | 0.43              |
| 2:M:643:VAL:HG13  | 2:M:647:GLN:NE2   | 2.33                     | 0.43              |
| 2:M:906:PHE:CD1   | 3:N:1067:VAL:HG13 | 2.53                     | 0.43              |
| 2:M:1000:MET:CE   | 2:M:1001:VAL:HG22 | 2.48                     | 0.43              |
| 2:M:1005:MET:SD   | 3:N:648:MET:HB2   | 2.58                     | 0.43              |
| 2:M:1052:MET:HE3  | 3:N:623:VAL:HG21  | 2.00                     | 0.43              |
| 3:N:13:ALA:O      | 3:N:511:TRP:HB3   | 2.18                     | 0.43              |
| 3:N:131:LYS:HE3   | 8:N:9947:HOH:O    | 2.17                     | 0.43              |
| 3:N:689:ASP:HA    | 8:N:2043:HOH:O    | 2.18                     | 0.43              |
| 5:P:411:HIS:CA    | 5:P:414:ARG:HE    | 2.31                     | 0.43              |
| 1:A:161:ARG:HG3   | 1:A:161:ARG:NH1   | 2.33                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:78:ILE:HG23   | 8:B:9503:HOH:O    | 2.17                     | 0.43              |
| 1:B:101:LEU:HA    | 8:B:9491:HOH:O    | 2.17                     | 0.43              |
| 1:B:137:ARG:HH12  | 1:B:139:ASN:HB3   | 1.83                     | 0.43              |
| 1:B:185:ARG:NH1   | 3:D:692:GLU:CD    | 2.76                     | 0.43              |
| 2:C:129:ILE:HB    | 2:C:134:ARG:HD2   | 2.00                     | 0.43              |
| 2:C:181:VAL:CG1   | 2:C:182:VAL:N     | 2.81                     | 0.43              |
| 2:C:369:PRO:HA    | 8:C:2227:HOH:O    | 2.18                     | 0.43              |
| 2:C:413:LEU:H     | 2:C:413:LEU:CD1   | 2.18                     | 0.43              |
| 2:C:676:ILE:HG22  | 2:C:988:VAL:HG13  | 1.99                     | 0.43              |
| 2:C:885:ILE:HG13  | 3:D:949:ILE:HG22  | 2.00                     | 0.43              |
| 2:C:987:ILE:HG12  | 3:D:948:THR:HG23  | 2.00                     | 0.43              |
| 2:C:1016:ILE:HD13 | 2:C:1016:ILE:H    | 1.82                     | 0.43              |
| 2:C:1019:GLN:HE21 | 2:C:1019:GLN:HB3  | 1.59                     | 0.43              |
| 3:D:22:SER:OG     | 3:D:23:TYR:N      | 2.51                     | 0.43              |
| 3:D:79:GLU:O      | 3:D:80:VAL:HB     | 2.18                     | 0.43              |
| 3:D:399:ARG:CZ    | 8:D:2498:HOH:O    | 2.66                     | 0.43              |
| 3:D:470:LEU:HB2   | 3:D:503:LEU:HD21  | 2.00                     | 0.43              |
| 3:D:500:ARG:HH22  | 3:D:1388:ARG:NH1  | 2.16                     | 0.43              |
| 3:D:584:ASN:HB3   | 8:D:9687:HOH:O    | 2.17                     | 0.43              |
| 3:D:618:LEU:HD23  | 3:D:618:LEU:HA    | 1.69                     | 0.43              |
| 3:D:796:ARG:NH1   | 3:D:859:ASP:HB2   | 2.33                     | 0.43              |
| 3:D:1042:ARG:HG3  | 3:D:1042:ARG:O    | 2.18                     | 0.43              |
| 3:D:1102:THR:HG22 | 3:D:1222:GLY:CA   | 2.49                     | 0.43              |
| 3:D:1465:ASN:ND2  | 8:D:9954:HOH:O    | 2.51                     | 0.43              |
| 1:L:88:ARG:CB     | 1:L:123:MET:HE2   | 2.48                     | 0.43              |
| 1:L:176:ARG:HH12  | 3:N:884:ARG:HD3   | 1.83                     | 0.43              |
| 2:M:29:ALA:HB2    | 2:M:337:GLY:HA3   | 2.01                     | 0.43              |
| 2:M:353:ARG:HB3   | 8:M:2122:HOH:O    | 2.18                     | 0.43              |
| 2:M:771:GLU:HB2   | 8:M:9723:HOH:O    | 2.17                     | 0.43              |
| 3:N:177:ALA:HB1   | 3:N:199:LEU:CB    | 2.47                     | 0.43              |
| 3:N:195:VAL:HG22  | 8:N:9862:HOH:O    | 2.18                     | 0.43              |
| 3:N:433:GLY:HA3   | 3:N:449:SER:O     | 2.17                     | 0.43              |
| 3:N:530:VAL:HG12  | 3:N:531:ASP:N     | 2.33                     | 0.43              |
| 3:N:1096:ARG:CG   | 3:N:1096:ARG:NH1  | 2.81                     | 0.43              |
| 3:N:1096:ARG:NH1  | 3:N:1096:ARG:HG2  | 2.33                     | 0.43              |
| 3:N:1115:THR:CG2  | 3:N:1151:ARG:HH21 | 2.31                     | 0.43              |
| 3:N:1247:ALA:O    | 3:N:1248:GLY:C    | 2.61                     | 0.43              |
| 3:N:1256:LEU:O    | 3:N:1257:PRO:C    | 2.60                     | 0.43              |
| 3:N:1385:GLY:HA2  | 3:N:1413:THR:HG21 | 1.99                     | 0.43              |
| 4:O:4:PRO:HA      | 8:O:1112:HOH:O    | 2.18                     | 0.43              |
| 4:O:40:LEU:CG     | 4:O:67:GLU:HG2    | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:18:ARG:NH1    | 1:A:88:ARG:NE     | 2.63                     | 0.43              |
| 1:A:39:PRO:HG2    | 1:B:39:PRO:CG     | 2.46                     | 0.43              |
| 1:A:70:GLY:HA2    | 1:A:133:GLU:CD    | 2.42                     | 0.43              |
| 1:A:133:GLU:CG    | 1:A:134:GLU:N     | 2.81                     | 0.43              |
| 1:A:198:ARG:NH2   | 2:C:934:PHE:HE1   | 2.16                     | 0.43              |
| 2:C:439:CYS:SG    | 2:C:441:VAL:N     | 2.91                     | 0.43              |
| 2:C:720:GLU:HG2   | 2:C:760:SER:HB3   | 2.00                     | 0.43              |
| 2:C:1034:GLU:HG3  | 2:C:1035:MET:H    | 1.82                     | 0.43              |
| 3:D:116:LEU:HB3   | 3:D:118:LEU:CD1   | 2.48                     | 0.43              |
| 3:D:148:GLU:HB3   | 3:D:151:GLN:HG3   | 2.00                     | 0.43              |
| 3:D:396:VAL:HG13  | 3:D:447:VAL:CA    | 2.45                     | 0.43              |
| 3:D:480:GLU:HG2   | 3:D:492:ALA:HB2   | 2.00                     | 0.43              |
| 3:D:709:HIS:HA    | 3:D:1227:GLN:CD   | 2.43                     | 0.43              |
| 3:D:947:ILE:HD12  | 3:D:947:ILE:O     | 2.19                     | 0.43              |
| 3:D:988:ARG:HH11  | 3:D:992:ILE:HD11  | 1.83                     | 0.43              |
| 3:D:1438:ALA:HB1  | 8:D:9745:HOH:O    | 2.17                     | 0.43              |
| 4:E:6:ILE:HA      | 4:E:9:LEU:HD12    | 2.00                     | 0.43              |
| 2:M:283:ILE:HG22  | 2:M:284:ARG:HG2   | 2.00                     | 0.43              |
| 2:M:578:VAL:HG11  | 2:M:991:GLN:OE1   | 2.18                     | 0.43              |
| 2:M:1014:SER:HA   | 2:M:1021:LEU:HD23 | 2.00                     | 0.43              |
| 2:M:1102:LEU:HD13 | 3:N:7:LYS:O       | 2.19                     | 0.43              |
| 3:N:420:VAL:HG22  | 8:N:2309:HOH:O    | 2.16                     | 0.43              |
| 3:N:568:ARG:NH2   | 8:N:2401:HOH:O    | 2.50                     | 0.43              |
| 3:N:1363:LEU:CD1  | 3:N:1368:ILE:HD11 | 2.49                     | 0.43              |
| 3:N:1406:ARG:HG2  | 8:N:9632:HOH:O    | 2.17                     | 0.43              |
| 3:N:1487:VAL:HB   | 4:O:74:VAL:HB     | 2.01                     | 0.43              |
| 5:P:410:TYR:HA    | 5:P:413:SER:HG    | 1.80                     | 0.43              |
| 2:C:533:ASP:HB3   | 2:C:538:GLN:NE2   | 2.33                     | 0.43              |
| 3:D:144:GLY:HA2   | 8:D:9643:HOH:O    | 2.18                     | 0.43              |
| 3:D:207:PHE:CB    | 3:D:208:PRO:HD2   | 2.41                     | 0.43              |
| 3:D:229:ALA:HB1   | 8:D:2446:HOH:O    | 2.18                     | 0.43              |
| 3:D:389:GLU:O     | 3:D:389:GLU:HG2   | 2.18                     | 0.43              |
| 3:D:527:MET:CE    | 3:D:535:PHE:HB3   | 2.44                     | 0.43              |
| 3:D:550:ARG:HG3   | 3:D:550:ARG:NH1   | 2.33                     | 0.43              |
| 3:D:553:ARG:HD2   | 3:D:570:GLU:CD    | 2.43                     | 0.43              |
| 3:D:613:ARG:HG3   | 3:D:613:ARG:NH1   | 2.31                     | 0.43              |
| 3:D:614:PHE:CZ    | 3:D:1439:SER:O    | 2.71                     | 0.43              |
| 3:D:700:VAL:HG22  | 3:D:718:PRO:HG3   | 2.00                     | 0.43              |
| 3:D:1240:THR:O    | 3:D:1257:PRO:HB3  | 2.17                     | 0.43              |
| 5:F:164:LYS:HA    | 5:F:171:LYS:HZ3   | 1.83                     | 0.43              |
| 5:F:365:GLU:OE1   | 5:F:365:GLU:N     | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:F:411:HIS:C    | 5:F:413:SER:N    | 2.76                     | 0.43              |
| 1:K:64:GLU:OE2   | 1:K:76:VAL:HG13  | 2.18                     | 0.43              |
| 1:L:188:GLN:H    | 1:L:188:GLN:HG2  | 1.52                     | 0.43              |
| 2:M:58:ASP:O     | 2:M:59:LYS:HG2   | 2.18                     | 0.43              |
| 2:M:207:LEU:HD22 | 2:M:221:LEU:CD1  | 2.49                     | 0.43              |
| 2:M:524:VAL:HG22 | 2:M:528:GLU:HB2  | 1.99                     | 0.43              |
| 2:M:559:LEU:HD22 | 8:M:9785:HOH:O   | 2.18                     | 0.43              |
| 2:M:1065:ALA:CB  | 2:M:1077:PRO:HG2 | 2.48                     | 0.43              |
| 3:N:97:THR:HB    | 3:N:571:LYS:HD3  | 2.00                     | 0.43              |
| 3:N:112:ILE:HG22 | 3:N:512:MET:CE   | 2.48                     | 0.43              |
| 3:N:427:VAL:HB   | 3:N:435:VAL:HB   | 2.01                     | 0.43              |
| 3:N:831:GLY:HA3  | 8:N:9675:HOH:O   | 2.18                     | 0.43              |
| 4:O:2:ALA:N      | 8:O:1102:HOH:O   | 2.50                     | 0.43              |
| 4:O:45:ARG:NE    | 8:O:5067:HOH:O   | 2.51                     | 0.43              |
| 5:P:85:LEU:HD22  | 5:P:193:ARG:CZ   | 2.48                     | 0.43              |
| 5:P:209:PHE:O    | 5:P:213:ILE:HG13 | 2.19                     | 0.43              |
| 5:P:259:ARG:N    | 8:P:9565:HOH:O   | 2.51                     | 0.43              |
| 5:P:410:TYR:O    | 5:P:413:SER:HB2  | 2.18                     | 0.43              |
| 1:B:88:ARG:NH1   | 8:B:9511:HOH:O   | 2.52                     | 0.43              |
| 2:C:110:GLU:CB   | 2:C:369:PRO:HG3  | 2.48                     | 0.43              |
| 2:C:204:GLN:NE2  | 2:C:228:ALA:CB   | 2.81                     | 0.43              |
| 2:C:576:ALA:H    | 2:C:662:GLU:CD   | 2.26                     | 0.43              |
| 2:C:638:ASP:HB2  | 8:C:2064:HOH:O   | 2.19                     | 0.43              |
| 3:D:456:MET:C    | 8:D:2363:HOH:O   | 2.60                     | 0.43              |
| 3:D:470:LEU:H    | 3:D:470:LEU:HG   | 1.57                     | 0.43              |
| 3:D:853:VAL:HG22 | 3:D:858:VAL:O    | 2.19                     | 0.43              |
| 3:D:996:TRP:CE2  | 3:D:1056:PRO:HG2 | 2.53                     | 0.43              |
| 3:D:1493:LYS:HG3 | 8:D:9756:HOH:O   | 2.17                     | 0.43              |
| 5:F:94:LEU:O     | 5:F:95:THR:C     | 2.62                     | 0.43              |
| 5:F:167:PRO:HB2  | 5:F:169:GLU:CD   | 2.44                     | 0.43              |
| 5:F:278:LEU:CD1  | 5:F:290:GLU:HB3  | 2.36                     | 0.43              |
| 1:K:83:LYS:HD3   | 8:M:9621:HOH:O   | 2.16                     | 0.43              |
| 1:K:219:ARG:NH1  | 1:K:220:GLU:HA   | 2.33                     | 0.43              |
| 2:M:181:VAL:HG12 | 2:M:182:VAL:N    | 2.32                     | 0.43              |
| 2:M:917:LEU:HD23 | 2:M:917:LEU:HA   | 1.73                     | 0.43              |
| 2:M:945:ARG:NH2  | 8:M:9941:HOH:O   | 2.50                     | 0.43              |
| 2:M:1044:GLY:O   | 2:M:1046:ALA:N   | 2.51                     | 0.43              |
| 3:N:154:THR:CG2  | 3:N:155:ASP:N    | 2.82                     | 0.43              |
| 3:N:521:PRO:O    | 3:N:525:ARG:NH1  | 2.50                     | 0.43              |
| 3:N:580:ALA:HA   | 3:N:584:ASN:OD1  | 2.19                     | 0.43              |
| 3:N:792:ILE:HA   | 8:N:9873:HOH:O   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:849:ALA:O     | 3:N:853:VAL:HG23  | 2.18                     | 0.43              |
| 3:N:889:ALA:HB1   | 3:N:930:LEU:HA    | 2.01                     | 0.43              |
| 3:N:908:LYS:CB    | 3:N:1027:GLY:HA3  | 2.43                     | 0.43              |
| 3:N:970:LYS:NZ    | 8:N:9576:HOH:O    | 2.51                     | 0.43              |
| 3:N:1326:THR:HG22 | 3:N:1327:ARG:N    | 2.28                     | 0.43              |
| 3:N:1471:LEU:HD23 | 8:N:9651:HOH:O    | 2.19                     | 0.43              |
| 4:O:54:LEU:CD2    | 4:O:63:TRP:HE1    | 2.31                     | 0.43              |
| 5:P:85:LEU:HB3    | 8:P:9542:HOH:O    | 2.19                     | 0.43              |
| 5:P:277:GLN:HB2   | 8:P:9578:HOH:O    | 2.18                     | 0.43              |
| 1:B:109:VAL:HG21  | 1:B:138:LEU:HD21  | 1.99                     | 0.43              |
| 2:C:22:GLN:HE21   | 2:C:22:GLN:HB3    | 1.70                     | 0.43              |
| 2:C:129:ILE:HD11  | 2:C:386:PHE:CD2   | 2.53                     | 0.43              |
| 2:C:479:VAL:HG21  | 2:C:503:LEU:HD11  | 2.00                     | 0.43              |
| 2:C:518:LYS:C     | 8:C:9604:HOH:O    | 2.62                     | 0.43              |
| 2:C:594:ALA:N     | 8:C:9533:HOH:O    | 2.51                     | 0.43              |
| 2:C:595:LEU:HD13  | 2:C:639:GLN:OE1   | 2.19                     | 0.43              |
| 2:C:602:GLU:HG2   | 2:C:603:VAL:N     | 2.34                     | 0.43              |
| 2:C:630:ARG:HH21  | 2:C:707:ARG:H     | 1.66                     | 0.43              |
| 2:C:643:VAL:HG22  | 8:C:2226:HOH:O    | 2.18                     | 0.43              |
| 2:C:669:GLY:O     | 2:C:670:GLN:HG3   | 2.19                     | 0.43              |
| 2:C:672:VAL:HG23  | 2:C:868:ASP:CB    | 2.42                     | 0.43              |
| 2:C:710:ILE:HD11  | 2:C:758:ARG:HH21  | 1.84                     | 0.43              |
| 2:C:1058:ASP:OD1  | 2:C:1083:GLU:N    | 2.52                     | 0.43              |
| 2:C:1070:ILE:HD13 | 3:D:751:LEU:HD22  | 2.00                     | 0.43              |
| 3:D:2:LYS:HB3     | 3:D:3:LYS:HD3     | 2.01                     | 0.43              |
| 3:D:28:LYS:HA     | 3:D:29:PRO:HD3    | 1.79                     | 0.43              |
| 3:D:126:VAL:HG11  | 3:D:152:LEU:HD12  | 2.00                     | 0.43              |
| 3:D:148:GLU:HB3   | 3:D:151:GLN:CG    | 2.48                     | 0.43              |
| 3:D:240:GLU:O     | 3:D:243:ALA:N     | 2.50                     | 0.43              |
| 3:D:521:PRO:HA    | 3:D:522:PRO:HD3   | 1.73                     | 0.43              |
| 3:D:605:ASP:OD1   | 3:D:605:ASP:N     | 2.50                     | 0.43              |
| 3:D:787:LEU:HD12  | 3:D:787:LEU:O     | 2.18                     | 0.43              |
| 3:D:827:ILE:O     | 3:D:837:GLY:HA3   | 2.19                     | 0.43              |
| 3:D:899:LEU:HD21  | 3:D:914:LEU:HD23  | 2.01                     | 0.43              |
| 3:D:1058:ARG:HH11 | 3:D:1058:ARG:CG   | 2.32                     | 0.43              |
| 3:D:1235:GLN:C    | 3:D:1359:GLN:HE22 | 2.27                     | 0.43              |
| 3:D:1243:THR:O    | 3:D:1269:LYS:HD2  | 2.18                     | 0.43              |
| 3:D:1476:THR:HG22 | 3:D:1476:THR:O    | 2.17                     | 0.43              |
| 5:F:402:ASN:OD1   | 5:F:402:ASN:N     | 2.50                     | 0.43              |
| 1:K:44:LEU:HD21   | 1:K:199:ILE:HD13  | 2.01                     | 0.43              |
| 1:K:161:ARG:HH11  | 1:K:161:ARG:HG3   | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:395:LYS:HE2  | 2:M:403:SER:HB2  | 2.01                     | 0.43              |
| 2:M:441:VAL:HG13 | 2:M:442:GLU:N    | 2.34                     | 0.43              |
| 2:M:611:ILE:HD11 | 2:M:641:PRO:HB3  | 2.01                     | 0.43              |
| 3:N:23:TYR:O     | 3:N:24:GLY:O     | 2.37                     | 0.43              |
| 3:N:171:LEU:HA   | 3:N:172:PRO:HD2  | 1.56                     | 0.43              |
| 4:O:5:GLY:O      | 4:O:9:LEU:HG     | 2.18                     | 0.43              |
| 5:P:144:ILE:CB   | 5:P:145:PRO:HD3  | 2.48                     | 0.43              |
| 5:P:282:LEU:HD22 | 5:P:282:LEU:HA   | 1.82                     | 0.43              |
| 1:A:61:VAL:HG11  | 1:A:75:VAL:HG21  | 2.01                     | 0.43              |
| 1:A:226:SER:HB2  | 8:A:9514:HOH:O   | 2.17                     | 0.43              |
| 2:C:94:LEU:HD11  | 8:C:9663:HOH:O   | 2.19                     | 0.43              |
| 2:C:264:PRO:CB   | 2:C:289:THR:HB   | 2.49                     | 0.43              |
| 2:C:281:LEU:HD11 | 2:C:306:THR:HA   | 2.00                     | 0.43              |
| 2:C:367:LEU:HA   | 2:C:371:LYS:CB   | 2.48                     | 0.43              |
| 2:C:479:VAL:HB   | 2:C:503:LEU:HD11 | 2.00                     | 0.43              |
| 2:C:885:ILE:HD12 | 3:D:949:ILE:O    | 2.18                     | 0.43              |
| 2:C:952:LEU:HD12 | 2:C:969:GLN:CD   | 2.43                     | 0.43              |
| 3:D:82:LYS:O     | 3:D:84:ILE:N     | 2.51                     | 0.43              |
| 3:D:103:TRP:HZ2  | 3:D:604:THR:HG1  | 1.63                     | 0.43              |
| 3:D:534:ARG:HG2  | 5:F:312:GLN:HE22 | 1.82                     | 0.43              |
| 3:D:684:LYS:HD3  | 3:D:686:GLU:OE2  | 2.18                     | 0.43              |
| 3:D:806:PHE:HE1  | 3:D:809:PRO:O    | 2.01                     | 0.43              |
| 3:D:1197:ARG:HD3 | 3:D:1396:GLU:CB  | 2.46                     | 0.43              |
| 3:D:1353:GLN:CD  | 3:D:1365:ASP:OD2 | 2.62                     | 0.43              |
| 1:K:45:LEU:HD21  | 1:K:177:VAL:HG23 | 2.00                     | 0.43              |
| 1:K:143:ARG:NH1  | 1:K:145:ASP:OD1  | 2.52                     | 0.43              |
| 1:K:156:HIS:CD2  | 1:K:158:ILE:HG12 | 2.53                     | 0.43              |
| 2:M:197:LEU:HB3  | 2:M:202:TYR:HB2  | 2.01                     | 0.43              |
| 2:M:216:GLU:O    | 2:M:218:VAL:N    | 2.51                     | 0.43              |
| 2:M:242:LEU:HD13 | 2:M:242:LEU:N    | 2.33                     | 0.43              |
| 2:M:330:ASN:HB3  | 8:M:2182:HOH:O   | 2.18                     | 0.43              |
| 2:M:454:SER:HB2  | 8:M:9853:HOH:O   | 2.18                     | 0.43              |
| 2:M:727:PRO:CG   | 2:M:785:VAL:HG12 | 2.44                     | 0.43              |
| 2:M:737:LEU:HD21 | 2:M:754:ILE:CG2  | 2.48                     | 0.43              |
| 2:M:774:LEU:HD22 | 2:M:774:LEU:C    | 2.43                     | 0.43              |
| 2:M:1002:GLU:HG3 | 2:M:1003:ASP:N   | 2.33                     | 0.43              |
| 2:M:1030:GLN:OE1 | 3:N:628:ARG:HB2  | 2.18                     | 0.43              |
| 2:M:1056:LYS:HE2 | 3:N:623:VAL:CG1  | 2.48                     | 0.43              |
| 3:N:96:ALA:CB    | 3:N:554:LEU:HD12 | 2.47                     | 0.43              |
| 3:N:481:MET:SD   | 3:N:1388:ARG:CG  | 2.96                     | 0.43              |
| 3:N:609:GLY:HA3  | 3:N:613:ARG:HB3  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1116:ASN:ND2  | 3:N:1116:ASN:N    | 2.52                     | 0.43              |
| 3:N:1372:VAL:HA   | 3:N:1375:MET:CE   | 2.48                     | 0.43              |
| 4:O:54:LEU:HG     | 4:O:58:PRO:CG     | 2.48                     | 0.43              |
| 1:A:55:SER:HB2    | 1:A:158:ILE:HG21  | 2.01                     | 0.43              |
| 1:B:62:LEU:H      | 1:B:62:LEU:HD12   | 1.83                     | 0.43              |
| 2:C:162:ILE:HB    | 2:C:172:ILE:CD1   | 2.49                     | 0.43              |
| 2:C:193:LEU:HG    | 2:C:307:LEU:HD22  | 2.01                     | 0.43              |
| 2:C:657:ASP:OD2   | 2:C:662:GLU:O     | 2.37                     | 0.43              |
| 2:C:759:THR:HB    | 2:C:785:VAL:CG1   | 2.48                     | 0.43              |
| 2:C:979:THR:HG23  | 2:C:981:GLU:N     | 2.25                     | 0.43              |
| 2:C:1072:LYS:HD2  | 8:C:9885:HOH:O    | 2.19                     | 0.43              |
| 3:D:421:LEU:HG    | 3:D:422:ALA:O     | 2.19                     | 0.43              |
| 3:D:580:ALA:O     | 3:D:602:SER:HB3   | 2.18                     | 0.43              |
| 3:D:799:LYS:HE2   | 3:D:824:ASN:O     | 2.18                     | 0.43              |
| 3:D:889:ALA:HB1   | 3:D:930:LEU:HA    | 2.01                     | 0.43              |
| 3:D:1079:LYS:NZ   | 8:D:9833:HOH:O    | 2.52                     | 0.43              |
| 3:D:1207:TYR:C    | 8:D:9589:HOH:O    | 2.62                     | 0.43              |
| 3:D:1275:SER:OG   | 3:D:1277:ILE:O    | 2.37                     | 0.43              |
| 3:D:1353:GLN:O    | 3:D:1357:ARG:HD2  | 2.19                     | 0.43              |
| 3:D:1354:LYS:HE3  | 8:D:9873:HOH:O    | 2.18                     | 0.43              |
| 4:E:46:PRO:CB     | 4:E:54:LEU:CD2    | 2.97                     | 0.43              |
| 1:L:186:LEU:HD23  | 1:L:186:LEU:HA    | 1.79                     | 0.43              |
| 2:M:3:ILE:O       | 2:M:3:ILE:HG22    | 2.19                     | 0.43              |
| 2:M:101:ILE:HG23  | 2:M:107:LEU:CD2   | 2.41                     | 0.43              |
| 2:M:569:VAL:O     | 2:M:569:VAL:HG13  | 2.18                     | 0.43              |
| 2:M:770:GLU:HG2   | 3:N:65:ARG:HH22   | 1.83                     | 0.43              |
| 2:M:854:PRO:C     | 2:M:856:GLU:H     | 2.25                     | 0.43              |
| 2:M:984:GLU:H     | 2:M:984:GLU:HG2   | 1.68                     | 0.43              |
| 3:N:112:ILE:HG13  | 3:N:124:GLU:OE2   | 2.18                     | 0.43              |
| 3:N:214:GLU:HG2   | 3:N:215:TYR:CD1   | 2.54                     | 0.43              |
| 3:N:820:GLU:HA    | 3:N:825:ALA:O     | 2.18                     | 0.43              |
| 3:N:1151:ARG:NH1  | 8:N:9821:HOH:O    | 2.52                     | 0.43              |
| 3:N:1340:GLY:O    | 3:N:1344:VAL:HG23 | 2.18                     | 0.43              |
| 3:N:1396:GLU:HG2  | 3:N:1399:ASP:OD2  | 2.19                     | 0.43              |
| 3:N:1487:VAL:HG12 | 3:N:1488:ASP:O    | 2.19                     | 0.43              |
| 5:P:166:LEU:HD13  | 5:P:170:HIS:HB2   | 2.00                     | 0.43              |
| 5:P:198:ILE:HD11  | 5:P:240:THR:HA    | 2.01                     | 0.43              |
| 5:P:232:ARG:O     | 5:P:233:PHE:C     | 2.61                     | 0.43              |
| 5:P:249:ARG:HG3   | 5:P:253:ASP:OD2   | 2.19                     | 0.43              |
| 1:A:182:GLU:OE2   | 2:C:934:PHE:HB3   | 2.17                     | 0.43              |
| 1:B:61:VAL:HG22   | 8:B:9525:HOH:O    | 2.19                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:63:GLY:HA3    | 2:C:103:LYS:HG2  | 1.99                     | 0.43              |
| 2:C:146:VAL:HB    | 2:C:281:LEU:HD22 | 2.01                     | 0.43              |
| 2:C:473:ARG:HG3   | 2:C:474:VAL:N    | 2.34                     | 0.43              |
| 2:C:748:GLU:CA    | 2:C:799:ILE:HG22 | 2.46                     | 0.43              |
| 2:C:950:LEU:HG    | 2:C:952:LEU:CD2  | 2.48                     | 0.43              |
| 2:C:957:LYS:HG2   | 2:C:961:GLU:HB3  | 2.00                     | 0.43              |
| 2:C:1102:LEU:HD23 | 2:C:1106:ASP:C   | 2.44                     | 0.43              |
| 3:D:19:ARG:HD2    | 8:D:9545:HOH:O   | 2.18                     | 0.43              |
| 3:D:434:ARG:CB    | 3:D:447:VAL:HG22 | 2.45                     | 0.43              |
| 3:D:704:ARG:HG3   | 3:D:705:ALA:N    | 2.34                     | 0.43              |
| 3:D:937:TYR:HB3   | 3:D:941:PHE:CE1  | 2.54                     | 0.43              |
| 3:D:1499:ARG:O    | 3:D:1502:ALA:HB3 | 2.19                     | 0.43              |
| 5:F:156:VAL:N     | 8:F:9476:HOH:O   | 2.47                     | 0.43              |
| 2:M:44:ILE:HG23   | 2:M:344:PHE:CE1  | 2.54                     | 0.43              |
| 2:M:238:LEU:HD23  | 8:M:9936:HOH:O   | 2.19                     | 0.43              |
| 2:M:525:SER:O     | 2:M:529:VAL:HG23 | 2.19                     | 0.43              |
| 2:M:732:ALA:HA    | 2:M:735:ARG:NE   | 2.34                     | 0.43              |
| 2:M:999:HIS:HD2   | 8:M:2181:HOH:O   | 2.01                     | 0.43              |
| 2:M:1031:ARG:HD3  | 3:N:620:GLY:C    | 2.44                     | 0.43              |
| 3:N:122:GLU:O     | 3:N:126:VAL:HB   | 2.19                     | 0.43              |
| 3:N:693:GLU:HA    | 4:O:48:MET:HE1   | 2.01                     | 0.43              |
| 3:N:1093:TYR:O    | 3:N:1097:LYS:HG2 | 2.18                     | 0.43              |
| 3:N:1105:ILE:HD11 | 3:N:1374:GLN:CD  | 2.44                     | 0.43              |
| 3:N:1107:VAL:HG12 | 3:N:1217:ILE:HA  | 2.00                     | 0.43              |
| 5:P:204:GLY:HA2   | 8:P:9767:HOH:O   | 2.19                     | 0.43              |
| 5:P:223:ALA:HB2   | 5:P:242:TRP:CB   | 2.49                     | 0.43              |
| 5:P:350:LEU:CD1   | 5:P:422:LEU:CB   | 2.92                     | 0.43              |
| 1:A:48:ILE:HG22   | 1:A:173:PRO:HD2  | 2.00                     | 0.43              |
| 2:C:200:LEU:HD22  | 2:C:300:ASP:OD1  | 2.19                     | 0.43              |
| 2:C:395:LYS:O     | 2:C:633:GLN:NE2  | 2.52                     | 0.43              |
| 2:C:1003:ASP:O    | 2:C:1004:LYS:C   | 2.62                     | 0.43              |
| 2:C:1081:VAL:HB   | 2:C:1086:ARG:CZ  | 2.49                     | 0.43              |
| 3:D:9:ARG:HD2     | 8:D:2198:HOH:O   | 2.18                     | 0.43              |
| 3:D:10:ILE:HG22   | 3:D:1451:ALA:HA  | 1.99                     | 0.43              |
| 3:D:42:ASP:O      | 3:D:46:ASP:HB2   | 2.19                     | 0.43              |
| 3:D:572:ARG:O     | 3:D:575:GLN:HB3  | 2.19                     | 0.43              |
| 3:D:894:LYS:HB2   | 8:D:9522:HOH:O   | 2.19                     | 0.43              |
| 3:D:1296:SER:C    | 3:D:1298:GLY:N   | 2.76                     | 0.43              |
| 3:D:1353:GLN:NE2  | 3:D:1365:ASP:OD2 | 2.52                     | 0.43              |
| 3:D:1416:ALA:HB2  | 8:D:9686:HOH:O   | 2.19                     | 0.43              |
| 3:D:1458:GLU:HB3  | 8:D:9556:HOH:O   | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:288:TYR:CE2   | 5:F:305:GLU:HA    | 2.53                     | 0.43              |
| 5:F:353:GLU:OE2   | 5:F:356:LYS:HD2   | 2.19                     | 0.43              |
| 5:F:372:ARG:HD2   | 5:F:372:ARG:HA    | 1.75                     | 0.43              |
| 1:L:137:ARG:HG2   | 1:L:137:ARG:NH1   | 2.30                     | 0.43              |
| 2:M:309:TYR:HA    | 2:M:312:ALA:HB3   | 2.01                     | 0.43              |
| 2:M:889:HIS:NE2   | 2:M:970:GLY:HA3   | 2.34                     | 0.43              |
| 2:M:906:PHE:CZ    | 3:N:1067:VAL:HA   | 2.53                     | 0.43              |
| 2:M:1055:LEU:HD23 | 2:M:1055:LEU:N    | 2.33                     | 0.43              |
| 3:N:141:ILE:HG22  | 3:N:142:LEU:N     | 2.34                     | 0.43              |
| 3:N:422:ALA:CB    | 5:P:178:ARG:HH22  | 2.32                     | 0.43              |
| 3:N:427:VAL:O     | 3:N:433:GLY:O     | 2.37                     | 0.43              |
| 3:N:598:ARG:HA    | 3:N:599:PRO:HD3   | 1.89                     | 0.43              |
| 3:N:693:GLU:HA    | 8:N:9582:HOH:O    | 2.19                     | 0.43              |
| 3:N:781:PRO:HB3   | 3:N:785:ILE:CG2   | 2.49                     | 0.43              |
| 3:N:794:GLN:CA    | 3:N:879:ARG:HH12  | 2.31                     | 0.43              |
| 3:N:1083:ASP:O    | 3:N:1087:ARG:CD   | 2.67                     | 0.43              |
| 3:N:1373:ARG:HG2  | 3:N:1374:GLN:HE21 | 1.84                     | 0.43              |
| 3:N:1425:THR:HG21 | 8:N:2233:HOH:O    | 2.18                     | 0.43              |
| 3:N:1447:LEU:O    | 3:N:1448:THR:C    | 2.62                     | 0.43              |
| 4:O:45:ARG:HH12   | 4:O:72:ARG:HH21   | 1.66                     | 0.43              |
| 5:P:170:HIS:HA    | 5:P:173:TYR:HD1   | 1.83                     | 0.43              |
| 1:A:9:PRO:HG2     | 1:B:224:TYR:CD2   | 2.54                     | 0.42              |
| 1:A:177:VAL:HG12  | 1:A:178:ALA:N     | 2.34                     | 0.42              |
| 1:A:219:ARG:HD3   | 8:A:9459:HOH:O    | 2.19                     | 0.42              |
| 2:C:207:LEU:HD22  | 2:C:221:LEU:CD2   | 2.49                     | 0.42              |
| 2:C:626:ARG:HG2   | 2:C:629:TYR:CE1   | 2.54                     | 0.42              |
| 2:C:673:LEU:HD23  | 2:C:867:VAL:HA    | 2.01                     | 0.42              |
| 2:C:1095:LEU:O    | 2:C:1096:ALA:C    | 2.62                     | 0.42              |
| 3:D:12:LEU:HD23   | 3:D:13:ALA:N      | 2.25                     | 0.42              |
| 3:D:169:TYR:HA    | 3:D:392:SER:HA    | 2.00                     | 0.42              |
| 3:D:661:MET:HE2   | 3:D:673:ALA:HB1   | 2.00                     | 0.42              |
| 3:D:696:HIS:HD2   | 8:E:9410:HOH:O    | 2.01                     | 0.42              |
| 3:D:729:HIS:ND1   | 3:D:730:PRO:CD    | 2.82                     | 0.42              |
| 3:D:1110:ALA:O    | 3:D:1111:ASP:C    | 2.59                     | 0.42              |
| 3:D:1138:ALA:O    | 3:D:1141:GLU:HB2  | 2.19                     | 0.42              |
| 3:D:1234:THR:HG23 | 8:D:2149:HOH:O    | 2.18                     | 0.42              |
| 4:E:54:LEU:HA     | 4:E:58:PRO:CG     | 2.49                     | 0.42              |
| 4:E:72:ARG:N      | 8:E:9366:HOH:O    | 2.45                     | 0.42              |
| 5:F:315:VAL:HG12  | 5:F:316:SER:N     | 2.34                     | 0.42              |
| 5:F:369:LEU:O     | 5:F:373:LYS:HG2   | 2.19                     | 0.42              |
| 1:K:107:LYS:HG2   | 1:K:108:GLU:N     | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:27:ARG:HG2    | 8:M:9618:HOH:O    | 2.18                     | 0.42              |
| 2:M:33:ASP:N      | 8:M:2159:HOH:O    | 2.52                     | 0.42              |
| 2:M:418:LEU:HD11  | 8:M:2225:HOH:O    | 2.19                     | 0.42              |
| 2:M:879:ARG:NH1   | 3:N:1029:ARG:HH12 | 2.17                     | 0.42              |
| 3:N:10:ILE:HG13   | 3:N:1434:TRP:CZ2  | 2.54                     | 0.42              |
| 3:N:240:GLU:O     | 3:N:241:ILE:C     | 2.62                     | 0.42              |
| 3:N:404:GLU:OE2   | 3:N:414:ARG:NH1   | 2.52                     | 0.42              |
| 3:N:827:ILE:HD12  | 3:N:828:LYS:HZ1   | 1.84                     | 0.42              |
| 5:P:74:LYS:HD3    | 5:P:74:LYS:HA     | 1.87                     | 0.42              |
| 1:A:96:THR:HG21   | 8:A:9543:HOH:O    | 2.19                     | 0.42              |
| 1:B:1:MET:H1      | 1:B:1:MET:HG3     | 1.66                     | 0.42              |
| 2:C:121:MET:HA    | 2:C:127:PHE:CD2   | 2.55                     | 0.42              |
| 2:C:196:LEU:HD11  | 2:C:303:PHE:CE1   | 2.54                     | 0.42              |
| 2:C:217:LEU:HD12  | 2:C:311:PHE:CD2   | 2.54                     | 0.42              |
| 2:C:265:ARG:HA    | 2:C:289:THR:OG1   | 2.18                     | 0.42              |
| 2:C:367:LEU:HD11  | 8:C:9627:HOH:O    | 2.18                     | 0.42              |
| 2:C:575:GLN:HA    | 2:C:662:GLU:HG3   | 2.00                     | 0.42              |
| 2:C:601:GLY:HA3   | 2:C:615:TYR:HA    | 2.01                     | 0.42              |
| 2:C:715:THR:HG22  | 2:C:717:LEU:HG    | 2.01                     | 0.42              |
| 2:C:739:GLU:O     | 2:C:740:GLU:C     | 2.62                     | 0.42              |
| 2:C:1105:LYS:O    | 2:C:1107:ASN:N    | 2.52                     | 0.42              |
| 3:D:54:LYS:HA     | 8:D:9647:HOH:O    | 2.19                     | 0.42              |
| 3:D:171:LEU:HA    | 3:D:172:PRO:HD3   | 1.59                     | 0.42              |
| 3:D:399:ARG:NH2   | 8:D:2498:HOH:O    | 2.51                     | 0.42              |
| 3:D:960:LYS:HG2   | 3:D:964:LEU:HD12  | 2.00                     | 0.42              |
| 3:D:1487:VAL:HG12 | 3:D:1488:ASP:O    | 2.19                     | 0.42              |
| 5:F:363:GLU:CG    | 5:F:364:ARG:N     | 2.82                     | 0.42              |
| 5:F:416:ARG:HD2   | 5:F:419:ARG:HB3   | 2.01                     | 0.42              |
| 1:K:218:LEU:HD12  | 1:K:222:LEU:HD23  | 2.00                     | 0.42              |
| 2:M:516:ARG:CD    | 2:M:521:PRO:HA    | 2.49                     | 0.42              |
| 2:M:555:ALA:HA    | 3:N:1070:TYR:HH   | 1.85                     | 0.42              |
| 2:M:691:SER:CB    | 2:M:858:MET:SD    | 3.07                     | 0.42              |
| 2:M:778:PHE:CE2   | 5:P:419:ARG:CD    | 2.98                     | 0.42              |
| 2:M:971:LYS:HZ2   | 3:N:950:GLY:HA3   | 1.84                     | 0.42              |
| 3:N:103:TRP:NE1   | 3:N:583:ASP:OD2   | 2.52                     | 0.42              |
| 3:N:166:GLN:N     | 8:N:9606:HOH:O    | 2.52                     | 0.42              |
| 3:N:172:PRO:HA    | 3:N:173:PRO:HD3   | 1.53                     | 0.42              |
| 3:N:1320:GLU:H    | 3:N:1323:GLN:NE2  | 2.17                     | 0.42              |
| 3:N:1481:VAL:HG11 | 4:O:18:ARG:CA     | 2.38                     | 0.42              |
| 4:O:41:GLU:C      | 4:O:45:ARG:HG3    | 2.44                     | 0.42              |
| 5:P:361:LEU:HD21  | 5:P:408:LEU:CB    | 2.49                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:222:LEU:HD13 | 1:A:222:LEU:HA    | 1.83                     | 0.42              |
| 1:B:108:GLU:HB3  | 1:B:128:HIS:CE1   | 2.54                     | 0.42              |
| 1:B:192:LEU:HD23 | 1:B:192:LEU:HA    | 1.84                     | 0.42              |
| 2:C:12:VAL:CG1   | 2:C:534:VAL:HG13  | 2.49                     | 0.42              |
| 2:C:103:LYS:HD3  | 2:C:103:LYS:HA    | 1.56                     | 0.42              |
| 2:C:203:ASP:O    | 2:C:207:LEU:HB2   | 2.18                     | 0.42              |
| 2:C:217:LEU:HB2  | 2:C:311:PHE:CE2   | 2.54                     | 0.42              |
| 2:C:346:VAL:O    | 2:C:350:ARG:HG3   | 2.19                     | 0.42              |
| 2:C:564:MET:SD   | 2:C:846:LYS:HD2   | 2.59                     | 0.42              |
| 2:C:572:ILE:CD1  | 2:C:701:THR:HB    | 2.49                     | 0.42              |
| 2:C:578:VAL:HG11 | 2:C:991:GLN:CD    | 2.45                     | 0.42              |
| 2:C:607:ASP:HB2  | 2:C:610:ARG:H     | 1.83                     | 0.42              |
| 3:D:411:THR:CG2  | 3:D:429:SER:HB3   | 2.46                     | 0.42              |
| 3:D:433:GLY:HA3  | 3:D:449:SER:O     | 2.18                     | 0.42              |
| 3:D:483:HIS:ND1  | 3:D:483:HIS:N     | 2.67                     | 0.42              |
| 3:D:601:ARG:HH22 | 3:D:611:GLN:H     | 1.68                     | 0.42              |
| 3:D:951:ILE:HG23 | 3:D:1062:ARG:NH2  | 2.34                     | 0.42              |
| 3:D:991:GLN:HG2  | 8:D:9698:HOH:O    | 2.19                     | 0.42              |
| 3:D:1144:LEU:HA  | 3:D:1147:ARG:HG3  | 2.01                     | 0.42              |
| 3:D:1228:SER:O   | 3:D:1232:PRO:HD2  | 2.19                     | 0.42              |
| 3:D:1266:ARG:O   | 3:D:1268:PRO:HD3  | 2.19                     | 0.42              |
| 3:D:1310:ARG:HG3 | 3:D:1327:ARG:HB3  | 2.01                     | 0.42              |
| 5:F:79:ASP:HB3   | 5:F:80:PRO:HD2    | 2.01                     | 0.42              |
| 5:F:408:LEU:HD23 | 5:F:408:LEU:C     | 2.43                     | 0.42              |
| 1:K:224:TYR:CG   | 1:L:9:PRO:HG2     | 2.55                     | 0.42              |
| 2:M:207:LEU:HB3  | 2:M:221:LEU:HD21  | 2.00                     | 0.42              |
| 2:M:279:GLU:HG3  | 2:M:280:LYS:N     | 2.33                     | 0.42              |
| 2:M:376:ARG:HH12 | 5:P:285:GLU:CG    | 2.31                     | 0.42              |
| 2:M:432:ARG:HH22 | 3:N:1047:LYS:CE   | 2.31                     | 0.42              |
| 2:M:695:LEU:HD21 | 2:M:833:LEU:O     | 2.19                     | 0.42              |
| 2:M:1008:ARG:C   | 8:M:9822:HOH:O    | 2.62                     | 0.42              |
| 3:N:55:ASP:OD2   | 3:N:82:LYS:HD3    | 2.18                     | 0.42              |
| 3:N:152:LEU:HD23 | 3:N:152:LEU:H     | 1.83                     | 0.42              |
| 3:N:194:GLY:O    | 3:N:196:VAL:HG23  | 2.19                     | 0.42              |
| 3:N:584:ASN:HD21 | 3:N:590:PRO:HB2   | 1.84                     | 0.42              |
| 3:N:845:ASN:CG   | 3:N:846:PRO:HD2   | 2.43                     | 0.42              |
| 3:N:1489:GLN:HA  | 3:N:1489:GLN:HE21 | 1.82                     | 0.42              |
| 5:P:149:GLU:N    | 8:P:9479:HOH:O    | 2.52                     | 0.42              |
| 1:B:54:THR:CG2   | 1:B:158:ILE:HG13  | 2.33                     | 0.42              |
| 1:B:95:GLN:HB3   | 8:B:9540:HOH:O    | 2.18                     | 0.42              |
| 1:B:223:THR:C    | 1:B:225:PHE:H     | 2.27                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:2:GLU:HG2    | 8:C:9758:HOH:O    | 2.18                     | 0.42              |
| 2:C:110:GLU:HB3  | 8:C:9664:HOH:O    | 2.18                     | 0.42              |
| 2:C:149:THR:HG23 | 2:C:150:PRO:HD2   | 2.02                     | 0.42              |
| 2:C:259:GLY:O    | 2:C:290:LEU:O     | 2.37                     | 0.42              |
| 2:C:578:VAL:HG11 | 2:C:991:GLN:HB3   | 2.01                     | 0.42              |
| 2:C:605:LYS:HB2  | 2:C:610:ARG:NH1   | 2.34                     | 0.42              |
| 2:C:722:ILE:O    | 2:C:722:ILE:HG23  | 2.19                     | 0.42              |
| 3:D:450:TYR:O    | 3:D:452:ILE:N     | 2.51                     | 0.42              |
| 3:D:459:GLU:O    | 3:D:463:GLN:HG2   | 2.19                     | 0.42              |
| 3:D:553:ARG:HD2  | 3:D:570:GLU:OE2   | 2.19                     | 0.42              |
| 3:D:884:ARG:HG3  | 8:D:9779:HOH:O    | 2.19                     | 0.42              |
| 3:D:1210:SER:HA  | 8:D:2016:HOH:O    | 2.20                     | 0.42              |
| 4:E:37:ASN:HA    | 8:E:9378:HOH:O    | 2.19                     | 0.42              |
| 4:E:95:GLY:HA3   | 8:E:9401:HOH:O    | 2.19                     | 0.42              |
| 1:K:1:MET:O      | 1:K:6:LEU:CB      | 2.47                     | 0.42              |
| 1:K:139:ASN:ND2  | 8:K:5059:HOH:O    | 2.52                     | 0.42              |
| 1:L:11:PHE:CE2   | 1:L:13:VAL:HG22   | 2.54                     | 0.42              |
| 2:M:118:ILE:HA   | 2:M:119:PRO:HD3   | 1.83                     | 0.42              |
| 2:M:182:VAL:HG23 | 8:M:2190:HOH:O    | 2.20                     | 0.42              |
| 2:M:276:LYS:CG   | 2:M:280:LYS:HE3   | 2.50                     | 0.42              |
| 2:M:630:ARG:HE   | 2:M:707:ARG:HB2   | 1.84                     | 0.42              |
| 2:M:1095:LEU:O   | 2:M:1096:ALA:C    | 2.62                     | 0.42              |
| 2:M:1101:THR:O   | 2:M:1102:LEU:HD12 | 2.20                     | 0.42              |
| 2:M:1106:ASP:HA  | 3:N:7:LYS:HE3     | 2.00                     | 0.42              |
| 3:N:119:SER:HB3  | 3:N:123:LEU:H     | 1.84                     | 0.42              |
| 3:N:186:VAL:O    | 3:N:211:VAL:HB    | 2.20                     | 0.42              |
| 3:N:447:VAL:HG23 | 3:N:448:GLU:N     | 2.33                     | 0.42              |
| 3:N:632:VAL:O    | 3:N:727:GLN:HA    | 2.19                     | 0.42              |
| 3:N:657:LEU:HD13 | 3:N:691:LEU:HA    | 2.02                     | 0.42              |
| 3:N:658:LEU:O    | 3:N:661:MET:HB2   | 2.19                     | 0.42              |
| 3:N:862:ASP:O    | 3:N:877:PRO:HD2   | 2.19                     | 0.42              |
| 3:N:936:TYR:HB2  | 8:N:9603:HOH:O    | 2.19                     | 0.42              |
| 3:N:1111:ASP:O   | 3:N:1112:CYS:C    | 2.62                     | 0.42              |
| 3:N:1114:THR:O   | 3:N:1114:THR:HG22 | 2.19                     | 0.42              |
| 3:N:1377:LYS:HG2 | 3:N:1378:TYR:CE1  | 2.54                     | 0.42              |
| 3:N:1422:MET:HE2 | 3:N:1427:SER:HA   | 1.98                     | 0.42              |
| 5:P:194:LEU:HD13 | 5:P:194:LEU:C     | 2.45                     | 0.42              |
| 1:A:7:LYS:NZ     | 8:A:9447:HOH:O    | 2.48                     | 0.42              |
| 1:A:42:ARG:CZ    | 2:C:857:ASP:HB3   | 2.50                     | 0.42              |
| 2:C:279:GLU:CD   | 2:C:489:THR:HG21  | 2.44                     | 0.42              |
| 2:C:696:LYS:NZ   | 8:C:9599:HOH:O    | 2.44                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:701:THR:HG23  | 2:C:832:LYS:HG2  | 2.02                     | 0.42              |
| 2:C:830:LYS:HD3   | 8:C:2071:HOH:O   | 2.18                     | 0.42              |
| 3:D:23:TYR:CE2    | 3:D:89:ARG:NH1   | 2.88                     | 0.42              |
| 3:D:147:VAL:HG11  | 8:D:2105:HOH:O   | 2.20                     | 0.42              |
| 3:D:168:THR:HB    | 3:D:393:ILE:CD1  | 2.49                     | 0.42              |
| 3:D:916:TYR:HD2   | 3:D:916:TYR:O    | 2.03                     | 0.42              |
| 3:D:1259:VAL:HG11 | 3:D:1356:TYR:OH  | 2.20                     | 0.42              |
| 3:D:1327:ARG:NH1  | 8:D:9696:HOH:O   | 2.52                     | 0.42              |
| 5:F:332:PHE:N     | 5:F:332:PHE:CD1  | 2.88                     | 0.42              |
| 5:F:370:LYS:O     | 5:F:374:GLY:N    | 2.46                     | 0.42              |
| 1:K:94:LEU:HD13   | 8:K:742:HOH:O    | 2.20                     | 0.42              |
| 1:K:180:GLN:HG3   | 8:K:2871:HOH:O   | 2.19                     | 0.42              |
| 2:M:29:ALA:HB2    | 2:M:337:GLY:CA   | 2.50                     | 0.42              |
| 2:M:129:ILE:CG2   | 2:M:130:ASN:N    | 2.82                     | 0.42              |
| 2:M:250:ARG:HE    | 2:M:253:ALA:HB1  | 1.85                     | 0.42              |
| 2:M:473:ARG:NH2   | 8:M:9920:HOH:O   | 2.48                     | 0.42              |
| 2:M:877:PRO:HG2   | 3:N:1023:MET:HE1 | 2.01                     | 0.42              |
| 2:M:1105:LYS:H    | 2:M:1105:LYS:HG2 | 1.52                     | 0.42              |
| 2:M:1109:VAL:HG22 | 3:N:3:LYS:CG     | 2.50                     | 0.42              |
| 3:N:33:ASN:HB2    | 3:N:40:GLU:OE1   | 2.20                     | 0.42              |
| 3:N:56:TYR:HA     | 3:N:80:VAL:CG2   | 2.49                     | 0.42              |
| 3:N:199:LEU:HD23  | 3:N:199:LEU:C    | 2.44                     | 0.42              |
| 3:N:462:GLN:CB    | 3:N:513:ILE:HD13 | 2.49                     | 0.42              |
| 3:N:543:LEU:HA    | 3:N:546:ARG:HG3  | 2.01                     | 0.42              |
| 3:N:607:LEU:HA    | 8:N:2216:HOH:O   | 2.19                     | 0.42              |
| 3:N:1097:LYS:HG2  | 3:N:1097:LYS:H   | 1.47                     | 0.42              |
| 3:N:1434:TRP:CZ3  | 3:N:1455:LYS:O   | 2.73                     | 0.42              |
| 5:P:394:ARG:HA    | 5:P:397:ILE:CD1  | 2.39                     | 0.42              |
| 1:B:86:VAL:HG23   | 8:B:9516:HOH:O   | 2.20                     | 0.42              |
| 1:B:86:VAL:O      | 1:B:86:VAL:HG13  | 2.20                     | 0.42              |
| 2:C:44:ILE:HB     | 8:C:9525:HOH:O   | 2.18                     | 0.42              |
| 2:C:80:GLN:O      | 2:C:83:CYS:HB2   | 2.19                     | 0.42              |
| 2:C:264:PRO:CB    | 2:C:289:THR:CB   | 2.97                     | 0.42              |
| 2:C:296:GLY:HA2   | 8:C:2264:HOH:O   | 2.19                     | 0.42              |
| 2:C:302:VAL:HG12  | 8:C:9742:HOH:O   | 2.19                     | 0.42              |
| 2:C:676:ILE:HG21  | 2:C:988:VAL:HG13 | 1.99                     | 0.42              |
| 2:C:683:ASN:CB    | 2:C:687:ALA:O    | 2.67                     | 0.42              |
| 2:C:1031:ARG:HD3  | 3:D:619:LEU:CD2  | 2.47                     | 0.42              |
| 3:D:207:PHE:HE2   | 8:D:2157:HOH:O   | 2.01                     | 0.42              |
| 3:D:412:GLY:O     | 3:D:421:LEU:HB3  | 2.20                     | 0.42              |
| 3:D:785:ILE:HG23  | 3:D:938:GLY:HA3  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:790:TYR:CE1   | 3:D:1022:VAL:HG13 | 2.54                     | 0.42              |
| 3:D:910:SER:HB3   | 8:D:9734:HOH:O    | 2.19                     | 0.42              |
| 3:D:1219:GLU:O    | 3:D:1221:VAL:N    | 2.53                     | 0.42              |
| 3:D:1320:GLU:O    | 3:D:1323:GLN:HB2  | 2.19                     | 0.42              |
| 3:D:1425:THR:HG22 | 3:D:1426:LYS:N    | 2.34                     | 0.42              |
| 4:E:29:GLN:HB2    | 4:E:33:HIS:HD2    | 1.84                     | 0.42              |
| 4:E:41:GLU:HB3    | 8:E:9389:HOH:O    | 2.18                     | 0.42              |
| 4:E:45:ARG:HB3    | 4:E:46:PRO:CD     | 2.49                     | 0.42              |
| 4:E:54:LEU:HG     | 4:E:58:PRO:CD     | 2.44                     | 0.42              |
| 4:E:54:LEU:CD1    | 4:E:58:PRO:HB2    | 2.49                     | 0.42              |
| 5:F:363:GLU:CB    | 8:F:9704:HOH:O    | 2.67                     | 0.42              |
| 1:K:81:ASN:ND2    | 1:K:128:HIS:O     | 2.53                     | 0.42              |
| 1:K:214:ALA:HA    | 1:K:217:ILE:HD12  | 2.00                     | 0.42              |
| 2:M:38:LYS:HD3    | 2:M:38:LYS:HA     | 1.89                     | 0.42              |
| 2:M:139:GLN:N     | 8:M:9656:HOH:O    | 2.52                     | 0.42              |
| 2:M:552:HIS:ND1   | 2:M:886:LEU:HD13  | 2.35                     | 0.42              |
| 2:M:625:LEU:HD11  | 2:M:641:PRO:HG3   | 2.02                     | 0.42              |
| 2:M:858:MET:HB2   | 2:M:859:PRO:CD    | 2.50                     | 0.42              |
| 2:M:1043:TYR:CE2  | 3:N:763:MET:HG3   | 2.55                     | 0.42              |
| 3:N:153:LEU:CD1   | 3:N:158:TYR:HB2   | 2.49                     | 0.42              |
| 3:N:228:ALA:HB2   | 8:N:9528:HOH:O    | 2.20                     | 0.42              |
| 3:N:552:ASN:HB3   | 8:N:9969:HOH:O    | 2.18                     | 0.42              |
| 3:N:786:ILE:HD11  | 3:N:908:LYS:CB    | 2.49                     | 0.42              |
| 3:N:1008:PHE:CZ   | 3:N:1032:PRO:HA   | 2.55                     | 0.42              |
| 3:N:1344:VAL:HG12 | 3:N:1348:LEU:HD23 | 2.00                     | 0.42              |
| 4:O:29:GLN:NE2    | 8:O:895:HOH:O     | 2.51                     | 0.42              |
| 5:P:288:TYR:HE2   | 5:P:305:GLU:HG3   | 1.85                     | 0.42              |
| 5:P:407:LYS:HG3   | 8:P:9714:HOH:O    | 2.19                     | 0.42              |
| 1:A:138:LEU:HB2   | 8:A:9482:HOH:O    | 2.19                     | 0.42              |
| 2:C:157:ARG:HD2   | 2:C:314:THR:HG22  | 2.02                     | 0.42              |
| 2:C:399:ASN:ND2   | 2:C:568:ALA:O     | 2.49                     | 0.42              |
| 2:C:440:PRO:HB3   | 8:D:9725:HOH:O    | 2.19                     | 0.42              |
| 2:C:516:ARG:CD    | 3:D:1068:LEU:HD13 | 2.49                     | 0.42              |
| 2:C:695:LEU:HD22  | 2:C:832:LYS:HE2   | 2.00                     | 0.42              |
| 3:D:437:VAL:N     | 8:D:2096:HOH:O    | 2.52                     | 0.42              |
| 3:D:792:ILE:HG12  | 3:D:793:THR:HG23  | 2.00                     | 0.42              |
| 3:D:853:VAL:HG22  | 3:D:858:VAL:HB    | 2.02                     | 0.42              |
| 3:D:1109:GLU:HG2  | 3:D:1201:CYS:CA   | 2.49                     | 0.42              |
| 3:D:1211:MET:HE2  | 8:D:9586:HOH:O    | 2.19                     | 0.42              |
| 3:D:1237:THR:HG22 | 3:D:1238:MET:N    | 2.35                     | 0.42              |
| 3:D:1342:GLU:HB2  | 8:D:2486:HOH:O    | 2.18                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:F:170:HIS:HA    | 5:F:173:TYR:HD1  | 1.84                     | 0.42              |
| 5:F:232:ARG:O     | 5:F:233:PHE:C    | 2.62                     | 0.42              |
| 1:L:44:LEU:HD23   | 1:L:48:ILE:CD1   | 2.50                     | 0.42              |
| 2:M:143:SER:HB2   | 2:M:276:LYS:HZ3  | 1.83                     | 0.42              |
| 2:M:431:HIS:CD2   | 2:M:433:THR:H    | 2.37                     | 0.42              |
| 2:M:578:VAL:HG11  | 2:M:991:GLN:HB3  | 2.01                     | 0.42              |
| 2:M:865:THR:HA    | 2:M:866:PRO:HD3  | 1.85                     | 0.42              |
| 2:M:1005:MET:HG3  | 2:M:1005:MET:O   | 2.20                     | 0.42              |
| 2:M:1009:SER:OG   | 3:N:655:PRO:HD3  | 2.20                     | 0.42              |
| 2:M:1037:VAL:HG11 | 8:M:9845:HOH:O   | 2.20                     | 0.42              |
| 3:N:51:GLY:HA3    | 8:N:9729:HOH:O   | 2.19                     | 0.42              |
| 3:N:426:LYS:HZ1   | 5:P:138:SER:CA   | 2.32                     | 0.42              |
| 3:N:645:PRO:HA    | 3:N:721:VAL:O    | 2.19                     | 0.42              |
| 3:N:701:LEU:O     | 3:N:747:VAL:HA   | 2.20                     | 0.42              |
| 3:N:739:ASP:HB2   | 8:N:2331:HOH:O   | 2.19                     | 0.42              |
| 3:N:1003:VAL:O    | 3:N:1006:ALA:HB3 | 2.19                     | 0.42              |
| 3:N:1106:VAL:O    | 3:N:1108:ARG:HG2 | 2.20                     | 0.42              |
| 5:P:113:ILE:HG23  | 5:P:127:ILE:HB   | 2.02                     | 0.42              |
| 1:A:198:ARG:HD3   | 1:A:200:TRP:HH2  | 1.85                     | 0.42              |
| 2:C:626:ARG:HB3   | 2:C:629:TYR:HD1  | 1.85                     | 0.42              |
| 2:C:866:PRO:HB2   | 8:C:9715:HOH:O   | 2.20                     | 0.42              |
| 2:C:966:LEU:HD21  | 2:C:986:PRO:HG2  | 2.01                     | 0.42              |
| 2:C:978:ARG:HG3   | 2:C:978:ARG:HH11 | 1.85                     | 0.42              |
| 2:C:1034:GLU:OE2  | 3:D:1096:ARG:NE  | 2.52                     | 0.42              |
| 2:C:1059:ASP:CG   | 2:C:1062:GLY:HA3 | 2.45                     | 0.42              |
| 3:D:79:GLU:HG2    | 3:D:80:VAL:H     | 1.84                     | 0.42              |
| 3:D:113:GLY:CA    | 3:D:124:GLU:OE2  | 2.68                     | 0.42              |
| 3:D:152:LEU:N     | 3:D:152:LEU:CD2  | 2.83                     | 0.42              |
| 3:D:427:VAL:O     | 3:D:433:GLY:O    | 2.38                     | 0.42              |
| 3:D:435:VAL:HG22  | 3:D:446:VAL:HG22 | 2.01                     | 0.42              |
| 3:D:569:ASN:OD1   | 5:F:80:PRO:HB3   | 2.20                     | 0.42              |
| 5:F:223:ALA:HB2   | 5:F:242:TRP:HB2  | 2.01                     | 0.42              |
| 1:K:32:PHE:CG     | 8:K:1204:HOH:O   | 2.69                     | 0.42              |
| 1:L:109:VAL:HA    | 1:L:113:ASP:OD2  | 2.19                     | 0.42              |
| 1:L:142:VAL:O     | 1:L:142:VAL:HG23 | 2.19                     | 0.42              |
| 1:L:226:SER:O     | 1:L:228:PRO:HD3  | 2.20                     | 0.42              |
| 2:M:203:ASP:O     | 2:M:206:THR:HG22 | 2.19                     | 0.42              |
| 2:M:292:ARG:HD2   | 2:M:299:LYS:CD   | 2.49                     | 0.42              |
| 2:M:683:ASN:HD22  | 2:M:872:ASN:N    | 2.18                     | 0.42              |
| 2:M:1052:MET:HE1  | 2:M:1056:LYS:NZ  | 2.35                     | 0.42              |
| 2:M:1071:ILE:HG23 | 3:N:670:VAL:CG2  | 2.47                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:195:VAL:HG22  | 8:N:9660:HOH:O    | 2.18                     | 0.42              |
| 3:N:708:LEU:HD21  | 3:N:1091:SER:OG   | 2.19                     | 0.42              |
| 3:N:978:TYR:CE1   | 3:N:985:ASP:HA    | 2.52                     | 0.42              |
| 3:N:1044:LEU:HD13 | 8:N:9593:HOH:O    | 2.19                     | 0.42              |
| 3:N:1104:GLU:O    | 3:N:1106:VAL:HG23 | 2.20                     | 0.42              |
| 3:N:1109:GLU:C    | 3:N:1109:GLU:CD   | 2.88                     | 0.42              |
| 3:N:1149:LEU:HD13 | 3:N:1153:VAL:HG23 | 2.01                     | 0.42              |
| 3:N:1380:GLU:OE2  | 3:N:1390:LEU:HD13 | 2.19                     | 0.42              |
| 3:N:1389:LEU:O    | 3:N:1391:GLU:N    | 2.52                     | 0.42              |
| 3:N:1398:TRP:HE3  | 3:N:1415:VAL:HG11 | 1.80                     | 0.42              |
| 1:A:79:ILE:HG21   | 1:A:165:ILE:HD11  | 2.01                     | 0.42              |
| 2:C:41:ASN:HD22   | 2:C:41:ASN:N      | 2.16                     | 0.42              |
| 2:C:99:GLN:HG3    | 2:C:99:GLN:O      | 2.20                     | 0.42              |
| 2:C:200:LEU:HD22  | 2:C:300:ASP:HB3   | 2.02                     | 0.42              |
| 2:C:287:GLY:HA2   | 8:C:2319:HOH:O    | 2.20                     | 0.42              |
| 2:C:299:LYS:HG3   | 2:C:299:LYS:O     | 2.19                     | 0.42              |
| 2:C:346:VAL:HG12  | 2:C:350:ARG:HE    | 1.85                     | 0.42              |
| 2:C:569:VAL:HG11  | 2:C:996:LYS:HE2   | 2.01                     | 0.42              |
| 2:C:623:TYR:N     | 8:C:9839:HOH:O    | 2.44                     | 0.42              |
| 2:C:718:GLY:HA3   | 2:C:761:PHE:CE1   | 2.55                     | 0.42              |
| 2:C:728:HIS:NE2   | 5:F:423:ASP:O     | 2.52                     | 0.42              |
| 2:C:1038:TRP:CH2  | 3:D:1096:ARG:HD2  | 2.55                     | 0.42              |
| 3:D:23:TYR:O      | 3:D:24:GLY:O      | 2.38                     | 0.42              |
| 3:D:116:LEU:HD22  | 3:D:464:LEU:HB3   | 2.02                     | 0.42              |
| 3:D:493:ARG:CD    | 8:D:9868:HOH:O    | 2.67                     | 0.42              |
| 3:D:503:LEU:HA    | 8:D:9521:HOH:O    | 2.19                     | 0.42              |
| 3:D:566:ILE:CG2   | 5:F:214:GLN:HE22  | 2.32                     | 0.42              |
| 3:D:798:GLU:CG    | 3:D:799:LYS:H     | 2.28                     | 0.42              |
| 3:D:1137:ARG:O    | 3:D:1141:GLU:HG3  | 2.20                     | 0.42              |
| 3:D:1171:VAL:O    | 3:D:1171:VAL:HG12 | 2.18                     | 0.42              |
| 3:D:1472:ILE:HD13 | 8:D:9619:HOH:O    | 2.19                     | 0.42              |
| 1:L:187:GLY:HA2   | 8:L:2254:HOH:O    | 2.19                     | 0.42              |
| 2:M:184:MET:HE2   | 2:M:186:VAL:HG22  | 2.02                     | 0.42              |
| 2:M:216:GLU:C     | 2:M:218:VAL:H     | 2.26                     | 0.42              |
| 2:M:630:ARG:HH11  | 2:M:630:ARG:CG    | 2.32                     | 0.42              |
| 2:M:659:PRO:HD3   | 8:M:9732:HOH:O    | 2.19                     | 0.42              |
| 2:M:690:ILE:HD13  | 2:M:690:ILE:HA    | 1.81                     | 0.42              |
| 2:M:707:ARG:HD2   | 2:M:824:ARG:NH1   | 2.33                     | 0.42              |
| 2:M:737:LEU:O     | 2:M:738:ASP:C     | 2.62                     | 0.42              |
| 2:M:816:LYS:HB2   | 2:M:819:VAL:CG2   | 2.49                     | 0.42              |
| 2:M:1012:PRO:HA   | 8:P:9485:HOH:O    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:1015:LEU:N    | 8:M:9633:HOH:O    | 2.53                     | 0.42              |
| 3:N:27:GLU:O      | 3:N:28:LYS:HG3    | 2.19                     | 0.42              |
| 3:N:131:LYS:HD3   | 3:N:456:MET:CE    | 2.50                     | 0.42              |
| 3:N:401:TYR:HD2   | 3:N:415:VAL:HG13  | 1.85                     | 0.42              |
| 3:N:422:ALA:HB3   | 3:N:427:VAL:CG1   | 2.50                     | 0.42              |
| 3:N:477:LEU:HD22  | 3:N:492:ALA:CB    | 2.45                     | 0.42              |
| 3:N:683:ILE:HG22  | 3:N:687:VAL:CG2   | 2.47                     | 0.42              |
| 3:N:887:ALA:HB1   | 3:N:893:GLU:HG3   | 2.01                     | 0.42              |
| 3:N:950:GLY:O     | 3:N:953:ASP:HB2   | 2.19                     | 0.42              |
| 3:N:993:LEU:O     | 3:N:997:THR:OG1   | 2.37                     | 0.42              |
| 3:N:1112:CYS:N    | 8:N:2258:HOH:O    | 2.53                     | 0.42              |
| 3:N:1205:TYR:CZ   | 3:N:1221:VAL:HG22 | 2.54                     | 0.42              |
| 3:N:1486:VAL:CG2  | 4:O:22:VAL:HG13   | 2.50                     | 0.42              |
| 1:A:66:SER:O      | 1:A:75:VAL:HG23   | 2.20                     | 0.42              |
| 1:A:86:VAL:HG23   | 1:A:202:ASP:OD1   | 2.20                     | 0.42              |
| 1:A:127:LEU:HD12  | 1:A:127:LEU:C     | 2.44                     | 0.42              |
| 2:C:30:LEU:HD22   | 2:C:118:ILE:HD11  | 2.01                     | 0.42              |
| 2:C:874:LEU:HD21  | 3:D:787:LEU:HD23  | 1.98                     | 0.42              |
| 2:C:933:GLY:HA3   | 8:C:2179:HOH:O    | 2.19                     | 0.42              |
| 2:C:1108:PRO:HB2  | 8:C:2213:HOH:O    | 2.19                     | 0.42              |
| 3:D:135:LEU:HD21  | 3:D:139:GLY:HA3   | 2.01                     | 0.42              |
| 3:D:714:GLN:HE22  | 3:D:735:ALA:HB3   | 1.85                     | 0.42              |
| 3:D:1122:LEU:HD12 | 3:D:1122:LEU:N    | 2.34                     | 0.42              |
| 3:D:1285:GLU:O    | 3:D:1286:THR:C    | 2.63                     | 0.42              |
| 3:D:1373:ARG:HG2  | 3:D:1374:GLN:NE2  | 2.33                     | 0.42              |
| 4:E:18:ARG:NH2    | 8:E:9450:HOH:O    | 2.51                     | 0.42              |
| 4:E:84:ARG:HD2    | 8:E:9390:HOH:O    | 2.18                     | 0.42              |
| 5:F:286:PRO:HA    | 5:F:290:GLU:OE1   | 2.19                     | 0.42              |
| 5:F:420:ASP:O     | 5:F:422:LEU:CD2   | 2.51                     | 0.42              |
| 2:M:243:ARG:HA    | 2:M:244:PRO:HD3   | 1.54                     | 0.42              |
| 2:M:374:ASN:O     | 2:M:377:PRO:HD2   | 2.20                     | 0.42              |
| 2:M:413:LEU:HD12  | 2:M:413:LEU:N     | 2.34                     | 0.42              |
| 2:M:520:GLU:HA    | 2:M:521:PRO:HD3   | 1.90                     | 0.42              |
| 2:M:610:ARG:HD2   | 2:M:612:VAL:HG23  | 2.02                     | 0.42              |
| 2:M:627:ARG:O     | 2:M:638:ASP:HB3   | 2.19                     | 0.42              |
| 3:N:18:ILE:HD12   | 3:N:518:PRO:HD3   | 2.01                     | 0.42              |
| 3:N:82:LYS:HB3    | 8:N:2103:HOH:O    | 2.19                     | 0.42              |
| 3:N:99:ALA:HB1    | 3:N:575:GLN:HA    | 2.01                     | 0.42              |
| 3:N:826:PRO:HB3   | 8:N:9926:HOH:O    | 2.19                     | 0.42              |
| 3:N:864:VAL:CG1   | 3:N:865:THR:N     | 2.83                     | 0.42              |
| 3:N:1319:VAL:O    | 3:N:1319:VAL:HG23 | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:O:48:MET:N      | 4:O:54:LEU:HB2    | 2.35                     | 0.42              |
| 5:P:94:LEU:CD1    | 5:P:96:LEU:H      | 2.13                     | 0.42              |
| 5:P:156:VAL:N     | 8:P:9471:HOH:O    | 2.46                     | 0.42              |
| 5:P:195:VAL:HG12  | 5:P:213:ILE:HG23  | 2.02                     | 0.42              |
| 5:P:361:LEU:HD12  | 5:P:366:ALA:CB    | 2.49                     | 0.42              |
| 1:A:209:GLU:O     | 1:A:213:GLN:HG3   | 2.20                     | 0.41              |
| 1:B:5:LYS:O       | 1:B:8:ALA:CB      | 2.64                     | 0.41              |
| 2:C:143:SER:HB3   | 2:C:332:ARG:HB2   | 2.01                     | 0.41              |
| 2:C:165:LEU:HD12  | 2:C:165:LEU:C     | 2.46                     | 0.41              |
| 2:C:168:ARG:N     | 2:C:168:ARG:HD2   | 2.33                     | 0.41              |
| 2:C:216:GLU:C     | 2:C:218:VAL:N     | 2.77                     | 0.41              |
| 2:C:217:LEU:HD12  | 2:C:311:PHE:HA    | 2.01                     | 0.41              |
| 2:C:690:ILE:HG21  | 2:C:833:LEU:CD2   | 2.47                     | 0.41              |
| 2:C:1067:TYR:CE2  | 5:F:345:ALA:HB2   | 2.55                     | 0.41              |
| 3:D:195:VAL:HG22  | 8:D:9592:HOH:O    | 2.20                     | 0.41              |
| 3:D:508:ARG:HA    | 3:D:509:PRO:HD2   | 1.28                     | 0.41              |
| 3:D:678:GLU:HB2   | 8:D:9785:HOH:O    | 2.19                     | 0.41              |
| 3:D:1099:VAL:HG13 | 3:D:1223:ILE:HG13 | 2.02                     | 0.41              |
| 3:D:1197:ARG:N    | 8:D:9488:HOH:O    | 2.53                     | 0.41              |
| 3:D:1217:ILE:HG21 | 3:D:1480:PHE:CD2  | 2.55                     | 0.41              |
| 3:D:1282:ARG:HD3  | 3:D:1295:GLU:CD   | 2.45                     | 0.41              |
| 1:K:186:LEU:HB2   | 1:K:192:LEU:HD11  | 2.01                     | 0.41              |
| 1:K:225:PHE:HB2   | 8:K:5027:HOH:O    | 2.19                     | 0.41              |
| 1:L:65:PHE:HD1    | 8:L:3952:HOH:O    | 2.03                     | 0.41              |
| 2:M:18:LEU:HD23   | 2:M:542:VAL:HG21  | 2.01                     | 0.41              |
| 2:M:52:PHE:O      | 2:M:54:ILE:N      | 2.53                     | 0.41              |
| 2:M:103:LYS:HD3   | 2:M:103:LYS:HA    | 1.58                     | 0.41              |
| 2:M:169:GLY:C     | 8:M:9843:HOH:O    | 2.63                     | 0.41              |
| 2:M:253:ALA:N     | 8:M:9827:HOH:O    | 2.53                     | 0.41              |
| 2:M:439:CYS:SG    | 2:M:541:SER:N     | 2.90                     | 0.41              |
| 2:M:536:PRO:HB2   | 2:M:905:ILE:HD12  | 2.00                     | 0.41              |
| 2:M:571:LEU:HD21  | 2:M:700:TYR:CD2   | 2.55                     | 0.41              |
| 2:M:614:ARG:HH11  | 2:M:614:ARG:CG    | 2.33                     | 0.41              |
| 2:M:639:GLN:HA    | 2:M:657:ASP:O     | 2.20                     | 0.41              |
| 2:M:650:ARG:HG2   | 2:M:653:ASP:HB2   | 2.01                     | 0.41              |
| 2:M:777:ILE:HG22  | 2:M:778:PHE:HD1   | 1.85                     | 0.41              |
| 2:M:778:PHE:HE2   | 5:P:419:ARG:HD3   | 1.79                     | 0.41              |
| 2:M:918:LEU:HD23  | 2:M:968:LEU:O     | 2.20                     | 0.41              |
| 2:M:1098:ASP:O    | 3:N:9:ARG:O       | 2.38                     | 0.41              |
| 3:N:91:GLY:O      | 3:N:519:VAL:N     | 2.53                     | 0.41              |
| 3:N:455:ARG:HH22  | 5:P:140:ARG:CB    | 2.33                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:469:ASP:C     | 8:N:9534:HOH:O   | 2.63                     | 0.41              |
| 3:N:628:ARG:HG2   | 3:N:629:SER:N    | 2.34                     | 0.41              |
| 3:N:654:LYS:O     | 3:N:658:LEU:HG   | 2.20                     | 0.41              |
| 3:N:1042:ARG:HH12 | 3:N:1045:MET:CE  | 2.32                     | 0.41              |
| 3:N:1476:THR:C    | 3:N:1478:SER:N   | 2.75                     | 0.41              |
| 5:P:79:ASP:HB3    | 5:P:80:PRO:HD3   | 2.02                     | 0.41              |
| 5:P:140:ARG:HG3   | 5:P:141:VAL:N    | 2.33                     | 0.41              |
| 1:A:5:LYS:O       | 1:A:8:ALA:CB     | 2.65                     | 0.41              |
| 2:C:279:GLU:HG3   | 2:C:280:LYS:N    | 2.35                     | 0.41              |
| 2:C:449:ILE:C     | 2:C:451:LEU:H    | 2.27                     | 0.41              |
| 2:C:749:VAL:O     | 2:C:749:VAL:HG23 | 2.20                     | 0.41              |
| 2:C:858:MET:HE2   | 2:C:858:MET:HB3  | 1.87                     | 0.41              |
| 2:C:1031:ARG:CD   | 3:D:619:LEU:HD21 | 2.49                     | 0.41              |
| 3:D:83:SER:HA     | 8:D:9655:HOH:O   | 2.19                     | 0.41              |
| 3:D:191:LEU:HD23  | 3:D:191:LEU:HA   | 1.87                     | 0.41              |
| 3:D:191:LEU:CG    | 3:D:211:VAL:HG21 | 2.50                     | 0.41              |
| 3:D:704:ARG:CG    | 3:D:705:ALA:N    | 2.83                     | 0.41              |
| 3:D:899:LEU:HD13  | 3:D:900:ILE:HG23 | 2.02                     | 0.41              |
| 3:D:1022:VAL:CG2  | 8:D:9500:HOH:O   | 2.66                     | 0.41              |
| 3:D:1106:VAL:O    | 3:D:1108:ARG:HG2 | 2.21                     | 0.41              |
| 5:F:286:PRO:HB3   | 8:F:9483:HOH:O   | 2.19                     | 0.41              |
| 1:K:150:TYR:CE2   | 1:K:152:PRO:HG3  | 2.49                     | 0.41              |
| 1:L:171:PHE:O     | 1:L:173:PRO:HD3  | 2.20                     | 0.41              |
| 1:L:191:ASP:O     | 1:L:192:LEU:HD23 | 2.21                     | 0.41              |
| 2:M:249:LYS:O     | 2:M:249:LYS:HE3  | 2.20                     | 0.41              |
| 2:M:274:ARG:NH2   | 8:M:9939:HOH:O   | 2.52                     | 0.41              |
| 2:M:548:PRO:CG    | 2:M:842:ARG:NH2  | 2.84                     | 0.41              |
| 2:M:553:ASP:OD1   | 2:M:843:HIS:ND1  | 2.53                     | 0.41              |
| 2:M:577:PRO:HG3   | 2:M:993:PHE:CD2  | 2.55                     | 0.41              |
| 2:M:954:THR:N     | 8:M:9892:HOH:O   | 2.53                     | 0.41              |
| 3:N:33:ASN:OD1    | 3:N:40:GLU:HG2   | 2.21                     | 0.41              |
| 3:N:91:GLY:O      | 3:N:519:VAL:HB   | 2.20                     | 0.41              |
| 3:N:670:VAL:O     | 3:N:671:LYS:C    | 2.63                     | 0.41              |
| 3:N:1047:LYS:HA   | 3:N:1053:PHE:CE1 | 2.54                     | 0.41              |
| 3:N:1335:LEU:HD23 | 3:N:1335:LEU:O   | 2.20                     | 0.41              |
| 3:N:1471:LEU:HB3  | 8:N:9651:HOH:O   | 2.19                     | 0.41              |
| 5:P:163:LEU:CB    | 5:P:174:LEU:HG   | 2.45                     | 0.41              |
| 5:P:284:ARG:O     | 5:P:285:GLU:C    | 2.63                     | 0.41              |
| 5:P:416:ARG:NH1   | 5:P:419:ARG:CD   | 2.70                     | 0.41              |
| 1:A:219:ARG:NH1   | 1:B:219:ARG:CG   | 2.84                     | 0.41              |
| 1:B:91:ASN:H      | 1:B:94:LEU:HD13  | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:190:LYS:H     | 2:C:190:LYS:HG3   | 1.51                     | 0.41              |
| 2:C:230:ARG:HB3   | 8:C:2241:HOH:O    | 2.20                     | 0.41              |
| 2:C:334:ARG:HB3   | 2:C:338:GLU:OE2   | 2.20                     | 0.41              |
| 2:C:589:ARG:HD3   | 2:C:596:TYR:CZ    | 2.54                     | 0.41              |
| 2:C:654:LEU:HD23  | 2:C:654:LEU:O     | 2.20                     | 0.41              |
| 2:C:949:LYS:HB2   | 3:D:796:ARG:HH21  | 1.85                     | 0.41              |
| 2:C:962:GLN:NE2   | 8:C:9534:HOH:O    | 2.52                     | 0.41              |
| 2:C:1067:TYR:CZ   | 2:C:1071:ILE:HD11 | 2.54                     | 0.41              |
| 2:C:1098:ASP:HB3  | 3:D:11:ALA:O      | 2.20                     | 0.41              |
| 3:D:6:ARG:HG2     | 8:D:2460:HOH:O    | 2.19                     | 0.41              |
| 3:D:12:LEU:HD13   | 3:D:511:TRP:HB2   | 2.02                     | 0.41              |
| 3:D:58:CYS:HA     | 3:D:78:VAL:HG11   | 2.01                     | 0.41              |
| 3:D:104:PHE:CD1   | 3:D:512:MET:HG2   | 2.54                     | 0.41              |
| 3:D:145:VAL:HG13  | 3:D:146:PRO:N     | 2.34                     | 0.41              |
| 3:D:1240:THR:O    | 3:D:1243:THR:HG23 | 2.21                     | 0.41              |
| 4:E:81:PRO:HB3    | 8:E:9387:HOH:O    | 2.19                     | 0.41              |
| 5:F:288:TYR:HE2   | 5:F:305:GLU:HA    | 1.85                     | 0.41              |
| 5:F:302:LYS:HE3   | 5:F:306:GLU:OE2   | 2.20                     | 0.41              |
| 1:K:176:ARG:HB2   | 8:M:2117:HOH:O    | 2.19                     | 0.41              |
| 2:M:17:PRO:CD     | 8:M:9519:HOH:O    | 2.61                     | 0.41              |
| 2:M:45:GLN:HB3    | 8:M:9520:HOH:O    | 2.19                     | 0.41              |
| 2:M:216:GLU:C     | 2:M:218:VAL:N     | 2.78                     | 0.41              |
| 2:M:290:LEU:HD23  | 2:M:290:LEU:N     | 2.35                     | 0.41              |
| 2:M:293:PHE:CD2   | 2:M:293:PHE:O     | 2.73                     | 0.41              |
| 2:M:304:LEU:HD23  | 2:M:304:LEU:C     | 2.45                     | 0.41              |
| 2:M:401:LEU:HD13  | 2:M:587:VAL:CG1   | 2.50                     | 0.41              |
| 2:M:721:ARG:HE    | 2:M:783:ARG:HH21  | 1.63                     | 0.41              |
| 2:M:762:LYS:HB2   | 8:M:9919:HOH:O    | 2.20                     | 0.41              |
| 2:M:913:GLU:N     | 8:M:9582:HOH:O    | 2.53                     | 0.41              |
| 8:M:9803:HOH:O    | 3:N:1054:GLU:HB2  | 2.19                     | 0.41              |
| 3:N:23:TYR:O      | 3:N:49:ILE:HG23   | 2.20                     | 0.41              |
| 3:N:97:THR:HG23   | 5:P:144:ILE:HG21  | 2.02                     | 0.41              |
| 3:N:119:SER:O     | 3:N:120:ALA:C     | 2.64                     | 0.41              |
| 3:N:181:ASP:OD2   | 3:N:198:ARG:HB2   | 2.20                     | 0.41              |
| 3:N:404:GLU:CD    | 3:N:414:ARG:CZ    | 2.92                     | 0.41              |
| 3:N:640:HIS:CD2   | 3:N:641:GLN:HG3   | 2.55                     | 0.41              |
| 3:N:783:ARG:HA    | 3:N:1028:ALA:HA   | 2.02                     | 0.41              |
| 3:N:1032:PRO:HG2  | 8:N:9991:HOH:O    | 2.19                     | 0.41              |
| 3:N:1099:VAL:O    | 3:N:1099:VAL:HG12 | 2.21                     | 0.41              |
| 3:N:1495:ILE:HD12 | 8:O:1862:HOH:O    | 2.20                     | 0.41              |
| 4:O:61:GLU:C      | 4:O:63:TRP:N      | 2.76                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:44:LEU:HD23   | 1:B:48:ILE:HD12   | 2.02                     | 0.41              |
| 1:B:220:GLU:O     | 1:B:223:THR:HG23  | 2.20                     | 0.41              |
| 2:C:58:ASP:O      | 2:C:59:LYS:HG3    | 2.19                     | 0.41              |
| 2:C:139:GLN:O     | 2:C:334:ARG:N     | 2.51                     | 0.41              |
| 2:C:285:LEU:N     | 8:C:9567:HOH:O    | 2.44                     | 0.41              |
| 2:C:298:PHE:H     | 2:C:298:PHE:HD1   | 1.68                     | 0.41              |
| 2:C:438:ILE:HD13  | 2:C:453:THR:CG2   | 2.50                     | 0.41              |
| 2:C:1008:ARG:HB2  | 2:C:1027:PHE:HB2  | 2.02                     | 0.41              |
| 2:C:1115:LEU:H    | 2:C:1115:LEU:CD1  | 2.07                     | 0.41              |
| 2:C:1117:SER:HB2  | 8:C:9543:HOH:O    | 2.20                     | 0.41              |
| 3:D:378:ILE:HA    | 8:D:2467:HOH:O    | 2.20                     | 0.41              |
| 3:D:428:LYS:HD3   | 3:D:451:ASP:OD1   | 2.20                     | 0.41              |
| 3:D:598:ARG:HA    | 3:D:599:PRO:HD3   | 1.92                     | 0.41              |
| 3:D:796:ARG:C     | 3:D:797:LYS:HG3   | 2.45                     | 0.41              |
| 3:D:804:LEU:HD12  | 3:D:804:LEU:C     | 2.45                     | 0.41              |
| 3:D:863:VAL:HG23  | 8:D:9732:HOH:O    | 2.21                     | 0.41              |
| 3:D:1010:ASN:ND2  | 8:D:2570:HOH:O    | 2.52                     | 0.41              |
| 3:D:1017:PHE:HA   | 8:D:9500:HOH:O    | 2.21                     | 0.41              |
| 3:D:1197:ARG:NH2  | 8:D:2227:HOH:O    | 2.53                     | 0.41              |
| 3:D:1241:PHE:CE2  | 3:D:1260:ILE:HG13 | 2.54                     | 0.41              |
| 3:D:1264:GLU:HB3  | 3:D:1266:ARG:CD   | 2.49                     | 0.41              |
| 3:D:1273:VAL:HG22 | 3:D:1326:THR:HG1  | 1.85                     | 0.41              |
| 3:D:1306:PRO:HB3  | 8:D:2459:HOH:O    | 2.21                     | 0.41              |
| 3:D:1447:LEU:O    | 3:D:1448:THR:C    | 2.63                     | 0.41              |
| 3:D:1458:GLU:O    | 3:D:1460:ILE:HG13 | 2.20                     | 0.41              |
| 3:D:1483:PHE:CD1  | 3:D:1483:PHE:N    | 2.87                     | 0.41              |
| 5:F:93:LEU:HD22   | 5:F:98:GLU:CB     | 2.40                     | 0.41              |
| 5:F:287:THR:C     | 5:F:289:GLU:N     | 2.78                     | 0.41              |
| 5:F:338:LEU:N     | 5:F:338:LEU:HD23  | 2.35                     | 0.41              |
| 1:K:50:GLY:HA3    | 1:K:171:PHE:O     | 2.20                     | 0.41              |
| 2:M:45:GLN:NE2    | 8:M:9520:HOH:O    | 2.52                     | 0.41              |
| 2:M:69:LEU:HD13   | 2:M:97:ARG:NE     | 2.35                     | 0.41              |
| 2:M:209:ARG:HB3   | 8:M:2238:HOH:O    | 2.19                     | 0.41              |
| 2:M:272:ALA:HB1   | 8:M:9764:HOH:O    | 2.19                     | 0.41              |
| 2:M:293:PHE:O     | 2:M:293:PHE:CG    | 2.73                     | 0.41              |
| 2:M:449:ILE:C     | 2:M:451:LEU:H     | 2.27                     | 0.41              |
| 2:M:568:ALA:CB    | 2:M:668:LEU:HD22  | 2.46                     | 0.41              |
| 3:N:72:VAL:HG22   | 3:N:79:GLU:HB2    | 2.03                     | 0.41              |
| 3:N:521:PRO:HB2   | 3:N:524:LEU:HD12  | 2.00                     | 0.41              |
| 3:N:556:LYS:HE2   | 3:N:556:LYS:HB3   | 1.92                     | 0.41              |
| 3:N:616:GLN:CG    | 5:P:326:ASP:HB2   | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1242:HIS:HE1  | 3:N:1261:GLU:HA   | 1.84                     | 0.41              |
| 5:P:93:LEU:HG     | 5:P:190:ALA:HB1   | 2.03                     | 0.41              |
| 5:P:264:MET:O     | 5:P:268:ILE:HG13  | 2.20                     | 0.41              |
| 5:P:401:GLU:CG    | 5:P:402:ASN:OD1   | 2.68                     | 0.41              |
| 1:A:42:ARG:HH12   | 2:C:857:ASP:HB3   | 1.84                     | 0.41              |
| 1:A:184:THR:HG23  | 1:A:192:LEU:HB2   | 2.01                     | 0.41              |
| 1:B:164:ALA:C     | 8:B:9647:HOH:O    | 2.63                     | 0.41              |
| 2:C:10:ARG:HD2    | 2:C:10:ARG:HA     | 1.57                     | 0.41              |
| 2:C:148:PHE:CZ    | 2:C:281:LEU:HD13  | 2.55                     | 0.41              |
| 2:C:926:PHE:HE1   | 2:C:929:ARG:NH2   | 2.19                     | 0.41              |
| 2:C:943:VAL:HG22  | 2:C:985:GLY:N     | 2.27                     | 0.41              |
| 3:D:124:GLU:O     | 3:D:125:GLN:C     | 2.64                     | 0.41              |
| 3:D:126:VAL:O     | 3:D:132:TYR:HD1   | 2.04                     | 0.41              |
| 3:D:162:ARG:HE    | 3:D:162:ARG:HB2   | 1.50                     | 0.41              |
| 3:D:214:GLU:HB3   | 3:D:390:PRO:HD2   | 2.02                     | 0.41              |
| 3:D:378:ILE:O     | 3:D:379:ALA:C     | 2.63                     | 0.41              |
| 3:D:644:LEU:HD23  | 3:D:718:PRO:HB3   | 2.03                     | 0.41              |
| 3:D:644:LEU:HD23  | 3:D:718:PRO:CG    | 2.50                     | 0.41              |
| 3:D:699:VAL:HB    | 3:D:716:PHE:O     | 2.20                     | 0.41              |
| 4:E:69:LEU:HD21   | 8:E:9379:HOH:O    | 2.21                     | 0.41              |
| 5:F:267:THR:HG23  | 5:F:299:TRP:CH2   | 2.56                     | 0.41              |
| 1:K:152:PRO:HA    | 1:K:168:ASP:OD1   | 2.20                     | 0.41              |
| 2:M:70:GLU:OE1    | 2:M:97:ARG:HD3    | 2.19                     | 0.41              |
| 2:M:80:GLN:O      | 2:M:83:CYS:HB2    | 2.21                     | 0.41              |
| 2:M:115:LEU:HD12  | 2:M:378:LEU:CD2   | 2.51                     | 0.41              |
| 2:M:415:PRO:HB2   | 8:M:9616:HOH:O    | 2.20                     | 0.41              |
| 2:M:549:PHE:N     | 2:M:549:PHE:CD2   | 2.88                     | 0.41              |
| 2:M:668:LEU:H     | 2:M:993:PHE:HZ    | 1.67                     | 0.41              |
| 3:N:6:ARG:C       | 3:N:7:LYS:HG3     | 2.44                     | 0.41              |
| 3:N:14:SER:HA     | 3:N:511:TRP:CD2   | 2.56                     | 0.41              |
| 3:N:116:LEU:O     | 3:N:118:LEU:N     | 2.54                     | 0.41              |
| 3:N:116:LEU:HB3   | 3:N:118:LEU:CD1   | 2.51                     | 0.41              |
| 3:N:122:GLU:HB3   | 8:N:2207:HOH:O    | 2.20                     | 0.41              |
| 3:N:166:GLN:HB3   | 3:N:395:VAL:HG21  | 2.02                     | 0.41              |
| 3:N:950:GLY:O     | 3:N:951:ILE:C     | 2.62                     | 0.41              |
| 3:N:1285:GLU:O    | 3:N:1286:THR:C    | 2.63                     | 0.41              |
| 3:N:1368:ILE:H    | 3:N:1368:ILE:HG13 | 1.69                     | 0.41              |
| 3:N:1413:THR:HG21 | 8:N:9997:HOH:O    | 2.20                     | 0.41              |
| 5:P:189:GLU:O     | 5:P:192:LEU:HD12  | 2.21                     | 0.41              |
| 5:P:256:ARG:N     | 8:P:9547:HOH:O    | 2.53                     | 0.41              |
| 5:P:264:MET:HE2   | 5:P:264:MET:HA    | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:267:THR:HG23  | 5:P:299:TRP:CH2   | 2.55                     | 0.41              |
| 5:P:370:LYS:HG2   | 5:P:371:LEU:N     | 2.35                     | 0.41              |
| 1:A:48:ILE:HD13   | 1:A:210:ALA:HB1   | 2.03                     | 0.41              |
| 1:A:133:GLU:OE1   | 2:C:605:LYS:HB3   | 2.21                     | 0.41              |
| 1:A:224:TYR:CG    | 1:B:9:PRO:HG2     | 2.55                     | 0.41              |
| 1:B:34:VAL:HG12   | 8:C:2221:HOH:O    | 2.21                     | 0.41              |
| 2:C:127:PHE:CE1   | 2:C:386:PHE:CE2   | 3.09                     | 0.41              |
| 2:C:197:LEU:HD13  | 2:C:207:LEU:HD21  | 2.03                     | 0.41              |
| 2:C:293:PHE:O     | 2:C:293:PHE:CG    | 2.74                     | 0.41              |
| 2:C:436:GLY:O     | 2:C:459:ALA:HB2   | 2.20                     | 0.41              |
| 2:C:510:ALA:O     | 2:C:513:VAL:HG23  | 2.21                     | 0.41              |
| 2:C:882:LEU:HD23  | 2:C:882:LEU:HA    | 1.72                     | 0.41              |
| 2:C:1005:MET:HE3  | 3:D:724:GLN:O     | 2.21                     | 0.41              |
| 2:C:1095:LEU:O    | 2:C:1097:LEU:N    | 2.54                     | 0.41              |
| 3:D:131:LYS:CG    | 3:D:568:ARG:HG2   | 2.43                     | 0.41              |
| 3:D:603:LEU:CD2   | 3:D:606:ILE:HD12  | 2.50                     | 0.41              |
| 3:D:631:ILE:HG21  | 3:D:745:MET:HB2   | 2.03                     | 0.41              |
| 3:D:825:ALA:HA    | 3:D:826:PRO:HD3   | 1.92                     | 0.41              |
| 3:D:866:VAL:CG1   | 3:D:867:ARG:N     | 2.83                     | 0.41              |
| 3:D:897:TRP:HA    | 3:D:900:ILE:HG12  | 2.02                     | 0.41              |
| 3:D:1124:GLN:NE2  | 8:D:2167:HOH:O    | 2.52                     | 0.41              |
| 5:F:113:ILE:HG23  | 5:F:127:ILE:HB    | 2.02                     | 0.41              |
| 5:F:284:ARG:O     | 5:F:286:PRO:N     | 2.54                     | 0.41              |
| 2:M:11:GLU:CD     | 2:M:537:LYS:NZ    | 2.78                     | 0.41              |
| 2:M:47:ALA:HB2    | 2:M:345:ARG:NH1   | 2.35                     | 0.41              |
| 2:M:328:LEU:HD13  | 2:M:433:THR:CB    | 2.27                     | 0.41              |
| 2:M:480:THR:HG22  | 2:M:482:GLU:N     | 2.31                     | 0.41              |
| 2:M:564:MET:HA    | 2:M:564:MET:HE3   | 2.03                     | 0.41              |
| 2:M:814:GLU:HB2   | 8:M:2118:HOH:O    | 2.21                     | 0.41              |
| 2:M:910:LYS:HB3   | 2:M:912:PRO:HD2   | 2.02                     | 0.41              |
| 2:M:1004:LYS:O    | 2:M:1005:MET:C    | 2.64                     | 0.41              |
| 2:M:1068:GLU:O    | 2:M:1071:ILE:HB   | 2.20                     | 0.41              |
| 2:M:1096:ALA:HB1  | 3:N:13:ALA:CB     | 2.50                     | 0.41              |
| 3:N:98:PRO:HB2    | 8:N:2256:HOH:O    | 2.20                     | 0.41              |
| 3:N:191:LEU:HD21  | 8:N:2354:HOH:O    | 2.21                     | 0.41              |
| 3:N:414:ARG:O     | 3:N:415:VAL:C     | 2.63                     | 0.41              |
| 3:N:1095:THR:HG23 | 3:N:1226:ALA:O    | 2.21                     | 0.41              |
| 3:N:1225:ALA:O    | 3:N:1229:ILE:HG13 | 2.21                     | 0.41              |
| 3:N:1281:VAL:HG12 | 3:N:1282:ARG:N    | 2.35                     | 0.41              |
| 3:N:1412:LYS:C    | 3:N:1414:PRO:HD3  | 2.44                     | 0.41              |
| 4:O:94:PRO:C      | 8:O:4683:HOH:O    | 2.63                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:41:ARG:HG3   | 1:B:41:ARG:NH1    | 2.35                     | 0.41              |
| 1:B:228:PRO:O    | 1:B:229:GLN:HB2   | 2.20                     | 0.41              |
| 2:C:23:VAL:HG11  | 8:C:2155:HOH:O    | 2.20                     | 0.41              |
| 2:C:49:ARG:CG    | 8:C:9834:HOH:O    | 2.69                     | 0.41              |
| 2:C:193:LEU:N    | 8:C:9548:HOH:O    | 2.53                     | 0.41              |
| 2:C:243:ARG:HG2  | 2:C:243:ARG:NH1   | 2.35                     | 0.41              |
| 2:C:252:LYS:O    | 2:C:256:TYR:CD2   | 2.73                     | 0.41              |
| 2:C:571:LEU:HD21 | 2:C:700:TYR:CD2   | 2.56                     | 0.41              |
| 2:C:626:ARG:NH2  | 8:C:2123:HOH:O    | 2.53                     | 0.41              |
| 2:C:725:ASP:CB   | 2:C:783:ARG:NH1   | 2.84                     | 0.41              |
| 2:C:767:PRO:HG2  | 8:C:2324:HOH:O    | 2.19                     | 0.41              |
| 2:C:862:PRO:HG2  | 2:C:925:TYR:OH    | 2.20                     | 0.41              |
| 2:C:897:LEU:HB3  | 2:C:899:GLN:CG    | 2.51                     | 0.41              |
| 2:C:947:ALA:O    | 2:C:950:LEU:HB3   | 2.20                     | 0.41              |
| 2:C:1019:GLN:HA  | 2:C:1020:PRO:HD3  | 1.88                     | 0.41              |
| 2:C:1075:ASP:HB2 | 8:E:9418:HOH:O    | 2.20                     | 0.41              |
| 2:C:1085:PHE:O   | 2:C:1089:VAL:HG23 | 2.21                     | 0.41              |
| 3:D:22:SER:HA    | 3:D:90:MET:O      | 2.21                     | 0.41              |
| 3:D:163:TYR:HD1  | 8:D:2510:HOH:O    | 2.04                     | 0.41              |
| 3:D:413:ASP:OD1  | 3:D:421:LEU:HD22  | 2.21                     | 0.41              |
| 3:D:421:LEU:HD12 | 3:D:435:VAL:CG1   | 2.50                     | 0.41              |
| 3:D:637:LEU:HD23 | 3:D:729:HIS:HA    | 2.01                     | 0.41              |
| 3:D:714:GLN:HB2  | 3:D:736:PHE:HZ    | 1.85                     | 0.41              |
| 4:E:30:LEU:HD21  | 4:E:63:TRP:CE3    | 2.55                     | 0.41              |
| 5:F:218:GLN:O    | 5:F:218:GLN:HG3   | 2.18                     | 0.41              |
| 5:F:292:ALA:HA   | 5:F:299:TRP:HB3   | 2.03                     | 0.41              |
| 5:F:351:SER:O    | 5:F:355:GLU:HB2   | 2.20                     | 0.41              |
| 1:K:19:GLU:HB2   | 8:K:2111:HOH:O    | 2.21                     | 0.41              |
| 1:K:222:LEU:CD1  | 1:L:215:VAL:HB    | 2.40                     | 0.41              |
| 1:L:86:VAL:HG13  | 1:L:86:VAL:O      | 2.21                     | 0.41              |
| 8:L:767:HOH:O    | 3:N:844:ALA:C     | 2.63                     | 0.41              |
| 2:M:112:GLU:HG3  | 8:M:9779:HOH:O    | 2.20                     | 0.41              |
| 2:M:204:GLN:HB3  | 8:M:9635:HOH:O    | 2.20                     | 0.41              |
| 2:M:211:LEU:HD21 | 2:M:311:PHE:CE1   | 2.55                     | 0.41              |
| 2:M:257:VAL:C    | 2:M:259:GLY:N     | 2.72                     | 0.41              |
| 2:M:448:ASN:CB   | 2:M:452:ILE:HD11  | 2.50                     | 0.41              |
| 2:M:548:PRO:HG2  | 2:M:842:ARG:NH2   | 2.36                     | 0.41              |
| 2:M:550:LEU:HD12 | 2:M:550:LEU:O     | 2.21                     | 0.41              |
| 2:M:843:HIS:CD2  | 2:M:884:GLN:CA    | 3.04                     | 0.41              |
| 2:M:946:ARG:CD   | 2:M:984:GLU:HB2   | 2.51                     | 0.41              |
| 2:M:1056:LYS:HD2 | 8:M:2051:HOH:O    | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:191:LEU:HA   | 8:N:9660:HOH:O    | 2.21                     | 0.41              |
| 3:N:240:GLU:O    | 3:N:243:ALA:N     | 2.53                     | 0.41              |
| 3:N:466:LYS:HE2  | 8:N:9669:HOH:O    | 2.20                     | 0.41              |
| 3:N:809:PRO:HB2  | 3:N:812:ALA:H     | 1.86                     | 0.41              |
| 3:N:930:LEU:O    | 3:N:933:ALA:HB3   | 2.21                     | 0.41              |
| 3:N:970:LYS:HB2  | 3:N:970:LYS:HE3   | 1.94                     | 0.41              |
| 3:N:1038:LEU:O   | 3:N:1060:SER:HB2  | 2.21                     | 0.41              |
| 5:P:416:ARG:HH11 | 5:P:419:ARG:CG    | 2.33                     | 0.41              |
| 1:A:88:ARG:CB    | 1:A:123:MET:HE2   | 2.51                     | 0.41              |
| 1:B:102:LYS:HD3  | 8:B:9575:HOH:O    | 2.19                     | 0.41              |
| 2:C:41:ASN:HB3   | 8:C:9503:HOH:O    | 2.20                     | 0.41              |
| 2:C:144:PRO:CG   | 2:C:165:LEU:HD23  | 2.50                     | 0.41              |
| 2:C:182:VAL:HG13 | 8:C:9517:HOH:O    | 2.19                     | 0.41              |
| 2:C:250:ARG:HE   | 2:C:253:ALA:HB1   | 1.80                     | 0.41              |
| 2:C:286:SER:HB3  | 2:C:299:LYS:HZ1   | 1.85                     | 0.41              |
| 2:C:516:ARG:CZ   | 3:D:1068:LEU:HB3  | 2.51                     | 0.41              |
| 2:C:557:ARG:CZ   | 2:C:879:ARG:HG2   | 2.51                     | 0.41              |
| 2:C:1049:LEU:O   | 2:C:1053:LEU:HD23 | 2.20                     | 0.41              |
| 3:D:675:ARG:HG2  | 3:D:678:GLU:OE2   | 2.21                     | 0.41              |
| 3:D:704:ARG:CZ   | 3:D:743:ASP:OD1   | 2.69                     | 0.41              |
| 3:D:1145:TYR:HD2 | 3:D:1146:GLY:N    | 2.19                     | 0.41              |
| 3:D:1169:ASP:HB3 | 8:D:2458:HOH:O    | 2.20                     | 0.41              |
| 3:D:1295:GLU:HB3 | 3:D:1300:SER:HB3  | 2.02                     | 0.41              |
| 4:E:61:GLU:C     | 4:E:63:TRP:N      | 2.76                     | 0.41              |
| 5:F:309:LYS:HA   | 8:F:9730:HOH:O    | 2.21                     | 0.41              |
| 1:K:88:ARG:NH1   | 8:K:1036:HOH:O    | 2.53                     | 0.41              |
| 1:K:186:LEU:H    | 1:K:192:LEU:HD12  | 1.86                     | 0.41              |
| 1:L:45:LEU:HD21  | 1:L:177:VAL:HG23  | 2.03                     | 0.41              |
| 2:M:207:LEU:HD22 | 2:M:221:LEU:CD2   | 2.51                     | 0.41              |
| 2:M:285:LEU:HD21 | 2:M:290:LEU:HD23  | 2.03                     | 0.41              |
| 2:M:349:ALA:O    | 2:M:353:ARG:HG3   | 2.20                     | 0.41              |
| 2:M:384:GLU:CG   | 2:M:388:ARG:HH21  | 2.33                     | 0.41              |
| 2:M:516:ARG:NE   | 3:N:1068:LEU:HD22 | 2.36                     | 0.41              |
| 2:M:560:MET:HE2  | 8:M:9949:HOH:O    | 2.20                     | 0.41              |
| 2:M:748:GLU:N    | 8:M:9997:HOH:O    | 2.53                     | 0.41              |
| 2:M:1102:LEU:O   | 3:N:5:VAL:HA      | 2.20                     | 0.41              |
| 3:N:181:ASP:OD1  | 3:N:198:ARG:HD2   | 2.20                     | 0.41              |
| 3:N:186:VAL:HG22 | 3:N:211:VAL:CG1   | 2.51                     | 0.41              |
| 3:N:693:GLU:CG   | 4:O:48:MET:SD     | 3.06                     | 0.41              |
| 3:N:895:VAL:O    | 3:N:895:VAL:HG12  | 2.21                     | 0.41              |
| 3:N:1050:GLY:HA3 | 8:N:2250:HOH:O    | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:1116:ASN:ND2 | 3:N:1116:ASN:O   | 2.51                     | 0.41              |
| 4:O:18:ARG:O     | 4:O:22:VAL:HG23  | 2.21                     | 0.41              |
| 4:O:45:ARG:HH22  | 4:O:72:ARG:NH2   | 2.18                     | 0.41              |
| 5:P:94:LEU:O     | 5:P:95:THR:C     | 2.62                     | 0.41              |
| 5:P:101:GLU:O    | 5:P:105:LYS:HG3  | 2.21                     | 0.41              |
| 5:P:120:THR:CG2  | 5:P:122:LEU:HD13 | 2.50                     | 0.41              |
| 5:P:392:VAL:HG12 | 5:P:396:ARG:HB2  | 2.02                     | 0.41              |
| 1:A:26:GLU:CB    | 1:A:194:LYS:HG3  | 2.49                     | 0.41              |
| 1:A:32:PHE:CZ    | 1:B:47:SER:OG    | 2.74                     | 0.41              |
| 1:A:33:GLY:CA    | 1:A:195:LEU:HB2  | 2.51                     | 0.41              |
| 1:A:133:GLU:CD   | 2:C:605:LYS:HB3  | 2.46                     | 0.41              |
| 1:A:183:ASP:HB2  | 8:A:9529:HOH:O   | 2.19                     | 0.41              |
| 1:B:75:VAL:O     | 1:B:79:ILE:HG12  | 2.21                     | 0.41              |
| 1:B:87:VAL:CG2   | 1:B:144:VAL:HG11 | 2.49                     | 0.41              |
| 1:B:115:LEU:HA   | 1:B:116:PRO:HD3  | 1.93                     | 0.41              |
| 2:C:2:GLU:CB     | 8:C:2326:HOH:O   | 2.68                     | 0.41              |
| 2:C:58:ASP:O     | 2:C:59:LYS:CG    | 2.69                     | 0.41              |
| 2:C:188:LYS:HE3  | 8:C:9927:HOH:O   | 2.20                     | 0.41              |
| 2:C:250:ARG:HB3  | 2:C:253:ALA:CB   | 2.50                     | 0.41              |
| 2:C:264:PRO:HB2  | 2:C:289:THR:HB   | 2.03                     | 0.41              |
| 2:C:498:GLN:NE2  | 2:C:533:ASP:OD2  | 2.53                     | 0.41              |
| 2:C:534:VAL:H    | 2:C:538:GLN:HE22 | 1.68                     | 0.41              |
| 2:C:545:ASN:HA   | 2:C:905:ILE:HD11 | 2.03                     | 0.41              |
| 2:C:573:ARG:HB3  | 2:C:670:GLN:HE21 | 1.85                     | 0.41              |
| 2:C:593:ALA:HB3  | 8:C:9533:HOH:O   | 2.20                     | 0.41              |
| 2:C:606:VAL:HG22 | 2:C:645:VAL:HG22 | 2.01                     | 0.41              |
| 2:C:611:ILE:N    | 8:C:9839:HOH:O   | 2.53                     | 0.41              |
| 2:C:678:PRO:HG3  | 2:C:873:PRO:HD2  | 2.03                     | 0.41              |
| 2:C:865:THR:HA   | 2:C:866:PRO:HD3  | 1.85                     | 0.41              |
| 2:C:957:LYS:HG3  | 8:C:9735:HOH:O   | 2.21                     | 0.41              |
| 3:D:6:ARG:CZ     | 8:D:2044:HOH:O   | 2.69                     | 0.41              |
| 3:D:57:GLU:HA    | 8:D:9598:HOH:O   | 2.20                     | 0.41              |
| 3:D:91:GLY:O     | 3:D:519:VAL:HB   | 2.21                     | 0.41              |
| 3:D:162:ARG:HB3  | 8:D:2585:HOH:O   | 2.21                     | 0.41              |
| 3:D:177:ALA:HB1  | 3:D:199:LEU:HB3  | 2.03                     | 0.41              |
| 3:D:192:ALA:HB1  | 3:D:193:PRO:CD   | 2.51                     | 0.41              |
| 3:D:243:ALA:HA   | 8:D:9999:HOH:O   | 2.21                     | 0.41              |
| 3:D:538:SER:C    | 8:D:2538:HOH:O   | 2.63                     | 0.41              |
| 3:D:583:ASP:HA   | 3:D:602:SER:CB   | 2.51                     | 0.41              |
| 3:D:850:LEU:O    | 3:D:853:VAL:HB   | 2.21                     | 0.41              |
| 3:D:863:VAL:HG12 | 8:D:9719:HOH:O   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:868:TYR:CE1   | 3:D:869:MET:SD   | 3.13                     | 0.41              |
| 3:D:954:ALA:HB3   | 8:D:2373:HOH:O   | 2.20                     | 0.41              |
| 3:D:999:THR:HA    | 3:D:1002:LYS:HD2 | 2.03                     | 0.41              |
| 3:D:1114:THR:CG2  | 3:D:1195:GLN:HB3 | 2.51                     | 0.41              |
| 3:D:1258:ARG:O    | 3:D:1259:VAL:C   | 2.62                     | 0.41              |
| 3:D:1283:ILE:HG22 | 3:D:1284:GLU:N   | 2.36                     | 0.41              |
| 3:D:1372:VAL:HG22 | 3:D:1375:MET:HE3 | 2.03                     | 0.41              |
| 3:D:1457:ASP:OD1  | 3:D:1457:ASP:C   | 2.64                     | 0.41              |
| 3:D:1476:THR:HG23 | 4:E:21:VAL:CG2   | 2.51                     | 0.41              |
| 5:F:78:SER:HB2    | 5:F:82:ARG:HH21  | 1.84                     | 0.41              |
| 5:F:160:ASP:O     | 5:F:163:LEU:HB2  | 2.21                     | 0.41              |
| 5:F:358:LEU:HD23  | 5:F:358:LEU:C    | 2.46                     | 0.41              |
| 5:F:416:ARG:CD    | 5:F:419:ARG:HB3  | 2.50                     | 0.41              |
| 1:K:179:PHE:HZ    | 2:M:980:GLY:HA3  | 1.86                     | 0.41              |
| 1:L:100:LEU:HB2   | 1:L:115:LEU:HD11 | 2.02                     | 0.41              |
| 1:L:138:LEU:O     | 1:L:138:LEU:HD23 | 2.21                     | 0.41              |
| 2:M:10:ARG:HA     | 2:M:10:ARG:HD3   | 1.71                     | 0.41              |
| 2:M:31:GLN:HE21   | 2:M:31:GLN:HB3   | 1.47                     | 0.41              |
| 2:M:119:PRO:HG2   | 2:M:386:PHE:CG   | 2.56                     | 0.41              |
| 2:M:158:TYR:CD1   | 2:M:313:LEU:HD11 | 2.55                     | 0.41              |
| 2:M:343:GLN:HG2   | 2:M:385:PHE:CB   | 2.46                     | 0.41              |
| 2:M:358:ARG:NH2   | 2:M:374:ASN:OD1  | 2.54                     | 0.41              |
| 2:M:495:THR:HG21  | 2:M:524:VAL:HG21 | 2.03                     | 0.41              |
| 2:M:555:ALA:HB3   | 8:N:9822:HOH:O   | 2.20                     | 0.41              |
| 2:M:564:MET:HA    | 2:M:564:MET:CE   | 2.51                     | 0.41              |
| 2:M:614:ARG:NH1   | 2:M:614:ARG:HG2  | 2.34                     | 0.41              |
| 2:M:626:ARG:N     | 8:M:9859:HOH:O   | 2.54                     | 0.41              |
| 2:M:670:GLN:O     | 2:M:672:VAL:HG12 | 2.20                     | 0.41              |
| 2:M:706:GLU:N     | 2:M:827:VAL:O    | 2.53                     | 0.41              |
| 2:M:749:VAL:HG23  | 2:M:792:VAL:HG21 | 2.03                     | 0.41              |
| 2:M:850:ALA:HA    | 3:N:632:VAL:CG1  | 2.51                     | 0.41              |
| 2:M:897:LEU:CG    | 2:M:899:GLN:HE21 | 2.34                     | 0.41              |
| 2:M:909:ALA:O     | 2:M:910:LYS:HD2  | 2.21                     | 0.41              |
| 2:M:915:LYS:HD3   | 2:M:968:LEU:O    | 2.21                     | 0.41              |
| 2:M:930:LYS:HG2   | 8:M:2243:HOH:O   | 2.20                     | 0.41              |
| 2:M:1078:GLU:HA   | 2:M:1079:PRO:HD3 | 1.84                     | 0.41              |
| 3:N:30:GLU:HG3    | 3:N:41:ARG:HG2   | 2.03                     | 0.41              |
| 3:N:49:ILE:HG22   | 3:N:50:PHE:CD1   | 2.56                     | 0.41              |
| 3:N:50:PHE:CB     | 3:N:522:PRO:HG2  | 2.45                     | 0.41              |
| 3:N:54:LYS:HG2    | 3:N:55:ASP:H     | 1.86                     | 0.41              |
| 3:N:112:ILE:HD12  | 3:N:112:ILE:O    | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:194:GLY:HA2   | 8:N:9727:HOH:O    | 2.20                     | 0.41              |
| 3:N:386:HIS:C     | 5:P:96:LEU:HD12   | 2.46                     | 0.41              |
| 3:N:572:ARG:HA    | 8:N:2401:HOH:O    | 2.21                     | 0.41              |
| 3:N:593:ASN:CG    | 5:P:206:GLY:HA2   | 2.46                     | 0.41              |
| 3:N:640:HIS:CE1   | 3:N:717:GLN:CD    | 2.99                     | 0.41              |
| 3:N:845:ASN:ND2   | 3:N:846:PRO:HD2   | 2.35                     | 0.41              |
| 3:N:925:GLU:HG2   | 3:N:926:LYS:N     | 2.36                     | 0.41              |
| 3:N:964:LEU:O     | 3:N:968:ASP:HB2   | 2.21                     | 0.41              |
| 3:N:978:TYR:HD1   | 3:N:988:ARG:HB2   | 1.85                     | 0.41              |
| 3:N:1019:PRO:O    | 3:N:1023:MET:HG3  | 2.20                     | 0.41              |
| 3:N:1057:VAL:HG13 | 3:N:1069:GLU:CB   | 2.50                     | 0.41              |
| 3:N:1087:ARG:HH22 | 3:N:1256:LEU:HD22 | 1.76                     | 0.41              |
| 3:N:1097:LYS:HA   | 8:N:9612:HOH:O    | 2.21                     | 0.41              |
| 3:N:1209:LEU:HD12 | 3:N:1219:GLU:CD   | 2.46                     | 0.41              |
| 3:N:1244:GLY:N    | 8:N:9796:HOH:O    | 2.52                     | 0.41              |
| 3:N:1283:ILE:HG22 | 3:N:1284:GLU:H    | 1.85                     | 0.41              |
| 3:N:1393:GLN:HB3  | 3:N:1398:TRP:HE1  | 1.84                     | 0.41              |
| 3:N:1396:GLU:HB3  | 8:N:9673:HOH:O    | 2.21                     | 0.41              |
| 5:P:209:PHE:CD2   | 5:P:213:ILE:HD11  | 2.56                     | 0.41              |
| 5:P:257:THR:CB    | 5:P:314:PRO:HG2   | 2.46                     | 0.41              |
| 5:P:319:THR:HG22  | 5:P:320:PRO:HD2   | 2.02                     | 0.41              |
| 5:P:372:ARG:HD3   | 5:P:388:ALA:HA    | 2.02                     | 0.41              |
| 1:B:48:ILE:HD13   | 1:B:210:ALA:HB1   | 2.02                     | 0.41              |
| 2:C:247:PRO:C     | 2:C:249:LYS:H     | 2.29                     | 0.41              |
| 2:C:355:VAL:HG23  | 2:C:372:LEU:CA    | 2.50                     | 0.41              |
| 2:C:405:ARG:HD3   | 2:C:543:ASN:OD1   | 2.21                     | 0.41              |
| 2:C:443:THR:HG21  | 2:C:449:ILE:HA    | 2.03                     | 0.41              |
| 2:C:569:VAL:O     | 2:C:569:VAL:HG13  | 2.21                     | 0.41              |
| 2:C:735:ARG:HH11  | 2:C:735:ARG:HG2   | 1.86                     | 0.41              |
| 3:D:47:GLU:H      | 3:D:47:GLU:HG2    | 1.28                     | 0.41              |
| 3:D:521:PRO:O     | 3:D:525:ARG:NH1   | 2.53                     | 0.41              |
| 3:D:809:PRO:O     | 3:D:812:ALA:HB3   | 2.20                     | 0.41              |
| 3:D:1101:VAL:HG21 | 3:D:1424:VAL:O    | 2.21                     | 0.41              |
| 3:D:1121:PRO:HD3  | 8:D:2230:HOH:O    | 2.20                     | 0.41              |
| 3:D:1288:GLU:N    | 8:D:9557:HOH:O    | 2.50                     | 0.41              |
| 3:D:1459:LEU:CD1  | 3:D:1468:LEU:HD12 | 2.50                     | 0.41              |
| 4:E:4:PRO:O       | 4:E:5:GLY:C       | 2.63                     | 0.41              |
| 4:E:93:TYR:HA     | 4:E:94:PRO:HD3    | 1.50                     | 0.41              |
| 5:F:271:LEU:HD12  | 5:F:307:THR:HG21  | 2.03                     | 0.41              |
| 1:K:26:GLU:HB3    | 1:K:194:LYS:HG3   | 2.03                     | 0.41              |
| 1:K:94:LEU:HD12   | 1:K:94:LEU:N      | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:115:LEU:HA    | 1:L:116:PRO:HD3   | 1.93                     | 0.41              |
| 2:M:206:THR:O     | 2:M:210:GLU:HG3   | 2.21                     | 0.41              |
| 2:M:370:ALA:HB3   | 8:P:9629:HOH:O    | 2.21                     | 0.41              |
| 2:M:376:ARG:HH12  | 5:P:285:GLU:CD    | 2.29                     | 0.41              |
| 2:M:588:VAL:HG23  | 2:M:596:TYR:OH    | 2.21                     | 0.41              |
| 2:M:673:LEU:HD21  | 2:M:895:TYR:CE2   | 2.56                     | 0.41              |
| 2:M:799:ILE:HD13  | 2:M:799:ILE:N     | 2.35                     | 0.41              |
| 2:M:910:LYS:HE3   | 8:M:9916:HOH:O    | 2.21                     | 0.41              |
| 3:N:54:LYS:HB3    | 3:N:57:GLU:HB2    | 2.03                     | 0.41              |
| 3:N:67:ARG:HD2    | 3:N:67:ARG:HA     | 1.89                     | 0.41              |
| 3:N:154:THR:HG22  | 3:N:156:GLU:H     | 1.86                     | 0.41              |
| 3:N:502:PHE:CE1   | 3:N:509:PRO:HB3   | 2.56                     | 0.41              |
| 3:N:827:ILE:O     | 3:N:837:GLY:HA3   | 2.21                     | 0.41              |
| 3:N:914:LEU:HD23  | 3:N:914:LEU:O     | 2.21                     | 0.41              |
| 3:N:1096:ARG:HB2  | 3:N:1096:ARG:HH11 | 1.85                     | 0.41              |
| 3:N:1209:LEU:HD23 | 4:O:16:LYS:HD2    | 2.02                     | 0.41              |
| 3:N:1458:GLU:HG2  | 8:N:9602:HOH:O    | 2.21                     | 0.41              |
| 5:P:403:LYS:HB3   | 8:P:9587:HOH:O    | 2.20                     | 0.41              |
| 1:B:223:THR:C     | 1:B:225:PHE:N     | 2.77                     | 0.40              |
| 2:C:12:VAL:HG22   | 2:C:13:ILE:HG23   | 2.04                     | 0.40              |
| 2:C:52:PHE:O      | 2:C:54:ILE:N      | 2.54                     | 0.40              |
| 2:C:66:LEU:HD13   | 2:C:100:LEU:CB    | 2.48                     | 0.40              |
| 2:C:166:PRO:HG2   | 8:C:9971:HOH:O    | 2.21                     | 0.40              |
| 2:C:418:LEU:HA    | 8:C:9500:HOH:O    | 2.22                     | 0.40              |
| 2:C:682:TYR:CD1   | 3:D:635:PRO:HG2   | 2.56                     | 0.40              |
| 3:D:12:LEU:CD2    | 3:D:13:ALA:N      | 2.82                     | 0.40              |
| 3:D:532:GLY:HA2   | 8:F:9594:HOH:O    | 2.22                     | 0.40              |
| 3:D:539:ASP:OD2   | 5:F:316:SER:OG    | 2.39                     | 0.40              |
| 3:D:562:ALA:HB1   | 3:D:567:ILE:CD1   | 2.50                     | 0.40              |
| 3:D:623:VAL:CG1   | 3:D:626:SER:HB3   | 2.51                     | 0.40              |
| 3:D:623:VAL:HG12  | 3:D:626:SER:HB3   | 2.03                     | 0.40              |
| 3:D:633:VAL:HB    | 3:D:740:PHE:CE1   | 2.56                     | 0.40              |
| 3:D:977:ALA:O     | 3:D:982:PHE:HB2   | 2.21                     | 0.40              |
| 3:D:1003:VAL:O    | 3:D:1006:ALA:HB3  | 2.21                     | 0.40              |
| 3:D:1147:ARG:HB2  | 3:D:1188:VAL:HG21 | 2.03                     | 0.40              |
| 3:D:1343:ALA:HB1  | 8:D:9912:HOH:O    | 2.20                     | 0.40              |
| 3:D:1434:TRP:CD1  | 3:D:1434:TRP:C    | 2.99                     | 0.40              |
| 5:F:364:ARG:CB    | 5:F:365:GLU:OE1   | 2.69                     | 0.40              |
| 1:K:206:THR:N     | 1:K:209:GLU:OE1   | 2.52                     | 0.40              |
| 1:K:219:ARG:HH12  | 1:K:220:GLU:HA    | 1.85                     | 0.40              |
| 1:L:11:PHE:HE2    | 1:L:13:VAL:HG22   | 1.86                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:200:LEU:HD22  | 2:M:300:ASP:HB3   | 2.03                     | 0.40              |
| 2:M:453:THR:HA    | 8:M:9508:HOH:O    | 2.21                     | 0.40              |
| 2:M:841:ASN:ND2   | 2:M:843:HIS:HD2   | 2.16                     | 0.40              |
| 2:M:969:GLN:HG2   | 3:N:952:ASP:OD2   | 2.21                     | 0.40              |
| 2:M:1015:LEU:CA   | 5:P:335:ASP:HB3   | 2.38                     | 0.40              |
| 3:N:26:VAL:HG13   | 3:N:43:GLY:C      | 2.46                     | 0.40              |
| 3:N:206:ARG:O     | 3:N:206:ARG:HD2   | 2.21                     | 0.40              |
| 3:N:427:VAL:HB    | 3:N:435:VAL:CG2   | 2.51                     | 0.40              |
| 3:N:564:GLU:HA    | 8:N:9738:HOH:O    | 2.21                     | 0.40              |
| 3:N:614:PHE:CZ    | 3:N:1439:SER:O    | 2.74                     | 0.40              |
| 3:N:677:LEU:CD2   | 3:N:683:ILE:HD13  | 2.51                     | 0.40              |
| 3:N:840:LYS:HD2   | 3:N:841:TYR:CZ    | 2.56                     | 0.40              |
| 3:N:1233:GLY:HA2  | 3:N:1236:LEU:CD1  | 2.51                     | 0.40              |
| 3:N:1465:ASN:OD1  | 3:N:1465:ASN:O    | 2.39                     | 0.40              |
| 4:O:5:GLY:HA3     | 4:O:8:LYS:HD2     | 2.03                     | 0.40              |
| 1:A:18:ARG:HH12   | 1:A:88:ARG:NE     | 2.19                     | 0.40              |
| 1:A:22:GLU:OE1    | 2:C:934:PHE:CZ    | 2.74                     | 0.40              |
| 1:A:70:GLY:HA2    | 1:A:133:GLU:OE2   | 2.21                     | 0.40              |
| 1:B:23:PHE:HB2    | 1:B:197:LEU:HD23  | 2.03                     | 0.40              |
| 2:C:129:ILE:HD12  | 8:C:2106:HOH:O    | 2.20                     | 0.40              |
| 2:C:205:GLU:HG3   | 2:C:206:THR:N     | 2.35                     | 0.40              |
| 2:C:252:LYS:NZ    | 8:C:2171:HOH:O    | 2.53                     | 0.40              |
| 2:C:328:LEU:HD13  | 2:C:433:THR:CG2   | 2.52                     | 0.40              |
| 2:C:445:GLU:OE2   | 2:C:559:LEU:HD23  | 2.22                     | 0.40              |
| 2:C:588:VAL:HG21  | 2:C:664:GLY:O     | 2.20                     | 0.40              |
| 2:C:715:THR:CG2   | 2:C:717:LEU:HG    | 2.51                     | 0.40              |
| 2:C:889:HIS:HE1   | 3:D:951:ILE:N     | 2.13                     | 0.40              |
| 2:C:1090:LYS:HZ2  | 3:D:90:MET:HG3    | 1.84                     | 0.40              |
| 2:C:1118:LYS:NZ   | 8:C:2317:HOH:O    | 2.48                     | 0.40              |
| 3:D:422:ALA:HB3   | 3:D:427:VAL:HG13  | 2.03                     | 0.40              |
| 3:D:601:ARG:HH22  | 3:D:611:GLN:N     | 2.19                     | 0.40              |
| 3:D:728:LEU:HD22  | 3:D:745:MET:CE    | 2.51                     | 0.40              |
| 3:D:1007:VAL:HG23 | 3:D:1008:PHE:N    | 2.35                     | 0.40              |
| 3:D:1145:TYR:HA   | 3:D:1171:VAL:HG21 | 2.03                     | 0.40              |
| 3:D:1256:LEU:O    | 3:D:1257:PRO:C    | 2.63                     | 0.40              |
| 4:E:12:MET:O      | 4:E:75:PHE:HZ     | 2.04                     | 0.40              |
| 5:F:234:LYS:HE3   | 5:F:236:SER:HB2   | 2.03                     | 0.40              |
| 1:K:106:PRO:HG2   | 1:K:134:GLU:OE1   | 2.21                     | 0.40              |
| 1:K:222:LEU:HD13  | 1:K:222:LEU:HA    | 1.93                     | 0.40              |
| 1:L:219:ARG:HD3   | 8:L:1203:HOH:O    | 2.21                     | 0.40              |
| 2:M:24:GLU:N      | 8:M:9500:HOH:O    | 2.54                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:190:LYS:H     | 2:M:190:LYS:HG3  | 1.47                     | 0.40              |
| 2:M:219:GLN:NE2   | 8:M:2204:HOH:O   | 2.55                     | 0.40              |
| 2:M:474:VAL:O     | 2:M:474:VAL:HG22 | 2.20                     | 0.40              |
| 2:M:585:GLU:N     | 8:M:9499:HOH:O   | 2.53                     | 0.40              |
| 2:M:736:ASP:C     | 2:M:738:ASP:H    | 2.29                     | 0.40              |
| 2:M:739:GLU:HA    | 8:M:2253:HOH:O   | 2.21                     | 0.40              |
| 2:M:841:ASN:CG    | 2:M:843:HIS:H    | 2.28                     | 0.40              |
| 2:M:859:PRO:O     | 2:M:867:VAL:HG22 | 2.21                     | 0.40              |
| 3:N:213:VAL:HG13  | 8:N:9497:HOH:O   | 2.20                     | 0.40              |
| 3:N:399:ARG:HB3   | 3:N:402:PRO:HG3  | 2.03                     | 0.40              |
| 3:N:442:ASN:HB3   | 8:N:9747:HOH:O   | 2.22                     | 0.40              |
| 3:N:1090:ASP:C    | 3:N:1093:TYR:H   | 2.26                     | 0.40              |
| 3:N:1240:THR:O    | 3:N:1257:PRO:HB3 | 2.22                     | 0.40              |
| 3:N:1268:PRO:O    | 3:N:1269:LYS:C   | 2.62                     | 0.40              |
| 3:N:1371:VAL:O    | 3:N:1375:MET:HG3 | 2.21                     | 0.40              |
| 3:N:1432:LYS:H    | 3:N:1432:LYS:HG3 | 1.41                     | 0.40              |
| 4:O:27:ALA:HB2    | 4:O:61:GLU:HB3   | 2.03                     | 0.40              |
| 4:O:58:PRO:HB2    | 8:O:1927:HOH:O   | 2.20                     | 0.40              |
| 1:A:20:TYR:CD2    | 1:A:21:GLY:N     | 2.89                     | 0.40              |
| 1:B:79:ILE:HG13   | 1:B:80:LEU:N     | 2.37                     | 0.40              |
| 2:C:89:THR:HG22   | 2:C:91:GLN:HG2   | 2.03                     | 0.40              |
| 2:C:516:ARG:CZ    | 3:D:1068:LEU:CB  | 2.99                     | 0.40              |
| 2:C:679:PHE:CE1   | 2:C:859:PRO:HD3  | 2.55                     | 0.40              |
| 2:C:720:GLU:OE1   | 2:C:758:ARG:NH1  | 2.54                     | 0.40              |
| 2:C:1115:LEU:HD22 | 3:D:88:TYR:CD1   | 2.56                     | 0.40              |
| 2:C:1119:ARG:HD3  | 2:C:1119:ARG:HA  | 1.72                     | 0.40              |
| 3:D:126:VAL:HG12  | 3:D:127:LEU:N    | 2.36                     | 0.40              |
| 3:D:209:ARG:NH2   | 3:D:397:LYS:HD2  | 2.36                     | 0.40              |
| 3:D:441:ARG:O     | 3:D:443:VAL:HG23 | 2.21                     | 0.40              |
| 3:D:578:VAL:O     | 3:D:578:VAL:HG12 | 2.22                     | 0.40              |
| 3:D:834:THR:HG22  | 3:D:838:ARG:CD   | 2.51                     | 0.40              |
| 3:D:1042:ARG:O    | 3:D:1057:VAL:HB  | 2.20                     | 0.40              |
| 3:D:1141:GLU:O    | 3:D:1145:TYR:HB2 | 2.22                     | 0.40              |
| 3:D:1283:ILE:HG22 | 3:D:1284:GLU:H   | 1.86                     | 0.40              |
| 3:D:1295:GLU:HB3  | 3:D:1300:SER:OG  | 2.21                     | 0.40              |
| 3:D:1354:LYS:HA   | 8:D:2377:HOH:O   | 2.21                     | 0.40              |
| 5:F:195:VAL:HG13  | 5:F:243:ILE:HD13 | 2.04                     | 0.40              |
| 5:F:267:THR:HG23  | 5:F:299:TRP:HH2  | 1.85                     | 0.40              |
| 1:K:34:VAL:CG1    | 8:L:4157:HOH:O   | 2.69                     | 0.40              |
| 2:M:20:GLU:HB2    | 8:M:9519:HOH:O   | 2.20                     | 0.40              |
| 2:M:456:ALA:O     | 2:M:459:ALA:HB3  | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:577:PRO:HG3   | 2:M:993:PHE:CG    | 2.56                     | 0.40              |
| 2:M:585:GLU:HB2   | 8:M:9499:HOH:O    | 2.21                     | 0.40              |
| 2:M:800:VAL:HG13  | 2:M:825:VAL:HG13  | 2.02                     | 0.40              |
| 2:M:805:ARG:HD2   | 8:M:9824:HOH:O    | 2.20                     | 0.40              |
| 2:M:1031:ARG:NH1  | 3:N:620:GLY:O     | 2.49                     | 0.40              |
| 2:M:1085:PHE:CE1  | 3:N:1468:LEU:HG   | 2.56                     | 0.40              |
| 3:N:83:SER:N      | 8:N:9939:HOH:O    | 2.55                     | 0.40              |
| 3:N:170:PRO:HD2   | 3:N:391:ALA:O     | 2.20                     | 0.40              |
| 3:N:186:VAL:CG1   | 3:N:187:LYS:N     | 2.83                     | 0.40              |
| 3:N:214:GLU:OE1   | 3:N:390:PRO:HG2   | 2.21                     | 0.40              |
| 3:N:572:ARG:CA    | 8:N:2401:HOH:O    | 2.69                     | 0.40              |
| 3:N:850:LEU:HD21  | 3:N:881:LEU:HD13  | 2.04                     | 0.40              |
| 3:N:919:PHE:HA    | 3:N:927:THR:OG1   | 2.20                     | 0.40              |
| 3:N:1055:VAL:HA   | 3:N:1056:PRO:HD3  | 1.94                     | 0.40              |
| 3:N:1103:HIS:ND1  | 3:N:1463:LYS:HE2  | 2.37                     | 0.40              |
| 5:P:256:ARG:HD3   | 5:P:260:ILE:HG21  | 2.03                     | 0.40              |
| 5:P:364:ARG:HE    | 5:P:364:ARG:HB3   | 1.64                     | 0.40              |
| 1:A:180:GLN:NE2   | 2:C:934:PHE:CB    | 2.67                     | 0.40              |
| 1:B:52:ALA:H      | 1:B:171:PHE:HE1   | 1.69                     | 0.40              |
| 1:B:80:LEU:HD11   | 3:D:842:VAL:CG1   | 2.51                     | 0.40              |
| 1:B:100:LEU:HB2   | 1:B:115:LEU:HD11  | 2.03                     | 0.40              |
| 2:C:250:ARG:CZ    | 2:C:253:ALA:HB1   | 2.50                     | 0.40              |
| 2:C:305:PRO:HG3   | 2:C:308:ARG:NH2   | 2.36                     | 0.40              |
| 2:C:769:PRO:HA    | 8:C:9563:HOH:O    | 2.22                     | 0.40              |
| 2:C:841:ASN:C     | 2:C:841:ASN:ND2   | 2.71                     | 0.40              |
| 2:C:878:SER:HA    | 3:D:1034:GLN:OE1  | 2.21                     | 0.40              |
| 2:C:971:LYS:HB3   | 2:C:988:VAL:N     | 2.36                     | 0.40              |
| 2:C:1003:ASP:O    | 2:C:1005:MET:N    | 2.54                     | 0.40              |
| 2:C:1032:PHE:CE1  | 2:C:1052:MET:HE2  | 2.57                     | 0.40              |
| 3:D:133:ILE:CG2   | 3:D:454:ALA:HB1   | 2.43                     | 0.40              |
| 3:D:447:VAL:HG13  | 8:D:9567:HOH:O    | 2.21                     | 0.40              |
| 3:D:495:ARG:HB2   | 8:D:9869:HOH:O    | 2.20                     | 0.40              |
| 3:D:670:VAL:O     | 3:D:671:LYS:C     | 2.65                     | 0.40              |
| 3:D:699:VAL:HG22  | 3:D:756:GLN:NE2   | 2.37                     | 0.40              |
| 3:D:708:LEU:CD1   | 3:D:1231:GLU:HG2  | 2.51                     | 0.40              |
| 3:D:940:THR:O     | 3:D:941:PHE:C     | 2.65                     | 0.40              |
| 3:D:1042:ARG:NH1  | 3:D:1061:PHE:CZ   | 2.89                     | 0.40              |
| 3:D:1121:PRO:C    | 3:D:1122:LEU:HD12 | 2.46                     | 0.40              |
| 3:D:1209:LEU:HD21 | 4:E:16:LYS:HD2    | 2.03                     | 0.40              |
| 3:D:1432:LYS:CD   | 3:D:1433:SER:H    | 2.32                     | 0.40              |
| 3:D:1496:GLU:HG3  | 3:D:1500:LYS:HE3  | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:304:VAL:O     | 5:F:308:LEU:HG    | 2.20                     | 0.40              |
| 5:F:325:LYS:HE3   | 8:F:9533:HOH:O    | 2.20                     | 0.40              |
| 5:F:419:ARG:O     | 5:F:421:PHE:CD1   | 2.75                     | 0.40              |
| 1:K:219:ARG:NH1   | 1:K:220:GLU:CA    | 2.84                     | 0.40              |
| 2:M:9:ILE:CG2     | 2:M:499:ALA:HB1   | 2.46                     | 0.40              |
| 2:M:11:GLU:CD     | 2:M:537:LYS:HZ2   | 2.29                     | 0.40              |
| 2:M:101:ILE:HD13  | 2:M:107:LEU:HB3   | 2.03                     | 0.40              |
| 2:M:107:LEU:HD21  | 8:M:9696:HOH:O    | 2.22                     | 0.40              |
| 2:M:173:ASP:C     | 2:M:174:LEU:HD23  | 2.47                     | 0.40              |
| 2:M:592:LEU:HA    | 2:M:592:LEU:HD23  | 1.74                     | 0.40              |
| 2:M:625:LEU:HD13  | 2:M:639:GLN:O     | 2.20                     | 0.40              |
| 2:M:682:TYR:CE1   | 2:M:851:LYS:HD2   | 2.57                     | 0.40              |
| 2:M:1032:PHE:CZ   | 2:M:1052:MET:HG2  | 2.56                     | 0.40              |
| 3:N:584:ASN:OD1   | 3:N:590:PRO:HG2   | 2.22                     | 0.40              |
| 3:N:702:LEU:HD12  | 3:N:747:VAL:HB    | 2.04                     | 0.40              |
| 3:N:838:ARG:HH11  | 3:N:838:ARG:CG    | 2.34                     | 0.40              |
| 3:N:1018:ASN:O    | 3:N:1022:VAL:HG23 | 2.21                     | 0.40              |
| 3:N:1148:VAL:HG12 | 3:N:1148:VAL:O    | 2.21                     | 0.40              |
| 3:N:1438:ALA:HB2  | 3:N:1447:LEU:HD11 | 2.03                     | 0.40              |
| 5:P:270:LYS:HB3   | 5:P:295:MET:SD    | 2.61                     | 0.40              |
| 5:P:279:GLN:HB2   | 8:P:9682:HOH:O    | 2.21                     | 0.40              |
| 5:P:311:ALA:O     | 5:P:312:GLN:C     | 2.65                     | 0.40              |
| 5:P:393:THR:CG2   | 5:P:394:ARG:H     | 2.35                     | 0.40              |
| 5:P:400:ILE:HD13  | 8:P:9478:HOH:O    | 2.22                     | 0.40              |
| 1:A:76:VAL:HG13   | 8:A:9592:HOH:O    | 2.21                     | 0.40              |
| 1:B:109:VAL:O     | 1:B:129:ILE:HB    | 2.22                     | 0.40              |
| 1:B:227:ASN:HA    | 1:B:228:PRO:HD2   | 1.92                     | 0.40              |
| 2:C:148:PHE:HB2   | 2:C:313:LEU:CD2   | 2.51                     | 0.40              |
| 2:C:153:ALA:O     | 2:C:155:PRO:HD3   | 2.22                     | 0.40              |
| 2:C:195:LEU:HG    | 2:C:238:LEU:CD1   | 2.50                     | 0.40              |
| 2:C:504:GLU:OE1   | 2:C:507:ARG:HD2   | 2.22                     | 0.40              |
| 2:C:677:MET:CB    | 2:C:987:ILE:HD13  | 2.51                     | 0.40              |
| 2:C:736:ASP:C     | 2:C:738:ASP:H     | 2.29                     | 0.40              |
| 2:C:897:LEU:HD11  | 2:C:920:GLN:HB3   | 2.03                     | 0.40              |
| 2:C:1043:TYR:CE1  | 3:D:710:ARG:O     | 2.75                     | 0.40              |
| 2:C:1073:GLY:N    | 8:C:9484:HOH:O    | 2.54                     | 0.40              |
| 8:C:2291:HOH:O    | 3:D:859:ASP:CA    | 2.68                     | 0.40              |
| 3:D:145:VAL:HG13  | 3:D:146:PRO:CD    | 2.52                     | 0.40              |
| 3:D:525:ARG:N     | 3:D:526:PRO:HD3   | 2.33                     | 0.40              |
| 3:D:559:ALA:O     | 3:D:561:GLY:N     | 2.55                     | 0.40              |
| 3:D:645:PRO:HA    | 3:D:721:VAL:O     | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:900:ILE:HB    | 8:D:9916:HOH:O    | 2.21                     | 0.40              |
| 3:D:1034:GLN:O    | 3:D:1038:LEU:HD12 | 2.21                     | 0.40              |
| 3:D:1333:HIS:O    | 3:D:1336:LEU:HB3  | 2.22                     | 0.40              |
| 3:D:1432:LYS:NZ   | 3:D:1464:GLU:OE1  | 2.51                     | 0.40              |
| 3:D:1458:GLU:N    | 8:D:9506:HOH:O    | 2.50                     | 0.40              |
| 5:F:94:LEU:HB3    | 5:F:98:GLU:H      | 1.87                     | 0.40              |
| 5:F:404:ALA:O     | 5:F:408:LEU:HB3   | 2.22                     | 0.40              |
| 1:K:48:ILE:HA     | 1:K:49:PRO:HD3    | 1.75                     | 0.40              |
| 1:K:74:ASP:O      | 1:K:78:ILE:HG13   | 2.22                     | 0.40              |
| 1:K:189:ARG:HD2   | 1:K:191:ASP:OD1   | 2.22                     | 0.40              |
| 2:M:129:ILE:HG13  | 2:M:386:PHE:HB3   | 2.03                     | 0.40              |
| 2:M:280:LYS:O     | 2:M:309:TYR:CZ    | 2.75                     | 0.40              |
| 2:M:346:VAL:O     | 2:M:350:ARG:HG3   | 2.22                     | 0.40              |
| 2:M:393:GLN:NE2   | 2:M:409:ARG:HH11  | 2.18                     | 0.40              |
| 2:M:559:LEU:HD11  | 2:M:563:ASN:ND2   | 2.37                     | 0.40              |
| 2:M:768:THR:CB    | 2:M:771:GLU:HB3   | 2.48                     | 0.40              |
| 2:M:1102:LEU:HD23 | 2:M:1106:ASP:HB3  | 2.04                     | 0.40              |
| 3:N:168:THR:HB    | 3:N:393:ILE:HG13  | 2.03                     | 0.40              |
| 3:N:776:GLU:HA    | 3:N:777:PRO:HD3   | 1.93                     | 0.40              |
| 3:N:796:ARG:C     | 3:N:797:LYS:HG3   | 2.46                     | 0.40              |
| 3:N:983:LEU:HA    | 3:N:987:GLU:OE2   | 2.22                     | 0.40              |
| 3:N:1152:GLU:HG3  | 3:N:1153:VAL:N    | 2.36                     | 0.40              |
| 5:P:82:ARG:HA     | 8:P:9599:HOH:O    | 2.21                     | 0.40              |
| 5:P:365:GLU:OE1   | 5:P:365:GLU:N     | 2.54                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles        |
|-----|-------|---------------|-----------|---------|----------|--------------------|
| 1   | A     | 227/315 (72%) | 201 (88%) | 21 (9%) | 5 (2%)   | <b>5</b> <b>10</b> |

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| Mol | Chain | Analysed         | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|------------------|------------|-----------|----------|-------------|----|
| 1   | B     | 227/315 (72%)    | 200 (88%)  | 24 (11%)  | 3 (1%)   | 9           | 21 |
| 1   | K     | 227/315 (72%)    | 199 (88%)  | 24 (11%)  | 4 (2%)   | 6           | 14 |
| 1   | L     | 227/315 (72%)    | 199 (88%)  | 25 (11%)  | 3 (1%)   | 9           | 21 |
| 2   | C     | 1117/1119 (100%) | 923 (83%)  | 139 (12%) | 55 (5%)  | 1           | 2  |
| 2   | M     | 1117/1119 (100%) | 928 (83%)  | 135 (12%) | 54 (5%)  | 2           | 2  |
| 3   | D     | 1388/1524 (91%)  | 1119 (81%) | 196 (14%) | 73 (5%)  | 1           | 1  |
| 3   | N     | 1388/1524 (91%)  | 1113 (80%) | 200 (14%) | 75 (5%)  | 1           | 1  |
| 4   | E     | 93/99 (94%)      | 72 (77%)   | 13 (14%)  | 8 (9%)   | 0           | 0  |
| 4   | O     | 93/99 (94%)      | 71 (76%)   | 15 (16%)  | 7 (8%)   | 1           | 1  |
| 5   | F     | 341/423 (81%)    | 295 (86%)  | 31 (9%)   | 15 (4%)  | 2           | 2  |
| 5   | P     | 341/423 (81%)    | 288 (84%)  | 34 (10%)  | 19 (6%)  | 1           | 1  |
| All | All   | 6786/7590 (89%)  | 5608 (83%) | 857 (13%) | 321 (5%) | 2           | 2  |

All (321) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 187  | GLY  |
| 2   | C     | 111  | ASP  |
| 2   | C     | 152  | PRO  |
| 2   | C     | 231  | PRO  |
| 2   | C     | 244  | PRO  |
| 2   | C     | 288  | ARG  |
| 2   | C     | 369  | PRO  |
| 2   | C     | 465  | GLY  |
| 2   | C     | 627  | ARG  |
| 2   | C     | 684  | PHE  |
| 2   | C     | 727  | PRO  |
| 2   | C     | 738  | ASP  |
| 2   | C     | 1045 | ALA  |
| 3   | D     | 43   | GLY  |
| 3   | D     | 55   | ASP  |
| 3   | D     | 83   | SER  |
| 3   | D     | 208  | PRO  |
| 3   | D     | 238  | PRO  |
| 3   | D     | 241  | ILE  |
| 3   | D     | 246  | PRO  |
| 3   | D     | 370  | ALA  |
| 3   | D     | 373  | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 417  | PRO  |
| 3   | D     | 440  | VAL  |
| 3   | D     | 487  | ALA  |
| 3   | D     | 1066 | THR  |
| 3   | D     | 1089 | ALA  |
| 3   | D     | 1125 | PRO  |
| 3   | D     | 1129 | THR  |
| 3   | D     | 1197 | ARG  |
| 4   | E     | 42   | PRO  |
| 4   | E     | 53   | GLY  |
| 4   | E     | 58   | PRO  |
| 5   | F     | 75   | ILE  |
| 5   | F     | 145  | PRO  |
| 5   | F     | 297  | PRO  |
| 5   | F     | 341  | PRO  |
| 5   | F     | 390  | PHE  |
| 2   | M     | 111  | ASP  |
| 2   | M     | 152  | PRO  |
| 2   | M     | 231  | PRO  |
| 2   | M     | 244  | PRO  |
| 2   | M     | 288  | ARG  |
| 2   | M     | 369  | PRO  |
| 2   | M     | 462  | ASP  |
| 2   | M     | 465  | GLY  |
| 2   | M     | 627  | ARG  |
| 2   | M     | 684  | PHE  |
| 2   | M     | 727  | PRO  |
| 2   | M     | 784  | ASP  |
| 2   | M     | 864  | GLY  |
| 2   | M     | 1045 | ALA  |
| 3   | N     | 43   | GLY  |
| 3   | N     | 208  | PRO  |
| 3   | N     | 238  | PRO  |
| 3   | N     | 241  | ILE  |
| 3   | N     | 246  | PRO  |
| 3   | N     | 370  | ALA  |
| 3   | N     | 373  | PRO  |
| 3   | N     | 385  | VAL  |
| 3   | N     | 417  | PRO  |
| 3   | N     | 440  | VAL  |
| 3   | N     | 487  | ALA  |
| 3   | N     | 1066 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 1089 | ALA  |
| 3   | N     | 1129 | THR  |
| 3   | N     | 1197 | ARG  |
| 3   | N     | 1213 | ARG  |
| 4   | O     | 42   | PRO  |
| 4   | O     | 53   | GLY  |
| 4   | O     | 58   | PRO  |
| 5   | P     | 145  | PRO  |
| 5   | P     | 167  | PRO  |
| 5   | P     | 297  | PRO  |
| 5   | P     | 341  | PRO  |
| 5   | P     | 390  | PHE  |
| 5   | P     | 416  | ARG  |
| 1   | A     | 59   | GLU  |
| 1   | B     | 59   | GLU  |
| 2   | C     | 129  | ILE  |
| 2   | C     | 217  | LEU  |
| 2   | C     | 290  | LEU  |
| 2   | C     | 316  | GLY  |
| 2   | C     | 368  | THR  |
| 2   | C     | 419  | THR  |
| 2   | C     | 434  | HIS  |
| 2   | C     | 462  | ASP  |
| 2   | C     | 529  | VAL  |
| 2   | C     | 548  | PRO  |
| 2   | C     | 626  | ARG  |
| 2   | C     | 735  | ARG  |
| 2   | C     | 740  | GLU  |
| 2   | C     | 864  | GLY  |
| 2   | C     | 1096 | ALA  |
| 3   | D     | 24   | GLY  |
| 3   | D     | 37   | LEU  |
| 3   | D     | 78   | VAL  |
| 3   | D     | 140  | ALA  |
| 3   | D     | 234  | GLU  |
| 3   | D     | 381  | ALA  |
| 3   | D     | 385  | VAL  |
| 3   | D     | 424  | GLY  |
| 3   | D     | 509  | PRO  |
| 3   | D     | 560  | GLN  |
| 3   | D     | 803  | GLY  |
| 3   | D     | 1028 | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1213 | ARG  |
| 3   | D     | 1241 | PHE  |
| 3   | D     | 1248 | GLY  |
| 3   | D     | 1385 | GLY  |
| 4   | E     | 5    | GLY  |
| 5   | F     | 148  | LYS  |
| 5   | F     | 153  | PRO  |
| 5   | F     | 167  | PRO  |
| 5   | F     | 329  | TYR  |
| 1   | K     | 59   | GLU  |
| 1   | L     | 59   | GLU  |
| 2   | M     | 178  | PRO  |
| 2   | M     | 290  | LEU  |
| 2   | M     | 316  | GLY  |
| 2   | M     | 434  | HIS  |
| 2   | M     | 529  | VAL  |
| 2   | M     | 548  | PRO  |
| 2   | M     | 735  | ARG  |
| 2   | M     | 738  | ASP  |
| 2   | M     | 740  | GLU  |
| 2   | M     | 1096 | ALA  |
| 3   | N     | 24   | GLY  |
| 3   | N     | 37   | LEU  |
| 3   | N     | 140  | ALA  |
| 3   | N     | 234  | GLU  |
| 3   | N     | 368  | VAL  |
| 3   | N     | 379  | ALA  |
| 3   | N     | 381  | ALA  |
| 3   | N     | 415  | VAL  |
| 3   | N     | 424  | GLY  |
| 3   | N     | 451  | ASP  |
| 3   | N     | 618  | LEU  |
| 3   | N     | 1028 | ALA  |
| 3   | N     | 1125 | PRO  |
| 3   | N     | 1241 | PHE  |
| 3   | N     | 1248 | GLY  |
| 3   | N     | 1385 | GLY  |
| 3   | N     | 1475 | GLY  |
| 4   | O     | 46   | PRO  |
| 5   | P     | 75   | ILE  |
| 5   | P     | 148  | LYS  |
| 5   | P     | 153  | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | P     | 329  | TYR  |
| 1   | A     | 106  | PRO  |
| 1   | B     | 106  | PRO  |
| 2   | C     | 11   | GLU  |
| 2   | C     | 79   | PRO  |
| 2   | C     | 178  | PRO  |
| 2   | C     | 265  | ARG  |
| 2   | C     | 517  | ARG  |
| 2   | C     | 598  | GLU  |
| 2   | C     | 842  | ARG  |
| 2   | C     | 1005 | MET  |
| 3   | D     | 136  | ASP  |
| 3   | D     | 233  | LYS  |
| 3   | D     | 379  | ALA  |
| 3   | D     | 415  | VAL  |
| 3   | D     | 451  | ASP  |
| 3   | D     | 521  | PRO  |
| 3   | D     | 594  | PRO  |
| 3   | D     | 601  | ARG  |
| 3   | D     | 782  | SER  |
| 3   | D     | 807  | ALA  |
| 3   | D     | 822  | ALA  |
| 3   | D     | 844  | ALA  |
| 4   | E     | 41   | GLU  |
| 4   | E     | 46   | PRO  |
| 5   | F     | 97   | GLU  |
| 5   | F     | 326  | ASP  |
| 1   | K     | 106  | PRO  |
| 1   | K     | 187  | GLY  |
| 1   | L     | 106  | PRO  |
| 2   | M     | 11   | GLU  |
| 2   | M     | 79   | PRO  |
| 2   | M     | 129  | ILE  |
| 2   | M     | 217  | LEU  |
| 2   | M     | 265  | ARG  |
| 2   | M     | 368  | THR  |
| 2   | M     | 419  | THR  |
| 2   | M     | 442  | GLU  |
| 2   | M     | 626  | ARG  |
| 2   | M     | 1004 | LYS  |
| 2   | M     | 1106 | ASP  |
| 3   | N     | 31   | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 98   | PRO  |
| 3   | N     | 233  | LYS  |
| 3   | N     | 509  | PRO  |
| 3   | N     | 521  | PRO  |
| 3   | N     | 539  | ASP  |
| 3   | N     | 560  | GLN  |
| 3   | N     | 594  | PRO  |
| 3   | N     | 807  | ALA  |
| 3   | N     | 822  | ALA  |
| 3   | N     | 844  | ALA  |
| 3   | N     | 1040 | GLY  |
| 3   | N     | 1208 | ASP  |
| 3   | N     | 1265 | ALA  |
| 4   | O     | 5    | GLY  |
| 4   | O     | 41   | GLU  |
| 5   | P     | 97   | GLU  |
| 5   | P     | 147  | LEU  |
| 2   | C     | 29   | ALA  |
| 2   | C     | 31   | GLN  |
| 2   | C     | 180  | GLY  |
| 3   | D     | 31   | THR  |
| 3   | D     | 40   | GLU  |
| 3   | D     | 88   | TYR  |
| 3   | D     | 96   | ALA  |
| 3   | D     | 368  | VAL  |
| 3   | D     | 387  | LEU  |
| 3   | D     | 416  | ALA  |
| 3   | D     | 486  | ARG  |
| 3   | D     | 539  | ASP  |
| 3   | D     | 808  | THR  |
| 3   | D     | 989  | TYR  |
| 3   | D     | 1265 | ALA  |
| 3   | D     | 1475 | GLY  |
| 4   | E     | 82   | GLU  |
| 5   | F     | 288  | TYR  |
| 1   | K     | 29   | GLU  |
| 2   | M     | 29   | ALA  |
| 2   | M     | 180  | GLY  |
| 2   | M     | 457  | ALA  |
| 2   | M     | 517  | ARG  |
| 2   | M     | 518  | LYS  |
| 2   | M     | 874  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 67   | ARG  |
| 3   | N     | 78   | VAL  |
| 3   | N     | 82   | LYS  |
| 3   | N     | 96   | ALA  |
| 3   | N     | 119  | SER  |
| 3   | N     | 136  | ASP  |
| 3   | N     | 177  | ALA  |
| 3   | N     | 486  | ARG  |
| 3   | N     | 601  | ARG  |
| 3   | N     | 808  | THR  |
| 3   | N     | 989  | TYR  |
| 3   | N     | 1243 | THR  |
| 5   | P     | 326  | ASP  |
| 5   | P     | 364  | ARG  |
| 1   | A     | 93   | SER  |
| 2   | C     | 7    | GLY  |
| 2   | C     | 59   | LYS  |
| 2   | C     | 144  | PRO  |
| 2   | C     | 202  | TYR  |
| 2   | C     | 442  | GLU  |
| 2   | C     | 457  | ALA  |
| 2   | C     | 1004 | LYS  |
| 3   | D     | 67   | ARG  |
| 3   | D     | 98   | PRO  |
| 3   | D     | 177  | ALA  |
| 3   | D     | 522  | PRO  |
| 3   | D     | 1040 | GLY  |
| 2   | M     | 7    | GLY  |
| 2   | M     | 598  | GLU  |
| 2   | M     | 762  | LYS  |
| 3   | N     | 40   | GLU  |
| 3   | N     | 416  | ALA  |
| 3   | N     | 522  | PRO  |
| 3   | N     | 617  | ASN  |
| 4   | O     | 82   | GLU  |
| 5   | P     | 286  | PRO  |
| 5   | P     | 288  | TYR  |
| 2   | C     | 876  | VAL  |
| 3   | D     | 137  | PRO  |
| 3   | D     | 170  | PRO  |
| 3   | D     | 705  | ALA  |
| 3   | D     | 1388 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | F     | 286  | PRO  |
| 5   | F     | 364  | ARG  |
| 2   | M     | 78   | PHE  |
| 2   | M     | 876  | VAL  |
| 3   | N     | 137  | PRO  |
| 3   | N     | 170  | PRO  |
| 3   | N     | 387  | LEU  |
| 5   | P     | 76   | SER  |
| 5   | P     | 324  | GLU  |
| 5   | P     | 393  | THR  |
| 1   | B     | 125  | PRO  |
| 3   | N     | 483  | HIS  |
| 3   | N     | 870  | GLY  |
| 2   | C     | 74   | GLY  |
| 2   | C     | 78   | PHE  |
| 2   | C     | 779  | GLY  |
| 2   | M     | 131  | GLY  |
| 2   | M     | 144  | PRO  |
| 2   | M     | 779  | GLY  |
| 2   | M     | 812  | GLY  |
| 2   | M     | 905  | ILE  |
| 3   | N     | 803  | GLY  |
| 2   | C     | 336  | VAL  |
| 2   | C     | 812  | GLY  |
| 3   | D     | 407  | VAL  |
| 3   | D     | 1157 | GLY  |
| 3   | D     | 1392 | GLY  |
| 3   | N     | 781  | PRO  |
| 3   | N     | 1157 | GLY  |
| 3   | D     | 483  | HIS  |
| 3   | D     | 781  | PRO  |
| 3   | D     | 1454 | GLY  |
| 5   | F     | 397  | ILE  |
| 1   | L     | 125  | PRO  |
| 2   | M     | 186  | VAL  |
| 2   | M     | 877  | PRO  |
| 3   | N     | 146  | PRO  |
| 3   | N     | 407  | VAL  |
| 3   | N     | 1454 | GLY  |
| 1   | A     | 124  | ASN  |
| 2   | C     | 131  | GLY  |
| 2   | C     | 186  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 877 | PRO  |
| 4   | E     | 57  | ASP  |
| 3   | N     | 742 | GLY  |
| 2   | C     | 166 | PRO  |
| 2   | M     | 166 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |   |
|-----|-------|-----------------|------------|------------|-------------|---|
| 1   | A     | 202/273 (74%)   | 162 (80%)  | 40 (20%)   | 1           | 2 |
| 1   | B     | 202/273 (74%)   | 164 (81%)  | 38 (19%)   | 1           | 2 |
| 1   | K     | 202/273 (74%)   | 160 (79%)  | 42 (21%)   | 1           | 2 |
| 1   | L     | 202/273 (74%)   | 163 (81%)  | 39 (19%)   | 1           | 2 |
| 2   | C     | 941/941 (100%)  | 712 (76%)  | 229 (24%)  | 1           | 1 |
| 2   | M     | 941/941 (100%)  | 694 (74%)  | 247 (26%)  | 0           | 1 |
| 3   | D     | 1123/1279 (88%) | 840 (75%)  | 283 (25%)  | 0           | 1 |
| 3   | N     | 1123/1279 (88%) | 810 (72%)  | 313 (28%)  | 0           | 1 |
| 4   | E     | 83/87 (95%)     | 65 (78%)   | 18 (22%)   | 1           | 2 |
| 4   | O     | 83/87 (95%)     | 68 (82%)   | 15 (18%)   | 2           | 3 |
| 5   | F     | 295/370 (80%)   | 220 (75%)  | 75 (25%)   | 0           | 1 |
| 5   | P     | 295/370 (80%)   | 232 (79%)  | 63 (21%)   | 1           | 2 |
| All | All   | 5692/6446 (88%) | 4290 (75%) | 1402 (25%) | 1           | 1 |

All (1402) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MET  |
| 1   | A     | 5   | LYS  |
| 1   | A     | 9   | PRO  |
| 1   | A     | 12  | THR  |
| 1   | A     | 15  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | ARG  |
| 1   | A     | 26  | GLU  |
| 1   | A     | 30  | ARG  |
| 1   | A     | 54  | THR  |
| 1   | A     | 62  | LEU  |
| 1   | A     | 73  | GLU  |
| 1   | A     | 74  | ASP  |
| 1   | A     | 80  | LEU  |
| 1   | A     | 88  | ARG  |
| 1   | A     | 89  | PHE  |
| 1   | A     | 92  | PRO  |
| 1   | A     | 93  | SER  |
| 1   | A     | 95  | GLN  |
| 1   | A     | 96  | THR  |
| 1   | A     | 99  | LEU  |
| 1   | A     | 112 | ARG  |
| 1   | A     | 121 | GLU  |
| 1   | A     | 126 | ASP  |
| 1   | A     | 127 | LEU  |
| 1   | A     | 133 | GLU  |
| 1   | A     | 143 | ARG  |
| 1   | A     | 146 | ARG  |
| 1   | A     | 160 | ASP  |
| 1   | A     | 167 | VAL  |
| 1   | A     | 170 | VAL  |
| 1   | A     | 185 | ARG  |
| 1   | A     | 197 | LEU  |
| 1   | A     | 198 | ARG  |
| 1   | A     | 206 | THR  |
| 1   | A     | 208 | LEU  |
| 1   | A     | 216 | GLU  |
| 1   | A     | 219 | ARG  |
| 1   | A     | 222 | LEU  |
| 1   | A     | 227 | ASN  |
| 1   | A     | 229 | GLN  |
| 1   | B     | 1   | MET  |
| 1   | B     | 5   | LYS  |
| 1   | B     | 9   | PRO  |
| 1   | B     | 12  | THR  |
| 1   | B     | 26  | GLU  |
| 1   | B     | 30  | ARG  |
| 1   | B     | 54  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 62  | LEU  |
| 1   | B     | 73  | GLU  |
| 1   | B     | 80  | LEU  |
| 1   | B     | 88  | ARG  |
| 1   | B     | 89  | PHE  |
| 1   | B     | 90  | LEU  |
| 1   | B     | 93  | SER  |
| 1   | B     | 95  | GLN  |
| 1   | B     | 96  | THR  |
| 1   | B     | 99  | LEU  |
| 1   | B     | 112 | ARG  |
| 1   | B     | 119 | ASP  |
| 1   | B     | 121 | GLU  |
| 1   | B     | 127 | LEU  |
| 1   | B     | 138 | LEU  |
| 1   | B     | 139 | ASN  |
| 1   | B     | 140 | MET  |
| 1   | B     | 142 | VAL  |
| 1   | B     | 155 | LYS  |
| 1   | B     | 160 | ASP  |
| 1   | B     | 162 | ILE  |
| 1   | B     | 167 | VAL  |
| 1   | B     | 186 | LEU  |
| 1   | B     | 188 | GLN  |
| 1   | B     | 197 | LEU  |
| 1   | B     | 205 | VAL  |
| 1   | B     | 206 | THR  |
| 1   | B     | 208 | LEU  |
| 1   | B     | 213 | GLN  |
| 1   | B     | 223 | THR  |
| 1   | B     | 229 | GLN  |
| 2   | C     | 8   | ARG  |
| 2   | C     | 15  | LEU  |
| 2   | C     | 26  | TYR  |
| 2   | C     | 31  | GLN  |
| 2   | C     | 41  | ASN  |
| 2   | C     | 48  | PHE  |
| 2   | C     | 49  | ARG  |
| 2   | C     | 52  | PHE  |
| 2   | C     | 65  | VAL  |
| 2   | C     | 70  | GLU  |
| 2   | C     | 71  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 76  | PRO  |
| 2   | C     | 77  | PRO  |
| 2   | C     | 82  | GLU  |
| 2   | C     | 86  | LYS  |
| 2   | C     | 88  | LEU  |
| 2   | C     | 95  | TYR  |
| 2   | C     | 100 | LEU  |
| 2   | C     | 104 | ASP  |
| 2   | C     | 105 | THR  |
| 2   | C     | 107 | LEU  |
| 2   | C     | 111 | ASP  |
| 2   | C     | 113 | VAL  |
| 2   | C     | 115 | LEU  |
| 2   | C     | 118 | ILE  |
| 2   | C     | 129 | ILE  |
| 2   | C     | 138 | SER  |
| 2   | C     | 140 | ILE  |
| 2   | C     | 144 | PRO  |
| 2   | C     | 149 | THR  |
| 2   | C     | 152 | PRO  |
| 2   | C     | 158 | TYR  |
| 2   | C     | 163 | ILE  |
| 2   | C     | 165 | LEU  |
| 2   | C     | 166 | PRO  |
| 2   | C     | 167 | LYS  |
| 2   | C     | 168 | ARG  |
| 2   | C     | 170 | PRO  |
| 2   | C     | 172 | ILE  |
| 2   | C     | 173 | ASP  |
| 2   | C     | 178 | PRO  |
| 2   | C     | 182 | VAL  |
| 2   | C     | 186 | VAL  |
| 2   | C     | 188 | LYS  |
| 2   | C     | 189 | ARG  |
| 2   | C     | 190 | LYS  |
| 2   | C     | 194 | VAL  |
| 2   | C     | 198 | ARG  |
| 2   | C     | 203 | ASP  |
| 2   | C     | 206 | THR  |
| 2   | C     | 207 | LEU  |
| 2   | C     | 209 | ARG  |
| 2   | C     | 211 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 217 | LEU  |
| 2   | C     | 218 | VAL  |
| 2   | C     | 222 | MET  |
| 2   | C     | 229 | MET  |
| 2   | C     | 230 | ARG  |
| 2   | C     | 235 | LEU  |
| 2   | C     | 237 | ARG  |
| 2   | C     | 238 | LEU  |
| 2   | C     | 243 | ARG  |
| 2   | C     | 251 | ASP  |
| 2   | C     | 254 | VAL  |
| 2   | C     | 256 | TYR  |
| 2   | C     | 257 | VAL  |
| 2   | C     | 266 | ARG  |
| 2   | C     | 279 | GLU  |
| 2   | C     | 281 | LEU  |
| 2   | C     | 289 | THR  |
| 2   | C     | 290 | LEU  |
| 2   | C     | 293 | PHE  |
| 2   | C     | 297 | GLU  |
| 2   | C     | 302 | VAL  |
| 2   | C     | 303 | PHE  |
| 2   | C     | 304 | LEU  |
| 2   | C     | 309 | TYR  |
| 2   | C     | 327 | HIS  |
| 2   | C     | 333 | ILE  |
| 2   | C     | 343 | GLN  |
| 2   | C     | 345 | ARG  |
| 2   | C     | 348 | LEU  |
| 2   | C     | 351 | LEU  |
| 2   | C     | 358 | ARG  |
| 2   | C     | 359 | MET  |
| 2   | C     | 360 | LEU  |
| 2   | C     | 367 | LEU  |
| 2   | C     | 368 | THR  |
| 2   | C     | 372 | LEU  |
| 2   | C     | 373 | VAL  |
| 2   | C     | 379 | GLU  |
| 2   | C     | 383 | ARG  |
| 2   | C     | 398 | THR  |
| 2   | C     | 407 | LYS  |
| 2   | C     | 415 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 418 | LEU  |
| 2   | C     | 419 | THR  |
| 2   | C     | 420 | ARG  |
| 2   | C     | 422 | ARG  |
| 2   | C     | 425 | PHE  |
| 2   | C     | 426 | ASP  |
| 2   | C     | 427 | VAL  |
| 2   | C     | 430 | VAL  |
| 2   | C     | 432 | ARG  |
| 2   | C     | 438 | ILE  |
| 2   | C     | 441 | VAL  |
| 2   | C     | 442 | GLU  |
| 2   | C     | 443 | THR  |
| 2   | C     | 449 | ILE  |
| 2   | C     | 452 | ILE  |
| 2   | C     | 455 | LEU  |
| 2   | C     | 460 | ARG  |
| 2   | C     | 469 | THR  |
| 2   | C     | 474 | VAL  |
| 2   | C     | 500 | ASN  |
| 2   | C     | 502 | PRO  |
| 2   | C     | 503 | LEU  |
| 2   | C     | 508 | ILE  |
| 2   | C     | 514 | VAL  |
| 2   | C     | 518 | LYS  |
| 2   | C     | 520 | GLU  |
| 2   | C     | 523 | ILE  |
| 2   | C     | 524 | VAL  |
| 2   | C     | 527 | GLU  |
| 2   | C     | 541 | SER  |
| 2   | C     | 543 | ASN  |
| 2   | C     | 544 | THR  |
| 2   | C     | 545 | ASN  |
| 2   | C     | 549 | PHE  |
| 2   | C     | 551 | GLU  |
| 2   | C     | 564 | MET  |
| 2   | C     | 579 | VAL  |
| 2   | C     | 584 | GLU  |
| 2   | C     | 586 | ARG  |
| 2   | C     | 588 | VAL  |
| 2   | C     | 589 | ARG  |
| 2   | C     | 595 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 599 | GLU  |
| 2   | C     | 600 | ASP  |
| 2   | C     | 614 | ARG  |
| 2   | C     | 617 | ASP  |
| 2   | C     | 620 | LEU  |
| 2   | C     | 633 | GLN  |
| 2   | C     | 637 | LEU  |
| 2   | C     | 640 | ARG  |
| 2   | C     | 644 | VAL  |
| 2   | C     | 645 | VAL  |
| 2   | C     | 648 | ARG  |
| 2   | C     | 650 | ARG  |
| 2   | C     | 654 | LEU  |
| 2   | C     | 657 | ASP  |
| 2   | C     | 659 | PRO  |
| 2   | C     | 672 | VAL  |
| 2   | C     | 673 | LEU  |
| 2   | C     | 677 | MET  |
| 2   | C     | 685 | GLU  |
| 2   | C     | 689 | VAL  |
| 2   | C     | 699 | PHE  |
| 2   | C     | 701 | THR  |
| 2   | C     | 708 | TYR  |
| 2   | C     | 713 | ARG  |
| 2   | C     | 722 | ILE  |
| 2   | C     | 726 | ILE  |
| 2   | C     | 727 | PRO  |
| 2   | C     | 729 | LEU  |
| 2   | C     | 744 | ARG  |
| 2   | C     | 754 | ILE  |
| 2   | C     | 762 | LYS  |
| 2   | C     | 766 | GLU  |
| 2   | C     | 774 | LEU  |
| 2   | C     | 785 | VAL  |
| 2   | C     | 799 | ILE  |
| 2   | C     | 813 | VAL  |
| 2   | C     | 815 | LEU  |
| 2   | C     | 821 | GLU  |
| 2   | C     | 831 | ARG  |
| 2   | C     | 839 | LEU  |
| 2   | C     | 841 | ASN  |
| 2   | C     | 853 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 862  | PRO  |
| 2   | C     | 863  | ASP  |
| 2   | C     | 870  | ILE  |
| 2   | C     | 871  | LEU  |
| 2   | C     | 881  | ASN  |
| 2   | C     | 897  | LEU  |
| 2   | C     | 900  | ARG  |
| 2   | C     | 904  | PRO  |
| 2   | C     | 905  | ILE  |
| 2   | C     | 916  | GLU  |
| 2   | C     | 928  | LYS  |
| 2   | C     | 934  | PHE  |
| 2   | C     | 937  | ASP  |
| 2   | C     | 941  | VAL  |
| 2   | C     | 943  | VAL  |
| 2   | C     | 950  | LEU  |
| 2   | C     | 952  | LEU  |
| 2   | C     | 958  | THR  |
| 2   | C     | 963  | LEU  |
| 2   | C     | 964  | LYS  |
| 2   | C     | 972  | VAL  |
| 2   | C     | 975  | TYR  |
| 2   | C     | 984  | GLU  |
| 2   | C     | 986  | PRO  |
| 2   | C     | 988  | VAL  |
| 2   | C     | 999  | HIS  |
| 2   | C     | 1000 | MET  |
| 2   | C     | 1015 | LEU  |
| 2   | C     | 1016 | ILE  |
| 2   | C     | 1017 | THR  |
| 2   | C     | 1019 | GLN  |
| 2   | C     | 1024 | LYS  |
| 2   | C     | 1035 | MET  |
| 2   | C     | 1036 | GLU  |
| 2   | C     | 1040 | LEU  |
| 2   | C     | 1052 | MET  |
| 2   | C     | 1057 | SER  |
| 2   | C     | 1061 | GLU  |
| 2   | C     | 1079 | PRO  |
| 2   | C     | 1091 | GLU  |
| 2   | C     | 1092 | LEU  |
| 2   | C     | 1095 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1099 | VAL  |
| 2   | C     | 1100 | GLN  |
| 2   | C     | 1102 | LEU  |
| 2   | C     | 1104 | GLU  |
| 2   | C     | 1106 | ASP  |
| 2   | C     | 1115 | LEU  |
| 2   | C     | 1117 | SER  |
| 2   | C     | 1119 | ARG  |
| 3   | D     | 3    | LYS  |
| 3   | D     | 9    | ARG  |
| 3   | D     | 12   | LEU  |
| 3   | D     | 14   | SER  |
| 3   | D     | 15   | PRO  |
| 3   | D     | 20   | SER  |
| 3   | D     | 25   | GLU  |
| 3   | D     | 27   | GLU  |
| 3   | D     | 32   | ILE  |
| 3   | D     | 35   | ARG  |
| 3   | D     | 37   | LEU  |
| 3   | D     | 39   | PRO  |
| 3   | D     | 47   | GLU  |
| 3   | D     | 53   | ILE  |
| 3   | D     | 55   | ASP  |
| 3   | D     | 56   | TYR  |
| 3   | D     | 60   | CYS  |
| 3   | D     | 68   | PHE  |
| 3   | D     | 72   | VAL  |
| 3   | D     | 74   | GLU  |
| 3   | D     | 80   | VAL  |
| 3   | D     | 85   | VAL  |
| 3   | D     | 87   | ARG  |
| 3   | D     | 97   | THR  |
| 3   | D     | 102  | ILE  |
| 3   | D     | 103  | TRP  |
| 3   | D     | 107  | ASP  |
| 3   | D     | 112  | ILE  |
| 3   | D     | 115  | LEU  |
| 3   | D     | 118  | LEU  |
| 3   | D     | 121  | THR  |
| 3   | D     | 122  | GLU  |
| 3   | D     | 126  | VAL  |
| 3   | D     | 130  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 134 | VAL  |
| 3   | D     | 135 | LEU  |
| 3   | D     | 136 | ASP  |
| 3   | D     | 137 | PRO  |
| 3   | D     | 142 | LEU  |
| 3   | D     | 145 | VAL  |
| 3   | D     | 147 | VAL  |
| 3   | D     | 149 | LYS  |
| 3   | D     | 152 | LEU  |
| 3   | D     | 153 | LEU  |
| 3   | D     | 159 | ARG  |
| 3   | D     | 160 | GLU  |
| 3   | D     | 161 | LEU  |
| 3   | D     | 162 | ARG  |
| 3   | D     | 169 | TYR  |
| 3   | D     | 178 | LEU  |
| 3   | D     | 184 | GLU  |
| 3   | D     | 185 | VAL  |
| 3   | D     | 199 | LEU  |
| 3   | D     | 208 | PRO  |
| 3   | D     | 209 | ARG  |
| 3   | D     | 211 | VAL  |
| 3   | D     | 216 | VAL  |
| 3   | D     | 393 | ILE  |
| 3   | D     | 394 | LEU  |
| 3   | D     | 397 | LYS  |
| 3   | D     | 400 | VAL  |
| 3   | D     | 410 | SER  |
| 3   | D     | 411 | THR  |
| 3   | D     | 413 | ASP  |
| 3   | D     | 419 | ASP  |
| 3   | D     | 421 | LEU  |
| 3   | D     | 423 | ASP  |
| 3   | D     | 426 | LYS  |
| 3   | D     | 427 | VAL  |
| 3   | D     | 428 | LYS  |
| 3   | D     | 431 | VAL  |
| 3   | D     | 432 | TYR  |
| 3   | D     | 435 | VAL  |
| 3   | D     | 444 | VAL  |
| 3   | D     | 445 | ARG  |
| 3   | D     | 447 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 450 | TYR  |
| 3   | D     | 452 | ILE  |
| 3   | D     | 453 | ASP  |
| 3   | D     | 456 | MET  |
| 3   | D     | 468 | LEU  |
| 3   | D     | 474 | GLU  |
| 3   | D     | 483 | HIS  |
| 3   | D     | 488 | ARG  |
| 3   | D     | 496 | LEU  |
| 3   | D     | 498 | VAL  |
| 3   | D     | 508 | ARG  |
| 3   | D     | 520 | LEU  |
| 3   | D     | 521 | PRO  |
| 3   | D     | 528 | VAL  |
| 3   | D     | 542 | ASP  |
| 3   | D     | 549 | ASN  |
| 3   | D     | 554 | LEU  |
| 3   | D     | 565 | ILE  |
| 3   | D     | 567 | ILE  |
| 3   | D     | 569 | ASN  |
| 3   | D     | 571 | LYS  |
| 3   | D     | 586 | ARG  |
| 3   | D     | 590 | PRO  |
| 3   | D     | 591 | VAL  |
| 3   | D     | 594 | PRO  |
| 3   | D     | 597 | ASP  |
| 3   | D     | 601 | ARG  |
| 3   | D     | 602 | SER  |
| 3   | D     | 603 | LEU  |
| 3   | D     | 604 | THR  |
| 3   | D     | 605 | ASP  |
| 3   | D     | 606 | ILE  |
| 3   | D     | 611 | GLN  |
| 3   | D     | 619 | LEU  |
| 3   | D     | 623 | VAL  |
| 3   | D     | 635 | PRO  |
| 3   | D     | 641 | GLN  |
| 3   | D     | 644 | LEU  |
| 3   | D     | 651 | GLU  |
| 3   | D     | 652 | LEU  |
| 3   | D     | 659 | LYS  |
| 3   | D     | 661 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 662 | GLU  |
| 3   | D     | 663 | GLU  |
| 3   | D     | 669 | ASN  |
| 3   | D     | 676 | MET  |
| 3   | D     | 677 | LEU  |
| 3   | D     | 681 | ARG  |
| 3   | D     | 683 | ILE  |
| 3   | D     | 695 | ILE  |
| 3   | D     | 709 | HIS  |
| 3   | D     | 711 | LEU  |
| 3   | D     | 721 | VAL  |
| 3   | D     | 725 | SER  |
| 3   | D     | 741 | ASP  |
| 3   | D     | 749 | VAL  |
| 3   | D     | 783 | ARG  |
| 3   | D     | 784 | ASP  |
| 3   | D     | 792 | ILE  |
| 3   | D     | 794 | GLN  |
| 3   | D     | 804 | LEU  |
| 3   | D     | 828 | LYS  |
| 3   | D     | 836 | VAL  |
| 3   | D     | 848 | GLU  |
| 3   | D     | 858 | VAL  |
| 3   | D     | 860 | LEU  |
| 3   | D     | 861 | GLN  |
| 3   | D     | 863 | VAL  |
| 3   | D     | 865 | THR  |
| 3   | D     | 869 | MET  |
| 3   | D     | 871 | LYS  |
| 3   | D     | 876 | SER  |
| 3   | D     | 877 | PRO  |
| 3   | D     | 879 | ARG  |
| 3   | D     | 880 | ILE  |
| 3   | D     | 888 | GLU  |
| 3   | D     | 890 | VAL  |
| 3   | D     | 892 | ASP  |
| 3   | D     | 897 | TRP  |
| 3   | D     | 899 | LEU  |
| 3   | D     | 901 | GLN  |
| 3   | D     | 902 | LEU  |
| 3   | D     | 903 | ASP  |
| 3   | D     | 904 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 912  | LYS  |
| 3   | D     | 917  | GLN  |
| 3   | D     | 920  | LEU  |
| 3   | D     | 922  | LEU  |
| 3   | D     | 925  | GLU  |
| 3   | D     | 931  | LEU  |
| 3   | D     | 940  | THR  |
| 3   | D     | 951  | ILE  |
| 3   | D     | 955  | VAL  |
| 3   | D     | 969  | ARG  |
| 3   | D     | 972  | LEU  |
| 3   | D     | 988  | ARG  |
| 3   | D     | 990  | ASP  |
| 3   | D     | 994  | GLN  |
| 3   | D     | 1001 | GLU  |
| 3   | D     | 1007 | VAL  |
| 3   | D     | 1029 | ARG  |
| 3   | D     | 1037 | GLN  |
| 3   | D     | 1039 | CYS  |
| 3   | D     | 1041 | LEU  |
| 3   | D     | 1042 | ARG  |
| 3   | D     | 1044 | LEU  |
| 3   | D     | 1045 | MET  |
| 3   | D     | 1058 | ARG  |
| 3   | D     | 1062 | ARG  |
| 3   | D     | 1066 | THR  |
| 3   | D     | 1068 | LEU  |
| 3   | D     | 1083 | ASP  |
| 3   | D     | 1086 | LEU  |
| 3   | D     | 1087 | ARG  |
| 3   | D     | 1088 | THR  |
| 3   | D     | 1090 | ASP  |
| 3   | D     | 1096 | ARG  |
| 3   | D     | 1097 | LYS  |
| 3   | D     | 1101 | VAL  |
| 3   | D     | 1109 | GLU  |
| 3   | D     | 1116 | ASN  |
| 3   | D     | 1118 | ILE  |
| 3   | D     | 1125 | PRO  |
| 3   | D     | 1134 | LEU  |
| 3   | D     | 1135 | ARG  |
| 3   | D     | 1147 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1151 | ARG  |
| 3   | D     | 1154 | GLU  |
| 3   | D     | 1160 | LEU  |
| 3   | D     | 1161 | GLU  |
| 3   | D     | 1166 | LEU  |
| 3   | D     | 1167 | SER  |
| 3   | D     | 1173 | LEU  |
| 3   | D     | 1182 | GLU  |
| 3   | D     | 1183 | ILE  |
| 3   | D     | 1190 | SER  |
| 3   | D     | 1195 | GLN  |
| 3   | D     | 1196 | THR  |
| 3   | D     | 1197 | ARG  |
| 3   | D     | 1201 | CYS  |
| 3   | D     | 1207 | TYR  |
| 3   | D     | 1208 | ASP  |
| 3   | D     | 1211 | MET  |
| 3   | D     | 1213 | ARG  |
| 3   | D     | 1219 | GLU  |
| 3   | D     | 1221 | VAL  |
| 3   | D     | 1223 | ILE  |
| 3   | D     | 1228 | SER  |
| 3   | D     | 1232 | PRO  |
| 3   | D     | 1234 | THR  |
| 3   | D     | 1235 | GLN  |
| 3   | D     | 1238 | MET  |
| 3   | D     | 1240 | THR  |
| 3   | D     | 1243 | THR  |
| 3   | D     | 1251 | ASP  |
| 3   | D     | 1252 | ILE  |
| 3   | D     | 1253 | THR  |
| 3   | D     | 1264 | GLU  |
| 3   | D     | 1269 | LYS  |
| 3   | D     | 1274 | ILE  |
| 3   | D     | 1278 | ASP  |
| 3   | D     | 1285 | GLU  |
| 3   | D     | 1288 | GLU  |
| 3   | D     | 1290 | LEU  |
| 3   | D     | 1302 | GLU  |
| 3   | D     | 1304 | LYS  |
| 3   | D     | 1305 | LEU  |
| 3   | D     | 1306 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1311 | LEU  |
| 3   | D     | 1312 | LEU  |
| 3   | D     | 1314 | LYS  |
| 3   | D     | 1315 | ASP  |
| 3   | D     | 1320 | GLU  |
| 3   | D     | 1331 | ASP  |
| 3   | D     | 1344 | VAL  |
| 3   | D     | 1346 | ARG  |
| 3   | D     | 1348 | LEU  |
| 3   | D     | 1350 | GLU  |
| 3   | D     | 1353 | GLN  |
| 3   | D     | 1372 | VAL  |
| 3   | D     | 1373 | ARG  |
| 3   | D     | 1382 | THR  |
| 3   | D     | 1387 | SER  |
| 3   | D     | 1389 | LEU  |
| 3   | D     | 1396 | GLU  |
| 3   | D     | 1403 | LEU  |
| 3   | D     | 1410 | GLU  |
| 3   | D     | 1415 | VAL  |
| 3   | D     | 1422 | MET  |
| 3   | D     | 1424 | VAL  |
| 3   | D     | 1425 | THR  |
| 3   | D     | 1426 | LYS  |
| 3   | D     | 1427 | SER  |
| 3   | D     | 1429 | LEU  |
| 3   | D     | 1431 | THR  |
| 3   | D     | 1432 | LYS  |
| 3   | D     | 1435 | LEU  |
| 3   | D     | 1441 | GLN  |
| 3   | D     | 1442 | ASN  |
| 3   | D     | 1452 | ILE  |
| 3   | D     | 1464 | GLU  |
| 3   | D     | 1478 | SER  |
| 3   | D     | 1481 | VAL  |
| 3   | D     | 1483 | PHE  |
| 3   | D     | 1485 | GLN  |
| 3   | D     | 1492 | LEU  |
| 3   | D     | 1504 | GLU  |
| 4   | E     | 6    | ILE  |
| 4   | E     | 23   | VAL  |
| 4   | E     | 30   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | E     | 32  | ARG  |
| 4   | E     | 42  | PRO  |
| 4   | E     | 51  | LEU  |
| 4   | E     | 55  | PHE  |
| 4   | E     | 57  | ASP  |
| 4   | E     | 59  | ASN  |
| 4   | E     | 61  | GLU  |
| 4   | E     | 66  | LYS  |
| 4   | E     | 72  | ARG  |
| 4   | E     | 77  | GLU  |
| 4   | E     | 78  | ASN  |
| 4   | E     | 79  | LEU  |
| 4   | E     | 81  | PRO  |
| 4   | E     | 82  | GLU  |
| 4   | E     | 96  | GLU  |
| 5   | F     | 75  | ILE  |
| 5   | F     | 77  | THR  |
| 5   | F     | 84  | TYR  |
| 5   | F     | 86  | HIS  |
| 5   | F     | 91  | VAL  |
| 5   | F     | 122 | LEU  |
| 5   | F     | 124 | PRO  |
| 5   | F     | 128 | ARG  |
| 5   | F     | 130 | VAL  |
| 5   | F     | 135 | ILE  |
| 5   | F     | 136 | LEU  |
| 5   | F     | 142 | ARG  |
| 5   | F     | 145 | PRO  |
| 5   | F     | 148 | LYS  |
| 5   | F     | 149 | GLU  |
| 5   | F     | 152 | ASP  |
| 5   | F     | 155 | THR  |
| 5   | F     | 156 | VAL  |
| 5   | F     | 174 | LEU  |
| 5   | F     | 181 | GLU  |
| 5   | F     | 187 | LEU  |
| 5   | F     | 192 | LEU  |
| 5   | F     | 197 | SER  |
| 5   | F     | 213 | ILE  |
| 5   | F     | 229 | TYR  |
| 5   | F     | 234 | LYS  |
| 5   | F     | 243 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 245 | GLN  |
| 5   | F     | 249 | ARG  |
| 5   | F     | 258 | ILE  |
| 5   | F     | 262 | VAL  |
| 5   | F     | 271 | LEU  |
| 5   | F     | 280 | GLN  |
| 5   | F     | 282 | LEU  |
| 5   | F     | 285 | GLU  |
| 5   | F     | 286 | PRO  |
| 5   | F     | 287 | THR  |
| 5   | F     | 288 | TYR  |
| 5   | F     | 289 | GLU  |
| 5   | F     | 291 | ILE  |
| 5   | F     | 295 | MET  |
| 5   | F     | 302 | LYS  |
| 5   | F     | 316 | SER  |
| 5   | F     | 318 | GLU  |
| 5   | F     | 320 | PRO  |
| 5   | F     | 321 | ILE  |
| 5   | F     | 324 | GLU  |
| 5   | F     | 326 | ASP  |
| 5   | F     | 328 | PHE  |
| 5   | F     | 338 | LEU  |
| 5   | F     | 341 | PRO  |
| 5   | F     | 347 | GLN  |
| 5   | F     | 350 | LEU  |
| 5   | F     | 351 | SER  |
| 5   | F     | 353 | GLU  |
| 5   | F     | 359 | SER  |
| 5   | F     | 361 | LEU  |
| 5   | F     | 362 | SER  |
| 5   | F     | 363 | GLU  |
| 5   | F     | 370 | LYS  |
| 5   | F     | 375 | LEU  |
| 5   | F     | 395 | GLU  |
| 5   | F     | 398 | ARG  |
| 5   | F     | 399 | GLN  |
| 5   | F     | 405 | LEU  |
| 5   | F     | 407 | LYS  |
| 5   | F     | 408 | LEU  |
| 5   | F     | 409 | LYS  |
| 5   | F     | 410 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 414 | ARG  |
| 5   | F     | 416 | ARG  |
| 5   | F     | 418 | LEU  |
| 5   | F     | 419 | ARG  |
| 5   | F     | 422 | LEU  |
| 5   | F     | 423 | ASP  |
| 1   | K     | 1   | MET  |
| 1   | K     | 5   | LYS  |
| 1   | K     | 9   | PRO  |
| 1   | K     | 12  | THR  |
| 1   | K     | 15  | THR  |
| 1   | K     | 26  | GLU  |
| 1   | K     | 30  | ARG  |
| 1   | K     | 54  | THR  |
| 1   | K     | 62  | LEU  |
| 1   | K     | 73  | GLU  |
| 1   | K     | 80  | LEU  |
| 1   | K     | 88  | ARG  |
| 1   | K     | 89  | PHE  |
| 1   | K     | 93  | SER  |
| 1   | K     | 95  | GLN  |
| 1   | K     | 96  | THR  |
| 1   | K     | 99  | LEU  |
| 1   | K     | 112 | ARG  |
| 1   | K     | 121 | GLU  |
| 1   | K     | 127 | LEU  |
| 1   | K     | 142 | VAL  |
| 1   | K     | 143 | ARG  |
| 1   | K     | 146 | ARG  |
| 1   | K     | 148 | VAL  |
| 1   | K     | 159 | LYS  |
| 1   | K     | 160 | ASP  |
| 1   | K     | 162 | ILE  |
| 1   | K     | 163 | ASN  |
| 1   | K     | 167 | VAL  |
| 1   | K     | 170 | VAL  |
| 1   | K     | 185 | ARG  |
| 1   | K     | 186 | LEU  |
| 1   | K     | 188 | GLN  |
| 1   | K     | 189 | ARG  |
| 1   | K     | 196 | THR  |
| 1   | K     | 205 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 206 | THR  |
| 1   | K     | 208 | LEU  |
| 1   | K     | 218 | LEU  |
| 1   | K     | 219 | ARG  |
| 1   | K     | 227 | ASN  |
| 1   | K     | 228 | PRO  |
| 1   | L     | 1   | MET  |
| 1   | L     | 2   | LEU  |
| 1   | L     | 5   | LYS  |
| 1   | L     | 9   | PRO  |
| 1   | L     | 12  | THR  |
| 1   | L     | 16  | GLN  |
| 1   | L     | 26  | GLU  |
| 1   | L     | 30  | ARG  |
| 1   | L     | 54  | THR  |
| 1   | L     | 62  | LEU  |
| 1   | L     | 73  | GLU  |
| 1   | L     | 80  | LEU  |
| 1   | L     | 88  | ARG  |
| 1   | L     | 89  | PHE  |
| 1   | L     | 93  | SER  |
| 1   | L     | 95  | GLN  |
| 1   | L     | 96  | THR  |
| 1   | L     | 99  | LEU  |
| 1   | L     | 112 | ARG  |
| 1   | L     | 119 | ASP  |
| 1   | L     | 121 | GLU  |
| 1   | L     | 137 | ARG  |
| 1   | L     | 138 | LEU  |
| 1   | L     | 140 | MET  |
| 1   | L     | 145 | ASP  |
| 1   | L     | 148 | VAL  |
| 1   | L     | 154 | GLU  |
| 1   | L     | 160 | ASP  |
| 1   | L     | 161 | ARG  |
| 1   | L     | 162 | ILE  |
| 1   | L     | 168 | ASP  |
| 1   | L     | 190 | THR  |
| 1   | L     | 197 | LEU  |
| 1   | L     | 204 | SER  |
| 1   | L     | 206 | THR  |
| 1   | L     | 213 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 223 | THR  |
| 1   | L     | 228 | PRO  |
| 1   | L     | 229 | GLN  |
| 2   | M     | 3   | ILE  |
| 2   | M     | 6   | PHE  |
| 2   | M     | 9   | ILE  |
| 2   | M     | 19  | THR  |
| 2   | M     | 24  | GLU  |
| 2   | M     | 31  | GLN  |
| 2   | M     | 41  | ASN  |
| 2   | M     | 48  | PHE  |
| 2   | M     | 49  | ARG  |
| 2   | M     | 52  | PHE  |
| 2   | M     | 54  | ILE  |
| 2   | M     | 57  | GLU  |
| 2   | M     | 58  | ASP  |
| 2   | M     | 65  | VAL  |
| 2   | M     | 70  | GLU  |
| 2   | M     | 73  | LEU  |
| 2   | M     | 76  | PRO  |
| 2   | M     | 77  | PRO  |
| 2   | M     | 82  | GLU  |
| 2   | M     | 85  | GLU  |
| 2   | M     | 86  | LYS  |
| 2   | M     | 87  | ASP  |
| 2   | M     | 88  | LEU  |
| 2   | M     | 95  | TYR  |
| 2   | M     | 100 | LEU  |
| 2   | M     | 104 | ASP  |
| 2   | M     | 107 | LEU  |
| 2   | M     | 113 | VAL  |
| 2   | M     | 115 | LEU  |
| 2   | M     | 117 | HIS  |
| 2   | M     | 118 | ILE  |
| 2   | M     | 129 | ILE  |
| 2   | M     | 134 | ARG  |
| 2   | M     | 138 | SER  |
| 2   | M     | 140 | ILE  |
| 2   | M     | 144 | PRO  |
| 2   | M     | 146 | VAL  |
| 2   | M     | 149 | THR  |
| 2   | M     | 150 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 152 | PRO  |
| 2   | M     | 154 | ARG  |
| 2   | M     | 158 | TYR  |
| 2   | M     | 165 | LEU  |
| 2   | M     | 166 | PRO  |
| 2   | M     | 167 | LYS  |
| 2   | M     | 170 | PRO  |
| 2   | M     | 174 | LEU  |
| 2   | M     | 178 | PRO  |
| 2   | M     | 181 | VAL  |
| 2   | M     | 186 | VAL  |
| 2   | M     | 189 | ARG  |
| 2   | M     | 190 | LYS  |
| 2   | M     | 191 | PHE  |
| 2   | M     | 193 | LEU  |
| 2   | M     | 194 | VAL  |
| 2   | M     | 195 | LEU  |
| 2   | M     | 196 | LEU  |
| 2   | M     | 198 | ARG  |
| 2   | M     | 203 | ASP  |
| 2   | M     | 204 | GLN  |
| 2   | M     | 207 | LEU  |
| 2   | M     | 209 | ARG  |
| 2   | M     | 211 | LEU  |
| 2   | M     | 218 | VAL  |
| 2   | M     | 221 | LEU  |
| 2   | M     | 226 | VAL  |
| 2   | M     | 230 | ARG  |
| 2   | M     | 240 | THR  |
| 2   | M     | 241 | LEU  |
| 2   | M     | 242 | LEU  |
| 2   | M     | 247 | PRO  |
| 2   | M     | 252 | LYS  |
| 2   | M     | 256 | TYR  |
| 2   | M     | 257 | VAL  |
| 2   | M     | 261 | ILE  |
| 2   | M     | 266 | ARG  |
| 2   | M     | 268 | ASP  |
| 2   | M     | 269 | LEU  |
| 2   | M     | 275 | TYR  |
| 2   | M     | 276 | LYS  |
| 2   | M     | 279 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 281 | LEU  |
| 2   | M     | 288 | ARG  |
| 2   | M     | 289 | THR  |
| 2   | M     | 290 | LEU  |
| 2   | M     | 293 | PHE  |
| 2   | M     | 297 | GLU  |
| 2   | M     | 301 | GLU  |
| 2   | M     | 302 | VAL  |
| 2   | M     | 303 | PHE  |
| 2   | M     | 304 | LEU  |
| 2   | M     | 309 | TYR  |
| 2   | M     | 321 | GLU  |
| 2   | M     | 323 | ASP  |
| 2   | M     | 333 | ILE  |
| 2   | M     | 334 | ARG  |
| 2   | M     | 340 | MET  |
| 2   | M     | 341 | THR  |
| 2   | M     | 348 | LEU  |
| 2   | M     | 358 | ARG  |
| 2   | M     | 359 | MET  |
| 2   | M     | 367 | LEU  |
| 2   | M     | 379 | GLU  |
| 2   | M     | 383 | ARG  |
| 2   | M     | 384 | GLU  |
| 2   | M     | 400 | PRO  |
| 2   | M     | 402 | SER  |
| 2   | M     | 403 | SER  |
| 2   | M     | 415 | PRO  |
| 2   | M     | 419 | THR  |
| 2   | M     | 420 | ARG  |
| 2   | M     | 422 | ARG  |
| 2   | M     | 425 | PHE  |
| 2   | M     | 426 | ASP  |
| 2   | M     | 430 | VAL  |
| 2   | M     | 433 | THR  |
| 2   | M     | 439 | CYS  |
| 2   | M     | 443 | THR  |
| 2   | M     | 452 | ILE  |
| 2   | M     | 455 | LEU  |
| 2   | M     | 460 | ARG  |
| 2   | M     | 474 | VAL  |
| 2   | M     | 487 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 489 | THR  |
| 2   | M     | 491 | GLU  |
| 2   | M     | 500 | ASN  |
| 2   | M     | 503 | LEU  |
| 2   | M     | 511 | GLU  |
| 2   | M     | 520 | GLU  |
| 2   | M     | 522 | VAL  |
| 2   | M     | 523 | ILE  |
| 2   | M     | 527 | GLU  |
| 2   | M     | 532 | MET  |
| 2   | M     | 535 | SER  |
| 2   | M     | 543 | ASN  |
| 2   | M     | 548 | PRO  |
| 2   | M     | 549 | PHE  |
| 2   | M     | 550 | LEU  |
| 2   | M     | 556 | ASN  |
| 2   | M     | 559 | LEU  |
| 2   | M     | 564 | MET  |
| 2   | M     | 565 | GLN  |
| 2   | M     | 566 | THR  |
| 2   | M     | 572 | ILE  |
| 2   | M     | 579 | VAL  |
| 2   | M     | 584 | GLU  |
| 2   | M     | 589 | ARG  |
| 2   | M     | 600 | ASP  |
| 2   | M     | 609 | ASN  |
| 2   | M     | 614 | ARG  |
| 2   | M     | 627 | ARG  |
| 2   | M     | 630 | ARG  |
| 2   | M     | 633 | GLN  |
| 2   | M     | 637 | LEU  |
| 2   | M     | 640 | ARG  |
| 2   | M     | 645 | VAL  |
| 2   | M     | 649 | VAL  |
| 2   | M     | 650 | ARG  |
| 2   | M     | 654 | LEU  |
| 2   | M     | 662 | GLU  |
| 2   | M     | 670 | GLN  |
| 2   | M     | 672 | VAL  |
| 2   | M     | 673 | LEU  |
| 2   | M     | 674 | VAL  |
| 2   | M     | 679 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 680 | ASP  |
| 2   | M     | 685 | GLU  |
| 2   | M     | 689 | VAL  |
| 2   | M     | 690 | ILE  |
| 2   | M     | 697 | ARG  |
| 2   | M     | 698 | ASP  |
| 2   | M     | 701 | THR  |
| 2   | M     | 714 | ASP  |
| 2   | M     | 722 | ILE  |
| 2   | M     | 726 | ILE  |
| 2   | M     | 727 | PRO  |
| 2   | M     | 729 | LEU  |
| 2   | M     | 744 | ARG  |
| 2   | M     | 749 | VAL  |
| 2   | M     | 750 | LYS  |
| 2   | M     | 762 | LYS  |
| 2   | M     | 766 | GLU  |
| 2   | M     | 767 | PRO  |
| 2   | M     | 768 | THR  |
| 2   | M     | 770 | GLU  |
| 2   | M     | 773 | LEU  |
| 2   | M     | 774 | LEU  |
| 2   | M     | 785 | VAL  |
| 2   | M     | 790 | LEU  |
| 2   | M     | 791 | ARG  |
| 2   | M     | 799 | ILE  |
| 2   | M     | 807 | ARG  |
| 2   | M     | 813 | VAL  |
| 2   | M     | 831 | ARG  |
| 2   | M     | 839 | LEU  |
| 2   | M     | 848 | VAL  |
| 2   | M     | 853 | LEU  |
| 2   | M     | 861 | LEU  |
| 2   | M     | 865 | THR  |
| 2   | M     | 869 | VAL  |
| 2   | M     | 871 | LEU  |
| 2   | M     | 878 | SER  |
| 2   | M     | 881 | ASN  |
| 2   | M     | 886 | LEU  |
| 2   | M     | 897 | LEU  |
| 2   | M     | 900 | ARG  |
| 2   | M     | 904 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 905  | ILE  |
| 2   | M     | 918  | LEU  |
| 2   | M     | 928  | LYS  |
| 2   | M     | 929  | ARG  |
| 2   | M     | 934  | PHE  |
| 2   | M     | 937  | ASP  |
| 2   | M     | 938  | LYS  |
| 2   | M     | 941  | VAL  |
| 2   | M     | 942  | GLU  |
| 2   | M     | 950  | LEU  |
| 2   | M     | 952  | LEU  |
| 2   | M     | 958  | THR  |
| 2   | M     | 959  | PRO  |
| 2   | M     | 962  | GLN  |
| 2   | M     | 971  | LYS  |
| 2   | M     | 973  | VAL  |
| 2   | M     | 983  | ILE  |
| 2   | M     | 984  | GLU  |
| 2   | M     | 988  | VAL  |
| 2   | M     | 995  | MET  |
| 2   | M     | 999  | HIS  |
| 2   | M     | 1000 | MET  |
| 2   | M     | 1005 | MET  |
| 2   | M     | 1014 | SER  |
| 2   | M     | 1015 | LEU  |
| 2   | M     | 1016 | ILE  |
| 2   | M     | 1017 | THR  |
| 2   | M     | 1018 | GLN  |
| 2   | M     | 1019 | GLN  |
| 2   | M     | 1021 | LEU  |
| 2   | M     | 1052 | MET  |
| 2   | M     | 1074 | GLU  |
| 2   | M     | 1075 | ASP  |
| 2   | M     | 1097 | LEU  |
| 2   | M     | 1100 | GLN  |
| 2   | M     | 1104 | GLU  |
| 2   | M     | 1105 | LYS  |
| 2   | M     | 1106 | ASP  |
| 2   | M     | 1107 | ASN  |
| 2   | M     | 1115 | LEU  |
| 3   | N     | 3    | LYS  |
| 3   | N     | 7    | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | N     | 14  | SER  |
| 3   | N     | 15  | PRO  |
| 3   | N     | 18  | ILE  |
| 3   | N     | 27  | GLU  |
| 3   | N     | 35  | ARG  |
| 3   | N     | 39  | PRO  |
| 3   | N     | 47  | GLU  |
| 3   | N     | 53  | ILE  |
| 3   | N     | 62  | LYS  |
| 3   | N     | 68  | PHE  |
| 3   | N     | 69  | GLU  |
| 3   | N     | 75  | ARG  |
| 3   | N     | 76  | CYS  |
| 3   | N     | 79  | GLU  |
| 3   | N     | 80  | VAL  |
| 3   | N     | 83  | SER  |
| 3   | N     | 85  | VAL  |
| 3   | N     | 90  | MET  |
| 3   | N     | 94  | GLU  |
| 3   | N     | 98  | PRO  |
| 3   | N     | 101 | HIS  |
| 3   | N     | 102 | ILE  |
| 3   | N     | 107 | ASP  |
| 3   | N     | 112 | ILE  |
| 3   | N     | 115 | LEU  |
| 3   | N     | 118 | LEU  |
| 3   | N     | 119 | SER  |
| 3   | N     | 121 | THR  |
| 3   | N     | 122 | GLU  |
| 3   | N     | 123 | LEU  |
| 3   | N     | 126 | VAL  |
| 3   | N     | 133 | ILE  |
| 3   | N     | 134 | VAL  |
| 3   | N     | 135 | LEU  |
| 3   | N     | 138 | LYS  |
| 3   | N     | 142 | LEU  |
| 3   | N     | 143 | ASN  |
| 3   | N     | 145 | VAL  |
| 3   | N     | 146 | PRO  |
| 3   | N     | 149 | LYS  |
| 3   | N     | 156 | GLU  |
| 3   | N     | 161 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | N     | 168 | THR  |
| 3   | N     | 169 | TYR  |
| 3   | N     | 171 | LEU  |
| 3   | N     | 178 | LEU  |
| 3   | N     | 185 | VAL  |
| 3   | N     | 186 | VAL  |
| 3   | N     | 190 | GLU  |
| 3   | N     | 199 | LEU  |
| 3   | N     | 200 | ASP  |
| 3   | N     | 202 | VAL  |
| 3   | N     | 206 | ARG  |
| 3   | N     | 208 | PRO  |
| 3   | N     | 213 | VAL  |
| 3   | N     | 389 | GLU  |
| 3   | N     | 393 | ILE  |
| 3   | N     | 394 | LEU  |
| 3   | N     | 400 | VAL  |
| 3   | N     | 402 | PRO  |
| 3   | N     | 406 | ASP  |
| 3   | N     | 409 | VAL  |
| 3   | N     | 411 | THR  |
| 3   | N     | 413 | ASP  |
| 3   | N     | 414 | ARG  |
| 3   | N     | 419 | ASP  |
| 3   | N     | 420 | VAL  |
| 3   | N     | 421 | LEU  |
| 3   | N     | 423 | ASP  |
| 3   | N     | 427 | VAL  |
| 3   | N     | 429 | SER  |
| 3   | N     | 431 | VAL  |
| 3   | N     | 432 | TYR  |
| 3   | N     | 444 | VAL  |
| 3   | N     | 447 | VAL  |
| 3   | N     | 452 | ILE  |
| 3   | N     | 456 | MET  |
| 3   | N     | 462 | GLN  |
| 3   | N     | 468 | LEU  |
| 3   | N     | 473 | LEU  |
| 3   | N     | 483 | HIS  |
| 3   | N     | 489 | ARG  |
| 3   | N     | 498 | VAL  |
| 3   | N     | 502 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | N     | 504 | ASP  |
| 3   | N     | 505 | SER  |
| 3   | N     | 507 | ASN  |
| 3   | N     | 508 | ARG  |
| 3   | N     | 510 | GLU  |
| 3   | N     | 513 | ILE  |
| 3   | N     | 521 | PRO  |
| 3   | N     | 525 | ARG  |
| 3   | N     | 538 | SER  |
| 3   | N     | 539 | ASP  |
| 3   | N     | 543 | LEU  |
| 3   | N     | 545 | ARG  |
| 3   | N     | 547 | LEU  |
| 3   | N     | 549 | ASN  |
| 3   | N     | 554 | LEU  |
| 3   | N     | 560 | GLN  |
| 3   | N     | 564 | GLU  |
| 3   | N     | 569 | ASN  |
| 3   | N     | 571 | LYS  |
| 3   | N     | 576 | GLU  |
| 3   | N     | 587 | ARG  |
| 3   | N     | 591 | VAL  |
| 3   | N     | 594 | PRO  |
| 3   | N     | 606 | ILE  |
| 3   | N     | 611 | GLN  |
| 3   | N     | 619 | LEU  |
| 3   | N     | 624 | ASP  |
| 3   | N     | 625 | TYR  |
| 3   | N     | 629 | SER  |
| 3   | N     | 636 | GLN  |
| 3   | N     | 640 | HIS  |
| 3   | N     | 641 | GLN  |
| 3   | N     | 642 | CYS  |
| 3   | N     | 645 | PRO  |
| 3   | N     | 651 | GLU  |
| 3   | N     | 652 | LEU  |
| 3   | N     | 664 | LYS  |
| 3   | N     | 676 | MET  |
| 3   | N     | 681 | ARG  |
| 3   | N     | 683 | ILE  |
| 3   | N     | 695 | ILE  |
| 3   | N     | 702 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | N     | 704 | ARG  |
| 3   | N     | 710 | ARG  |
| 3   | N     | 719 | VAL  |
| 3   | N     | 733 | CYS  |
| 3   | N     | 734 | GLU  |
| 3   | N     | 747 | VAL  |
| 3   | N     | 749 | VAL  |
| 3   | N     | 752 | SER  |
| 3   | N     | 754 | PHE  |
| 3   | N     | 761 | ILE  |
| 3   | N     | 769 | LEU  |
| 3   | N     | 783 | ARG  |
| 3   | N     | 784 | ASP  |
| 3   | N     | 794 | GLN  |
| 3   | N     | 796 | ARG  |
| 3   | N     | 804 | LEU  |
| 3   | N     | 817 | GLU  |
| 3   | N     | 827 | ILE  |
| 3   | N     | 828 | LYS  |
| 3   | N     | 833 | GLU  |
| 3   | N     | 835 | SER  |
| 3   | N     | 836 | VAL  |
| 3   | N     | 838 | ARG  |
| 3   | N     | 841 | TYR  |
| 3   | N     | 842 | VAL  |
| 3   | N     | 848 | GLU  |
| 3   | N     | 851 | LEU  |
| 3   | N     | 861 | GLN  |
| 3   | N     | 862 | ASP  |
| 3   | N     | 863 | VAL  |
| 3   | N     | 865 | THR  |
| 3   | N     | 866 | VAL  |
| 3   | N     | 875 | THR  |
| 3   | N     | 877 | PRO  |
| 3   | N     | 879 | ARG  |
| 3   | N     | 897 | TRP  |
| 3   | N     | 899 | LEU  |
| 3   | N     | 901 | GLN  |
| 3   | N     | 903 | ASP  |
| 3   | N     | 904 | VAL  |
| 3   | N     | 911 | LEU  |
| 3   | N     | 912 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 922  | LEU  |
| 3   | N     | 932  | ASP  |
| 3   | N     | 934  | LEU  |
| 3   | N     | 940  | THR  |
| 3   | N     | 944  | THR  |
| 3   | N     | 948  | THR  |
| 3   | N     | 951  | ILE  |
| 3   | N     | 952  | ASP  |
| 3   | N     | 964  | LEU  |
| 3   | N     | 965  | GLU  |
| 3   | N     | 972  | LEU  |
| 3   | N     | 997  | THR  |
| 3   | N     | 1001 | GLU  |
| 3   | N     | 1003 | VAL  |
| 3   | N     | 1005 | GLN  |
| 3   | N     | 1007 | VAL  |
| 3   | N     | 1019 | PRO  |
| 3   | N     | 1020 | LEU  |
| 3   | N     | 1041 | LEU  |
| 3   | N     | 1042 | ARG  |
| 3   | N     | 1044 | LEU  |
| 3   | N     | 1045 | MET  |
| 3   | N     | 1049 | SER  |
| 3   | N     | 1055 | VAL  |
| 3   | N     | 1058 | ARG  |
| 3   | N     | 1062 | ARG  |
| 3   | N     | 1063 | GLU  |
| 3   | N     | 1066 | THR  |
| 3   | N     | 1068 | LEU  |
| 3   | N     | 1072 | ILE  |
| 3   | N     | 1073 | SER  |
| 3   | N     | 1086 | LEU  |
| 3   | N     | 1088 | THR  |
| 3   | N     | 1096 | ARG  |
| 3   | N     | 1097 | LYS  |
| 3   | N     | 1101 | VAL  |
| 3   | N     | 1109 | GLU  |
| 3   | N     | 1111 | ASP  |
| 3   | N     | 1114 | THR  |
| 3   | N     | 1116 | ASN  |
| 3   | N     | 1118 | ILE  |
| 3   | N     | 1119 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 1126 | ASP  |
| 3   | N     | 1131 | SER  |
| 3   | N     | 1134 | LEU  |
| 3   | N     | 1135 | ARG  |
| 3   | N     | 1147 | ARG  |
| 3   | N     | 1148 | VAL  |
| 3   | N     | 1152 | GLU  |
| 3   | N     | 1153 | VAL  |
| 3   | N     | 1156 | LEU  |
| 3   | N     | 1160 | LEU  |
| 3   | N     | 1161 | GLU  |
| 3   | N     | 1166 | LEU  |
| 3   | N     | 1168 | MET  |
| 3   | N     | 1169 | ASP  |
| 3   | N     | 1173 | LEU  |
| 3   | N     | 1176 | LYS  |
| 3   | N     | 1182 | GLU  |
| 3   | N     | 1183 | ILE  |
| 3   | N     | 1188 | VAL  |
| 3   | N     | 1189 | ARG  |
| 3   | N     | 1190 | SER  |
| 3   | N     | 1191 | PRO  |
| 3   | N     | 1197 | ARG  |
| 3   | N     | 1200 | VAL  |
| 3   | N     | 1201 | CYS  |
| 3   | N     | 1204 | CYS  |
| 3   | N     | 1207 | TYR  |
| 3   | N     | 1208 | ASP  |
| 3   | N     | 1211 | MET  |
| 3   | N     | 1219 | GLU  |
| 3   | N     | 1221 | VAL  |
| 3   | N     | 1223 | ILE  |
| 3   | N     | 1224 | VAL  |
| 3   | N     | 1231 | GLU  |
| 3   | N     | 1235 | GLN  |
| 3   | N     | 1238 | MET  |
| 3   | N     | 1243 | THR  |
| 3   | N     | 1251 | ASP  |
| 3   | N     | 1252 | ILE  |
| 3   | N     | 1253 | THR  |
| 3   | N     | 1256 | LEU  |
| 3   | N     | 1257 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 1262 | LEU  |
| 3   | N     | 1264 | GLU  |
| 3   | N     | 1274 | ILE  |
| 3   | N     | 1275 | SER  |
| 3   | N     | 1283 | ILE  |
| 3   | N     | 1284 | GLU  |
| 3   | N     | 1285 | GLU  |
| 3   | N     | 1290 | LEU  |
| 3   | N     | 1295 | GLU  |
| 3   | N     | 1297 | GLU  |
| 3   | N     | 1304 | LYS  |
| 3   | N     | 1306 | PRO  |
| 3   | N     | 1308 | GLU  |
| 3   | N     | 1310 | ARG  |
| 3   | N     | 1311 | LEU  |
| 3   | N     | 1312 | LEU  |
| 3   | N     | 1314 | LYS  |
| 3   | N     | 1323 | GLN  |
| 3   | N     | 1331 | ASP  |
| 3   | N     | 1332 | PRO  |
| 3   | N     | 1334 | GLN  |
| 3   | N     | 1337 | GLU  |
| 3   | N     | 1342 | GLU  |
| 3   | N     | 1346 | ARG  |
| 3   | N     | 1348 | LEU  |
| 3   | N     | 1352 | ILE  |
| 3   | N     | 1363 | LEU  |
| 3   | N     | 1375 | MET  |
| 3   | N     | 1377 | LYS  |
| 3   | N     | 1382 | THR  |
| 3   | N     | 1383 | ASP  |
| 3   | N     | 1387 | SER  |
| 3   | N     | 1388 | ARG  |
| 3   | N     | 1389 | LEU  |
| 3   | N     | 1390 | LEU  |
| 3   | N     | 1396 | GLU  |
| 3   | N     | 1403 | LEU  |
| 3   | N     | 1407 | LEU  |
| 3   | N     | 1408 | ILE  |
| 3   | N     | 1410 | GLU  |
| 3   | N     | 1419 | PRO  |
| 3   | N     | 1422 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 1424 | VAL  |
| 3   | N     | 1426 | LYS  |
| 3   | N     | 1429 | LEU  |
| 3   | N     | 1430 | SER  |
| 3   | N     | 1431 | THR  |
| 3   | N     | 1432 | LYS  |
| 3   | N     | 1442 | ASN  |
| 3   | N     | 1452 | ILE  |
| 3   | N     | 1464 | GLU  |
| 3   | N     | 1466 | VAL  |
| 3   | N     | 1468 | LEU  |
| 3   | N     | 1472 | ILE  |
| 3   | N     | 1481 | VAL  |
| 3   | N     | 1484 | THR  |
| 3   | N     | 1485 | GLN  |
| 3   | N     | 1492 | LEU  |
| 3   | N     | 1504 | GLU  |
| 4   | O     | 20   | THR  |
| 4   | O     | 30   | LEU  |
| 4   | O     | 42   | PRO  |
| 4   | O     | 43   | GLU  |
| 4   | O     | 44   | GLU  |
| 4   | O     | 51   | LEU  |
| 4   | O     | 56   | ASP  |
| 4   | O     | 58   | PRO  |
| 4   | O     | 59   | ASN  |
| 4   | O     | 61   | GLU  |
| 4   | O     | 66   | LYS  |
| 4   | O     | 69   | LEU  |
| 4   | O     | 77   | GLU  |
| 4   | O     | 79   | LEU  |
| 4   | O     | 81   | PRO  |
| 5   | P     | 77   | THR  |
| 5   | P     | 78   | SER  |
| 5   | P     | 80   | PRO  |
| 5   | P     | 84   | TYR  |
| 5   | P     | 86   | HIS  |
| 5   | P     | 88   | ILE  |
| 5   | P     | 91   | VAL  |
| 5   | P     | 117  | SER  |
| 5   | P     | 118  | GLU  |
| 5   | P     | 122  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | P     | 125 | ASP  |
| 5   | P     | 128 | ARG  |
| 5   | P     | 134 | LYS  |
| 5   | P     | 141 | VAL  |
| 5   | P     | 145 | PRO  |
| 5   | P     | 149 | GLU  |
| 5   | P     | 154 | LYS  |
| 5   | P     | 161 | GLN  |
| 5   | P     | 169 | GLU  |
| 5   | P     | 170 | HIS  |
| 5   | P     | 174 | LEU  |
| 5   | P     | 181 | GLU  |
| 5   | P     | 187 | LEU  |
| 5   | P     | 214 | GLN  |
| 5   | P     | 236 | SER  |
| 5   | P     | 245 | GLN  |
| 5   | P     | 263 | HIS  |
| 5   | P     | 264 | MET  |
| 5   | P     | 267 | THR  |
| 5   | P     | 271 | LEU  |
| 5   | P     | 274 | THR  |
| 5   | P     | 279 | GLN  |
| 5   | P     | 282 | LEU  |
| 5   | P     | 286 | PRO  |
| 5   | P     | 287 | THR  |
| 5   | P     | 288 | TYR  |
| 5   | P     | 289 | GLU  |
| 5   | P     | 295 | MET  |
| 5   | P     | 308 | LEU  |
| 5   | P     | 315 | VAL  |
| 5   | P     | 324 | GLU  |
| 5   | P     | 326 | ASP  |
| 5   | P     | 327 | SER  |
| 5   | P     | 341 | PRO  |
| 5   | P     | 343 | ASP  |
| 5   | P     | 347 | GLN  |
| 5   | P     | 350 | LEU  |
| 5   | P     | 351 | SER  |
| 5   | P     | 361 | LEU  |
| 5   | P     | 364 | ARG  |
| 5   | P     | 370 | LYS  |
| 5   | P     | 375 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | P     | 398 | ARG  |
| 5   | P     | 405 | LEU  |
| 5   | P     | 406 | ARG  |
| 5   | P     | 408 | LEU  |
| 5   | P     | 409 | LYS  |
| 5   | P     | 410 | TYR  |
| 5   | P     | 411 | HIS  |
| 5   | P     | 414 | ARG  |
| 5   | P     | 418 | LEU  |
| 5   | P     | 420 | ASP  |
| 5   | P     | 422 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (180) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 81  | ASN  |
| 1   | A     | 95  | GLN  |
| 1   | A     | 124 | ASN  |
| 1   | A     | 139 | ASN  |
| 1   | A     | 156 | HIS  |
| 1   | A     | 163 | ASN  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 227 | ASN  |
| 1   | A     | 229 | GLN  |
| 1   | B     | 16  | GLN  |
| 1   | B     | 81  | ASN  |
| 1   | B     | 95  | GLN  |
| 1   | B     | 124 | ASN  |
| 1   | B     | 128 | HIS  |
| 1   | B     | 156 | HIS  |
| 1   | B     | 163 | ASN  |
| 1   | B     | 212 | ASN  |
| 1   | B     | 227 | ASN  |
| 1   | B     | 229 | GLN  |
| 2   | C     | 22  | GLN  |
| 2   | C     | 31  | GLN  |
| 2   | C     | 41  | ASN  |
| 2   | C     | 99  | GLN  |
| 2   | C     | 320 | HIS  |
| 2   | C     | 406 | HIS  |
| 2   | C     | 498 | GLN  |
| 2   | C     | 538 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 565  | GLN  |
| 2   | C     | 609  | ASN  |
| 2   | C     | 647  | GLN  |
| 2   | C     | 671  | ASN  |
| 2   | C     | 704  | HIS  |
| 2   | C     | 829  | GLN  |
| 2   | C     | 834  | GLN  |
| 2   | C     | 841  | ASN  |
| 2   | C     | 843  | HIS  |
| 2   | C     | 881  | ASN  |
| 2   | C     | 889  | HIS  |
| 2   | C     | 969  | GLN  |
| 2   | C     | 1018 | GLN  |
| 2   | C     | 1019 | GLN  |
| 2   | C     | 1047 | HIS  |
| 2   | C     | 1100 | GLN  |
| 3   | D     | 101  | HIS  |
| 3   | D     | 462  | GLN  |
| 3   | D     | 549  | ASN  |
| 3   | D     | 560  | GLN  |
| 3   | D     | 569  | ASN  |
| 3   | D     | 575  | GLN  |
| 3   | D     | 617  | ASN  |
| 3   | D     | 669  | ASN  |
| 3   | D     | 680  | GLN  |
| 3   | D     | 703  | ASN  |
| 3   | D     | 717  | GLN  |
| 3   | D     | 724  | GLN  |
| 3   | D     | 727  | GLN  |
| 3   | D     | 756  | GLN  |
| 3   | D     | 762  | GLN  |
| 3   | D     | 794  | GLN  |
| 3   | D     | 816  | HIS  |
| 3   | D     | 845  | ASN  |
| 3   | D     | 855  | HIS  |
| 3   | D     | 861  | GLN  |
| 3   | D     | 917  | GLN  |
| 3   | D     | 976  | GLN  |
| 3   | D     | 1033 | GLN  |
| 3   | D     | 1103 | HIS  |
| 3   | D     | 1116 | ASN  |
| 3   | D     | 1184 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1323 | GLN  |
| 3   | D     | 1333 | HIS  |
| 3   | D     | 1353 | GLN  |
| 3   | D     | 1359 | GLN  |
| 3   | D     | 1374 | GLN  |
| 3   | D     | 1393 | GLN  |
| 3   | D     | 1441 | GLN  |
| 3   | D     | 1465 | ASN  |
| 3   | D     | 1489 | GLN  |
| 4   | E     | 29   | GLN  |
| 4   | E     | 33   | HIS  |
| 5   | F     | 83   | GLN  |
| 5   | F     | 90   | GLN  |
| 5   | F     | 191  | ASN  |
| 5   | F     | 218  | GLN  |
| 5   | F     | 245  | GLN  |
| 5   | F     | 254  | GLN  |
| 5   | F     | 269  | ASN  |
| 5   | F     | 279  | GLN  |
| 5   | F     | 312  | GLN  |
| 5   | F     | 411  | HIS  |
| 1   | K     | 38   | ASN  |
| 1   | K     | 81   | ASN  |
| 1   | K     | 95   | GLN  |
| 1   | K     | 124  | ASN  |
| 1   | K     | 163  | ASN  |
| 1   | K     | 180  | GLN  |
| 1   | K     | 188  | GLN  |
| 1   | K     | 212  | ASN  |
| 1   | K     | 213  | GLN  |
| 1   | K     | 227  | ASN  |
| 1   | L     | 95   | GLN  |
| 1   | L     | 124  | ASN  |
| 1   | L     | 128  | HIS  |
| 1   | L     | 156  | HIS  |
| 1   | L     | 163  | ASN  |
| 1   | L     | 212  | ASN  |
| 1   | L     | 221  | HIS  |
| 2   | M     | 31   | GLN  |
| 2   | M     | 41   | ASN  |
| 2   | M     | 45   | GLN  |
| 2   | M     | 117  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 187  | ASN  |
| 2   | M     | 320  | HIS  |
| 2   | M     | 343  | GLN  |
| 2   | M     | 390  | GLN  |
| 2   | M     | 431  | HIS  |
| 2   | M     | 552  | HIS  |
| 2   | M     | 647  | GLN  |
| 2   | M     | 671  | ASN  |
| 2   | M     | 834  | GLN  |
| 2   | M     | 841  | ASN  |
| 2   | M     | 843  | HIS  |
| 2   | M     | 845  | ASN  |
| 2   | M     | 881  | ASN  |
| 2   | M     | 884  | GLN  |
| 2   | M     | 889  | HIS  |
| 2   | M     | 899  | GLN  |
| 2   | M     | 920  | GLN  |
| 2   | M     | 1018 | GLN  |
| 2   | M     | 1019 | GLN  |
| 2   | M     | 1064 | ASN  |
| 2   | M     | 1100 | GLN  |
| 3   | N     | 101  | HIS  |
| 3   | N     | 151  | GLN  |
| 3   | N     | 507  | ASN  |
| 3   | N     | 541  | ASN  |
| 3   | N     | 549  | ASN  |
| 3   | N     | 551  | ASN  |
| 3   | N     | 636  | GLN  |
| 3   | N     | 640  | HIS  |
| 3   | N     | 680  | GLN  |
| 3   | N     | 703  | ASN  |
| 3   | N     | 709  | HIS  |
| 3   | N     | 714  | GLN  |
| 3   | N     | 727  | GLN  |
| 3   | N     | 756  | GLN  |
| 3   | N     | 768  | ASN  |
| 3   | N     | 824  | ASN  |
| 3   | N     | 845  | ASN  |
| 3   | N     | 861  | GLN  |
| 3   | N     | 962  | GLN  |
| 3   | N     | 994  | GLN  |
| 3   | N     | 1046 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 1116 | ASN  |
| 3   | N     | 1124 | GLN  |
| 3   | N     | 1195 | GLN  |
| 3   | N     | 1202 | GLN  |
| 3   | N     | 1242 | HIS  |
| 3   | N     | 1254 | GLN  |
| 3   | N     | 1323 | GLN  |
| 3   | N     | 1334 | GLN  |
| 3   | N     | 1353 | GLN  |
| 3   | N     | 1359 | GLN  |
| 3   | N     | 1367 | HIS  |
| 3   | N     | 1374 | GLN  |
| 3   | N     | 1441 | GLN  |
| 3   | N     | 1485 | GLN  |
| 3   | N     | 1489 | GLN  |
| 4   | O     | 28   | GLN  |
| 4   | O     | 29   | GLN  |
| 4   | O     | 59   | ASN  |
| 4   | O     | 86   | GLN  |
| 5   | P     | 90   | GLN  |
| 5   | P     | 161  | GLN  |
| 5   | P     | 214  | GLN  |
| 5   | P     | 218  | GLN  |
| 5   | P     | 245  | GLN  |
| 5   | P     | 277  | GLN  |
| 5   | P     | 279  | GLN  |
| 5   | P     | 337  | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 489 ligands modelled in this entry, 489 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 3   | D     | 1                |
| 3   | N     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | D     | 380:GLU   | C      | 381:ALA   | N      | 1.17         |
| 1     | N     | 380:GLU   | C      | 381:ALA   | N      | 1.17         |

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.