



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:38 PM UTC

PDB ID : 4WQS / pdb\_00004wqs  
Title : Thermus thermophilus RNA polymerase backtracked complex  
Authors : Murayama, Y.; Sekine, S.; Yokoyama, S.  
Deposited on : 2014-10-22  
Resolution : 4.31 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)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

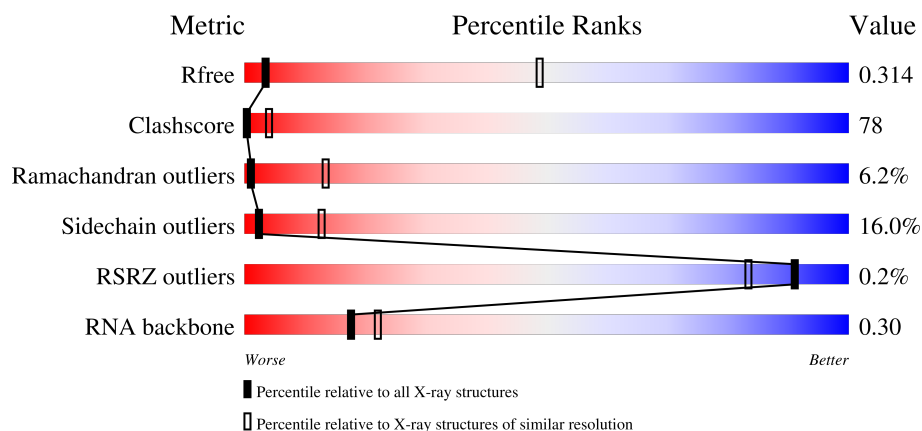
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.31 Å.

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



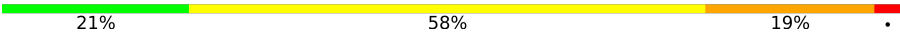
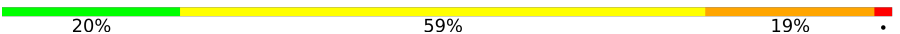
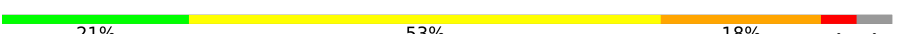
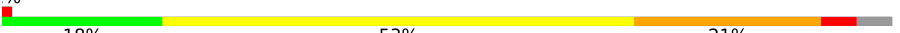
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1052 (4.70-3.90)                                      |
| Clashscore            | 190562                      | 1097 (4.70-3.90)                                      |
| Ramachandran outliers | 187476                      | 1001 (4.70-3.90)                                      |
| Sidechain outliers    | 187428                      | 1007 (4.72-3.88)                                      |
| RSRZ outliers         | 180081                      | 1049 (4.70-3.90)                                      |
| RNA backbone          | 3983                        | 1036 (5.50-3.10)                                      |

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 315    |                  |
| 1   | B     | 315    |                  |
| 1   | K     | 315    |                  |
| 1   | L     | 315    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 2   | C     | 1119   |  |
| 2   | M     | 1119   |  |
| 3   | D     | 1524   |  |
| 3   | N     | 1524   |  |
| 4   | E     | 99     |  |
| 4   | O     | 99     |  |
| 5   | G     | 28     |  |
| 5   | X     | 28     |  |
| 6   | H     | 16     |  |
| 6   | Y     | 16     |  |
| 7   | I     | 21     |  |
| 7   | Z     | 21     |  |

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 48166 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 DNA-directed RNA polymerase subunit alpha.

| 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 DNA-directed RNA polymerase subunit beta.

| 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 DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | D     | 1151     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9097  | 5753 | 1629 | 1682 | 33 |         |         |       |
| 3   | N     | 1288     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10175 | 6441 | 1804 | 1899 | 31 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | E     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 770   | 491 | 133 | 142 | 4 |         |         |       |
| 4   | O     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 770   | 491 | 133 | 142 | 4 |         |         |       |

- Molecule 5 is a DNA chain called DNA (28-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 5   | G     | 27       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 548   | 259 | 104 | 158 | 27 |         |         |       |
| 5   | X     | 27       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 548   | 259 | 104 | 158 | 27 |         |         |       |

- Molecule 6 is a RNA chain called RNA (5'-R(P\*CP\*CP\*AP\*GP\*CP\*CP\*GP\*GP\*CP\*GP\*CP\*UP\*CP\*GP\*CP\*A)-3').

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 6   | H     | 16       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 340   | 151 | 61 | 112 | 16 |         |         |       |
| 6   | Y     | 15       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 318   | 141 | 56 | 106 | 15 |         |         |       |

- Molecule 7 is a DNA chain called DNA (5'-D(P\*GP\*TP\*AP\*GP\*CP\*TP\*TP\*GP\*TP\*GP\*GP\*TP\*AP\*GP\*TP\*GP\*AP\*CP\*GP\*AP\*G)-3').

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 7   | I     | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 357   | 169 | 65 | 106 | 17 |         |         |       |
| 7   | Z     | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 357   | 169 | 65 | 106 | 17 |         |         |       |

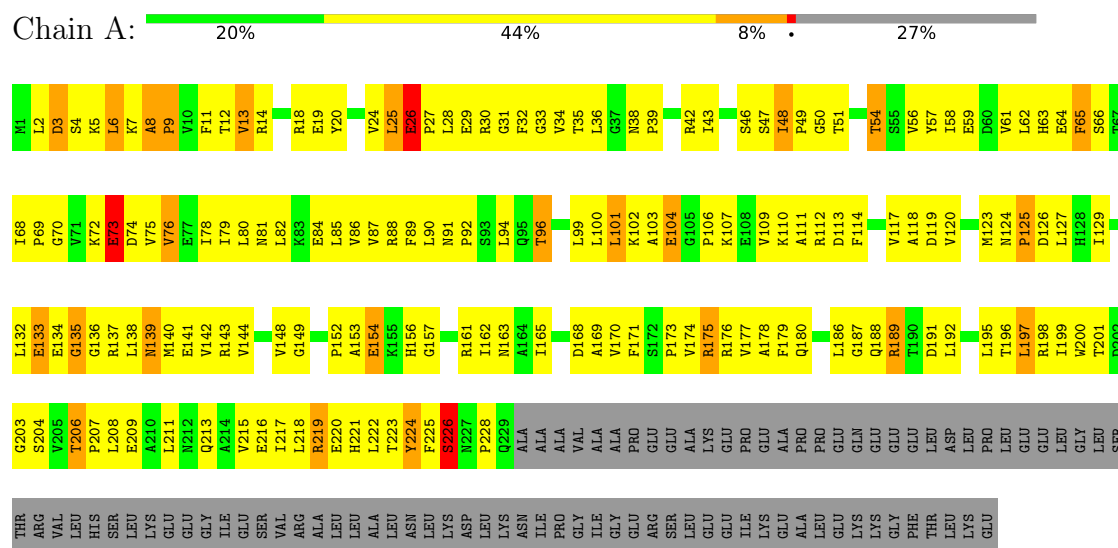
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 8   | D     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 8   | N     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

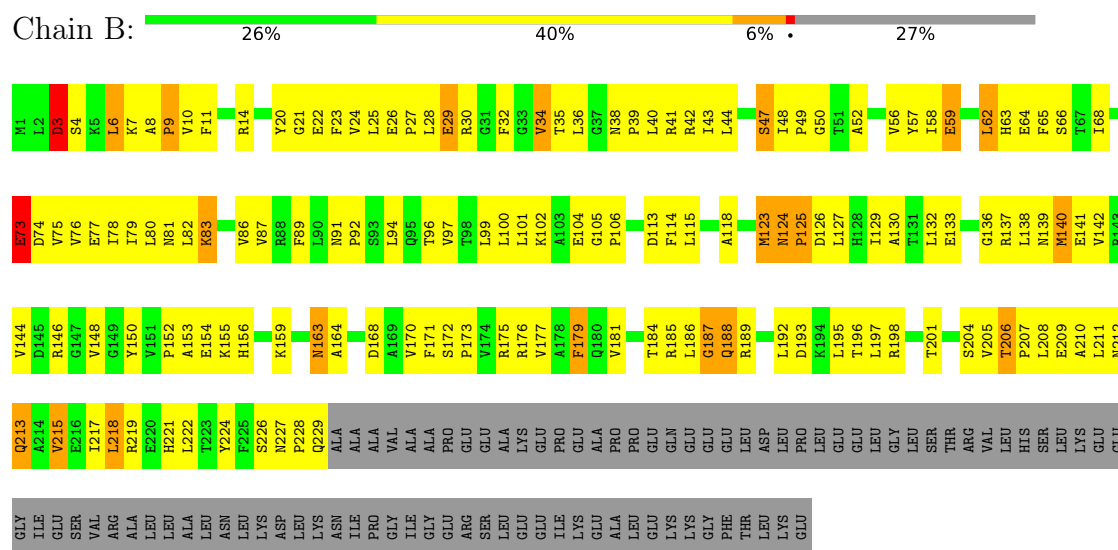
### 3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

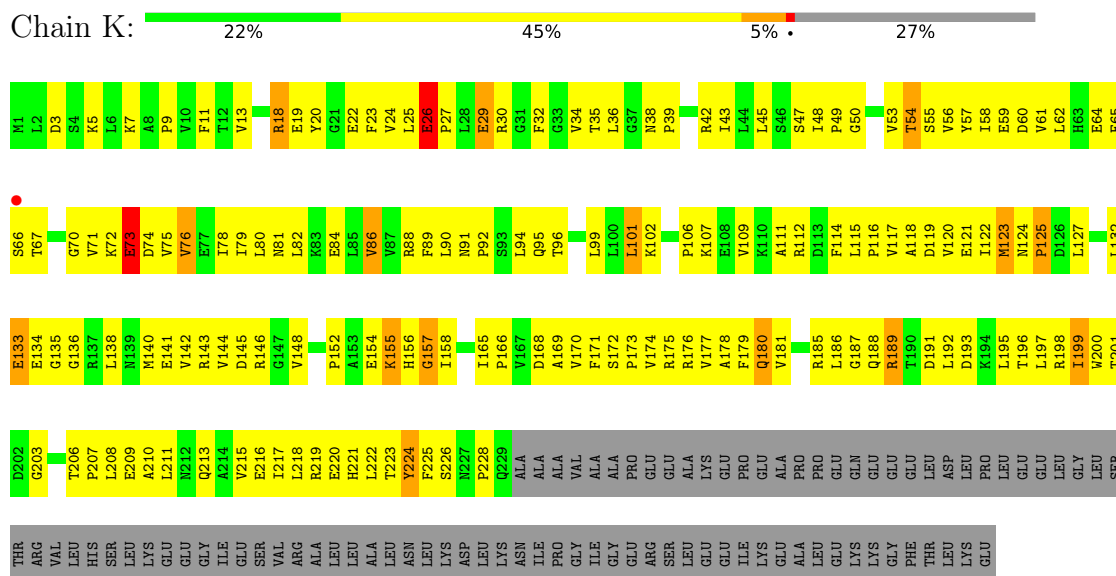
- Molecule 1: DNA-directed RNA polymerase subunit alpha



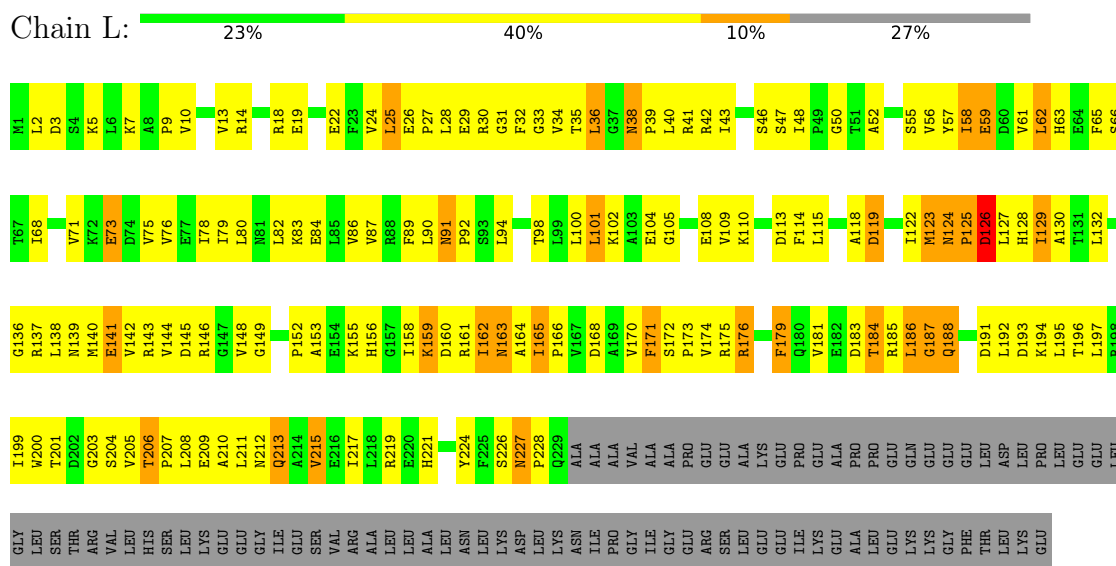
- Molecule 1: DNA-directed RNA polymerase subunit alpha



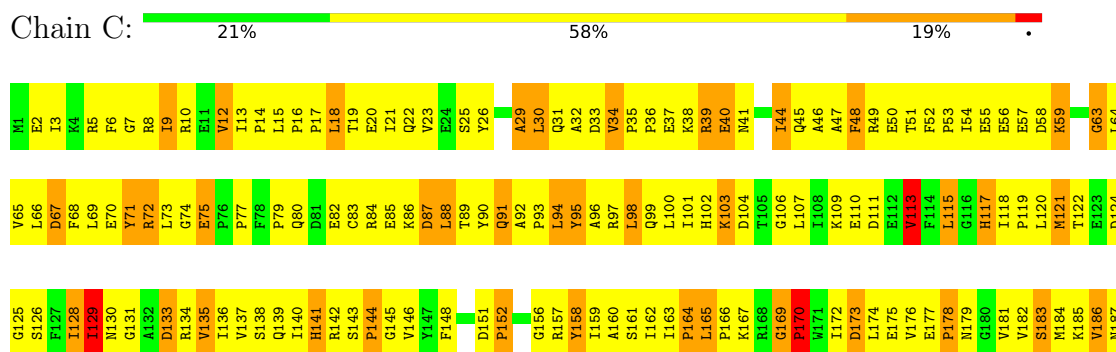
- Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta

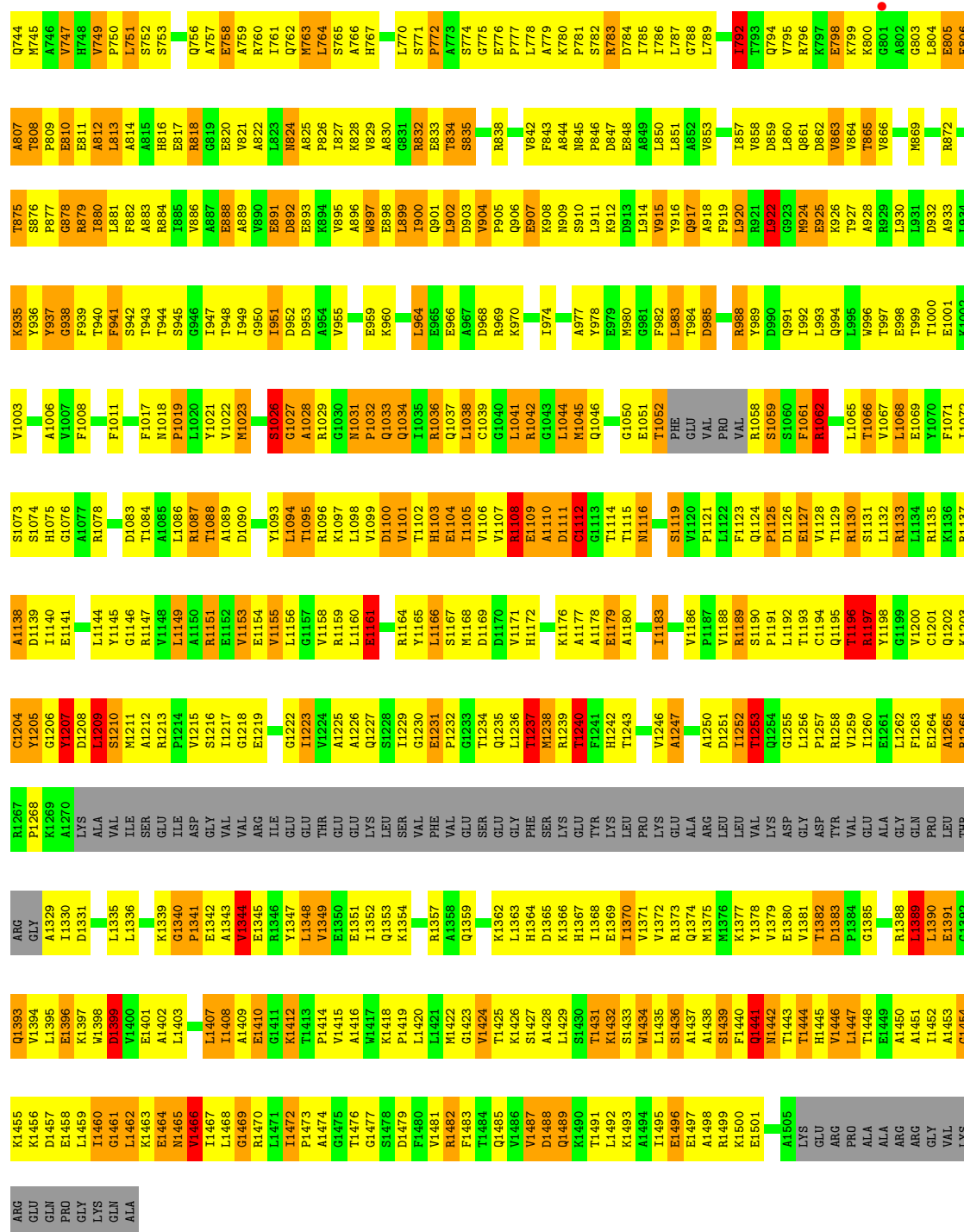


|       |       |       |      |      |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|
| S1084 | P1020 | E960  | A893 | R831 | S760 | D698 | L637 | P577 | E511 | E442 | T314 | K252 | K188 |
| F1085 | L1021 | E961  | G894 | K832 | F761 | F699 | D638 | V578 | R512 | T443 | V317 | A253 | R189 |
| R1086 | G1022 | Q962  | F896 | L833 | K762 | T700 | Q639 | V579 | V513 | P444 | V317 | Y256 | K190 |
| V1087 | L963  | Q963  | F896 | Q834 | G763 | T701 | Q639 | M580 | V514 |      |      | Y256 | F191 |
| L1088 | L1023 | Q964  | L897 | G835 | E764 | S702 | P641 | T581 | A515 | L451 | H320 | Y258 | L193 |
| V1089 | A1025 | E965  | G898 | G836 | S765 | I703 | R642 | G582 | R516 | T453 | E321 | G259 | V194 |
| K1090 | Q1026 | L966  | Q899 | D837 | E766 | H704 | V643 | L583 | R517 |      | V322 | L260 | L195 |
| E1091 | F1027 | L967  | R900 | K838 | P767 | I705 | V644 | E584 | K518 | S454 | D323 | L260 | L196 |
| L1092 | G1028 | L968  | Y901 | L839 | T768 | E706 | V645 | E585 | G519 | L455 | V322 |      |      |
| Q1093 | Q1029 | Q969  | I902 | A840 | P769 | R707 | Q646 | R586 | E520 | A456 | D324 |      |      |
| A1094 | G1030 | G970  | S903 | R841 | E770 | Y708 | Q647 | V587 | P521 | A457 | I325 |      |      |
| L1095 | R1031 | K971  | P904 | R842 | E771 | E709 | R648 | V588 | I522 | Y458 | D326 |      |      |
| A1096 | F1032 | R972  | I905 | R843 | R772 | I710 | V649 | R589 | I523 | A459 | H327 |      |      |
| L1097 | G1033 | V973  | P906 |      |      |      | R650 | D590 | V524 | R460 | L328 |      |      |
| V1098 | E1034 | L974  | D907 | K946 | S776 | R713 | R651 | S525 | S525 | V461 | G329 |      |      |
| V1099 | M1035 | Y975  | G908 | G847 | E780 | R714 | D652 | L592 | P526 | D462 | G330 |      |      |
| Q1100 | O1036 | D976  |      |      |      |      | D653 | A593 | F531 | E463 | R331 |      |      |
| T1101 | V1037 | G977  | E911 | A850 | R783 | L717 | L654 | A594 | F531 | L464 | R332 |      |      |
| L1102 | W1038 | R978  | P912 | K851 | D784 | G718 | L655 | L595 | M532 | G465 | I333 |      |      |
| D1103 | A1039 | T979  |      | L852 | V785 | P719 | L656 | V596 | D533 | F466 | R334 |      |      |
| E1104 | L980  | G980  | L918 | L853 | D787 | R721 | D657 | A597 | L401 | R468 | T335 |      |      |
| K1105 | E981  | P982  | A919 | P854 | D787 | R722 | D658 | E598 | S402 | T469 | V336 |      |      |
| D1106 | A1042 | P982  | Q920 | V855 | T788 | I722 |      | E599 | S403 | Y275 | G337 |      |      |
| N1107 | Y1043 | I983  | A921 | E856 | T788 | T723 |      | D600 | R405 | P470 | E338 |      |      |
| P1108 | G1044 | E984  | F922 | D857 | S789 | R724 | A667 | V606 | L404 | Y471 | L339 |      |      |
| V1109 | A1045 | G985  | E923 | R858 | L790 | D725 | L668 | D607 | R405 | R472 | K340 |      |      |
| D1110 | A1046 | P986  | V924 | P859 | T726 | I726 | Q670 | R609 | R406 | R473 | T341 |      |      |
| I1111 | H1047 | P987  | Y925 | H860 | R792 | F727 | L676 | R610 | R408 | V474 | D342 |      |      |
| E1112 | T1048 | V988  | F926 | L861 | T793 | R728 | L666 | R605 | R409 |      | Q343 |      |      |
| L1113 | L1049 | V989  | G927 | P862 | P794 | L729 | A667 | V606 | I410 | V478 | F344 |      |      |
| G1114 | O1050 | G990  | K928 | D863 | G795 | S730 | L668 | D607 | R409 | V479 | R345 |      |      |
| L1115 |       | Q991  | R929 | G864 | E796 | E732 | Q670 | R609 | A412 | T480 | R346 |      |      |
| A1116 |       | M992  | K930 | T865 | G797 | A732 | Q671 | R610 | L413 | D481 | G347 |      |      |
|       |       | F993  | G931 | P866 | T798 | A733 | N671 | R610 | G414 | E482 | L348 |      |      |
|       |       | I994  | E932 | V867 | L799 | L734 | L672 | I611 | P415 | V483 | A349 |      |      |
|       |       | M995  | G933 | D868 | V800 | R735 | L673 | V612 | G416 | V484 | R350 |      |      |
|       |       | K996  |      | V869 | V801 | D735 | V674 | V613 | G417 | Y485 | L351 |      |      |
|       |       | L997  | V936 | L870 | R802 | L737 | A675 | R614 | L418 | M486 | A352 |      |      |
|       |       | Y998  | D937 | L871 | T803 | D738 | L676 | V615 | T419 | T487 | R353 |      |      |
|       |       | H999  | K938 | N872 | G804 | E739 | E616 | A555 | R420 | A488 | G354 |      |      |
|       |       | M1000 | R939 | P873 | R805 | E740 | P678 | D617 | E421 | T489 | V355 |      |      |
|       |       | V1001 | E940 | L874 |      | G741 | F679 | G618 | R490 | E490 | R356 |      |      |
|       |       | R1063 | V941 | G875 | P811 | V742 | D680 | R619 | E491 | E491 | E357 |      |      |
|       |       | D1003 | E942 | V876 | G812 | V743 | G681 | L620 | G423 | D492 | R358 |      |      |
|       |       | K1004 | V943 | P877 | V613 | R744 | V682 | V621 | G424 | R493 | M359 |      |      |
|       |       | M1005 | L944 | S878 | E814 | I745 | N683 | E622 | F425 |      |      |      |      |
|       |       | A1007 | R946 | R879 | L815 | G746 | E684 | P624 | D426 |      |      |      |      |
|       |       | R1008 | A947 | N880 | K816 | A747 | E685 | P624 |      |      |      |      |      |
|       |       | T1009 | E948 | N881 | P817 | E748 | D686 | L625 | N563 | Q498 | V430 |      |      |
|       |       | T1010 | K949 | L882 | G818 | V749 | A687 | R626 | M564 | A499 | T368 |      |      |
|       |       | G1011 | L950 | Q884 | V619 | K750 | L688 | R627 | O565 | N500 | P369 |      |      |
|       |       | P1012 | V953 | L885 | R820 | P751 | V689 | F628 | Q567 |      |      |      |      |
|       |       | Y1013 |      | L886 | R824 | G752 | L690 | V629 | P570 |      |      |      |      |
|       |       | S1014 | T954 | E887 | G826 | D753 | S691 | R630 | L503 |      |      |      |      |
|       |       | L1015 | V826 | T883 | Y826 | I754 | E692 | R631 |      |      |      |      |      |
|       |       | I1016 | G956 | T889 | V827 | V755 | E693 | N632 |      |      |      |      |      |
|       |       | Q1017 | K957 | H889 | V827 | V756 | L694 | Q633 |      |      |      |      |      |
|       |       | T1018 | T958 | L890 | A828 | G757 | L695 | G634 |      |      |      |      |      |
|       |       | P1082 | G891 | G891 | R829 | R758 | K696 | T635 |      |      |      |      |      |
|       |       | E1083 | P959 | L892 | K830 | T759 | R697 | A636 |      |      |      |      |      |

- Molecule 2: DNA-directed RNA polymerase subunit beta





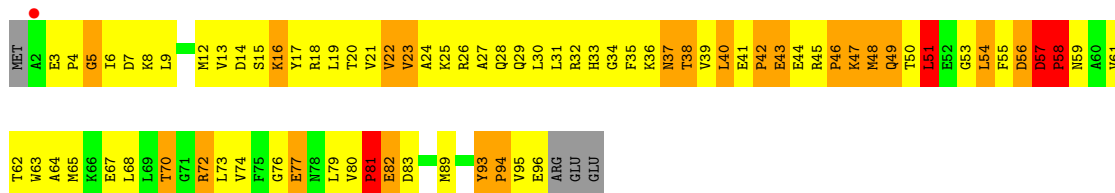
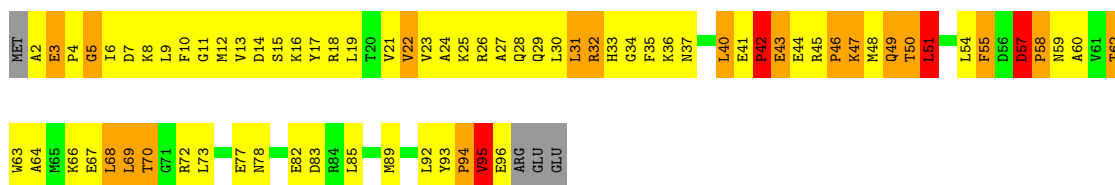


### • Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain N: 18% 49% 16% 15%

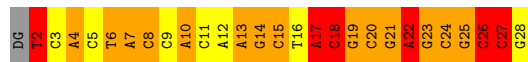


|       |      |      |      |      |      |      |      |      |      |      |     |     |      |      |      |
|-------|------|------|------|------|------|------|------|------|------|------|-----|-----|------|------|------|
| E1001 | L934 | G870 | P809 | V749 | E686 | V623 | G561 | A501 | R441 | PRO  | MET | ALA | G194 | V126 | K64  |
| G1007 | K935 | K871 | E810 | P750 | V687 | D624 | A562 | F502 | R442 | GLU  | PRO | GLU | G199 | L127 | K65  |
| F1008 | Y936 | R872 | E811 | L751 | W688 | Y625 | P563 | L503 | V443 | GLU  | ARG | GLU | V196 | F128 | Q66  |
| K1009 | Y937 | L873 | A812 | S752 | D689 | S626 | E564 | D504 | V444 | GLN  | GLN | GLU | F196 | F129 | R67  |
| G1010 | G938 | E874 | L813 | S753 | A690 | G627 | I565 | S505 | V445 | VAL  | VAL | GLY | S197 | F68  | F68  |
| N1010 | F939 | T875 | A814 | F754 | L691 | R628 | I566 | G506 | R445 | ILE  | ARG | VAL | R198 | K131 | E69  |
| F1011 | T940 | S876 | A815 | A755 | E692 | S693 | I567 | N507 | V446 | ALA  | ALA | VAL | L199 | Y132 |      |
| E1012 | P941 | P877 | H816 | Q756 | E693 | V630 | R568 | R508 | V447 | GLU  | ALA | GLU | D200 | I133 | V72  |
| E1013 | S942 | G878 | E817 | A757 | V694 | I631 | R569 | P509 | E448 | ALA  | GLN | LEU | G201 | V134 | C73  |
| N1014 | T943 | R879 | G819 | E758 | I695 | V632 | E570 | E510 | S449 | GLY  | VAL | GLY | V202 | L135 | E74  |
| Y1015 | T944 | I880 | G819 | A759 | R696 | V633 | K571 | W511 |      | GLY  | GLU | GLU | A203 | D136 | R75  |
| P1016 | S945 | L881 | E820 | R760 | G697 | G634 | B572 | R512 | I452 | VAL  | ALA | LEU | L204 | P137 | C76  |
| F1017 | G946 | F882 | V821 | I761 | K698 |      | R573 | I513 | D453 | VAL  | GLU | GLU | Y205 | G138 | G77  |
| F1018 | T947 | A883 | R821 | Q762 | V699 | L637 | L574 | L514 | A454 | HIS  | GLU | GLU | R206 | G139 | V78  |
| P1019 | T948 | R884 | L823 | M763 | V700 | K638 | Q575 | E515 | R455 | LEU  | GLU | GLY | F207 | A140 | E79  |
| L1020 | T949 | I885 | N824 | L764 | L701 | L639 | E576 | A516 | R456 | LEU  | GLY | ALA | PRO  | I141 | R80  |
| G1021 | G950 | V886 | A825 | S765 | L702 | K640 | A577 | G457 | R457 | GLU  | THR | PHE | ARG  | L142 | T81  |
| Y1022 | P951 | A887 | P826 | A766 | N703 | R641 | V578 | P518 | C457 | PRO  | THR | LEU | ARG  | N143 | K82  |
| M1023 | D952 | E888 | I827 | H767 | R704 | C642 | D579 | W519 | E459 | VAL  | VAL | VAL | VAL  | G144 | S83  |
|       | D953 | A889 | K828 | V768 | A705 | R643 | R586 | L520 | A460 | S392 | TYR | LEU | ARG  | V145 |      |
|       |      | V990 | K828 | L769 | P706 | L644 | L581 | P521 | I461 | I393 | LEU | ARG | VAL  | P146 | V85  |
|       | P957 | E891 | A830 | L770 | T707 | L650 | L582 | P522 | R462 | L394 | THR | ARG | GLU  | V147 | R86  |
|       | E958 | D892 | G831 | S771 | L708 | K646 | D583 | D523 | Q463 | V395 | LEU | GLU | TYR  | E148 | R87  |
|       | E959 | E893 | R832 | P772 | H709 | R647 | N584 | L524 | L464 | V396 | PHE | ASP | VAL  | K149 | Y88  |
|       | K960 | K894 | E833 | A773 | R710 | M648 | G585 | R525 | I465 | K397 | LEU | GLU | LYS  | R150 | R89  |
|       | K961 | V895 | T834 | S774 | L711 | L649 | R586 | P526 | K466 | A398 | GLU | PRO | LYS  | Q151 | M90  |
|       | Q962 | A996 | S835 | G775 | G712 | L650 | R587 | M527 | E467 | R399 | THR | VAL | GLU  | L152 | G91  |
|       | Y963 | W897 | V836 | E776 | L713 | E651 | G588 | W528 | L468 | V400 | THR | ALA | ARG  | L153 | H92  |
|       | L964 | E898 | G837 | P777 | Q714 | L652 | A589 | Q529 | D469 | Y401 | GLU | THR | ALA  | T154 |      |
|       | E965 | L899 | R838 | L778 | A715 | F653 | P590 | W530 | L470 |      | PRO | TYR | GLY  | D155 | L95  |
|       | E966 | I900 | L839 | A779 | F716 | K654 |      | D531 | E471 | D405 | LYS | PHE | LEU  | E156 | A96  |
|       | A967 | Q901 | K840 | K780 | Q717 | P655 | N593 | G532 | A472 | D406 | ASP | LEU | ARG  | E157 | T97  |
|       | D968 | L902 | R841 | P781 | P718 | F656 | P594 | G533 | L473 | V407 | TYR | PRO | LEU  | Y158 | P98  |
|       | R969 | E907 | V842 | S782 | V719 | L657 | G595 | R534 | E474 | E408 | ARG | VAL | LEU  | R159 | A99  |
|       | K970 | K908 | R843 | K783 | L720 | L658 | S596 | F535 | K475 | V409 | VAL | GLY | PRO  | E160 | A100 |
|       | L971 |      | A844 | D784 | V721 | K659 | D597 | A536 | E476 | S410 | GLN | MET | ALA  | L161 | H101 |
|       | L972 |      | N845 | I785 | E722 | K660 | R598 | T537 | L477 | T411 | PRO | THR | ALA  | R162 | I102 |
|       | Q973 |      | P846 | L786 | G723 | M661 | P599 | S538 | L478 | G412 | HIS | PRO | TRP  | Y163 | M103 |
|       | T974 |      | D847 | L787 |      | E662 | L600 | D539 | E479 | D413 | MET | LEU | VAL  | K164 | F104 |
|       | E975 |      | E848 | G788 | Q727 | E663 |      | L540 | M481 | R414 | ASN | VAL | GLU  | K165 | V105 |
|       | Q976 |      | A849 | L789 | L728 | K664 | L603 | N541 | K482 | V415 | VAL | VAL | GLY  | Q166 | D107 |
|       | A977 |      | L850 | Y790 | H729 | G665 | T604 | D542 | R486 | A416 | VAL | HIS | LYS  | E167 |      |
|       |      |      | L851 | Y791 | P730 | I666 | D605 | L543 | P484 | P417 | VAL | GLY | ALA  | V108 |      |
|       |      |      | L852 | L792 | L731 | L667 | L606 | Y544 |      |      | PRO | GLU | TYR  | P109 |      |
|       |      |      | V853 | T793 | V732 | P668 | L607 | R545 | S485 | V420 | GLU | ILE | LYS  | S110 |      |
|       |      |      | A854 | Q794 | C733 | R669 | S608 | R546 | R487 | L421 | GLY | VAL | PRO  | V175 |      |
|       |      |      | H855 | V795 | E734 | V670 | G609 | L547 | R488 | A422 | ALA | GLU | GLY  | D176 |      |
|       |      |      |      | R796 | A735 | K671 | K610 | I548 | R498 | D423 | ARG | LYS | GLU  | A177 |      |
|       |      |      |      | K797 | F736 |      | D611 | N549 | R499 |      | VAL | VAL | ILE  | L178 |      |
|       |      |      | V858 | L798 | F737 | R675 | G612 | R550 | A490 | V427 | GLU | GLN | LEU  | V179 |      |
|       |      |      | D859 | E798 | A738 | H676 | R613 | N551 | K491 |      | ALA | PRO | ALA  | K180 |      |
|       |      |      | L860 | K799 | L736 | H677 | R614 | N552 | A492 |      | GLY | LEU | GLU  | D181 |      |
|       |      |      | Q861 | K900 | D739 | L677 | F614 | R553 | R493 | V431 | ASP | ALA | LEU  | D117 |      |
|       |      |      | V862 | G801 | F740 | E678 | R615 | R553 | R493 |      | ASP | ALA | LEU  | L118 |      |
|       |      |      | V863 | A802 | D741 | R679 | Q616 | L554 | K494 | Y432 | LYS | GLU | PRO  | S119 |      |
|       |      |      | V864 | G803 | G742 | G680 | N617 | K555 | R495 | G433 | ILE | ALA | GLU  | E184 |      |
|       |      |      | T865 | L804 | D743 | R681 | L618 | K566 | L496 | R434 | VAL | LYS | PRO  | V185 |      |
|       |      |      | V866 | E805 | Q744 | D682 | L619 | L557 | S497 | V435 | ALA | GLY | TYR  | V186 |      |
|       |      |      | R867 | F806 | M745 | L683 | G620 | L558 | V498 | E436 | ALA | LEU | LEU  | K187 |      |
|       |      |      | L931 | A807 |      | K684 | K621 | A559 | V499 | V437 | ILE | LEU | PHE  | E122 |      |
|       |      |      | E933 | T808 | H748 | D685 | R622 | Q560 | R500 | D438 | ASP | ARG |      | E123 |      |
|       |      |      |      |      |      |      |      |      |      |      |     |     |      |      | Q125 |

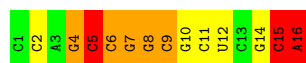




- Molecule 5: DNA (28-MER)



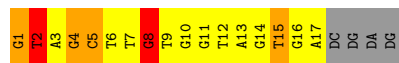
- Molecule 6: RNA (5'-R(P\*CP\*CP\*AP\*GP\*CP\*CP\*GP\*GP\*CP\*GP\*CP\*UP\*CP\*GP\*CP\*A)-3')



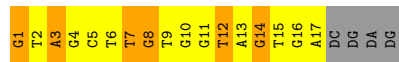
- Molecule 6: RNA (5'-R(P\*CP\*CP\*AP\*GP\*CP\*CP\*GP\*GP\*CP\*GP\*CP\*UP\*CP\*GP\*CP\*A)-3')



- Molecule 7: DNA (5'-D(P\*GP\*TP\*AP\*GP\*CP\*TP\*TP\*GP\*TP\*GP\*GP\*TP\*AP\*GP\*TP\*GP\*AP\*CP\*GP\*AP\*G)-3')



- Molecule 7: DNA (5'-D(P\*GP\*TP\*AP\*GP\*CP\*TP\*TP\*GP\*TP\*GP\*GP\*TP\*AP\*GP\*TP\*GP\*AP\*CP\*GP\*AP\*G)-3')



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 41                                                        | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 155.98Å 155.98Å 495.00Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 44.15 – 4.31<br>44.15 – 4.31                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (44.15-4.31)<br>99.4 (44.15-4.31)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.17                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.82 (at 4.28Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.9_1692)                            | Depositor        |
| R, $R_{free}$                                                           | 0.281 , 0.311<br>0.284 , 0.314                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3821 reflections (1.96%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 106.1                                                       | Xtriage          |
| Anisotropy                                                              | 0.046                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.10 , 156.3                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.30$ , $\langle L^2 \rangle = 0.14$ | Xtriage          |
| Estimated twinning fraction                                             | 0.499 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 48166                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 250.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.51         | 0/1838         | 1.09        | 14/2498 (0.6%)   |
| 1   | B     | 0.53         | 0/1838         | 1.07        | 7/2498 (0.3%)    |
| 1   | K     | 0.57         | 1/1838 (0.1%)  | 1.09        | 10/2498 (0.4%)   |
| 1   | L     | 0.53         | 0/1838         | 1.10        | 15/2498 (0.6%)   |
| 2   | C     | 0.63         | 1/8997 (0.0%)  | 1.25        | 110/12164 (0.9%) |
| 2   | M     | 0.61         | 0/8997         | 1.23        | 93/12164 (0.8%)  |
| 3   | D     | 0.65         | 2/9249 (0.0%)  | 1.30        | 126/12482 (1.0%) |
| 3   | N     | 0.66         | 0/10344        | 1.27        | 118/13968 (0.8%) |
| 4   | E     | 0.63         | 0/784          | 1.45        | 11/1057 (1.0%)   |
| 4   | O     | 0.57         | 0/784          | 1.30        | 9/1057 (0.9%)    |
| 5   | G     | 0.56         | 0/614          | 1.46        | 14/943 (1.5%)    |
| 5   | X     | 0.53         | 0/614          | 1.52        | 17/943 (1.8%)    |
| 6   | H     | 0.75         | 0/378          | 1.34        | 5/585 (0.9%)     |
| 6   | Y     | 0.75         | 0/353          | 1.17        | 4/546 (0.7%)     |
| 7   | I     | 0.49         | 0/400          | 1.21        | 3/616 (0.5%)     |
| 7   | Z     | 0.46         | 0/400          | 1.04        | 2/616 (0.3%)     |
| All | All   | 0.62         | 4/49266 (0.0%) | 1.25        | 558/67133 (0.8%) |

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 |
|-----|-------|---------------------|---------------------|
| 5   | G     | 0                   | 10                  |
| 5   | X     | 0                   | 11                  |
| 6   | H     | 0                   | 4                   |
| 6   | Y     | 0                   | 5                   |
| 7   | I     | 0                   | 6                   |
| 7   | Z     | 0                   | 4                   |
| All | All   | 0                   | 40                  |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | D     | 1246 | VAL  | CA-CB | 5.50  | 1.61        | 1.54     |
| 3   | D     | 726  | ILE  | CA-CB | -5.21 | 1.48        | 1.54     |
| 1   | K     | 76   | VAL  | CA-CB | -5.04 | 1.48        | 1.54     |
| 2   | C     | 702  | SER  | CA-C  | -5.01 | 1.46        | 1.52     |

All (558) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 4   | E     | 93   | TYR  | CA-C-N      | 17.64  | 137.32      | 118.97   |
| 4   | E     | 93   | TYR  | C-N-CA      | 17.64  | 137.32      | 118.97   |
| 3   | D     | 1247 | ALA  | N-CA-C      | -16.96 | 92.82       | 111.14   |
| 3   | N     | 1209 | LEU  | N-CA-C      | -15.19 | 85.96       | 109.96   |
| 3   | D     | 1209 | LEU  | N-CA-C      | -15.05 | 86.17       | 109.96   |
| 3   | N     | 621  | LYS  | N-CA-C      | 12.93  | 130.08      | 114.04   |
| 3   | D     | 621  | LYS  | N-CA-C      | 12.93  | 130.07      | 114.04   |
| 2   | C     | 177  | GLU  | CA-C-N      | 11.98  | 134.82      | 119.84   |
| 2   | C     | 177  | GLU  | C-N-CA      | 11.98  | 134.82      | 119.84   |
| 6   | H     | 5    | C    | N1-C1'-C2'  | -11.73 | 94.41       | 112.00   |
| 3   | N     | 143  | ASN  | N-CA-C      | -11.68 | 101.31      | 114.62   |
| 2   | C     | 728  | HIS  | N-CA-C      | 11.58  | 128.39      | 114.04   |
| 3   | D     | 508  | ARG  | CA-C-N      | 11.30  | 131.09      | 119.56   |
| 3   | D     | 508  | ARG  | C-N-CA      | 11.30  | 131.09      | 119.56   |
| 4   | O     | 93   | TYR  | CA-C-N      | 11.08  | 130.68      | 119.82   |
| 4   | O     | 93   | TYR  | C-N-CA      | 11.08  | 130.68      | 119.82   |
| 2   | M     | 728  | HIS  | N-CA-C      | 11.02  | 128.52      | 114.31   |
| 5   | X     | 26   | DC   | C2'-C3'-O3' | -10.92 | 95.12       | 111.50   |
| 3   | N     | 517  | VAL  | N-CA-C      | 10.88  | 119.24      | 107.60   |
| 3   | N     | 729  | HIS  | CA-C-N      | 10.85  | 133.40      | 119.84   |
| 3   | N     | 729  | HIS  | C-N-CA      | 10.85  | 133.40      | 119.84   |
| 3   | N     | 1127 | GLU  | N-CA-C      | -10.84 | 99.06       | 114.12   |
| 3   | N     | 1383 | ASP  | CA-C-N      | 10.73  | 131.40      | 119.92   |
| 3   | N     | 1383 | ASP  | C-N-CA      | 10.73  | 131.40      | 119.92   |
| 2   | M     | 177  | GLU  | CA-C-N      | 10.63  | 133.12      | 119.84   |
| 2   | M     | 177  | GLU  | C-N-CA      | 10.63  | 133.12      | 119.84   |
| 2   | C     | 318  | PRO  | N-CA-C      | -10.56 | 100.66      | 113.86   |
| 3   | N     | 1110 | ALA  | N-CA-C      | -10.50 | 90.08       | 108.13   |
| 3   | D     | 1110 | ALA  | N-CA-C      | -10.39 | 90.26       | 108.13   |
| 2   | M     | 729  | LEU  | N-CA-C      | 10.37  | 126.80      | 111.34   |
| 2   | M     | 1091 | GLU  | N-CA-C      | -10.31 | 100.04      | 111.07   |
| 2   | C     | 542  | VAL  | N-CA-C      | -10.30 | 100.85      | 110.53   |
| 4   | E     | 49   | GLN  | N-CA-C      | 10.19  | 128.90      | 113.61   |
| 2   | M     | 726  | ILE  | CA-C-N      | 10.06  | 132.42      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | M     | 726  | ILE  | C-N-CA      | 10.06 | 132.42      | 119.84   |
| 3   | N     | 508  | ARG  | CA-C-N      | 10.00 | 130.27      | 119.87   |
| 3   | N     | 508  | ARG  | C-N-CA      | 10.00 | 130.27      | 119.87   |
| 3   | N     | 1109 | GLU  | N-CA-C      | 9.83  | 120.91      | 107.73   |
| 2   | C     | 1091 | GLU  | N-CA-C      | -9.72 | 100.67      | 111.07   |
| 3   | D     | 143  | ASN  | N-CA-C      | -9.71 | 102.52      | 114.75   |
| 3   | D     | 1252 | ILE  | N-CA-C      | 9.63  | 120.11      | 106.53   |
| 4   | O     | 51   | LEU  | N-CA-C      | -9.61 | 94.86       | 107.73   |
| 5   | G     | 21   | DG   | C2'-C3'-O3' | -9.57 | 97.15       | 111.50   |
| 2   | M     | 165  | LEU  | N-CA-C      | -9.40 | 99.32       | 110.13   |
| 5   | X     | 21   | DG   | C2'-C3'-O3' | -9.36 | 97.46       | 111.50   |
| 3   | N     | 615  | ARG  | N-CA-C      | -9.34 | 101.10      | 111.28   |
| 4   | O     | 49   | GLN  | N-CA-C      | 9.29  | 128.57      | 113.89   |
| 3   | D     | 1498 | ALA  | N-CA-C      | -9.19 | 101.49      | 112.89   |
| 4   | E     | 51   | LEU  | N-CA-C      | -9.19 | 95.42       | 107.73   |
| 3   | D     | 81   | THR  | N-CA-C      | -9.16 | 91.28       | 110.80   |
| 2   | M     | 318  | PRO  | N-CA-C      | -9.08 | 102.51      | 113.86   |
| 2   | C     | 726  | ILE  | CA-C-N      | 9.03  | 131.13      | 119.84   |
| 2   | C     | 726  | ILE  | C-N-CA      | 9.03  | 131.13      | 119.84   |
| 2   | C     | 266  | ARG  | N-CA-C      | -9.01 | 102.43      | 113.15   |
| 2   | M     | 1111 | ILE  | N-CA-C      | -8.82 | 102.13      | 110.42   |
| 2   | C     | 279  | GLU  | N-CA-C      | 8.81  | 120.81      | 111.03   |
| 3   | D     | 1109 | GLU  | N-CA-C      | 8.73  | 120.17      | 108.38   |
| 5   | X     | 18   | DC   | C4'-C3'-O3' | 8.72  | 123.08      | 110.00   |
| 3   | N     | 922  | LEU  | N-CA-C      | 8.66  | 122.35      | 111.69   |
| 3   | N     | 80   | VAL  | N-CA-C      | 8.66  | 122.83      | 108.81   |
| 3   | D     | 142  | LEU  | N-CA-C      | 8.49  | 120.85      | 110.41   |
| 2   | M     | 266  | ARG  | N-CA-C      | -8.47 | 103.07      | 113.15   |
| 2   | M     | 32   | ALA  | N-CA-C      | 8.39  | 121.49      | 111.33   |
| 1   | L     | 172  | SER  | CA-C-N      | 8.31  | 128.51      | 119.87   |
| 1   | L     | 172  | SER  | C-N-CA      | 8.31  | 128.51      | 119.87   |
| 3   | N     | 525  | ARG  | CA-C-N      | 8.31  | 130.22      | 119.84   |
| 3   | N     | 525  | ARG  | C-N-CA      | 8.31  | 130.22      | 119.84   |
| 4   | O     | 94   | PRO  | N-CA-C      | 8.30  | 124.69      | 113.98   |
| 2   | M     | 591  | SER  | N-CA-C      | -8.29 | 99.84       | 110.53   |
| 3   | D     | 811  | GLU  | N-CA-C      | -8.26 | 103.20      | 113.28   |
| 2   | M     | 301  | GLU  | N-CA-C      | -8.22 | 103.76      | 113.21   |
| 3   | D     | 525  | ARG  | CA-C-N      | 8.20  | 128.25      | 119.89   |
| 3   | D     | 525  | ARG  | C-N-CA      | 8.20  | 128.25      | 119.89   |
| 3   | D     | 1383 | ASP  | CA-C-N      | 8.15  | 128.64      | 119.92   |
| 3   | D     | 1383 | ASP  | C-N-CA      | 8.15  | 128.64      | 119.92   |
| 2   | M     | 275  | TYR  | N-CA-C      | -8.13 | 102.49      | 111.36   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | N     | 1260 | ILE  | N-CA-C      | -8.12 | 103.35      | 110.74   |
| 2   | C     | 32   | ALA  | N-CA-C      | 8.11  | 121.03      | 111.71   |
| 2   | M     | 118  | ILE  | CA-C-N      | 8.09  | 128.14      | 119.89   |
| 2   | M     | 118  | ILE  | C-N-CA      | 8.09  | 128.14      | 119.89   |
| 3   | N     | 753  | SER  | N-CA-C      | -8.06 | 102.71      | 112.54   |
| 2   | C     | 591  | SER  | N-CA-C      | -8.00 | 100.21      | 110.53   |
| 3   | N     | 1206 | GLY  | N-CA-C      | 7.97  | 121.34      | 110.58   |
| 3   | N     | 131  | LYS  | N-CA-C      | 7.94  | 124.64      | 107.49   |
| 3   | N     | 622  | ARG  | N-CA-C      | 7.93  | 121.51      | 107.80   |
| 3   | D     | 1101 | VAL  | N-CA-C      | 7.91  | 118.31      | 111.90   |
| 3   | N     | 141  | ILE  | N-CA-C      | 7.89  | 119.13      | 110.21   |
| 3   | D     | 622  | ARG  | N-CA-C      | 7.89  | 121.45      | 107.80   |
| 2   | M     | 12   | VAL  | N-CA-C      | 7.89  | 118.64      | 110.36   |
| 3   | D     | 517  | VAL  | N-CA-C      | 7.87  | 116.70      | 107.73   |
| 2   | C     | 729  | LEU  | N-CA-C      | 7.87  | 127.56      | 110.80   |
| 3   | D     | 753  | SER  | N-CA-C      | -7.86 | 102.70      | 111.82   |
| 5   | G     | 27   | DC   | C2'-C3'-O3' | -7.85 | 99.73       | 111.50   |
| 2   | M     | 63   | GLY  | N-CA-C      | -7.83 | 104.21      | 115.64   |
| 3   | N     | 1034 | GLN  | N-CA-C      | 7.82  | 119.89      | 111.36   |
| 5   | G     | 18   | DC   | C4'-C3'-O3' | 7.81  | 121.71      | 110.00   |
| 2   | M     | 542  | VAL  | N-CA-C      | -7.79 | 102.74      | 110.30   |
| 2   | M     | 858  | MET  | CA-C-N      | 7.71  | 129.48      | 119.84   |
| 2   | M     | 858  | MET  | C-N-CA      | 7.71  | 129.48      | 119.84   |
| 4   | E     | 94   | PRO  | N-CA-C      | 7.68  | 124.45      | 113.47   |
| 3   | N     | 812  | ALA  | N-CA-C      | -7.67 | 103.92      | 113.28   |
| 3   | D     | 730  | PRO  | N-CA-C      | 7.65  | 124.17      | 113.53   |
| 3   | D     | 1331 | ASP  | CA-C-N      | 7.62  | 127.16      | 119.24   |
| 3   | D     | 1331 | ASP  | C-N-CA      | 7.62  | 127.16      | 119.24   |
| 5   | X     | 24   | DC   | C2'-C3'-O3' | -7.62 | 100.07      | 111.50   |
| 3   | D     | 80   | VAL  | N-CA-C      | 7.59  | 119.28      | 108.42   |
| 2   | C     | 1081 | VAL  | N-CA-C      | 7.57  | 116.37      | 108.95   |
| 5   | X     | 7    | DA   | C4'-C3'-O3' | 7.55  | 121.32      | 110.00   |
| 3   | D     | 798  | GLU  | N-CA-C      | 7.53  | 120.91      | 108.48   |
| 3   | N     | 811  | GLU  | N-CA-C      | -7.49 | 104.15      | 113.28   |
| 2   | C     | 1078 | GLU  | CA-C-N      | 7.48  | 129.19      | 119.84   |
| 2   | C     | 1078 | GLU  | C-N-CA      | 7.48  | 129.19      | 119.84   |
| 6   | H     | 15   | C    | C5'-C4'-C3' | -7.47 | 104.79      | 116.00   |
| 3   | N     | 490  | ALA  | N-CA-C      | -7.46 | 101.62      | 111.24   |
| 3   | N     | 1399 | ASP  | N-CA-C      | -7.45 | 103.17      | 111.82   |
| 5   | X     | 25   | DG   | C2'-C3'-O3' | -7.43 | 100.35      | 111.50   |
| 3   | N     | 1340 | GLY  | CA-C-N      | 7.43  | 129.13      | 119.84   |
| 3   | N     | 1340 | GLY  | C-N-CA      | 7.43  | 129.13      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | D     | 1340 | GLY  | CA-C-N      | 7.42  | 129.12      | 119.84   |
| 3   | D     | 1340 | GLY  | C-N-CA      | 7.42  | 129.12      | 119.84   |
| 3   | D     | 1027 | GLY  | N-CA-C      | -7.41 | 104.50      | 113.99   |
| 4   | E     | 50   | THR  | N-CA-C      | -7.40 | 103.52      | 112.54   |
| 2   | M     | 1078 | GLU  | CA-C-N      | 7.39  | 129.08      | 119.84   |
| 2   | M     | 1078 | GLU  | C-N-CA      | 7.39  | 129.08      | 119.84   |
| 2   | M     | 260  | LEU  | N-CA-C      | 7.34  | 122.80      | 113.55   |
| 6   | Y     | 5    | C    | N1-C1'-C2'  | -7.32 | 101.02      | 112.00   |
| 2   | C     | 301  | GLU  | N-CA-C      | -7.32 | 104.80      | 113.21   |
| 3   | D     | 1112 | CYS  | N-CA-C      | -7.30 | 99.35       | 110.30   |
| 4   | O     | 50   | THR  | N-CA-C      | -7.30 | 103.64      | 112.54   |
| 3   | N     | 832  | ARG  | N-CA-C      | 7.29  | 118.88      | 111.07   |
| 1   | L     | 227  | ASN  | N-CA-C      | 7.28  | 119.36      | 109.24   |
| 3   | N     | 81   | THR  | N-CA-C      | -7.27 | 95.31       | 110.80   |
| 5   | G     | 20   | DC   | C5'-C4'-C3' | -7.27 | 103.99      | 114.90   |
| 3   | N     | 1469 | GLY  | N-CA-C      | -7.25 | 105.23      | 115.30   |
| 5   | G     | 18   | DC   | C2'-C3'-O3' | 7.23  | 122.34      | 111.50   |
| 3   | N     | 1236 | LEU  | N-CA-C      | 7.22  | 120.35      | 109.95   |
| 3   | D     | 118  | LEU  | N-CA-C      | -7.19 | 98.43       | 109.14   |
| 2   | C     | 275  | TYR  | N-CA-C      | -7.19 | 103.48      | 111.82   |
| 2   | M     | 687  | ALA  | N-CA-C      | -7.17 | 100.88      | 110.55   |
| 3   | D     | 108  | VAL  | CA-C-N      | -7.14 | 110.92      | 119.84   |
| 3   | D     | 108  | VAL  | C-N-CA      | -7.14 | 110.92      | 119.84   |
| 3   | N     | 1393 | GLN  | N-CA-C      | 7.12  | 119.90      | 109.07   |
| 2   | C     | 547  | ILE  | CA-C-N      | 7.11  | 128.73      | 119.84   |
| 2   | C     | 547  | ILE  | C-N-CA      | 7.11  | 128.73      | 119.84   |
| 2   | C     | 373  | VAL  | N-CA-C      | 7.08  | 119.26      | 108.71   |
| 2   | C     | 302  | VAL  | CB-CA-C     | -7.07 | 105.70      | 111.71   |
| 3   | N     | 1107 | VAL  | CB-CA-C     | -7.06 | 105.31      | 113.22   |
| 3   | D     | 592  | THR  | N-CA-C      | -7.04 | 99.86       | 110.28   |
| 3   | D     | 528  | VAL  | N-CA-C      | 7.02  | 119.26      | 109.29   |
| 1   | B     | 6    | LEU  | N-CA-C      | -7.01 | 103.65      | 111.71   |
| 2   | C     | 12   | VAL  | N-CA-C      | 7.01  | 117.72      | 110.36   |
| 2   | C     | 260  | LEU  | N-CA-C      | 7.01  | 122.38      | 113.55   |
| 2   | C     | 481  | ASP  | N-CA-C      | -7.00 | 105.09      | 112.93   |
| 3   | D     | 1399 | ASP  | N-CA-C      | -7.00 | 104.00      | 112.54   |
| 2   | M     | 1081 | VAL  | N-CA-C      | 7.00  | 115.81      | 108.95   |
| 2   | M     | 730  | SER  | N-CA-C      | 6.98  | 120.02      | 109.41   |
| 1   | A     | 59   | GLU  | N-CA-C      | 6.97  | 119.52      | 111.02   |
| 5   | G     | 18   | DC   | C5'-C4'-C3' | -6.96 | 104.47      | 114.90   |
| 3   | D     | 1460 | ILE  | N-CA-C      | -6.95 | 98.11       | 108.12   |
| 3   | N     | 1107 | VAL  | N-CA-C      | 6.95  | 113.64      | 106.21   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | C     | 1095 | LEU  | N-CA-C      | -6.93 | 100.22      | 110.48   |
| 7   | I     | 1    | DG   | O5'-P-OP1   | -6.92 | 88.24       | 109.00   |
| 5   | G     | 22   | DA   | C2'-C3'-O3' | -6.92 | 101.13      | 111.50   |
| 1   | A     | 76   | VAL  | N-CA-C      | 6.91  | 117.67      | 110.62   |
| 2   | M     | 731  | GLU  | N-CA-C      | -6.90 | 104.89      | 113.38   |
| 3   | N     | 1126 | ASP  | N-CA-C      | 6.89  | 120.57      | 107.75   |
| 5   | G     | 23   | DG   | C2'-C3'-O3' | -6.88 | 101.19      | 111.50   |
| 2   | C     | 319  | GLY  | N-CA-C      | -6.87 | 100.67      | 110.63   |
| 3   | N     | 159  | ARG  | N-CA-C      | -6.87 | 103.72      | 111.07   |
| 2   | C     | 442  | GLU  | N-CA-C      | 6.84  | 119.58      | 111.71   |
| 2   | C     | 304  | LEU  | CA-C-N      | 6.81  | 126.77      | 119.28   |
| 2   | C     | 304  | LEU  | C-N-CA      | 6.81  | 126.77      | 119.28   |
| 2   | M     | 481  | ASP  | N-CA-C      | -6.81 | 105.30      | 112.93   |
| 2   | M     | 310  | LEU  | N-CA-C      | -6.80 | 103.80      | 111.07   |
| 7   | I     | 2    | DT   | C5'-C4'-C3' | -6.79 | 104.72      | 114.90   |
| 3   | N     | 448  | GLU  | N-CA-C      | 6.77  | 119.50      | 111.71   |
| 2   | C     | 265  | ARG  | N-CA-C      | 6.76  | 120.53      | 109.24   |
| 5   | G     | 2    | DT   | C4'-C3'-O3' | 6.75  | 120.12      | 110.00   |
| 2   | C     | 730  | SER  | N-CA-C      | 6.75  | 119.66      | 109.41   |
| 2   | M     | 373  | VAL  | N-CA-C      | 6.75  | 118.76      | 108.71   |
| 2   | C     | 393  | GLN  | N-CA-C      | 6.73  | 119.64      | 109.41   |
| 3   | D     | 1393 | GLN  | N-CA-C      | 6.73  | 119.30      | 109.07   |
| 3   | D     | 65   | ARG  | N-CA-C      | 6.72  | 117.34      | 108.07   |
| 3   | N     | 1287 | GLU  | N-CA-C      | 6.71  | 118.38      | 111.14   |
| 3   | N     | 891  | GLU  | N-CA-C      | 6.71  | 119.42      | 111.71   |
| 2   | C     | 1110 | ASP  | N-CA-C      | 6.70  | 119.32      | 108.41   |
| 2   | M     | 243  | ARG  | N-CA-C      | 6.67  | 122.41      | 108.39   |
| 7   | I     | 8    | DG   | C5'-C4'-C3' | -6.67 | 104.90      | 114.90   |
| 2   | C     | 302  | VAL  | N-CA-C      | 6.67  | 117.75      | 111.48   |
| 3   | N     | 806  | PHE  | N-CA-C      | -6.66 | 105.02      | 113.01   |
| 3   | D     | 922  | LEU  | N-CA-C      | 6.64  | 121.60      | 112.90   |
| 2   | M     | 393  | GLN  | N-CA-C      | 6.63  | 119.02      | 109.14   |
| 3   | D     | 1033 | GLN  | N-CA-C      | -6.60 | 104.08      | 111.28   |
| 3   | N     | 433  | GLY  | N-CA-C      | 6.60  | 119.87      | 111.09   |
| 6   | Y     | 7    | G    | N9-C1'-C2'  | -6.60 | 102.11      | 112.00   |
| 3   | N     | 1035 | ILE  | N-CA-C      | -6.60 | 103.89      | 110.62   |
| 2   | M     | 398  | THR  | N-CA-C      | -6.58 | 103.00      | 111.02   |
| 5   | G     | 26   | DC   | C2'-C3'-O3' | -6.58 | 101.63      | 111.50   |
| 3   | D     | 521  | PRO  | CA-C-N      | 6.55  | 128.03      | 119.84   |
| 3   | D     | 521  | PRO  | C-N-CA      | 6.55  | 128.03      | 119.84   |
| 2   | C     | 409  | ARG  | N-CA-C      | 6.55  | 120.96      | 109.96   |
| 1   | A     | 13   | VAL  | N-CA-C      | 6.54  | 119.76      | 108.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | C     | 800  | VAL  | CB-CA-C     | -6.52 | 103.45      | 111.08   |
| 3   | D     | 633  | VAL  | N-CA-C      | 6.51  | 118.82      | 109.51   |
| 2   | M     | 319  | GLY  | N-CA-C      | -6.50 | 101.20      | 110.63   |
| 3   | D     | 544  | TYR  | N-CA-C      | -6.50 | 104.28      | 111.82   |
| 2   | C     | 731  | GLU  | N-CA-C      | -6.48 | 105.41      | 113.38   |
| 3   | D     | 806  | PHE  | N-CA-C      | -6.48 | 104.63      | 112.54   |
| 3   | D     | 126  | VAL  | N-CA-C      | 6.47  | 116.96      | 110.23   |
| 6   | H     | 16   | A    | C2'-C3'-O3' | 6.47  | 123.41      | 113.70   |
| 3   | N     | 133  | ILE  | N-CA-C      | 6.47  | 118.38      | 109.46   |
| 2   | C     | 1017 | THR  | N-CA-C      | -6.46 | 99.98       | 110.20   |
| 3   | D     | 122  | GLU  | N-CA-C      | 6.46  | 118.41      | 111.36   |
| 3   | D     | 824  | ASN  | N-CA-C      | 6.46  | 118.01      | 110.97   |
| 3   | N     | 142  | LEU  | N-CA-C      | 6.46  | 119.27      | 110.35   |
| 3   | N     | 875  | THR  | N-CA-C      | 6.46  | 118.89      | 109.07   |
| 3   | D     | 1126 | ASP  | N-CA-C      | 6.44  | 119.21      | 108.20   |
| 3   | N     | 1112 | CYS  | N-CA-C      | -6.43 | 100.65      | 110.30   |
| 2   | C     | 346  | VAL  | N-CA-C      | -6.43 | 103.99      | 111.00   |
| 2   | C     | 297  | GLU  | N-CA-C      | -6.43 | 99.22       | 109.76   |
| 2   | C     | 1037 | VAL  | CB-CA-C     | -6.42 | 103.48      | 111.70   |
| 3   | N     | 586  | ARG  | N-CA-C      | -6.42 | 103.53      | 111.75   |
| 3   | D     | 609  | GLY  | N-CA-C      | 6.42  | 118.58      | 112.04   |
| 5   | X     | 27   | DC   | C2'-C3'-O3' | -6.40 | 101.90      | 111.50   |
| 1   | A     | 135  | GLY  | N-CA-C      | -6.39 | 105.09      | 114.61   |
| 5   | X     | 23   | DG   | C2'-C3'-O3' | -6.38 | 101.93      | 111.50   |
| 2   | M     | 1084 | SER  | N-CA-C      | -6.37 | 104.34      | 111.28   |
| 1   | L     | 227  | ASN  | CA-C-N      | 6.37  | 126.55      | 120.31   |
| 1   | L     | 227  | ASN  | C-N-CA      | 6.37  | 126.55      | 120.31   |
| 3   | N     | 1129 | THR  | CB-CA-C     | -6.36 | 109.23      | 116.54   |
| 2   | M     | 265  | ARG  | N-CA-C      | 6.36  | 119.50      | 108.76   |
| 5   | G     | 4    | DA   | C2'-C3'-O3' | 6.35  | 121.03      | 111.50   |
| 2   | M     | 690  | ILE  | N-CA-C      | 6.35  | 118.54      | 108.89   |
| 1   | K     | 59   | GLU  | N-CA-C      | 6.35  | 118.72      | 111.11   |
| 1   | L     | 171  | PHE  | N-CA-C      | 6.34  | 117.88      | 110.97   |
| 3   | N     | 515  | GLU  | N-CA-C      | -6.33 | 103.18      | 113.19   |
| 2   | C     | 686  | ASP  | N-CA-C      | -6.32 | 103.75      | 112.03   |
| 3   | D     | 1469 | GLY  | N-CA-C      | -6.32 | 105.35      | 115.08   |
| 3   | D     | 1034 | GLN  | CA-C-N      | -6.32 | 113.01      | 120.72   |
| 3   | D     | 1034 | GLN  | C-N-CA      | -6.32 | 113.01      | 120.72   |
| 2   | M     | 938  | LYS  | N-CA-C      | -6.31 | 104.40      | 111.28   |
| 2   | M     | 178  | PRO  | N-CA-C      | 6.31  | 125.47      | 112.47   |
| 3   | D     | 832  | ARG  | N-CA-C      | 6.31  | 117.95      | 111.14   |
| 2   | C     | 702  | SER  | CA-C-N      | -6.30 | 114.49      | 122.37   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | C     | 702  | SER  | C-N-CA    | -6.30 | 114.49      | 122.37   |
| 2   | C     | 797  | GLY  | N-CA-C    | -6.30 | 101.94      | 111.14   |
| 2   | M     | 686  | ASP  | N-CA-C    | -6.29 | 103.78      | 112.03   |
| 2   | C     | 165  | LEU  | N-CA-C    | -6.29 | 102.90      | 110.13   |
| 3   | D     | 812  | ALA  | N-CA-C    | -6.28 | 105.44      | 113.23   |
| 3   | N     | 798  | GLU  | N-CA-C    | 6.28  | 118.84      | 108.48   |
| 3   | N     | 818  | ARG  | N-CA-C    | -6.28 | 105.44      | 113.23   |
| 1   | K     | 135  | GLY  | N-CA-C    | -6.28 | 105.26      | 114.61   |
| 2   | C     | 284  | ARG  | N-CA-C    | 6.27  | 120.27      | 110.17   |
| 2   | C     | 406  | HIS  | N-CA-C    | -6.26 | 104.20      | 112.34   |
| 3   | D     | 1178 | ALA  | N-CA-C    | -6.26 | 104.54      | 111.36   |
| 3   | D     | 1246 | VAL  | N-CA-C    | 6.26  | 117.82      | 111.00   |
| 3   | D     | 1066 | THR  | N-CA-C    | 6.25  | 118.37      | 110.24   |
| 2   | M     | 749  | VAL  | N-CA-C    | 6.24  | 116.85      | 108.11   |
| 3   | D     | 19   | ARG  | N-CA-C    | -6.24 | 104.54      | 111.71   |
| 2   | M     | 58   | ASP  | N-CA-C    | 6.24  | 118.87      | 108.20   |
| 3   | N     | 1032 | PRO  | N-CA-C    | -6.24 | 105.73      | 113.84   |
| 2   | M     | 67   | ASP  | N-CA-C    | 6.24  | 119.18      | 109.52   |
| 2   | C     | 296  | GLY  | N-CA-C    | -6.23 | 105.89      | 114.67   |
| 3   | D     | 509  | PRO  | N-CA-C    | 6.23  | 121.94      | 113.84   |
| 3   | N     | 201  | GLY  | N-CA-C    | 6.22  | 118.53      | 110.45   |
| 1   | B     | 188  | GLN  | N-CA-C    | 6.21  | 117.74      | 110.97   |
| 3   | N     | 1210 | SER  | N-CA-C    | -6.20 | 104.81      | 112.38   |
| 3   | D     | 121  | THR  | N-CA-C    | 6.20  | 124.01      | 110.80   |
| 3   | D     | 683  | ILE  | N-CA-C    | 6.20  | 117.08      | 108.89   |
| 1   | L     | 188  | GLN  | N-CA-C    | 6.19  | 117.91      | 111.03   |
| 2   | C     | 687  | ALA  | N-CA-C    | -6.19 | 102.20      | 110.55   |
| 2   | M     | 135  | VAL  | N-CA-C    | 6.18  | 117.03      | 108.12   |
| 3   | D     | 875  | THR  | N-CA-C    | 6.18  | 118.47      | 109.07   |
| 7   | Z     | 1    | DG   | O5'-P-OP1 | -6.17 | 90.48       | 109.00   |
| 3   | N     | 28   | LYS  | CA-C-N    | 6.17  | 127.55      | 119.84   |
| 3   | N     | 28   | LYS  | C-N-CA    | 6.17  | 127.55      | 119.84   |
| 3   | N     | 1297 | GLU  | N-CA-C    | -6.16 | 105.82      | 113.15   |
| 2   | C     | 44   | ILE  | N-CA-C    | 6.14  | 116.89      | 110.62   |
| 3   | N     | 824  | ASN  | N-CA-C    | 6.13  | 117.65      | 110.97   |
| 2   | C     | 264  | PRO  | CA-C-N    | -6.12 | 112.81      | 122.73   |
| 2   | C     | 264  | PRO  | C-N-CA    | -6.12 | 112.81      | 122.73   |
| 3   | D     | 520  | LEU  | CA-C-N    | -6.12 | 114.08      | 120.38   |
| 3   | D     | 520  | LEU  | C-N-CA    | -6.12 | 114.08      | 120.38   |
| 3   | N     | 723  | GLY  | N-CA-C    | 6.12  | 121.93      | 112.45   |
| 2   | M     | 1017 | THR  | N-CA-C    | -6.12 | 100.53      | 110.20   |
| 2   | C     | 67   | ASP  | N-CA-C    | 6.11  | 118.99      | 109.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | M     | 717  | LEU  | N-CA-C      | -6.10 | 105.84      | 113.28   |
| 3   | D     | 1210 | SER  | N-CA-C      | -6.10 | 104.70      | 111.71   |
| 2   | M     | 297  | GLU  | N-CA-C      | -6.09 | 99.74       | 109.96   |
| 2   | C     | 243  | ARG  | N-CA-C      | 6.08  | 121.17      | 108.39   |
| 4   | E     | 95   | VAL  | N-CA-C      | 6.08  | 121.98      | 109.34   |
| 1   | K     | 47   | SER  | N-CA-C      | 6.07  | 118.81      | 111.40   |
| 6   | Y     | 5    | C    | OP2-P-O3'   | -6.05 | 89.84       | 108.00   |
| 2   | M     | 1118 | LYS  | N-CA-C      | 6.05  | 119.94      | 110.32   |
| 5   | X     | 17   | DA   | C5'-C4'-C3' | -6.04 | 105.84      | 114.90   |
| 3   | D     | 805  | GLU  | N-CA-C      | 6.03  | 117.68      | 109.11   |
| 3   | D     | 1368 | ILE  | CB-CA-C     | -6.02 | 104.17      | 111.88   |
| 3   | N     | 1101 | VAL  | CB-CA-C     | -6.02 | 105.52      | 111.30   |
| 3   | N     | 1460 | ILE  | N-CA-C      | -6.02 | 99.38       | 108.17   |
| 2   | C     | 727  | PRO  | N-CA-C      | 6.01  | 124.86      | 112.47   |
| 3   | N     | 1178 | ALA  | N-CA-C      | -6.01 | 104.73      | 111.28   |
| 3   | N     | 1062 | ARG  | N-CA-C      | -6.01 | 104.65      | 111.14   |
| 3   | N     | 1194 | CYS  | N-CA-C      | -5.98 | 102.06      | 110.50   |
| 2   | C     | 230  | ARG  | CA-C-N      | 5.98  | 127.32      | 119.84   |
| 2   | C     | 230  | ARG  | C-N-CA      | 5.98  | 127.32      | 119.84   |
| 2   | C     | 673  | LEU  | N-CA-C      | -5.98 | 100.99      | 109.96   |
| 3   | D     | 100  | ALA  | N-CA-C      | 5.97  | 118.49      | 109.23   |
| 2   | M     | 284  | ARG  | N-CA-C      | 5.97  | 119.79      | 110.17   |
| 3   | D     | 688  | TRP  | N-CA-C      | -5.97 | 104.84      | 111.71   |
| 5   | X     | 2    | DT   | C4'-C3'-O3' | 5.96  | 118.94      | 110.00   |
| 2   | M     | 632  | ASN  | N-CA-C      | -5.96 | 105.11      | 112.38   |
| 1   | B     | 171  | PHE  | N-CA-C      | 5.96  | 117.58      | 111.14   |
| 2   | C     | 135  | VAL  | N-CA-C      | 5.95  | 116.86      | 108.17   |
| 3   | D     | 1059 | SER  | N-CA-C      | 5.95  | 118.58      | 110.55   |
| 3   | D     | 1108 | ARG  | N-CA-C      | -5.95 | 97.62       | 108.02   |
| 3   | D     | 58   | CYS  | N-CA-C      | 5.94  | 114.45      | 108.75   |
| 3   | D     | 1116 | ASN  | N-CA-C      | -5.94 | 97.48       | 107.99   |
| 3   | D     | 1031 | ASN  | C-N-CD      | -5.93 | 100.69      | 125.00   |
| 3   | N     | 1059 | SER  | N-CA-C      | 5.92  | 118.55      | 110.55   |
| 2   | C     | 1094 | ALA  | N-CA-C      | -5.92 | 104.83      | 111.28   |
| 3   | N     | 779  | ALA  | N-CA-C      | -5.91 | 105.38      | 112.59   |
| 2   | C     | 365  | ASP  | N-CA-C      | 5.90  | 118.46      | 111.33   |
| 1   | K     | 169  | ALA  | N-CA-C      | 5.89  | 118.55      | 109.07   |
| 3   | D     | 747  | VAL  | N-CA-C      | 5.88  | 116.12      | 108.35   |
| 1   | L     | 59   | GLU  | N-CA-C      | 5.88  | 117.69      | 111.28   |
| 3   | D     | 1127 | GLU  | N-CA-C      | -5.87 | 98.30       | 110.80   |
| 3   | D     | 792  | ILE  | N-CA-C      | 5.87  | 116.60      | 110.62   |
| 2   | C     | 690  | ILE  | N-CA-C      | 5.86  | 117.80      | 108.89   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | C     | 1109 | VAL  | CA-C-N      | -5.83 | 114.79      | 123.00   |
| 2   | C     | 1109 | VAL  | C-N-CA      | -5.83 | 114.79      | 123.00   |
| 3   | D     | 1265 | ALA  | N-CA-C      | -5.82 | 101.43      | 110.10   |
| 2   | C     | 421  | GLU  | N-CA-C      | 5.81  | 119.55      | 112.23   |
| 2   | C     | 858  | MET  | CA-C-N      | 5.81  | 127.10      | 119.84   |
| 2   | C     | 858  | MET  | C-N-CA      | 5.81  | 127.10      | 119.84   |
| 3   | D     | 133  | ILE  | N-CA-C      | 5.80  | 118.10      | 109.17   |
| 3   | D     | 891  | GLU  | N-CA-C      | 5.79  | 118.36      | 111.71   |
| 2   | M     | 406  | HIS  | N-CA-C      | -5.78 | 104.82      | 112.34   |
| 3   | N     | 1459 | LEU  | N-CA-C      | 5.76  | 118.83      | 108.17   |
| 2   | C     | 443  | THR  | CA-C-N      | 5.76  | 125.52      | 119.76   |
| 2   | C     | 443  | THR  | C-N-CA      | 5.76  | 125.52      | 119.76   |
| 1   | K     | 172  | SER  | CA-C-N      | 5.75  | 126.83      | 120.45   |
| 1   | K     | 172  | SER  | C-N-CA      | 5.75  | 126.83      | 120.45   |
| 2   | M     | 302  | VAL  | N-CA-C      | 5.74  | 116.50      | 111.56   |
| 5   | G     | 19   | DG   | C2'-C3'-O3' | -5.74 | 102.89      | 111.50   |
| 3   | N     | 1234 | THR  | N-CA-C      | -5.73 | 105.93      | 114.64   |
| 2   | M     | 559  | LEU  | N-CA-C      | -5.72 | 104.95      | 111.07   |
| 5   | G     | 25   | DG   | C2'-C3'-O3' | -5.71 | 102.94      | 111.50   |
| 2   | C     | 183  | SER  | N-CA-C      | 5.70  | 118.44      | 107.44   |
| 2   | C     | 717  | LEU  | N-CA-C      | -5.70 | 106.33      | 113.28   |
| 3   | D     | 818  | ARG  | N-CA-C      | -5.69 | 106.17      | 113.23   |
| 2   | M     | 261  | ILE  | N-CA-C      | 5.69  | 121.17      | 109.34   |
| 3   | N     | 136  | ASP  | CA-C-N      | -5.68 | 112.74      | 119.84   |
| 3   | N     | 136  | ASP  | C-N-CA      | -5.68 | 112.74      | 119.84   |
| 2   | M     | 797  | GLY  | N-CA-C      | -5.67 | 102.86      | 111.14   |
| 3   | N     | 1188 | VAL  | N-CA-C      | 5.66  | 116.90      | 108.46   |
| 1   | K     | 13   | VAL  | N-CA-C      | 5.66  | 117.98      | 108.81   |
| 1   | B     | 68   | ILE  | N-CA-C      | 5.66  | 114.72      | 108.05   |
| 1   | A     | 8    | ALA  | CA-C-N      | 5.65  | 126.90      | 119.84   |
| 1   | A     | 8    | ALA  | C-N-CA      | 5.65  | 126.90      | 119.84   |
| 3   | N     | 1371 | VAL  | N-CA-C      | 5.65  | 116.10      | 110.23   |
| 3   | D     | 18   | ILE  | N-CA-C      | -5.64 | 105.00      | 110.42   |
| 3   | D     | 131  | LYS  | N-CA-C      | 5.64  | 118.73      | 107.62   |
| 3   | N     | 471  | GLU  | N-CA-C      | 5.63  | 117.42      | 111.28   |
| 3   | N     | 65   | ARG  | N-CA-C      | 5.63  | 115.84      | 108.07   |
| 2   | M     | 442  | GLU  | N-CA-C      | 5.63  | 118.18      | 111.71   |
| 3   | N     | 466  | LYS  | N-CA-C      | 5.63  | 117.09      | 111.07   |
| 2   | M     | 727  | PRO  | N-CA-C      | 5.62  | 124.05      | 112.47   |
| 3   | D     | 140  | ALA  | N-CA-C      | 5.62  | 122.76      | 110.80   |
| 2   | C     | 768  | THR  | CA-C-N      | 5.61  | 125.14      | 119.19   |
| 2   | C     | 768  | THR  | C-N-CA      | 5.61  | 125.14      | 119.19   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | M     | 183  | SER  | N-CA-C      | 5.61  | 118.27      | 107.44   |
| 5   | X     | 13   | DA   | C5'-C4'-C3' | -5.61 | 106.48      | 114.90   |
| 3   | N     | 512  | MET  | N-CA-C      | -5.60 | 105.55      | 112.38   |
| 3   | N     | 792  | ILE  | N-CA-C      | 5.60  | 116.38      | 110.72   |
| 5   | X     | 22   | DA   | C2'-C3'-O3' | -5.60 | 103.10      | 111.50   |
| 2   | C     | 178  | PRO  | N-CA-C      | 5.60  | 124.00      | 112.47   |
| 3   | N     | 140  | ALA  | N-CA-C      | 5.60  | 122.72      | 110.80   |
| 3   | D     | 79   | GLU  | N-CA-C      | -5.60 | 101.42      | 110.32   |
| 3   | N     | 641  | GLN  | N-CA-C      | 5.59  | 118.00      | 109.95   |
| 2   | C     | 1002 | GLU  | N-CA-C      | -5.59 | 105.96      | 112.89   |
| 2   | C     | 310  | LEU  | N-CA-C      | -5.59 | 105.19      | 111.28   |
| 2   | C     | 261  | ILE  | N-CA-C      | 5.58  | 120.95      | 109.34   |
| 2   | M     | 976  | ASP  | N-CA-C      | 5.58  | 118.12      | 111.71   |
| 5   | X     | 20   | DC   | C2'-C3'-O3' | -5.58 | 103.14      | 111.50   |
| 2   | C     | 398  | THR  | N-CA-C      | -5.57 | 104.23      | 111.02   |
| 3   | D     | 141  | ILE  | N-CA-C      | 5.56  | 117.91      | 109.12   |
| 3   | D     | 1026 | SER  | N-CA-C      | -5.56 | 103.19      | 110.53   |
| 3   | N     | 1317 | ASP  | N-CA-C      | 5.56  | 118.34      | 110.50   |
| 1   | A     | 169  | ALA  | N-CA-C      | 5.55  | 118.01      | 109.07   |
| 3   | N     | 51   | GLY  | N-CA-C      | 5.55  | 123.66      | 112.34   |
| 2   | M     | 296  | GLY  | N-CA-C      | -5.55 | 106.85      | 114.67   |
| 3   | D     | 779  | ALA  | N-CA-C      | -5.53 | 105.84      | 112.59   |
| 2   | M     | 264  | PRO  | CA-C-N      | -5.53 | 114.23      | 122.74   |
| 2   | M     | 264  | PRO  | C-N-CA      | -5.53 | 114.23      | 122.74   |
| 3   | N     | 654  | LYS  | N-CA-C      | -5.53 | 105.31      | 113.16   |
| 1   | A     | 26   | GLU  | N-CA-C      | 5.50  | 112.97      | 108.07   |
| 3   | D     | 456  | MET  | N-CA-C      | 5.50  | 116.62      | 108.86   |
| 3   | N     | 527  | MET  | N-CA-C      | -5.50 | 96.78       | 107.62   |
| 2   | C     | 1011 | GLY  | CA-C-N      | 5.50  | 125.47      | 120.03   |
| 2   | C     | 1011 | GLY  | C-N-CA      | 5.50  | 125.47      | 120.03   |
| 1   | L     | 68   | ILE  | N-CA-C      | 5.50  | 114.54      | 108.05   |
| 5   | X     | 7    | DA   | C2'-C3'-O3' | 5.48  | 119.73      | 111.50   |
| 3   | D     | 736  | PHE  | N-CA-C      | -5.47 | 101.56      | 109.59   |
| 3   | D     | 1105 | ILE  | N-CA-C      | 5.46  | 115.44      | 108.12   |
| 6   | H     | 15   | C    | N1-C1'-C2'  | 5.46  | 120.19      | 112.00   |
| 5   | G     | 20   | DC   | C2'-C3'-O3' | -5.46 | 103.31      | 111.50   |
| 2   | C     | 455  | LEU  | N-CA-C      | 5.45  | 118.50      | 110.59   |
| 1   | A     | 226  | SER  | N-CA-C      | 5.45  | 119.49      | 111.04   |
| 2   | M     | 323  | ASP  | N-CA-C      | 5.45  | 117.60      | 109.59   |
| 3   | N     | 1001 | GLU  | N-CA-C      | -5.43 | 106.16      | 112.89   |
| 3   | N     | 175  | VAL  | N-CA-C      | 5.43  | 116.12      | 108.36   |
| 3   | D     | 1252 | ILE  | N-CA-CB     | -5.42 | 106.05      | 112.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | N     | 1237 | THR  | N-CA-C      | 5.42  | 122.35      | 110.80   |
| 2   | C     | 882  | LEU  | N-CA-C      | -5.42 | 106.51      | 113.01   |
| 3   | N     | 664  | LYS  | N-CA-C      | -5.41 | 103.55      | 110.53   |
| 2   | C     | 431  | HIS  | N-CA-C      | 5.41  | 117.52      | 110.43   |
| 1   | A     | 73   | GLU  | N-CA-C      | 5.40  | 117.51      | 110.43   |
| 2   | M     | 811  | PRO  | N-CA-C      | -5.40 | 105.75      | 113.47   |
| 3   | N     | 1268 | PRO  | N-CA-C      | 5.40  | 119.18      | 111.13   |
| 4   | E     | 57   | ASP  | N-CA-C      | 5.40  | 121.74      | 109.81   |
| 2   | M     | 455  | LEU  | N-CA-C      | 5.40  | 117.49      | 110.53   |
| 1   | K     | 26   | GLU  | N-CA-C      | 5.40  | 112.87      | 108.07   |
| 3   | N     | 1061 | PHE  | N-CA-C      | -5.39 | 106.54      | 113.23   |
| 3   | D     | 1101 | VAL  | CB-CA-C     | -5.38 | 106.14      | 111.30   |
| 3   | D     | 458  | ALA  | N-CA-C      | -5.38 | 106.67      | 113.18   |
| 3   | N     | 449  | SER  | N-CA-C      | 5.38  | 118.70      | 110.20   |
| 3   | D     | 572  | ARG  | N-CA-C      | -5.36 | 105.08      | 111.03   |
| 1   | A     | 48   | ILE  | N-CA-C      | 5.35  | 114.85      | 108.96   |
| 2   | M     | 346  | VAL  | N-CA-C      | -5.35 | 105.17      | 111.00   |
| 5   | X     | 19   | DG   | C2'-C3'-O3' | -5.34 | 103.48      | 111.50   |
| 1   | B     | 59   | GLU  | N-CA-C      | 5.34  | 117.79      | 111.33   |
| 3   | D     | 18   | ILE  | CB-CA-C     | -5.33 | 105.15      | 111.97   |
| 2   | M     | 535  | SER  | CA-C-N      | 5.32  | 125.64      | 119.47   |
| 2   | M     | 535  | SER  | C-N-CA      | 5.32  | 125.64      | 119.47   |
| 2   | M     | 303  | PHE  | N-CA-C      | 5.31  | 117.07      | 111.28   |
| 2   | M     | 936  | VAL  | N-CA-C      | 5.31  | 117.03      | 108.85   |
| 3   | N     | 66   | GLN  | N-CA-C      | 5.30  | 118.21      | 111.69   |
| 4   | O     | 57   | ASP  | N-CA-C      | 5.30  | 121.53      | 109.81   |
| 2   | C     | 408  | ARG  | CA-C-N      | -5.29 | 114.25      | 122.09   |
| 2   | C     | 408  | ARG  | C-N-CA      | -5.29 | 114.25      | 122.09   |
| 3   | D     | 772  | PRO  | N-CA-C      | -5.29 | 107.52      | 114.03   |
| 1   | L     | 38   | ASN  | CA-C-N      | 5.29  | 126.45      | 119.84   |
| 1   | L     | 38   | ASN  | C-N-CA      | 5.29  | 126.45      | 119.84   |
| 1   | K     | 199  | ILE  | N-CA-C      | 5.29  | 116.10      | 108.48   |
| 1   | B     | 91   | ASN  | N-CA-C      | 5.29  | 114.39      | 108.25   |
| 1   | L     | 91   | ASN  | N-CA-C      | 5.29  | 114.39      | 108.25   |
| 1   | A     | 6    | LEU  | N-CA-C      | -5.28 | 105.52      | 111.28   |
| 3   | N     | 736  | PHE  | N-CA-C      | -5.28 | 101.55      | 109.15   |
| 2   | C     | 1092 | LEU  | CA-CB-CG    | -5.27 | 97.84       | 116.30   |
| 1   | L     | 165  | ILE  | CA-C-N      | 5.27  | 125.21      | 119.78   |
| 1   | L     | 165  | ILE  | C-N-CA      | 5.27  | 125.21      | 119.78   |
| 2   | M     | 882  | LEU  | N-CA-C      | -5.27 | 106.69      | 113.01   |
| 3   | D     | 9    | ARG  | N-CA-C      | 5.26  | 117.00      | 108.26   |
| 1   | A     | 12   | THR  | N-CA-C      | 5.26  | 117.67      | 109.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 68   | ILE  | N-CA-C      | 5.25  | 113.72      | 107.73   |
| 3   | D     | 561  | GLY  | N-CA-C      | -5.25 | 100.73      | 113.18   |
| 2   | C     | 323  | ASP  | N-CA-C      | 5.25  | 117.29      | 109.25   |
| 3   | D     | 1461 | GLY  | N-CA-C      | -5.25 | 106.96      | 111.95   |
| 2   | C     | 226  | VAL  | N-CA-C      | 5.25  | 115.46      | 110.42   |
| 3   | N     | 810  | GLU  | N-CA-C      | -5.25 | 106.93      | 113.38   |
| 4   | O     | 82   | GLU  | N-CA-C      | 5.25  | 121.97      | 110.80   |
| 6   | H     | 5    | C    | C2'-C3'-O3' | 5.25  | 121.57      | 113.70   |
| 3   | D     | 1034 | GLN  | N-CA-C      | 5.24  | 117.00      | 111.28   |
| 2   | C     | 242  | LEU  | N-CA-C      | -5.24 | 103.97      | 110.41   |
| 3   | D     | 617  | ASN  | N-CA-C      | 5.23  | 117.78      | 111.40   |
| 3   | N     | 509  | PRO  | N-CA-C      | 5.23  | 120.47      | 114.03   |
| 2   | C     | 525  | SER  | CA-C-N      | 5.23  | 124.89      | 119.56   |
| 2   | C     | 525  | SER  | C-N-CA      | 5.23  | 124.89      | 119.56   |
| 3   | D     | 915  | VAL  | CB-CA-C     | -5.23 | 105.28      | 111.97   |
| 2   | M     | 704  | HIS  | N-CA-C      | 5.23  | 117.97      | 109.24   |
| 3   | D     | 1112 | CYS  | N-CA-CB     | 5.22  | 117.84      | 109.28   |
| 3   | N     | 1467 | ILE  | N-CA-C      | -5.22 | 104.67      | 110.62   |
| 3   | D     | 1062 | ARG  | N-CA-C      | -5.22 | 105.50      | 111.14   |
| 1   | K     | 73   | GLU  | N-CA-C      | 5.22  | 117.42      | 110.53   |
| 2   | M     | 1019 | GLN  | CA-C-N      | 5.21  | 125.15      | 119.78   |
| 2   | M     | 1019 | GLN  | C-N-CA      | 5.21  | 125.15      | 119.78   |
| 3   | N     | 99   | ALA  | N-CA-C      | -5.21 | 101.37      | 109.14   |
| 3   | N     | 835  | SER  | N-CA-C      | -5.21 | 103.65      | 110.53   |
| 3   | N     | 617  | ASN  | N-CA-C      | 5.21  | 117.76      | 111.40   |
| 2   | M     | 3    | ILE  | N-CA-C      | 5.21  | 115.40      | 108.11   |
| 2   | M     | 1011 | GLY  | CA-C-N      | 5.21  | 125.19      | 120.03   |
| 2   | M     | 1011 | GLY  | C-N-CA      | 5.21  | 125.19      | 120.03   |
| 2   | M     | 1073 | GLY  | N-CA-C      | -5.21 | 105.91      | 114.76   |
| 7   | Z     | 3    | DA   | C5'-C4'-C3' | -5.21 | 107.09      | 114.90   |
| 2   | C     | 683  | ASN  | N-CA-C      | -5.19 | 102.63      | 110.06   |
| 2   | C     | 456  | ALA  | N-CA-C      | 5.19  | 116.63      | 110.19   |
| 2   | C     | 749  | VAL  | N-CA-C      | 5.19  | 115.32      | 107.80   |
| 2   | M     | 508  | ILE  | N-CA-C      | -5.19 | 104.35      | 110.21   |
| 5   | X     | 6    | DT   | C4'-C3'-O3' | 5.19  | 117.78      | 110.00   |
| 3   | D     | 878  | GLY  | CA-C-N      | 5.19  | 127.23      | 120.28   |
| 3   | D     | 878  | GLY  | C-N-CA      | 5.19  | 127.23      | 120.28   |
| 2   | M     | 865  | THR  | CA-C-N      | 5.18  | 127.04      | 120.51   |
| 2   | M     | 865  | THR  | C-N-CA      | 5.18  | 127.04      | 120.51   |
| 2   | C     | 169  | GLY  | CA-C-N      | 5.18  | 126.31      | 119.84   |
| 2   | C     | 169  | GLY  | C-N-CA      | 5.18  | 126.31      | 119.84   |
| 3   | D     | 1266 | ARG  | N-CA-C      | 5.18  | 115.88      | 108.74   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | D     | 938  | GLY  | N-CA-C     | -5.17 | 107.90      | 114.16   |
| 4   | E     | 47   | LYS  | N-CA-C     | 5.17  | 117.11      | 108.99   |
| 3   | D     | 810  | GLU  | N-CA-C     | -5.17 | 107.03      | 113.38   |
| 6   | Y     | 12   | U    | N1-C1'-C2' | -5.17 | 104.25      | 112.00   |
| 3   | N     | 1116 | ASN  | N-CA-C     | -5.16 | 98.99       | 108.02   |
| 2   | M     | 59   | LYS  | N-CA-C     | -5.15 | 99.82       | 110.80   |
| 3   | D     | 1253 | THR  | N-CA-C     | 5.15  | 117.84      | 109.24   |
| 2   | M     | 169  | GLY  | CA-C-N     | 5.15  | 126.28      | 119.84   |
| 2   | M     | 169  | GLY  | C-N-CA     | 5.15  | 126.28      | 119.84   |
| 1   | L     | 13   | VAL  | N-CA-C     | 5.14  | 115.68      | 108.17   |
| 3   | D     | 1188 | VAL  | N-CA-C     | 5.14  | 116.12      | 108.46   |
| 3   | D     | 1444 | THR  | CB-CA-C    | -5.14 | 102.80      | 112.00   |
| 3   | N     | 792  | ILE  | CB-CA-C    | -5.14 | 105.12      | 112.22   |
| 2   | C     | 422  | ARG  | N-CA-C     | 5.14  | 118.38      | 112.57   |
| 3   | D     | 1061 | PHE  | N-CA-C     | -5.14 | 106.86      | 113.23   |
| 3   | N     | 593  | ASN  | CA-C-N     | 5.14  | 126.27      | 119.84   |
| 3   | N     | 593  | ASN  | C-N-CA     | 5.14  | 126.27      | 119.84   |
| 3   | D     | 641  | GLN  | N-CA-C     | 5.14  | 118.08      | 109.96   |
| 2   | M     | 776  | SER  | N-CA-C     | 5.13  | 117.54      | 111.33   |
| 3   | N     | 118  | LEU  | N-CA-C     | -5.13 | 101.49      | 109.14   |
| 1   | B     | 97   | VAL  | N-CA-C     | 5.13  | 115.30      | 108.11   |
| 3   | N     | 144  | GLY  | N-CA-C     | -5.13 | 101.02      | 113.18   |
| 3   | N     | 1101 | VAL  | N-CA-C     | 5.13  | 116.06      | 111.90   |
| 5   | X     | 7    | DA   | N9-C1'-C2' | -5.13 | 105.80      | 113.50   |
| 2   | C     | 936  | VAL  | N-CA-C     | 5.12  | 116.98      | 108.99   |
| 3   | D     | 904  | VAL  | N-CA-C     | 5.11  | 114.58      | 108.45   |
| 4   | O     | 47   | LYS  | N-CA-C     | 5.11  | 117.00      | 108.99   |
| 3   | D     | 1434 | TRP  | N-CA-C     | -5.10 | 107.09      | 113.72   |
| 4   | E     | 3    | GLU  | CA-C-N     | 5.10  | 125.10      | 119.90   |
| 4   | E     | 3    | GLU  | C-N-CA     | 5.10  | 125.10      | 119.90   |
| 3   | N     | 53   | ILE  | N-CA-C     | -5.10 | 104.61      | 111.44   |
| 2   | M     | 494  | TYR  | N-CA-C     | 5.08  | 117.01      | 109.69   |
| 3   | N     | 727  | GLN  | N-CA-C     | 5.08  | 116.55      | 108.67   |
| 2   | C     | 242  | LEU  | CA-C-N     | -5.08 | 116.91      | 123.16   |
| 2   | C     | 242  | LEU  | C-N-CA     | -5.08 | 116.91      | 123.16   |
| 3   | N     | 708  | LEU  | N-CA-C     | 5.08  | 117.94      | 111.69   |
| 2   | C     | 854  | PRO  | N-CA-C     | -5.08 | 103.22      | 111.19   |
| 3   | N     | 1077 | ALA  | N-CA-C     | -5.07 | 106.19      | 112.38   |
| 2   | C     | 503  | LEU  | N-CA-C     | 5.07  | 117.42      | 108.75   |
| 2   | C     | 742  | VAL  | N-CA-C     | 5.06  | 116.09      | 109.21   |
| 2   | C     | 811  | PRO  | N-CA-C     | -5.06 | 106.50      | 113.53   |
| 2   | C     | 63   | GLY  | N-CA-C     | -5.06 | 108.08      | 115.72   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | D     | 109  | PRO  | N-CA-C  | -5.05 | 102.06      | 112.47   |
| 3   | N     | 997  | THR  | N-CA-C  | -5.05 | 107.25      | 113.41   |
| 2   | C     | 29   | ALA  | N-CA-C  | -5.05 | 105.47      | 110.97   |
| 3   | D     | 64   | LYS  | N-CA-C  | 5.05  | 121.17      | 113.19   |
| 2   | M     | 422  | ARG  | N-CA-C  | 5.05  | 118.28      | 112.57   |
| 3   | N     | 1445 | HIS  | N-CA-C  | -5.05 | 105.67      | 111.07   |
| 2   | M     | 705  | ILE  | N-CA-C  | 5.04  | 115.17      | 108.11   |
| 2   | C     | 546  | LEU  | CA-C-N  | -5.04 | 118.97      | 122.59   |
| 2   | C     | 546  | LEU  | C-N-CA  | -5.04 | 118.97      | 122.59   |
| 3   | N     | 938  | GLY  | N-CA-C  | -5.03 | 108.08      | 114.16   |
| 3   | D     | 1344 | VAL  | N-CA-C  | -5.02 | 105.00      | 110.23   |
| 3   | D     | 1487 | VAL  | N-CA-C  | 5.02  | 115.60      | 108.42   |
| 2   | M     | 230  | ARG  | CA-C-N  | 5.02  | 126.11      | 119.84   |
| 2   | M     | 230  | ARG  | C-N-CA  | 5.02  | 126.11      | 119.84   |
| 3   | D     | 482  | LYS  | N-CA-C  | 5.02  | 117.64      | 111.82   |
| 3   | N     | 1108 | ARG  | N-CA-C  | -5.02 | 99.24       | 108.02   |
| 3   | D     | 1466 | VAL  | CB-CA-C | -5.01 | 105.48      | 112.04   |
| 2   | M     | 258  | TYR  | N-CA-C  | -5.01 | 107.66      | 112.97   |
| 3   | D     | 1006 | ALA  | N-CA-C  | 5.00  | 116.73      | 111.28   |
| 3   | N     | 1331 | ASP  | C-N-CD  | -5.00 | 104.49      | 125.00   |

There are no chirality outliers.

All (40) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 5   | G     | 10  | DA   | Sidechain |
| 5   | G     | 11  | DC   | Sidechain |
| 5   | G     | 14  | DG   | Sidechain |
| 5   | G     | 15  | DC   | Sidechain |
| 5   | G     | 17  | DA   | Sidechain |
| 5   | G     | 18  | DC   | Sidechain |
| 5   | G     | 2   | DT   | Sidechain |
| 5   | G     | 3   | DC   | Sidechain |
| 5   | G     | 4   | DA   | Sidechain |
| 5   | G     | 9   | DC   | Sidechain |
| 6   | H     | 5   | C    | Sidechain |
| 6   | H     | 7   | G    | Sidechain |
| 6   | H     | 8   | G    | Sidechain |
| 6   | H     | 9   | C    | Sidechain |
| 7   | I     | 14  | DG   | Sidechain |
| 7   | I     | 15  | DT   | Sidechain |
| 7   | I     | 2   | DT   | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 7   | I     | 4   | DG   | Sidechain |
| 7   | I     | 5   | DC   | Sidechain |
| 7   | I     | 8   | DG   | Sidechain |
| 5   | X     | 10  | DA   | Sidechain |
| 5   | X     | 14  | DG   | Sidechain |
| 5   | X     | 15  | DC   | Sidechain |
| 5   | X     | 17  | DA   | Sidechain |
| 5   | X     | 18  | DC   | Sidechain |
| 5   | X     | 2   | DT   | Sidechain |
| 5   | X     | 22  | DA   | Sidechain |
| 5   | X     | 26  | DC   | Sidechain |
| 5   | X     | 27  | DC   | Sidechain |
| 5   | X     | 4   | DA   | Sidechain |
| 5   | X     | 8   | DC   | Sidechain |
| 6   | Y     | 10  | G    | Sidechain |
| 6   | Y     | 11  | C    | Sidechain |
| 6   | Y     | 15  | C    | Sidechain |
| 6   | Y     | 7   | G    | Sidechain |
| 6   | Y     | 9   | C    | Sidechain |
| 7   | Z     | 12  | DT   | Sidechain |
| 7   | Z     | 14  | DG   | Sidechain |
| 7   | Z     | 7   | DT   | Sidechain |
| 7   | Z     | 8   | DG   | Sidechain |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1806  | 0        | 1861     | 267     | 0            |
| 1   | B     | 1806  | 0        | 1861     | 189     | 0            |
| 1   | K     | 1806  | 0        | 1861     | 205     | 0            |
| 1   | L     | 1806  | 0        | 1861     | 213     | 0            |
| 2   | C     | 8829  | 0        | 8933     | 1477    | 0            |
| 2   | M     | 8829  | 0        | 8933     | 1485    | 0            |
| 3   | D     | 9097  | 0        | 9316     | 1681    | 0            |
| 3   | N     | 10175 | 0        | 10401    | 1839    | 0            |
| 4   | E     | 770   | 0        | 784      | 130     | 0            |
| 4   | O     | 770   | 0        | 784      | 159     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | G     | 548   | 0        | 301      | 114     | 0            |
| 5   | X     | 548   | 0        | 301      | 93      | 0            |
| 6   | H     | 340   | 0        | 176      | 78      | 0            |
| 6   | Y     | 318   | 0        | 165      | 58      | 0            |
| 7   | I     | 357   | 0        | 194      | 68      | 0            |
| 7   | Z     | 357   | 0        | 194      | 71      | 0            |
| 8   | D     | 2     | 0        | 0        | 0       | 0            |
| 8   | N     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 48166 | 0        | 47926    | 7443    | 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 78.

All (7443) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:52:PHE:CZ     | 2:C:68:PHE:HB2    | 1.22                     | 1.67              |
| 3:D:897:TRP:HA    | 3:D:900:ILE:CG1   | 1.33                     | 1.56              |
| 3:D:1041:LEU:HD11 | 3:D:1045:MET:SD   | 1.55                     | 1.44              |
| 3:D:705:ALA:HB1   | 6:H:14:G:N2       | 1.24                     | 1.40              |
| 3:D:744:GLN:CD    | 5:G:21:DG:H21     | 1.34                     | 1.34              |
| 3:D:705:ALA:CB    | 6:H:14:G:H21      | 1.40                     | 1.32              |
| 2:C:52:PHE:CZ     | 2:C:68:PHE:CB     | 2.12                     | 1.31              |
| 3:N:610:LYS:O     | 3:N:615:ARG:HG2   | 1.18                     | 1.29              |
| 2:M:486:MET:SD    | 2:M:490:GLU:HB2   | 1.72                     | 1.28              |
| 3:N:610:LYS:C     | 3:N:615:ARG:HG2   | 1.58                     | 1.27              |
| 3:D:897:TRP:CA    | 3:D:900:ILE:HG12  | 1.62                     | 1.27              |
| 3:D:1033:GLN:O    | 3:D:1037:GLN:CB   | 1.82                     | 1.26              |
| 3:N:1033:GLN:OE1  | 3:N:1240:THR:HG21 | 1.31                     | 1.26              |
| 2:M:265:ARG:N     | 2:M:289:THR:HG21  | 1.49                     | 1.26              |
| 1:A:28:LEU:HD22   | 1:A:32:PHE:CD1    | 1.70                     | 1.25              |
| 3:D:1033:GLN:O    | 3:D:1037:GLN:HB2  | 1.29                     | 1.24              |
| 3:D:1041:LEU:CD1  | 3:D:1045:MET:SD   | 2.24                     | 1.24              |
| 3:D:1042:ARG:NH2  | 3:D:1073:SER:HB2  | 1.52                     | 1.24              |
| 3:N:618:LEU:HD12  | 3:N:1467:ILE:CG1  | 1.66                     | 1.24              |
| 3:D:989:TYR:OH    | 3:D:1051:GLU:HG3  | 1.07                     | 1.24              |
| 2:C:50:GLU:HA     | 2:C:266:ARG:CZ    | 1.70                     | 1.21              |
| 3:N:625:TYR:OH    | 3:N:655:PRO:HG2   | 1.33                     | 1.20              |
| 3:N:1129:THR:HB   | 3:N:1320:GLU:CG   | 1.73                     | 1.18              |
| 3:N:1485:GLN:HG3  | 4:O:79:LEU:H      | 1.08                     | 1.18              |
| 2:C:336:VAL:HA    | 2:C:339:LEU:HD12  | 1.20                     | 1.18              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:265:ARG:H     | 2:M:289:THR:CG2   | 1.55                     | 1.17              |
| 2:M:1109:VAL:HG11 | 3:N:5:VAL:HG22    | 1.22                     | 1.17              |
| 3:N:705:ALA:HB3   | 3:N:706:PRO:HD3   | 1.27                     | 1.16              |
| 3:N:1435:LEU:HD23 | 3:N:1464:GLU:HB2  | 1.16                     | 1.15              |
| 4:E:36:LYS:H      | 4:E:95:VAL:HG21   | 1.09                     | 1.15              |
| 3:N:19:ARG:HH21   | 3:N:516:ALA:HB2   | 1.08                     | 1.15              |
| 3:N:477:LEU:HD12  | 3:N:496:LEU:HD13  | 1.29                     | 1.15              |
| 2:C:52:PHE:CE2    | 2:C:68:PHE:HB2    | 1.81                     | 1.15              |
| 1:L:185:ARG:NH2   | 3:N:688:TRP:HB3   | 1.59                     | 1.15              |
| 2:C:48:PHE:O      | 2:C:52:PHE:HB2    | 1.46                     | 1.14              |
| 3:D:1034:GLN:O    | 3:D:1038:LEU:HB2  | 1.46                     | 1.14              |
| 1:L:185:ARG:HH22  | 3:N:688:TRP:CB    | 1.58                     | 1.14              |
| 3:N:833:GLU:O     | 3:N:834:THR:HG23  | 1.45                     | 1.14              |
| 1:K:178:ALA:HB2   | 2:M:864:GLY:H     | 1.11                     | 1.13              |
| 2:M:490:GLU:HA    | 2:M:493:ARG:HD3   | 1.28                     | 1.13              |
| 3:D:897:TRP:HB2   | 3:D:900:ILE:HD11  | 1.14                     | 1.13              |
| 2:M:1056:LYS:HE3  | 3:N:751:LEU:HD11  | 1.31                     | 1.13              |
| 3:N:618:LEU:CD1   | 3:N:1467:ILE:HG12 | 1.77                     | 1.13              |
| 3:D:833:GLU:O     | 3:D:834:THR:HG23  | 1.47                     | 1.12              |
| 3:N:814:ALA:HB1   | 3:N:818:ARG:HH21  | 1.08                     | 1.12              |
| 7:I:3:DA:H1'      | 7:I:4:DG:H5'      | 1.30                     | 1.12              |
| 2:C:266:ARG:HA    | 2:C:288:ARG:HD3   | 1.29                     | 1.12              |
| 2:M:455:LEU:HD13  | 2:M:459:ALA:HB3   | 1.25                     | 1.12              |
| 3:N:754:PHE:HA    | 4:O:24:ALA:HB1    | 1.22                     | 1.12              |
| 3:D:897:TRP:CA    | 3:D:900:ILE:CG1   | 2.24                     | 1.12              |
| 1:K:156:HIS:HE1   | 1:K:166:PRO:HB3   | 1.04                     | 1.12              |
| 3:N:98:PRO:HG2    | 3:N:462:GLN:NE2   | 1.65                     | 1.11              |
| 3:N:697:GLY:HA2   | 3:N:717:GLN:CD    | 1.73                     | 1.11              |
| 2:C:423:ALA:HB1   | 7:I:1:DG:H5''     | 1.33                     | 1.11              |
| 2:C:630:ARG:HD2   | 2:C:634:GLY:HA2   | 1.27                     | 1.11              |
| 2:C:1024:LYS:HB2  | 6:H:4:G:H21       | 1.14                     | 1.11              |
| 2:C:409:ARG:HB3   | 2:C:454:SER:OG    | 1.51                     | 1.11              |
| 3:N:483:HIS:HB2   | 3:N:484:PRO:HD3   | 1.21                     | 1.11              |
| 3:D:993:LEU:O     | 3:D:997:THR:HG23  | 1.51                     | 1.10              |
| 1:K:156:HIS:CE1   | 1:K:166:PRO:HB3   | 1.87                     | 1.10              |
| 3:N:783:ARG:HE    | 3:N:1029:ARG:CD   | 1.64                     | 1.10              |
| 3:N:1442:ASN:O    | 3:N:1446:VAL:HG23 | 1.51                     | 1.10              |
| 2:C:692:GLU:HG2   | 2:C:696:LYS:HE3   | 1.29                     | 1.10              |
| 3:D:126:VAL:O     | 3:D:130:SER:HB2   | 1.51                     | 1.10              |
| 2:M:490:GLU:HB3   | 2:M:493:ARG:HH11  | 1.17                     | 1.10              |
| 2:C:1042:ALA:HB2  | 3:D:1227:GLN:HE22 | 0.95                     | 1.09              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:50:GLU:HG3    | 2:C:266:ARG:HD2   | 1.13                     | 1.09              |
| 3:D:608:SER:HB3   | 3:D:1442:ASN:O    | 1.53                     | 1.09              |
| 3:N:957:PRO:HG2   | 3:N:1007:VAL:HG22 | 1.34                     | 1.09              |
| 3:D:1112:CYS:HB3  | 3:D:1195:GLN:HG2  | 1.17                     | 1.09              |
| 7:Z:11:DG:H2''    | 7:Z:12:DT:H71     | 1.24                     | 1.09              |
| 1:A:28:LEU:CD2    | 1:A:32:PHE:HD1    | 1.66                     | 1.08              |
| 2:C:861:LEU:HD23  | 2:C:863:ASP:H     | 0.99                     | 1.08              |
| 2:M:89:THR:HG21   | 2:M:383:ARG:HH22  | 1.14                     | 1.08              |
| 5:X:4:DA:H2''     | 5:X:5:DC:H5''     | 1.10                     | 1.08              |
| 3:N:925:GLU:HB3   | 4:O:6:ILE:HG22    | 1.25                     | 1.08              |
| 3:D:989:TYR:OH    | 3:D:1051:GLU:CG   | 2.00                     | 1.08              |
| 3:D:1112:CYS:H    | 3:D:1201:CYS:CB   | 1.66                     | 1.08              |
| 2:M:857:ASP:HB2   | 2:M:978:ARG:HG2   | 1.34                     | 1.08              |
| 3:N:704:ARG:HA    | 3:N:745:MET:HG2   | 1.30                     | 1.08              |
| 5:G:17:DA:H2''    | 5:G:18:DC:H5'     | 1.26                     | 1.08              |
| 3:N:1238:MET:O    | 3:N:1239:ARG:HG2  | 1.53                     | 1.08              |
| 3:D:1042:ARG:HH21 | 3:D:1073:SER:CB   | 1.65                     | 1.07              |
| 2:M:675:ALA:HA    | 2:M:989:VAL:HG12  | 1.11                     | 1.07              |
| 2:C:328:LEU:HD13  | 2:C:433:THR:HB    | 1.33                     | 1.07              |
| 3:N:1238:MET:O    | 3:N:1239:ARG:CG   | 2.02                     | 1.07              |
| 3:D:1472:ILE:HD13 | 3:D:1472:ILE:H    | 1.15                     | 1.07              |
| 3:N:760:ARG:HH11  | 4:O:61:VAL:HG23   | 1.15                     | 1.07              |
| 3:D:520:LEU:HD23  | 3:D:525:ARG:HD2   | 1.37                     | 1.06              |
| 3:D:696:HIS:CD2   | 4:E:59:ASN:HB2    | 1.90                     | 1.06              |
| 2:C:69:LEU:HD12   | 2:C:97:ARG:HB3    | 1.37                     | 1.06              |
| 3:D:1045:MET:CE   | 3:D:1076:GLY:HA3  | 1.85                     | 1.06              |
| 2:M:431:HIS:HB3   | 2:M:434:HIS:CE1   | 1.91                     | 1.06              |
| 3:D:783:ARG:HA    | 3:D:1028:ALA:HA   | 1.33                     | 1.05              |
| 3:N:957:PRO:CG    | 3:N:1007:VAL:HG22 | 1.85                     | 1.05              |
| 3:N:1128:VAL:HB   | 3:N:1133:ARG:HH22 | 1.21                     | 1.05              |
| 3:N:181:ASP:HB3   | 3:N:441:ARG:HD3   | 1.35                     | 1.05              |
| 3:N:783:ARG:NE    | 3:N:1029:ARG:HD2  | 1.70                     | 1.05              |
| 2:C:50:GLU:HG3    | 2:C:266:ARG:CD    | 1.87                     | 1.05              |
| 3:D:899:LEU:HD22  | 3:D:917:GLN:CG    | 1.86                     | 1.05              |
| 7:Z:3:DA:H1'      | 7:Z:4:DG:H5'      | 1.33                     | 1.05              |
| 2:C:89:THR:HA     | 2:C:129:ILE:O     | 1.57                     | 1.05              |
| 3:D:989:TYR:CZ    | 3:D:1051:GLU:HG3  | 1.91                     | 1.05              |
| 3:D:1481:VAL:HG11 | 4:E:18:ARG:HA     | 1.30                     | 1.05              |
| 1:L:185:ARG:CZ    | 3:N:688:TRP:HB3   | 1.85                     | 1.05              |
| 1:A:32:PHE:CE1    | 1:B:221:HIS:NE2   | 2.25                     | 1.04              |
| 3:N:1274:ILE:HD13 | 3:N:1276:GLU:HG2  | 1.36                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1472:ILE:HD13 | 3:N:1472:ILE:H    | 1.16                     | 1.04              |
| 2:C:165:LEU:HG    | 2:C:166:PRO:HA    | 1.34                     | 1.04              |
| 3:N:521:PRO:HB2   | 3:N:524:LEU:HD13  | 1.37                     | 1.04              |
| 3:N:1109:GLU:HG2  | 3:N:1201:CYS:HA   | 1.39                     | 1.04              |
| 3:N:157:GLU:HA    | 3:N:160:GLU:OE1   | 1.56                     | 1.04              |
| 3:D:1262:LEU:HD23 | 3:D:1352:ILE:HG12 | 1.39                     | 1.04              |
| 3:N:783:ARG:NH2   | 3:N:1029:ARG:HB3  | 1.72                     | 1.04              |
| 3:D:1410:GLU:HG2  | 2:M:374:ASN:HA    | 1.40                     | 1.04              |
| 2:M:939:ARG:HA    | 2:M:939:ARG:HE    | 1.19                     | 1.04              |
| 3:N:171:LEU:HD11  | 3:N:195:VAL:HG23  | 1.38                     | 1.04              |
| 2:C:48:PHE:C      | 2:C:52:PHE:HB2    | 1.81                     | 1.03              |
| 3:D:704:ARG:HA    | 3:D:745:MET:HG2   | 1.37                     | 1.03              |
| 3:D:1258:ARG:HH12 | 3:D:1329:ALA:HB1  | 1.20                     | 1.03              |
| 3:N:62:LYS:HG3    | 3:N:75:ARG:HD2    | 1.37                     | 1.03              |
| 3:N:610:LYS:O     | 3:N:615:ARG:CG    | 2.05                     | 1.03              |
| 2:C:987:ILE:HG23  | 3:D:948:THR:HG21  | 1.40                     | 1.03              |
| 2:M:89:THR:HA     | 2:M:129:ILE:O     | 1.57                     | 1.03              |
| 5:G:13:DA:H2"     | 5:G:14:DG:OP2     | 1.59                     | 1.03              |
| 3:D:28:LYS:HG3    | 3:D:29:PRO:HD2    | 1.41                     | 1.03              |
| 3:N:1216:SER:HB3  | 4:O:15:SER:CB     | 1.89                     | 1.03              |
| 3:N:171:LEU:CD1   | 3:N:195:VAL:HG23  | 1.88                     | 1.02              |
| 3:D:744:GLN:CD    | 5:G:21:DG:N2      | 2.15                     | 1.02              |
| 3:D:1003:VAL:CG1  | 3:D:1036:ARG:HD2  | 1.90                     | 1.02              |
| 2:M:455:LEU:HD12  | 2:M:456:ALA:O     | 1.60                     | 1.02              |
| 2:C:739:GLU:HG3   | 2:C:742:VAL:HB    | 1.39                     | 1.02              |
| 3:D:136:ASP:HB3   | 3:D:137:PRO:HD3   | 1.40                     | 1.02              |
| 2:M:409:ARG:HA    | 2:M:454:SER:HA    | 1.42                     | 1.02              |
| 3:N:783:ARG:HH21  | 3:N:1029:ARG:HB3  | 0.89                     | 1.02              |
| 4:O:54:LEU:HD23   | 4:O:58:PRO:HD2    | 1.41                     | 1.02              |
| 1:L:185:ARG:NH2   | 3:N:688:TRP:CB    | 2.19                     | 1.02              |
| 3:N:525:ARG:HB2   | 3:N:538:SER:HB3   | 1.41                     | 1.02              |
| 3:N:698:LYS:HG2   | 4:O:59:ASN:ND2    | 1.74                     | 1.02              |
| 3:N:1294:VAL:HG12 | 3:N:1319:VAL:HG21 | 1.42                     | 1.01              |
| 1:A:28:LEU:HD22   | 1:A:32:PHE:HD1    | 0.84                     | 1.01              |
| 3:N:603:LEU:O     | 3:N:606:ILE:HG22  | 1.60                     | 1.01              |
| 3:N:1018:ASN:HB3  | 3:N:1021:TYR:HB3  | 1.41                     | 1.01              |
| 2:C:1036:GLU:HA   | 3:D:707:THR:HG21  | 1.42                     | 1.01              |
| 1:L:188:GLN:HG3   | 3:N:685:ASP:OD2   | 1.61                     | 1.01              |
| 1:A:28:LEU:HD13   | 1:A:32:PHE:HB3    | 1.42                     | 1.01              |
| 2:C:1097:LEU:HD22 | 2:C:1097:LEU:H    | 1.22                     | 1.01              |
| 3:D:764:LEU:HD23  | 3:D:767:HIS:CE1   | 1.96                     | 1.01              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:960:LYS:HE3   | 3:D:964:LEU:HD12  | 1.41                     | 1.01              |
| 3:N:398:ALA:HB2   | 3:N:447:VAL:HA    | 1.43                     | 1.01              |
| 7:I:5:DC:H2"      | 7:I:6:DT:OP2      | 1.59                     | 1.01              |
| 2:C:423:ALA:CB    | 7:I:1:DG:H5"      | 1.91                     | 1.00              |
| 3:D:860:LEU:HA    | 3:D:877:PRO:HB2   | 1.43                     | 1.00              |
| 3:N:166:GLN:O     | 3:N:167:GLU:HB2   | 1.60                     | 1.00              |
| 3:N:1294:VAL:HG12 | 3:N:1319:VAL:CG2  | 1.90                     | 1.00              |
| 3:D:1087:ARG:HG3  | 3:D:1236:LEU:HD22 | 1.03                     | 1.00              |
| 2:M:768:THR:HB    | 2:M:771:GLU:HB3   | 1.43                     | 1.00              |
| 3:D:705:ALA:HB3   | 3:D:706:PRO:HD3   | 1.39                     | 1.00              |
| 3:N:771:SER:HB3   | 3:N:778:LEU:HD13  | 1.43                     | 1.00              |
| 3:N:1468:LEU:HD22 | 3:N:1470:ARG:HB2  | 1.41                     | 1.00              |
| 1:A:39:PRO:HG3    | 1:B:39:PRO:HG3    | 1.43                     | 1.00              |
| 3:D:1045:MET:HE2  | 3:D:1076:GLY:CA   | 1.91                     | 1.00              |
| 3:N:1101:VAL:HG13 | 3:N:1428:ALA:HB2  | 1.43                     | 1.00              |
| 3:D:600:LEU:H     | 3:D:600:LEU:HD12  | 1.25                     | 1.00              |
| 3:N:711:LEU:HD12  | 3:N:778:LEU:HD23  | 1.44                     | 1.00              |
| 2:C:675:ALA:HA    | 2:C:989:VAL:HG12  | 1.44                     | 0.99              |
| 2:C:1115:LEU:HG   | 3:D:85:VAL:HG12   | 1.43                     | 0.99              |
| 3:D:456:MET:HA    | 3:D:460:ALA:HB2   | 1.43                     | 0.99              |
| 2:M:1040:LEU:HD23 | 2:M:1049:LEU:HD13 | 1.43                     | 0.99              |
| 1:A:63:HIS:HB3    | 2:C:746:GLY:CA    | 1.93                     | 0.99              |
| 3:N:1216:SER:HB3  | 4:O:15:SER:OG     | 1.61                     | 0.99              |
| 3:N:1033:GLN:OE1  | 3:N:1240:THR:CG2  | 2.09                     | 0.99              |
| 7:Z:4:DG:H2"      | 7:Z:5:DC:OP2      | 1.59                     | 0.99              |
| 2:C:1036:GLU:HG3  | 3:D:707:THR:OG1   | 1.62                     | 0.99              |
| 2:M:64:LEU:HD22   | 2:M:359:MET:HG3   | 1.43                     | 0.99              |
| 2:M:754:ILE:HD13  | 2:M:791:ARG:HG2   | 1.44                     | 0.99              |
| 2:M:889:HIS:HE1   | 2:M:988:VAL:HG21  | 1.24                     | 0.99              |
| 3:N:1129:THR:HB   | 3:N:1320:GLU:CD   | 1.88                     | 0.98              |
| 3:D:708:LEU:HD22  | 3:D:1231:GLU:HA   | 1.41                     | 0.98              |
| 2:M:706:GLU:HG2   | 2:M:708:TYR:CZ    | 1.97                     | 0.98              |
| 3:N:1463:LYS:O    | 3:N:1467:ILE:HG13 | 1.63                     | 0.98              |
| 7:I:4:DG:H2"      | 7:I:5:DC:OP2      | 1.64                     | 0.98              |
| 3:N:453:ASP:HB3   | 3:N:455:ARG:HH21  | 1.25                     | 0.98              |
| 2:C:292:ARG:HG2   | 2:C:298:PHE:HA    | 1.42                     | 0.98              |
| 1:L:185:ARG:NH1   | 3:N:688:TRP:HB3   | 1.78                     | 0.98              |
| 3:N:810:GLU:O     | 3:N:813:LEU:HG    | 1.63                     | 0.98              |
| 3:D:902:LEU:HD23  | 3:D:902:LEU:H     | 1.29                     | 0.97              |
| 3:D:1087:ARG:CG   | 3:D:1236:LEU:HD22 | 1.94                     | 0.97              |
| 3:N:18:ILE:HG23   | 3:N:518:PRO:HG3   | 1.43                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1129:THR:HB   | 3:N:1320:GLU:HG3  | 1.42                     | 0.97              |
| 3:D:539:ASP:HB3   | 3:D:600:LEU:HB3   | 1.46                     | 0.97              |
| 3:D:522:PRO:HA    | 3:D:525:ARG:HH11  | 1.26                     | 0.97              |
| 3:N:157:GLU:HA    | 3:N:160:GLU:CD    | 1.89                     | 0.97              |
| 2:C:399:ASN:ND2   | 2:C:402:SER:HB3   | 1.78                     | 0.97              |
| 2:C:399:ASN:HD21  | 2:C:402:SER:HB3   | 1.29                     | 0.97              |
| 1:A:63:HIS:HB3    | 2:C:746:GLY:HA2   | 1.46                     | 0.97              |
| 2:M:422:ARG:HB3   | 7:Z:1:DG:C2       | 1.99                     | 0.97              |
| 3:N:1129:THR:HG23 | 3:N:1130:ARG:N    | 1.79                     | 0.97              |
| 2:C:1042:ALA:HB2  | 3:D:1227:GLN:NE2  | 1.80                     | 0.96              |
| 3:N:618:LEU:HD12  | 3:N:1467:ILE:HG12 | 0.97                     | 0.96              |
| 2:C:694:LEU:HD21  | 2:C:868:ASP:HB3   | 1.47                     | 0.96              |
| 3:N:1442:ASN:O    | 3:N:1446:VAL:CG2  | 2.12                     | 0.96              |
| 3:D:1211:MET:HG2  | 3:D:1212:ALA:H    | 1.29                     | 0.96              |
| 3:N:783:ARG:HE    | 3:N:1029:ARG:HD3  | 1.30                     | 0.96              |
| 3:D:1109:GLU:HG2  | 3:D:1201:CYS:HA   | 1.46                     | 0.96              |
| 3:N:843:PHE:HB2   | 3:N:866:VAL:HG22  | 1.48                     | 0.96              |
| 3:D:900:ILE:O     | 3:D:902:LEU:CD2   | 2.14                     | 0.96              |
| 3:D:1096:ARG:HH21 | 3:D:1440:PHE:HD2  | 1.01                     | 0.96              |
| 3:N:1268:PRO:HG3  | 3:N:1329:ALA:HB1  | 1.47                     | 0.96              |
| 2:C:50:GLU:HB2    | 2:C:266:ARG:NH1   | 1.80                     | 0.96              |
| 2:C:336:VAL:CA    | 2:C:339:LEU:HD12  | 1.94                     | 0.96              |
| 3:D:565:ILE:H     | 3:D:565:ILE:HD12  | 1.30                     | 0.96              |
| 2:C:630:ARG:CD    | 2:C:634:GLY:HA2   | 1.95                     | 0.95              |
| 2:M:861:LEU:HD22  | 2:M:863:ASP:HB3   | 1.44                     | 0.95              |
| 3:N:783:ARG:HH21  | 3:N:1029:ARG:CB   | 1.79                     | 0.95              |
| 2:C:89:THR:HG21   | 2:C:383:ARG:HH12  | 1.29                     | 0.95              |
| 3:D:1209:LEU:HD23 | 3:D:1211:MET:H    | 1.28                     | 0.95              |
| 2:C:409:ARG:HA    | 2:C:454:SER:HA    | 1.48                     | 0.95              |
| 3:N:483:HIS:CB    | 3:N:484:PRO:HD3   | 1.97                     | 0.95              |
| 3:N:764:LEU:HD23  | 3:N:767:HIS:CE1   | 2.01                     | 0.95              |
| 3:N:1220:ALA:HB1  | 3:N:1223:ILE:HD13 | 1.47                     | 0.95              |
| 2:M:395:LYS:HE2   | 2:M:403:SER:HB2   | 1.46                     | 0.95              |
| 3:D:899:LEU:HD22  | 3:D:917:GLN:CB    | 1.97                     | 0.95              |
| 1:A:43:ILE:HG23   | 1:A:47:SER:OG     | 1.66                     | 0.95              |
| 2:M:973:VAL:O     | 2:M:974:LEU:HD12  | 1.65                     | 0.95              |
| 3:N:646:LYS:HB2   | 3:N:688:TRP:CZ3   | 2.02                     | 0.95              |
| 3:N:695:ILE:HD11  | 3:N:718:PRO:HB2   | 1.44                     | 0.95              |
| 2:C:260:LEU:HB3   | 2:C:291:ALA:HB1   | 1.46                     | 0.94              |
| 2:M:329:GLY:HA3   | 2:M:489:THR:HG23  | 1.49                     | 0.94              |
| 2:C:861:LEU:HG    | 2:C:862:PRO:HD2   | 1.49                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:86:LYS:HD3    | 2:M:813:VAL:HB    | 1.46                     | 0.94              |
| 3:N:1462:LEU:HD23 | 3:N:1473:PRO:HD2  | 1.49                     | 0.94              |
| 3:D:814:ALA:HB1   | 3:D:818:ARG:HH21  | 1.32                     | 0.94              |
| 2:M:7:GLY:H       | 2:M:904:PRO:HD2   | 1.31                     | 0.94              |
| 2:M:260:LEU:HB3   | 2:M:291:ALA:HB1   | 1.50                     | 0.94              |
| 2:M:1115:LEU:H    | 2:M:1115:LEU:HD12 | 1.29                     | 0.94              |
| 3:D:660:LYS:HD2   | 3:D:694:VAL:HG22  | 1.48                     | 0.94              |
| 3:D:1045:MET:HE2  | 3:D:1076:GLY:HA3  | 0.97                     | 0.94              |
| 2:M:861:LEU:CD2   | 2:M:863:ASP:H     | 1.80                     | 0.94              |
| 2:M:1016:ILE:HG12 | 2:M:1017:THR:H    | 1.31                     | 0.94              |
| 7:I:10:DG:H2''    | 7:I:11:DG:OP2     | 1.65                     | 0.94              |
| 5:G:5:DC:H2''     | 5:G:6:DT:O5'      | 1.65                     | 0.94              |
| 5:X:12:DA:H2''    | 5:X:13:DA:OP2     | 1.62                     | 0.94              |
| 3:D:1112:CYS:CB   | 3:D:1195:GLN:HG2  | 1.97                     | 0.94              |
| 1:L:28:LEU:HB2    | 1:L:193:ASP:HB2   | 1.48                     | 0.94              |
| 1:K:176:ARG:HH11  | 2:M:865:THR:HB    | 1.32                     | 0.94              |
| 2:M:1046:ALA:HB1  | 3:N:1471:LEU:HD11 | 1.47                     | 0.94              |
| 3:N:98:PRO:HG2    | 3:N:462:GLN:CD    | 1.92                     | 0.94              |
| 5:X:4:DA:H2''     | 5:X:5:DC:C5'      | 1.97                     | 0.94              |
| 1:A:32:PHE:HE1    | 1:B:221:HIS:HE2   | 1.06                     | 0.94              |
| 2:M:36:PRO:HG2    | 2:M:70:GLU:HB3    | 1.50                     | 0.94              |
| 2:M:971:LYS:HE3   | 2:M:988:VAL:HG12  | 1.49                     | 0.94              |
| 3:N:136:ASP:HB3   | 3:N:137:PRO:HD3   | 1.48                     | 0.94              |
| 3:N:754:PHE:HA    | 4:O:24:ALA:CB     | 1.98                     | 0.94              |
| 3:N:1271:LYS:NZ   | 3:N:1331:ASP:HB2  | 1.83                     | 0.94              |
| 2:C:439:CYS:SG    | 2:C:541:SER:N     | 2.41                     | 0.94              |
| 3:D:1042:ARG:HH21 | 3:D:1073:SER:HB2  | 0.77                     | 0.94              |
| 2:M:405:ARG:CZ    | 2:M:566:THR:HG21  | 1.98                     | 0.94              |
| 2:M:409:ARG:HB3   | 2:M:454:SER:OG    | 1.68                     | 0.94              |
| 3:D:1042:ARG:HG2  | 3:D:1061:PHE:HE1  | 1.33                     | 0.93              |
| 3:N:693:GLU:HA    | 4:O:48:MET:CE     | 1.98                     | 0.93              |
| 2:C:227:PHE:HD2   | 2:C:237:ARG:HE    | 1.12                     | 0.93              |
| 3:D:960:LYS:HE3   | 3:D:964:LEU:CD1   | 1.97                     | 0.93              |
| 2:M:1015:LEU:H    | 6:Y:5:C:N4        | 1.66                     | 0.93              |
| 3:N:521:PRO:HD2   | 3:N:524:LEU:HD22  | 1.49                     | 0.93              |
| 3:D:899:LEU:HD22  | 3:D:917:GLN:HB3   | 1.48                     | 0.93              |
| 3:N:1109:GLU:CG   | 3:N:1201:CYS:HA   | 1.97                     | 0.93              |
| 3:D:603:LEU:O     | 3:D:606:ILE:HG22  | 1.67                     | 0.93              |
| 3:D:739:ASP:H     | 6:H:15:C:H5''     | 1.33                     | 0.93              |
| 3:D:1095:THR:HG21 | 3:D:1230:GLY:HA3  | 1.49                     | 0.93              |
| 3:D:1256:LEU:HG   | 3:D:1260:ILE:HD11 | 1.50                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:144:PRO:HG2   | 2:M:265:ARG:NH1   | 1.83                     | 0.93              |
| 2:M:964:LYS:O     | 2:M:968:LEU:HG    | 1.69                     | 0.93              |
| 3:N:783:ARG:NE    | 3:N:1029:ARG:CD   | 2.29                     | 0.93              |
| 2:C:65:VAL:HB     | 2:C:101:ILE:HB    | 1.50                     | 0.93              |
| 3:D:1101:VAL:HG13 | 3:D:1428:ALA:HB2  | 1.47                     | 0.93              |
| 2:C:50:GLU:CA     | 2:C:266:ARG:CZ    | 2.46                     | 0.92              |
| 3:N:646:LYS:NZ    | 3:N:688:TRP:NE1   | 2.17                     | 0.92              |
| 3:N:1098:LEU:HD23 | 3:N:1226:ALA:HA   | 1.48                     | 0.92              |
| 3:N:1277:ILE:HD12 | 3:N:1301:LYS:HB2  | 1.51                     | 0.92              |
| 2:C:50:GLU:HA     | 2:C:266:ARG:NH2   | 1.83                     | 0.92              |
| 5:X:27:DC:OP2     | 5:X:27:DC:H6      | 1.51                     | 0.92              |
| 2:M:762:LYS:HA    | 2:M:786:LYS:HD2   | 1.50                     | 0.92              |
| 5:G:6:DT:H2''     | 5:G:7:DA:OP2      | 1.67                     | 0.92              |
| 5:X:4:DA:C2''     | 5:X:5:DC:H5''     | 1.98                     | 0.92              |
| 1:A:27:PRO:HG2    | 1:A:186:LEU:HD13  | 1.49                     | 0.92              |
| 2:M:157:ARG:NH1   | 2:M:314:THR:HB    | 1.84                     | 0.92              |
| 2:M:404:LEU:HA    | 2:M:407:LYS:CD    | 1.99                     | 0.92              |
| 3:N:455:ARG:HD3   | 3:N:463:GLN:HG3   | 1.51                     | 0.92              |
| 2:C:1034:GLU:HA   | 2:C:1037:VAL:HG23 | 1.51                     | 0.92              |
| 3:D:108:VAL:HB    | 3:D:109:PRO:HD3   | 1.51                     | 0.92              |
| 3:D:610:LYS:C     | 3:D:615:ARG:HG2   | 1.94                     | 0.92              |
| 3:N:600:LEU:HD12  | 3:N:600:LEU:H     | 1.33                     | 0.92              |
| 3:N:1435:LEU:CD2  | 3:N:1464:GLU:HB2  | 2.00                     | 0.92              |
| 3:D:1003:VAL:HG11 | 3:D:1036:ARG:HD2  | 1.51                     | 0.92              |
| 2:M:1097:LEU:H    | 2:M:1097:LEU:HD22 | 1.35                     | 0.92              |
| 3:D:864:VAL:HG12  | 3:D:865:THR:H     | 1.34                     | 0.92              |
| 3:N:701:LEU:HD12  | 3:N:701:LEU:H     | 1.32                     | 0.92              |
| 2:M:753:ASP:O     | 2:M:792:VAL:HG23  | 1.69                     | 0.91              |
| 3:N:618:LEU:CD1   | 3:N:1467:ILE:CD1  | 2.48                     | 0.91              |
| 3:N:783:ARG:CZ    | 3:N:1029:ARG:HD2  | 2.00                     | 0.91              |
| 1:A:176:ARG:NH1   | 2:C:865:THR:HB    | 1.85                     | 0.91              |
| 1:A:39:PRO:HG3    | 1:B:39:PRO:CG     | 2.00                     | 0.91              |
| 2:M:157:ARG:CZ    | 2:M:314:THR:HB    | 1.99                     | 0.91              |
| 2:M:843:HIS:CE1   | 2:M:884:GLN:HA    | 2.05                     | 0.91              |
| 1:A:222:LEU:HD23  | 1:B:219:ARG:HB2   | 1.49                     | 0.91              |
| 2:C:674:VAL:HG23  | 2:C:869:VAL:HG13  | 1.53                     | 0.91              |
| 3:D:882:PHE:O     | 3:D:886:VAL:HG23  | 1.70                     | 0.91              |
| 3:D:1095:THR:CG2  | 3:D:1230:GLY:HA3  | 2.00                     | 0.91              |
| 3:D:109:PRO:HB3   | 3:D:494:LYS:NZ    | 1.86                     | 0.91              |
| 3:D:1087:ARG:HG3  | 3:D:1236:LEU:CD2  | 1.97                     | 0.91              |
| 2:M:73:LEU:HB2    | 2:M:93:PRO:O      | 1.69                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:705:ALA:HB1   | 6:Y:14:G:H21      | 1.32                     | 0.91              |
| 3:N:882:PHE:O     | 3:N:886:VAL:HG23  | 1.70                     | 0.91              |
| 2:C:395:LYS:HE2   | 2:C:403:SER:HB2   | 1.50                     | 0.91              |
| 3:D:654:LYS:HB3   | 3:D:655:PRO:HD3   | 1.51                     | 0.91              |
| 4:E:54:LEU:HG     | 4:E:58:PRO:HG2    | 1.50                     | 0.91              |
| 3:N:860:LEU:HA    | 3:N:877:PRO:HB2   | 1.50                     | 0.91              |
| 3:D:897:TRP:CB    | 3:D:900:ILE:HD11  | 1.99                     | 0.91              |
| 2:C:861:LEU:HD23  | 2:C:863:ASP:N     | 1.85                     | 0.91              |
| 2:M:312:ALA:HB1   | 2:M:318:PRO:HG2   | 1.52                     | 0.91              |
| 3:D:610:LYS:O     | 3:D:615:ARG:HG2   | 1.70                     | 0.90              |
| 3:D:615:ARG:HH12  | 3:D:1096:ARG:NE   | 1.69                     | 0.90              |
| 3:D:1195:GLN:HG3  | 3:D:1196:THR:N    | 1.85                     | 0.90              |
| 4:E:40:LEU:HD21   | 4:E:67:GLU:HA     | 1.51                     | 0.90              |
| 2:M:490:GLU:HB3   | 2:M:493:ARG:NH1   | 1.84                     | 0.90              |
| 2:M:492:ASP:HB3   | 2:M:518:LYS:HD2   | 1.51                     | 0.90              |
| 3:N:698:LYS:HG2   | 4:O:59:ASN:CG     | 1.96                     | 0.90              |
| 2:M:490:GLU:HA    | 2:M:493:ARG:CD    | 2.00                     | 0.90              |
| 3:N:925:GLU:HB3   | 4:O:6:ILE:CG2     | 2.01                     | 0.90              |
| 3:N:1465:ASN:OD1  | 3:N:1473:PRO:HG3  | 1.71                     | 0.90              |
| 3:D:1066:THR:HG22 | 3:D:1069:GLU:CD   | 1.95                     | 0.90              |
| 2:M:631:SER:HB3   | 2:M:635:THR:H     | 1.36                     | 0.90              |
| 3:N:181:ASP:CB    | 3:N:441:ARG:HD3   | 2.01                     | 0.90              |
| 1:A:154:GLU:H     | 1:A:154:GLU:CD    | 1.77                     | 0.90              |
| 3:N:646:LYS:HZ2   | 3:N:688:TRP:NE1   | 1.69                     | 0.90              |
| 3:D:1112:CYS:H    | 3:D:1201:CYS:HB3  | 1.36                     | 0.90              |
| 3:D:1372:VAL:HA   | 3:D:1375:MET:HE3  | 1.52                     | 0.90              |
| 2:M:402:SER:HA    | 2:M:566:THR:HG23  | 1.52                     | 0.90              |
| 2:M:404:LEU:HA    | 2:M:407:LYS:HD2   | 1.51                     | 0.90              |
| 2:M:675:ALA:CA    | 2:M:989:VAL:HG12  | 2.02                     | 0.90              |
| 5:G:23:DG:N2      | 6:H:11:C:O2       | 2.05                     | 0.90              |
| 2:C:162:ILE:HB    | 2:C:172:ILE:HB    | 1.54                     | 0.90              |
| 3:D:1256:LEU:CG   | 3:D:1260:ILE:HD11 | 2.02                     | 0.90              |
| 3:D:1083:ASP:O    | 3:D:1087:ARG:HG2  | 1.70                     | 0.90              |
| 2:M:861:LEU:HD23  | 2:M:863:ASP:H     | 1.36                     | 0.90              |
| 3:D:900:ILE:O     | 3:D:902:LEU:HD23  | 1.70                     | 0.90              |
| 3:N:522:PRO:HA    | 3:N:525:ARG:NH1   | 1.86                     | 0.90              |
| 2:C:64:LEU:HD22   | 2:C:359:MET:HG3   | 1.51                     | 0.90              |
| 2:C:247:PRO:HD2   | 2:C:250:ARG:HH12  | 1.36                     | 0.89              |
| 1:K:7:LYS:HD2     | 1:K:186:LEU:HD21  | 1.51                     | 0.89              |
| 2:M:691:SER:OG    | 2:M:693:GLU:HB3   | 1.71                     | 0.89              |
| 3:N:108:VAL:HB    | 3:N:109:PRO:HD3   | 1.54                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1024:LYS:HB2  | 6:H:4:G:N2        | 1.86                     | 0.89              |
| 3:D:554:LEU:O     | 3:D:558:LEU:HG    | 1.71                     | 0.89              |
| 2:M:537:LYS:HD2   | 2:M:905:ILE:HD13  | 1.53                     | 0.89              |
| 7:Z:11:DG:H2''    | 7:Z:12:DT:OP2     | 1.70                     | 0.89              |
| 2:C:58:ASP:O      | 2:C:59:LYS:HB2    | 1.72                     | 0.89              |
| 3:D:1087:ARG:HE   | 3:D:1236:LEU:CD2  | 1.84                     | 0.89              |
| 3:N:1236:LEU:HD12 | 3:N:1256:LEU:HB2  | 1.54                     | 0.89              |
| 2:C:720:GLU:HG2   | 2:C:760:SER:HB3   | 1.54                     | 0.89              |
| 3:N:1280:VAL:HA   | 3:N:1318:TYR:HA   | 1.54                     | 0.89              |
| 1:L:28:LEU:HG     | 1:L:193:ASP:O     | 1.72                     | 0.89              |
| 1:K:178:ALA:HB2   | 2:M:864:GLY:N     | 1.88                     | 0.89              |
| 2:M:79:PRO:HG2    | 2:M:82:GLU:HB2    | 1.55                     | 0.89              |
| 2:M:328:LEU:HD13  | 2:M:433:THR:HB    | 1.53                     | 0.89              |
| 3:D:705:ALA:CB    | 3:D:706:PRO:HD3   | 2.02                     | 0.89              |
| 2:M:313:LEU:HD13  | 2:M:321:GLU:HG2   | 1.54                     | 0.89              |
| 2:M:650:ARG:HG2   | 2:M:653:ASP:HB2   | 1.53                     | 0.89              |
| 3:D:632:VAL:O     | 3:D:727:GLN:HA    | 1.73                     | 0.89              |
| 3:D:1109:GLU:CG   | 3:D:1201:CYS:HA   | 2.03                     | 0.89              |
| 2:C:312:ALA:HB1   | 2:C:318:PRO:HG2   | 1.54                     | 0.89              |
| 3:D:1438:ALA:N    | 3:D:1446:VAL:HG11 | 1.87                     | 0.89              |
| 2:M:676:ILE:HG22  | 2:M:988:VAL:O     | 1.73                     | 0.89              |
| 2:M:687:ALA:O     | 2:M:688:ILE:HD12  | 1.73                     | 0.89              |
| 2:M:918:LEU:HD23  | 2:M:968:LEU:HA    | 1.52                     | 0.89              |
| 5:X:14:DG:H2''    | 5:X:15:DC:OP2     | 1.72                     | 0.89              |
| 2:C:857:ASP:HB2   | 2:C:978:ARG:HG2   | 1.55                     | 0.89              |
| 3:N:1281:VAL:HG11 | 3:N:1313:VAL:HG13 | 1.54                     | 0.89              |
| 3:D:26:VAL:HG11   | 3:D:44:LEU:HD23   | 1.55                     | 0.88              |
| 2:M:437:ARG:C     | 2:M:438:ILE:HD12  | 1.98                     | 0.88              |
| 6:H:9:C:H2'       | 6:H:10:G:O4'      | 1.72                     | 0.88              |
| 3:N:697:GLY:HA2   | 3:N:717:GLN:NE2   | 1.87                     | 0.88              |
| 3:N:1305:LEU:HD12 | 3:N:1311:LEU:HD22 | 1.54                     | 0.88              |
| 3:N:27:GLU:HB3    | 3:N:41:ARG:HH12   | 1.36                     | 0.88              |
| 3:D:483:HIS:HB2   | 3:D:484:PRO:HD3   | 1.54                     | 0.88              |
| 2:M:688:ILE:HG22  | 2:M:849:VAL:HA    | 1.53                     | 0.88              |
| 3:D:582:LEU:HA    | 3:D:603:LEU:HD12  | 1.55                     | 0.88              |
| 2:M:445:GLU:HA    | 2:M:449:ILE:HD12  | 1.54                     | 0.88              |
| 5:X:19:DG:H2''    | 5:X:20:DC:H5'     | 1.56                     | 0.88              |
| 3:D:703:ASN:O     | 3:D:745:MET:HB3   | 1.74                     | 0.88              |
| 2:M:1095:LEU:HD11 | 3:N:603:LEU:HB3   | 1.55                     | 0.88              |
| 3:N:1128:VAL:HB   | 3:N:1133:ARG:NH2  | 1.88                     | 0.88              |
| 2:M:431:HIS:HB3   | 2:M:434:HIS:NE2   | 1.87                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:98:PRO:HG2    | 3:N:462:GLN:HE22  | 1.34                     | 0.88              |
| 4:O:54:LEU:HA     | 4:O:58:PRO:HG2    | 1.56                     | 0.88              |
| 5:X:7:DA:H2''     | 5:X:8:DC:H5'      | 1.54                     | 0.88              |
| 1:L:185:ARG:HH22  | 3:N:688:TRP:HB3   | 1.18                     | 0.88              |
| 2:M:273:GLY:HA2   | 2:M:276:LYS:HD2   | 1.56                     | 0.88              |
| 2:C:1045:ALA:HB1  | 2:C:1048:THR:HB   | 1.54                     | 0.88              |
| 2:C:1089:VAL:HG13 | 2:C:1099:VAL:HB   | 1.54                     | 0.88              |
| 3:D:136:ASP:CB    | 3:D:137:PRO:HD3   | 2.04                     | 0.88              |
| 3:D:1397:LYS:HZ1  | 3:D:1432:LYS:HE3  | 1.39                     | 0.88              |
| 6:H:7:G:O2'       | 6:H:8:G:H5'       | 1.73                     | 0.88              |
| 2:C:52:PHE:CE1    | 2:C:68:PHE:HB2    | 2.04                     | 0.87              |
| 3:D:1379:VAL:HG12 | 3:D:1419:PRO:HA   | 1.56                     | 0.87              |
| 2:M:1090:LYS:HZ3  | 2:M:1112:PHE:HE1  | 1.16                     | 0.87              |
| 1:A:42:ARG:HD3    | 1:B:35:THR:HA     | 1.54                     | 0.87              |
| 3:D:615:ARG:O     | 3:D:619:LEU:HG    | 1.74                     | 0.87              |
| 2:C:300:ASP:CG    | 2:C:300:ASP:O     | 2.16                     | 0.87              |
| 3:N:160:GLU:HG2   | 3:N:165:LYS:HG3   | 1.56                     | 0.87              |
| 3:N:456:MET:HA    | 3:N:460:ALA:HB2   | 1.55                     | 0.87              |
| 3:N:482:LYS:HE2   | 3:N:1384:PRO:HD2  | 1.56                     | 0.87              |
| 5:X:15:DC:H1'     | 5:X:16:DT:H5'     | 1.56                     | 0.87              |
| 2:M:31:GLN:HB3    | 2:M:71:TYR:OH     | 1.72                     | 0.87              |
| 2:M:328:LEU:HD22  | 2:M:433:THR:HG22  | 1.55                     | 0.87              |
| 3:N:132:TYR:HD2   | 3:N:154:THR:HB    | 1.39                     | 0.87              |
| 3:N:465:LEU:HD22  | 3:N:510:GLU:HA    | 1.54                     | 0.87              |
| 3:N:897:TRP:HA    | 3:N:900:ILE:HG12  | 1.55                     | 0.87              |
| 2:M:65:VAL:HB     | 2:M:101:ILE:HB    | 1.56                     | 0.87              |
| 2:M:211:LEU:HB2   | 2:M:308:ARG:HD2   | 1.55                     | 0.87              |
| 3:N:520:LEU:HD23  | 3:N:525:ARG:HD2   | 1.56                     | 0.87              |
| 3:N:952:ASP:HA    | 3:N:1062:ARG:HH21 | 1.36                     | 0.87              |
| 7:Z:1:DG:H3'      | 7:Z:1:DG:P        | 2.15                     | 0.87              |
| 3:D:796:ARG:HB2   | 3:D:828:LYS:HD3   | 1.57                     | 0.87              |
| 3:D:799:LYS:HB3   | 3:D:826:PRO:HG2   | 1.57                     | 0.87              |
| 3:N:646:LYS:HE3   | 3:N:688:TRP:CZ2   | 2.09                     | 0.87              |
| 5:G:19:DG:H2''    | 5:G:20:DC:O5'     | 1.74                     | 0.87              |
| 2:C:796:GLU:HB2   | 2:C:1004:LYS:HZ3  | 1.40                     | 0.87              |
| 3:D:900:ILE:HD12  | 3:D:902:LEU:CD2   | 2.04                     | 0.87              |
| 3:N:814:ALA:HB1   | 3:N:818:ARG:NH2   | 1.88                     | 0.87              |
| 3:N:1295:GLU:HG2  | 3:N:1300:SER:HB3  | 1.54                     | 0.87              |
| 2:C:31:GLN:CD     | 2:C:71:TYR:HH     | 1.83                     | 0.86              |
| 2:M:143:SER:HB2   | 2:M:276:LYS:HE2   | 1.55                     | 0.86              |
| 3:N:1486:VAL:HA   | 4:O:74:VAL:O      | 1.74                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:36:PRO:HG2    | 2:C:70:GLU:HB3    | 1.55                     | 0.86              |
| 3:D:1434:TRP:CZ3  | 3:D:1455:LYS:HB3  | 2.10                     | 0.86              |
| 2:M:328:LEU:HD23  | 2:M:437:ARG:HD3   | 1.55                     | 0.86              |
| 4:O:9:LEU:HA      | 4:O:12:MET:SD     | 2.15                     | 0.86              |
| 7:Z:1:DG:H3'      | 7:Z:1:DG:OP3      | 1.75                     | 0.86              |
| 1:A:104:GLU:HA    | 1:A:136:GLY:O     | 1.75                     | 0.86              |
| 3:D:522:PRO:HA    | 3:D:525:ARG:NH1   | 1.90                     | 0.86              |
| 2:M:260:LEU:HB3   | 2:M:291:ALA:CB    | 2.06                     | 0.86              |
| 2:M:479:VAL:HG22  | 2:M:506:ASN:HA    | 1.57                     | 0.86              |
| 3:N:1129:THR:HG23 | 3:N:1130:ARG:H    | 1.39                     | 0.86              |
| 2:C:129:ILE:HD12  | 2:C:129:ILE:N     | 1.90                     | 0.86              |
| 3:N:693:GLU:HA    | 4:O:48:MET:HE2    | 1.55                     | 0.86              |
| 2:C:90:TYR:O      | 2:C:119:PRO:HA    | 1.74                     | 0.86              |
| 3:D:1330:ILE:HD13 | 3:D:1347:TYR:OH   | 1.74                     | 0.86              |
| 2:M:987:ILE:HG23  | 3:N:948:THR:HG21  | 1.54                     | 0.86              |
| 2:M:1016:ILE:H    | 2:M:1016:ILE:HD13 | 1.37                     | 0.86              |
| 2:C:270:GLY:O     | 2:C:274:ARG:HB3   | 1.76                     | 0.86              |
| 3:D:1426:LYS:HA   | 3:D:1429:LEU:HD22 | 1.57                     | 0.86              |
| 2:M:139:GLN:OE1   | 2:M:415:PRO:HD3   | 1.76                     | 0.86              |
| 3:N:1209:LEU:HD23 | 3:N:1210:SER:H    | 1.41                     | 0.86              |
| 5:G:17:DA:H2''    | 5:G:18:DC:C5'     | 2.04                     | 0.86              |
| 3:D:834:THR:HG22  | 3:D:838:ARG:HH11  | 1.39                     | 0.86              |
| 4:E:36:LYS:N      | 4:E:95:VAL:HG21   | 1.91                     | 0.86              |
| 3:N:524:LEU:O     | 3:N:526:PRO:HD3   | 1.75                     | 0.86              |
| 3:N:632:VAL:O     | 3:N:727:GLN:HA    | 1.75                     | 0.86              |
| 3:N:899:LEU:CB    | 3:N:917:GLN:HG2   | 2.05                     | 0.86              |
| 2:C:326:ASP:HB2   | 2:C:431:HIS:ND1   | 1.91                     | 0.86              |
| 2:C:579:VAL:HG13  | 2:C:842:ARG:HH22  | 1.39                     | 0.86              |
| 2:C:690:ILE:HG12  | 2:C:691:SER:N     | 1.91                     | 0.86              |
| 2:M:808:ARG:HH21  | 2:M:820:ARG:HH21  | 1.17                     | 0.86              |
| 3:N:73:CYS:HB3    | 3:N:76:CYS:O      | 1.75                     | 0.86              |
| 3:N:522:PRO:HA    | 3:N:525:ARG:HH11  | 1.37                     | 0.86              |
| 7:Z:11:DG:C2'     | 7:Z:12:DT:H71     | 2.06                     | 0.86              |
| 2:C:872:ASN:OD1   | 2:C:874:LEU:HB2   | 1.76                     | 0.86              |
| 3:D:1103:HIS:CG   | 3:D:1104:GLU:H    | 1.94                     | 0.86              |
| 2:C:49:ARG:HA     | 2:C:52:PHE:HB3    | 1.57                     | 0.85              |
| 3:D:628:ARG:HE    | 5:G:22:DA:H4'     | 1.41                     | 0.85              |
| 1:B:74:ASP:HB3    | 3:D:872:ARG:HH22  | 1.39                     | 0.85              |
| 2:M:679:PHE:C     | 3:N:943:THR:HG22  | 2.00                     | 0.85              |
| 3:N:166:GLN:O     | 3:N:167:GLU:CB    | 2.21                     | 0.85              |
| 3:N:498:VAL:O     | 3:N:501:ALA:HB3   | 1.77                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:660:LYS:HD2   | 3:N:694:VAL:HG22  | 1.56                     | 0.85              |
| 4:O:40:LEU:HD21   | 4:O:67:GLU:HA     | 1.57                     | 0.85              |
| 3:D:486:ARG:HA    | 3:D:489:ARG:HG2   | 1.57                     | 0.85              |
| 3:D:1093:TYR:CE1  | 5:G:17:DA:H1'     | 2.10                     | 0.85              |
| 3:N:1485:GLN:HG3  | 4:O:79:LEU:N      | 1.91                     | 0.85              |
| 3:N:618:LEU:HD12  | 3:N:1467:ILE:CD1  | 2.07                     | 0.85              |
| 2:M:342:ASP:O     | 2:M:346:VAL:HG23  | 1.77                     | 0.85              |
| 3:N:693:GLU:HG3   | 4:O:48:MET:SD     | 2.16                     | 0.85              |
| 3:N:1094:LEU:HD12 | 3:N:1097:LYS:HD2  | 1.57                     | 0.85              |
| 2:C:18:LEU:H      | 2:C:18:LEU:HD12   | 1.41                     | 0.85              |
| 2:M:270:GLY:O     | 2:M:274:ARG:HB3   | 1.76                     | 0.85              |
| 3:N:1093:TYR:CE1  | 5:X:18:DC:H5''    | 2.11                     | 0.85              |
| 7:Z:12:DT:H2''    | 7:Z:13:DA:C8      | 2.11                     | 0.85              |
| 1:A:178:ALA:HB2   | 2:C:864:GLY:H     | 1.38                     | 0.85              |
| 2:C:16:PRO:HD3    | 2:C:458:TYR:CD2   | 2.12                     | 0.85              |
| 3:D:906:GLN:HB3   | 3:D:911:LEU:HD11  | 1.56                     | 0.85              |
| 1:L:24:VAL:HG13   | 1:L:196:THR:HG22  | 1.59                     | 0.85              |
| 3:N:1114:THR:HB   | 3:N:1195:GLN:HB3  | 1.59                     | 0.85              |
| 3:D:1194:CYS:HB2  | 3:D:1204:CYS:SG   | 2.17                     | 0.85              |
| 3:D:52:PRO:HD2    | 3:D:85:VAL:HG21   | 1.59                     | 0.85              |
| 1:B:228:PRO:O     | 1:B:229:GLN:HG3   | 1.77                     | 0.84              |
| 2:C:918:LEU:HB3   | 2:C:968:LEU:HD23  | 1.58                     | 0.84              |
| 3:D:1438:ALA:CA   | 3:D:1446:VAL:HG11 | 2.05                     | 0.84              |
| 4:E:54:LEU:HA     | 4:E:58:PRO:HG2    | 1.58                     | 0.84              |
| 2:M:758:ARG:HB3   | 2:M:788:THR:O     | 1.76                     | 0.84              |
| 4:O:54:LEU:CD2    | 4:O:63:TRP:HE1    | 1.90                     | 0.84              |
| 3:N:1128:VAL:HG12 | 3:N:1129:THR:HG22 | 1.59                     | 0.84              |
| 5:X:24:DC:H2''    | 5:X:25:DG:H5'     | 1.59                     | 0.84              |
| 2:C:281:LEU:HD12  | 2:C:309:TYR:HB2   | 1.58                     | 0.84              |
| 2:M:862:PRO:HB3   | 2:M:929:ARG:HH22  | 1.40                     | 0.84              |
| 3:N:864:VAL:HG12  | 3:N:865:THR:H     | 1.40                     | 0.84              |
| 2:M:165:LEU:HG    | 2:M:166:PRO:HA    | 1.58                     | 0.84              |
| 6:Y:6:C:H3'       | 6:Y:7:G:C8        | 2.13                     | 0.84              |
| 2:M:63:GLY:HA3    | 2:M:103:LYS:HG3   | 1.58                     | 0.84              |
| 3:D:52:PRO:HG2    | 3:D:80:VAL:HG13   | 1.58                     | 0.84              |
| 3:D:1216:SER:CB   | 4:E:16:LYS:H      | 1.89                     | 0.84              |
| 2:M:887:GLU:OE2   | 2:M:992:MET:HE2   | 1.76                     | 0.84              |
| 2:C:302:VAL:O     | 2:C:305:PRO:HD2   | 1.77                     | 0.84              |
| 3:D:117:ASP:HB2   | 3:D:495:ARG:NH1   | 1.93                     | 0.84              |
| 2:M:396:ASP:HB3   | 2:M:406:HIS:CD2   | 2.11                     | 0.84              |
| 2:M:936:VAL:HA    | 2:M:940:GLU:OE2   | 1.77                     | 0.84              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:19:ARG:NH2    | 3:N:516:ALA:HB2  | 1.93                     | 0.84              |
| 3:N:1274:ILE:HG22 | 3:N:1301:LYS:HZ1 | 1.43                     | 0.84              |
| 1:A:106:PRO:HG3   | 1:A:134:GLU:CD   | 2.03                     | 0.84              |
| 2:C:1081:VAL:HB   | 2:C:1086:ARG:HE  | 1.40                     | 0.84              |
| 3:D:737:ASN:HB3   | 6:H:15:C:O2'     | 1.77                     | 0.84              |
| 3:D:743:ASP:OD2   | 6:H:14:G:H4'     | 1.76                     | 0.84              |
| 2:M:676:ILE:HG12  | 2:M:873:PRO:HG3  | 1.59                     | 0.84              |
| 3:N:767:HIS:CD2   | 4:O:6:ILE:HG12   | 2.11                     | 0.84              |
| 2:C:1090:LYS:NZ   | 3:D:21:TRP:HB3   | 1.93                     | 0.84              |
| 1:B:100:LEU:HD12  | 1:B:115:LEU:HD21 | 1.57                     | 0.83              |
| 2:C:395:LYS:HE3   | 2:C:407:LYS:HD2  | 1.59                     | 0.83              |
| 1:K:76:VAL:O      | 1:K:79:ILE:HG13  | 1.77                     | 0.83              |
| 3:N:477:LEU:CD1   | 3:N:496:LEU:HD13 | 2.07                     | 0.83              |
| 3:N:483:HIS:HB2   | 3:N:484:PRO:CD   | 2.07                     | 0.83              |
| 3:D:10:ILE:HG22   | 3:D:1451:ALA:HA  | 1.60                     | 0.83              |
| 1:K:178:ALA:CB    | 2:M:864:GLY:H    | 1.89                     | 0.83              |
| 2:M:1083:GLU:OE1  | 2:M:1086:ARG:HD2 | 1.78                     | 0.83              |
| 3:N:12:LEU:HD22   | 3:N:511:TRP:HB2  | 1.61                     | 0.83              |
| 3:N:1292:VAL:HG23 | 3:N:1305:LEU:HG  | 1.60                     | 0.83              |
| 2:M:490:GLU:CA    | 2:M:493:ARG:HD3  | 2.06                     | 0.83              |
| 1:K:9:PRO:HB3     | 1:K:25:LEU:HG    | 1.60                     | 0.83              |
| 1:K:176:ARG:NH1   | 2:M:865:THR:HB   | 1.92                     | 0.83              |
| 1:L:185:ARG:HH22  | 3:N:688:TRP:HB2  | 1.43                     | 0.83              |
| 2:M:44:ILE:HG22   | 2:M:45:GLN:N     | 1.94                     | 0.83              |
| 1:A:112:ARG:HH21  | 1:A:125:PRO:HB2  | 1.43                     | 0.83              |
| 2:C:144:PRO:HG2   | 2:C:265:ARG:HH11 | 1.43                     | 0.83              |
| 3:D:1033:GLN:O    | 3:D:1037:GLN:HB3 | 1.78                     | 0.83              |
| 2:M:313:LEU:HB2   | 2:M:321:GLU:HG3  | 1.59                     | 0.83              |
| 2:M:675:ALA:HA    | 2:M:989:VAL:CG1  | 2.04                     | 0.83              |
| 2:C:20:GLU:HG2    | 2:C:21:ILE:HD12  | 1.58                     | 0.83              |
| 2:C:1034:GLU:HA   | 2:C:1037:VAL:CG2 | 2.08                     | 0.83              |
| 3:D:614:PHE:CE2   | 3:D:1443:THR:HB  | 2.14                     | 0.83              |
| 2:M:404:LEU:O     | 2:M:407:LYS:HB2  | 1.78                     | 0.83              |
| 2:C:260:LEU:HB3   | 2:C:291:ALA:CB   | 2.08                     | 0.83              |
| 2:C:388:ARG:HD2   | 5:G:27:DC:H4'    | 1.58                     | 0.83              |
| 2:C:684:PHE:N     | 2:C:687:ALA:HB3  | 1.92                     | 0.83              |
| 2:C:861:LEU:HD21  | 2:C:925:TYR:CE2  | 2.14                     | 0.83              |
| 3:D:65:ARG:HG3    | 3:D:66:GLN:H     | 1.44                     | 0.83              |
| 3:D:1472:ILE:H    | 3:D:1472:ILE:CD1 | 1.83                     | 0.83              |
| 2:M:162:ILE:HB    | 2:M:172:ILE:HB   | 1.60                     | 0.83              |
| 7:Z:1:DG:H2''     | 7:Z:2:DT:OP2     | 1.78                     | 0.83              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:922:PHE:HB3   | 2:C:964:LYS:NZ   | 1.94                     | 0.83              |
| 3:D:705:ALA:HB3   | 3:D:706:PRO:CD   | 2.08                     | 0.83              |
| 4:E:41:GLU:HG2    | 4:E:42:PRO:HD3   | 1.61                     | 0.83              |
| 2:M:186:VAL:HG23  | 2:M:187:ASN:H    | 1.43                     | 0.83              |
| 3:N:796:ARG:HH21  | 3:N:862:ASP:CG   | 1.86                     | 0.83              |
| 3:D:738:ALA:HA    | 6:H:15:C:H4'     | 1.60                     | 0.83              |
| 2:M:34:VAL:HB     | 2:M:38:LYS:HG3   | 1.58                     | 0.83              |
| 3:N:675:ARG:O     | 3:N:678:GLU:HG2  | 1.79                     | 0.83              |
| 3:N:1128:VAL:HG13 | 3:N:1320:GLU:OE2 | 1.79                     | 0.83              |
| 3:D:646:LYS:HG3   | 3:D:647:ARG:H    | 1.43                     | 0.82              |
| 4:E:28:GLN:HB3    | 4:E:32:ARG:HH12  | 1.43                     | 0.82              |
| 3:N:646:LYS:HD2   | 3:N:688:TRP:CE2  | 2.13                     | 0.82              |
| 5:X:13:DA:H2''    | 5:X:14:DG:OP2    | 1.77                     | 0.82              |
| 3:D:728:LEU:HD11  | 3:D:732:VAL:HG21 | 1.58                     | 0.82              |
| 3:D:1211:MET:HG2  | 3:D:1212:ALA:N   | 1.90                     | 0.82              |
| 3:N:1201:CYS:SG   | 3:N:1204:CYS:N   | 2.51                     | 0.82              |
| 3:D:1046:GLN:HA   | 3:D:1052:THR:HA  | 1.61                     | 0.82              |
| 3:N:625:TYR:CZ    | 3:N:655:PRO:HG2  | 2.13                     | 0.82              |
| 2:C:199:VAL:HG13  | 2:C:235:LEU:HG   | 1.62                     | 0.82              |
| 3:D:899:LEU:HD22  | 3:D:917:GLN:HG3  | 1.60                     | 0.82              |
| 3:N:758:GLU:HB3   | 4:O:20:THR:HG21  | 1.61                     | 0.82              |
| 5:X:11:DC:H2''    | 5:X:12:DA:OP2    | 1.77                     | 0.82              |
| 2:C:739:GLU:CG    | 2:C:742:VAL:HB   | 2.08                     | 0.82              |
| 2:C:861:LEU:CD2   | 2:C:863:ASP:H    | 1.89                     | 0.82              |
| 3:N:625:TYR:OH    | 3:N:655:PRO:CG   | 2.23                     | 0.82              |
| 2:C:191:PHE:HB2   | 2:C:241:LEU:HD11 | 1.62                     | 0.82              |
| 2:C:945:ARG:HG2   | 2:C:949:LYS:HE3  | 1.59                     | 0.82              |
| 3:D:530:VAL:O     | 6:H:4:G:H5'      | 1.80                     | 0.82              |
| 3:D:951:ILE:HD12  | 3:D:1062:ARG:HE  | 1.43                     | 0.82              |
| 2:M:403:SER:O     | 2:M:407:LYS:HG3  | 1.79                     | 0.82              |
| 3:N:486:ARG:HA    | 3:N:489:ARG:HG2  | 1.62                     | 0.82              |
| 6:Y:5:C:H2'       | 6:Y:5:C:O2       | 1.77                     | 0.82              |
| 7:Z:5:DC:H2''     | 7:Z:6:DT:OP2     | 1.79                     | 0.82              |
| 1:A:152:PRO:HB3   | 1:A:154:GLU:OE1  | 1.80                     | 0.82              |
| 2:C:15:LEU:HD12   | 2:C:15:LEU:H     | 1.44                     | 0.82              |
| 2:C:724:ARG:HG3   | 2:C:737:LEU:HD22 | 1.60                     | 0.82              |
| 3:D:54:LYS:NZ     | 6:H:2:C:OP1      | 2.12                     | 0.82              |
| 3:N:607:LEU:HD23  | 3:N:613:ARG:HB3  | 1.61                     | 0.82              |
| 3:D:907:GLU:HG2   | 3:D:908:LYS:N    | 1.93                     | 0.82              |
| 3:D:1189:ARG:HD2  | 3:D:1204:CYS:SG  | 2.20                     | 0.82              |
| 2:C:129:ILE:N     | 2:C:129:ILE:CD1  | 2.42                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:628:ARG:NE    | 5:G:22:DA:H4'     | 1.95                     | 0.82              |
| 2:M:1040:LEU:HD23 | 2:M:1049:LEU:CD1  | 2.10                     | 0.82              |
| 3:N:646:LYS:HZ2   | 3:N:688:TRP:CD1   | 1.97                     | 0.82              |
| 2:C:404:LEU:HA    | 2:C:407:LYS:HD3   | 1.62                     | 0.82              |
| 3:D:656:PHE:HB3   | 3:D:694:VAL:HG11  | 1.62                     | 0.82              |
| 2:M:338:GLU:O     | 2:M:341:THR:HG22  | 1.79                     | 0.82              |
| 2:M:579:VAL:HG13  | 2:M:842:ARG:HH22  | 1.44                     | 0.82              |
| 2:C:328:LEU:HD11  | 2:C:434:HIS:CD2   | 2.15                     | 0.81              |
| 3:D:641:GLN:HB3   | 3:D:717:GLN:O     | 1.79                     | 0.81              |
| 3:N:899:LEU:HB2   | 3:N:917:GLN:HG2   | 1.62                     | 0.81              |
| 3:N:1059:SER:HB2  | 3:N:1065:LEU:HD12 | 1.62                     | 0.81              |
| 4:O:54:LEU:HD21   | 4:O:63:TRP:HE1    | 1.42                     | 0.81              |
| 2:C:265:ARG:HB3   | 2:C:267:TYR:CD2   | 2.15                     | 0.81              |
| 2:C:674:VAL:HG12  | 2:C:990:GLY:O     | 1.80                     | 0.81              |
| 2:C:1016:ILE:HG12 | 2:C:1017:THR:N    | 1.95                     | 0.81              |
| 3:D:631:ILE:CD1   | 3:D:743:ASP:HB2   | 2.09                     | 0.81              |
| 3:D:1041:LEU:HD13 | 3:D:1045:MET:SD   | 2.18                     | 0.81              |
| 1:L:110:LYS:HD3   | 1:L:126:ASP:HA    | 1.62                     | 0.81              |
| 3:N:609:GLY:O     | 3:N:615:ARG:HB2   | 1.79                     | 0.81              |
| 5:G:5:DC:H2''     | 5:G:6:DT:C5'      | 2.09                     | 0.81              |
| 3:D:631:ILE:HD11  | 3:D:743:ASP:HB2   | 1.62                     | 0.81              |
| 3:D:1410:GLU:CG   | 2:M:374:ASN:HA    | 2.10                     | 0.81              |
| 2:M:617:ASP:CG    | 2:M:619:ARG:HE    | 1.88                     | 0.81              |
| 3:N:183:GLU:HG2   | 3:N:184:GLU:N     | 1.95                     | 0.81              |
| 3:N:1389:LEU:CG   | 3:N:1390:LEU:H    | 1.93                     | 0.81              |
| 3:D:711:LEU:HD12  | 3:D:778:LEU:HD23  | 1.61                     | 0.81              |
| 7:Z:11:DG:H8      | 7:Z:11:DG:OP2     | 1.61                     | 0.81              |
| 3:D:744:GLN:NE2   | 5:G:21:DG:H21     | 1.79                     | 0.81              |
| 2:M:1014:SER:HB3  | 2:M:1017:THR:O    | 1.80                     | 0.81              |
| 5:G:21:DG:H2''    | 5:G:22:DA:C5'     | 2.11                     | 0.81              |
| 3:D:1087:ARG:HE   | 3:D:1236:LEU:HD21 | 1.43                     | 0.81              |
| 3:D:1098:LEU:HD23 | 3:D:1226:ALA:HA   | 1.61                     | 0.81              |
| 1:L:80:LEU:HG     | 3:N:844:ALA:HA    | 1.63                     | 0.81              |
| 1:L:185:ARG:HH12  | 3:N:688:TRP:HB3   | 1.43                     | 0.81              |
| 5:X:7:DA:H2'      | 5:X:8:DC:C6       | 2.15                     | 0.81              |
| 2:C:1041:GLU:HB3  | 3:D:1223:ILE:HG12 | 1.61                     | 0.81              |
| 2:C:1060:ILE:HG23 | 2:C:1061:GLU:H    | 1.43                     | 0.81              |
| 3:D:52:PRO:HD2    | 3:D:85:VAL:CG2    | 2.11                     | 0.81              |
| 3:D:1460:ILE:O    | 3:D:1460:ILE:HG13 | 1.78                     | 0.81              |
| 1:B:24:VAL:HG13   | 1:B:196:THR:HG22  | 1.63                     | 0.81              |
| 2:C:49:ARG:HA     | 2:C:52:PHE:CB     | 2.11                     | 0.81              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:263:ASP:HB2   | 2:C:264:PRO:HD3  | 1.60                     | 0.81              |
| 3:D:1109:GLU:CD   | 3:D:1202:GLN:H   | 1.88                     | 0.81              |
| 3:N:581:LEU:HD23  | 3:N:581:LEU:H    | 1.43                     | 0.81              |
| 2:C:186:VAL:HG23  | 2:C:187:ASN:H    | 1.44                     | 0.81              |
| 2:C:928:LYS:NZ    | 2:C:932:GLU:HG3  | 1.96                     | 0.81              |
| 2:C:1014:SER:HB3  | 2:C:1017:THR:O   | 1.80                     | 0.81              |
| 3:D:696:HIS:CD2   | 4:E:59:ASN:N     | 2.48                     | 0.81              |
| 3:D:897:TRP:HA    | 3:D:900:ILE:CD1  | 2.11                     | 0.81              |
| 2:M:611:ILE:HD11  | 2:M:641:PRO:HG3  | 1.63                     | 0.81              |
| 2:M:875:GLY:HA2   | 3:N:1029:ARG:NH2 | 1.96                     | 0.81              |
| 3:N:481:MET:HE2   | 3:N:493:ARG:HA   | 1.61                     | 0.81              |
| 3:N:639:LEU:HD12  | 3:N:640:HIS:H    | 1.45                     | 0.81              |
| 2:C:918:LEU:HD23  | 2:C:968:LEU:HA   | 1.62                     | 0.80              |
| 3:D:637:LEU:HD11  | 3:D:642:CYS:HA   | 1.61                     | 0.80              |
| 3:D:1216:SER:HB3  | 4:E:16:LYS:H     | 1.44                     | 0.80              |
| 3:D:1472:ILE:HD13 | 3:D:1472:ILE:N   | 1.94                     | 0.80              |
| 3:N:1435:LEU:HD23 | 3:N:1464:GLU:CB  | 2.06                     | 0.80              |
| 2:C:141:HIS:NE2   | 2:C:332:ARG:HB3  | 1.97                     | 0.80              |
| 2:C:328:LEU:HD13  | 2:C:433:THR:CB   | 2.09                     | 0.80              |
| 2:C:328:LEU:CD1   | 2:C:433:THR:HB   | 2.09                     | 0.80              |
| 2:C:457:ALA:HB3   | 2:C:538:GLN:HA   | 1.64                     | 0.80              |
| 2:C:1115:LEU:CG   | 3:D:85:VAL:HG12  | 2.10                     | 0.80              |
| 3:D:671:LYS:O     | 3:D:675:ARG:HG3  | 1.80                     | 0.80              |
| 3:D:989:TYR:HH    | 3:D:1051:GLU:HG3 | 1.44                     | 0.80              |
| 2:M:157:ARG:HD3   | 2:M:314:THR:CG2  | 2.11                     | 0.80              |
| 2:M:437:ARG:NH2   | 2:M:488:ALA:HA   | 1.96                     | 0.80              |
| 3:N:638:LYS:HD3   | 3:N:932:ASP:OD2  | 1.81                     | 0.80              |
| 3:N:728:LEU:HD12  | 3:N:729:HIS:H    | 1.46                     | 0.80              |
| 5:G:17:DA:C2'     | 5:G:18:DC:H5'    | 2.11                     | 0.80              |
| 2:C:31:GLN:HB3    | 2:C:71:TYR:OH    | 1.82                     | 0.80              |
| 3:D:610:LYS:HB2   | 5:G:18:DC:OP2    | 1.81                     | 0.80              |
| 2:M:304:LEU:HD23  | 2:M:305:PRO:HD3  | 1.60                     | 0.80              |
| 3:N:36:THR:C      | 3:N:38:LYS:H     | 1.89                     | 0.80              |
| 7:I:3:DA:H1'      | 7:I:4:DG:C5'     | 2.10                     | 0.80              |
| 2:C:831:ARG:HH12  | 2:C:1004:LYS:HG2 | 1.46                     | 0.80              |
| 2:C:676:ILE:HG22  | 2:C:988:VAL:O    | 1.82                     | 0.80              |
| 2:C:697:ARG:O     | 2:C:699:PHE:N    | 2.14                     | 0.80              |
| 3:D:50:PHE:O      | 3:D:86:ARG:HA    | 1.81                     | 0.80              |
| 3:D:899:LEU:CD2   | 3:D:917:GLN:HG3  | 2.10                     | 0.80              |
| 3:D:1191:PRO:O    | 3:D:1373:ARG:NH1 | 2.14                     | 0.80              |
| 2:C:266:ARG:HA    | 2:C:288:ARG:CD   | 2.10                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:431:HIS:H     | 2:C:434:HIS:CE1   | 2.00                     | 0.80              |
| 2:C:683:ASN:O     | 2:C:872:ASN:HB2   | 1.80                     | 0.80              |
| 3:D:771:SER:HB3   | 3:D:778:LEU:HD13  | 1.64                     | 0.80              |
| 1:A:42:ARG:NH1    | 1:B:34:VAL:HB     | 1.97                     | 0.80              |
| 3:D:1088:THR:HG23 | 3:D:1234:THR:CG2  | 2.12                     | 0.80              |
| 3:D:1242:HIS:HB2  | 3:D:1251:ASP:HB2  | 1.64                     | 0.80              |
| 3:D:1425:THR:O    | 3:D:1429:LEU:HD13 | 1.81                     | 0.80              |
| 3:N:181:ASP:HB3   | 3:N:441:ARG:CD    | 2.11                     | 0.80              |
| 3:N:615:ARG:O     | 3:N:619:LEU:HG    | 1.82                     | 0.80              |
| 3:N:1213:ARG:HH22 | 4:O:14:ASP:HA     | 1.44                     | 0.80              |
| 1:B:212:ASN:O     | 1:B:215:VAL:HG22  | 1.80                     | 0.80              |
| 3:N:693:GLU:O     | 4:O:48:MET:HE1    | 1.82                     | 0.80              |
| 2:C:52:PHE:HZ     | 2:C:68:PHE:HB2    | 1.37                     | 0.79              |
| 3:D:565:ILE:HD12  | 3:D:565:ILE:N     | 1.97                     | 0.79              |
| 3:D:792:ILE:O     | 3:D:878:GLY:HA3   | 1.82                     | 0.79              |
| 3:D:1088:THR:HG23 | 3:D:1234:THR:HG23 | 1.63                     | 0.79              |
| 3:N:136:ASP:CB    | 3:N:137:PRO:HD3   | 2.11                     | 0.79              |
| 3:N:1472:ILE:H    | 3:N:1472:ILE:CD1  | 1.85                     | 0.79              |
| 4:O:34:GLY:HA3    | 4:O:95:VAL:HB     | 1.64                     | 0.79              |
| 5:X:8:DC:H2"      | 5:X:9:DC:OP2      | 1.82                     | 0.79              |
| 1:A:88:ARG:HD2    | 1:A:204:SER:O     | 1.82                     | 0.79              |
| 2:M:89:THR:HG21   | 2:M:383:ARG:NH2   | 1.94                     | 0.79              |
| 2:M:1067:TYR:O    | 2:M:1071:ILE:HG12 | 1.82                     | 0.79              |
| 3:N:493:ARG:CZ    | 3:N:1391:GLU:HA   | 2.12                     | 0.79              |
| 2:C:976:ASP:CG    | 2:C:979:THR:HG22  | 2.06                     | 0.79              |
| 1:L:92:PRO:HA     | 1:L:146:ARG:HH12  | 1.45                     | 0.79              |
| 3:D:1096:ARG:NH2  | 3:D:1440:PHE:HD2  | 1.77                     | 0.79              |
| 1:K:177:VAL:O     | 2:M:864:GLY:HA2   | 1.82                     | 0.79              |
| 3:N:1166:LEU:H    | 3:N:1166:LEU:HD23 | 1.48                     | 0.79              |
| 6:H:15:C:OP2      | 6:H:15:C:H6       | 1.66                     | 0.79              |
| 2:C:831:ARG:NH1   | 2:C:1004:LYS:HG2  | 1.98                     | 0.79              |
| 2:M:693:GLU:CG    | 2:M:697:ARG:HH21  | 1.95                     | 0.79              |
| 2:M:1000:MET:HB2  | 2:M:1002:GLU:HG2  | 1.63                     | 0.79              |
| 3:N:646:LYS:CD    | 3:N:688:TRP:CZ2   | 2.66                     | 0.79              |
| 3:N:1389:LEU:HG   | 3:N:1390:LEU:H    | 1.47                     | 0.79              |
| 2:C:498:GLN:OE1   | 3:D:1067:VAL:HB   | 1.81                     | 0.79              |
| 1:L:137:ARG:NH2   | 1:L:139:ASN:HB3   | 1.97                     | 0.79              |
| 2:M:445:GLU:HA    | 2:M:449:ILE:CD1   | 2.11                     | 0.79              |
| 3:N:111:LYS:HG2   | 3:N:1448:THR:HG22 | 1.63                     | 0.79              |
| 3:D:700:VAL:O     | 3:D:715:ALA:HA    | 1.82                     | 0.79              |
| 1:L:26:GLU:HB2    | 1:L:27:PRO:HA     | 1.61                     | 0.79              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:398:THR:N     | 2:M:633:GLN:HG2  | 1.97                     | 0.79              |
| 2:M:939:ARG:HA    | 2:M:939:ARG:NE   | 1.97                     | 0.79              |
| 3:N:1200:VAL:HG13 | 3:N:1204:CYS:HB2 | 1.64                     | 0.79              |
| 7:Z:2:DT:H1'      | 7:Z:3:DA:H5'     | 1.63                     | 0.79              |
| 3:D:704:ARG:HB2   | 3:D:745:MET:HE3  | 1.62                     | 0.79              |
| 3:D:960:LYS:CE    | 3:D:964:LEU:HD12 | 2.12                     | 0.79              |
| 3:N:754:PHE:CA    | 4:O:24:ALA:HB1   | 2.08                     | 0.79              |
| 3:D:17:LYS:O      | 3:D:20:SER:HB3   | 1.81                     | 0.79              |
| 4:O:43:GLU:HG3    | 4:O:44:GLU:H     | 1.47                     | 0.79              |
| 3:D:1096:ARG:NH2  | 3:D:1440:PHE:CD2 | 2.50                     | 0.79              |
| 3:D:1112:CYS:N    | 3:D:1201:CYS:HB3 | 1.98                     | 0.79              |
| 2:M:396:ASP:HB3   | 2:M:406:HIS:CG   | 2.17                     | 0.79              |
| 3:N:675:ARG:HA    | 3:N:678:GLU:CD   | 2.08                     | 0.79              |
| 2:C:332:ARG:CZ    | 2:C:464:LEU:HG   | 2.13                     | 0.78              |
| 2:C:1016:ILE:HG12 | 2:C:1017:THR:H   | 1.48                     | 0.78              |
| 3:D:1003:VAL:HG13 | 3:D:1036:ARG:HD2 | 1.65                     | 0.78              |
| 3:N:27:GLU:HB3    | 3:N:41:ARG:NH1   | 1.97                     | 0.78              |
| 3:N:760:ARG:NH1   | 4:O:61:VAL:HG23  | 1.96                     | 0.78              |
| 3:N:1016:PRO:HA   | 3:N:1021:TYR:HE1 | 1.48                     | 0.78              |
| 6:Y:6:C:O5'       | 6:Y:6:C:H6       | 1.66                     | 0.78              |
| 2:C:338:GLU:O     | 2:C:341:THR:HG22 | 1.84                     | 0.78              |
| 3:D:10:ILE:HG22   | 3:D:1451:ALA:CA  | 2.13                     | 0.78              |
| 3:D:10:ILE:HG13   | 3:D:1434:TRP:CZ2 | 2.18                     | 0.78              |
| 3:D:1093:TYR:CZ   | 5:G:17:DA:H1'    | 2.19                     | 0.78              |
| 4:E:70:THR:HB     | 4:E:72:ARG:HG2   | 1.63                     | 0.78              |
| 1:K:197:LEU:HD23  | 1:K:197:LEU:H    | 1.47                     | 0.78              |
| 2:M:927:GLY:HA2   | 2:M:930:LYS:HD3  | 1.63                     | 0.78              |
| 3:N:501:ALA:HB1   | 3:N:1453:ALA:HB2 | 1.64                     | 0.78              |
| 7:Z:16:DG:H2''    | 7:Z:17:DA:OP2    | 1.83                     | 0.78              |
| 2:C:52:PHE:CE1    | 2:C:68:PHE:N     | 2.51                     | 0.78              |
| 2:C:436:GLY:HA2   | 2:C:539:VAL:HA   | 1.65                     | 0.78              |
| 3:D:902:LEU:HD23  | 3:D:902:LEU:N    | 1.98                     | 0.78              |
| 3:N:1018:ASN:HB3  | 3:N:1021:TYR:CB  | 2.13                     | 0.78              |
| 3:N:1277:ILE:HD12 | 3:N:1301:LYS:N   | 1.99                     | 0.78              |
| 3:N:1383:ASP:HB2  | 3:N:1416:ALA:HB3 | 1.65                     | 0.78              |
| 5:G:2:DT:H2'      | 5:G:3:DC:C5      | 2.18                     | 0.78              |
| 3:D:637:LEU:HD11  | 3:D:642:CYS:CA   | 2.14                     | 0.78              |
| 2:M:1019:GLN:NE2  | 2:M:1058:ASP:OD1 | 2.17                     | 0.78              |
| 3:N:705:ALA:CB    | 3:N:706:PRO:HD3  | 2.10                     | 0.78              |
| 3:N:1277:ILE:CD1  | 3:N:1301:LYS:HB2 | 2.13                     | 0.78              |
| 1:A:46:SER:HB3    | 2:C:856:GLU:OE2  | 1.84                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:758:ARG:HB3   | 2:C:788:THR:O     | 1.82                     | 0.78              |
| 3:D:743:ASP:CG    | 6:H:14:G:O2'      | 2.26                     | 0.78              |
| 3:D:1205:TYR:CE2  | 3:D:1215:VAL:HG21 | 2.19                     | 0.78              |
| 3:N:833:GLU:O     | 3:N:834:THR:CG2   | 2.30                     | 0.78              |
| 4:E:59:ASN:HB3    | 4:E:62:THR:OG1    | 1.83                     | 0.78              |
| 2:M:140:ILE:O     | 2:M:418:LEU:HD23  | 1.84                     | 0.78              |
| 2:M:808:ARG:HH21  | 2:M:820:ARG:NH2   | 1.81                     | 0.78              |
| 2:M:1074:GLU:HG2  | 2:M:1075:ASP:H    | 1.48                     | 0.78              |
| 7:I:6:DT:H2''     | 7:I:7:DT:OP2      | 1.82                     | 0.78              |
| 2:C:48:PHE:O      | 2:C:52:PHE:CB     | 2.29                     | 0.78              |
| 2:C:367:LEU:HB3   | 2:C:371:LYS:HE3   | 1.65                     | 0.78              |
| 3:D:1112:CYS:N    | 3:D:1201:CYS:SG   | 2.57                     | 0.78              |
| 2:M:129:ILE:HG22  | 2:M:130:ASN:N     | 1.97                     | 0.78              |
| 2:M:683:ASN:O     | 2:M:872:ASN:HB2   | 1.84                     | 0.78              |
| 2:M:889:HIS:HE1   | 2:M:988:VAL:CG2   | 1.96                     | 0.78              |
| 3:N:163:TYR:HD1   | 3:N:165:LYS:H     | 1.31                     | 0.78              |
| 3:N:171:LEU:CD1   | 3:N:195:VAL:CG2   | 2.61                     | 0.78              |
| 3:N:1098:LEU:O    | 3:N:1102:THR:HG23 | 1.84                     | 0.78              |
| 3:N:1240:THR:O    | 3:N:1241:PHE:HB2  | 1.82                     | 0.78              |
| 3:D:1195:GLN:CG   | 3:D:1196:THR:N    | 2.47                     | 0.78              |
| 2:M:603:VAL:HB    | 2:M:647:GLN:H     | 1.49                     | 0.78              |
| 3:N:1131:SER:CB   | 3:N:1133:ARG:HH21 | 1.96                     | 0.78              |
| 3:N:1438:ALA:O    | 3:N:1443:THR:HG22 | 1.83                     | 0.78              |
| 2:M:300:ASP:OD2   | 2:M:303:PHE:HB2   | 1.82                     | 0.78              |
| 2:M:705:ILE:HG12  | 2:M:828:ALA:HB2   | 1.64                     | 0.78              |
| 2:M:707:ARG:HD2   | 2:M:824:ARG:HD2   | 1.66                     | 0.78              |
| 2:M:1109:VAL:HG11 | 3:N:5:VAL:CG2     | 2.10                     | 0.78              |
| 2:C:684:PHE:H     | 2:C:687:ALA:HB3   | 1.47                     | 0.78              |
| 1:L:201:THR:HG21  | 1:L:205:VAL:O     | 1.84                     | 0.78              |
| 2:M:626:ARG:HG3   | 2:M:639:GLN:HE21  | 1.49                     | 0.78              |
| 3:N:501:ALA:CB    | 3:N:1453:ALA:HB2  | 2.14                     | 0.78              |
| 2:M:332:ARG:C     | 2:M:333:ILE:HD12  | 2.09                     | 0.77              |
| 2:M:1095:LEU:CD2  | 3:N:603:LEU:HD13  | 2.15                     | 0.77              |
| 3:N:646:LYS:CE    | 3:N:688:TRP:CZ2   | 2.66                     | 0.77              |
| 3:N:1106:VAL:HG11 | 3:N:1474:ALA:CB   | 2.14                     | 0.77              |
| 2:C:487:THR:HG22  | 2:C:489:THR:HG23  | 1.65                     | 0.77              |
| 3:D:1018:ASN:HB3  | 3:D:1021:TYR:HB3  | 1.66                     | 0.77              |
| 3:D:1197:ARG:HA   | 3:D:1396:GLU:HG3  | 1.66                     | 0.77              |
| 2:M:1045:ALA:HB1  | 2:M:1048:THR:HB   | 1.66                     | 0.77              |
| 3:N:1425:THR:O    | 3:N:1429:LEU:HD13 | 1.84                     | 0.77              |
| 7:Z:10:DG:H2''    | 7:Z:11:DG:OP2     | 1.85                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:408:ARG:HG3   | 2:C:454:SER:HB3   | 1.65                     | 0.77              |
| 2:C:796:GLU:HB2   | 2:C:1004:LYS:NZ   | 1.99                     | 0.77              |
| 2:C:1103:ASP:CG   | 2:C:1104:GLU:H    | 1.92                     | 0.77              |
| 3:D:136:ASP:HB3   | 3:D:137:PRO:CD    | 2.13                     | 0.77              |
| 3:D:498:VAL:O     | 3:D:501:ALA:HB3   | 1.84                     | 0.77              |
| 1:L:212:ASN:O     | 1:L:215:VAL:HG22  | 1.84                     | 0.77              |
| 2:M:881:ASN:N     | 2:M:881:ASN:HD22  | 1.81                     | 0.77              |
| 3:N:457:GLY:O     | 3:N:460:ALA:N     | 2.18                     | 0.77              |
| 3:N:704:ARG:HE    | 3:N:706:PRO:HD2   | 1.50                     | 0.77              |
| 3:N:1381:VAL:HG12 | 3:N:1382:THR:N    | 1.99                     | 0.77              |
| 1:A:43:ILE:HG22   | 1:A:47:SER:HB2    | 1.67                     | 0.77              |
| 2:C:274:ARG:HG3   | 2:C:274:ARG:HH11  | 1.47                     | 0.77              |
| 3:N:41:ARG:HD3    | 3:N:42:ASP:N      | 1.99                     | 0.77              |
| 3:N:1468:LEU:HD23 | 3:N:1468:LEU:O    | 1.83                     | 0.77              |
| 1:A:102:LYS:HB3   | 1:A:139:ASN:CG    | 2.09                     | 0.77              |
| 1:B:218:LEU:O     | 1:B:222:LEU:HG    | 1.85                     | 0.77              |
| 2:C:688:ILE:CD1   | 2:C:847:GLY:HA3   | 2.15                     | 0.77              |
| 2:C:861:LEU:CD2   | 2:C:863:ASP:HB3   | 2.15                     | 0.77              |
| 2:C:966:LEU:HD21  | 2:C:986:PRO:HG2   | 1.65                     | 0.77              |
| 3:D:1033:GLN:C    | 3:D:1037:GLN:HB2  | 2.09                     | 0.77              |
| 2:M:697:ARG:O     | 2:M:699:PHE:N     | 2.17                     | 0.77              |
| 3:N:646:LYS:CE    | 3:N:688:TRP:CE2   | 2.68                     | 0.77              |
| 5:G:20:DC:H2''    | 5:G:21:DG:H5'     | 1.66                     | 0.77              |
| 5:G:21:DG:H2''    | 5:G:22:DA:H5'     | 1.66                     | 0.77              |
| 1:B:34:VAL:HG22   | 1:B:181:VAL:HG21  | 1.65                     | 0.77              |
| 2:C:265:ARG:H     | 2:C:289:THR:HG21  | 1.47                     | 0.77              |
| 2:M:5:ARG:HB3     | 2:M:902:ILE:HB    | 1.66                     | 0.77              |
| 2:M:334:ARG:HB2   | 2:M:339:LEU:HD21  | 1.67                     | 0.77              |
| 3:N:1438:ALA:CA   | 3:N:1446:VAL:HG11 | 2.15                     | 0.77              |
| 3:D:639:LEU:HD12  | 3:D:640:HIS:H     | 1.49                     | 0.77              |
| 2:M:532:MET:HG2   | 2:M:533:ASP:N     | 1.98                     | 0.77              |
| 3:N:654:LYS:O     | 3:N:658:LEU:HG    | 1.84                     | 0.77              |
| 3:N:792:ILE:O     | 3:N:878:GLY:HA3   | 1.85                     | 0.77              |
| 5:G:28:DG:OP2     | 5:G:28:DG:H8      | 1.66                     | 0.77              |
| 2:C:559:LEU:HD23  | 2:C:563:ASN:OD1   | 1.84                     | 0.77              |
| 2:C:693:GLU:HG2   | 2:C:697:ARG:HH21  | 1.48                     | 0.77              |
| 2:C:185:LYS:CG    | 2:C:190:LYS:HG3   | 2.14                     | 0.77              |
| 2:C:266:ARG:CA    | 2:C:288:ARG:HD3   | 2.14                     | 0.77              |
| 2:C:368:THR:HB    | 2:C:369:PRO:HD3   | 1.66                     | 0.77              |
| 2:C:1095:LEU:HB3  | 2:C:1097:LEU:HD23 | 1.65                     | 0.77              |
| 3:N:660:LYS:CD    | 3:N:694:VAL:HG22  | 2.14                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:Z:13:DA:H2''    | 7:Z:14:DG:OP2     | 1.82                     | 0.77              |
| 2:C:151:ASP:OD1   | 2:C:152:PRO:HD2   | 1.84                     | 0.77              |
| 2:C:1042:ALA:CB   | 3:D:710:ARG:HB3   | 2.15                     | 0.77              |
| 3:D:6:ARG:O       | 3:D:7:LYS:HG3     | 1.85                     | 0.77              |
| 3:D:1440:PHE:O    | 3:D:1441:GLN:HB2  | 1.85                     | 0.77              |
| 2:M:1082:PRO:O    | 2:M:1086:ARG:HG3  | 1.84                     | 0.77              |
| 3:N:98:PRO:HG3    | 3:N:515:GLU:HB3   | 1.67                     | 0.77              |
| 1:A:103:ALA:O     | 1:A:138:LEU:HB3   | 1.85                     | 0.76              |
| 1:A:175:ARG:HD3   | 1:A:176:ARG:HG2   | 1.67                     | 0.76              |
| 2:C:683:ASN:HA    | 2:C:687:ALA:C     | 2.10                     | 0.76              |
| 3:D:7:LYS:HG2     | 3:D:1458:GLU:HA   | 1.67                     | 0.76              |
| 1:K:86:VAL:CG1    | 1:K:124:ASN:HB2   | 2.14                     | 0.76              |
| 2:C:1003:ASP:CG   | 2:C:1004:LYS:N    | 2.43                     | 0.76              |
| 1:L:101:LEU:CD1   | 1:L:113:ASP:HB3   | 2.16                     | 0.76              |
| 2:M:85:GLU:O      | 2:M:824:ARG:NH2   | 2.18                     | 0.76              |
| 3:N:618:LEU:CD1   | 3:N:1467:ILE:CG1  | 2.47                     | 0.76              |
| 3:N:1426:LYS:HA   | 3:N:1429:LEU:HD22 | 1.68                     | 0.76              |
| 7:I:11:DG:H2'     | 7:I:12:DT:H72     | 1.65                     | 0.76              |
| 2:C:1094:ALA:HA   | 3:D:518:PRO:HB2   | 1.65                     | 0.76              |
| 1:K:112:ARG:HG2   | 1:K:112:ARG:HH11  | 1.50                     | 0.76              |
| 3:N:167:GLU:OE1   | 3:N:198:ARG:NH2   | 2.18                     | 0.76              |
| 2:C:904:PRO:HD2   | 2:C:908:GLY:HA2   | 1.67                     | 0.76              |
| 2:C:1111:ILE:HG13 | 2:C:1112:PHE:H    | 1.49                     | 0.76              |
| 3:D:897:TRP:HB2   | 3:D:900:ILE:CD1   | 2.07                     | 0.76              |
| 3:N:131:LYS:HG3   | 3:N:568:ARG:HG2   | 1.68                     | 0.76              |
| 2:C:1032:PHE:O    | 2:C:1036:GLU:HB2  | 1.84                     | 0.76              |
| 3:N:638:LYS:HD3   | 3:N:932:ASP:CG    | 2.11                     | 0.76              |
| 3:N:1216:SER:HB3  | 4:O:15:SER:CA     | 2.15                     | 0.76              |
| 3:D:705:ALA:CB    | 6:H:14:G:N2       | 2.15                     | 0.76              |
| 3:D:1154:GLU:O    | 3:N:562:ALA:N     | 2.17                     | 0.76              |
| 3:D:1194:CYS:HB3  | 3:D:1373:ARG:HH12 | 1.48                     | 0.76              |
| 3:N:171:LEU:CG    | 3:N:195:VAL:HG23  | 2.15                     | 0.76              |
| 3:N:1238:MET:O    | 3:N:1239:ARG:HG3  | 1.84                     | 0.76              |
| 2:C:304:LEU:CG    | 2:C:305:PRO:HD3   | 2.15                     | 0.76              |
| 2:C:328:LEU:HD22  | 2:C:433:THR:O     | 1.85                     | 0.76              |
| 2:C:404:LEU:HD22  | 2:C:591:SER:HB3   | 1.68                     | 0.76              |
| 3:D:600:LEU:H     | 3:D:600:LEU:CD1   | 1.99                     | 0.76              |
| 1:A:72:LYS:HE3    | 2:C:641:PRO:O     | 1.86                     | 0.76              |
| 3:D:615:ARG:HH12  | 3:D:1096:ARG:CZ   | 1.99                     | 0.76              |
| 3:D:1112:CYS:N    | 3:D:1201:CYS:CB   | 2.47                     | 0.76              |
| 1:K:181:VAL:N     | 2:M:937:ASP:OD1   | 2.18                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:703:ILE:H     | 2:M:703:ILE:HD12  | 1.51                     | 0.76              |
| 2:M:876:VAL:HG11  | 2:M:885:ILE:HD11  | 1.67                     | 0.76              |
| 3:N:796:ARG:HG3   | 3:N:861:GLN:O     | 1.85                     | 0.76              |
| 1:A:188:GLN:HG3   | 1:A:189:ARG:H     | 1.51                     | 0.76              |
| 2:C:939:ARG:HA    | 2:C:939:ARG:HE    | 1.49                     | 0.76              |
| 3:D:897:TRP:HA    | 3:D:900:ILE:HG13  | 1.62                     | 0.76              |
| 3:D:1231:GLU:HB3  | 3:D:1232:PRO:HD3  | 1.66                     | 0.76              |
| 2:C:48:PHE:O      | 2:C:52:PHE:N      | 2.19                     | 0.76              |
| 2:C:679:PHE:H     | 2:C:683:ASN:HD21  | 1.32                     | 0.76              |
| 2:C:687:ALA:C     | 2:C:688:ILE:HD12  | 2.10                     | 0.76              |
| 3:D:1380:GLU:HG2  | 3:D:1381:VAL:H    | 1.50                     | 0.76              |
| 4:E:36:LYS:H      | 4:E:95:VAL:CG2    | 1.96                     | 0.76              |
| 2:M:735:ARG:HG2   | 2:M:735:ARG:HH11  | 1.49                     | 0.76              |
| 2:M:1012:PRO:HD3  | 2:M:1026:GLN:HG2  | 1.68                     | 0.76              |
| 3:N:702:LEU:O     | 3:N:713:ILE:HA    | 1.86                     | 0.76              |
| 2:C:943:VAL:HG23  | 2:C:985:GLY:H     | 1.51                     | 0.75              |
| 3:D:522:PRO:CA    | 3:D:525:ARG:HH11  | 1.99                     | 0.75              |
| 2:M:966:LEU:HD21  | 2:M:986:PRO:HG2   | 1.66                     | 0.75              |
| 3:N:102:ILE:HD12  | 3:N:579:ASP:HB3   | 1.68                     | 0.75              |
| 3:D:847:ASP:O     | 3:D:851:LEU:HG    | 1.85                     | 0.75              |
| 2:M:129:ILE:HD13  | 2:M:134:ARG:HB2   | 1.68                     | 0.75              |
| 2:M:677:MET:HB3   | 3:N:948:THR:HG21  | 1.68                     | 0.75              |
| 2:M:684:PHE:CG    | 2:M:685:GLU:N     | 2.53                     | 0.75              |
| 3:N:166:GLN:HA    | 3:N:198:ARG:HB3   | 1.69                     | 0.75              |
| 2:C:739:GLU:HG3   | 2:C:742:VAL:CB    | 2.16                     | 0.75              |
| 3:D:618:LEU:HD13  | 3:D:1439:SER:HB3  | 1.67                     | 0.75              |
| 2:M:42:VAL:HA     | 2:M:46:ALA:HB2    | 1.68                     | 0.75              |
| 2:M:52:PHE:HE1    | 2:M:66:LEU:HG     | 1.51                     | 0.75              |
| 3:N:646:LYS:HD2   | 3:N:688:TRP:CZ2   | 2.22                     | 0.75              |
| 1:A:43:ILE:HG22   | 1:A:47:SER:CB     | 2.16                     | 0.75              |
| 3:D:614:PHE:HE2   | 3:D:1443:THR:HB   | 1.51                     | 0.75              |
| 3:D:1446:VAL:HB   | 3:D:1447:LEU:HD13 | 1.67                     | 0.75              |
| 2:M:946:ARG:CZ    | 2:M:984:GLU:HB2   | 2.17                     | 0.75              |
| 2:M:1095:LEU:O    | 2:M:1096:ALA:C    | 2.30                     | 0.75              |
| 3:N:166:GLN:CB    | 3:N:198:ARG:HB3   | 2.16                     | 0.75              |
| 3:N:646:LYS:HD2   | 3:N:688:TRP:CD2   | 2.22                     | 0.75              |
| 2:C:285:LEU:HD23  | 2:C:285:LEU:O     | 1.86                     | 0.75              |
| 3:D:900:ILE:HD12  | 3:D:902:LEU:HD22  | 1.68                     | 0.75              |
| 3:D:1209:LEU:HD21 | 4:E:16:LYS:NZ     | 2.00                     | 0.75              |
| 3:N:1274:ILE:HG22 | 3:N:1301:LYS:NZ   | 2.01                     | 0.75              |
| 5:G:8:DC:H2"      | 5:G:9:DC:OP2      | 1.85                     | 0.75              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:1190:SER:O    | 3:D:1204:CYS:SG  | 2.44                     | 0.75              |
| 3:D:1481:VAL:HG12 | 4:E:21:VAL:HG21  | 1.68                     | 0.75              |
| 3:N:1109:GLU:CD   | 3:N:1202:GLN:H   | 1.95                     | 0.75              |
| 2:C:928:LYS:HZ2   | 2:C:932:GLU:HG3  | 1.51                     | 0.75              |
| 3:D:704:ARG:HA    | 3:D:745:MET:CG   | 2.13                     | 0.75              |
| 3:D:737:ASN:HB3   | 6:H:15:C:HO2'    | 1.52                     | 0.75              |
| 2:M:1021:LEU:HD22 | 6:Y:5:C:O2       | 1.86                     | 0.75              |
| 3:N:996:TRP:HA    | 3:N:999:THR:HG22 | 1.69                     | 0.75              |
| 3:N:1197:ARG:HB3  | 3:N:1396:GLU:CD  | 2.11                     | 0.75              |
| 3:D:696:HIS:CD2   | 4:E:59:ASN:CB    | 2.69                     | 0.75              |
| 2:M:129:ILE:HG22  | 2:M:130:ASN:H    | 1.49                     | 0.75              |
| 2:M:724:ARG:HG3   | 2:M:737:LEU:HD22 | 1.68                     | 0.75              |
| 3:N:696:HIS:ND1   | 3:N:697:GLY:N    | 2.35                     | 0.75              |
| 3:N:1211:MET:HG2  | 3:N:1212:ALA:H   | 1.52                     | 0.75              |
| 3:D:608:SER:CB    | 3:D:1442:ASN:O   | 2.35                     | 0.75              |
| 3:D:1042:ARG:HG2  | 3:D:1061:PHE:CE1 | 2.19                     | 0.75              |
| 1:L:185:ARG:NH2   | 3:N:688:TRP:HB2  | 2.00                     | 0.75              |
| 2:M:265:ARG:HB3   | 2:M:267:TYR:CG   | 2.22                     | 0.75              |
| 2:M:732:ALA:HA    | 2:M:735:ARG:CZ   | 2.17                     | 0.75              |
| 3:N:1239:ARG:NH1  | 3:N:1239:ARG:HB2 | 2.02                     | 0.75              |
| 2:C:304:LEU:HG    | 2:C:305:PRO:HD3  | 1.68                     | 0.74              |
| 2:C:395:LYS:HZ1   | 2:C:407:LYS:NZ   | 1.85                     | 0.74              |
| 1:L:52:ALA:HB1    | 1:L:170:VAL:H    | 1.52                     | 0.74              |
| 2:M:889:HIS:O     | 2:M:892:LEU:HB3  | 1.87                     | 0.74              |
| 3:N:1224:VAL:HA   | 3:N:1227:GLN:OE1 | 1.87                     | 0.74              |
| 3:N:1270:ALA:O    | 3:N:1329:ALA:HB3 | 1.86                     | 0.74              |
| 7:I:11:DG:H2''    | 7:I:12:DT:OP2    | 1.86                     | 0.74              |
| 2:C:326:ASP:HB3   | 2:C:431:HIS:HB2  | 1.69                     | 0.74              |
| 3:D:85:VAL:HB     | 3:D:89:ARG:CZ    | 2.17                     | 0.74              |
| 3:D:473:LEU:HG    | 3:D:476:GLU:OE2  | 1.87                     | 0.74              |
| 2:M:57:GLU:O      | 2:M:62:GLY:HA3   | 1.87                     | 0.74              |
| 2:M:479:VAL:HG11  | 2:M:503:LEU:HD11 | 1.70                     | 0.74              |
| 2:M:580:MET:HB3   | 2:M:584:GLU:OE2  | 1.86                     | 0.74              |
| 3:N:1267:ARG:HG3  | 3:N:1271:LYS:HE2 | 1.68                     | 0.74              |
| 3:N:1465:ASN:OD1  | 3:N:1473:PRO:CG  | 2.34                     | 0.74              |
| 4:O:5:GLY:HA3     | 4:O:8:LYS:HD2    | 1.69                     | 0.74              |
| 2:C:52:PHE:CZ     | 2:C:68:PHE:CA    | 2.71                     | 0.74              |
| 2:C:759:THR:HB    | 2:C:785:VAL:HG22 | 1.69                     | 0.74              |
| 3:D:7:LYS:HA      | 3:D:1457:ASP:O   | 1.87                     | 0.74              |
| 1:L:62:LEU:HD12   | 1:L:63:HIS:H     | 1.52                     | 0.74              |
| 2:M:893:ALA:HB1   | 2:M:897:LEU:HD12 | 1.69                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:695:ILE:CD1   | 3:N:718:PRO:HB2   | 2.17                     | 0.74              |
| 3:N:1369:GLU:O    | 3:N:1372:VAL:HG12 | 1.87                     | 0.74              |
| 2:C:165:LEU:HG    | 2:C:166:PRO:CA    | 2.15                     | 0.74              |
| 2:C:1032:PHE:CE2  | 2:C:1037:VAL:HA   | 2.22                     | 0.74              |
| 2:M:415:PRO:HD2   | 2:M:418:LEU:HD13  | 1.70                     | 0.74              |
| 3:N:182:GLY:HA2   | 3:N:203:ALA:O     | 1.87                     | 0.74              |
| 3:N:553:ARG:O     | 3:N:557:LEU:HG    | 1.86                     | 0.74              |
| 3:N:653:PHE:HB3   | 3:N:656:PHE:HB2   | 1.67                     | 0.74              |
| 3:N:902:LEU:HD23  | 3:N:902:LEU:H     | 1.52                     | 0.74              |
| 3:N:1262:LEU:HD23 | 3:N:1352:ILE:HG12 | 1.70                     | 0.74              |
| 2:C:930:LYS:HD2   | 2:C:960:GLU:OE1   | 1.88                     | 0.74              |
| 3:D:899:LEU:CD2   | 3:D:917:GLN:CG    | 2.64                     | 0.74              |
| 1:L:124:ASN:ND2   | 1:L:127:LEU:HB2   | 2.00                     | 0.74              |
| 3:N:87:ARG:HD3    | 3:N:524:LEU:HD11  | 1.68                     | 0.74              |
| 1:A:87:VAL:HG21   | 1:A:144:VAL:HG11  | 1.70                     | 0.74              |
| 2:C:759:THR:HB    | 2:C:785:VAL:CG2   | 2.17                     | 0.74              |
| 2:C:911:GLU:HB3   | 2:C:912:PRO:HD3   | 1.70                     | 0.74              |
| 2:M:328:LEU:HD11  | 2:M:434:HIS:CE1   | 2.22                     | 0.74              |
| 2:M:1054:THR:OG1  | 2:M:1055:LEU:HG   | 1.87                     | 0.74              |
| 3:N:607:LEU:HA    | 3:N:613:ARG:CB    | 2.18                     | 0.74              |
| 3:D:907:GLU:O     | 3:D:911:LEU:HD13  | 1.88                     | 0.74              |
| 2:M:889:HIS:CE1   | 2:M:988:VAL:HG21  | 2.16                     | 0.74              |
| 2:M:1046:ALA:HB2  | 3:N:1476:THR:HB   | 1.69                     | 0.74              |
| 4:O:37:ASN:HD22   | 4:O:37:ASN:N      | 1.85                     | 0.74              |
| 1:A:94:LEU:HD21   | 1:A:119:ASP:HB2   | 1.67                     | 0.74              |
| 2:C:537:LYS:HD2   | 2:C:905:ILE:HD13  | 1.69                     | 0.74              |
| 2:C:939:ARG:HD3   | 2:C:982:PRO:HD3   | 1.69                     | 0.74              |
| 3:D:641:GLN:HG2   | 3:D:717:GLN:HE21  | 1.51                     | 0.74              |
| 3:D:785:ILE:H     | 3:D:785:ILE:HD12  | 1.51                     | 0.74              |
| 3:D:1166:LEU:HD23 | 3:D:1166:LEU:H    | 1.53                     | 0.74              |
| 2:M:110:GLU:HG3   | 2:M:369:PRO:HG3   | 1.68                     | 0.74              |
| 2:C:12:VAL:HB     | 2:C:472:ARG:HH11  | 1.53                     | 0.74              |
| 2:C:292:ARG:CG    | 2:C:298:PHE:HA    | 2.15                     | 0.74              |
| 2:C:492:ASP:OD2   | 2:C:518:LYS:HB3   | 1.88                     | 0.74              |
| 2:C:1090:LYS:HZ1  | 3:D:21:TRP:HB3    | 1.53                     | 0.74              |
| 3:D:764:LEU:CD2   | 3:D:767:HIS:CE1   | 2.69                     | 0.74              |
| 1:K:188:GLN:HG3   | 1:K:189:ARG:H     | 1.52                     | 0.74              |
| 2:M:541:SER:O     | 2:M:545:ASN:ND2   | 2.21                     | 0.74              |
| 2:M:1060:ILE:HG23 | 2:M:1061:GLU:H    | 1.52                     | 0.74              |
| 3:N:171:LEU:HD11  | 3:N:195:VAL:CG2   | 2.18                     | 0.74              |
| 3:N:925:GLU:OE1   | 4:O:7:ASP:OD2     | 2.06                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:G:11:DC:H2''    | 5:G:12:DA:OP2     | 1.86                     | 0.74              |
| 1:A:43:ILE:CG2    | 1:A:47:SER:CB     | 2.66                     | 0.74              |
| 1:B:26:GLU:HB2    | 1:B:27:PRO:HA     | 1.68                     | 0.74              |
| 1:B:52:ALA:HB1    | 1:B:170:VAL:H     | 1.53                     | 0.74              |
| 3:D:531:ASP:OD1   | 6:H:4:G:H4'       | 1.88                     | 0.74              |
| 2:M:1114:GLY:H    | 2:M:1115:LEU:HD12 | 1.53                     | 0.74              |
| 3:N:950:GLY:O     | 3:N:953:ASP:HB2   | 1.87                     | 0.74              |
| 3:N:1461:GLY:O    | 3:N:1465:ASN:HB2  | 1.88                     | 0.74              |
| 1:A:222:LEU:HD23  | 1:B:219:ARG:CB    | 2.18                     | 0.73              |
| 1:B:30:ARG:HG2    | 1:B:30:ARG:HH11   | 1.52                     | 0.73              |
| 2:C:423:ALA:HB1   | 7:I:1:DG:C5'      | 2.15                     | 0.73              |
| 3:D:102:ILE:HB    | 3:D:579:ASP:OD1   | 1.88                     | 0.73              |
| 3:D:600:LEU:HD12  | 3:D:600:LEU:N     | 2.02                     | 0.73              |
| 3:D:864:VAL:HG12  | 3:D:865:THR:N     | 2.04                     | 0.73              |
| 3:D:1412:LYS:HB2  | 2:M:376:ARG:NH2   | 2.03                     | 0.73              |
| 2:M:328:LEU:HD11  | 2:M:434:HIS:ND1   | 2.03                     | 0.73              |
| 2:M:684:PHE:N     | 2:M:687:ALA:HB3   | 2.02                     | 0.73              |
| 2:M:987:ILE:CG2   | 3:N:948:THR:HG21  | 2.17                     | 0.73              |
| 3:N:97:THR:CG2    | 3:N:459:GLU:HB2   | 2.17                     | 0.73              |
| 3:N:149:LYS:HE3   | 3:N:150:ARG:H     | 1.52                     | 0.73              |
| 3:N:1152:GLU:OE2  | 3:N:1154:GLU:HG3  | 1.88                     | 0.73              |
| 2:C:588:VAL:HG21  | 2:C:664:GLY:O     | 1.89                     | 0.73              |
| 3:D:6:ARG:HD2     | 3:D:1470:ARG:HH12 | 1.51                     | 0.73              |
| 3:D:11:ALA:HB1    | 3:D:507:ASN:OD1   | 1.89                     | 0.73              |
| 3:D:829:VAL:O     | 3:D:835:SER:HB3   | 1.88                     | 0.73              |
| 3:D:897:TRP:O     | 3:D:900:ILE:HG13  | 1.88                     | 0.73              |
| 3:D:996:TRP:HA    | 3:D:999:THR:HG22  | 1.69                     | 0.73              |
| 1:K:56:VAL:HG22   | 1:K:142:VAL:HG12  | 1.70                     | 0.73              |
| 2:M:157:ARG:HD3   | 2:M:314:THR:HG21  | 1.71                     | 0.73              |
| 3:N:1216:SER:CB   | 4:O:15:SER:OG     | 2.35                     | 0.73              |
| 3:N:1274:ILE:CG2  | 3:N:1301:LYS:NZ   | 2.51                     | 0.73              |
| 3:N:1294:VAL:HG12 | 3:N:1319:VAL:HG23 | 1.70                     | 0.73              |
| 2:C:52:PHE:HB3    | 2:C:53:PRO:HD3    | 1.69                     | 0.73              |
| 2:C:345:ARG:HA    | 2:C:348:LEU:HD22  | 1.67                     | 0.73              |
| 2:C:922:PHE:HB3   | 2:C:964:LYS:HZ2   | 1.52                     | 0.73              |
| 3:D:729:HIS:O     | 3:D:732:VAL:HG22  | 1.88                     | 0.73              |
| 4:O:25:LYS:O      | 4:O:29:GLN:HG3    | 1.89                     | 0.73              |
| 7:Z:9:DT:H2''     | 7:Z:10:DG:OP2     | 1.88                     | 0.73              |
| 2:C:139:GLN:O     | 2:C:333:ILE:HA    | 1.89                     | 0.73              |
| 2:C:685:GLU:HG2   | 3:D:739:ASP:HB2   | 1.69                     | 0.73              |
| 3:D:65:ARG:H      | 3:D:68:PHE:HE1    | 1.34                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1216:SER:HB3  | 4:E:16:LYS:N      | 2.01                     | 0.73              |
| 3:D:1225:ALA:HA   | 3:D:1367:HIS:ND1  | 2.02                     | 0.73              |
| 3:D:1465:ASN:HD21 | 3:D:1470:ARG:HB3  | 1.52                     | 0.73              |
| 1:L:56:VAL:HG13   | 1:L:142:VAL:HG12  | 1.68                     | 0.73              |
| 2:M:603:VAL:HB    | 2:M:647:GLN:N     | 2.03                     | 0.73              |
| 3:N:87:ARG:CB     | 3:N:523:ASP:HB2   | 2.19                     | 0.73              |
| 3:N:699:VAL:HG21  | 3:N:760:ARG:HB3   | 1.70                     | 0.73              |
| 3:N:1200:VAL:CG1  | 3:N:1204:CYS:HB2  | 2.17                     | 0.73              |
| 2:C:749:VAL:HG22  | 2:C:798:GLY:O     | 1.89                     | 0.73              |
| 2:C:1097:LEU:H    | 2:C:1097:LEU:CD2  | 1.98                     | 0.73              |
| 3:D:702:LEU:O     | 3:D:713:ILE:HA    | 1.89                     | 0.73              |
| 2:M:861:LEU:HD23  | 2:M:862:PRO:N     | 2.03                     | 0.73              |
| 2:M:1095:LEU:HD21 | 3:N:603:LEU:CD1   | 2.17                     | 0.73              |
| 3:N:478:LEU:CD2   | 3:N:1388:ARG:HD3  | 2.19                     | 0.73              |
| 3:N:520:LEU:HD11  | 3:N:524:LEU:HD23  | 1.68                     | 0.73              |
| 3:N:705:ALA:HB3   | 3:N:706:PRO:CD    | 2.14                     | 0.73              |
| 1:A:42:ARG:HB2    | 1:B:35:THR:HG23   | 1.69                     | 0.73              |
| 2:C:16:PRO:O      | 2:C:18:LEU:HD12   | 1.89                     | 0.73              |
| 2:C:18:LEU:H      | 2:C:18:LEU:CD1    | 2.00                     | 0.73              |
| 2:C:50:GLU:HB2    | 2:C:266:ARG:HH11  | 1.54                     | 0.73              |
| 2:M:113:VAL:HG11  | 2:M:373:VAL:HG11  | 1.70                     | 0.73              |
| 2:M:460:ARG:HG2   | 2:M:485:TYR:CE2   | 2.23                     | 0.73              |
| 2:M:762:LYS:HE3   | 2:M:786:LYS:HE2   | 1.68                     | 0.73              |
| 3:N:639:LEU:HA    | 3:N:729:HIS:CD2   | 2.24                     | 0.73              |
| 2:C:1035:MET:SD   | 5:G:20:DC:H5'     | 2.28                     | 0.73              |
| 3:D:1034:GLN:O    | 3:D:1038:LEU:CB   | 2.34                     | 0.73              |
| 2:M:265:ARG:H     | 2:M:289:THR:HG21  | 0.64                     | 0.73              |
| 2:M:674:VAL:HG23  | 2:M:869:VAL:HG13  | 1.69                     | 0.73              |
| 3:N:1294:VAL:CG2  | 3:N:1301:LYS:HB3  | 2.18                     | 0.73              |
| 2:C:352:ALA:O     | 2:C:355:VAL:HG12  | 1.89                     | 0.73              |
| 2:C:673:LEU:HB3   | 2:C:868:ASP:OD1   | 1.88                     | 0.73              |
| 2:C:679:PHE:C     | 3:D:943:THR:HG22  | 2.14                     | 0.73              |
| 3:D:8:VAL:HG21    | 3:D:1435:LEU:HD21 | 1.69                     | 0.73              |
| 3:D:739:ASP:N     | 6:H:15:C:H5''     | 2.04                     | 0.73              |
| 3:D:1168:MET:HE3  | 3:D:1171:VAL:HB   | 1.69                     | 0.73              |
| 3:D:1438:ALA:HA   | 3:D:1446:VAL:HG11 | 1.68                     | 0.73              |
| 4:E:64:ALA:O      | 4:E:68:LEU:HD22   | 1.88                     | 0.73              |
| 2:M:922:PHE:HB3   | 2:M:964:LYS:NZ    | 2.04                     | 0.73              |
| 2:M:1016:ILE:HG12 | 2:M:1017:THR:N    | 2.03                     | 0.73              |
| 3:N:87:ARG:HB2    | 3:N:523:ASP:HB2   | 1.71                     | 0.73              |
| 3:N:481:MET:SD    | 3:N:493:ARG:HB2   | 2.28                     | 0.73              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:703:ASN:O    | 3:N:745:MET:HB3   | 1.89                     | 0.73              |
| 3:N:958:GLU:OE2  | 3:N:961:LYS:HD3   | 1.89                     | 0.73              |
| 3:N:1111:ASP:HA  | 3:N:1201:CYS:HB2  | 1.69                     | 0.73              |
| 3:D:128:TYR:HE2  | 3:D:458:ALA:HA    | 1.52                     | 0.73              |
| 3:D:1342:GLU:HA  | 3:D:1345:GLU:OE1  | 1.89                     | 0.73              |
| 1:L:179:PHE:HB2  | 1:L:195:LEU:HD11  | 1.70                     | 0.73              |
| 2:M:328:LEU:CD2  | 2:M:437:ARG:HD3   | 2.18                     | 0.73              |
| 3:N:1107:VAL:HB  | 3:N:1218:GLY:H    | 1.53                     | 0.73              |
| 1:B:102:LYS:HE2  | 1:B:139:ASN:HB2   | 1.70                     | 0.73              |
| 2:C:329:GLY:C    | 2:C:330:ASN:ND2   | 2.47                     | 0.73              |
| 3:D:615:ARG:HH22 | 3:D:1096:ARG:HD2  | 1.51                     | 0.73              |
| 2:M:587:VAL:HG11 | 2:M:666:LEU:HD22  | 1.68                     | 0.73              |
| 7:I:16:DG:H2''   | 7:I:17:DA:OP2     | 1.89                     | 0.73              |
| 1:B:28:LEU:HB2   | 1:B:193:ASP:HB2   | 1.69                     | 0.72              |
| 1:B:58:ILE:HD13  | 1:B:140:MET:HB3   | 1.70                     | 0.72              |
| 2:C:630:ARG:HH21 | 2:C:707:ARG:H     | 1.37                     | 0.72              |
| 2:C:688:ILE:HD13 | 2:C:847:GLY:HA3   | 1.70                     | 0.72              |
| 2:C:692:GLU:O    | 2:C:696:LYS:HG3   | 1.89                     | 0.72              |
| 2:M:90:TYR:HE1   | 2:M:120:LEU:HD12  | 1.54                     | 0.72              |
| 2:M:139:GLN:O    | 2:M:333:ILE:HA    | 1.89                     | 0.72              |
| 1:A:43:ILE:HD13  | 1:B:32:PHE:HE2    | 1.53                     | 0.72              |
| 2:C:460:ARG:HH22 | 2:C:468:ARG:NH1   | 1.87                     | 0.72              |
| 3:D:1447:LEU:N   | 3:D:1447:LEU:CD1  | 2.52                     | 0.72              |
| 1:K:86:VAL:HG12  | 1:K:124:ASN:HB2   | 1.71                     | 0.72              |
| 2:M:626:ARG:HG3  | 2:M:639:GLN:NE2   | 2.04                     | 0.72              |
| 3:N:23:TYR:O     | 3:N:49:ILE:HG23   | 1.89                     | 0.72              |
| 3:N:610:LYS:C    | 3:N:615:ARG:CG    | 2.52                     | 0.72              |
| 3:N:899:LEU:HD23 | 3:N:921:ARG:HG3   | 1.72                     | 0.72              |
| 3:N:1194:CYS:SG  | 3:N:1200:VAL:HG13 | 2.29                     | 0.72              |
| 3:N:1484:THR:HA  | 4:O:76:GLY:O      | 1.88                     | 0.72              |
| 6:H:5:C:O5'      | 6:H:5:C:C6        | 2.42                     | 0.72              |
| 1:A:48:ILE:O     | 1:A:148:VAL:HG13  | 1.87                     | 0.72              |
| 2:C:64:LEU:HD12  | 2:C:100:LEU:HD11  | 1.71                     | 0.72              |
| 2:C:281:LEU:HD12 | 2:C:309:TYR:CB    | 2.19                     | 0.72              |
| 2:C:333:ILE:O    | 2:C:465:GLY:HA3   | 1.90                     | 0.72              |
| 4:E:54:LEU:HD21  | 4:E:63:TRP:HE1    | 1.53                     | 0.72              |
| 2:M:106:GLY:O    | 2:M:107:LEU:HD23  | 1.89                     | 0.72              |
| 3:N:434:ARG:HH11 | 3:N:434:ARG:HB3   | 1.54                     | 0.72              |
| 1:A:176:ARG:HH11 | 2:C:865:THR:HB    | 1.54                     | 0.72              |
| 2:C:143:SER:HB2  | 2:C:276:LYS:HE2   | 1.70                     | 0.72              |
| 2:C:678:PRO:HG3  | 2:C:873:PRO:HD2   | 1.71                     | 0.72              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:486:ARG:HB2  | 5:G:8:DC:OP1      | 1.88                     | 0.72              |
| 3:D:714:GLN:HE21 | 3:D:765:SER:CB    | 2.02                     | 0.72              |
| 3:D:739:ASP:O    | 3:D:743:ASP:CG    | 2.32                     | 0.72              |
| 2:M:393:GLN:HG2  | 6:Y:10:G:H4'      | 1.72                     | 0.72              |
| 2:M:627:ARG:HG3  | 2:M:628:PHE:H     | 1.52                     | 0.72              |
| 3:N:104:PHE:HD2  | 3:N:1448:THR:HG23 | 1.53                     | 0.72              |
| 3:N:1097:LYS:O   | 3:N:1101:VAL:HG22 | 1.89                     | 0.72              |
| 5:G:6:DT:H4'     | 5:G:6:DT:OP1      | 1.87                     | 0.72              |
| 5:X:3:DC:H2''    | 5:X:4:DA:OP2      | 1.89                     | 0.72              |
| 2:C:292:ARG:HB2  | 2:C:299:LYS:HG2   | 1.71                     | 0.72              |
| 2:C:479:VAL:HG22 | 2:C:506:ASN:HA    | 1.72                     | 0.72              |
| 3:D:1388:ARG:HD2 | 3:D:1388:ARG:N    | 2.05                     | 0.72              |
| 3:D:1465:ASN:ND2 | 3:D:1470:ARG:HB3  | 2.04                     | 0.72              |
| 2:M:304:LEU:CD2  | 2:M:305:PRO:HD3   | 2.19                     | 0.72              |
| 2:M:630:ARG:HD2  | 2:M:634:GLY:HA2   | 1.71                     | 0.72              |
| 2:M:684:PHE:H    | 2:M:687:ALA:HB3   | 1.53                     | 0.72              |
| 3:N:1023:MET:O   | 3:N:1028:ALA:HB3  | 1.90                     | 0.72              |
| 1:A:5:LYS:O      | 1:A:8:ALA:HB2     | 1.90                     | 0.72              |
| 2:C:274:ARG:HG3  | 2:C:274:ARG:NH1   | 2.02                     | 0.72              |
| 2:C:395:LYS:NZ   | 2:C:407:LYS:NZ    | 2.38                     | 0.72              |
| 3:D:645:PRO:HG2  | 3:D:724:GLN:O     | 1.90                     | 0.72              |
| 3:D:900:ILE:HD12 | 3:D:902:LEU:HD21  | 1.70                     | 0.72              |
| 2:M:678:PRO:HG3  | 2:M:873:PRO:HD2   | 1.70                     | 0.72              |
| 2:M:694:LEU:HD11 | 2:M:868:ASP:HB3   | 1.70                     | 0.72              |
| 2:M:720:GLU:HG2  | 2:M:760:SER:CB    | 2.19                     | 0.72              |
| 3:N:776:GLU:OE1  | 3:N:912:LYS:HE2   | 1.89                     | 0.72              |
| 7:I:11:DG:C8     | 7:I:12:DT:H72     | 2.24                     | 0.72              |
| 2:C:89:THR:CA    | 2:C:129:ILE:O     | 2.36                     | 0.72              |
| 2:C:183:SER:OG   | 2:C:190:LYS:HG2   | 1.89                     | 0.72              |
| 2:C:444:PRO:HB3  | 6:H:12:U:OP1      | 1.90                     | 0.72              |
| 3:D:41:ARG:C     | 3:D:43:GLY:H      | 1.97                     | 0.72              |
| 3:D:974:ILE:O    | 3:D:977:ALA:HB3   | 1.89                     | 0.72              |
| 3:D:1031:ASN:HB3 | 3:D:1034:GLN:HB2  | 1.72                     | 0.72              |
| 2:M:687:ALA:O    | 2:M:688:ILE:CD1   | 2.37                     | 0.72              |
| 3:N:134:VAL:HG12 | 3:N:152:LEU:HB3   | 1.72                     | 0.72              |
| 3:N:477:LEU:HD12 | 3:N:496:LEU:CD1   | 2.14                     | 0.72              |
| 3:N:806:PHE:CE1  | 3:N:813:LEU:HB3   | 2.25                     | 0.72              |
| 7:I:2:DT:H2''    | 7:I:3:DA:OP2      | 1.90                     | 0.72              |
| 5:X:16:DT:H2''   | 5:X:17:DA:OP2     | 1.89                     | 0.72              |
| 1:B:221:HIS:HA   | 1:B:224:TYR:CD2   | 2.25                     | 0.72              |
| 2:C:344:PHE:O    | 2:C:348:LEU:HD13  | 1.88                     | 0.72              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:1040:LEU:HG   | 2:C:1045:ALA:HB3 | 1.70                     | 0.72              |
| 3:D:95:LEU:HD23   | 3:D:96:ALA:H     | 1.54                     | 0.72              |
| 3:D:613:ARG:O     | 3:D:616:GLN:HB3  | 1.89                     | 0.72              |
| 3:D:810:GLU:O     | 3:D:813:LEU:HG   | 1.90                     | 0.72              |
| 3:D:1258:ARG:HH12 | 3:D:1329:ALA:CB  | 1.98                     | 0.72              |
| 1:L:14:ARG:HB2    | 1:L:22:GLU:HB2   | 1.71                     | 0.72              |
| 2:M:274:ARG:O     | 2:M:274:ARG:HD3  | 1.89                     | 0.72              |
| 2:M:580:MET:HB3   | 2:M:584:GLU:CD   | 2.15                     | 0.72              |
| 3:N:502:PHE:CE1   | 3:N:509:PRO:HB3  | 2.25                     | 0.72              |
| 3:N:917:GLN:HA    | 3:N:920:LEU:HD12 | 1.70                     | 0.72              |
| 3:N:1197:ARG:HA   | 3:N:1396:GLU:HG3 | 1.70                     | 0.72              |
| 3:N:1330:ILE:HD13 | 3:N:1347:TYR:CE1 | 2.25                     | 0.72              |
| 4:O:26:ARG:O      | 4:O:30:LEU:HD13  | 1.89                     | 0.72              |
| 2:C:86:LYS:HB3    | 2:C:813:VAL:HG23 | 1.70                     | 0.72              |
| 2:C:1005:MET:HE3  | 3:D:648:MET:HG3  | 1.72                     | 0.72              |
| 1:L:101:LEU:HD11  | 1:L:113:ASP:HB3  | 1.72                     | 0.72              |
| 2:M:260:LEU:HD12  | 2:M:261:ILE:N    | 2.05                     | 0.72              |
| 2:M:887:GLU:OE1   | 2:M:992:MET:HG3  | 1.90                     | 0.72              |
| 3:N:513:ILE:HD12  | 3:N:513:ILE:O    | 1.90                     | 0.72              |
| 3:N:1277:ILE:HD12 | 3:N:1301:LYS:CB  | 2.19                     | 0.72              |
| 2:C:397:GLU:OE2   | 2:C:632:ASN:HB2  | 1.90                     | 0.72              |
| 2:C:979:THR:HG23  | 2:C:981:GLU:H    | 1.53                     | 0.72              |
| 3:D:708:LEU:HB3   | 3:D:1231:GLU:HB2 | 1.72                     | 0.72              |
| 3:D:1380:GLU:HG2  | 3:D:1381:VAL:N   | 2.05                     | 0.72              |
| 3:D:1447:LEU:HD13 | 3:D:1447:LEU:H   | 1.55                     | 0.72              |
| 1:L:78:ILE:O      | 1:L:82:LEU:HG    | 1.89                     | 0.72              |
| 2:M:580:MET:SD    | 2:M:584:GLU:HG3  | 2.30                     | 0.72              |
| 2:M:1054:THR:OG1  | 2:M:1055:LEU:N   | 2.19                     | 0.72              |
| 3:N:1322:GLY:O    | 3:N:1323:GLN:HB2 | 1.89                     | 0.72              |
| 2:C:44:ILE:O      | 2:C:48:PHE:CD2   | 2.43                     | 0.71              |
| 2:C:252:LYS:HD3   | 2:C:296:GLY:HA2  | 1.71                     | 0.71              |
| 2:C:358:ARG:HH12  | 2:C:374:ASN:CG   | 1.98                     | 0.71              |
| 3:D:153:LEU:HD13  | 3:D:158:TYR:HB2  | 1.70                     | 0.71              |
| 3:D:1033:GLN:CB   | 3:D:1037:GLN:OE1 | 2.38                     | 0.71              |
| 3:D:1042:ARG:CZ   | 3:D:1073:SER:HB2 | 2.19                     | 0.71              |
| 1:L:7:LYS:NZ      | 1:L:186:LEU:HD13 | 2.04                     | 0.71              |
| 2:M:642:ARG:HG3   | 2:M:657:ASP:OD2  | 1.90                     | 0.71              |
| 2:M:1002:GLU:HA   | 5:X:23:DG:H5''   | 1.72                     | 0.71              |
| 2:M:1013:TYR:CE1  | 2:M:1020:PRO:HG3 | 2.24                     | 0.71              |
| 3:N:83:SER:O      | 3:N:86:ARG:HB3   | 1.90                     | 0.71              |
| 2:C:110:GLU:HG3   | 2:C:369:PRO:HG3  | 1.72                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1095:LEU:HG   | 3:D:603:LEU:HD13  | 1.71                     | 0.71              |
| 3:D:554:LEU:HD11  | 3:D:558:LEU:HD21  | 1.72                     | 0.71              |
| 3:D:744:GLN:OE1   | 5:G:21:DG:N2      | 2.23                     | 0.71              |
| 3:D:1265:ALA:O    | 3:D:1266:ARG:HG3  | 1.89                     | 0.71              |
| 3:N:1258:ARG:O    | 3:N:1262:LEU:HD13 | 1.89                     | 0.71              |
| 1:A:57:TYR:CE2    | 1:A:161:ARG:HD2   | 2.26                     | 0.71              |
| 2:C:410:ILE:HG22  | 2:C:453:THR:O     | 1.90                     | 0.71              |
| 2:C:541:SER:O     | 2:C:545:ASN:ND2   | 2.24                     | 0.71              |
| 4:E:68:LEU:HD12   | 4:E:73:LEU:HD13   | 1.71                     | 0.71              |
| 2:M:598:GLU:O     | 2:M:651:LYS:HG3   | 1.90                     | 0.71              |
| 2:M:754:ILE:CD1   | 2:M:791:ARG:HG2   | 2.17                     | 0.71              |
| 3:N:141:ILE:HD11  | 3:N:448:GLU:HG2   | 1.72                     | 0.71              |
| 3:N:525:ARG:HB3   | 3:N:540:LEU:HD12  | 1.71                     | 0.71              |
| 3:N:645:PRO:HA    | 3:N:721:VAL:O     | 1.90                     | 0.71              |
| 3:N:1129:THR:CB   | 3:N:1320:GLU:CG   | 2.62                     | 0.71              |
| 7:I:1:DG:OP3      | 7:I:1:DG:H3'      | 1.90                     | 0.71              |
| 2:C:861:LEU:HD22  | 2:C:863:ASP:HB3   | 1.73                     | 0.71              |
| 3:D:524:LEU:N     | 3:D:524:LEU:HD12  | 2.05                     | 0.71              |
| 2:M:90:TYR:O      | 2:M:119:PRO:HA    | 1.89                     | 0.71              |
| 2:M:284:ARG:HG2   | 2:M:301:GLU:OE1   | 1.90                     | 0.71              |
| 2:M:720:GLU:HG2   | 2:M:760:SER:HB3   | 1.71                     | 0.71              |
| 3:N:809:PRO:HB2   | 3:N:812:ALA:HB2   | 1.73                     | 0.71              |
| 3:N:1462:LEU:CD2  | 3:N:1473:PRO:HD2  | 2.20                     | 0.71              |
| 5:G:21:DG:H2''    | 5:G:22:DA:O5'     | 1.88                     | 0.71              |
| 6:H:8:G:H2'       | 6:H:9:C:C6        | 2.25                     | 0.71              |
| 1:B:123:MET:C     | 1:B:125:PRO:HD3   | 2.16                     | 0.71              |
| 2:C:1037:VAL:HG12 | 2:C:1041:GLU:OE2  | 1.89                     | 0.71              |
| 3:D:799:LYS:O     | 3:D:829:VAL:HG22  | 1.90                     | 0.71              |
| 2:M:122:THR:HB    | 2:M:124:ASP:OD1   | 1.91                     | 0.71              |
| 2:M:276:LYS:HA    | 2:M:280:LYS:HD2   | 1.71                     | 0.71              |
| 2:M:334:ARG:O     | 2:M:339:LEU:HD11  | 1.91                     | 0.71              |
| 2:M:536:PRO:HB3   | 2:M:906:PHE:HD1   | 1.54                     | 0.71              |
| 2:M:570:PRO:HD2   | 2:M:635:THR:HG21  | 1.72                     | 0.71              |
| 3:N:696:HIS:CG    | 3:N:697:GLY:H     | 2.07                     | 0.71              |
| 3:N:1209:LEU:HD12 | 3:N:1216:SER:H    | 1.56                     | 0.71              |
| 1:A:86:VAL:CG2    | 1:A:204:SER:HB2   | 2.21                     | 0.71              |
| 1:A:86:VAL:HG12   | 1:A:124:ASN:HB2   | 1.71                     | 0.71              |
| 2:C:122:THR:HB    | 2:C:124:ASP:OD1   | 1.91                     | 0.71              |
| 2:C:415:PRO:HD2   | 2:C:418:LEU:HD13  | 1.72                     | 0.71              |
| 3:D:122:GLU:O     | 3:D:126:VAL:HG23  | 1.91                     | 0.71              |
| 2:M:21:ILE:H      | 2:M:21:ILE:HD12   | 1.56                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:107:ASP:OD1   | 3:N:1445:HIS:HB2  | 1.90                     | 0.71              |
| 3:N:133:ILE:HG23  | 3:N:456:MET:HB3   | 1.71                     | 0.71              |
| 3:N:1109:GLU:HG2  | 3:N:1201:CYS:CA   | 2.19                     | 0.71              |
| 5:G:19:DG:C2'     | 5:G:20:DC:O5'     | 2.38                     | 0.71              |
| 2:C:88:LEU:HD13   | 2:C:89:THR:H      | 1.56                     | 0.71              |
| 3:D:1095:THR:HA   | 3:D:1098:LEU:HD13 | 1.73                     | 0.71              |
| 3:D:1255:GLY:C    | 3:D:1257:PRO:HD2  | 2.16                     | 0.71              |
| 3:D:1256:LEU:HG   | 3:D:1260:ILE:CD1  | 2.21                     | 0.71              |
| 3:N:646:LYS:CG    | 3:N:688:TRP:CH2   | 2.73                     | 0.71              |
| 6:Y:8:G:H2'       | 6:Y:9:C:O4'       | 1.91                     | 0.71              |
| 2:C:395:LYS:HZ1   | 2:C:407:LYS:HZ3   | 1.37                     | 0.71              |
| 2:C:409:ARG:HH12  | 2:C:444:PRO:HG3   | 1.55                     | 0.71              |
| 2:C:674:VAL:CG2   | 2:C:869:VAL:HG13  | 2.20                     | 0.71              |
| 3:D:1114:THR:HG23 | 3:D:1114:THR:O    | 1.90                     | 0.71              |
| 2:M:511:GLU:O     | 2:M:526:PRO:HD3   | 1.90                     | 0.71              |
| 2:M:578:VAL:HG13  | 2:M:671:ASN:ND2   | 2.05                     | 0.71              |
| 2:M:1046:ALA:HA   | 3:N:1472:ILE:HD11 | 1.73                     | 0.71              |
| 3:D:30:GLU:HB3    | 3:D:40:GLU:HG2    | 1.73                     | 0.71              |
| 3:D:1177:ALA:O    | 3:D:1180:ALA:HB3  | 1.91                     | 0.71              |
| 3:D:1340:GLY:O    | 3:D:1344:VAL:HG23 | 1.90                     | 0.71              |
| 2:M:352:ALA:O     | 2:M:355:VAL:HG12  | 1.90                     | 0.71              |
| 3:N:646:LYS:NZ    | 3:N:688:TRP:CE2   | 2.59                     | 0.71              |
| 3:N:840:LYS:HD3   | 3:N:841:TYR:OH    | 1.90                     | 0.71              |
| 3:N:847:ASP:O     | 3:N:851:LEU:HG    | 1.90                     | 0.71              |
| 1:B:52:ALA:HB2    | 1:B:170:VAL:C     | 2.16                     | 0.71              |
| 2:C:144:PRO:HG2   | 2:C:265:ARG:NH1   | 2.05                     | 0.71              |
| 2:C:227:PHE:HD2   | 2:C:237:ARG:NE    | 1.88                     | 0.71              |
| 2:C:433:THR:C     | 2:C:435:TYR:H     | 1.99                     | 0.71              |
| 3:D:586:ARG:NH2   | 3:D:1442:ASN:OD1  | 2.24                     | 0.71              |
| 2:M:236:ILE:HA    | 2:M:239:PHE:HD2   | 1.56                     | 0.71              |
| 3:N:57:GLU:HG2    | 3:N:58:CYS:N      | 2.05                     | 0.71              |
| 3:N:136:ASP:HB3   | 3:N:137:PRO:CD    | 2.21                     | 0.71              |
| 2:C:244:PRO:HD2   | 2:C:245:GLY:H     | 1.56                     | 0.70              |
| 2:C:431:HIS:CD2   | 2:C:433:THR:H     | 2.08                     | 0.70              |
| 3:D:17:LYS:HG2    | 3:D:21:TRP:NE1    | 2.05                     | 0.70              |
| 3:D:487:ALA:HB2   | 5:G:7:DA:C2'      | 2.21                     | 0.70              |
| 3:D:633:VAL:HG22  | 3:D:635:PRO:HD3   | 1.73                     | 0.70              |
| 3:D:1434:TRP:CZ3  | 3:D:1457:ASP:HB2  | 2.25                     | 0.70              |
| 2:M:677:MET:CB    | 2:M:987:ILE:HD13  | 2.21                     | 0.70              |
| 2:M:754:ILE:HD12  | 2:M:789:SER:HB2   | 1.72                     | 0.70              |
| 3:N:478:LEU:HD22  | 3:N:1388:ARG:HD3  | 1.73                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:35:THR:O      | 1:A:39:PRO:HG2    | 1.90                     | 0.70              |
| 2:C:190:LYS:H     | 2:C:190:LYS:HD2   | 1.56                     | 0.70              |
| 1:K:72:LYS:O      | 2:M:608:GLY:HA2   | 1.91                     | 0.70              |
| 2:M:140:ILE:HD13  | 2:M:331:ARG:HH21  | 1.56                     | 0.70              |
| 2:M:455:LEU:CD1   | 2:M:456:ALA:O     | 2.37                     | 0.70              |
| 2:M:496:ILE:HA    | 2:M:531:PHE:O     | 1.92                     | 0.70              |
| 2:M:676:ILE:CG2   | 2:M:988:VAL:HG22  | 2.21                     | 0.70              |
| 2:M:753:ASP:HB2   | 2:M:792:VAL:HG21  | 1.72                     | 0.70              |
| 3:N:101:HIS:ND1   | 3:N:103:TRP:HB2   | 2.06                     | 0.70              |
| 3:N:653:PHE:CZ    | 3:N:749:VAL:CG1   | 2.73                     | 0.70              |
| 3:N:758:GLU:HB3   | 4:O:20:THR:CG2    | 2.21                     | 0.70              |
| 5:X:23:DG:H2'     | 5:X:24:DC:C6      | 2.26                     | 0.70              |
| 1:A:18:ARG:O      | 1:A:201:THR:OG1   | 2.09                     | 0.70              |
| 2:C:1045:ALA:HB2  | 3:D:763:MET:HE1   | 1.73                     | 0.70              |
| 2:M:676:ILE:HG21  | 2:M:988:VAL:HG22  | 1.72                     | 0.70              |
| 2:M:1040:LEU:CD2  | 2:M:1049:LEU:HD13 | 2.21                     | 0.70              |
| 3:N:520:LEU:HD21  | 3:N:524:LEU:HB3   | 1.73                     | 0.70              |
| 3:N:783:ARG:NH2   | 3:N:1029:ARG:HD2  | 2.06                     | 0.70              |
| 3:N:1366:LYS:HA   | 3:N:1369:GLU:OE1  | 1.91                     | 0.70              |
| 2:C:1008:ARG:HD2  | 2:C:1028:GLY:H    | 1.56                     | 0.70              |
| 3:D:1380:GLU:HB2  | 3:D:1420:LEU:HD11 | 1.73                     | 0.70              |
| 1:L:52:ALA:HB2    | 1:L:170:VAL:C     | 2.16                     | 0.70              |
| 1:L:101:LEU:HD23  | 1:L:101:LEU:C     | 2.16                     | 0.70              |
| 2:M:903:SER:OG    | 2:M:908:GLY:HA3   | 1.91                     | 0.70              |
| 3:N:650:LEU:O     | 3:N:654:LYS:HB2   | 1.90                     | 0.70              |
| 2:C:273:GLY:HA2   | 2:C:276:LYS:HD2   | 1.72                     | 0.70              |
| 2:C:1007:ALA:HB1  | 3:D:652:LEU:CD1   | 2.21                     | 0.70              |
| 3:D:528:VAL:HG12  | 3:D:529:GLN:N     | 2.06                     | 0.70              |
| 3:D:1256:LEU:CD2  | 3:D:1260:ILE:HD11 | 2.21                     | 0.70              |
| 3:N:1084:THR:HG22 | 3:N:1087:ARG:HH22 | 1.57                     | 0.70              |
| 3:D:843:PHE:HB2   | 3:D:866:VAL:HG22  | 1.73                     | 0.70              |
| 2:M:399:ASN:OD1   | 2:M:401:LEU:HB3   | 1.92                     | 0.70              |
| 2:M:605:LYS:HD3   | 2:M:610:ARG:NH1   | 2.07                     | 0.70              |
| 2:C:88:LEU:O      | 2:C:129:ILE:O     | 2.08                     | 0.70              |
| 2:C:336:VAL:HA    | 2:C:339:LEU:CD1   | 2.12                     | 0.70              |
| 2:C:347:GLY:HA3   | 2:C:378:LEU:HD12  | 1.73                     | 0.70              |
| 3:D:72:VAL:HG23   | 3:D:78:VAL:N      | 2.06                     | 0.70              |
| 4:E:27:ALA:O      | 4:E:31:LEU:HG     | 1.90                     | 0.70              |
| 2:M:52:PHE:HB3    | 2:M:53:PRO:HD3    | 1.74                     | 0.70              |
| 2:M:959:PRO:HA    | 2:M:962:GLN:HG3   | 1.73                     | 0.70              |
| 3:N:1093:TYR:CZ   | 5:X:18:DC:H5"     | 2.27                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:63:HIS:CB     | 2:C:746:GLY:HA2   | 2.21                     | 0.70              |
| 3:D:1109:GLU:CB   | 3:D:1201:CYS:HA   | 2.22                     | 0.70              |
| 4:E:13:VAL:HG21   | 4:E:19:LEU:HD13   | 1.74                     | 0.70              |
| 2:M:90:TYR:CE1    | 2:M:120:LEU:HD12  | 2.26                     | 0.70              |
| 3:N:1292:VAL:CG2  | 3:N:1311:LEU:HD13 | 2.21                     | 0.70              |
| 3:N:1379:VAL:HG12 | 3:N:1419:PRO:HA   | 1.72                     | 0.70              |
| 6:Y:10:G:H2'      | 6:Y:11:C:C6       | 2.26                     | 0.70              |
| 2:C:21:ILE:HD12   | 2:C:21:ILE:H      | 1.57                     | 0.70              |
| 2:C:332:ARG:NH2   | 2:C:464:LEU:HG    | 2.07                     | 0.70              |
| 3:D:103:TRP:CH2   | 3:D:1444:THR:HA   | 2.27                     | 0.70              |
| 3:D:103:TRP:CZ3   | 3:D:1444:THR:HA   | 2.27                     | 0.70              |
| 3:D:127:LEU:C     | 3:D:127:LEU:HD12  | 2.16                     | 0.70              |
| 3:D:1003:VAL:HG11 | 3:D:1036:ARG:HH11 | 1.56                     | 0.70              |
| 3:D:1046:GLN:HG2  | 3:D:1052:THR:HG22 | 1.74                     | 0.70              |
| 3:D:1100:ASP:HA   | 3:D:1463:LYS:NZ   | 2.06                     | 0.70              |
| 2:M:861:LEU:HD21  | 2:M:925:TYR:CE2   | 2.27                     | 0.70              |
| 3:N:206:ARG:HG2   | 3:N:394:LEU:HD22  | 1.72                     | 0.70              |
| 4:O:54:LEU:HD23   | 4:O:58:PRO:CD     | 2.19                     | 0.70              |
| 2:C:1092:LEU:HD13 | 2:C:1099:VAL:HG21 | 1.74                     | 0.70              |
| 4:E:27:ALA:HA     | 4:E:30:LEU:HD13   | 1.74                     | 0.70              |
| 1:L:137:ARG:HH21  | 1:L:139:ASN:HB3   | 1.56                     | 0.70              |
| 2:M:328:LEU:HB2   | 2:M:488:ALA:CB    | 2.21                     | 0.70              |
| 3:N:56:TYR:OH     | 3:N:69:GLU:HB2    | 1.91                     | 0.70              |
| 5:G:24:DC:OP2     | 5:G:24:DC:H6      | 1.74                     | 0.70              |
| 3:D:615:ARG:HH22  | 3:D:1096:ARG:CD   | 2.04                     | 0.69              |
| 3:D:809:PRO:HB2   | 3:D:812:ALA:HB2   | 1.74                     | 0.69              |
| 1:L:100:LEU:HB2   | 1:L:115:LEU:HD21  | 1.73                     | 0.69              |
| 2:M:374:ASN:O     | 2:M:377:PRO:HD2   | 1.92                     | 0.69              |
| 3:N:480:GLU:OE1   | 3:N:488:ARG:HG3   | 1.91                     | 0.69              |
| 2:C:12:VAL:HB     | 2:C:472:ARG:NH1   | 2.07                     | 0.69              |
| 3:D:30:GLU:HB3    | 3:D:40:GLU:CG     | 2.22                     | 0.69              |
| 2:M:685:GLU:OE2   | 3:N:783:ARG:HD2   | 1.92                     | 0.69              |
| 2:M:1006:HIS:CE1  | 2:M:1027:PHE:HA   | 2.26                     | 0.69              |
| 2:M:1101:THR:HG21 | 2:M:1111:ILE:HG23 | 1.71                     | 0.69              |
| 3:N:809:PRO:HB2   | 3:N:812:ALA:CB    | 2.22                     | 0.69              |
| 2:C:66:LEU:HD13   | 2:C:100:LEU:HB2   | 1.74                     | 0.69              |
| 2:C:173:ASP:OD1   | 2:C:185:LYS:HB2   | 1.92                     | 0.69              |
| 2:C:759:THR:HA    | 2:C:786:LYS:O     | 1.92                     | 0.69              |
| 3:D:9:ARG:NH1     | 3:D:11:ALA:HB2    | 2.07                     | 0.69              |
| 3:D:1146:GLY:HA3  | 3:D:1207:TYR:HB2  | 1.74                     | 0.69              |
| 3:N:1066:THR:HG22 | 3:N:1069:GLU:CD   | 2.17                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1129:THR:CG2  | 3:N:1130:ARG:N    | 2.49                     | 0.69              |
| 5:X:27:DC:P       | 5:X:27:DC:H3'     | 2.33                     | 0.69              |
| 1:A:65:PHE:CE1    | 2:C:799:ILE:HB    | 2.27                     | 0.69              |
| 1:B:211:LEU:O     | 1:B:215:VAL:HG13  | 1.92                     | 0.69              |
| 2:C:328:LEU:HD21  | 2:C:434:HIS:HA    | 1.74                     | 0.69              |
| 3:D:72:VAL:HG23   | 3:D:78:VAL:H      | 1.56                     | 0.69              |
| 3:D:525:ARG:HB2   | 3:D:538:SER:HB3   | 1.73                     | 0.69              |
| 2:M:532:MET:HE3   | 2:M:533:ASP:O     | 1.92                     | 0.69              |
| 2:M:584:GLU:HB2   | 2:M:666:LEU:H     | 1.56                     | 0.69              |
| 3:N:465:LEU:CD2   | 3:N:510:GLU:HA    | 2.22                     | 0.69              |
| 3:N:1353:GLN:O    | 3:N:1357:ARG:HG3  | 1.93                     | 0.69              |
| 3:D:1089:ALA:HA   | 5:G:19:DG:H5'     | 1.74                     | 0.69              |
| 1:L:92:PRO:HA     | 1:L:146:ARG:NH1   | 2.06                     | 0.69              |
| 2:M:267:TYR:HD2   | 2:M:267:TYR:O     | 1.73                     | 0.69              |
| 2:M:557:ARG:HD2   | 2:M:560:MET:HG3   | 1.73                     | 0.69              |
| 3:N:699:VAL:CG2   | 3:N:760:ARG:HB3   | 2.22                     | 0.69              |
| 3:N:1239:ARG:HB2  | 3:N:1239:ARG:HH11 | 1.58                     | 0.69              |
| 2:C:274:ARG:NH1   | 2:C:285:LEU:HD22  | 2.07                     | 0.69              |
| 3:D:678:GLU:HG3   | 3:D:679:ARG:HG3   | 1.74                     | 0.69              |
| 3:D:696:HIS:NE2   | 4:E:59:ASN:HB2    | 2.06                     | 0.69              |
| 3:D:1197:ARG:HD3  | 3:D:1198:TYR:H    | 1.58                     | 0.69              |
| 2:M:290:LEU:HG    | 2:M:290:LEU:O     | 1.92                     | 0.69              |
| 2:M:969:GLN:OE1   | 3:N:952:ASP:HB2   | 1.93                     | 0.69              |
| 2:M:1115:LEU:HD12 | 2:M:1115:LEU:N    | 2.06                     | 0.69              |
| 5:G:7:DA:OP2      | 5:G:7:DA:H8       | 1.74                     | 0.69              |
| 2:C:554:ASP:OD2   | 2:C:556:ASN:HB3   | 1.92                     | 0.69              |
| 2:C:776:SER:HA    | 2:C:780:GLU:HB3   | 1.75                     | 0.69              |
| 2:M:237:ARG:HB2   | 2:M:237:ARG:HH11  | 1.56                     | 0.69              |
| 3:N:198:ARG:HG3   | 3:N:198:ARG:O     | 1.92                     | 0.69              |
| 3:N:502:PHE:CE1   | 3:N:1452:ILE:HG23 | 2.28                     | 0.69              |
| 3:N:715:ALA:HB3   | 3:N:764:LEU:HA    | 1.73                     | 0.69              |
| 3:N:925:GLU:OE2   | 4:O:5:GLY:HA2     | 1.93                     | 0.69              |
| 3:N:1031:ASN:OD1  | 3:N:1033:GLN:HB2  | 1.91                     | 0.69              |
| 1:A:106:PRO:CG    | 1:A:134:GLU:OE1   | 2.41                     | 0.69              |
| 1:B:57:TYR:HE1    | 1:B:163:ASN:HB2   | 1.58                     | 0.69              |
| 2:C:399:ASN:OD1   | 2:C:402:SER:N     | 2.23                     | 0.69              |
| 2:C:971:LYS:HA    | 2:C:988:VAL:HA    | 1.73                     | 0.69              |
| 3:D:1041:LEU:O    | 3:D:1045:MET:HB2  | 1.93                     | 0.69              |
| 4:E:45:ARG:HG2    | 4:E:46:PRO:HD2    | 1.74                     | 0.69              |
| 4:E:54:LEU:HA     | 4:E:58:PRO:CG     | 2.22                     | 0.69              |
| 2:M:433:THR:C     | 2:M:435:TYR:H     | 2.00                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:442:GLU:HG2   | 2:M:454:SER:HB2   | 1.73                     | 0.69              |
| 2:M:567:GLN:HE22  | 6:Y:13:C:H5''     | 1.58                     | 0.69              |
| 2:M:888:THR:O     | 2:M:990:GLY:HA3   | 1.93                     | 0.69              |
| 3:N:957:PRO:HG2   | 3:N:1007:VAL:CG2  | 2.18                     | 0.69              |
| 3:N:1106:VAL:HG11 | 3:N:1474:ALA:HB2  | 1.75                     | 0.69              |
| 3:N:1281:VAL:N    | 3:N:1317:ASP:O    | 2.26                     | 0.69              |
| 2:C:564:MET:HE2   | 2:C:995:MET:HE3   | 1.74                     | 0.69              |
| 2:C:725:ASP:O     | 2:C:727:PRO:HD3   | 1.92                     | 0.69              |
| 2:C:830:LYS:O     | 2:C:832:LYS:N     | 2.26                     | 0.69              |
| 3:D:758:GLU:HB3   | 3:D:762:GLN:HE21  | 1.57                     | 0.69              |
| 3:D:1111:ASP:HA   | 3:D:1201:CYS:HB2  | 1.75                     | 0.69              |
| 1:L:38:ASN:HB3    | 1:L:39:PRO:HD3    | 1.75                     | 0.69              |
| 2:M:644:VAL:HG22  | 2:M:647:GLN:OE1   | 1.92                     | 0.69              |
| 2:M:674:VAL:HG12  | 2:M:990:GLY:O     | 1.93                     | 0.69              |
| 2:C:129:ILE:CD1   | 2:C:129:ILE:H     | 2.06                     | 0.69              |
| 2:C:723:THR:HG23  | 2:C:725:ASP:H     | 1.57                     | 0.69              |
| 3:D:1239:ARG:O    | 3:D:1240:THR:HG23 | 1.92                     | 0.69              |
| 3:N:153:LEU:O     | 3:N:153:LEU:HD12  | 1.93                     | 0.69              |
| 3:N:179:VAL:HG13  | 3:N:183:GLU:HB3   | 1.75                     | 0.69              |
| 3:N:567:ILE:O     | 3:N:571:LYS:HG2   | 1.93                     | 0.69              |
| 3:N:625:TYR:HH    | 3:N:655:PRO:HG2   | 1.58                     | 0.69              |
| 5:G:5:DC:H2''     | 5:G:6:DT:C4'      | 2.23                     | 0.69              |
| 7:I:11:DG:C2'     | 7:I:12:DT:H72     | 2.22                     | 0.69              |
| 1:B:38:ASN:HB3    | 1:B:39:PRO:HD3    | 1.73                     | 0.68              |
| 1:K:96:THR:OG1    | 1:K:143:ARG:HD2   | 1.92                     | 0.68              |
| 1:L:195:LEU:HD12  | 1:L:196:THR:N     | 2.08                     | 0.68              |
| 2:M:64:LEU:CD2    | 2:M:359:MET:HG3   | 2.23                     | 0.68              |
| 2:M:1038:TRP:HA   | 2:M:1041:GLU:OE1  | 1.93                     | 0.68              |
| 2:M:1090:LYS:NZ   | 2:M:1112:PHE:HE1  | 1.90                     | 0.68              |
| 3:N:710:ARG:HH12  | 4:O:16:LYS:NZ     | 1.91                     | 0.68              |
| 3:N:916:TYR:O     | 3:N:920:LEU:HG    | 1.93                     | 0.68              |
| 3:N:1225:ALA:HA   | 3:N:1367:HIS:ND1  | 2.08                     | 0.68              |
| 6:Y:9:C:O2'       | 6:Y:10:G:H5'      | 1.93                     | 0.68              |
| 2:C:50:GLU:CB     | 2:C:266:ARG:NH1   | 2.56                     | 0.68              |
| 2:C:212:GLY:HA3   | 2:C:218:VAL:HG21  | 1.74                     | 0.68              |
| 3:D:28:LYS:CG     | 3:D:29:PRO:HD2    | 2.23                     | 0.68              |
| 3:D:528:VAL:HG12  | 3:D:529:GLN:H     | 1.58                     | 0.68              |
| 3:D:638:LYS:HB2   | 3:D:641:GLN:NE2   | 2.08                     | 0.68              |
| 3:D:1335:LEU:HD21 | 3:D:1344:VAL:HA   | 1.76                     | 0.68              |
| 2:M:86:LYS:HB3    | 2:M:813:VAL:HG23  | 1.76                     | 0.68              |
| 2:M:332:ARG:HG2   | 2:M:333:ILE:N     | 2.07                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:979:THR:HG23  | 2:M:981:GLU:H     | 1.58                     | 0.68              |
| 3:N:156:GLU:O     | 3:N:160:GLU:HG3   | 1.93                     | 0.68              |
| 3:N:1216:SER:HB3  | 4:O:15:SER:HA     | 1.75                     | 0.68              |
| 1:A:154:GLU:CD    | 1:A:154:GLU:N     | 2.51                     | 0.68              |
| 1:A:162:ILE:HG13  | 1:A:163:ASN:H     | 1.57                     | 0.68              |
| 1:A:206:THR:HG22  | 1:A:209:GLU:HG3   | 1.75                     | 0.68              |
| 2:C:274:ARG:HG2   | 2:C:285:LEU:HD13  | 1.76                     | 0.68              |
| 2:C:598:GLU:O     | 2:C:651:LYS:HG3   | 1.94                     | 0.68              |
| 2:C:1042:ALA:CB   | 3:D:1227:GLN:HE22 | 1.90                     | 0.68              |
| 2:C:1101:THR:C    | 2:C:1102:LEU:HD12 | 2.17                     | 0.68              |
| 2:M:455:LEU:CD1   | 2:M:459:ALA:HB3   | 2.14                     | 0.68              |
| 2:M:1062:GLY:O    | 2:M:1066:ALA:HB2  | 1.93                     | 0.68              |
| 3:N:1129:THR:HB   | 3:N:1320:GLU:OE1  | 1.92                     | 0.68              |
| 3:N:1129:THR:CB   | 3:N:1320:GLU:HG3  | 2.21                     | 0.68              |
| 2:C:290:LEU:HB3   | 2:C:302:VAL:HG11  | 1.76                     | 0.68              |
| 2:C:1034:GLU:CD   | 3:D:619:LEU:HD22  | 2.17                     | 0.68              |
| 3:D:799:LYS:CB    | 3:D:826:PRO:HG2   | 2.23                     | 0.68              |
| 3:D:1167:SER:O    | 3:D:1171:VAL:HG23 | 1.93                     | 0.68              |
| 3:N:122:GLU:O     | 3:N:126:VAL:HG23  | 1.93                     | 0.68              |
| 1:B:87:VAL:HG21   | 1:B:144:VAL:HG11  | 1.75                     | 0.68              |
| 2:C:690:ILE:HG13  | 2:C:694:LEU:HD12  | 1.75                     | 0.68              |
| 2:C:1062:GLY:O    | 2:C:1066:ALA:HB2  | 1.93                     | 0.68              |
| 3:D:133:ILE:O     | 3:D:152:LEU:HB2   | 1.92                     | 0.68              |
| 3:D:897:TRP:HA    | 3:D:900:ILE:HG12  | 0.69                     | 0.68              |
| 2:M:266:ARG:HA    | 2:M:288:ARG:HD3   | 1.75                     | 0.68              |
| 2:M:725:ASP:O     | 2:M:727:PRO:HD3   | 1.93                     | 0.68              |
| 3:N:1109:GLU:HG2  | 3:N:1200:VAL:O    | 1.94                     | 0.68              |
| 3:N:1283:ILE:HD11 | 3:N:1314:LYS:HA   | 1.75                     | 0.68              |
| 3:N:1292:VAL:HG22 | 3:N:1311:LEU:HD13 | 1.74                     | 0.68              |
| 2:C:185:LYS:HG2   | 2:C:190:LYS:HG3   | 1.75                     | 0.68              |
| 2:C:1006:HIS:HD1  | 2:C:1027:PHE:HD1  | 1.40                     | 0.68              |
| 3:D:28:LYS:HB3    | 3:D:41:ARG:HD2    | 1.74                     | 0.68              |
| 3:D:540:LEU:H     | 3:D:540:LEU:HD12  | 1.58                     | 0.68              |
| 3:D:1256:LEU:N    | 3:D:1257:PRO:CD   | 2.57                     | 0.68              |
| 3:N:695:ILE:O     | 3:N:696:HIS:C     | 2.37                     | 0.68              |
| 1:B:49:PRO:HA     | 1:B:148:VAL:HG12  | 1.75                     | 0.68              |
| 2:C:946:ARG:HA    | 2:C:949:LYS:HD2   | 1.75                     | 0.68              |
| 2:C:1097:LEU:HD22 | 2:C:1097:LEU:N    | 2.04                     | 0.68              |
| 3:D:109:PRO:HB3   | 3:D:494:LYS:HZ3   | 1.57                     | 0.68              |
| 3:D:704:ARG:CA    | 3:D:745:MET:HG2   | 2.21                     | 0.68              |
| 2:M:367:LEU:HB3   | 2:M:371:LYS:HE3   | 1.76                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:152:LEU:HD23  | 3:N:152:LEU:H     | 1.59                     | 0.68              |
| 3:N:457:GLY:C     | 3:N:459:GLU:N     | 2.49                     | 0.68              |
| 3:N:508:ARG:HB3   | 3:N:510:GLU:OE2   | 1.94                     | 0.68              |
| 3:N:845:ASN:CG    | 3:N:846:PRO:HD2   | 2.18                     | 0.68              |
| 3:N:1394:VAL:HB   | 3:N:1397:LYS:HE2  | 1.76                     | 0.68              |
| 1:A:42:ARG:CZ     | 1:B:34:VAL:HB     | 2.24                     | 0.68              |
| 2:C:630:ARG:HD3   | 2:C:705:ILE:CG2   | 2.24                     | 0.68              |
| 3:D:9:ARG:HA      | 3:D:1434:TRP:HH2  | 1.58                     | 0.68              |
| 3:D:47:GLU:HG2    | 3:D:53:ILE:HB     | 1.74                     | 0.68              |
| 2:M:1109:VAL:HG21 | 3:N:5:VAL:HG13    | 1.76                     | 0.68              |
| 3:N:115:LEU:C     | 3:N:115:LEU:HD23  | 2.19                     | 0.68              |
| 5:G:25:DG:H2'     | 5:G:26:DC:C6      | 2.28                     | 0.68              |
| 7:I:1:DG:H3'      | 7:I:1:DG:P        | 2.33                     | 0.68              |
| 1:A:13:VAL:HG12   | 1:A:14:ARG:N      | 2.08                     | 0.68              |
| 2:C:274:ARG:NE    | 2:C:278:GLU:OE2   | 2.27                     | 0.68              |
| 2:C:358:ARG:HH22  | 2:C:374:ASN:HB3   | 1.59                     | 0.68              |
| 2:C:1016:ILE:HG12 | 2:C:1017:THR:HG23 | 1.76                     | 0.68              |
| 3:D:554:LEU:HA    | 3:D:557:LEU:HD12  | 1.76                     | 0.68              |
| 1:K:171:PHE:O     | 1:K:173:PRO:HD3   | 1.94                     | 0.68              |
| 1:L:123:MET:C     | 1:L:125:PRO:HD3   | 2.19                     | 0.68              |
| 2:M:710:ILE:HD11  | 2:M:758:ARG:HE    | 1.56                     | 0.68              |
| 2:M:710:ILE:HD12  | 2:M:790:LEU:HB2   | 1.75                     | 0.68              |
| 4:O:25:LYS:HA     | 4:O:28:GLN:NE2    | 2.09                     | 0.68              |
| 2:C:73:LEU:HB2    | 2:C:93:PRO:O      | 1.94                     | 0.68              |
| 2:C:396:ASP:HA    | 2:C:633:GLN:NE2   | 2.09                     | 0.68              |
| 2:C:571:LEU:HD21  | 2:C:700:TYR:HA    | 1.75                     | 0.68              |
| 2:C:889:HIS:O     | 2:C:892:LEU:HB3   | 1.94                     | 0.68              |
| 3:D:9:ARG:HA      | 3:D:1455:LYS:O    | 1.94                     | 0.68              |
| 3:D:642:CYS:SG    | 3:D:716:PHE:HB2   | 2.34                     | 0.68              |
| 4:E:26:ARG:O      | 4:E:30:LEU:HD12   | 1.94                     | 0.68              |
| 3:N:720:LEU:H     | 3:N:720:LEU:HD12  | 1.57                     | 0.68              |
| 3:N:1223:ILE:O    | 3:N:1227:GLN:HG3  | 1.94                     | 0.68              |
| 3:D:701:LEU:H     | 3:D:701:LEU:HD12  | 1.59                     | 0.67              |
| 3:D:1109:GLU:HG2  | 3:D:1201:CYS:CA   | 2.21                     | 0.67              |
| 2:M:7:GLY:HA3     | 2:M:904:PRO:HG2   | 1.76                     | 0.67              |
| 2:M:274:ARG:HH11  | 2:M:274:ARG:HG3   | 1.58                     | 0.67              |
| 2:M:971:LYS:HA    | 2:M:988:VAL:HA    | 1.76                     | 0.67              |
| 7:I:11:DG:H8      | 7:I:11:DG:O5'     | 1.77                     | 0.67              |
| 1:B:102:LYS:HD2   | 1:B:139:ASN:OD1   | 1.94                     | 0.67              |
| 2:C:435:TYR:O     | 2:C:437:ARG:HD2   | 1.93                     | 0.67              |
| 2:M:378:LEU:HG    | 2:M:382:ILE:HD11  | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:80:VAL:HG12   | 3:N:81:THR:O      | 1.94                     | 0.67              |
| 3:N:1263:PHE:O    | 3:N:1424:VAL:HG12 | 1.94                     | 0.67              |
| 2:C:52:PHE:HE1    | 2:C:68:PHE:N      | 1.91                     | 0.67              |
| 2:C:304:LEU:HD23  | 2:C:305:PRO:HD3   | 1.77                     | 0.67              |
| 2:C:838:LYS:C     | 2:C:839:LEU:HD23  | 2.20                     | 0.67              |
| 3:D:505:SER:CB    | 3:D:1453:ALA:HA   | 2.24                     | 0.67              |
| 3:D:619:LEU:HB2   | 3:D:621:LYS:NZ    | 2.10                     | 0.67              |
| 3:D:827:ILE:H     | 3:D:827:ILE:HD12  | 1.60                     | 0.67              |
| 3:D:1448:THR:O    | 3:D:1452:ILE:HD13 | 1.95                     | 0.67              |
| 3:N:104:PHE:CD2   | 3:N:1448:THR:HG23 | 2.29                     | 0.67              |
| 3:N:1209:LEU:HD23 | 3:N:1210:SER:N    | 2.08                     | 0.67              |
| 6:H:4:G:H2'       | 6:H:5:C:C6        | 2.29                     | 0.67              |
| 7:Z:15:DT:H2''    | 7:Z:16:DG:OP2     | 1.94                     | 0.67              |
| 1:A:31:GLY:O      | 1:A:34:VAL:CG1    | 2.42                     | 0.67              |
| 2:C:58:ASP:O      | 2:C:59:LYS:CB     | 2.42                     | 0.67              |
| 2:C:218:VAL:HG13  | 2:C:221:LEU:HD21  | 1.77                     | 0.67              |
| 3:D:785:ILE:HG23  | 3:D:938:GLY:HA3   | 1.76                     | 0.67              |
| 3:D:1447:LEU:CD1  | 3:D:1447:LEU:H    | 2.07                     | 0.67              |
| 3:D:1457:ASP:O    | 3:D:1459:LEU:HD12 | 1.93                     | 0.67              |
| 2:M:69:LEU:HB2    | 2:M:97:ARG:HB2    | 1.75                     | 0.67              |
| 2:M:189:ARG:HD3   | 2:M:190:LYS:H     | 1.60                     | 0.67              |
| 2:M:289:THR:O     | 2:M:291:ALA:N     | 2.28                     | 0.67              |
| 2:M:300:ASP:C     | 2:M:302:VAL:H     | 2.02                     | 0.67              |
| 2:M:420:ARG:HD2   | 7:Z:1:DG:C5'      | 2.24                     | 0.67              |
| 2:M:430:VAL:HG11  | 3:N:1075:HIS:HA   | 1.75                     | 0.67              |
| 2:M:760:SER:O     | 2:M:785:VAL:HG22  | 1.95                     | 0.67              |
| 2:M:862:PRO:CB    | 2:M:929:ARG:HH22  | 2.05                     | 0.67              |
| 2:M:1040:LEU:HG   | 2:M:1045:ALA:HB3  | 1.76                     | 0.67              |
| 2:M:1053:LEU:HD12 | 3:N:1469:GLY:HA2  | 1.76                     | 0.67              |
| 3:N:206:ARG:HB2   | 3:N:392:SER:O     | 1.94                     | 0.67              |
| 3:N:486:ARG:O     | 3:N:490:ALA:HB2   | 1.94                     | 0.67              |
| 3:N:493:ARG:NH1   | 3:N:1391:GLU:HG2  | 2.09                     | 0.67              |
| 3:N:732:VAL:HB    | 3:N:736:PHE:HE1   | 1.59                     | 0.67              |
| 1:A:63:HIS:HB3    | 2:C:746:GLY:HA3   | 1.77                     | 0.67              |
| 1:A:178:ALA:HB2   | 2:C:864:GLY:N     | 2.10                     | 0.67              |
| 2:C:151:ASP:HB2   | 2:C:157:ARG:O     | 1.95                     | 0.67              |
| 2:C:693:GLU:CG    | 2:C:697:ARG:HH21  | 2.08                     | 0.67              |
| 2:C:939:ARG:HA    | 2:C:939:ARG:NE    | 2.10                     | 0.67              |
| 2:C:957:LYS:HB3   | 2:C:962:GLN:HG2   | 1.77                     | 0.67              |
| 2:C:1046:ALA:C    | 3:D:1472:ILE:HD11 | 2.19                     | 0.67              |
| 3:D:1031:ASN:HB3  | 3:D:1034:GLN:CB   | 2.25                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:690:ILE:HG23  | 2:M:852:ILE:HA    | 1.77                     | 0.67              |
| 2:M:887:GLU:CD    | 2:M:992:MET:HE2   | 2.18                     | 0.67              |
| 2:M:887:GLU:CD    | 2:M:992:MET:HG3   | 2.19                     | 0.67              |
| 3:N:1481:VAL:HG13 | 4:O:18:ARG:HE     | 1.58                     | 0.67              |
| 2:C:595:LEU:O     | 2:C:655:LEU:HG    | 1.95                     | 0.67              |
| 2:C:682:TYR:CZ    | 3:D:635:PRO:HG2   | 2.29                     | 0.67              |
| 2:C:937:ASP:HB3   | 2:C:940:GLU:HG3   | 1.76                     | 0.67              |
| 3:D:646:LYS:HG3   | 3:D:647:ARG:N     | 2.10                     | 0.67              |
| 3:D:714:GLN:HE21  | 3:D:765:SER:HB3   | 1.60                     | 0.67              |
| 2:M:683:ASN:HA    | 2:M:687:ALA:C     | 2.20                     | 0.67              |
| 2:M:841:ASN:HD21  | 2:M:884:GLN:HB3   | 1.60                     | 0.67              |
| 3:N:1128:VAL:CB   | 3:N:1133:ARG:HH22 | 2.04                     | 0.67              |
| 3:N:1293:PHE:HB3  | 3:N:1295:GLU:HG3  | 1.74                     | 0.67              |
| 3:N:1377:LYS:O    | 3:N:1377:LYS:HG2  | 1.93                     | 0.67              |
| 2:C:304:LEU:CD2   | 2:C:305:PRO:HD3   | 2.25                     | 0.67              |
| 2:C:690:ILE:HG23  | 2:C:852:ILE:HA    | 1.76                     | 0.67              |
| 3:D:1103:HIS:CG   | 3:D:1104:GLU:N    | 2.57                     | 0.67              |
| 1:L:87:VAL:HG21   | 1:L:144:VAL:HG11  | 1.75                     | 0.67              |
| 2:M:668:LEU:HD12  | 2:M:668:LEU:N     | 2.09                     | 0.67              |
| 2:M:690:ILE:HG12  | 2:M:691:SER:N     | 2.08                     | 0.67              |
| 3:N:166:GLN:CA    | 3:N:198:ARG:HB3   | 2.24                     | 0.67              |
| 6:H:5:C:C6        | 6:H:5:C:H3'       | 2.30                     | 0.67              |
| 2:C:89:THR:HG21   | 2:C:383:ARG:NH1   | 2.06                     | 0.67              |
| 2:C:987:ILE:CG2   | 3:D:948:THR:HG21  | 2.23                     | 0.67              |
| 3:D:950:GLY:O     | 3:D:953:ASP:HB2   | 1.95                     | 0.67              |
| 4:E:28:GLN:O      | 4:E:32:ARG:NH1    | 2.27                     | 0.67              |
| 1:L:80:LEU:HD12   | 1:L:83:LYS:NZ     | 2.10                     | 0.67              |
| 2:M:22:GLN:C      | 2:M:121:MET:HE1   | 2.20                     | 0.67              |
| 2:M:163:ILE:HD13  | 2:M:171:TRP:CH2   | 2.29                     | 0.67              |
| 2:M:195:LEU:CD2   | 2:M:238:LEU:HG    | 2.25                     | 0.67              |
| 2:M:265:ARG:HB3   | 2:M:267:TYR:CD1   | 2.29                     | 0.67              |
| 2:M:588:VAL:HG23  | 2:M:596:TYR:OH    | 1.95                     | 0.67              |
| 3:N:1061:PHE:HE1  | 3:N:1065:LEU:HD22 | 1.60                     | 0.67              |
| 2:C:69:LEU:CD1    | 2:C:97:ARG:HB3    | 2.20                     | 0.67              |
| 2:M:267:TYR:O     | 2:M:267:TYR:CD2   | 2.47                     | 0.67              |
| 2:M:393:GLN:HE21  | 6:Y:10:G:H4'      | 1.58                     | 0.67              |
| 2:M:673:LEU:HD22  | 2:M:867:VAL:HG12  | 1.77                     | 0.67              |
| 3:N:157:GLU:O     | 3:N:160:GLU:HB2   | 1.95                     | 0.67              |
| 3:N:434:ARG:HD2   | 3:N:435:VAL:H     | 1.60                     | 0.67              |
| 3:N:646:LYS:HG3   | 3:N:688:TRP:CH2   | 2.30                     | 0.67              |
| 3:N:1259:VAL:HA   | 3:N:1262:LEU:HD22 | 1.77                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:139:GLN:CD    | 2:C:418:LEU:HD22  | 2.20                     | 0.67              |
| 2:C:1000:MET:C    | 2:C:1002:GLU:H    | 2.01                     | 0.67              |
| 3:D:952:ASP:HA    | 3:D:1062:ARG:NH2  | 2.10                     | 0.67              |
| 2:M:144:PRO:HG2   | 2:M:265:ARG:HH11  | 1.59                     | 0.67              |
| 2:M:941:VAL:HA    | 2:M:944:LEU:HB2   | 1.75                     | 0.67              |
| 3:N:639:LEU:HD12  | 3:N:640:HIS:N     | 2.09                     | 0.67              |
| 2:C:152:PRO:HD3   | 2:C:159:ILE:HD11  | 1.77                     | 0.66              |
| 2:C:654:LEU:HD23  | 2:C:654:LEU:H     | 1.59                     | 0.66              |
| 3:D:1381:VAL:HB   | 3:D:1389:LEU:O    | 1.93                     | 0.66              |
| 1:K:88:ARG:HH22   | 1:K:90:LEU:HG     | 1.59                     | 0.66              |
| 1:K:177:VAL:O     | 2:M:864:GLY:CA    | 2.43                     | 0.66              |
| 2:M:703:ILE:HD12  | 2:M:703:ILE:N     | 2.09                     | 0.66              |
| 3:N:1431:THR:HG23 | 3:N:1433:SER:O    | 1.96                     | 0.66              |
| 2:C:800:VAL:HA    | 2:C:827:VAL:HG22  | 1.78                     | 0.66              |
| 3:D:30:GLU:HB2    | 3:D:41:ARG:HG3    | 1.75                     | 0.66              |
| 3:D:785:ILE:CG2   | 3:D:938:GLY:HA3   | 2.25                     | 0.66              |
| 3:D:1412:LYS:O    | 3:D:1414:PRO:HD3  | 1.95                     | 0.66              |
| 2:M:143:SER:CB    | 2:M:276:LYS:HE2   | 2.24                     | 0.66              |
| 2:M:643:VAL:HG13  | 2:M:647:GLN:CD    | 2.20                     | 0.66              |
| 3:N:525:ARG:HB2   | 3:N:538:SER:CB    | 2.23                     | 0.66              |
| 3:N:1229:ILE:HD11 | 3:N:1367:HIS:HB3  | 1.78                     | 0.66              |
| 5:X:27:DC:H2'     | 5:X:28:DG:C8      | 2.31                     | 0.66              |
| 1:A:50:GLY:HA3    | 1:A:173:PRO:HG3   | 1.77                     | 0.66              |
| 1:B:56:VAL:HG13   | 1:B:142:VAL:HG12  | 1.77                     | 0.66              |
| 2:C:140:ILE:HG23  | 2:C:410:ILE:CD1   | 2.25                     | 0.66              |
| 2:C:537:LYS:CD    | 2:C:905:ILE:HD13  | 2.25                     | 0.66              |
| 3:D:919:PHE:HA    | 3:D:927:THR:OG1   | 1.95                     | 0.66              |
| 3:D:1094:LEU:HD11 | 3:D:1260:ILE:HD12 | 1.77                     | 0.66              |
| 3:D:1488:ASP:OD1  | 4:E:89:MET:HE1    | 1.95                     | 0.66              |
| 1:L:19:GLU:HG3    | 1:L:201:THR:O     | 1.94                     | 0.66              |
| 1:L:38:ASN:O      | 1:L:41:ARG:HB3    | 1.95                     | 0.66              |
| 2:M:580:MET:O     | 2:M:902:ILE:HA    | 1.95                     | 0.66              |
| 2:M:905:ILE:HG22  | 2:M:906:PHE:N     | 2.10                     | 0.66              |
| 3:N:116:LEU:HB3   | 3:N:118:LEU:HD11  | 1.76                     | 0.66              |
| 3:N:619:LEU:HB2   | 3:N:621:LYS:NZ    | 2.10                     | 0.66              |
| 3:N:646:LYS:CD    | 3:N:688:TRP:CE2   | 2.78                     | 0.66              |
| 3:N:697:GLY:CA    | 3:N:717:GLN:CD    | 2.60                     | 0.66              |
| 3:N:1263:PHE:HA   | 3:N:1375:MET:HE1  | 1.75                     | 0.66              |
| 2:C:148:PHE:HZ    | 2:C:281:LEU:HD13  | 1.59                     | 0.66              |
| 2:C:939:ARG:HD3   | 2:C:982:PRO:CD    | 2.24                     | 0.66              |
| 3:D:1213:ARG:HH12 | 4:E:11:GLY:HA2    | 1.59                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:102:LYS:HE2   | 1:L:139:ASN:HB2   | 1.77                     | 0.66              |
| 3:N:166:GLN:HA    | 3:N:198:ARG:CB    | 2.26                     | 0.66              |
| 3:N:1110:ALA:O    | 3:N:1111:ASP:C    | 2.38                     | 0.66              |
| 3:N:1213:ARG:NH2  | 4:O:14:ASP:HA     | 2.11                     | 0.66              |
| 2:C:289:THR:O     | 2:C:291:ALA:N     | 2.28                     | 0.66              |
| 3:D:57:GLU:HG2    | 3:D:58:CYS:N      | 2.10                     | 0.66              |
| 3:D:750:PRO:HB2   | 3:D:756:GLN:HA    | 1.78                     | 0.66              |
| 3:N:25:GLU:HB2    | 3:N:92:HIS:CE1    | 2.30                     | 0.66              |
| 3:N:1476:THR:HG23 | 4:O:21:VAL:HG22   | 1.78                     | 0.66              |
| 2:C:326:ASP:HB2   | 2:C:431:HIS:HD1   | 1.58                     | 0.66              |
| 2:C:532:MET:HG2   | 2:C:533:ASP:N     | 2.09                     | 0.66              |
| 2:C:642:ARG:HG3   | 2:C:657:ASP:OD2   | 1.95                     | 0.66              |
| 2:C:1045:ALA:HB2  | 3:D:763:MET:CE    | 2.26                     | 0.66              |
| 1:K:9:PRO:HB3     | 1:K:25:LEU:CG     | 2.24                     | 0.66              |
| 2:M:579:VAL:HG13  | 2:M:842:ARG:NH2   | 2.10                     | 0.66              |
| 2:M:751:PRO:HB3   | 2:M:794:PRO:HA    | 1.78                     | 0.66              |
| 2:M:1087:VAL:O    | 2:M:1091:GLU:HG3  | 1.96                     | 0.66              |
| 3:N:28:LYS:HB2    | 3:N:41:ARG:HD2    | 1.77                     | 0.66              |
| 3:N:1137:ARG:O    | 3:N:1141:GLU:HG3  | 1.95                     | 0.66              |
| 3:D:574:LEU:O     | 3:D:578:VAL:HG23  | 1.96                     | 0.66              |
| 3:D:613:ARG:HH11  | 3:D:616:GLN:HG2   | 1.59                     | 0.66              |
| 3:D:1097:LYS:O    | 3:D:1101:VAL:HG22 | 1.95                     | 0.66              |
| 3:D:1481:VAL:CG1  | 4:E:21:VAL:HG21   | 2.25                     | 0.66              |
| 2:M:676:ILE:O     | 2:M:676:ILE:HG23  | 1.95                     | 0.66              |
| 2:M:1105:LYS:HD2  | 2:M:1105:LYS:O    | 1.95                     | 0.66              |
| 1:A:153:ALA:HA    | 1:A:156:HIS:NE2   | 2.11                     | 0.66              |
| 3:D:526:PRO:O     | 3:D:537:THR:HA    | 1.94                     | 0.66              |
| 3:D:774:SER:C     | 3:D:776:GLU:H     | 2.02                     | 0.66              |
| 3:N:646:LYS:HB2   | 3:N:688:TRP:CH2   | 2.29                     | 0.66              |
| 3:N:785:ILE:H     | 3:N:785:ILE:HD12  | 1.61                     | 0.66              |
| 3:N:1292:VAL:O    | 3:N:1303:TYR:HB2  | 1.95                     | 0.66              |
| 4:O:54:LEU:HA     | 4:O:58:PRO:CG     | 2.24                     | 0.66              |
| 1:A:43:ILE:CG2    | 1:A:47:SER:OG     | 2.44                     | 0.66              |
| 1:A:197:LEU:HD23  | 1:A:197:LEU:H     | 1.61                     | 0.66              |
| 2:C:1013:TYR:HA   | 2:C:1020:PRO:HA   | 1.76                     | 0.66              |
| 2:C:1089:VAL:O    | 2:C:1092:LEU:HB2  | 1.96                     | 0.66              |
| 3:D:1084:THR:HA   | 3:D:1087:ARG:HG2  | 1.78                     | 0.66              |
| 3:D:1111:ASP:HB2  | 3:D:1203:LYS:HG3  | 1.78                     | 0.66              |
| 2:M:237:ARG:HH11  | 2:M:237:ARG:CB    | 2.09                     | 0.66              |
| 3:N:15:PRO:HA     | 3:N:18:ILE:HG12   | 1.78                     | 0.66              |
| 1:A:18:ARG:O      | 1:A:207:PRO:HD3   | 1.95                     | 0.66              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:73:LEU:HB3    | 2:C:94:LEU:HA    | 1.78                     | 0.66              |
| 2:C:799:ILE:C     | 2:C:827:VAL:HG13 | 2.21                     | 0.66              |
| 2:C:939:ARG:HB3   | 2:C:982:PRO:HG3  | 1.78                     | 0.66              |
| 3:D:1110:ALA:O    | 3:D:1111:ASP:C   | 2.38                     | 0.66              |
| 3:D:1258:ARG:NH1  | 3:D:1329:ALA:HB1 | 2.04                     | 0.66              |
| 1:L:80:LEU:HG     | 3:N:844:ALA:CA   | 2.25                     | 0.66              |
| 2:M:1001:VAL:HG11 | 5:X:24:DC:OP1    | 1.96                     | 0.66              |
| 3:N:477:LEU:HD13  | 3:N:496:LEU:HB2  | 1.77                     | 0.66              |
| 3:N:637:LEU:HD11  | 3:N:642:CYS:N    | 2.11                     | 0.66              |
| 3:N:1268:PRO:HG3  | 3:N:1329:ALA:CB  | 2.22                     | 0.66              |
| 1:A:42:ARG:HH12   | 1:B:34:VAL:HB    | 1.59                     | 0.65              |
| 2:C:8:ARG:HH21    | 2:C:10:ARG:NH2   | 1.94                     | 0.65              |
| 2:C:459:ALA:HB1   | 2:C:467:ILE:CG2  | 2.25                     | 0.65              |
| 2:C:957:LYS:HG2   | 2:C:961:GLU:HB2  | 1.77                     | 0.65              |
| 3:D:10:ILE:CD1    | 3:D:1434:TRP:NE1 | 2.59                     | 0.65              |
| 3:D:108:VAL:CB    | 3:D:109:PRO:HD3  | 2.26                     | 0.65              |
| 3:D:1194:CYS:HB3  | 3:D:1373:ARG:NH1 | 2.09                     | 0.65              |
| 3:D:1408:ILE:O    | 2:M:370:ALA:HB1  | 1.95                     | 0.65              |
| 2:M:1009:SER:HB3  | 3:N:651:GLU:OE1  | 1.96                     | 0.65              |
| 3:N:646:LYS:HD2   | 3:N:688:TRP:CH2  | 2.31                     | 0.65              |
| 3:N:752:SER:OG    | 3:N:754:PHE:HB3  | 1.96                     | 0.65              |
| 3:N:882:PHE:HA    | 3:N:885:ILE:HD12 | 1.78                     | 0.65              |
| 3:N:1375:MET:HB3  | 3:N:1422:MET:O   | 1.96                     | 0.65              |
| 3:N:1380:GLU:HA   | 3:N:1391:GLU:O   | 1.95                     | 0.65              |
| 2:C:134:ARG:NH1   | 2:C:387:SER:HA   | 2.11                     | 0.65              |
| 3:D:89:ARG:O      | 3:D:521:PRO:HG3  | 1.96                     | 0.65              |
| 3:D:1033:GLN:C    | 3:D:1037:GLN:CB  | 2.69                     | 0.65              |
| 3:D:1380:GLU:HA   | 3:D:1391:GLU:O   | 1.96                     | 0.65              |
| 1:L:79:ILE:HA     | 1:L:82:LEU:HD12  | 1.78                     | 0.65              |
| 2:M:313:LEU:HB2   | 2:M:321:GLU:CG   | 2.25                     | 0.65              |
| 2:M:445:GLU:CA    | 2:M:449:ILE:HD12 | 2.25                     | 0.65              |
| 2:M:732:ALA:HA    | 2:M:735:ARG:NH2  | 2.10                     | 0.65              |
| 3:N:41:ARG:HD3    | 3:N:42:ASP:H     | 1.61                     | 0.65              |
| 3:N:544:TYR:O     | 3:N:548:ILE:HG12 | 1.96                     | 0.65              |
| 3:N:693:GLU:CG    | 4:O:48:MET:SD    | 2.84                     | 0.65              |
| 5:G:7:DA:H2"      | 5:G:8:DC:OP2     | 1.94                     | 0.65              |
| 2:C:34:VAL:HB     | 2:C:38:LYS:HG3   | 1.78                     | 0.65              |
| 2:C:63:GLY:HA3    | 2:C:103:LYS:HG3  | 1.78                     | 0.65              |
| 2:C:152:PRO:HD3   | 2:C:159:ILE:CD1  | 2.27                     | 0.65              |
| 2:C:265:ARG:H     | 2:C:289:THR:CG2  | 2.09                     | 0.65              |
| 2:C:374:ASN:O     | 2:C:377:PRO:HD2  | 1.96                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1081:VAL:HB   | 2:C:1086:ARG:NE   | 2.11                     | 0.65              |
| 3:D:46:ASP:OD2    | 3:D:48:ARG:HB3    | 1.95                     | 0.65              |
| 3:D:1237:THR:HG22 | 3:D:1238:MET:H    | 1.61                     | 0.65              |
| 4:E:23:VAL:HG22   | 4:E:68:LEU:HD23   | 1.78                     | 0.65              |
| 1:L:188:GLN:CG    | 3:N:685:ASP:OD2   | 2.41                     | 0.65              |
| 2:M:86:LYS:O      | 2:M:88:LEU:N      | 2.28                     | 0.65              |
| 2:M:286:SER:HB3   | 2:M:299:LYS:HE3   | 1.78                     | 0.65              |
| 2:M:1092:LEU:HD13 | 2:M:1099:VAL:HG21 | 1.76                     | 0.65              |
| 3:N:73:CYS:SG     | 3:N:75:ARG:HG3    | 2.35                     | 0.65              |
| 3:N:792:ILE:HG12  | 3:N:878:GLY:CA    | 2.27                     | 0.65              |
| 3:N:1239:ARG:HG3  | 3:N:1240:THR:H    | 1.62                     | 0.65              |
| 3:N:1448:THR:O    | 3:N:1452:ILE:HD13 | 1.96                     | 0.65              |
| 1:A:63:HIS:CE1    | 1:A:65:PHE:C      | 2.74                     | 0.65              |
| 2:C:831:ARG:CZ    | 2:C:1004:LYS:HZ2  | 2.08                     | 0.65              |
| 3:D:86:ARG:HG2    | 3:D:522:PRO:HG2   | 1.78                     | 0.65              |
| 3:D:715:ALA:HB3   | 3:D:764:LEU:HA    | 1.79                     | 0.65              |
| 1:L:83:LYS:HD2    | 3:N:848:GLU:OE1   | 1.97                     | 0.65              |
| 2:M:567:GLN:HE22  | 6:Y:13:C:C5'      | 2.10                     | 0.65              |
| 2:M:857:ASP:HB2   | 2:M:978:ARG:CG    | 2.21                     | 0.65              |
| 2:M:1095:LEU:O    | 2:M:1097:LEU:N    | 2.29                     | 0.65              |
| 3:N:86:ARG:O      | 3:N:522:PRO:HD2   | 1.96                     | 0.65              |
| 3:N:774:SER:C     | 3:N:776:GLU:H     | 2.04                     | 0.65              |
| 3:N:1129:THR:N    | 3:N:1320:GLU:HG2  | 2.10                     | 0.65              |
| 3:N:1441:GLN:CG   | 3:N:1442:ASN:H    | 2.09                     | 0.65              |
| 6:H:5:C:O5'       | 6:H:5:C:H6        | 1.80                     | 0.65              |
| 5:X:6:DT:H2''     | 5:X:7:DA:C8       | 2.30                     | 0.65              |
| 2:C:165:LEU:HB3   | 2:C:265:ARG:NH1   | 2.12                     | 0.65              |
| 2:C:300:ASP:C     | 2:C:302:VAL:H     | 2.04                     | 0.65              |
| 2:C:729:LEU:HD13  | 3:D:675:ARG:NH1   | 2.11                     | 0.65              |
| 2:C:903:SER:OG    | 2:C:908:GLY:HA3   | 1.95                     | 0.65              |
| 3:D:97:THR:HB     | 3:D:571:LYS:HE2   | 1.76                     | 0.65              |
| 3:D:645:PRO:HA    | 3:D:721:VAL:O     | 1.97                     | 0.65              |
| 2:M:653:ASP:OD1   | 2:M:654:LEU:HD23  | 1.97                     | 0.65              |
| 3:N:784:ASP:HB3   | 3:N:939:PHE:HE2   | 1.60                     | 0.65              |
| 3:D:95:LEU:HD23   | 3:D:96:ALA:N      | 2.11                     | 0.65              |
| 3:D:728:LEU:HD11  | 3:D:732:VAL:CG2   | 2.26                     | 0.65              |
| 3:D:1083:ASP:O    | 3:D:1087:ARG:CG   | 2.45                     | 0.65              |
| 1:L:80:LEU:O      | 3:N:844:ALA:HB2   | 1.96                     | 0.65              |
| 2:M:486:MET:SD    | 2:M:490:GLU:CB    | 2.68                     | 0.65              |
| 2:M:1095:LEU:HD21 | 3:N:603:LEU:HD13  | 1.74                     | 0.65              |
| 3:N:24:GLY:HA3    | 3:N:49:ILE:HG12   | 1.78                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:394:LEU:HD23  | 3:N:394:LEU:H     | 1.61                     | 0.65              |
| 3:N:433:GLY:HA3   | 3:N:447:VAL:O     | 1.97                     | 0.65              |
| 3:N:1033:GLN:CD   | 3:N:1240:THR:CG2  | 2.68                     | 0.65              |
| 3:N:1100:ASP:OD2  | 3:N:1440:PHE:CB   | 2.44                     | 0.65              |
| 3:N:1238:MET:C    | 3:N:1239:ARG:HG2  | 2.22                     | 0.65              |
| 3:N:1284:GLU:HG3  | 3:N:1285:GLU:N    | 2.12                     | 0.65              |
| 3:N:1381:VAL:HG12 | 3:N:1382:THR:H    | 1.60                     | 0.65              |
| 3:N:1465:ASN:OD1  | 3:N:1473:PRO:HD3  | 1.96                     | 0.65              |
| 1:A:123:MET:C     | 1:A:125:PRO:HD3   | 2.22                     | 0.65              |
| 2:C:537:LYS:NZ    | 2:C:904:PRO:HB3   | 2.10                     | 0.65              |
| 3:D:696:HIS:CG    | 3:D:697:GLY:H     | 2.13                     | 0.65              |
| 3:D:741:ASP:O     | 6:H:14:G:H5"      | 1.96                     | 0.65              |
| 3:D:808:THR:OG1   | 3:D:809:PRO:HD3   | 1.96                     | 0.65              |
| 3:D:1033:GLN:O    | 3:D:1037:GLN:N    | 2.30                     | 0.65              |
| 2:M:145:GLY:HA3   | 2:M:276:LYS:HD3   | 1.77                     | 0.65              |
| 2:M:451:LEU:HB2   | 2:M:452:ILE:HD12  | 1.78                     | 0.65              |
| 2:M:611:ILE:HD11  | 2:M:641:PRO:CG    | 2.27                     | 0.65              |
| 3:N:462:GLN:HG3   | 3:N:513:ILE:HG12  | 1.78                     | 0.65              |
| 3:N:607:LEU:HA    | 3:N:613:ARG:HB2   | 1.77                     | 0.65              |
| 3:N:1264:GLU:O    | 3:N:1266:ARG:N    | 2.30                     | 0.65              |
| 7:I:5:DC:C6       | 7:I:6:DT:H72      | 2.31                     | 0.65              |
| 1:A:102:LYS:HA    | 1:A:138:LEU:O     | 1.97                     | 0.65              |
| 2:C:86:LYS:O      | 2:C:88:LEU:N      | 2.29                     | 0.65              |
| 2:C:145:GLY:HA3   | 2:C:276:LYS:HD3   | 1.78                     | 0.65              |
| 2:C:1016:ILE:HG22 | 3:D:523:ASP:O     | 1.97                     | 0.65              |
| 3:D:52:PRO:CG     | 3:D:80:VAL:HG13   | 2.27                     | 0.65              |
| 3:D:615:ARG:NH2   | 3:D:1096:ARG:HD2  | 2.11                     | 0.65              |
| 3:D:862:ASP:O     | 3:D:876:SER:HA    | 1.96                     | 0.65              |
| 3:D:1044:LEU:O    | 3:D:1045:MET:C    | 2.39                     | 0.65              |
| 3:D:1496:GLU:O    | 3:D:1499:ARG:HB2  | 1.97                     | 0.65              |
| 2:M:1038:TRP:O    | 2:M:1041:GLU:HB2  | 1.97                     | 0.65              |
| 2:M:1056:LYS:HE3  | 3:N:751:LEU:CD1   | 2.18                     | 0.65              |
| 3:N:1331:ASP:O    | 3:N:1335:LEU:HB2  | 1.96                     | 0.65              |
| 3:N:1438:ALA:HA   | 3:N:1446:VAL:HG11 | 1.77                     | 0.65              |
| 2:C:1042:ALA:HB3  | 3:D:710:ARG:HB3   | 1.78                     | 0.65              |
| 3:D:10:ILE:HG13   | 3:D:1434:TRP:CE2  | 2.32                     | 0.65              |
| 1:L:101:LEU:HB2   | 1:L:114:PHE:HA    | 1.79                     | 0.65              |
| 2:M:183:SER:HB2   | 2:M:190:LYS:HD3   | 1.78                     | 0.65              |
| 3:N:87:ARG:HD3    | 3:N:524:LEU:CD1   | 2.26                     | 0.65              |
| 3:N:924:MET:N     | 4:O:7:ASP:OD2     | 2.29                     | 0.65              |
| 3:N:1114:THR:O    | 3:N:1189:ARG:NH2  | 2.21                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:I:12:DT:H2"     | 7:I:13:DA:OP2     | 1.97                     | 0.65              |
| 1:A:31:GLY:O      | 1:A:34:VAL:HG12   | 1.96                     | 0.65              |
| 2:C:165:LEU:HA    | 2:C:166:PRO:O     | 1.97                     | 0.65              |
| 2:C:276:LYS:HA    | 2:C:280:LYS:HD2   | 1.78                     | 0.65              |
| 2:C:342:ASP:O     | 2:C:346:VAL:HG23  | 1.97                     | 0.65              |
| 2:C:676:ILE:CG2   | 2:C:988:VAL:HG13  | 2.27                     | 0.65              |
| 2:C:1093:GLN:HB3  | 3:D:21:TRP:CE3    | 2.31                     | 0.65              |
| 3:D:1154:GLU:HB2  | 3:N:562:ALA:C     | 2.22                     | 0.65              |
| 3:D:1237:THR:HB   | 3:D:1359:GLN:NE2  | 2.11                     | 0.65              |
| 4:E:54:LEU:HG     | 4:E:58:PRO:CG     | 2.24                     | 0.65              |
| 1:K:58:ILE:HD13   | 1:K:140:MET:HB3   | 1.77                     | 0.65              |
| 2:M:1032:PHE:O    | 2:M:1036:GLU:HB2  | 1.97                     | 0.65              |
| 3:N:87:ARG:HB3    | 3:N:523:ASP:OD2   | 1.96                     | 0.65              |
| 3:N:501:ALA:CB    | 3:N:1452:ILE:HG22 | 2.26                     | 0.65              |
| 3:N:693:GLU:O     | 4:O:48:MET:SD     | 2.55                     | 0.65              |
| 6:H:6:C:N4        | 6:H:7:G:C6        | 2.65                     | 0.65              |
| 1:A:88:ARG:HG2    | 1:A:88:ARG:HH11   | 1.62                     | 0.64              |
| 2:C:468:ARG:HD3   | 2:C:485:TYR:HB3   | 1.78                     | 0.64              |
| 2:C:524:VAL:HG12  | 2:C:525:SER:H     | 1.62                     | 0.64              |
| 2:C:762:LYS:HD2   | 2:C:786:LYS:HB2   | 1.77                     | 0.64              |
| 2:C:877:PRO:HG3   | 3:D:1023:MET:SD   | 2.37                     | 0.64              |
| 3:D:8:VAL:CG2     | 3:D:1435:LEU:HD21 | 2.26                     | 0.64              |
| 3:D:614:PHE:CZ    | 3:D:1438:ALA:HB1  | 2.31                     | 0.64              |
| 3:D:716:PHE:O     | 3:D:718:PRO:HD3   | 1.97                     | 0.64              |
| 3:D:1412:LYS:CB   | 2:M:376:ARG:HH21  | 2.09                     | 0.64              |
| 1:K:53:VAL:HG21   | 1:K:82:LEU:HB3    | 1.78                     | 0.64              |
| 2:M:583:LEU:O     | 2:M:587:VAL:HG23  | 1.96                     | 0.64              |
| 2:M:937:ASP:OD2   | 2:M:939:ARG:HG2   | 1.97                     | 0.64              |
| 3:N:30:GLU:HB3    | 3:N:40:GLU:HG2    | 1.79                     | 0.64              |
| 3:N:785:ILE:HD12  | 3:N:785:ILE:N     | 2.12                     | 0.64              |
| 3:N:862:ASP:O     | 3:N:877:PRO:HD3   | 1.96                     | 0.64              |
| 1:A:102:LYS:HB3   | 1:A:139:ASN:OD1   | 1.97                     | 0.64              |
| 2:C:244:PRO:CD    | 2:C:245:GLY:H     | 2.09                     | 0.64              |
| 2:C:496:ILE:HA    | 2:C:531:PHE:O     | 1.97                     | 0.64              |
| 2:C:899:GLN:HG3   | 2:C:901:TYR:OH    | 1.97                     | 0.64              |
| 2:C:1048:THR:OG1  | 3:D:758:GLU:HG3   | 1.96                     | 0.64              |
| 2:C:1060:ILE:HG23 | 2:C:1061:GLU:N    | 2.12                     | 0.64              |
| 3:D:7:LYS:CG      | 3:D:1458:GLU:HA   | 2.26                     | 0.64              |
| 3:D:927:THR:O     | 3:D:930:LEU:HB3   | 1.97                     | 0.64              |
| 2:M:260:LEU:HD12  | 2:M:261:ILE:HG13  | 1.77                     | 0.64              |
| 2:M:487:THR:HB    | 2:M:490:GLU:HG3   | 1.78                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:861:LEU:HD22 | 2:M:863:ASP:H     | 1.60                     | 0.64              |
| 2:M:1008:ARG:HD2 | 2:M:1028:GLY:H    | 1.61                     | 0.64              |
| 3:N:98:PRO:HG2   | 3:N:462:GLN:OE1   | 1.97                     | 0.64              |
| 3:N:1111:ASP:CG  | 3:N:1203:LYS:HD2  | 2.22                     | 0.64              |
| 1:A:32:PHE:HE1   | 1:B:221:HIS:NE2   | 1.80                     | 0.64              |
| 2:C:30:LEU:HD12  | 2:C:30:LEU:O      | 1.97                     | 0.64              |
| 2:C:267:TYR:O    | 2:C:268:ASP:C     | 2.39                     | 0.64              |
| 2:C:328:LEU:C    | 2:C:330:ASN:H     | 2.05                     | 0.64              |
| 2:C:1036:GLU:N   | 2:C:1036:GLU:OE1  | 2.30                     | 0.64              |
| 3:D:111:LYS:HE2  | 3:D:1445:HIS:NE2  | 2.12                     | 0.64              |
| 3:D:809:PRO:HB2  | 3:D:812:ALA:CB    | 2.27                     | 0.64              |
| 3:D:1442:ASN:C   | 3:D:1443:THR:HG23 | 2.22                     | 0.64              |
| 1:K:88:ARG:HH12  | 1:K:90:LEU:HD11   | 1.62                     | 0.64              |
| 2:M:692:GLU:OE1  | 2:M:854:PRO:HB3   | 1.97                     | 0.64              |
| 3:N:584:ASN:OD1  | 3:N:590:PRO:HD2   | 1.96                     | 0.64              |
| 5:G:21:DG:C2'    | 5:G:22:DA:O5'     | 2.45                     | 0.64              |
| 1:B:38:ASN:O     | 1:B:41:ARG:HB3    | 1.97                     | 0.64              |
| 2:C:1000:MET:C   | 2:C:1002:GLU:N    | 2.55                     | 0.64              |
| 2:M:129:ILE:N    | 2:M:129:ILE:HD12  | 2.13                     | 0.64              |
| 2:M:193:LEU:HD23 | 2:M:307:LEU:HD11  | 1.79                     | 0.64              |
| 2:M:267:TYR:HB2  | 2:M:272:ALA:HB1   | 1.78                     | 0.64              |
| 2:M:918:LEU:HD23 | 2:M:968:LEU:CA    | 2.25                     | 0.64              |
| 3:N:160:GLU:O    | 3:N:163:TYR:N     | 2.30                     | 0.64              |
| 3:N:653:PHE:CZ   | 3:N:749:VAL:HG13  | 2.32                     | 0.64              |
| 3:N:840:LYS:HD3  | 3:N:841:TYR:CZ    | 2.32                     | 0.64              |
| 6:Y:9:C:C2'      | 6:Y:10:G:H5'      | 2.28                     | 0.64              |
| 1:A:106:PRO:HG2  | 1:A:134:GLU:OE1   | 1.98                     | 0.64              |
| 2:C:541:SER:OG   | 2:C:543:ASN:N     | 2.30                     | 0.64              |
| 2:C:1090:LYS:HD2 | 3:D:90:MET:CG     | 2.27                     | 0.64              |
| 2:M:462:ASP:HB3  | 2:M:468:ARG:HD2   | 1.79                     | 0.64              |
| 2:M:486:MET:HG3  | 2:M:487:THR:O     | 1.98                     | 0.64              |
| 2:M:817:PRO:O    | 3:N:532:GLY:HA2   | 1.97                     | 0.64              |
| 2:M:1032:PHE:CE2 | 2:M:1037:VAL:HA   | 2.33                     | 0.64              |
| 3:N:73:CYS:SG    | 3:N:76:CYS:N      | 2.70                     | 0.64              |
| 3:N:153:LEU:HD13 | 3:N:158:TYR:HB2   | 1.78                     | 0.64              |
| 3:N:464:LEU:O    | 3:N:468:LEU:HG    | 1.97                     | 0.64              |
| 1:A:75:VAL:O     | 1:A:79:ILE:HG23   | 1.98                     | 0.64              |
| 2:C:148:PHE:CZ   | 2:C:281:LEU:HD13  | 2.33                     | 0.64              |
| 2:C:611:ILE:HD11 | 2:C:641:PRO:HG3   | 1.78                     | 0.64              |
| 2:C:685:GLU:OE1  | 3:D:739:ASP:HB3   | 1.97                     | 0.64              |
| 2:C:854:PRO:HB2  | 2:C:856:GLU:HG3   | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:33:ASN:HB2    | 3:D:40:GLU:CD     | 2.23                     | 0.64              |
| 3:D:639:LEU:HG    | 3:D:932:ASP:OD1   | 1.97                     | 0.64              |
| 3:D:1229:ILE:HD11 | 3:D:1367:HIS:HB3  | 1.79                     | 0.64              |
| 1:K:42:ARG:HH12   | 1:L:34:VAL:CG1    | 2.11                     | 0.64              |
| 1:K:42:ARG:CZ     | 2:M:857:ASP:HB3   | 2.27                     | 0.64              |
| 1:L:132:LEU:HG    | 1:L:136:GLY:HA3   | 1.79                     | 0.64              |
| 2:M:41:ASN:HB2    | 2:M:45:GLN:HG2    | 1.79                     | 0.64              |
| 2:M:626:ARG:O     | 2:M:638:ASP:HA    | 1.98                     | 0.64              |
| 3:N:619:LEU:HB2   | 3:N:621:LYS:HZ3   | 1.63                     | 0.64              |
| 3:N:714:GLN:HE22  | 3:N:732:VAL:HG11  | 1.63                     | 0.64              |
| 3:N:813:LEU:O     | 3:N:817:GLU:HB2   | 1.97                     | 0.64              |
| 5:X:27:DC:OP2     | 5:X:27:DC:C6      | 2.43                     | 0.64              |
| 1:A:110:LYS:O     | 1:A:111:ALA:C     | 2.41                     | 0.64              |
| 3:D:619:LEU:HD12  | 3:D:621:LYS:HZ1   | 1.62                     | 0.64              |
| 3:D:709:HIS:HA    | 3:D:1227:GLN:HB3  | 1.78                     | 0.64              |
| 3:D:951:ILE:CD1   | 3:D:1062:ARG:HE   | 2.09                     | 0.64              |
| 2:M:269:LEU:HG    | 2:M:288:ARG:HG2   | 1.79                     | 0.64              |
| 2:M:1047:HIS:O    | 2:M:1051:GLU:HG3  | 1.98                     | 0.64              |
| 3:N:116:LEU:HB3   | 3:N:118:LEU:CD1   | 2.28                     | 0.64              |
| 3:N:628:ARG:HH11  | 3:N:628:ARG:HG3   | 1.63                     | 0.64              |
| 3:N:1101:VAL:HG13 | 3:N:1428:ALA:CB   | 2.24                     | 0.64              |
| 7:I:17:DA:H8      | 7:I:17:DA:O5'     | 1.80                     | 0.64              |
| 2:C:1005:MET:HE3  | 3:D:648:MET:CG    | 2.28                     | 0.64              |
| 3:D:562:ALA:HB1   | 3:D:567:ILE:HD11  | 1.80                     | 0.64              |
| 3:D:758:GLU:HB3   | 3:D:762:GLN:NE2   | 2.13                     | 0.64              |
| 3:D:832:ARG:HD2   | 3:D:832:ARG:O     | 1.97                     | 0.64              |
| 3:D:1033:GLN:HB3  | 3:D:1037:GLN:OE1  | 1.98                     | 0.64              |
| 3:D:1402:ALA:HB2  | 3:D:1415:VAL:HG21 | 1.79                     | 0.64              |
| 3:D:1493:LYS:O    | 3:D:1497:GLU:HG2  | 1.98                     | 0.64              |
| 1:K:70:GLY:N      | 2:M:607:ASP:OD1   | 2.28                     | 0.64              |
| 2:M:292:ARG:HB2   | 2:M:299:LYS:HG2   | 1.80                     | 0.64              |
| 2:M:911:GLU:HA    | 2:M:914:ILE:HD12  | 1.80                     | 0.64              |
| 2:M:1058:ASP:OD1  | 2:M:1084:SER:HB3  | 1.98                     | 0.64              |
| 3:N:187:LYS:HE2   | 3:N:199:LEU:HA    | 1.80                     | 0.64              |
| 3:N:619:LEU:HD12  | 3:N:621:LYS:HZ1   | 1.62                     | 0.64              |
| 7:I:15:DT:H2''    | 7:I:16:DG:OP2     | 1.98                     | 0.64              |
| 1:A:165:ILE:O     | 1:A:165:ILE:HG13  | 1.97                     | 0.64              |
| 2:C:327:HIS:HA    | 2:C:431:HIS:NE2   | 2.13                     | 0.64              |
| 3:D:480:GLU:O     | 3:D:484:PRO:HD2   | 1.98                     | 0.64              |
| 3:D:704:ARG:HE    | 3:D:705:ALA:HB3   | 1.62                     | 0.64              |
| 3:D:1238:MET:O    | 3:D:1253:THR:HG21 | 1.98                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1239:ARG:HA   | 3:D:1253:THR:HB   | 1.80                     | 0.64              |
| 2:M:396:ASP:CB    | 2:M:406:HIS:CD2   | 2.80                     | 0.64              |
| 3:N:52:PRO:HB2    | 3:N:83:SER:HA     | 1.79                     | 0.64              |
| 3:N:696:HIS:CE1   | 4:O:62:THR:HG21   | 2.32                     | 0.64              |
| 3:N:860:LEU:HD23  | 3:N:877:PRO:HB2   | 1.80                     | 0.64              |
| 1:A:50:GLY:CA     | 1:A:173:PRO:HG3   | 2.28                     | 0.64              |
| 2:C:15:LEU:HD12   | 2:C:15:LEU:N      | 2.11                     | 0.64              |
| 2:C:602:GLU:OE1   | 2:C:648:ARG:HG2   | 1.98                     | 0.64              |
| 2:C:622:GLU:O     | 2:C:624:PRO:HD3   | 1.98                     | 0.64              |
| 2:C:888:THR:O     | 2:C:990:GLY:HA3   | 1.98                     | 0.64              |
| 3:D:133:ILE:HG12  | 3:D:456:MET:HB3   | 1.79                     | 0.64              |
| 2:M:124:ASP:OD1   | 2:M:126:SER:OG    | 2.10                     | 0.64              |
| 2:M:263:ASP:O     | 2:M:264:PRO:O     | 2.15                     | 0.64              |
| 2:M:264:PRO:HB3   | 2:M:289:THR:HB    | 1.78                     | 0.64              |
| 2:M:397:GLU:CD    | 2:M:632:ASN:HB2   | 2.22                     | 0.64              |
| 2:M:1032:PHE:O    | 2:M:1033:GLY:O    | 2.16                     | 0.64              |
| 2:M:1111:ILE:HG13 | 2:M:1112:PHE:H    | 1.62                     | 0.64              |
| 3:N:45:PHE:CD1    | 3:N:522:PRO:HB3   | 2.33                     | 0.64              |
| 3:N:456:MET:O     | 3:N:459:GLU:HB3   | 1.98                     | 0.64              |
| 3:N:550:ARG:HD3   | 3:N:570:GLU:OE1   | 1.97                     | 0.64              |
| 3:N:1088:THR:HG21 | 5:X:19:DG:N2      | 2.13                     | 0.64              |
| 6:H:12:U:O5'      | 6:H:12:U:H6       | 1.81                     | 0.64              |
| 1:B:179:PHE:HB2   | 1:B:195:LEU:HD11  | 1.80                     | 0.63              |
| 2:C:85:GLU:O      | 2:C:824:ARG:NH2   | 2.31                     | 0.63              |
| 2:C:683:ASN:OD1   | 2:C:872:ASN:HB2   | 1.98                     | 0.63              |
| 3:D:1412:LYS:HB2  | 2:M:376:ARG:HH21  | 1.61                     | 0.63              |
| 2:M:267:TYR:O     | 2:M:268:ASP:C     | 2.40                     | 0.63              |
| 2:M:683:ASN:O     | 2:M:683:ASN:ND2   | 2.24                     | 0.63              |
| 2:M:854:PRO:HB2   | 2:M:856:GLU:HG3   | 1.79                     | 0.63              |
| 3:N:137:PRO:HD2   | 3:N:453:ASP:CG    | 2.23                     | 0.63              |
| 3:N:484:PRO:HB3   | 3:N:488:ARG:NH2   | 2.13                     | 0.63              |
| 3:N:862:ASP:O     | 3:N:876:SER:HA    | 1.97                     | 0.63              |
| 3:N:937:TYR:O     | 3:N:941:PHE:HB2   | 1.98                     | 0.63              |
| 3:N:1274:ILE:HD12 | 3:N:1274:ILE:O    | 1.98                     | 0.63              |
| 3:N:1345:GLU:O    | 3:N:1349:VAL:HG23 | 1.98                     | 0.63              |
| 3:N:1380:GLU:HG3  | 3:N:1381:VAL:H    | 1.63                     | 0.63              |
| 7:I:11:DG:C2'     | 7:I:12:DT:C7      | 2.77                     | 0.63              |
| 3:D:54:LYS:O      | 3:D:55:ASP:O      | 2.17                     | 0.63              |
| 3:D:104:PHE:CD2   | 3:D:1448:THR:HG23 | 2.33                     | 0.63              |
| 3:D:704:ARG:HG3   | 3:D:705:ALA:N     | 2.12                     | 0.63              |
| 4:E:46:PRO:HB2    | 4:E:54:LEU:HD22   | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:33:ASN:OD1    | 3:N:35:ARG:HG3    | 1.98                     | 0.63              |
| 3:N:899:LEU:HB3   | 3:N:917:GLN:HG2   | 1.80                     | 0.63              |
| 3:N:1389:LEU:HD12 | 3:N:1390:LEU:N    | 2.13                     | 0.63              |
| 3:N:1472:ILE:HD13 | 3:N:1472:ILE:N    | 2.00                     | 0.63              |
| 3:N:1485:GLN:HB2  | 4:O:79:LEU:HB3    | 1.80                     | 0.63              |
| 6:H:11:C:H2'      | 6:H:12:U:C6       | 2.33                     | 0.63              |
| 1:B:101:LEU:HB2   | 1:B:114:PHE:HA    | 1.79                     | 0.63              |
| 2:C:12:VAL:HG11   | 2:C:472:ARG:HD3   | 1.79                     | 0.63              |
| 2:C:157:ARG:NH2   | 2:C:158:TYR:CE1   | 2.65                     | 0.63              |
| 2:C:460:ARG:HG2   | 2:C:485:TYR:CE2   | 2.33                     | 0.63              |
| 2:C:1083:GLU:O    | 2:C:1087:VAL:HG12 | 1.98                     | 0.63              |
| 3:D:1410:GLU:OE2  | 2:M:373:VAL:HG12  | 1.98                     | 0.63              |
| 3:D:1432:LYS:HB2  | 3:D:1432:LYS:NZ   | 2.13                     | 0.63              |
| 2:M:630:ARG:HH11  | 2:M:630:ARG:HG3   | 1.63                     | 0.63              |
| 2:M:906:PHE:CD1   | 3:N:1067:VAL:HG22 | 2.32                     | 0.63              |
| 3:N:1149:LEU:HD22 | 3:N:1151:ARG:O    | 1.97                     | 0.63              |
| 5:G:16:DT:H2''    | 5:G:17:DA:OP1     | 1.99                     | 0.63              |
| 2:C:129:ILE:HG22  | 2:C:130:ASN:N     | 2.13                     | 0.63              |
| 2:C:216:GLU:HG2   | 2:C:219:GLN:OE1   | 1.98                     | 0.63              |
| 2:C:264:PRO:HB3   | 2:C:289:THR:HB    | 1.80                     | 0.63              |
| 2:C:694:LEU:HD21  | 2:C:868:ASP:CB    | 2.27                     | 0.63              |
| 2:C:720:GLU:HG2   | 2:C:760:SER:CB    | 2.28                     | 0.63              |
| 2:C:836:GLY:HA3   | 3:D:724:GLN:OE1   | 1.98                     | 0.63              |
| 2:C:1115:LEU:CD2  | 3:D:85:VAL:HG12   | 2.27                     | 0.63              |
| 3:D:1200:VAL:HG22 | 3:D:1373:ARG:HH12 | 1.62                     | 0.63              |
| 2:M:217:LEU:HD12  | 2:M:311:PHE:CD2   | 2.33                     | 0.63              |
| 2:M:631:SER:HB3   | 2:M:635:THR:N     | 2.11                     | 0.63              |
| 3:N:521:PRO:CD    | 3:N:524:LEU:HD22  | 2.26                     | 0.63              |
| 3:N:565:ILE:H     | 3:N:565:ILE:HD12  | 1.64                     | 0.63              |
| 3:N:690:ALA:O     | 3:N:694:VAL:HG23  | 1.98                     | 0.63              |
| 3:N:834:THR:HA    | 3:N:838:ARG:NH1   | 2.13                     | 0.63              |
| 3:N:853:VAL:HA    | 3:N:858:VAL:O     | 1.99                     | 0.63              |
| 5:X:7:DA:H2''     | 5:X:8:DC:C5'      | 2.27                     | 0.63              |
| 2:C:31:GLN:HB3    | 2:C:71:TYR:HH     | 1.64                     | 0.63              |
| 2:C:572:ILE:HG13  | 2:C:573:ARG:H     | 1.64                     | 0.63              |
| 2:C:582:GLY:C     | 2:C:583:LEU:HD12  | 2.23                     | 0.63              |
| 3:D:1442:ASN:O    | 3:D:1443:THR:HG23 | 1.99                     | 0.63              |
| 2:M:694:LEU:HD21  | 2:M:868:ASP:OD2   | 1.98                     | 0.63              |
| 2:M:1013:TYR:HE1  | 2:M:1020:PRO:HG3  | 1.63                     | 0.63              |
| 2:M:1032:PHE:HE2  | 2:M:1037:VAL:HA   | 1.64                     | 0.63              |
| 3:N:97:THR:HG23   | 3:N:459:GLU:HB2   | 1.81                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:398:ALA:CB   | 3:N:447:VAL:HA    | 2.26                     | 0.63              |
| 3:N:477:LEU:HD22 | 3:N:492:ALA:HB1   | 1.80                     | 0.63              |
| 3:N:659:LYS:HE3  | 3:N:663:GLU:OE2   | 1.98                     | 0.63              |
| 2:C:302:VAL:C    | 2:C:305:PRO:HD2   | 2.23                     | 0.63              |
| 3:D:18:ILE:HD12  | 3:D:518:PRO:HG3   | 1.80                     | 0.63              |
| 3:D:618:LEU:HD11 | 3:D:1463:LYS:HG3  | 1.80                     | 0.63              |
| 3:D:731:LEU:HD21 | 3:D:782:SER:H     | 1.63                     | 0.63              |
| 2:M:496:ILE:N    | 2:M:496:ILE:HD12  | 2.13                     | 0.63              |
| 2:M:1013:TYR:HA  | 2:M:1020:PRO:HA   | 1.81                     | 0.63              |
| 2:M:1085:PHE:O   | 2:M:1088:LEU:HB3  | 1.99                     | 0.63              |
| 3:N:130:SER:O    | 3:N:568:ARG:HD3   | 1.99                     | 0.63              |
| 3:N:704:ARG:HG2  | 3:N:736:PHE:HB3   | 1.80                     | 0.63              |
| 4:O:47:LYS:N     | 4:O:54:LEU:HD13   | 2.13                     | 0.63              |
| 1:B:9:PRO:HB3    | 1:B:25:LEU:HD21   | 1.79                     | 0.63              |
| 2:C:50:GLU:CB    | 2:C:266:ARG:CZ    | 2.76                     | 0.63              |
| 2:C:265:ARG:HG2  | 2:C:267:TYR:H     | 1.64                     | 0.63              |
| 2:C:300:ASP:OD2  | 2:C:303:PHE:HB2   | 1.99                     | 0.63              |
| 2:C:1047:HIS:HB2 | 3:D:758:GLU:OE1   | 1.99                     | 0.63              |
| 3:D:654:LYS:HB3  | 3:D:655:PRO:CD    | 2.28                     | 0.63              |
| 2:M:77:PRO:HD3   | 2:M:93:PRO:HD3    | 1.80                     | 0.63              |
| 2:M:473:ARG:HG3  | 2:M:474:VAL:N     | 2.11                     | 0.63              |
| 2:M:498:GLN:CG   | 2:M:516:ARG:HH21  | 2.12                     | 0.63              |
| 3:N:693:GLU:O    | 4:O:48:MET:CE     | 2.46                     | 0.63              |
| 5:X:3:DC:H6      | 5:X:3:DC:O5'      | 1.81                     | 0.63              |
| 2:C:328:LEU:HD22 | 2:C:433:THR:C     | 2.23                     | 0.63              |
| 2:C:692:GLU:CG   | 2:C:696:LYS:HE3   | 2.20                     | 0.63              |
| 3:D:1453:ALA:O   | 3:D:1455:LYS:N    | 2.31                     | 0.63              |
| 1:K:75:VAL:O     | 1:K:79:ILE:HG23   | 1.97                     | 0.63              |
| 2:M:422:ARG:HB3  | 7:Z:1:DG:N2       | 2.14                     | 0.63              |
| 2:M:516:ARG:NH2  | 3:N:1068:LEU:HB2  | 2.14                     | 0.63              |
| 3:N:12:LEU:HD23  | 3:N:13:ALA:H      | 1.64                     | 0.63              |
| 3:N:1126:ASP:OD1 | 3:N:1129:THR:N    | 2.32                     | 0.63              |
| 3:N:1240:THR:O   | 3:N:1241:PHE:CB   | 2.47                     | 0.63              |
| 2:C:516:ARG:HE   | 3:D:1068:LEU:HD13 | 1.63                     | 0.63              |
| 2:C:580:MET:O    | 2:C:902:ILE:HA    | 1.98                     | 0.63              |
| 3:D:850:LEU:HD12 | 3:D:850:LEU:H     | 1.63                     | 0.63              |
| 3:D:1083:ASP:O   | 3:D:1087:ARG:HD3  | 1.99                     | 0.63              |
| 3:D:1191:PRO:C   | 3:D:1373:ARG:HH11 | 2.07                     | 0.63              |
| 1:K:88:ARG:NH2   | 1:K:90:LEU:HG     | 2.13                     | 0.63              |
| 2:M:22:GLN:O     | 2:M:121:MET:HE1   | 1.99                     | 0.63              |
| 2:M:252:LYS:HD3  | 2:M:296:GLY:HA2   | 1.81                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:666:LEU:HG    | 2:M:668:LEU:HD11  | 1.80                     | 0.63              |
| 3:N:23:TYR:CE1    | 3:N:89:ARG:HG2    | 2.34                     | 0.63              |
| 3:N:607:LEU:HA    | 3:N:613:ARG:HB3   | 1.79                     | 0.63              |
| 3:N:1111:ASP:OD1  | 3:N:1203:LYS:HB2  | 1.99                     | 0.63              |
| 2:C:185:LYS:HD3   | 2:C:190:LYS:HZ3   | 1.64                     | 0.62              |
| 3:D:33:ASN:HB2    | 3:D:40:GLU:OE1    | 1.99                     | 0.62              |
| 3:D:902:LEU:H     | 3:D:902:LEU:CD2   | 2.05                     | 0.62              |
| 3:D:1242:HIS:O    | 3:D:1250:ALA:HA   | 1.98                     | 0.62              |
| 2:M:263:ASP:C     | 2:M:264:PRO:O     | 2.42                     | 0.62              |
| 3:N:1093:TYR:CE1  | 5:X:18:DC:C5'     | 2.82                     | 0.62              |
| 7:I:11:DG:C8      | 7:I:11:DG:O5'     | 2.52                     | 0.62              |
| 1:A:42:ARG:HB2    | 1:B:35:THR:CG2    | 2.29                     | 0.62              |
| 2:C:557:ARG:NH2   | 2:C:879:ARG:HE    | 1.97                     | 0.62              |
| 2:C:682:TYR:CE2   | 3:D:635:PRO:HG2   | 2.34                     | 0.62              |
| 2:C:831:ARG:NH2   | 2:C:1004:LYS:HZ2  | 1.96                     | 0.62              |
| 2:C:893:ALA:O     | 2:C:897:LEU:HG    | 1.99                     | 0.62              |
| 3:D:542:ASP:HB2   | 3:D:600:LEU:HD23  | 1.80                     | 0.62              |
| 3:D:1003:VAL:HG13 | 3:D:1036:ARG:CD   | 2.28                     | 0.62              |
| 1:L:89:PHE:HB3    | 1:L:94:LEU:HD13   | 1.81                     | 0.62              |
| 2:M:987:ILE:HD11  | 3:N:946:GLY:HA2   | 1.81                     | 0.62              |
| 3:N:703:ASN:OD1   | 3:N:707:THR:HG23  | 1.99                     | 0.62              |
| 3:N:750:PRO:HB2   | 3:N:756:GLN:HA    | 1.81                     | 0.62              |
| 3:N:770:LEU:HD22  | 3:N:775:GLY:O     | 2.00                     | 0.62              |
| 3:N:785:ILE:HG23  | 3:N:938:GLY:HA3   | 1.81                     | 0.62              |
| 1:A:43:ILE:HD13   | 1:B:32:PHE:CE2    | 2.34                     | 0.62              |
| 1:B:206:THR:HG23  | 1:B:208:LEU:H     | 1.61                     | 0.62              |
| 2:C:45:GLN:O      | 2:C:48:PHE:HB2    | 1.99                     | 0.62              |
| 2:C:263:ASP:O     | 2:C:264:PRO:O     | 2.17                     | 0.62              |
| 2:C:577:PRO:HG3   | 2:C:993:PHE:CE1   | 2.34                     | 0.62              |
| 2:C:1102:LEU:O    | 3:D:5:VAL:HG13    | 1.99                     | 0.62              |
| 3:D:148:GLU:HB3   | 3:D:151:GLN:CB    | 2.30                     | 0.62              |
| 3:D:615:ARG:NH1   | 3:D:1096:ARG:CZ   | 2.61                     | 0.62              |
| 3:D:908:LYS:HB2   | 3:D:1027:GLY:HA3  | 1.79                     | 0.62              |
| 3:D:1112:CYS:HB3  | 3:D:1195:GLN:CG   | 2.11                     | 0.62              |
| 3:D:1463:LYS:O    | 3:D:1467:ILE:HG13 | 2.00                     | 0.62              |
| 1:L:100:LEU:HB2   | 1:L:115:LEU:CD2   | 2.28                     | 0.62              |
| 2:M:10:ARG:HH11   | 2:M:10:ARG:HA     | 1.64                     | 0.62              |
| 2:M:52:PHE:CD2    | 2:M:68:PHE:HB2    | 2.34                     | 0.62              |
| 2:M:431:HIS:NE2   | 2:M:433:THR:OG1   | 2.32                     | 0.62              |
| 2:M:524:VAL:HG12  | 2:M:525:SER:N     | 2.14                     | 0.62              |
| 2:M:1094:ALA:HB2  | 3:N:90:MET:HE1    | 1.80                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:98:PRO:O     | 3:N:458:ALA:HB3   | 1.99                     | 0.62              |
| 1:A:109:VAL:O    | 1:A:110:LYS:HD3   | 1.98                     | 0.62              |
| 2:C:617:ASP:CG   | 2:C:619:ARG:HE    | 2.07                     | 0.62              |
| 3:D:119:SER:O    | 3:D:121:THR:N     | 2.33                     | 0.62              |
| 3:D:474:GLU:O    | 3:D:478:LEU:HG    | 2.00                     | 0.62              |
| 3:D:1033:GLN:HB2 | 3:D:1037:GLN:OE1  | 1.99                     | 0.62              |
| 2:M:263:ASP:HB2  | 2:M:264:PRO:HD3   | 1.81                     | 0.62              |
| 2:M:680:ASP:OD1  | 3:N:943:THR:HG21  | 1.98                     | 0.62              |
| 3:N:501:ALA:HB1  | 3:N:1453:ALA:CB   | 2.29                     | 0.62              |
| 3:N:700:VAL:HG22 | 3:N:718:PRO:CG    | 2.29                     | 0.62              |
| 3:N:1367:HIS:O   | 3:N:1370:ILE:HG12 | 1.99                     | 0.62              |
| 3:N:1483:PHE:HB2 | 4:O:77:GLU:OE1    | 1.99                     | 0.62              |
| 6:Y:4:G:H2'      | 6:Y:5:C:H6        | 1.63                     | 0.62              |
| 6:Y:6:C:H3'      | 6:Y:7:G:H8        | 1.64                     | 0.62              |
| 1:A:70:GLY:H     | 2:C:607:ASP:CG    | 2.06                     | 0.62              |
| 1:A:162:ILE:HG13 | 1:A:163:ASN:N     | 2.15                     | 0.62              |
| 1:B:175:ARG:HB3  | 3:D:847:ASP:OD2   | 1.99                     | 0.62              |
| 2:C:490:GLU:HA   | 2:C:493:ARG:HD3   | 1.82                     | 0.62              |
| 2:C:836:GLY:HA2  | 3:D:725:SER:HB3   | 1.80                     | 0.62              |
| 2:C:897:LEU:HD21 | 2:C:921:ALA:HA    | 1.82                     | 0.62              |
| 3:D:1206:GLY:HA3 | 3:D:1366:LYS:NZ   | 2.15                     | 0.62              |
| 1:K:101:LEU:HD13 | 1:K:114:PHE:CE1   | 2.35                     | 0.62              |
| 1:L:101:LEU:HD12 | 1:L:113:ASP:C     | 2.25                     | 0.62              |
| 3:N:132:TYR:HD2  | 3:N:154:THR:CB    | 2.10                     | 0.62              |
| 3:N:799:LYS:HB3  | 3:N:826:PRO:HG2   | 1.81                     | 0.62              |
| 3:N:1459:LEU:HA  | 3:N:1464:GLU:OE1  | 1.99                     | 0.62              |
| 1:A:11:PHE:HA    | 1:A:25:LEU:HD12   | 1.81                     | 0.62              |
| 1:A:64:GLU:O     | 1:A:75:VAL:HB     | 1.98                     | 0.62              |
| 2:C:393:GLN:HG2  | 6:H:10:G:O2'      | 1.99                     | 0.62              |
| 2:C:470:PRO:HD3  | 2:C:485:TYR:CE2   | 2.35                     | 0.62              |
| 2:C:729:LEU:HD13 | 3:D:675:ARG:HD2   | 1.81                     | 0.62              |
| 2:C:1032:PHE:CZ  | 2:C:1037:VAL:HA   | 2.35                     | 0.62              |
| 2:C:1087:VAL:O   | 2:C:1091:GLU:HG3  | 2.00                     | 0.62              |
| 3:D:56:TYR:O     | 3:D:80:VAL:HG21   | 1.99                     | 0.62              |
| 3:D:530:VAL:HG13 | 6:H:5:C:OP1       | 1.99                     | 0.62              |
| 3:D:639:LEU:HD12 | 3:D:640:HIS:N     | 2.15                     | 0.62              |
| 3:D:704:ARG:HD3  | 3:D:738:ALA:HB2   | 1.82                     | 0.62              |
| 2:M:15:LEU:HB2   | 2:M:586:ARG:HH12  | 1.65                     | 0.62              |
| 2:M:274:ARG:NH2  | 2:M:284:ARG:HA    | 2.15                     | 0.62              |
| 2:M:683:ASN:HD22 | 2:M:683:ASN:C     | 2.05                     | 0.62              |
| 2:M:1058:ASP:OD1 | 2:M:1084:SER:OG   | 2.16                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:63:TYR:CE1    | 3:N:73:CYS:HA     | 2.35                     | 0.62              |
| 3:N:119:SER:HB2   | 3:N:123:LEU:H     | 1.65                     | 0.62              |
| 3:N:703:ASN:CG    | 3:N:713:ILE:HD11  | 2.24                     | 0.62              |
| 3:N:1465:ASN:OD1  | 3:N:1473:PRO:CD   | 2.46                     | 0.62              |
| 5:G:3:DC:H2''     | 5:G:4:DA:O5'      | 2.00                     | 0.62              |
| 1:B:99:LEU:HB3    | 1:B:114:PHE:CD2   | 2.35                     | 0.62              |
| 2:C:90:TYR:HB2    | 2:C:128:ILE:HB    | 1.82                     | 0.62              |
| 2:C:708:TYR:CE2   | 2:C:793:PRO:HG2   | 2.35                     | 0.62              |
| 3:D:464:LEU:O     | 3:D:468:LEU:HG    | 1.99                     | 0.62              |
| 1:L:25:LEU:O      | 1:L:28:LEU:HD21   | 1.99                     | 0.62              |
| 1:L:201:THR:HG21  | 1:L:205:VAL:HG23  | 1.80                     | 0.62              |
| 3:N:62:LYS:CG     | 3:N:75:ARG:HD2    | 2.23                     | 0.62              |
| 3:N:160:GLU:O     | 3:N:164:GLY:N     | 2.32                     | 0.62              |
| 3:N:646:LYS:HD2   | 3:N:688:TRP:CE3   | 2.34                     | 0.62              |
| 3:N:1131:SER:HB2  | 3:N:1133:ARG:NH2  | 2.15                     | 0.62              |
| 5:G:5:DC:C2'      | 5:G:6:DT:O5'      | 2.46                     | 0.62              |
| 2:C:286:SER:HB3   | 2:C:299:LYS:HE3   | 1.80                     | 0.62              |
| 2:C:524:VAL:HG12  | 2:C:525:SER:N     | 2.15                     | 0.62              |
| 3:D:487:ALA:HB2   | 5:G:7:DA:H2'      | 1.80                     | 0.62              |
| 3:D:1149:LEU:HD22 | 3:D:1151:ARG:O    | 2.00                     | 0.62              |
| 1:K:35:THR:O      | 1:K:39:PRO:HG2    | 1.99                     | 0.62              |
| 2:M:163:ILE:HD12  | 2:M:164:PRO:N     | 2.13                     | 0.62              |
| 2:M:172:ILE:H     | 2:M:172:ILE:HD12  | 1.64                     | 0.62              |
| 3:N:759:ALA:HA    | 3:N:763:MET:HE2   | 1.81                     | 0.62              |
| 2:C:302:VAL:HG13  | 2:C:303:PHE:H     | 1.65                     | 0.62              |
| 3:D:619:LEU:HB2   | 3:D:621:LYS:HZ3   | 1.65                     | 0.62              |
| 3:D:1388:ARG:HD2  | 3:D:1388:ARG:H    | 1.65                     | 0.62              |
| 1:K:73:GLU:H      | 1:K:73:GLU:CD     | 2.05                     | 0.62              |
| 2:M:395:LYS:HB3   | 2:M:397:GLU:OE2   | 2.00                     | 0.62              |
| 2:M:679:PHE:O     | 2:M:680:ASP:O     | 2.18                     | 0.62              |
| 3:N:143:ASN:HA    | 3:N:161:LEU:HD12  | 1.81                     | 0.62              |
| 3:N:486:ARG:HG2   | 3:N:1390:LEU:HD11 | 1.82                     | 0.62              |
| 1:B:24:VAL:HG22   | 1:B:196:THR:HG22  | 1.81                     | 0.62              |
| 2:C:41:ASN:HB3    | 2:C:45:GLN:OE1    | 1.99                     | 0.62              |
| 2:C:328:LEU:HB2   | 2:C:433:THR:HB    | 1.80                     | 0.62              |
| 2:C:650:ARG:HG2   | 2:C:653:ASP:HB2   | 1.82                     | 0.62              |
| 2:C:988:VAL:HG11  | 3:D:949:ILE:O     | 1.98                     | 0.62              |
| 2:C:1046:ALA:O    | 3:D:1472:ILE:HD11 | 1.99                     | 0.62              |
| 2:C:1095:LEU:O    | 2:C:1096:ALA:C    | 2.43                     | 0.62              |
| 3:D:506:GLY:O     | 3:D:507:ASN:C     | 2.43                     | 0.62              |
| 1:L:58:ILE:HD13   | 1:L:140:MET:HB3   | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:1058:ASP:OD1  | 2:M:1084:SER:CB   | 2.47                     | 0.62              |
| 3:N:62:LYS:HG3    | 3:N:75:ARG:CD     | 2.23                     | 0.62              |
| 3:N:834:THR:HG22  | 3:N:838:ARG:HH11  | 1.64                     | 0.62              |
| 3:N:1131:SER:HB2  | 3:N:1133:ARG:HH21 | 1.65                     | 0.62              |
| 3:N:1323:GLN:N    | 3:N:1324:PRO:CD   | 2.63                     | 0.62              |
| 4:O:70:THR:HG21   | 4:O:72:ARG:CZ     | 2.30                     | 0.62              |
| 1:A:188:GLN:HG3   | 1:A:189:ARG:N     | 2.15                     | 0.61              |
| 1:B:57:TYR:HB2    | 1:B:164:ALA:HB2   | 1.82                     | 0.61              |
| 2:C:634:GLY:HA3   | 2:C:705:ILE:O     | 2.00                     | 0.61              |
| 2:C:710:ILE:HD12  | 2:C:790:LEU:HB2   | 1.82                     | 0.61              |
| 2:C:945:ARG:O     | 2:C:949:LYS:HG3   | 2.00                     | 0.61              |
| 3:D:498:VAL:HG12  | 3:D:502:PHE:HE1   | 1.64                     | 0.61              |
| 3:D:879:ARG:HH12  | 3:D:905:PRO:HD3   | 1.65                     | 0.61              |
| 3:D:1103:HIS:HA   | 3:D:1223:ILE:HD11 | 1.81                     | 0.61              |
| 3:D:1114:THR:HG22 | 3:D:1195:GLN:HB3  | 1.80                     | 0.61              |
| 1:K:7:LYS:HD2     | 1:K:186:LEU:CD2   | 2.29                     | 0.61              |
| 1:K:217:ILE:HG22  | 1:K:221:HIS:NE2   | 2.15                     | 0.61              |
| 2:M:98:LEU:N      | 2:M:98:LEU:HD12   | 2.15                     | 0.61              |
| 2:M:110:GLU:CG    | 2:M:369:PRO:HG3   | 2.30                     | 0.61              |
| 2:M:140:ILE:HG22  | 2:M:333:ILE:HG13  | 1.82                     | 0.61              |
| 3:N:95:LEU:HB2    | 3:N:515:GLU:HA    | 1.82                     | 0.61              |
| 3:N:744:GLN:HG3   | 3:N:744:GLN:O     | 1.99                     | 0.61              |
| 2:C:335:THR:O     | 2:C:339:LEU:HG    | 2.00                     | 0.61              |
| 2:C:613:VAL:O     | 2:C:620:LEU:HA    | 2.00                     | 0.61              |
| 3:D:897:TRP:C     | 3:D:900:ILE:HG13  | 2.24                     | 0.61              |
| 3:D:1183:ILE:HG22 | 3:N:559:ALA:O     | 2.00                     | 0.61              |
| 4:E:54:LEU:CG     | 4:E:58:PRO:HG2    | 2.26                     | 0.61              |
| 2:M:211:LEU:HD12  | 2:M:211:LEU:O     | 2.00                     | 0.61              |
| 2:M:586:ARG:HD2   | 2:M:590:ASP:OD2   | 2.00                     | 0.61              |
| 2:M:647:GLN:O     | 2:M:649:VAL:HG13  | 2.00                     | 0.61              |
| 2:M:1088:LEU:HA   | 2:M:1091:GLU:OE1  | 2.01                     | 0.61              |
| 3:N:764:LEU:HD12  | 3:N:765:SER:N     | 2.15                     | 0.61              |
| 3:N:939:PHE:O     | 3:N:942:SER:OG    | 2.16                     | 0.61              |
| 7:I:8:DG:H2''     | 7:I:9:DT:OP2      | 1.99                     | 0.61              |
| 2:C:172:ILE:H     | 2:C:172:ILE:HD12  | 1.64                     | 0.61              |
| 2:C:265:ARG:HB3   | 2:C:267:TYR:CE2   | 2.35                     | 0.61              |
| 2:C:492:ASP:HB3   | 2:C:518:LYS:HD2   | 1.81                     | 0.61              |
| 2:C:714:ASP:OD2   | 2:C:820:ARG:HB2   | 2.00                     | 0.61              |
| 3:D:41:ARG:C      | 3:D:43:GLY:N      | 2.58                     | 0.61              |
| 3:D:774:SER:HB2   | 3:D:776:GLU:HG2   | 1.82                     | 0.61              |
| 3:D:1195:GLN:CG   | 3:D:1196:THR:H    | 2.11                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:84:GLU:CD     | 3:N:845:ASN:HB2   | 2.25                     | 0.61              |
| 2:M:911:GLU:HB3   | 2:M:912:PRO:HD3   | 1.82                     | 0.61              |
| 2:M:1050:GLN:O    | 2:M:1054:THR:HG23 | 2.00                     | 0.61              |
| 2:M:1053:LEU:HD23 | 2:M:1053:LEU:N    | 2.15                     | 0.61              |
| 3:N:132:TYR:HA    | 3:N:154:THR:HA    | 1.82                     | 0.61              |
| 3:N:171:LEU:HG    | 3:N:195:VAL:HG23  | 1.80                     | 0.61              |
| 3:N:457:GLY:O     | 3:N:459:GLU:N     | 2.34                     | 0.61              |
| 3:N:952:ASP:HA    | 3:N:1062:ARG:NH2  | 2.14                     | 0.61              |
| 2:C:52:PHE:CE1    | 2:C:68:PHE:CB     | 2.74                     | 0.61              |
| 2:C:516:ARG:CZ    | 3:D:1068:LEU:HD22 | 2.31                     | 0.61              |
| 3:D:676:MET:HE1   | 3:D:683:ILE:HA    | 1.81                     | 0.61              |
| 3:D:1109:GLU:OE1  | 3:D:1201:CYS:HB2  | 2.00                     | 0.61              |
| 2:M:52:PHE:CE1    | 2:M:66:LEU:HG     | 2.33                     | 0.61              |
| 2:M:170:PRO:HD2   | 2:M:263:ASP:HB3   | 1.82                     | 0.61              |
| 2:M:350:ARG:O     | 2:M:353:ARG:HB3   | 2.01                     | 0.61              |
| 3:N:502:PHE:CD1   | 3:N:1452:ILE:HG23 | 2.36                     | 0.61              |
| 3:N:1379:VAL:HA   | 3:N:1420:LEU:HB2  | 1.82                     | 0.61              |
| 3:D:524:LEU:N     | 3:D:524:LEU:CD1   | 2.62                     | 0.61              |
| 3:D:583:ASP:OD1   | 3:D:586:ARG:HG2   | 2.01                     | 0.61              |
| 3:D:833:GLU:O     | 3:D:834:THR:CG2   | 2.36                     | 0.61              |
| 3:D:983:LEU:CD1   | 3:D:988:ARG:HB2   | 2.30                     | 0.61              |
| 1:K:156:HIS:ND1   | 1:K:157:GLY:N     | 2.48                     | 0.61              |
| 2:M:165:LEU:HA    | 2:M:166:PRO:O     | 1.99                     | 0.61              |
| 2:M:332:ARG:CZ    | 2:M:464:LEU:HD11  | 2.30                     | 0.61              |
| 2:M:569:VAL:HG21  | 2:M:702:SER:OG    | 2.01                     | 0.61              |
| 2:M:1052:MET:N    | 2:M:1052:MET:SD   | 2.72                     | 0.61              |
| 3:N:625:TYR:CD2   | 3:N:652:LEU:O     | 2.54                     | 0.61              |
| 1:A:43:ILE:O      | 1:A:47:SER:N      | 2.18                     | 0.61              |
| 2:C:73:LEU:C      | 2:C:73:LEU:HD12   | 2.25                     | 0.61              |
| 2:C:946:ARG:HB3   | 2:C:946:ARG:HH11  | 1.66                     | 0.61              |
| 2:C:1032:PHE:O    | 2:C:1033:GLY:O    | 2.17                     | 0.61              |
| 2:C:1115:LEU:HD23 | 3:D:85:VAL:HA     | 1.83                     | 0.61              |
| 3:D:87:ARG:HB2    | 3:D:524:LEU:HD11  | 1.81                     | 0.61              |
| 3:D:93:ILE:HD12   | 3:D:517:VAL:HB    | 1.83                     | 0.61              |
| 3:D:131:LYS:HG3   | 3:D:568:ARG:HG2   | 1.80                     | 0.61              |
| 3:D:163:TYR:HD1   | 3:D:163:TYR:H     | 1.46                     | 0.61              |
| 3:D:743:ASP:OD1   | 6:H:14:G:O2'      | 2.18                     | 0.61              |
| 3:D:750:PRO:CB    | 3:D:756:GLN:HA    | 2.30                     | 0.61              |
| 1:K:42:ARG:HH12   | 1:L:34:VAL:HB     | 1.64                     | 0.61              |
| 1:K:72:LYS:HE3    | 2:M:641:PRO:HB2   | 1.81                     | 0.61              |
| 2:M:95:TYR:HD2    | 2:M:114:PHE:HB3   | 1.65                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:532:MET:CG    | 2:M:533:ASP:N     | 2.64                     | 0.61              |
| 2:M:1046:ALA:HB1  | 3:N:1471:LEU:CD1  | 2.26                     | 0.61              |
| 2:M:1056:LYS:HD3  | 3:N:623:VAL:HG13  | 1.82                     | 0.61              |
| 3:N:90:MET:HE2    | 3:N:520:LEU:HA    | 1.82                     | 0.61              |
| 3:N:619:LEU:N     | 3:N:619:LEU:HD23  | 2.16                     | 0.61              |
| 3:N:1256:LEU:HG   | 3:N:1260:ILE:HD11 | 1.82                     | 0.61              |
| 1:B:150:TYR:HE2   | 1:B:168:ASP:HB3   | 1.66                     | 0.61              |
| 2:C:239:PHE:CZ    | 2:C:250:ARG:HD2   | 2.35                     | 0.61              |
| 2:C:267:TYR:CG    | 2:C:272:ALA:HB1   | 2.36                     | 0.61              |
| 2:C:678:PRO:O     | 3:D:943:THR:HA    | 2.01                     | 0.61              |
| 3:D:86:ARG:O      | 3:D:521:PRO:HB3   | 1.99                     | 0.61              |
| 3:D:101:HIS:O     | 3:D:105:VAL:HG23  | 2.01                     | 0.61              |
| 3:D:1106:VAL:HG11 | 3:D:1474:ALA:CB   | 2.30                     | 0.61              |
| 1:L:32:PHE:O      | 1:L:36:LEU:HG     | 2.00                     | 0.61              |
| 2:M:16:PRO:O      | 2:M:18:LEU:HD12   | 2.00                     | 0.61              |
| 2:M:36:PRO:HB2    | 2:M:70:GLU:HG2    | 1.82                     | 0.61              |
| 2:M:68:PHE:HE1    | 2:M:96:ALA:HB1    | 1.64                     | 0.61              |
| 2:M:143:SER:HB2   | 2:M:276:LYS:CE    | 2.28                     | 0.61              |
| 2:M:394:PHE:CE1   | 2:M:632:ASN:HB3   | 2.36                     | 0.61              |
| 2:M:418:LEU:N     | 2:M:418:LEU:HD12  | 2.16                     | 0.61              |
| 2:M:613:VAL:O     | 2:M:620:LEU:HA    | 2.01                     | 0.61              |
| 3:N:503:LEU:O     | 3:N:504:ASP:C     | 2.44                     | 0.61              |
| 3:N:716:PHE:O     | 3:N:718:PRO:HD3   | 2.01                     | 0.61              |
| 2:C:897:LEU:HD22  | 2:C:920:GLN:HE22  | 1.66                     | 0.61              |
| 2:C:1090:LYS:HD2  | 3:D:90:MET:SD     | 2.41                     | 0.61              |
| 3:D:781:PRO:HB2   | 3:D:786:ILE:CG1   | 2.31                     | 0.61              |
| 4:E:64:ALA:O      | 4:E:68:LEU:HD13   | 2.01                     | 0.61              |
| 1:K:221:HIS:HA    | 1:K:224:TYR:CD2   | 2.36                     | 0.61              |
| 2:M:20:GLU:HG2    | 2:M:21:ILE:HD12   | 1.82                     | 0.61              |
| 2:M:30:LEU:O      | 2:M:30:LEU:HD12   | 2.00                     | 0.61              |
| 2:M:66:LEU:HD12   | 2:M:99:GLN:O      | 2.01                     | 0.61              |
| 2:M:577:PRO:HG3   | 2:M:993:PHE:CE2   | 2.36                     | 0.61              |
| 2:M:630:ARG:CD    | 2:M:634:GLY:HA2   | 2.30                     | 0.61              |
| 3:N:105:VAL:HG22  | 3:N:112:ILE:HG21  | 1.82                     | 0.61              |
| 3:N:187:LYS:CE    | 3:N:199:LEU:HA    | 2.30                     | 0.61              |
| 3:N:661:MET:O     | 3:N:664:LYS:O     | 2.18                     | 0.61              |
| 3:N:711:LEU:HD21  | 3:N:768:ASN:HB3   | 1.81                     | 0.61              |
| 4:O:34:GLY:CA     | 4:O:95:VAL:HB     | 2.29                     | 0.61              |
| 5:X:13:DA:C2'     | 5:X:14:DG:OP2     | 2.44                     | 0.61              |
| 1:A:56:VAL:HG13   | 1:A:142:VAL:HG12  | 1.83                     | 0.61              |
| 1:A:226:SER:O     | 1:A:228:PRO:HD3   | 1.99                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1056:LYS:NZ   | 3:D:749:VAL:H     | 1.99                     | 0.61              |
| 3:D:32:ILE:HG12   | 3:D:39:PRO:HA     | 1.81                     | 0.61              |
| 3:D:105:VAL:HA    | 3:D:112:ILE:CG2   | 2.31                     | 0.61              |
| 3:D:119:SER:HB2   | 3:D:123:LEU:HB2   | 1.83                     | 0.61              |
| 3:D:521:PRO:HD2   | 3:D:524:LEU:HD22  | 1.82                     | 0.61              |
| 3:D:542:ASP:HA    | 3:D:545:ARG:HH21  | 1.64                     | 0.61              |
| 3:D:937:TYR:O     | 3:D:941:PHE:HB2   | 2.01                     | 0.61              |
| 3:D:1129:THR:HG23 | 3:D:1130:ARG:N    | 2.16                     | 0.61              |
| 3:D:1264:GLU:HB3  | 3:D:1266:ARG:HD2  | 1.82                     | 0.61              |
| 2:M:226:VAL:HG13  | 2:M:227:PHE:CD1   | 2.36                     | 0.61              |
| 3:N:119:SER:HB2   | 3:N:123:LEU:CB    | 2.30                     | 0.61              |
| 3:N:1177:ALA:O    | 3:N:1180:ALA:HB3  | 1.99                     | 0.61              |
| 3:N:1238:MET:C    | 3:N:1239:ARG:CG   | 2.74                     | 0.61              |
| 7:I:4:DG:C2'      | 7:I:5:DC:OP2      | 2.44                     | 0.61              |
| 1:A:211:LEU:O     | 1:A:215:VAL:HG23  | 2.01                     | 0.61              |
| 1:B:101:LEU:HD11  | 1:B:113:ASP:HB3   | 1.83                     | 0.61              |
| 2:C:15:LEU:H      | 2:C:15:LEU:CD1    | 2.12                     | 0.61              |
| 2:C:98:LEU:HD12   | 2:C:98:LEU:N      | 2.16                     | 0.61              |
| 2:C:604:ALA:HB3   | 2:C:612:VAL:O     | 2.01                     | 0.61              |
| 3:D:623:VAL:HG12  | 3:D:624:ASP:N     | 2.16                     | 0.61              |
| 3:D:1398:TRP:HA   | 3:D:1398:TRP:CE3  | 2.36                     | 0.61              |
| 3:D:1447:LEU:O    | 3:D:1448:THR:C    | 2.44                     | 0.61              |
| 1:K:121:GLU:HG2   | 1:K:122:ILE:N     | 2.14                     | 0.61              |
| 1:L:89:PHE:HB3    | 1:L:94:LEU:CD1    | 2.31                     | 0.61              |
| 2:M:775:ARG:NH1   | 2:M:782:ALA:HB1   | 2.16                     | 0.61              |
| 3:N:609:GLY:O     | 3:N:615:ARG:CB    | 2.49                     | 0.61              |
| 3:N:804:LEU:HD23  | 3:N:804:LEU:H     | 1.64                     | 0.61              |
| 3:N:1103:HIS:CE1  | 3:N:1463:LYS:HB3  | 2.36                     | 0.61              |
| 3:N:1220:ALA:O    | 3:N:1224:VAL:HG23 | 2.01                     | 0.61              |
| 7:Z:12:DT:H2''    | 7:Z:13:DA:H8      | 1.63                     | 0.61              |
| 2:C:133:ASP:OD2   | 2:C:133:ASP:N     | 2.33                     | 0.60              |
| 2:C:395:LYS:CE    | 2:C:407:LYS:HD2   | 2.31                     | 0.60              |
| 2:C:409:ARG:HH12  | 2:C:444:PRO:CG    | 2.14                     | 0.60              |
| 3:D:490:ALA:O     | 3:D:493:ARG:HG3   | 2.01                     | 0.60              |
| 3:D:739:ASP:OD1   | 3:D:741:ASP:OD2   | 2.19                     | 0.60              |
| 3:D:1153:VAL:HG13 | 3:N:560:GLN:O     | 2.00                     | 0.60              |
| 4:E:54:LEU:HD23   | 4:E:54:LEU:O      | 2.00                     | 0.60              |
| 2:M:604:ALA:HB3   | 2:M:612:VAL:O     | 2.02                     | 0.60              |
| 2:M:606:VAL:HG22  | 2:M:645:VAL:HG13  | 1.83                     | 0.60              |
| 2:M:677:MET:HB3   | 2:M:987:ILE:HG21  | 1.82                     | 0.60              |
| 3:N:9:ARG:HH12    | 3:N:11:ALA:HB2    | 1.65                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:111:LYS:CG    | 3:N:1448:THR:HG22 | 2.31                     | 0.60              |
| 3:N:623:VAL:HG12  | 3:N:624:ASP:N     | 2.16                     | 0.60              |
| 3:N:690:ALA:O     | 3:N:693:GLU:HB3   | 2.01                     | 0.60              |
| 5:X:15:DC:O5'     | 5:X:15:DC:H6      | 1.84                     | 0.60              |
| 1:A:106:PRO:HA    | 1:A:133:GLU:O     | 2.01                     | 0.60              |
| 1:B:101:LEU:HD23  | 1:B:101:LEU:C     | 2.26                     | 0.60              |
| 3:D:713:ILE:O     | 3:D:714:GLN:HG3   | 2.01                     | 0.60              |
| 3:D:1161:GLU:HG2  | 3:D:1164:ARG:HB2  | 1.83                     | 0.60              |
| 2:M:15:LEU:HB2    | 2:M:586:ARG:NH1   | 2.15                     | 0.60              |
| 2:M:1075:ASP:CB   | 4:O:32:ARG:NH2    | 2.64                     | 0.60              |
| 3:N:171:LEU:HG    | 3:N:195:VAL:CG2   | 2.31                     | 0.60              |
| 3:N:845:ASN:O     | 3:N:848:GLU:HB2   | 2.00                     | 0.60              |
| 2:C:50:GLU:HB2    | 2:C:266:ARG:CZ    | 2.31                     | 0.60              |
| 2:C:409:ARG:NH1   | 2:C:444:PRO:HG3   | 2.15                     | 0.60              |
| 2:C:690:ILE:CG1   | 2:C:691:SER:N     | 2.63                     | 0.60              |
| 2:C:757:GLY:HA2   | 2:C:789:SER:HB3   | 1.82                     | 0.60              |
| 3:D:739:ASP:O     | 3:D:743:ASP:OD1   | 2.18                     | 0.60              |
| 3:D:813:LEU:HD12  | 3:D:813:LEU:C     | 2.26                     | 0.60              |
| 3:D:994:GLN:HG2   | 3:D:1243:THR:O    | 2.01                     | 0.60              |
| 3:D:1109:GLU:OE1  | 3:D:1111:ASP:N    | 2.35                     | 0.60              |
| 3:D:1378:TYR:OH   | 3:D:1431:THR:HA   | 2.00                     | 0.60              |
| 1:L:176:ARG:NH1   | 3:N:884:ARG:HD3   | 2.15                     | 0.60              |
| 2:M:44:ILE:CG2    | 2:M:45:GLN:N      | 2.64                     | 0.60              |
| 3:N:143:ASN:OD1   | 3:N:145:VAL:O     | 2.19                     | 0.60              |
| 1:A:112:ARG:HH21  | 1:A:125:PRO:CB    | 2.13                     | 0.60              |
| 3:D:54:LYS:HG2    | 3:D:57:GLU:CD     | 2.26                     | 0.60              |
| 3:D:84:ILE:HG13   | 3:D:85:VAL:N      | 2.16                     | 0.60              |
| 3:D:134:VAL:HG12  | 3:D:152:LEU:HB3   | 1.82                     | 0.60              |
| 2:M:89:THR:CA     | 2:M:129:ILE:O     | 2.43                     | 0.60              |
| 2:M:677:MET:HB3   | 2:M:987:ILE:HD13  | 1.83                     | 0.60              |
| 2:M:853:LEU:HB2   | 2:M:858:MET:HE3   | 1.83                     | 0.60              |
| 2:M:1001:VAL:HG21 | 5:X:24:DC:H5'     | 1.83                     | 0.60              |
| 3:N:87:ARG:HG3    | 3:N:88:TYR:CD2    | 2.36                     | 0.60              |
| 3:N:166:GLN:HB3   | 3:N:198:ARG:HB3   | 1.83                     | 0.60              |
| 3:N:919:PHE:HA    | 3:N:927:THR:OG1   | 2.02                     | 0.60              |
| 3:N:1061:PHE:CE1  | 3:N:1065:LEU:HD22 | 2.36                     | 0.60              |
| 1:B:78:ILE:O      | 1:B:82:LEU:HG     | 2.01                     | 0.60              |
| 2:C:1016:ILE:CG1  | 2:C:1017:THR:H    | 2.12                     | 0.60              |
| 3:D:520:LEU:HD11  | 3:D:524:LEU:HD23  | 1.82                     | 0.60              |
| 3:D:770:LEU:HD22  | 3:D:775:GLY:O     | 2.01                     | 0.60              |
| 1:K:50:GLY:HA3    | 1:K:173:PRO:HG3   | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:101:ILE:HG23  | 2:M:107:LEU:HD22  | 1.81                     | 0.60              |
| 2:M:264:PRO:CB    | 2:M:289:THR:HB    | 2.32                     | 0.60              |
| 2:M:1031:ARG:HB3  | 5:X:22:DA:OP1     | 2.01                     | 0.60              |
| 2:M:1036:GLU:OE1  | 2:M:1036:GLU:N    | 2.35                     | 0.60              |
| 3:N:52:PRO:HG2    | 3:N:85:VAL:CG2    | 2.31                     | 0.60              |
| 3:N:578:VAL:O     | 3:N:582:LEU:HG    | 2.00                     | 0.60              |
| 3:N:1453:ALA:O    | 3:N:1455:LYS:N    | 2.33                     | 0.60              |
| 4:O:36:LYS:HG2    | 4:O:95:VAL:CG2    | 2.31                     | 0.60              |
| 1:A:106:PRO:CG    | 1:A:134:GLU:CD    | 2.74                     | 0.60              |
| 1:B:30:ARG:HG2    | 1:B:30:ARG:NH1    | 2.12                     | 0.60              |
| 1:B:170:VAL:HG11  | 3:D:848:GLU:OE2   | 2.01                     | 0.60              |
| 3:D:136:ASP:CG    | 3:D:137:PRO:HD3   | 2.26                     | 0.60              |
| 3:D:619:LEU:N     | 3:D:619:LEU:HD23  | 2.16                     | 0.60              |
| 3:D:641:GLN:HG2   | 3:D:717:GLN:NE2   | 2.15                     | 0.60              |
| 3:D:804:LEU:HD12  | 3:D:830:ALA:O     | 2.01                     | 0.60              |
| 3:D:907:GLU:HG2   | 3:D:908:LYS:H     | 1.66                     | 0.60              |
| 2:M:305:PRO:HA    | 2:M:308:ARG:HB2   | 1.83                     | 0.60              |
| 2:M:690:ILE:HG22  | 2:M:851:LYS:O     | 2.00                     | 0.60              |
| 2:M:874:LEU:CD1   | 3:N:783:ARG:HB2   | 2.32                     | 0.60              |
| 3:N:501:ALA:HB1   | 3:N:1453:ALA:CA   | 2.31                     | 0.60              |
| 3:N:526:PRO:O     | 3:N:537:THR:HA    | 2.00                     | 0.60              |
| 3:N:642:CYS:SG    | 3:N:716:PHE:HB2   | 2.42                     | 0.60              |
| 3:N:712:GLY:O     | 3:N:713:ILE:HG13  | 2.00                     | 0.60              |
| 3:N:1216:SER:CB   | 4:O:15:SER:HA     | 2.31                     | 0.60              |
| 3:N:1468:LEU:HD22 | 3:N:1470:ARG:CB   | 2.23                     | 0.60              |
| 5:X:26:DC:C2      | 5:X:27:DC:C5      | 2.89                     | 0.60              |
| 7:Z:4:DG:C2'      | 7:Z:5:DC:OP2      | 2.37                     | 0.60              |
| 1:A:206:THR:HG23  | 1:A:208:LEU:H     | 1.67                     | 0.60              |
| 2:C:850:ALA:HA    | 3:D:632:VAL:HG13  | 1.83                     | 0.60              |
| 3:D:706:PRO:CG    | 5:G:19:DG:N2      | 2.64                     | 0.60              |
| 3:D:845:ASN:O     | 3:D:848:GLU:HB2   | 2.01                     | 0.60              |
| 3:D:853:VAL:HA    | 3:D:858:VAL:O     | 2.01                     | 0.60              |
| 3:D:1059:SER:HB2  | 3:D:1065:LEU:HD12 | 1.84                     | 0.60              |
| 3:D:1116:ASN:O    | 3:D:1193:THR:HB   | 2.01                     | 0.60              |
| 3:D:1496:GLU:HA   | 3:D:1499:ARG:NE   | 2.15                     | 0.60              |
| 1:L:7:LYS:O       | 1:L:7:LYS:HD3     | 2.01                     | 0.60              |
| 2:M:227:PHE:HD2   | 2:M:237:ARG:HD3   | 1.66                     | 0.60              |
| 2:M:508:ILE:HD13  | 2:M:508:ILE:N     | 2.16                     | 0.60              |
| 2:M:692:GLU:HB2   | 2:M:853:LEU:O     | 2.02                     | 0.60              |
| 2:M:861:LEU:CD2   | 2:M:863:ASP:HB3   | 2.26                     | 0.60              |
| 2:M:875:GLY:HA2   | 3:N:1029:ARG:HH21 | 1.67                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:939:ARG:HE    | 2:M:939:ARG:CA    | 1.96                     | 0.60              |
| 3:N:457:GLY:O     | 3:N:458:ALA:C     | 2.44                     | 0.60              |
| 3:N:488:ARG:HG2   | 3:N:488:ARG:HH11  | 1.66                     | 0.60              |
| 3:N:682:ASP:O     | 3:N:683:ILE:HG13  | 2.01                     | 0.60              |
| 3:D:522:PRO:CA    | 3:D:525:ARG:NH1   | 2.61                     | 0.60              |
| 3:D:1003:VAL:HG13 | 3:D:1036:ARG:HG3  | 1.84                     | 0.60              |
| 3:D:1353:GLN:O    | 3:D:1357:ARG:HG3  | 2.01                     | 0.60              |
| 3:D:1448:THR:O    | 3:D:1452:ILE:CD1  | 2.50                     | 0.60              |
| 1:L:48:ILE:HD13   | 1:L:210:ALA:HB1   | 1.84                     | 0.60              |
| 2:M:64:LEU:HD22   | 2:M:359:MET:CG    | 2.25                     | 0.60              |
| 2:M:147:TYR:CE2   | 2:M:330:ASN:HB3   | 2.37                     | 0.60              |
| 2:M:265:ARG:C     | 2:M:267:TYR:H     | 2.10                     | 0.60              |
| 2:M:457:ALA:HB3   | 2:M:538:GLN:HA    | 1.82                     | 0.60              |
| 2:M:1060:ILE:O    | 2:M:1063:ARG:HG2  | 2.01                     | 0.60              |
| 3:N:637:LEU:HD11  | 3:N:642:CYS:CA    | 2.31                     | 0.60              |
| 3:N:730:PRO:HG2   | 3:N:731:LEU:H     | 1.67                     | 0.60              |
| 3:N:1377:LYS:HE2  | 3:N:1394:VAL:HG22 | 1.82                     | 0.60              |
| 2:M:22:GLN:OE1    | 2:M:336:VAL:HG21  | 2.02                     | 0.60              |
| 2:M:426:ASP:HA    | 2:M:429:ASP:OD2   | 2.02                     | 0.60              |
| 2:M:841:ASN:ND2   | 2:M:884:GLN:HB3   | 2.16                     | 0.60              |
| 3:N:41:ARG:C      | 3:N:43:GLY:H      | 2.09                     | 0.60              |
| 3:N:98:PRO:HA     | 3:N:514:LEU:O     | 2.01                     | 0.60              |
| 3:N:637:LEU:HD21  | 3:N:642:CYS:HA    | 1.84                     | 0.60              |
| 3:N:646:LYS:CD    | 3:N:688:TRP:CH2   | 2.85                     | 0.60              |
| 3:N:704:ARG:CG    | 3:N:736:PHE:HB3   | 2.31                     | 0.60              |
| 3:N:732:VAL:HB    | 3:N:736:PHE:CE1   | 2.37                     | 0.60              |
| 3:N:1447:LEU:N    | 3:N:1447:LEU:HD12 | 2.17                     | 0.60              |
| 4:O:32:ARG:NH1    | 4:O:32:ARG:HB2    | 2.17                     | 0.60              |
| 2:C:384:GLU:O     | 2:C:388:ARG:HB2   | 2.02                     | 0.60              |
| 2:C:751:PRO:HB3   | 2:C:794:PRO:HA    | 1.83                     | 0.60              |
| 3:D:776:GLU:HB3   | 3:D:912:LYS:HE2   | 1.84                     | 0.60              |
| 3:D:817:GLU:O     | 3:D:821:VAL:HG23  | 2.02                     | 0.60              |
| 3:D:1348:LEU:O    | 3:D:1352:ILE:HG13 | 2.01                     | 0.60              |
| 1:K:140:MET:HE3   | 1:K:142:VAL:HG13  | 1.84                     | 0.60              |
| 1:L:115:LEU:HD12  | 1:L:115:LEU:O     | 2.01                     | 0.60              |
| 2:M:266:ARG:HA    | 2:M:288:ARG:CD    | 2.31                     | 0.60              |
| 2:M:269:LEU:HG    | 2:M:288:ARG:HA    | 1.83                     | 0.60              |
| 2:M:334:ARG:HA    | 2:M:338:GLU:OE2   | 2.01                     | 0.60              |
| 2:M:423:ALA:HB2   | 7:Z:1:DG:O4'      | 2.02                     | 0.60              |
| 2:M:492:ASP:HB3   | 2:M:518:LYS:CD    | 2.29                     | 0.60              |
| 2:M:843:HIS:CE1   | 2:M:884:GLN:CA    | 2.84                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:1097:LEU:H    | 2:M:1097:LEU:CD2  | 2.11                     | 0.60              |
| 3:N:704:ARG:CB    | 3:N:736:PHE:HB3   | 2.32                     | 0.60              |
| 3:N:1301:LYS:HG3  | 3:N:1303:TYR:CE1  | 2.37                     | 0.60              |
| 3:N:1382:THR:HG21 | 3:N:1418:LYS:HE3  | 1.83                     | 0.60              |
| 3:N:1462:LEU:HD22 | 3:N:1472:ILE:HG22 | 1.83                     | 0.60              |
| 1:A:43:ILE:C      | 1:A:47:SER:HB2    | 2.27                     | 0.59              |
| 1:B:57:TYR:CE1    | 1:B:163:ASN:HB2   | 2.35                     | 0.59              |
| 2:C:56:GLU:HB3    | 2:C:359:MET:SD    | 2.43                     | 0.59              |
| 2:C:140:ILE:HG23  | 2:C:410:ILE:HD11  | 1.84                     | 0.59              |
| 2:C:1045:ALA:HB2  | 3:D:763:MET:SD    | 2.42                     | 0.59              |
| 3:D:108:VAL:HB    | 3:D:109:PRO:CD    | 2.25                     | 0.59              |
| 3:D:577:ALA:O     | 3:D:580:ALA:HB3   | 2.01                     | 0.59              |
| 3:D:584:ASN:ND2   | 3:D:590:PRO:HD2   | 2.17                     | 0.59              |
| 3:D:613:ARG:NE    | 3:D:613:ARG:HA    | 2.14                     | 0.59              |
| 3:D:704:ARG:HH11  | 3:D:738:ALA:CB    | 2.13                     | 0.59              |
| 3:D:918:ALA:CB    | 3:D:927:THR:HG23  | 2.31                     | 0.59              |
| 3:D:1252:ILE:HG23 | 3:D:1252:ILE:O    | 2.02                     | 0.59              |
| 4:E:30:LEU:HB3    | 4:E:35:PHE:CE1    | 2.37                     | 0.59              |
| 1:L:56:VAL:HG12   | 1:L:57:TYR:N      | 2.17                     | 0.59              |
| 2:M:52:PHE:O      | 2:M:54:ILE:N      | 2.35                     | 0.59              |
| 2:M:260:LEU:HD12  | 2:M:261:ILE:H     | 1.67                     | 0.59              |
| 2:M:274:ARG:HG2   | 2:M:285:LEU:HD13  | 1.83                     | 0.59              |
| 2:M:498:GLN:HG2   | 2:M:516:ARG:HH21  | 1.67                     | 0.59              |
| 2:M:735:ARG:HG2   | 2:M:735:ARG:NH1   | 2.14                     | 0.59              |
| 2:M:825:VAL:HG12  | 2:M:827:VAL:HG23  | 1.83                     | 0.59              |
| 2:M:1101:THR:C    | 2:M:1102:LEU:HD12 | 2.26                     | 0.59              |
| 3:N:539:ASP:HB3   | 3:N:600:LEU:HB3   | 1.84                     | 0.59              |
| 3:N:646:LYS:HD2   | 3:N:688:TRP:CZ3   | 2.37                     | 0.59              |
| 3:N:1136:LYS:HB2  | 3:N:1139:ASP:OD2  | 2.02                     | 0.59              |
| 2:C:679:PHE:O     | 2:C:680:ASP:C     | 2.45                     | 0.59              |
| 2:C:1012:PRO:HD3  | 2:C:1026:GLN:HG2  | 1.82                     | 0.59              |
| 2:C:1060:ILE:O    | 2:C:1063:ARG:HG2  | 2.02                     | 0.59              |
| 3:D:1027:GLY:O    | 3:D:1028:ALA:O    | 2.20                     | 0.59              |
| 3:D:1168:MET:HG3  | 3:D:1172:HIS:NE2  | 2.16                     | 0.59              |
| 2:M:950:LEU:HB3   | 2:M:952:LEU:HD23  | 1.83                     | 0.59              |
| 2:M:1115:LEU:H    | 2:M:1115:LEU:CD1  | 2.06                     | 0.59              |
| 3:N:1167:SER:O    | 3:N:1171:VAL:HG23 | 2.02                     | 0.59              |
| 3:N:1496:GLU:O    | 3:N:1500:LYS:HG3  | 2.02                     | 0.59              |
| 5:G:20:DC:H2''    | 5:G:21:DG:C5'     | 2.30                     | 0.59              |
| 2:C:296:GLY:O     | 2:C:298:PHE:CZ    | 2.55                     | 0.59              |
| 2:C:304:LEU:HD23  | 2:C:304:LEU:H     | 1.67                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:516:ARG:NE    | 3:D:1068:LEU:HD13 | 2.17                     | 0.59              |
| 2:C:559:LEU:CD2   | 2:C:563:ASN:OD1   | 2.50                     | 0.59              |
| 2:C:1092:LEU:O    | 2:C:1097:LEU:O    | 2.20                     | 0.59              |
| 2:C:1110:ASP:OD2  | 2:C:1112:PHE:O    | 2.19                     | 0.59              |
| 3:D:879:ARG:NH2   | 3:D:903:ASP:O     | 2.35                     | 0.59              |
| 4:E:9:LEU:HD11    | 4:E:69:LEU:HD12   | 1.84                     | 0.59              |
| 1:L:211:LEU:O     | 1:L:215:VAL:HG13  | 2.02                     | 0.59              |
| 2:M:172:ILE:HD12  | 2:M:172:ILE:N     | 2.18                     | 0.59              |
| 2:M:474:VAL:HG23  | 2:M:478:VAL:O     | 2.02                     | 0.59              |
| 2:M:684:PHE:CE2   | 2:M:685:GLU:HB2   | 2.37                     | 0.59              |
| 2:M:799:ILE:C     | 2:M:827:VAL:HG13  | 2.25                     | 0.59              |
| 3:N:752:SER:HB3   | 3:N:755:ALA:HB3   | 1.84                     | 0.59              |
| 3:N:774:SER:C     | 3:N:776:GLU:N     | 2.57                     | 0.59              |
| 3:N:800:LYS:HD2   | 3:N:804:LEU:HD13  | 1.85                     | 0.59              |
| 3:N:1211:MET:HE2  | 3:N:1213:ARG:HB3  | 1.84                     | 0.59              |
| 3:N:1446:VAL:CG1  | 3:N:1447:LEU:HD12 | 2.32                     | 0.59              |
| 4:O:13:VAL:HG12   | 4:O:15:SER:H      | 1.66                     | 0.59              |
| 5:X:9:DC:H2"      | 5:X:10:DA:H8      | 1.67                     | 0.59              |
| 1:A:46:SER:CB     | 2:C:856:GLU:OE2   | 2.50                     | 0.59              |
| 2:C:50:GLU:CG     | 2:C:266:ARG:CD    | 2.73                     | 0.59              |
| 2:C:650:ARG:CG    | 2:C:653:ASP:HB2   | 2.32                     | 0.59              |
| 2:C:881:ASN:O     | 2:C:884:GLN:HG3   | 2.02                     | 0.59              |
| 2:C:1016:ILE:CG1  | 2:C:1017:THR:N    | 2.66                     | 0.59              |
| 3:D:109:PRO:HB3   | 3:D:494:LYS:HZ1   | 1.63                     | 0.59              |
| 3:D:984:THR:OG1   | 3:D:985:ASP:N     | 2.36                     | 0.59              |
| 3:D:1041:LEU:HD12 | 3:D:1042:ARG:CZ   | 2.33                     | 0.59              |
| 3:D:1256:LEU:HD21 | 3:D:1260:ILE:HD11 | 1.84                     | 0.59              |
| 4:E:4:PRO:HG2     | 4:E:66:LYS:NZ     | 2.17                     | 0.59              |
| 2:M:69:LEU:HD12   | 2:M:97:ARG:HB3    | 1.83                     | 0.59              |
| 2:M:211:LEU:HD13  | 2:M:308:ARG:HA    | 1.85                     | 0.59              |
| 2:M:333:ILE:HD12  | 2:M:333:ILE:N     | 2.17                     | 0.59              |
| 2:M:584:GLU:CB    | 2:M:666:LEU:HB3   | 2.33                     | 0.59              |
| 2:M:876:VAL:H     | 2:M:877:PRO:HD2   | 1.66                     | 0.59              |
| 3:N:166:GLN:HA    | 3:N:198:ARG:HG2   | 1.84                     | 0.59              |
| 3:N:1207:TYR:O    | 3:N:1215:VAL:HG23 | 2.02                     | 0.59              |
| 1:A:117:VAL:HB    | 1:A:120:VAL:CG1   | 2.33                     | 0.59              |
| 1:B:58:ILE:CD1    | 1:B:140:MET:HB3   | 2.31                     | 0.59              |
| 2:C:110:GLU:OE1   | 2:C:113:VAL:HG22  | 2.02                     | 0.59              |
| 3:D:862:ASP:O     | 3:D:877:PRO:HD3   | 2.03                     | 0.59              |
| 3:D:1100:ASP:HA   | 3:D:1463:LYS:HZ1  | 1.66                     | 0.59              |
| 1:K:92:PRO:HG3    | 1:K:146:ARG:NH2   | 2.17                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:184:MET:O     | 2:M:190:LYS:HA   | 2.01                     | 0.59              |
| 2:M:328:LEU:HB2   | 2:M:488:ALA:HB2  | 1.83                     | 0.59              |
| 2:M:404:LEU:HA    | 2:M:407:LYS:HD3  | 1.81                     | 0.59              |
| 3:N:792:ILE:HG23  | 3:N:793:THR:HG23 | 1.84                     | 0.59              |
| 3:N:939:PHE:O     | 3:N:943:THR:HG23 | 2.01                     | 0.59              |
| 3:N:1189:ARG:HD2  | 3:N:1204:CYS:HA  | 1.83                     | 0.59              |
| 3:N:1209:LEU:HD21 | 4:O:16:LYS:HE3   | 1.84                     | 0.59              |
| 5:G:15:DC:H1'     | 5:G:16:DT:H5'    | 1.84                     | 0.59              |
| 7:I:3:DA:H2''     | 7:I:4:DG:O5'     | 2.03                     | 0.59              |
| 6:Y:11:C:O5'      | 6:Y:11:C:H6      | 1.85                     | 0.59              |
| 1:A:73:GLU:CD     | 1:A:73:GLU:H     | 2.11                     | 0.59              |
| 2:C:170:PRO:HD2   | 2:C:263:ASP:HB3  | 1.83                     | 0.59              |
| 2:C:490:GLU:HA    | 2:C:493:ARG:CD   | 2.32                     | 0.59              |
| 2:C:796:GLU:HB3   | 2:C:829:GLN:OE1  | 2.02                     | 0.59              |
| 2:C:824:ARG:HD2   | 2:C:826:TYR:OH   | 2.03                     | 0.59              |
| 2:C:946:ARG:HB3   | 2:C:946:ARG:NH1  | 2.18                     | 0.59              |
| 3:D:30:GLU:CD     | 3:D:40:GLU:HG2   | 2.27                     | 0.59              |
| 3:D:505:SER:HB3   | 3:D:1454:GLY:H   | 1.67                     | 0.59              |
| 3:D:989:TYR:CZ    | 3:D:1051:GLU:CG  | 2.76                     | 0.59              |
| 3:D:1154:GLU:N    | 3:N:561:GLY:HA3  | 2.18                     | 0.59              |
| 3:D:1154:GLU:C    | 3:N:562:ALA:H    | 2.11                     | 0.59              |
| 3:D:1223:ILE:HD12 | 3:D:1223:ILE:N   | 2.17                     | 0.59              |
| 2:M:715:THR:HG23  | 2:M:720:GLU:OE2  | 2.01                     | 0.59              |
| 2:M:775:ARG:HD2   | 2:M:782:ALA:CB   | 2.33                     | 0.59              |
| 3:N:199:LEU:HD23  | 3:N:200:ASP:N    | 2.17                     | 0.59              |
| 3:N:900:ILE:O     | 3:N:900:ILE:HG13 | 2.01                     | 0.59              |
| 3:N:1175:ILE:O    | 3:N:1179:GLU:HG3 | 2.02                     | 0.59              |
| 3:N:1330:ILE:HD13 | 3:N:1347:TYR:HE1 | 1.67                     | 0.59              |
| 3:N:1422:MET:HE3  | 3:N:1427:SER:HA  | 1.84                     | 0.59              |
| 3:N:1435:LEU:HD22 | 3:N:1457:ASP:CG  | 2.28                     | 0.59              |
| 3:N:1441:GLN:CD   | 3:N:1442:ASN:H   | 2.10                     | 0.59              |
| 3:N:1447:LEU:O    | 3:N:1448:THR:C   | 2.45                     | 0.59              |
| 2:C:106:GLY:O     | 2:C:107:LEU:HD23 | 2.03                     | 0.59              |
| 2:C:630:ARG:NE    | 2:C:634:GLY:HA2  | 2.18                     | 0.59              |
| 3:D:465:LEU:HD13  | 3:D:510:GLU:HA   | 1.83                     | 0.59              |
| 3:D:1431:THR:HG23 | 3:D:1433:SER:O   | 2.02                     | 0.59              |
| 1:K:24:VAL:HG22   | 1:K:196:THR:HG22 | 1.84                     | 0.59              |
| 2:M:8:ARG:N       | 2:M:907:ASP:OD2  | 2.35                     | 0.59              |
| 2:M:10:ARG:HH11   | 2:M:10:ARG:CA    | 2.14                     | 0.59              |
| 2:M:160:ALA:HB3   | 2:M:174:LEU:HB2  | 1.84                     | 0.59              |
| 2:M:605:LYS:HD3   | 2:M:610:ARG:HH12 | 1.68                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:653:PHE:CZ    | 3:N:749:VAL:HG11  | 2.38                     | 0.59              |
| 3:N:907:GLU:HG2   | 3:N:908:LYS:N     | 2.17                     | 0.59              |
| 5:G:2:DT:C2'      | 5:G:3:DC:C5       | 2.85                     | 0.59              |
| 6:H:9:C:H2'       | 6:H:10:G:C1'      | 2.33                     | 0.59              |
| 2:C:90:TYR:C      | 2:C:91:GLN:HG3    | 2.27                     | 0.59              |
| 2:C:408:ARG:HH21  | 2:C:455:LEU:HD12  | 1.67                     | 0.59              |
| 2:C:455:LEU:HD13  | 2:C:459:ALA:HB3   | 1.85                     | 0.59              |
| 2:C:752:GLY:HA3   | 3:D:679:ARG:HA    | 1.85                     | 0.59              |
| 3:D:23:TYR:O      | 3:D:49:ILE:HG23   | 2.02                     | 0.59              |
| 3:D:484:PRO:HB3   | 3:D:488:ARG:NE    | 2.18                     | 0.59              |
| 3:D:695:ILE:HD11  | 3:D:718:PRO:HB2   | 1.85                     | 0.59              |
| 2:M:143:SER:O     | 2:M:145:GLY:N     | 2.36                     | 0.59              |
| 2:M:753:ASP:HB2   | 2:M:792:VAL:CG2   | 2.32                     | 0.59              |
| 2:M:906:PHE:CG    | 3:N:1067:VAL:HG22 | 2.37                     | 0.59              |
| 2:M:1082:PRO:O    | 2:M:1085:PHE:HB3  | 2.02                     | 0.59              |
| 2:M:1089:VAL:O    | 2:M:1092:LEU:HB2  | 2.02                     | 0.59              |
| 3:N:750:PRO:HB3   | 3:N:755:ALA:O     | 2.03                     | 0.59              |
| 3:N:1370:ILE:O    | 3:N:1374:GLN:HG2  | 2.03                     | 0.59              |
| 7:Z:12:DT:H71     | 7:Z:12:DT:OP2     | 2.02                     | 0.59              |
| 1:A:87:VAL:HG21   | 1:A:144:VAL:CG1   | 2.33                     | 0.59              |
| 2:C:130:ASN:HD21  | 2:C:383:ARG:NH2   | 2.01                     | 0.59              |
| 3:D:564:GLU:HA    | 3:D:567:ILE:HD12  | 1.83                     | 0.59              |
| 3:D:1146:GLY:CA   | 3:D:1207:TYR:HB2  | 2.32                     | 0.59              |
| 3:D:1442:ASN:ND2  | 5:G:16:DT:OP1     | 2.35                     | 0.59              |
| 2:M:1048:THR:OG1  | 3:N:755:ALA:HB1   | 2.03                     | 0.59              |
| 3:N:112:ILE:HD11  | 3:N:116:LEU:HD12  | 1.83                     | 0.59              |
| 3:N:135:LEU:HD11  | 3:N:147:VAL:HG23  | 1.85                     | 0.59              |
| 3:N:785:ILE:CD1   | 3:N:939:PHE:CE2   | 2.86                     | 0.59              |
| 3:N:896:ALA:O     | 3:N:900:ILE:HG23  | 2.03                     | 0.59              |
| 1:A:179:PHE:HB2   | 1:A:195:LEU:HD11  | 1.85                     | 0.59              |
| 2:C:679:PHE:O     | 2:C:680:ASP:O     | 2.20                     | 0.59              |
| 2:C:1008:ARG:HG2  | 2:C:1008:ARG:HH11 | 1.66                     | 0.59              |
| 2:C:1093:GLN:O    | 3:D:21:TRP:HZ3    | 1.86                     | 0.59              |
| 3:D:1096:ARG:HH12 | 5:G:18:DC:P       | 2.25                     | 0.59              |
| 3:D:1106:VAL:HG12 | 3:D:1107:VAL:N    | 2.18                     | 0.59              |
| 2:M:304:LEU:CG    | 2:M:305:PRO:HD3   | 2.33                     | 0.59              |
| 2:M:340:MET:O     | 2:M:340:MET:SD    | 2.61                     | 0.59              |
| 2:M:504:GLU:HB2   | 2:M:507:ARG:HB3   | 1.85                     | 0.59              |
| 2:M:869:VAL:HG22  | 2:M:870:ILE:N     | 2.17                     | 0.59              |
| 2:M:889:HIS:CE1   | 2:M:988:VAL:CG2   | 2.81                     | 0.59              |
| 2:M:1092:LEU:HB3  | 2:M:1099:VAL:HG23 | 1.85                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:33:ASN:HB2    | 3:N:40:GLU:OE1    | 2.02                     | 0.59              |
| 3:N:133:ILE:HG12  | 3:N:456:MET:HE2   | 1.83                     | 0.59              |
| 3:N:683:ILE:HG22  | 3:N:684:LYS:N     | 2.17                     | 0.59              |
| 3:N:792:ILE:HD11  | 3:N:881:LEU:HB3   | 1.85                     | 0.59              |
| 3:N:1446:VAL:HG12 | 3:N:1447:LEU:HD12 | 1.85                     | 0.59              |
| 5:G:17:DA:OP1     | 5:G:17:DA:O4'     | 2.21                     | 0.59              |
| 2:C:2:GLU:O       | 2:C:3:ILE:HD13    | 2.03                     | 0.58              |
| 2:C:269:LEU:HD12  | 2:C:288:ARG:HG3   | 1.84                     | 0.58              |
| 2:C:346:VAL:O     | 2:C:350:ARG:HG3   | 2.03                     | 0.58              |
| 2:C:541:SER:OG    | 2:C:542:VAL:N     | 2.36                     | 0.58              |
| 2:C:647:GLN:O     | 2:C:649:VAL:HG13  | 2.04                     | 0.58              |
| 2:C:753:ASP:O     | 2:C:792:VAL:HG23  | 2.02                     | 0.58              |
| 3:D:19:ARG:HH11   | 3:D:19:ARG:HG3    | 1.67                     | 0.58              |
| 3:D:36:THR:C      | 3:D:38:LYS:H      | 2.09                     | 0.58              |
| 3:D:1256:LEU:O    | 3:D:1257:PRO:C    | 2.46                     | 0.58              |
| 3:D:1347:TYR:CE2  | 3:D:1351:GLU:HG2  | 2.38                     | 0.58              |
| 3:D:1468:LEU:HD22 | 3:D:1470:ARG:HG3  | 1.85                     | 0.58              |
| 3:D:1492:LEU:HD12 | 3:D:1493:LYS:HE3  | 1.85                     | 0.58              |
| 1:L:206:THR:HG23  | 1:L:208:LEU:H     | 1.67                     | 0.58              |
| 2:M:680:ASP:N     | 3:N:943:THR:HG22  | 2.18                     | 0.58              |
| 3:N:581:LEU:H     | 3:N:581:LEU:CD2   | 2.15                     | 0.58              |
| 3:N:583:ASP:OD1   | 3:N:586:ARG:HG2   | 2.03                     | 0.58              |
| 3:N:671:LYS:O     | 3:N:675:ARG:HG3   | 2.03                     | 0.58              |
| 6:H:6:C:C5        | 6:H:7:G:N7        | 2.71                     | 0.58              |
| 5:X:12:DA:C2      | 5:X:13:DA:C4      | 2.91                     | 0.58              |
| 2:C:263:ASP:C     | 2:C:264:PRO:O     | 2.46                     | 0.58              |
| 2:C:272:ALA:O     | 2:C:276:LYS:HE3   | 2.03                     | 0.58              |
| 2:C:290:LEU:HD23  | 2:C:290:LEU:H     | 1.67                     | 0.58              |
| 2:C:496:ILE:HD12  | 2:C:496:ILE:N     | 2.18                     | 0.58              |
| 2:C:555:ALA:O     | 2:C:558:ALA:HB3   | 2.03                     | 0.58              |
| 2:C:999:HIS:ND1   | 2:C:1003:ASP:HB2  | 2.18                     | 0.58              |
| 3:D:741:ASP:O     | 6:H:14:G:C5'      | 2.50                     | 0.58              |
| 3:D:1033:GLN:O    | 3:D:1037:GLN:CA   | 2.51                     | 0.58              |
| 3:D:1236:LEU:HD23 | 3:D:1236:LEU:O    | 2.03                     | 0.58              |
| 1:L:7:LYS:HZ1     | 1:L:186:LEU:HD13  | 1.68                     | 0.58              |
| 2:M:684:PHE:CZ    | 2:M:685:GLU:HB2   | 2.38                     | 0.58              |
| 3:N:139:GLY:O     | 3:N:147:VAL:HB    | 2.04                     | 0.58              |
| 1:A:89:PHE:C      | 1:A:90:LEU:HD12   | 2.29                     | 0.58              |
| 1:A:177:VAL:O     | 2:C:864:GLY:HA2   | 2.03                     | 0.58              |
| 2:C:682:TYR:O     | 2:C:850:ALA:HB3   | 2.02                     | 0.58              |
| 2:C:756:VAL:HB    | 2:C:790:LEU:HB3   | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1010:THR:HA   | 3:D:624:ASP:OD1   | 2.03                     | 0.58              |
| 2:C:1034:GLU:HB3  | 3:D:619:LEU:HB3   | 1.86                     | 0.58              |
| 2:C:1063:ARG:HG3  | 2:C:1064:ASN:N    | 2.17                     | 0.58              |
| 3:D:33:ASN:HB2    | 3:D:40:GLU:OE2    | 2.04                     | 0.58              |
| 3:D:473:LEU:HD12  | 3:D:473:LEU:N     | 2.19                     | 0.58              |
| 3:D:1198:TYR:OH   | 3:D:1432:LYS:NZ   | 2.36                     | 0.58              |
| 2:M:170:PRO:HG2   | 2:M:258:TYR:CE2   | 2.38                     | 0.58              |
| 2:M:405:ARG:C     | 2:M:407:LYS:N     | 2.60                     | 0.58              |
| 2:M:430:VAL:CG1   | 3:N:1075:HIS:HA   | 2.33                     | 0.58              |
| 2:M:510:ALA:HB3   | 2:M:513:VAL:CG2   | 2.32                     | 0.58              |
| 2:M:873:PRO:O     | 2:M:877:PRO:HD2   | 2.03                     | 0.58              |
| 2:M:1013:TYR:O    | 6:Y:4:G:O6        | 2.21                     | 0.58              |
| 2:M:1022:GLY:HA3  | 2:M:1026:GLN:O    | 2.03                     | 0.58              |
| 3:N:465:LEU:HD22  | 3:N:510:GLU:CA    | 2.32                     | 0.58              |
| 3:N:619:LEU:HD12  | 3:N:621:LYS:NZ    | 2.18                     | 0.58              |
| 3:N:686:GLU:HA    | 3:N:689:ASP:OD2   | 2.02                     | 0.58              |
| 3:N:701:LEU:C     | 3:N:702:LEU:HD12  | 2.29                     | 0.58              |
| 3:N:1114:THR:O    | 3:N:1114:THR:CG2  | 2.50                     | 0.58              |
| 2:C:345:ARG:HA    | 2:C:348:LEU:HB2   | 1.85                     | 0.58              |
| 2:C:431:HIS:CG    | 2:C:432:ARG:N     | 2.71                     | 0.58              |
| 2:C:1039:ALA:HA   | 3:D:1227:GLN:OE1  | 2.03                     | 0.58              |
| 2:C:1056:LYS:HE2  | 3:D:625:TYR:HB2   | 1.86                     | 0.58              |
| 3:D:917:GLN:HA    | 3:D:920:LEU:HD12  | 1.84                     | 0.58              |
| 3:D:1115:THR:HG22 | 3:D:1151:ARG:HH21 | 1.67                     | 0.58              |
| 3:D:1266:ARG:HH22 | 7:I:4:DG:H4'      | 1.68                     | 0.58              |
| 4:E:50:THR:HB     | 4:E:51:LEU:HD23   | 1.85                     | 0.58              |
| 2:M:762:LYS:HD3   | 2:M:784:ASP:O     | 2.03                     | 0.58              |
| 3:N:618:LEU:CD1   | 3:N:1467:ILE:HD11 | 2.32                     | 0.58              |
| 3:N:641:GLN:HB3   | 3:N:717:GLN:O     | 2.04                     | 0.58              |
| 3:N:1293:PHE:CD2  | 3:N:1300:SER:HB2  | 2.39                     | 0.58              |
| 3:N:1422:MET:CE   | 3:N:1427:SER:HA   | 2.34                     | 0.58              |
| 2:C:122:THR:HB    | 2:C:124:ASP:CG    | 2.29                     | 0.58              |
| 3:D:152:LEU:HD23  | 3:D:152:LEU:H     | 1.66                     | 0.58              |
| 1:K:223:THR:C     | 1:K:225:PHE:H     | 2.11                     | 0.58              |
| 2:M:108:ILE:HD11  | 2:M:365:ASP:OD1   | 2.03                     | 0.58              |
| 2:M:676:ILE:HG12  | 2:M:676:ILE:O     | 2.04                     | 0.58              |
| 2:M:679:PHE:O     | 2:M:680:ASP:C     | 2.46                     | 0.58              |
| 2:M:1021:LEU:HD22 | 6:Y:5:C:H2'       | 1.86                     | 0.58              |
| 2:M:1098:ASP:HB2  | 3:N:21:TRP:HZ2    | 1.68                     | 0.58              |
| 1:A:88:ARG:HG2    | 1:A:88:ARG:NH1    | 2.15                     | 0.58              |
| 2:C:151:ASP:OD2   | 2:C:175:GLU:OE2   | 2.22                     | 0.58              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:436:GLY:H     | 2:C:539:VAL:HG13 | 1.69                     | 0.58              |
| 2:C:944:LEU:O     | 2:C:948:GLU:HG3  | 2.03                     | 0.58              |
| 2:C:1090:LYS:HE2  | 2:C:1112:PHE:CE1 | 2.38                     | 0.58              |
| 3:D:619:LEU:HD12  | 3:D:621:LYS:NZ   | 2.18                     | 0.58              |
| 3:D:1190:SER:OG   | 3:D:1369:GLU:OE2 | 2.21                     | 0.58              |
| 3:D:1194:CYS:SG   | 3:D:1200:VAL:HA  | 2.44                     | 0.58              |
| 3:D:1465:ASN:ND2  | 3:D:1470:ARG:CB  | 2.66                     | 0.58              |
| 2:M:479:VAL:CG2   | 2:M:506:ASN:HA   | 2.33                     | 0.58              |
| 2:M:493:ARG:HB2   | 2:M:494:TYR:CE1  | 2.38                     | 0.58              |
| 2:M:570:PRO:HD2   | 2:M:635:THR:CG2  | 2.33                     | 0.58              |
| 2:M:752:GLY:H     | 2:M:792:VAL:HB   | 1.68                     | 0.58              |
| 2:M:791:ARG:HB3   | 2:M:791:ARG:HH11 | 1.68                     | 0.58              |
| 3:N:412:GLY:O     | 3:N:434:ARG:HD3  | 2.04                     | 0.58              |
| 3:N:662:GLU:O     | 3:N:664:LYS:O    | 2.21                     | 0.58              |
| 3:N:1109:GLU:CD   | 3:N:1202:GLN:N   | 2.61                     | 0.58              |
| 3:N:1389:LEU:CD1  | 3:N:1390:LEU:H   | 2.15                     | 0.58              |
| 3:N:1484:THR:HG23 | 4:O:76:GLY:C     | 2.29                     | 0.58              |
| 1:A:38:ASN:O      | 1:A:42:ARG:HG3   | 2.03                     | 0.58              |
| 1:B:101:LEU:HD12  | 1:B:113:ASP:C    | 2.27                     | 0.58              |
| 2:C:94:LEU:HD12   | 2:C:95:TYR:N     | 2.19                     | 0.58              |
| 2:C:423:ALA:HB2   | 7:I:1:DG:H5"     | 1.84                     | 0.58              |
| 2:C:695:LEU:HD21  | 2:C:832:LYS:HG2  | 1.85                     | 0.58              |
| 3:D:107:ASP:O     | 3:D:108:VAL:C    | 2.46                     | 0.58              |
| 3:D:486:ARG:HA    | 3:D:489:ARG:CG   | 2.32                     | 0.58              |
| 3:D:701:LEU:HD12  | 3:D:701:LEU:N    | 2.17                     | 0.58              |
| 3:D:1377:LYS:HE2  | 3:D:1378:TYR:CZ  | 2.39                     | 0.58              |
| 3:D:1440:PHE:O    | 3:D:1441:GLN:CB  | 2.52                     | 0.58              |
| 1:L:36:LEU:O      | 1:L:39:PRO:HD2   | 2.04                     | 0.58              |
| 2:M:18:LEU:HD12   | 2:M:18:LEU:H     | 1.68                     | 0.58              |
| 2:M:439:CYS:SG    | 2:M:541:SER:N    | 2.71                     | 0.58              |
| 4:O:54:LEU:HG     | 4:O:58:PRO:HG2   | 1.84                     | 0.58              |
| 2:C:211:LEU:CD1   | 2:C:308:ARG:HA   | 2.32                     | 0.58              |
| 2:C:422:ARG:O     | 7:I:1:DG:C4      | 2.57                     | 0.58              |
| 2:C:502:PRO:HB2   | 2:C:509:ALA:HB3  | 1.85                     | 0.58              |
| 2:C:1056:LYS:HB3  | 3:D:623:VAL:HG13 | 1.86                     | 0.58              |
| 3:D:41:ARG:HD3    | 3:D:43:GLY:N     | 2.19                     | 0.58              |
| 3:D:1213:ARG:NH1  | 4:E:11:GLY:HA2   | 2.18                     | 0.58              |
| 3:D:1371:VAL:O    | 3:D:1374:GLN:HB2 | 2.04                     | 0.58              |
| 3:D:1422:MET:HE2  | 3:D:1427:SER:HA  | 1.86                     | 0.58              |
| 1:L:153:ALA:HA    | 1:L:156:HIS:CE1  | 2.38                     | 0.58              |
| 2:M:88:LEU:O      | 2:M:129:ILE:O    | 2.20                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:493:ARG:NH2  | 2:M:494:TYR:OH    | 2.37                     | 0.58              |
| 2:M:1075:ASP:HB2 | 4:O:32:ARG:NH2    | 2.19                     | 0.58              |
| 3:N:412:GLY:HA2  | 3:N:434:ARG:NE    | 2.19                     | 0.58              |
| 3:N:489:ARG:NH2  | 3:N:1389:LEU:HD21 | 2.19                     | 0.58              |
| 3:N:696:HIS:CG   | 3:N:697:GLY:N     | 2.67                     | 0.58              |
| 3:N:1236:LEU:O   | 3:N:1237:THR:OG1  | 2.21                     | 0.58              |
| 3:N:1440:PHE:O   | 3:N:1441:GLN:HB3  | 2.04                     | 0.58              |
| 4:O:61:VAL:O     | 4:O:65:MET:HG3    | 2.03                     | 0.58              |
| 6:Y:5:C:O2       | 6:Y:5:C:C2'       | 2.48                     | 0.58              |
| 1:A:223:THR:C    | 1:A:225:PHE:H     | 2.11                     | 0.58              |
| 1:B:153:ALA:HA   | 1:B:156:HIS:CE1   | 2.38                     | 0.58              |
| 1:B:179:PHE:N    | 1:B:179:PHE:CD2   | 2.72                     | 0.58              |
| 2:C:185:LYS:HD3  | 2:C:190:LYS:NZ    | 2.18                     | 0.58              |
| 2:C:1022:GLY:HA3 | 2:C:1026:GLN:O    | 2.03                     | 0.58              |
| 3:D:493:ARG:HD2  | 3:D:493:ARG:C     | 2.29                     | 0.58              |
| 3:D:641:GLN:HA   | 3:D:717:GLN:H     | 1.68                     | 0.58              |
| 3:D:695:ILE:O    | 3:D:696:HIS:C     | 2.46                     | 0.58              |
| 3:D:1147:ARG:NH2 | 3:D:1369:GLU:OE2  | 2.36                     | 0.58              |
| 2:M:141:HIS:HD2  | 2:M:332:ARG:O     | 1.87                     | 0.58              |
| 2:M:1101:THR:HB  | 2:M:1109:VAL:HB   | 1.86                     | 0.58              |
| 3:N:1403:LEU:O   | 3:N:1407:LEU:HB2  | 2.03                     | 0.58              |
| 1:A:43:ILE:HG23  | 1:A:47:SER:CB     | 2.34                     | 0.58              |
| 2:C:54:ILE:HG12  | 2:C:64:LEU:HD23   | 1.86                     | 0.58              |
| 2:C:110:GLU:CG   | 2:C:369:PRO:HG3   | 2.33                     | 0.58              |
| 2:C:919:ALA:CA   | 2:C:968:LEU:HD21  | 2.34                     | 0.58              |
| 2:C:953:VAL:HG11 | 2:C:962:GLN:HB3   | 1.86                     | 0.58              |
| 3:D:918:ALA:HB1  | 3:D:927:THR:HG23  | 1.84                     | 0.58              |
| 3:D:1102:THR:O   | 3:D:1103:HIS:C    | 2.46                     | 0.58              |
| 3:D:1433:SER:HB2 | 3:D:1457:ASP:OD1  | 2.04                     | 0.58              |
| 1:K:106:PRO:HA   | 1:K:133:GLU:O     | 2.04                     | 0.58              |
| 1:L:25:LEU:O     | 1:L:25:LEU:HD23   | 2.04                     | 0.58              |
| 2:M:113:VAL:HG12 | 2:M:115:LEU:HD23  | 1.86                     | 0.58              |
| 2:M:139:GLN:CD   | 2:M:415:PRO:HD3   | 2.29                     | 0.58              |
| 2:M:677:MET:HB3  | 3:N:948:THR:CG2   | 2.33                     | 0.58              |
| 2:M:871:LEU:O    | 2:M:873:PRO:HD3   | 2.04                     | 0.58              |
| 2:M:872:ASN:OD1  | 2:M:874:LEU:HB2   | 2.03                     | 0.58              |
| 3:N:58:CYS:SG    | 3:N:62:LYS:N      | 2.77                     | 0.58              |
| 3:N:843:PHE:HB2  | 3:N:866:VAL:CG2   | 2.29                     | 0.58              |
| 3:N:1296:SER:C   | 3:N:1298:GLY:H    | 2.10                     | 0.58              |
| 6:H:9:C:C2'      | 6:H:10:G:O4'      | 2.47                     | 0.58              |
| 2:C:617:ASP:CG   | 2:C:619:ARG:HH21  | 2.12                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:688:ILE:HG22 | 2:C:689:VAL:N     | 2.19                     | 0.57              |
| 2:C:694:LEU:O    | 2:C:699:PHE:HB2   | 2.03                     | 0.57              |
| 2:C:896:PHE:O    | 2:C:924:VAL:HG11  | 2.03                     | 0.57              |
| 3:D:524:LEU:O    | 3:D:526:PRO:HD3   | 2.04                     | 0.57              |
| 3:D:774:SER:C    | 3:D:776:GLU:N     | 2.57                     | 0.57              |
| 3:D:1019:PRO:O   | 3:D:1023:MET:HB2  | 2.03                     | 0.57              |
| 3:D:1087:ARG:NE  | 3:D:1236:LEU:CD1  | 2.67                     | 0.57              |
| 4:E:28:GLN:C     | 4:E:32:ARG:HH12   | 2.12                     | 0.57              |
| 2:M:101:ILE:HD12 | 2:M:107:LEU:HD22  | 1.84                     | 0.57              |
| 2:M:189:ARG:HD3  | 2:M:190:LYS:N     | 2.18                     | 0.57              |
| 2:M:581:THR:C    | 2:M:902:ILE:HG23  | 2.29                     | 0.57              |
| 2:M:713:ARG:HB3  | 2:M:720:GLU:OE2   | 2.03                     | 0.57              |
| 2:M:984:GLU:HG2  | 3:N:944:THR:O     | 2.04                     | 0.57              |
| 3:N:659:LYS:O    | 3:N:663:GLU:HG2   | 2.04                     | 0.57              |
| 3:N:695:ILE:O    | 3:N:698:LYS:N     | 2.37                     | 0.57              |
| 3:N:918:ALA:CB   | 3:N:927:THR:HG23  | 2.33                     | 0.57              |
| 1:A:86:VAL:HG23  | 1:A:204:SER:HB2   | 1.87                     | 0.57              |
| 2:C:18:LEU:HD13  | 2:C:590:ASP:CG    | 2.29                     | 0.57              |
| 2:C:136:ILE:HD13 | 2:C:392:SER:OG    | 2.03                     | 0.57              |
| 2:C:498:GLN:HE22 | 3:D:1067:VAL:HG11 | 1.69                     | 0.57              |
| 2:C:976:ASP:OD1  | 2:C:978:ARG:HB2   | 2.04                     | 0.57              |
| 2:C:1067:TYR:O   | 2:C:1071:ILE:HG12 | 2.03                     | 0.57              |
| 3:D:6:ARG:C      | 3:D:7:LYS:HG3     | 2.29                     | 0.57              |
| 3:D:47:GLU:HB3   | 3:D:51:GLY:O      | 2.05                     | 0.57              |
| 3:D:526:PRO:HD2  | 3:D:538:SER:HB2   | 1.85                     | 0.57              |
| 2:M:251:ASP:C    | 2:M:252:LYS:HG3   | 2.28                     | 0.57              |
| 2:M:706:GLU:CG   | 2:M:708:TYR:CZ    | 2.82                     | 0.57              |
| 2:M:971:LYS:HG2  | 2:M:988:VAL:HG12  | 1.86                     | 0.57              |
| 2:M:1031:ARG:HG2 | 5:X:21:DG:H5"     | 1.85                     | 0.57              |
| 3:N:136:ASP:CG   | 3:N:137:PRO:HD3   | 2.29                     | 0.57              |
| 3:N:453:ASP:HB3  | 3:N:455:ARG:NH2   | 2.08                     | 0.57              |
| 3:N:646:LYS:HZ1  | 3:N:688:TRP:NE1   | 2.02                     | 0.57              |
| 3:N:807:ALA:HA   | 3:N:833:GLU:HG3   | 1.86                     | 0.57              |
| 3:N:814:ALA:CB   | 3:N:818:ARG:HH21  | 2.00                     | 0.57              |
| 3:N:860:LEU:O    | 3:N:877:PRO:HD2   | 2.04                     | 0.57              |
| 1:A:42:ARG:NH2   | 1:B:34:VAL:HB     | 2.19                     | 0.57              |
| 2:C:799:ILE:O    | 2:C:827:VAL:HG13  | 2.04                     | 0.57              |
| 2:C:1003:ASP:O   | 3:D:724:GLN:NE2   | 2.37                     | 0.57              |
| 2:C:1046:ALA:CA  | 3:D:1472:ILE:HD11 | 2.34                     | 0.57              |
| 2:C:1095:LEU:CD2 | 3:D:603:LEU:HD13  | 2.34                     | 0.57              |
| 3:D:45:PHE:CD1   | 3:D:522:PRO:HB3   | 2.39                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1093:TYR:OH   | 3:D:1440:PHE:CE2  | 2.56                     | 0.57              |
| 1:L:34:VAL:HG22   | 1:L:181:VAL:HG21  | 1.85                     | 0.57              |
| 2:M:302:VAL:O     | 2:M:305:PRO:HD2   | 2.04                     | 0.57              |
| 2:M:328:LEU:CD1   | 2:M:433:THR:HB    | 2.28                     | 0.57              |
| 2:M:384:GLU:HA    | 2:M:388:ARG:HD3   | 1.86                     | 0.57              |
| 2:M:1083:GLU:O    | 2:M:1087:VAL:HG12 | 2.04                     | 0.57              |
| 3:N:850:LEU:H     | 3:N:850:LEU:HD12  | 1.69                     | 0.57              |
| 1:B:115:LEU:HD12  | 1:B:115:LEU:O     | 2.04                     | 0.57              |
| 2:C:9:ILE:HD12    | 2:C:9:ILE:O       | 2.05                     | 0.57              |
| 2:C:12:VAL:CB     | 2:C:472:ARG:HH11  | 2.15                     | 0.57              |
| 2:C:143:SER:O     | 2:C:145:GLY:N     | 2.38                     | 0.57              |
| 2:C:405:ARG:C     | 2:C:407:LYS:N     | 2.59                     | 0.57              |
| 2:C:460:ARG:NH2   | 2:C:468:ARG:HH11  | 2.02                     | 0.57              |
| 2:C:487:THR:CG2   | 2:C:489:THR:HG23  | 2.35                     | 0.57              |
| 2:C:683:ASN:HA    | 2:C:687:ALA:O     | 2.03                     | 0.57              |
| 3:D:85:VAL:HB     | 3:D:89:ARG:NH1    | 2.19                     | 0.57              |
| 3:D:87:ARG:HB2    | 3:D:524:LEU:CD1   | 2.35                     | 0.57              |
| 3:D:549:ASN:HB2   | 3:D:550:ARG:HH21  | 1.69                     | 0.57              |
| 3:D:575:GLN:O     | 3:D:578:VAL:HB    | 2.05                     | 0.57              |
| 3:D:1424:VAL:HG13 | 3:D:1425:THR:N    | 2.20                     | 0.57              |
| 4:E:34:GLY:CA     | 4:E:95:VAL:HB     | 2.34                     | 0.57              |
| 2:M:816:LYS:HB2   | 2:M:819:VAL:HG21  | 1.86                     | 0.57              |
| 3:N:6:ARG:O       | 3:N:7:LYS:HG3     | 2.05                     | 0.57              |
| 3:N:107:ASP:CG    | 3:N:109:PRO:HD2   | 2.28                     | 0.57              |
| 3:N:117:ASP:CG    | 3:N:117:ASP:O     | 2.48                     | 0.57              |
| 3:N:417:PRO:HD2   | 3:N:432:TYR:CZ    | 2.40                     | 0.57              |
| 3:N:443:VAL:HG13  | 3:N:445:ARG:NH2   | 2.20                     | 0.57              |
| 3:N:1381:VAL:CG1  | 3:N:1382:THR:N    | 2.67                     | 0.57              |
| 6:H:6:C:O5'       | 6:H:6:C:H6        | 1.87                     | 0.57              |
| 6:H:7:G:H2'       | 6:H:8:G:O4'       | 2.04                     | 0.57              |
| 1:A:153:ALA:HA    | 1:A:156:HIS:CE1   | 2.39                     | 0.57              |
| 2:C:1092:LEU:HB3  | 2:C:1099:VAL:HG23 | 1.87                     | 0.57              |
| 3:D:785:ILE:HG22  | 3:D:789:LEU:HD11  | 1.87                     | 0.57              |
| 3:D:919:PHE:HZ    | 3:D:1211:MET:HG3  | 1.67                     | 0.57              |
| 1:K:67:THR:HG21   | 2:M:609:ASN:OD1   | 2.04                     | 0.57              |
| 2:M:137:VAL:O     | 2:M:391:LEU:HD21  | 2.04                     | 0.57              |
| 2:M:203:ASP:O     | 2:M:207:LEU:HB2   | 2.04                     | 0.57              |
| 2:M:584:GLU:HB3   | 2:M:666:LEU:HB3   | 1.86                     | 0.57              |
| 3:N:36:THR:C      | 3:N:38:LYS:N      | 2.58                     | 0.57              |
| 3:N:134:VAL:HG12  | 3:N:152:LEU:CB    | 2.34                     | 0.57              |
| 3:N:1389:LEU:CG   | 3:N:1390:LEU:N    | 2.66                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:171:PHE:O     | 1:A:173:PRO:HD3   | 2.04                     | 0.57              |
| 2:C:676:ILE:HG23  | 2:C:676:ILE:O     | 2.05                     | 0.57              |
| 2:C:1103:ASP:CG   | 2:C:1104:GLU:N    | 2.63                     | 0.57              |
| 3:D:644:LEU:HD12  | 3:D:645:PRO:N     | 2.19                     | 0.57              |
| 3:D:649:ALA:HA    | 3:D:652:LEU:HD22  | 1.87                     | 0.57              |
| 3:D:704:ARG:HG2   | 3:D:736:PHE:HB3   | 1.85                     | 0.57              |
| 2:M:1091:GLU:OE1  | 3:N:613:ARG:HG2   | 2.05                     | 0.57              |
| 3:N:927:THR:O     | 3:N:930:LEU:HB3   | 2.04                     | 0.57              |
| 3:N:1176:LYS:HA   | 3:N:1179:GLU:OE1  | 2.05                     | 0.57              |
| 3:N:1239:ARG:HG3  | 3:N:1240:THR:N    | 2.19                     | 0.57              |
| 3:N:1380:GLU:O    | 3:N:1417:TRP:HB2  | 2.04                     | 0.57              |
| 5:G:28:DG:OP2     | 5:G:28:DG:C8      | 2.54                     | 0.57              |
| 2:C:183:SER:CB    | 2:C:190:LYS:HG2   | 2.35                     | 0.57              |
| 2:C:462:ASP:HB3   | 2:C:468:ARG:NE    | 2.20                     | 0.57              |
| 2:C:676:ILE:O     | 2:C:676:ILE:HG12  | 2.03                     | 0.57              |
| 2:C:1031:ARG:HE   | 3:D:621:LYS:HD2   | 1.70                     | 0.57              |
| 2:C:1046:ALA:HB2  | 3:D:1476:THR:H    | 1.68                     | 0.57              |
| 3:D:638:LYS:HZ3   | 3:D:932:ASP:HB3   | 1.69                     | 0.57              |
| 3:D:936:TYR:O     | 3:D:939:PHE:HB2   | 2.03                     | 0.57              |
| 3:D:1207:TYR:O    | 3:D:1215:VAL:HG23 | 2.03                     | 0.57              |
| 4:E:30:LEU:O      | 4:E:35:PHE:HA     | 2.04                     | 0.57              |
| 2:M:221:LEU:HG    | 2:M:222:MET:HG3   | 1.86                     | 0.57              |
| 2:M:431:HIS:CD2   | 2:M:433:THR:HG1   | 2.21                     | 0.57              |
| 2:M:839:LEU:HD23  | 2:M:996:LYS:HA    | 1.86                     | 0.57              |
| 2:M:1115:LEU:HD22 | 3:N:88:TYR:HD1    | 1.70                     | 0.57              |
| 3:N:456:MET:CA    | 3:N:460:ALA:HB2   | 2.30                     | 0.57              |
| 3:N:792:ILE:HG12  | 3:N:878:GLY:HA3   | 1.85                     | 0.57              |
| 3:N:1106:VAL:HG11 | 3:N:1474:ALA:HB1  | 1.87                     | 0.57              |
| 5:X:13:DA:H2'     | 5:X:13:DA:O5'     | 2.04                     | 0.57              |
| 5:X:17:DA:H2''    | 5:X:18:DC:OP2     | 2.03                     | 0.57              |
| 1:B:89:PHE:HB3    | 1:B:94:LEU:HD12   | 1.86                     | 0.57              |
| 1:B:221:HIS:HA    | 1:B:224:TYR:HD2   | 1.66                     | 0.57              |
| 2:C:226:VAL:HG13  | 2:C:227:PHE:CD1   | 2.39                     | 0.57              |
| 2:C:301:GLU:O     | 2:C:305:PRO:HG2   | 2.04                     | 0.57              |
| 2:C:367:LEU:HB3   | 2:C:371:LYS:CE    | 2.35                     | 0.57              |
| 2:C:1042:ALA:HB3  | 3:D:710:ARG:CB    | 2.35                     | 0.57              |
| 2:C:1056:LYS:HD3  | 3:D:623:VAL:HG13  | 1.86                     | 0.57              |
| 3:D:22:SER:OG     | 3:D:92:HIS:ND1    | 2.37                     | 0.57              |
| 3:D:1192:LEU:HD23 | 3:D:1373:ARG:HB2  | 1.86                     | 0.57              |
| 3:D:1205:TYR:HE2  | 3:D:1215:VAL:HG21 | 1.67                     | 0.57              |
| 1:L:73:GLU:HG3    | 1:L:130:ALA:CB    | 2.35                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:174:LEU:HD22  | 2:M:193:LEU:HD21  | 1.87                     | 0.57              |
| 2:M:367:LEU:O     | 2:M:372:LEU:HD13  | 2.05                     | 0.57              |
| 3:N:109:PRO:HG2   | 3:N:1445:HIS:CE1  | 2.40                     | 0.57              |
| 3:N:159:ARG:HG2   | 3:N:163:TYR:CE2   | 2.40                     | 0.57              |
| 3:N:628:ARG:HG3   | 3:N:628:ARG:NH1   | 2.18                     | 0.57              |
| 3:N:767:HIS:HA    | 3:N:924:MET:SD    | 2.45                     | 0.57              |
| 3:N:899:LEU:HD22  | 3:N:917:GLN:CG    | 2.34                     | 0.57              |
| 3:N:1147:ARG:HH22 | 3:N:1369:GLU:CD   | 2.13                     | 0.57              |
| 3:N:1274:ILE:HG21 | 3:N:1301:LYS:HZ2  | 1.70                     | 0.57              |
| 5:G:22:DA:H2'     | 5:G:23:DG:C8      | 2.39                     | 0.57              |
| 1:A:107:LYS:O     | 1:A:132:LEU:HB2   | 2.05                     | 0.57              |
| 1:A:180:GLN:CD    | 2:C:937:ASP:HB2   | 2.29                     | 0.57              |
| 2:C:88:LEU:CD1    | 2:C:89:THR:H      | 2.17                     | 0.57              |
| 2:C:184:MET:HE2   | 2:C:186:VAL:HG13  | 1.87                     | 0.57              |
| 3:D:524:LEU:CD1   | 3:D:524:LEU:H     | 2.17                     | 0.57              |
| 3:D:1209:LEU:HD21 | 4:E:16:LYS:CE     | 2.34                     | 0.57              |
| 3:D:1236:LEU:O    | 3:D:1237:THR:O    | 2.22                     | 0.57              |
| 2:M:285:LEU:HD23  | 2:M:285:LEU:O     | 2.03                     | 0.57              |
| 2:M:397:GLU:C     | 2:M:633:GLN:HG2   | 2.30                     | 0.57              |
| 2:M:452:ILE:HD12  | 2:M:452:ILE:N     | 2.19                     | 0.57              |
| 2:M:643:VAL:HG13  | 2:M:647:GLN:OE1   | 2.05                     | 0.57              |
| 2:M:843:HIS:HE1   | 2:M:887:GLU:OE2   | 1.88                     | 0.57              |
| 2:M:1094:ALA:CB   | 3:N:90:MET:HE1    | 2.35                     | 0.57              |
| 2:M:1105:LYS:NZ   | 2:M:1107:ASN:HB2  | 2.20                     | 0.57              |
| 3:N:87:ARG:HB2    | 3:N:524:LEU:CD1   | 2.34                     | 0.57              |
| 3:N:183:GLU:HG2   | 3:N:184:GLU:H     | 1.66                     | 0.57              |
| 3:N:563:PRO:CG    | 3:N:566:ILE:HD12  | 2.35                     | 0.57              |
| 3:N:1017:PHE:HA   | 3:N:1022:VAL:HG21 | 1.85                     | 0.57              |
| 3:N:1396:GLU:O    | 3:N:1400:VAL:HG23 | 2.05                     | 0.57              |
| 1:B:41:ARG:HG3    | 1:B:177:VAL:HG21  | 1.87                     | 0.57              |
| 2:C:274:ARG:HG3   | 2:C:285:LEU:HD22  | 1.86                     | 0.57              |
| 2:C:304:LEU:HG    | 2:C:305:PRO:CD    | 2.33                     | 0.57              |
| 2:C:409:ARG:NH2   | 6:H:11:C:H5''     | 2.20                     | 0.57              |
| 3:D:477:LEU:HD22  | 3:D:492:ALA:HB1   | 1.86                     | 0.57              |
| 3:D:1206:GLY:HA3  | 3:D:1366:LYS:HZ1  | 1.70                     | 0.57              |
| 3:D:1403:LEU:O    | 3:D:1407:LEU:HB2  | 2.05                     | 0.57              |
| 2:M:41:ASN:HB2    | 2:M:45:GLN:CG     | 2.35                     | 0.57              |
| 2:M:312:ALA:CB    | 2:M:318:PRO:HG2   | 2.32                     | 0.57              |
| 3:N:52:PRO:HG2    | 3:N:85:VAL:HG23   | 1.87                     | 0.57              |
| 3:N:199:LEU:HD23  | 3:N:200:ASP:H     | 1.70                     | 0.57              |
| 3:N:1102:THR:O    | 3:N:1103:HIS:C    | 2.46                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:O:57:ASP:H      | 4:O:58:PRO:HD3    | 1.69                     | 0.57              |
| 7:Z:1:DG:P        | 7:Z:1:DG:C3'      | 2.92                     | 0.57              |
| 2:C:50:GLU:CA     | 2:C:266:ARG:NH1   | 2.68                     | 0.56              |
| 2:C:489:THR:OG1   | 2:C:490:GLU:N     | 2.37                     | 0.56              |
| 2:C:584:GLU:HB3   | 2:C:666:LEU:HB3   | 1.87                     | 0.56              |
| 2:C:957:LYS:HD3   | 2:C:961:GLU:HB3   | 1.85                     | 0.56              |
| 2:C:1081:VAL:CB   | 2:C:1086:ARG:HE   | 2.15                     | 0.56              |
| 3:D:45:PHE:HD1    | 3:D:522:PRO:HB3   | 1.69                     | 0.56              |
| 3:D:505:SER:OG    | 3:D:1453:ALA:HA   | 2.05                     | 0.56              |
| 3:D:883:ALA:O     | 3:D:886:VAL:HB    | 2.05                     | 0.56              |
| 3:D:1044:LEU:O    | 3:D:1044:LEU:HD23 | 2.05                     | 0.56              |
| 3:D:1135:ARG:HD2  | 3:D:1140:ILE:HG13 | 1.86                     | 0.56              |
| 1:K:197:LEU:HD23  | 1:K:197:LEU:N     | 2.18                     | 0.56              |
| 3:N:143:ASN:CG    | 3:N:145:VAL:H     | 2.12                     | 0.56              |
| 3:N:574:LEU:O     | 3:N:578:VAL:HG23  | 2.04                     | 0.56              |
| 3:N:625:TYR:CE2   | 3:N:655:PRO:HG2   | 2.39                     | 0.56              |
| 3:N:700:VAL:HG22  | 3:N:718:PRO:HG3   | 1.87                     | 0.56              |
| 3:N:701:LEU:H     | 3:N:701:LEU:CD1   | 2.12                     | 0.56              |
| 3:N:752:SER:HB3   | 3:N:755:ALA:CB    | 2.35                     | 0.56              |
| 3:N:843:PHE:HD2   | 3:N:848:GLU:HB3   | 1.70                     | 0.56              |
| 3:N:947:ILE:O     | 3:N:947:ILE:HD12  | 2.04                     | 0.56              |
| 3:N:1326:THR:C    | 3:N:1327:ARG:HG3  | 2.29                     | 0.56              |
| 7:I:11:DG:H2''    | 7:I:12:DT:C6      | 2.40                     | 0.56              |
| 1:A:65:PHE:CD1    | 1:A:65:PHE:N      | 2.73                     | 0.56              |
| 2:C:44:ILE:O      | 2:C:48:PHE:CG     | 2.57                     | 0.56              |
| 2:C:48:PHE:HB3    | 2:C:52:PHE:CD2    | 2.40                     | 0.56              |
| 2:C:350:ARG:O     | 2:C:353:ARG:HB3   | 2.05                     | 0.56              |
| 2:C:757:GLY:HA2   | 2:C:789:SER:CB    | 2.35                     | 0.56              |
| 2:C:861:LEU:HG    | 2:C:862:PRO:CD    | 2.31                     | 0.56              |
| 2:C:966:LEU:CD2   | 2:C:986:PRO:HG2   | 2.35                     | 0.56              |
| 3:D:9:ARG:HA      | 3:D:1434:TRP:CH2  | 2.40                     | 0.56              |
| 3:D:576:GLU:C     | 3:D:576:GLU:CD    | 2.72                     | 0.56              |
| 3:D:983:LEU:HD12  | 3:D:988:ARG:HB2   | 1.86                     | 0.56              |
| 3:D:1041:LEU:HD12 | 3:D:1042:ARG:NH2  | 2.20                     | 0.56              |
| 3:D:1066:THR:HG22 | 3:D:1069:GLU:CG   | 2.35                     | 0.56              |
| 3:D:1108:ARG:HD3  | 3:D:1108:ARG:N    | 2.20                     | 0.56              |
| 3:D:1205:TYR:CD2  | 3:D:1215:VAL:HG21 | 2.40                     | 0.56              |
| 1:K:107:LYS:O     | 1:K:132:LEU:HB2   | 2.05                     | 0.56              |
| 1:K:111:ALA:HB3   | 1:K:124:ASN:O     | 2.05                     | 0.56              |
| 1:K:176:ARG:HG3   | 1:K:200:TRP:CE3   | 2.39                     | 0.56              |
| 2:M:148:PHE:HE1   | 2:M:309:TYR:HD2   | 1.53                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:495:ARG:O    | 3:N:499:VAL:HG23  | 2.04                     | 0.56              |
| 3:N:666:ILE:HG23 | 3:N:684:LYS:NZ    | 2.19                     | 0.56              |
| 3:N:1146:GLY:CA  | 3:N:1207:TYR:HB2  | 2.35                     | 0.56              |
| 5:G:3:DC:O5'     | 5:G:3:DC:H6       | 1.88                     | 0.56              |
| 1:A:38:ASN:HB3   | 1:A:39:PRO:HD3    | 1.86                     | 0.56              |
| 1:A:222:LEU:HD22 | 1:B:219:ARG:HG3   | 1.86                     | 0.56              |
| 1:B:83:LYS:HD3   | 1:B:168:ASP:O     | 2.06                     | 0.56              |
| 2:C:26:TYR:O     | 2:C:30:LEU:HG     | 2.06                     | 0.56              |
| 2:C:44:ILE:HG23  | 2:C:344:PHE:CE1   | 2.40                     | 0.56              |
| 2:C:52:PHE:HZ    | 2:C:68:PHE:CB     | 2.00                     | 0.56              |
| 2:C:218:VAL:HG13 | 2:C:221:LEU:CD2   | 2.36                     | 0.56              |
| 2:C:939:ARG:HE   | 2:C:939:ARG:CA    | 2.16                     | 0.56              |
| 3:D:30:GLU:HB3   | 3:D:40:GLU:HB3    | 1.87                     | 0.56              |
| 3:D:54:LYS:O     | 3:D:55:ASP:C      | 2.48                     | 0.56              |
| 3:D:72:VAL:CG2   | 3:D:77:GLY:HA2    | 2.35                     | 0.56              |
| 3:D:95:LEU:CD2   | 3:D:96:ALA:N      | 2.68                     | 0.56              |
| 3:D:897:TRP:CA   | 3:D:900:ILE:HG13  | 2.24                     | 0.56              |
| 3:D:1111:ASP:CG  | 3:D:1203:LYS:HD2  | 2.31                     | 0.56              |
| 3:D:1330:ILE:CD1 | 3:D:1347:TYR:OH   | 2.50                     | 0.56              |
| 3:D:1379:VAL:CG1 | 3:D:1419:PRO:HA   | 2.33                     | 0.56              |
| 3:D:1435:LEU:CD2 | 3:D:1459:LEU:HD11 | 2.35                     | 0.56              |
| 4:E:25:LYS:HA    | 4:E:28:GLN:OE1    | 2.04                     | 0.56              |
| 4:E:34:GLY:HA3   | 4:E:95:VAL:HB     | 1.86                     | 0.56              |
| 1:K:123:MET:C    | 1:K:125:PRO:HD3   | 2.30                     | 0.56              |
| 1:K:132:LEU:HD23 | 1:K:136:GLY:O     | 2.04                     | 0.56              |
| 1:L:47:SER:OG    | 1:L:217:ILE:HG12  | 2.05                     | 0.56              |
| 2:M:343:GLN:HG2  | 2:M:385:PHE:CG    | 2.40                     | 0.56              |
| 2:M:396:ASP:CG   | 2:M:396:ASP:O     | 2.48                     | 0.56              |
| 2:M:627:ARG:O    | 2:M:638:ASP:HB3   | 2.05                     | 0.56              |
| 2:M:753:ASP:O    | 2:M:792:VAL:N     | 2.33                     | 0.56              |
| 2:M:1000:MET:O   | 2:M:1003:ASP:HB3  | 2.05                     | 0.56              |
| 2:M:1035:MET:HA  | 2:M:1038:TRP:CE3  | 2.40                     | 0.56              |
| 3:N:119:SER:HB2  | 3:N:123:LEU:HB2   | 1.88                     | 0.56              |
| 3:N:600:LEU:H    | 3:N:600:LEU:CD1   | 2.09                     | 0.56              |
| 3:N:613:ARG:NE   | 3:N:613:ARG:HA    | 2.20                     | 0.56              |
| 3:N:752:SER:O    | 3:N:756:GLN:N     | 2.37                     | 0.56              |
| 3:N:764:LEU:HD23 | 3:N:767:HIS:HE1   | 1.66                     | 0.56              |
| 3:N:804:LEU:HD23 | 3:N:804:LEU:N     | 2.20                     | 0.56              |
| 3:N:834:THR:HG22 | 3:N:838:ARG:NH1   | 2.18                     | 0.56              |
| 3:N:1023:MET:O   | 3:N:1028:ALA:CB   | 2.53                     | 0.56              |
| 3:N:1124:GLN:OE1 | 3:N:1135:ARG:HG2  | 2.06                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:I:1:DG:H2''     | 7:I:2:DT:OP2     | 2.05                     | 0.56              |
| 6:Y:8:G:C8        | 6:Y:8:G:H3'      | 2.41                     | 0.56              |
| 7:Z:7:DT:H2''     | 7:Z:8:DG:C8      | 2.40                     | 0.56              |
| 1:A:88:ARG:CD     | 1:A:204:SER:O    | 2.53                     | 0.56              |
| 1:A:222:LEU:CD2   | 1:B:219:ARG:HG3  | 2.34                     | 0.56              |
| 3:D:32:ILE:HG23   | 3:D:38:LYS:O     | 2.06                     | 0.56              |
| 3:D:133:ILE:HA    | 3:D:456:MET:HB2  | 1.86                     | 0.56              |
| 3:D:133:ILE:HG22  | 3:D:134:VAL:N    | 2.20                     | 0.56              |
| 3:D:455:ARG:HB3   | 3:D:459:GLU:HG2  | 1.88                     | 0.56              |
| 3:D:640:HIS:HE2   | 3:D:717:GLN:CD   | 2.13                     | 0.56              |
| 3:D:1044:LEU:O    | 3:D:1045:MET:O   | 2.23                     | 0.56              |
| 3:D:1461:GLY:O    | 3:D:1473:PRO:HG2 | 2.04                     | 0.56              |
| 4:E:45:ARG:HD3    | 4:E:55:PHE:CD2   | 2.41                     | 0.56              |
| 2:M:36:PRO:CG     | 2:M:70:GLU:HB3   | 2.30                     | 0.56              |
| 2:M:181:VAL:HG12  | 2:M:182:VAL:N    | 2.21                     | 0.56              |
| 2:M:420:ARG:HD2   | 7:Z:1:DG:H5'     | 1.87                     | 0.56              |
| 2:M:578:VAL:HG13  | 2:M:671:ASN:CG   | 2.31                     | 0.56              |
| 2:M:848:VAL:HG23  | 3:N:740:PHE:O    | 2.04                     | 0.56              |
| 3:N:72:VAL:HG23   | 3:N:78:VAL:H     | 1.70                     | 0.56              |
| 3:N:154:THR:HG21  | 3:N:157:GLU:OE2  | 2.06                     | 0.56              |
| 3:N:1192:LEU:HD13 | 3:N:1345:GLU:HG2 | 1.86                     | 0.56              |
| 3:N:1274:ILE:CG2  | 3:N:1301:LYS:HZ2 | 2.19                     | 0.56              |
| 4:O:26:ARG:CZ     | 4:O:73:LEU:HD21  | 2.36                     | 0.56              |
| 2:C:184:MET:O     | 2:C:190:LYS:HA   | 2.05                     | 0.56              |
| 2:C:195:LEU:CD2   | 2:C:238:LEU:HG   | 2.36                     | 0.56              |
| 2:C:265:ARG:HB3   | 2:C:267:TYR:CG   | 2.39                     | 0.56              |
| 2:C:356:ARG:NH1   | 2:C:356:ARG:HB2  | 2.20                     | 0.56              |
| 2:C:395:LYS:NZ    | 2:C:407:LYS:HZ3  | 1.99                     | 0.56              |
| 3:D:1237:THR:HB   | 3:D:1359:GLN:CD  | 2.31                     | 0.56              |
| 1:K:112:ARG:HG2   | 1:K:112:ARG:NH1  | 2.19                     | 0.56              |
| 2:M:393:GLN:HE21  | 6:Y:10:G:C4'     | 2.18                     | 0.56              |
| 2:M:681:GLY:HA3   | 3:N:939:PHE:CE1  | 2.40                     | 0.56              |
| 2:M:706:GLU:HG2   | 2:M:708:TYR:CE2  | 2.38                     | 0.56              |
| 2:M:1016:ILE:H    | 2:M:1016:ILE:CD1 | 2.09                     | 0.56              |
| 2:M:1090:LYS:HA   | 2:M:1093:GLN:HB2 | 1.87                     | 0.56              |
| 3:N:116:LEU:HD22  | 3:N:118:LEU:HD21 | 1.87                     | 0.56              |
| 3:N:584:ASN:CG    | 3:N:590:PRO:HD2  | 2.30                     | 0.56              |
| 3:N:1016:PRO:HA   | 3:N:1021:TYR:CE1 | 2.36                     | 0.56              |
| 5:G:2:DT:H2''     | 5:G:3:DC:C6      | 2.41                     | 0.56              |
| 5:G:6:DT:C2'      | 5:G:7:DA:OP2     | 2.41                     | 0.56              |
| 7:Z:14:DG:H2''    | 7:Z:15:DT:OP2    | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:48:ILE:CD1    | 1:A:174:VAL:HG21  | 2.36                     | 0.56              |
| 1:A:106:PRO:HG3   | 1:A:134:GLU:OE1   | 2.04                     | 0.56              |
| 1:B:32:PHE:O      | 1:B:36:LEU:HG     | 2.04                     | 0.56              |
| 2:C:6:PHE:O       | 2:C:8:ARG:HD2     | 2.05                     | 0.56              |
| 2:C:84:ARG:HA     | 2:C:131:GLY:HA2   | 1.87                     | 0.56              |
| 2:C:135:VAL:O     | 2:C:392:SER:HA    | 2.06                     | 0.56              |
| 2:C:144:PRO:HA    | 2:C:163:ILE:O     | 2.05                     | 0.56              |
| 2:C:627:ARG:HG3   | 2:C:628:PHE:H     | 1.70                     | 0.56              |
| 2:C:878:SER:CB    | 3:D:1029:ARG:NH1  | 2.68                     | 0.56              |
| 3:D:9:ARG:HH11    | 3:D:1454:GLY:CA   | 2.19                     | 0.56              |
| 3:D:658:LEU:HA    | 3:D:661:MET:HG3   | 1.87                     | 0.56              |
| 3:D:1088:THR:HG23 | 3:D:1234:THR:HG21 | 1.88                     | 0.56              |
| 3:D:1135:ARG:HB3  | 3:D:1140:ILE:HD11 | 1.86                     | 0.56              |
| 3:D:1382:THR:OG1  | 3:D:1418:LYS:HE3  | 2.06                     | 0.56              |
| 2:M:328:LEU:HD22  | 2:M:433:THR:CG2   | 2.30                     | 0.56              |
| 2:M:1051:GLU:OE2  | 3:N:755:ALA:HB3   | 2.05                     | 0.56              |
| 2:M:1103:ASP:CG   | 2:M:1104:GLU:H    | 2.13                     | 0.56              |
| 3:N:443:VAL:HG13  | 3:N:445:ARG:HH22  | 1.70                     | 0.56              |
| 6:H:5:C:C6        | 6:H:5:C:C3'       | 2.88                     | 0.56              |
| 7:I:5:DC:C2'      | 7:I:6:DT:OP2      | 2.41                     | 0.56              |
| 2:C:79:PRO:HG2    | 2:C:82:GLU:CG     | 2.35                     | 0.56              |
| 2:C:399:ASN:O     | 2:C:402:SER:N     | 2.39                     | 0.56              |
| 3:D:752:SER:O     | 3:D:756:GLN:N     | 2.38                     | 0.56              |
| 3:D:1106:VAL:O    | 3:D:1108:ARG:HD3  | 2.06                     | 0.56              |
| 3:D:1223:ILE:N    | 3:D:1223:ILE:CD1  | 2.69                     | 0.56              |
| 4:E:28:GLN:CB     | 4:E:32:ARG:HH12   | 2.18                     | 0.56              |
| 1:L:102:LYS:CD    | 1:L:139:ASN:HB2   | 2.36                     | 0.56              |
| 2:M:63:GLY:CA     | 2:M:103:LYS:HG3   | 2.35                     | 0.56              |
| 2:M:191:PHE:HB2   | 2:M:241:LEU:HD11  | 1.87                     | 0.56              |
| 2:M:200:LEU:HD13  | 2:M:300:ASP:OD1   | 2.05                     | 0.56              |
| 2:M:261:ILE:CD1   | 2:M:262:ALA:H     | 2.18                     | 0.56              |
| 2:M:328:LEU:HD13  | 2:M:433:THR:CB    | 2.30                     | 0.56              |
| 2:M:420:ARG:HD2   | 7:Z:1:DG:H5''     | 1.88                     | 0.56              |
| 2:M:682:TYR:O     | 2:M:850:ALA:HB3   | 2.05                     | 0.56              |
| 2:M:700:TYR:HB3   | 2:M:833:LEU:HD13  | 1.86                     | 0.56              |
| 2:M:723:THR:HG23  | 2:M:725:ASP:HB2   | 1.87                     | 0.56              |
| 3:N:875:THR:CG2   | 3:N:876:SER:N     | 2.69                     | 0.56              |
| 7:Z:11:DG:OP2     | 7:Z:11:DG:H2'     | 2.06                     | 0.56              |
| 1:A:102:LYS:HG3   | 1:A:102:LYS:O     | 2.05                     | 0.56              |
| 1:B:73:GLU:OE1    | 1:B:130:ALA:HA    | 2.06                     | 0.56              |
| 2:C:162:ILE:CB    | 2:C:172:ILE:HB    | 2.33                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:354:GLY:HA2   | 2:C:357:GLU:OE2   | 2.06                     | 0.56              |
| 2:C:728:HIS:O     | 2:C:729:LEU:HG    | 2.06                     | 0.56              |
| 3:D:1138:ALA:HB1  | 3:D:1362:LYS:HE3  | 1.87                     | 0.56              |
| 1:K:86:VAL:HG13   | 1:K:124:ASN:HB2   | 1.88                     | 0.56              |
| 1:K:213:GLN:O     | 1:K:217:ILE:HG13  | 2.06                     | 0.56              |
| 1:L:28:LEU:HD12   | 1:L:193:ASP:HB3   | 1.88                     | 0.56              |
| 2:M:176:VAL:HG12  | 2:M:182:VAL:HG13  | 1.88                     | 0.56              |
| 2:M:195:LEU:HD21  | 2:M:238:LEU:HG    | 1.87                     | 0.56              |
| 2:M:394:PHE:CZ    | 2:M:632:ASN:OD1   | 2.58                     | 0.56              |
| 2:M:754:ILE:HD11  | 2:M:791:ARG:CZ    | 2.35                     | 0.56              |
| 2:M:1038:TRP:HA   | 2:M:1041:GLU:CG   | 2.35                     | 0.56              |
| 3:N:107:ASP:CG    | 3:N:1445:HIS:HA   | 2.31                     | 0.56              |
| 3:N:551:ASN:O     | 3:N:554:LEU:HB3   | 2.05                     | 0.56              |
| 3:N:1115:THR:HG21 | 3:N:1151:ARG:HH21 | 1.70                     | 0.56              |
| 3:N:1280:VAL:HA   | 3:N:1318:TYR:CA   | 2.32                     | 0.56              |
| 5:G:7:DA:OP2      | 5:G:7:DA:C8       | 2.58                     | 0.56              |
| 6:Y:6:C:O5'       | 6:Y:6:C:C6        | 2.53                     | 0.56              |
| 2:C:12:VAL:HG11   | 2:C:472:ARG:CD    | 2.36                     | 0.56              |
| 2:C:265:ARG:C     | 2:C:267:TYR:H     | 2.11                     | 0.56              |
| 2:C:396:ASP:HB2   | 2:C:406:HIS:CD2   | 2.41                     | 0.56              |
| 3:D:525:ARG:O     | 3:D:525:ARG:HG2   | 2.06                     | 0.56              |
| 3:D:828:LYS:HE2   | 3:D:862:ASP:OD2   | 2.06                     | 0.56              |
| 3:D:1344:VAL:O    | 3:D:1348:LEU:HD13 | 2.06                     | 0.56              |
| 3:D:1446:VAL:HB   | 3:D:1447:LEU:CD1  | 2.36                     | 0.56              |
| 1:L:102:LYS:HG3   | 1:L:138:LEU:O     | 2.06                     | 0.56              |
| 2:M:394:PHE:HE1   | 2:M:632:ASN:HB3   | 1.70                     | 0.56              |
| 2:M:438:ILE:HD12  | 2:M:438:ILE:N     | 2.21                     | 0.56              |
| 2:M:1101:THR:OG1  | 2:M:1109:VAL:O    | 2.24                     | 0.56              |
| 3:N:107:ASP:O     | 3:N:108:VAL:C     | 2.46                     | 0.56              |
| 3:N:501:ALA:HB1   | 3:N:1452:ILE:HG22 | 1.86                     | 0.56              |
| 3:N:989:TYR:O     | 3:N:993:LEU:HG    | 2.06                     | 0.56              |
| 3:N:1103:HIS:CG   | 3:N:1104:GLU:H    | 2.24                     | 0.56              |
| 3:N:1211:MET:HG2  | 3:N:1212:ALA:N    | 2.19                     | 0.56              |
| 3:N:1236:LEU:C    | 3:N:1237:THR:OG1  | 2.49                     | 0.56              |
| 3:N:1274:ILE:CD1  | 3:N:1276:GLU:HG2  | 2.22                     | 0.56              |
| 3:N:1281:VAL:HG23 | 3:N:1319:VAL:HG21 | 1.87                     | 0.56              |
| 2:C:49:ARG:N      | 2:C:52:PHE:HB2    | 2.21                     | 0.56              |
| 2:C:196:LEU:O     | 2:C:199:VAL:HB    | 2.06                     | 0.56              |
| 2:C:281:LEU:HD11  | 2:C:306:THR:HA    | 1.88                     | 0.56              |
| 2:C:460:ARG:HH22  | 2:C:468:ARG:HH11  | 1.49                     | 0.56              |
| 2:C:737:LEU:HD21  | 2:C:741:GLY:C     | 2.30                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:128:TYR:CE2   | 3:D:458:ALA:HB2   | 2.41                     | 0.56              |
| 3:D:1377:LYS:HG2  | 3:D:1378:TYR:CE1  | 2.40                     | 0.56              |
| 4:E:25:LYS:O      | 4:E:29:GLN:HG3    | 2.06                     | 0.56              |
| 1:K:193:ASP:HA    | 2:M:938:LYS:HZ3   | 1.71                     | 0.56              |
| 2:M:141:HIS:O     | 2:M:331:ARG:HA    | 2.05                     | 0.56              |
| 3:N:33:ASN:HB2    | 3:N:40:GLU:CD     | 2.30                     | 0.56              |
| 3:N:87:ARG:HB3    | 3:N:523:ASP:HB2   | 1.89                     | 0.56              |
| 3:N:525:ARG:O     | 3:N:525:ARG:HG2   | 2.06                     | 0.56              |
| 3:N:902:LEU:HD23  | 3:N:902:LEU:N     | 2.21                     | 0.56              |
| 3:N:957:PRO:HG3   | 3:N:1007:VAL:HG22 | 1.85                     | 0.56              |
| 3:N:1268:PRO:HG2  | 3:N:1270:ALA:O    | 2.06                     | 0.56              |
| 4:O:80:VAL:HG13   | 4:O:81:PRO:HD2    | 1.88                     | 0.56              |
| 2:C:876:VAL:HG11  | 2:C:885:ILE:HD11  | 1.87                     | 0.55              |
| 3:D:696:HIS:HD2   | 4:E:59:ASN:N      | 2.01                     | 0.55              |
| 3:D:899:LEU:HD23  | 3:D:917:GLN:HG3   | 1.86                     | 0.55              |
| 3:D:925:GLU:HB3   | 4:E:6:ILE:HG22    | 1.87                     | 0.55              |
| 3:D:1125:PRO:O    | 3:D:1131:SER:O    | 2.23                     | 0.55              |
| 2:M:74:GLY:O      | 2:M:76:PRO:HD3    | 2.06                     | 0.55              |
| 2:M:368:THR:HB    | 2:M:369:PRO:HD3   | 1.87                     | 0.55              |
| 2:M:757:GLY:HA2   | 2:M:789:SER:HB3   | 1.88                     | 0.55              |
| 3:N:502:PHE:CZ    | 3:N:509:PRO:HB3   | 2.41                     | 0.55              |
| 3:N:767:HIS:CD2   | 4:O:6:ILE:CG1     | 2.87                     | 0.55              |
| 3:N:1191:PRO:O    | 3:N:1373:ARG:NH1  | 2.39                     | 0.55              |
| 2:C:265:ARG:HD3   | 2:C:267:TYR:HB3   | 1.88                     | 0.55              |
| 2:C:975:TYR:HA    | 2:C:982:PRO:HA    | 1.87                     | 0.55              |
| 3:D:521:PRO:HB2   | 3:D:524:LEU:HD13  | 1.87                     | 0.55              |
| 3:D:1003:VAL:HG21 | 3:D:1036:ARG:NH1  | 2.21                     | 0.55              |
| 4:E:54:LEU:HD23   | 4:E:58:PRO:HD2    | 1.88                     | 0.55              |
| 2:M:584:GLU:O     | 2:M:588:VAL:HG13  | 2.05                     | 0.55              |
| 3:N:465:LEU:HD13  | 3:N:510:GLU:HA    | 1.88                     | 0.55              |
| 3:N:482:LYS:HE2   | 3:N:1384:PRO:CD   | 2.31                     | 0.55              |
| 3:N:1146:GLY:HA3  | 3:N:1207:TYR:HB2  | 1.88                     | 0.55              |
| 3:N:1445:HIS:O    | 3:N:1446:VAL:C    | 2.49                     | 0.55              |
| 3:N:1484:THR:HG23 | 4:O:76:GLY:O      | 2.06                     | 0.55              |
| 1:A:110:LYS:O     | 1:A:112:ARG:N     | 2.39                     | 0.55              |
| 2:C:433:THR:O     | 2:C:435:TYR:N     | 2.37                     | 0.55              |
| 2:C:688:ILE:CG2   | 2:C:689:VAL:N     | 2.70                     | 0.55              |
| 2:C:833:LEU:CD1   | 2:C:996:LYS:HE2   | 2.36                     | 0.55              |
| 2:C:1058:ASP:HB3  | 2:C:1082:PRO:HB3  | 1.88                     | 0.55              |
| 3:D:62:LYS:HE2    | 3:D:62:LYS:HA     | 1.88                     | 0.55              |
| 3:D:994:GLN:HA    | 3:D:997:THR:OG1   | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1183:ILE:HA   | 3:N:559:ALA:O     | 2.06                     | 0.55              |
| 3:D:1223:ILE:HD11 | 3:D:1462:LEU:HD11 | 1.88                     | 0.55              |
| 1:K:38:ASN:ND2    | 2:M:978:ARG:O     | 2.40                     | 0.55              |
| 3:N:638:LYS:HB2   | 3:N:641:GLN:OE1   | 2.06                     | 0.55              |
| 3:N:701:LEU:HD23  | 3:N:763:MET:HE3   | 1.89                     | 0.55              |
| 3:N:711:LEU:C     | 3:N:713:ILE:H     | 2.14                     | 0.55              |
| 3:N:786:ILE:HG21  | 3:N:1027:GLY:H    | 1.70                     | 0.55              |
| 3:N:1277:ILE:HD12 | 3:N:1301:LYS:CA   | 2.37                     | 0.55              |
| 2:C:157:ARG:NH2   | 2:C:158:TYR:HE1   | 2.05                     | 0.55              |
| 2:C:274:ARG:CG    | 2:C:285:LEU:HD13  | 2.36                     | 0.55              |
| 2:C:395:LYS:NZ    | 2:C:407:LYS:HZ2   | 2.04                     | 0.55              |
| 2:C:430:VAL:HB    | 3:D:1078:ARG:CZ   | 2.36                     | 0.55              |
| 2:C:930:LYS:HD2   | 2:C:960:GLU:CD    | 2.31                     | 0.55              |
| 2:C:958:THR:OG1   | 2:C:961:GLU:HG2   | 2.06                     | 0.55              |
| 2:C:1085:PHE:CE2  | 3:D:1468:LEU:HA   | 2.42                     | 0.55              |
| 3:D:118:LEU:O     | 3:D:120:ALA:N     | 2.39                     | 0.55              |
| 3:D:826:PRO:HD2   | 3:D:829:VAL:CG2   | 2.35                     | 0.55              |
| 3:D:897:TRP:C     | 3:D:900:ILE:CG1   | 2.80                     | 0.55              |
| 3:D:1003:VAL:HG13 | 3:D:1036:ARG:CG   | 2.36                     | 0.55              |
| 3:D:1147:ARG:HH12 | 3:D:1190:SER:HA   | 1.71                     | 0.55              |
| 3:D:1465:ASN:HD21 | 3:D:1470:ARG:CB   | 2.19                     | 0.55              |
| 1:L:26:GLU:N      | 1:L:26:GLU:OE2    | 2.39                     | 0.55              |
| 1:L:174:VAL:HG13  | 1:L:200:TRP:O     | 2.06                     | 0.55              |
| 2:M:5:ARG:CB      | 2:M:902:ILE:HB    | 2.33                     | 0.55              |
| 2:M:881:ASN:N     | 2:M:881:ASN:ND2   | 2.49                     | 0.55              |
| 2:M:1046:ALA:CB   | 3:N:1476:THR:HB   | 2.36                     | 0.55              |
| 2:M:1058:ASP:HB3  | 2:M:1082:PRO:HB3  | 1.88                     | 0.55              |
| 3:N:163:TYR:CE1   | 3:N:165:LYS:HA    | 2.42                     | 0.55              |
| 3:N:493:ARG:NH2   | 3:N:1391:GLU:HA   | 2.21                     | 0.55              |
| 3:N:1277:ILE:CG1  | 3:N:1301:LYS:HB2  | 2.35                     | 0.55              |
| 5:G:12:DA:H2''    | 5:G:13:DA:OP2     | 2.05                     | 0.55              |
| 7:Z:11:DG:C2'     | 7:Z:12:DT:OP2     | 2.49                     | 0.55              |
| 1:A:65:PHE:CD1    | 2:C:801:VAL:HG12  | 2.40                     | 0.55              |
| 1:A:117:VAL:HB    | 1:A:120:VAL:HG12  | 1.89                     | 0.55              |
| 2:C:181:VAL:HG12  | 2:C:182:VAL:N     | 2.20                     | 0.55              |
| 2:C:1045:ALA:CB   | 3:D:763:MET:HE1   | 2.35                     | 0.55              |
| 3:D:684:LYS:O     | 3:D:687:VAL:HG23  | 2.07                     | 0.55              |
| 3:D:764:LEU:HD23  | 3:D:767:HIS:HE1   | 1.60                     | 0.55              |
| 4:E:46:PRO:CB     | 4:E:54:LEU:HD22   | 2.36                     | 0.55              |
| 1:L:102:LYS:HG2   | 1:L:104:GLU:OE2   | 2.06                     | 0.55              |
| 2:M:45:GLN:O      | 2:M:48:PHE:HB2    | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:211:LEU:CD1   | 2:M:308:ARG:HA    | 2.37                     | 0.55              |
| 2:M:269:LEU:CG    | 2:M:288:ARG:HG2   | 2.37                     | 0.55              |
| 2:M:274:ARG:HH21  | 2:M:284:ARG:HA    | 1.72                     | 0.55              |
| 2:M:409:ARG:HA    | 2:M:454:SER:CA    | 2.26                     | 0.55              |
| 2:M:422:ARG:CB    | 7:Z:1:DG:C2       | 2.85                     | 0.55              |
| 2:M:466:PHE:O     | 2:M:468:ARG:HG3   | 2.06                     | 0.55              |
| 3:N:583:ASP:CG    | 3:N:586:ARG:HG2   | 2.32                     | 0.55              |
| 3:N:584:ASN:ND2   | 3:N:590:PRO:HD2   | 2.22                     | 0.55              |
| 3:N:625:TYR:HE2   | 3:N:655:PRO:HD2   | 1.72                     | 0.55              |
| 3:N:1084:THR:CG2  | 3:N:1087:ARG:HH22 | 2.18                     | 0.55              |
| 5:X:16:DT:C2'     | 5:X:17:DA:OP2     | 2.51                     | 0.55              |
| 1:A:180:GLN:NE2   | 2:C:937:ASP:HB2   | 2.21                     | 0.55              |
| 2:C:205:GLU:OE2   | 2:C:206:THR:HG22  | 2.07                     | 0.55              |
| 2:C:243:ARG:HH11  | 2:C:243:ARG:HG3   | 1.71                     | 0.55              |
| 3:D:18:ILE:O      | 3:D:22:SER:HB3    | 2.07                     | 0.55              |
| 3:D:781:PRO:HB2   | 3:D:786:ILE:HG12  | 1.87                     | 0.55              |
| 3:D:1095:THR:HG22 | 3:D:1098:LEU:HD22 | 1.89                     | 0.55              |
| 3:D:1256:LEU:N    | 3:D:1257:PRO:HD2  | 2.21                     | 0.55              |
| 1:K:156:HIS:ND1   | 1:K:158:ILE:HG12  | 2.21                     | 0.55              |
| 1:L:79:ILE:HA     | 1:L:82:LEU:CD1    | 2.36                     | 0.55              |
| 1:L:102:LYS:CE    | 1:L:139:ASN:HB2   | 2.37                     | 0.55              |
| 2:M:861:LEU:HD23  | 2:M:863:ASP:N     | 2.16                     | 0.55              |
| 3:N:133:ILE:HG12  | 3:N:456:MET:HB3   | 1.89                     | 0.55              |
| 3:N:666:ILE:HG23  | 3:N:684:LYS:HZ2   | 1.71                     | 0.55              |
| 3:N:703:ASN:CB    | 3:N:713:ILE:HG12  | 2.36                     | 0.55              |
| 3:N:711:LEU:CD1   | 3:N:778:LEU:HD23  | 2.27                     | 0.55              |
| 3:N:1271:LYS:HZ1  | 3:N:1331:ASP:HB2  | 1.69                     | 0.55              |
| 5:X:2:DT:H2'      | 5:X:3:DC:C5       | 2.42                     | 0.55              |
| 1:A:65:PHE:CZ     | 2:C:799:ILE:HB    | 2.41                     | 0.55              |
| 1:B:25:LEU:O      | 1:B:28:LEU:HD21   | 2.07                     | 0.55              |
| 2:C:44:ILE:HG22   | 2:C:48:PHE:CE2    | 2.42                     | 0.55              |
| 2:C:385:PHE:O     | 2:C:389:SER:HB3   | 2.07                     | 0.55              |
| 2:C:431:HIS:N     | 2:C:434:HIS:ND1   | 2.55                     | 0.55              |
| 2:C:474:VAL:HG23  | 2:C:478:VAL:O     | 2.07                     | 0.55              |
| 3:D:9:ARG:HH11    | 3:D:1454:GLY:HA3  | 1.71                     | 0.55              |
| 3:D:925:GLU:HB2   | 4:E:2:ALA:HB3     | 1.89                     | 0.55              |
| 3:D:1154:GLU:HB2  | 3:N:562:ALA:N     | 2.22                     | 0.55              |
| 3:D:1340:GLY:O    | 3:D:1343:ALA:HB3  | 2.07                     | 0.55              |
| 3:D:1397:LYS:HZ1  | 3:D:1432:LYS:CE   | 2.16                     | 0.55              |
| 1:L:84:GLU:OE1    | 3:N:845:ASN:HB2   | 2.07                     | 0.55              |
| 2:M:409:ARG:NH2   | 6:Y:12:U:OP1      | 2.40                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:707:ARG:HD2   | 2:M:824:ARG:CD   | 2.37                     | 0.55              |
| 2:M:739:GLU:HB2   | 2:M:742:VAL:HB   | 1.89                     | 0.55              |
| 3:N:513:ILE:HD12  | 3:N:513:ILE:C    | 2.31                     | 0.55              |
| 3:N:1372:VAL:HG13 | 3:N:1373:ARG:N   | 2.21                     | 0.55              |
| 5:X:19:DG:C2'     | 5:X:20:DC:H5'    | 2.33                     | 0.55              |
| 2:C:41:ASN:CB     | 2:C:45:GLN:OE1   | 2.53                     | 0.55              |
| 2:C:580:MET:HB3   | 2:C:584:GLU:CD   | 2.32                     | 0.55              |
| 2:C:673:LEU:HD22  | 2:C:867:VAL:HG12 | 1.89                     | 0.55              |
| 2:C:756:VAL:O     | 2:C:789:SER:HB3  | 2.06                     | 0.55              |
| 2:C:1090:LYS:HZ2  | 3:D:21:TRP:HB3   | 1.71                     | 0.55              |
| 3:D:23:TYR:CE1    | 3:D:89:ARG:HG2   | 2.42                     | 0.55              |
| 3:D:552:ASN:O     | 3:D:556:LYS:HG3  | 2.07                     | 0.55              |
| 3:D:606:ILE:O     | 3:D:613:ARG:HB2  | 2.06                     | 0.55              |
| 3:D:704:ARG:NE    | 3:D:705:ALA:HB3  | 2.22                     | 0.55              |
| 3:D:826:PRO:HD2   | 3:D:829:VAL:HG22 | 1.89                     | 0.55              |
| 4:E:60:ALA:O      | 4:E:63:TRP:HB2   | 2.07                     | 0.55              |
| 2:M:163:ILE:HD13  | 2:M:171:TRP:CZ3  | 2.42                     | 0.55              |
| 2:M:680:ASP:N     | 3:N:943:THR:CG2  | 2.70                     | 0.55              |
| 2:M:693:GLU:HG2   | 2:M:697:ARG:HH21 | 1.69                     | 0.55              |
| 2:M:854:PRO:HB2   | 2:M:856:GLU:CG   | 2.37                     | 0.55              |
| 2:M:936:VAL:CA    | 2:M:940:GLU:OE2  | 2.52                     | 0.55              |
| 3:N:81:THR:HB     | 3:N:85:VAL:HG22  | 1.88                     | 0.55              |
| 3:N:111:LYS:NZ    | 3:N:1449:GLU:HG3 | 2.22                     | 0.55              |
| 3:N:112:ILE:O     | 3:N:116:LEU:N    | 2.33                     | 0.55              |
| 3:N:728:LEU:CD1   | 3:N:729:HIS:H    | 2.16                     | 0.55              |
| 3:N:1059:SER:CB   | 3:N:1065:LEU:HA  | 2.36                     | 0.55              |
| 5:X:9:DC:O5'      | 5:X:9:DC:H6      | 1.90                     | 0.55              |
| 1:A:102:LYS:CB    | 1:A:139:ASN:OD1  | 2.55                     | 0.55              |
| 2:C:52:PHE:HZ     | 2:C:68:PHE:CA    | 2.19                     | 0.55              |
| 2:C:267:TYR:HB2   | 2:C:272:ALA:HB1  | 1.89                     | 0.55              |
| 2:C:575:GLN:C     | 2:C:667:ALA:HB1  | 2.32                     | 0.55              |
| 2:C:905:ILE:HG22  | 2:C:906:PHE:N    | 2.22                     | 0.55              |
| 2:C:976:ASP:CB    | 2:C:979:THR:HG22 | 2.37                     | 0.55              |
| 3:D:704:ARG:HD2   | 3:D:745:MET:SD   | 2.47                     | 0.55              |
| 3:D:708:LEU:HB3   | 3:D:1231:GLU:CB  | 2.35                     | 0.55              |
| 1:K:96:THR:HB     | 1:K:145:ASP:OD2  | 2.06                     | 0.55              |
| 2:M:145:GLY:CA    | 2:M:276:LYS:HD3  | 2.37                     | 0.55              |
| 2:M:750:LYS:HD2   | 2:M:750:LYS:N    | 2.21                     | 0.55              |
| 2:M:905:ILE:N     | 2:M:905:ILE:CD1  | 2.70                     | 0.55              |
| 3:N:26:VAL:HG13   | 3:N:43:GLY:O     | 2.06                     | 0.55              |
| 3:N:72:VAL:HG23   | 3:N:78:VAL:N     | 2.22                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:135:LEU:HA    | 3:N:453:ASP:O     | 2.07                     | 0.55              |
| 3:N:171:LEU:HD21  | 3:N:194:GLY:HA3   | 1.89                     | 0.55              |
| 3:N:618:LEU:CD1   | 3:N:1467:ILE:HD13 | 2.36                     | 0.55              |
| 3:N:703:ASN:HA    | 3:N:713:ILE:HG12  | 1.88                     | 0.55              |
| 3:N:827:ILE:N     | 3:N:827:ILE:HD12  | 2.22                     | 0.55              |
| 3:N:1281:VAL:HG21 | 3:N:1313:VAL:HG21 | 1.88                     | 0.55              |
| 3:N:1461:GLY:O    | 3:N:1473:PRO:HG2  | 2.07                     | 0.55              |
| 2:C:141:HIS:O     | 2:C:331:ARG:HA    | 2.06                     | 0.55              |
| 2:C:394:PHE:CZ    | 5:G:25:DG:H4'     | 2.42                     | 0.55              |
| 3:D:704:ARG:NH1   | 3:D:738:ALA:CB    | 2.70                     | 0.55              |
| 3:D:798:GLU:HG2   | 3:D:799:LYS:N     | 2.22                     | 0.55              |
| 3:D:960:LYS:O     | 3:D:964:LEU:HB2   | 2.07                     | 0.55              |
| 3:D:1034:GLN:O    | 3:D:1038:LEU:N    | 2.39                     | 0.55              |
| 3:D:1154:GLU:H    | 3:N:561:GLY:HA3   | 1.72                     | 0.55              |
| 3:D:1189:ARG:HH11 | 3:D:1189:ARG:HG3  | 1.72                     | 0.55              |
| 3:N:907:GLU:O     | 3:N:911:LEU:HD12  | 2.07                     | 0.55              |
| 3:N:1274:ILE:HG21 | 3:N:1301:LYS:HD2  | 1.88                     | 0.55              |
| 7:I:11:DG:C2'     | 7:I:12:DT:OP2     | 2.49                     | 0.55              |
| 7:Z:3:DA:C1'      | 7:Z:4:DG:H5'      | 2.23                     | 0.55              |
| 1:A:13:VAL:CG1    | 1:A:14:ARG:N      | 2.70                     | 0.54              |
| 1:B:9:PRO:HB3     | 1:B:25:LEU:CD2    | 2.36                     | 0.54              |
| 1:B:100:LEU:HB2   | 1:B:115:LEU:CD2   | 2.37                     | 0.54              |
| 2:C:79:PRO:HG2    | 2:C:82:GLU:HG3    | 1.89                     | 0.54              |
| 2:C:739:GLU:HB2   | 2:C:742:VAL:HB    | 1.89                     | 0.54              |
| 2:M:713:ARG:HG2   | 2:M:714:ASP:N     | 2.22                     | 0.54              |
| 2:M:1074:GLU:CG   | 2:M:1075:ASP:H    | 2.18                     | 0.54              |
| 2:M:1092:LEU:O    | 2:M:1097:LEU:O    | 2.25                     | 0.54              |
| 3:N:98:PRO:CG     | 3:N:462:GLN:OE1   | 2.55                     | 0.54              |
| 3:N:631:ILE:HG12  | 3:N:743:ASP:O     | 2.07                     | 0.54              |
| 3:N:1384:PRO:HG3  | 3:N:1389:LEU:N    | 2.22                     | 0.54              |
| 1:B:92:PRO:HA     | 1:B:146:ARG:NH1   | 2.23                     | 0.54              |
| 2:C:31:GLN:NE2    | 2:C:38:LYS:O      | 2.40                     | 0.54              |
| 2:C:141:HIS:CD2   | 2:C:332:ARG:HB3   | 2.43                     | 0.54              |
| 2:C:160:ALA:HB3   | 2:C:174:LEU:HD12  | 1.90                     | 0.54              |
| 3:D:9:ARG:HG3     | 3:D:1455:LYS:O    | 2.06                     | 0.54              |
| 3:D:770:LEU:HB2   | 3:D:1210:SER:O    | 2.08                     | 0.54              |
| 4:E:28:GLN:C      | 4:E:32:ARG:NH1    | 2.65                     | 0.54              |
| 1:L:152:PRO:HB2   | 1:L:155:LYS:HB2   | 1.88                     | 0.54              |
| 2:M:393:GLN:CG    | 6:Y:10:G:H4'      | 2.37                     | 0.54              |
| 2:M:433:THR:O     | 2:M:435:TYR:N     | 2.37                     | 0.54              |
| 2:M:490:GLU:CB    | 2:M:493:ARG:HH11  | 2.04                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:13:ALA:O      | 3:N:511:TRP:HB3   | 2.07                     | 0.54              |
| 3:N:134:VAL:O     | 3:N:454:ALA:HA    | 2.07                     | 0.54              |
| 3:N:135:LEU:CD1   | 3:N:147:VAL:HG23  | 2.37                     | 0.54              |
| 3:N:478:LEU:HD23  | 3:N:1388:ARG:HD3  | 1.88                     | 0.54              |
| 3:N:1033:GLN:CD   | 3:N:1240:THR:HG22 | 2.32                     | 0.54              |
| 3:N:1276:GLU:HA   | 3:N:1301:LYS:HG2  | 1.88                     | 0.54              |
| 3:N:1393:GLN:HB2  | 3:N:1398:TRP:CZ2  | 2.42                     | 0.54              |
| 1:A:43:ILE:O      | 1:A:47:SER:HB2    | 2.06                     | 0.54              |
| 1:A:154:GLU:N     | 1:A:154:GLU:OE2   | 2.39                     | 0.54              |
| 2:C:49:ARG:HA     | 2:C:52:PHE:HB2    | 1.88                     | 0.54              |
| 2:C:49:ARG:CA     | 2:C:52:PHE:HB2    | 2.37                     | 0.54              |
| 2:C:400:PRO:HA    | 2:C:403:SER:OG    | 2.07                     | 0.54              |
| 2:C:442:GLU:OE2   | 2:C:543:ASN:HB3   | 2.08                     | 0.54              |
| 2:C:676:ILE:HG23  | 3:D:948:THR:HB    | 1.90                     | 0.54              |
| 2:C:1007:ALA:HB1  | 3:D:652:LEU:HD13  | 1.88                     | 0.54              |
| 3:D:741:ASP:OD2   | 6:H:14:G:O3'      | 2.25                     | 0.54              |
| 2:M:550:LEU:HG    | 3:N:1070:TYR:HE1  | 1.71                     | 0.54              |
| 2:M:767:PRO:HB3   | 2:M:772:ARG:NH2   | 2.23                     | 0.54              |
| 3:N:660:LYS:HD2   | 3:N:694:VAL:CG2   | 2.35                     | 0.54              |
| 3:N:867:ARG:HD2   | 3:N:867:ARG:C     | 2.31                     | 0.54              |
| 3:N:1281:VAL:HG21 | 3:N:1313:VAL:HG11 | 1.89                     | 0.54              |
| 6:H:7:G:C2'       | 6:H:8:G:H5'       | 2.36                     | 0.54              |
| 6:Y:4:G:H8        | 6:Y:4:G:O5'       | 1.90                     | 0.54              |
| 1:A:50:GLY:HA3    | 1:A:171:PHE:O     | 2.06                     | 0.54              |
| 2:C:48:PHE:HB3    | 2:C:52:PHE:HD2    | 1.72                     | 0.54              |
| 2:C:223:ASP:OD2   | 2:C:224:GLU:HG2   | 2.07                     | 0.54              |
| 2:C:290:LEU:HD23  | 2:C:290:LEU:N     | 2.22                     | 0.54              |
| 2:C:996:LYS:C     | 2:C:997:LEU:HD22  | 2.32                     | 0.54              |
| 2:C:1013:TYR:HD1  | 2:C:1020:PRO:HG3  | 1.72                     | 0.54              |
| 3:D:42:ASP:O      | 3:D:43:GLY:O      | 2.25                     | 0.54              |
| 3:D:1472:ILE:C    | 3:D:1474:ALA:H    | 2.15                     | 0.54              |
| 2:M:183:SER:OG    | 2:M:190:LYS:HG2   | 2.08                     | 0.54              |
| 2:M:757:GLY:HA2   | 2:M:789:SER:CB    | 2.37                     | 0.54              |
| 2:M:1000:MET:CB   | 2:M:1002:GLU:HG2  | 2.33                     | 0.54              |
| 3:N:14:SER:O      | 3:N:17:LYS:N      | 2.41                     | 0.54              |
| 3:N:136:ASP:CB    | 3:N:137:PRO:CD    | 2.81                     | 0.54              |
| 3:N:433:GLY:HA2   | 3:N:449:SER:O     | 2.08                     | 0.54              |
| 3:N:608:SER:C     | 3:N:612:GLY:HA3   | 2.32                     | 0.54              |
| 7:Z:13:DA:C2'     | 7:Z:14:DG:OP2     | 2.53                     | 0.54              |
| 1:A:57:TYR:HE1    | 1:A:163:ASN:HB2   | 1.72                     | 0.54              |
| 2:C:55:GLU:OE2    | 2:C:57:GLU:HB2    | 2.08                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:118:ILE:HG22  | 2:C:382:ILE:HD13 | 1.89                     | 0.54              |
| 2:C:410:ILE:HG22  | 2:C:453:THR:HG23 | 1.89                     | 0.54              |
| 2:C:458:TYR:HB3   | 2:C:485:TYR:OH   | 2.08                     | 0.54              |
| 2:C:557:ARG:NH1   | 2:C:560:MET:HG3  | 2.23                     | 0.54              |
| 2:C:796:GLU:CB    | 2:C:1004:LYS:HZ3 | 2.16                     | 0.54              |
| 2:C:896:PHE:CE2   | 2:C:925:TYR:HA   | 2.42                     | 0.54              |
| 3:D:47:GLU:CG     | 3:D:53:ILE:HB    | 2.38                     | 0.54              |
| 3:D:1472:ILE:O    | 3:D:1477:GLY:HA3 | 2.07                     | 0.54              |
| 1:K:89:PHE:HB3    | 1:K:94:LEU:HD13  | 1.89                     | 0.54              |
| 2:M:243:ARG:N     | 2:M:244:PRO:HD3  | 2.21                     | 0.54              |
| 2:M:1001:VAL:CG2  | 5:X:24:DC:H5'    | 2.38                     | 0.54              |
| 2:M:1115:LEU:HD22 | 3:N:88:TYR:CD1   | 2.42                     | 0.54              |
| 3:N:82:LYS:HA     | 3:N:82:LYS:CE    | 2.37                     | 0.54              |
| 3:N:631:ILE:HB    | 3:N:740:PHE:HE2  | 1.73                     | 0.54              |
| 3:N:918:ALA:HB1   | 3:N:927:THR:HG23 | 1.88                     | 0.54              |
| 5:X:26:DC:C4      | 5:X:27:DC:N4     | 2.75                     | 0.54              |
| 1:A:4:SER:HA      | 1:A:7:LYS:HE2    | 1.90                     | 0.54              |
| 2:C:693:GLU:HA    | 2:C:696:LYS:HD2  | 1.90                     | 0.54              |
| 3:D:502:PHE:CE2   | 3:D:509:PRO:HB3  | 2.43                     | 0.54              |
| 3:D:690:ALA:O     | 3:D:694:VAL:HG23 | 2.07                     | 0.54              |
| 3:D:711:LEU:C     | 3:D:713:ILE:H    | 2.15                     | 0.54              |
| 1:L:58:ILE:HD11   | 1:L:140:MET:SD   | 2.47                     | 0.54              |
| 2:M:202:TYR:OH    | 2:M:304:LEU:HD22 | 2.08                     | 0.54              |
| 2:M:402:SER:HA    | 2:M:566:THR:CG2  | 2.33                     | 0.54              |
| 2:M:709:GLU:HG3   | 2:M:824:ARG:HG3  | 1.90                     | 0.54              |
| 3:N:41:ARG:NH1    | 3:N:42:ASP:HB3   | 2.23                     | 0.54              |
| 3:N:63:TYR:CD1    | 3:N:73:CYS:HA    | 2.43                     | 0.54              |
| 3:N:181:ASP:HA    | 3:N:205:TYR:CD1  | 2.43                     | 0.54              |
| 3:N:1031:ASN:O    | 3:N:1033:GLN:N   | 2.39                     | 0.54              |
| 1:B:14:ARG:HB2    | 1:B:22:GLU:HB2   | 1.90                     | 0.54              |
| 1:B:25:LEU:HD23   | 1:B:28:LEU:HD21  | 1.89                     | 0.54              |
| 2:C:36:PRO:HB2    | 2:C:70:GLU:CG    | 2.38                     | 0.54              |
| 2:C:352:ALA:C     | 2:C:355:VAL:HG12 | 2.32                     | 0.54              |
| 2:C:435:TYR:CE1   | 2:C:539:VAL:HG21 | 2.42                     | 0.54              |
| 2:C:510:ALA:O     | 2:C:513:VAL:HG23 | 2.08                     | 0.54              |
| 2:C:1087:VAL:HG23 | 3:D:524:LEU:CD2  | 2.38                     | 0.54              |
| 3:D:16:GLU:H      | 3:D:16:GLU:CD    | 2.16                     | 0.54              |
| 3:D:50:PHE:C      | 3:D:86:ARG:HA    | 2.32                     | 0.54              |
| 3:D:704:ARG:HH11  | 3:D:738:ALA:HB2  | 1.72                     | 0.54              |
| 2:M:405:ARG:C     | 2:M:407:LYS:H    | 2.16                     | 0.54              |
| 2:M:512:ARG:HD3   | 2:M:523:ILE:CD1  | 2.38                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:622:GLU:O     | 2:M:624:PRO:HD3  | 2.08                     | 0.54              |
| 2:M:630:ARG:HG3   | 2:M:630:ARG:O    | 2.08                     | 0.54              |
| 2:M:758:ARG:NH1   | 2:M:788:THR:HB   | 2.22                     | 0.54              |
| 3:N:154:THR:CG2   | 3:N:157:GLU:OE2  | 2.56                     | 0.54              |
| 3:N:503:LEU:O     | 3:N:506:GLY:N    | 2.40                     | 0.54              |
| 3:N:834:THR:HB    | 3:N:838:ARG:HB2  | 1.90                     | 0.54              |
| 3:N:1096:ARG:NH2  | 5:X:18:DC:OP1    | 2.37                     | 0.54              |
| 3:N:1432:LYS:HZ3  | 3:N:1432:LYS:HB2 | 1.73                     | 0.54              |
| 4:O:30:LEU:O      | 4:O:35:PHE:HA    | 2.08                     | 0.54              |
| 5:G:10:DA:H2''    | 5:G:11:DC:OP2    | 2.08                     | 0.54              |
| 6:Y:5:C:C6        | 6:Y:5:C:O5'      | 2.61                     | 0.54              |
| 1:A:222:LEU:CD2   | 1:B:219:ARG:CB   | 2.86                     | 0.54              |
| 2:C:185:LYS:HG3   | 2:C:190:LYS:HG3  | 1.90                     | 0.54              |
| 2:C:897:LEU:O     | 2:C:899:GLN:HG2  | 2.08                     | 0.54              |
| 3:D:683:ILE:N     | 3:D:683:ILE:HD12 | 2.23                     | 0.54              |
| 3:D:1066:THR:HG23 | 3:D:1069:GLU:H   | 1.72                     | 0.54              |
| 3:D:1106:VAL:HG11 | 3:D:1474:ALA:HB1 | 1.88                     | 0.54              |
| 3:D:1398:TRP:HA   | 3:D:1398:TRP:HE3 | 1.73                     | 0.54              |
| 1:K:19:GLU:HA     | 1:K:201:THR:O    | 2.07                     | 0.54              |
| 1:K:185:ARG:HG3   | 1:K:185:ARG:O    | 2.08                     | 0.54              |
| 1:L:55:SER:OG     | 1:L:166:PRO:HA   | 2.07                     | 0.54              |
| 2:M:5:ARG:HA      | 2:M:902:ILE:O    | 2.08                     | 0.54              |
| 2:M:73:LEU:HD12   | 2:M:74:GLY:N     | 2.23                     | 0.54              |
| 2:M:148:PHE:CE1   | 2:M:309:TYR:HD2  | 2.26                     | 0.54              |
| 2:M:267:TYR:CE1   | 2:M:273:GLY:HA3  | 2.43                     | 0.54              |
| 2:M:975:TYR:HA    | 2:M:982:PRO:HA   | 1.90                     | 0.54              |
| 3:N:65:ARG:HG3    | 3:N:66:GLN:H     | 1.72                     | 0.54              |
| 3:N:493:ARG:HH22  | 3:N:1392:GLY:H   | 1.54                     | 0.54              |
| 3:N:1211:MET:CE   | 3:N:1213:ARG:HB3 | 2.38                     | 0.54              |
| 3:N:1283:ILE:HB   | 3:N:1315:ASP:OD1 | 2.08                     | 0.54              |
| 5:G:2:DT:OP2      | 5:G:2:DT:H4'     | 2.07                     | 0.54              |
| 1:A:39:PRO:HG3    | 1:B:39:PRO:HG2   | 1.87                     | 0.54              |
| 3:D:1492:LEU:HD12 | 3:D:1493:LYS:CE  | 2.38                     | 0.54              |
| 2:M:157:ARG:HD3   | 2:M:314:THR:HG22 | 1.90                     | 0.54              |
| 2:M:399:ASN:O     | 2:M:402:SER:N    | 2.41                     | 0.54              |
| 2:M:503:LEU:HD23  | 2:M:507:ARG:O    | 2.07                     | 0.54              |
| 2:M:512:ARG:HD3   | 2:M:523:ILE:HD11 | 1.89                     | 0.54              |
| 3:N:964:LEU:O     | 3:N:968:ASP:HB2  | 2.08                     | 0.54              |
| 3:N:970:LYS:HD3   | 3:N:995:LEU:HD13 | 1.89                     | 0.54              |
| 3:N:1031:ASN:ND2  | 3:N:1034:GLN:HG3 | 2.23                     | 0.54              |
| 2:C:18:LEU:HD12   | 2:C:18:LEU:N     | 2.15                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:739:GLU:CB    | 2:C:742:VAL:HB    | 2.37                     | 0.54              |
| 2:C:926:PHE:CD2   | 2:C:960:GLU:OE2   | 2.61                     | 0.54              |
| 2:C:1081:VAL:HB   | 2:C:1086:ARG:HH21 | 1.73                     | 0.54              |
| 3:D:117:ASP:HB2   | 3:D:495:ARG:CZ    | 2.37                     | 0.54              |
| 3:D:487:ALA:N     | 5:G:8:DC:OP2      | 2.41                     | 0.54              |
| 3:D:1031:ASN:CB   | 3:D:1034:GLN:HB3  | 2.38                     | 0.54              |
| 3:D:1197:ARG:HB3  | 3:D:1396:GLU:OE2  | 2.08                     | 0.54              |
| 2:M:91:GLN:HB3    | 2:M:118:ILE:C     | 2.33                     | 0.54              |
| 2:M:471:TYR:CE2   | 2:M:496:ILE:HG21  | 2.42                     | 0.54              |
| 2:M:754:ILE:HD12  | 2:M:789:SER:CB    | 2.37                     | 0.54              |
| 3:N:148:GLU:HG2   | 3:N:151:GLN:HB2   | 1.90                     | 0.54              |
| 3:N:568:ARG:HE    | 3:N:572:ARG:HG2   | 1.73                     | 0.54              |
| 3:N:683:ILE:CG2   | 3:N:684:LYS:N     | 2.71                     | 0.54              |
| 3:N:845:ASN:ND2   | 3:N:846:PRO:HD2   | 2.22                     | 0.54              |
| 3:N:1098:LEU:HD23 | 3:N:1226:ALA:CA   | 2.30                     | 0.54              |
| 5:G:16:DT:C2      | 5:G:17:DA:N7      | 2.75                     | 0.54              |
| 1:A:124:ASN:OD1   | 1:A:127:LEU:HB2   | 2.08                     | 0.53              |
| 1:B:179:PHE:N     | 1:B:179:PHE:HD2   | 2.06                     | 0.53              |
| 1:B:184:THR:O     | 1:B:192:LEU:HB2   | 2.08                     | 0.53              |
| 2:C:433:THR:HG21  | 2:C:488:ALA:HB1   | 1.90                     | 0.53              |
| 2:C:460:ARG:HH11  | 2:C:460:ARG:HG3   | 1.74                     | 0.53              |
| 2:C:1018:GLN:HG2  | 3:D:87:ARG:NH2    | 2.23                     | 0.53              |
| 3:D:41:ARG:HD3    | 3:D:42:ASP:N      | 2.23                     | 0.53              |
| 3:D:583:ASP:CG    | 3:D:586:ARG:HG2   | 2.34                     | 0.53              |
| 3:D:814:ALA:HB1   | 3:D:818:ARG:NH2   | 2.13                     | 0.53              |
| 3:D:1114:THR:O    | 3:D:1114:THR:CG2  | 2.56                     | 0.53              |
| 3:D:1197:ARG:HB3  | 3:D:1396:GLU:CD   | 2.33                     | 0.53              |
| 1:K:99:LEU:HB2    | 1:K:142:VAL:HG23  | 1.90                     | 0.53              |
| 1:L:179:PHE:N     | 1:L:179:PHE:CD2   | 2.74                     | 0.53              |
| 2:M:198:ARG:HD2   | 2:M:204:GLN:OE1   | 2.07                     | 0.53              |
| 2:M:1102:LEU:O    | 3:N:5:VAL:CG1     | 2.56                     | 0.53              |
| 3:N:36:THR:O      | 3:N:38:LYS:N      | 2.39                     | 0.53              |
| 3:N:117:ASP:HB2   | 3:N:495:ARG:HH12  | 1.73                     | 0.53              |
| 4:O:45:ARG:HG2    | 4:O:46:PRO:HD2    | 1.90                     | 0.53              |
| 1:A:36:LEU:C      | 1:A:39:PRO:HD2    | 2.34                     | 0.53              |
| 1:B:52:ALA:HB2    | 1:B:170:VAL:O     | 2.07                     | 0.53              |
| 2:C:265:ARG:HG2   | 2:C:267:TYR:N     | 2.22                     | 0.53              |
| 2:C:274:ARG:HH21  | 2:C:284:ARG:HA    | 1.73                     | 0.53              |
| 2:C:516:ARG:NE    | 3:D:1068:LEU:HD22 | 2.22                     | 0.53              |
| 2:C:580:MET:HE2   | 2:C:902:ILE:HG12  | 1.90                     | 0.53              |
| 2:C:714:ASP:OD1   | 2:C:719:PRO:HG3   | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:893:ALA:HB1   | 2:C:897:LEU:HD12  | 1.90                     | 0.53              |
| 2:C:1006:HIS:HA   | 2:C:1027:PHE:HD1  | 1.73                     | 0.53              |
| 2:C:1040:LEU:HD23 | 2:C:1049:LEU:CD1  | 2.37                     | 0.53              |
| 3:D:54:LYS:HG2    | 3:D:57:GLU:OE1    | 2.08                     | 0.53              |
| 3:D:1472:ILE:C    | 3:D:1474:ALA:N    | 2.66                     | 0.53              |
| 4:E:57:ASP:H      | 4:E:58:PRO:HD3    | 1.73                     | 0.53              |
| 1:K:42:ARG:HH12   | 1:L:34:VAL:CB     | 2.21                     | 0.53              |
| 1:K:174:VAL:HG22  | 1:K:201:THR:HG22  | 1.89                     | 0.53              |
| 1:L:26:GLU:HB3    | 1:L:194:LYS:HA    | 1.90                     | 0.53              |
| 2:M:143:SER:OG    | 2:M:147:TYR:OH    | 2.24                     | 0.53              |
| 2:M:1075:ASP:OD2  | 4:O:31:LEU:HD13   | 2.07                     | 0.53              |
| 3:N:505:SER:OG    | 3:N:1454:GLY:N    | 2.41                     | 0.53              |
| 1:A:49:PRO:HB3    | 1:A:148:VAL:HG22  | 1.91                     | 0.53              |
| 1:B:206:THR:HG22  | 1:B:209:GLU:H     | 1.73                     | 0.53              |
| 2:C:31:GLN:NE2    | 2:C:38:LYS:HB2    | 2.24                     | 0.53              |
| 2:C:327:HIS:HA    | 2:C:431:HIS:CD2   | 2.44                     | 0.53              |
| 2:C:395:LYS:O     | 2:C:397:GLU:HG3   | 2.08                     | 0.53              |
| 2:C:693:GLU:O     | 2:C:697:ARG:HG2   | 2.08                     | 0.53              |
| 2:C:1040:LEU:HD23 | 2:C:1049:LEU:HD13 | 1.90                     | 0.53              |
| 3:D:741:ASP:OD2   | 6:H:14:G:H5'      | 2.09                     | 0.53              |
| 3:D:1107:VAL:HG12 | 3:D:1217:ILE:HG23 | 1.90                     | 0.53              |
| 3:D:1200:VAL:HG12 | 3:D:1201:CYS:O    | 2.09                     | 0.53              |
| 3:D:1397:LYS:NZ   | 3:D:1432:LYS:HE3  | 2.18                     | 0.53              |
| 3:D:1442:ASN:CG   | 3:D:1444:THR:OG1  | 2.52                     | 0.53              |
| 4:E:23:VAL:O      | 4:E:26:ARG:HB3    | 2.08                     | 0.53              |
| 2:M:406:HIS:CD2   | 2:M:409:ARG:HH21  | 2.26                     | 0.53              |
| 2:M:437:ARG:CZ    | 2:M:488:ALA:HA    | 2.38                     | 0.53              |
| 2:M:697:ARG:O     | 2:M:697:ARG:HG3   | 2.09                     | 0.53              |
| 2:M:939:ARG:HD3   | 2:M:982:PRO:HD3   | 1.89                     | 0.53              |
| 2:M:1034:GLU:HA   | 2:M:1037:VAL:HG23 | 1.90                     | 0.53              |
| 4:O:54:LEU:HD23   | 4:O:54:LEU:O      | 2.08                     | 0.53              |
| 7:I:11:DG:H2'     | 7:I:12:DT:C7      | 2.37                     | 0.53              |
| 7:Z:1:DG:H3'      | 7:Z:1:DG:OP1      | 2.08                     | 0.53              |
| 2:C:172:ILE:HD12  | 2:C:172:ILE:N     | 2.23                     | 0.53              |
| 2:C:676:ILE:HG21  | 2:C:988:VAL:HG13  | 1.88                     | 0.53              |
| 2:C:1035:MET:C    | 3:D:707:THR:HB    | 2.33                     | 0.53              |
| 3:D:701:LEU:O     | 3:D:747:VAL:HG23  | 2.08                     | 0.53              |
| 3:D:744:GLN:C     | 3:D:745:MET:HG3   | 2.34                     | 0.53              |
| 3:D:857:ILE:HG22  | 3:D:858:VAL:HG13  | 1.91                     | 0.53              |
| 1:K:34:VAL:HG13   | 1:K:35:THR:N      | 2.22                     | 0.53              |
| 2:M:17:PRO:O      | 2:M:20:GLU:HB3    | 2.08                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:1048:THR:O    | 2:M:1052:MET:SD  | 2.66                     | 0.53              |
| 3:N:55:ASP:HB3    | 3:N:82:LYS:NZ    | 2.24                     | 0.53              |
| 3:N:482:LYS:CE    | 3:N:1384:PRO:HD2 | 2.34                     | 0.53              |
| 3:N:520:LEU:CD1   | 3:N:521:PRO:HD2  | 2.38                     | 0.53              |
| 3:N:1122:LEU:HD13 | 3:N:1184:GLN:O   | 2.08                     | 0.53              |
| 3:N:1496:GLU:CD   | 3:N:1500:LYS:HE3 | 2.33                     | 0.53              |
| 1:A:63:HIS:HE1    | 1:A:65:PHE:O     | 1.91                     | 0.53              |
| 1:B:36:LEU:O      | 1:B:39:PRO:HD2   | 2.09                     | 0.53              |
| 1:B:48:ILE:HD13   | 1:B:210:ALA:HB1  | 1.91                     | 0.53              |
| 2:C:124:ASP:OD1   | 2:C:126:SER:N    | 2.25                     | 0.53              |
| 2:C:140:ILE:HG23  | 2:C:410:ILE:HD13 | 1.90                     | 0.53              |
| 2:C:164:PRO:HD2   | 2:C:170:PRO:O    | 2.08                     | 0.53              |
| 2:C:277:ALA:O     | 2:C:278:GLU:C    | 2.51                     | 0.53              |
| 2:C:336:VAL:N     | 2:C:339:LEU:HD12 | 2.23                     | 0.53              |
| 2:C:431:HIS:N     | 2:C:434:HIS:CE1  | 2.72                     | 0.53              |
| 2:C:854:PRO:HB2   | 2:C:856:GLU:CD   | 2.32                     | 0.53              |
| 3:D:133:ILE:HA    | 3:D:456:MET:CB   | 2.37                     | 0.53              |
| 3:D:880:ILE:HD13  | 3:D:880:ILE:O    | 2.08                     | 0.53              |
| 3:D:1161:GLU:CD   | 3:D:1161:GLU:H   | 2.17                     | 0.53              |
| 3:D:1197:ARG:CD   | 3:D:1198:TYR:H   | 2.21                     | 0.53              |
| 1:K:152:PRO:HD2   | 1:K:155:LYS:HB2  | 1.90                     | 0.53              |
| 1:L:59:GLU:HB2    | 1:L:137:ARG:HH22 | 1.73                     | 0.53              |
| 2:M:570:PRO:CD    | 2:M:635:THR:HG21 | 2.36                     | 0.53              |
| 2:M:758:ARG:HG2   | 2:M:788:THR:OG1  | 2.08                     | 0.53              |
| 2:M:854:PRO:HB2   | 2:M:856:GLU:CD   | 2.33                     | 0.53              |
| 2:M:972:VAL:HG23  | 2:M:974:LEU:HD13 | 1.90                     | 0.53              |
| 3:N:6:ARG:C       | 3:N:7:LYS:HG3    | 2.33                     | 0.53              |
| 3:N:111:LYS:HE2   | 3:N:1445:HIS:CD2 | 2.44                     | 0.53              |
| 3:N:113:GLY:O     | 3:N:116:LEU:O    | 2.26                     | 0.53              |
| 3:N:143:ASN:OD1   | 3:N:145:VAL:HG12 | 2.08                     | 0.53              |
| 3:N:701:LEU:HD12  | 3:N:701:LEU:N    | 2.12                     | 0.53              |
| 3:N:1019:PRO:O    | 3:N:1023:MET:HB2 | 2.08                     | 0.53              |
| 3:N:1365:ASP:O    | 3:N:1369:GLU:HG3 | 2.09                     | 0.53              |
| 3:N:1472:ILE:O    | 3:N:1477:GLY:HA3 | 2.08                     | 0.53              |
| 5:X:26:DC:N3      | 5:X:27:DC:N4     | 2.56                     | 0.53              |
| 2:C:503:LEU:HD23  | 2:C:507:ARG:O    | 2.08                     | 0.53              |
| 2:C:537:LYS:HZ1   | 2:C:904:PRO:HB3  | 1.74                     | 0.53              |
| 2:C:572:ILE:HG23  | 2:C:703:ILE:HD13 | 1.89                     | 0.53              |
| 2:C:1062:GLY:O    | 2:C:1066:ALA:CB  | 2.57                     | 0.53              |
| 2:M:292:ARG:HH11  | 2:M:299:LYS:HD3  | 1.74                     | 0.53              |
| 2:M:460:ARG:HG2   | 2:M:485:TYR:CD2  | 2.43                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:683:ASN:HB2   | 2:M:872:ASN:HB2   | 1.89                     | 0.53              |
| 2:M:1013:TYR:CD2  | 2:M:1063:ARG:NH2  | 2.77                     | 0.53              |
| 3:N:400:VAL:HG22  | 3:N:443:VAL:HG21  | 1.91                     | 0.53              |
| 3:N:682:ASP:C     | 3:N:683:ILE:HG13  | 2.34                     | 0.53              |
| 3:N:688:TRP:CE3   | 3:N:688:TRP:HA    | 2.44                     | 0.53              |
| 3:N:756:GLN:HG3   | 4:O:61:VAL:HG21   | 1.90                     | 0.53              |
| 3:N:1441:GLN:HG2  | 3:N:1442:ASN:H    | 1.73                     | 0.53              |
| 5:G:9:DC:O5'      | 5:G:9:DC:H6       | 1.89                     | 0.53              |
| 6:Y:1:C:H2'       | 6:Y:2:C:C6        | 2.44                     | 0.53              |
| 1:A:57:TYR:CZ     | 1:A:161:ARG:HG2   | 2.43                     | 0.53              |
| 1:A:62:LEU:HD12   | 1:A:62:LEU:N      | 2.23                     | 0.53              |
| 1:A:199:ILE:HD12  | 1:A:199:ILE:N     | 2.24                     | 0.53              |
| 1:B:24:VAL:CG1    | 1:B:196:THR:HG22  | 2.36                     | 0.53              |
| 2:C:195:LEU:O     | 2:C:199:VAL:HG23  | 2.08                     | 0.53              |
| 2:C:561:GLY:O     | 2:C:565:GLN:HG3   | 2.07                     | 0.53              |
| 2:C:762:LYS:NZ    | 2:C:786:LYS:HG3   | 2.24                     | 0.53              |
| 3:D:465:LEU:HA    | 3:D:468:LEU:HD12  | 1.91                     | 0.53              |
| 3:D:720:LEU:H     | 3:D:720:LEU:HD12  | 1.74                     | 0.53              |
| 3:D:983:LEU:H     | 3:D:983:LEU:CD2   | 2.22                     | 0.53              |
| 1:L:105:GLY:O     | 1:L:132:LEU:HB3   | 2.08                     | 0.53              |
| 2:M:295:ASP:HB2   | 2:M:297:GLU:OE2   | 2.09                     | 0.53              |
| 2:M:1033:GLY:O    | 2:M:1037:VAL:HG23 | 2.08                     | 0.53              |
| 2:M:1081:VAL:HB   | 2:M:1086:ARG:HE   | 1.74                     | 0.53              |
| 2:M:1088:LEU:HD23 | 2:M:1088:LEU:C    | 2.33                     | 0.53              |
| 3:N:568:ARG:HG3   | 3:N:572:ARG:HE    | 1.72                     | 0.53              |
| 3:N:871:LYS:CB    | 3:N:873:LEU:HD21  | 2.39                     | 0.53              |
| 3:N:1118:ILE:HG13 | 3:N:1192:LEU:HD12 | 1.90                     | 0.53              |
| 3:N:1132:LEU:N    | 3:N:1132:LEU:HD12 | 2.24                     | 0.53              |
| 6:Y:9:C:H2'       | 6:Y:10:G:H5'      | 1.91                     | 0.53              |
| 2:C:68:PHE:C      | 2:C:69:LEU:HD23   | 2.33                     | 0.53              |
| 2:C:1037:VAL:O    | 2:C:1041:GLU:HG3  | 2.09                     | 0.53              |
| 3:D:16:GLU:HA     | 3:D:19:ARG:HG2    | 1.89                     | 0.53              |
| 3:D:483:HIS:HB2   | 3:D:484:PRO:CD    | 2.34                     | 0.53              |
| 3:D:698:LYS:HD2   | 4:E:59:ASN:OD1    | 2.09                     | 0.53              |
| 2:M:7:GLY:HA2     | 2:M:907:ASP:O     | 2.09                     | 0.53              |
| 2:M:135:VAL:O     | 2:M:392:SER:HA    | 2.08                     | 0.53              |
| 2:M:195:LEU:HG    | 2:M:238:LEU:HG    | 1.90                     | 0.53              |
| 2:M:244:PRO:HG2   | 2:M:246:ASP:OD2   | 2.08                     | 0.53              |
| 2:M:603:VAL:O     | 2:M:646:GLY:HA2   | 2.09                     | 0.53              |
| 2:M:714:ASP:OD2   | 2:M:820:ARG:HB2   | 2.09                     | 0.53              |
| 2:M:878:SER:OG    | 3:N:1029:ARG:NH2  | 2.42                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1093:TYR:HE2  | 3:N:1440:PHE:HE2  | 1.57                     | 0.53              |
| 3:N:1096:ARG:HH22 | 5:X:18:DC:P       | 2.32                     | 0.53              |
| 3:N:1504:GLU:O    | 3:N:1505:ALA:C    | 2.52                     | 0.53              |
| 7:I:3:DA:C1'      | 7:I:4:DG:H5'      | 2.21                     | 0.53              |
| 5:X:13:DA:C2'     | 5:X:13:DA:O5'     | 2.55                     | 0.53              |
| 1:A:170:VAL:HG23  | 1:A:170:VAL:O     | 2.09                     | 0.53              |
| 2:C:145:GLY:CA    | 2:C:276:LYS:HD3   | 2.39                     | 0.53              |
| 2:C:332:ARG:HG2   | 2:C:333:ILE:N     | 2.23                     | 0.53              |
| 2:C:688:ILE:HD11  | 2:C:847:GLY:HA3   | 1.90                     | 0.53              |
| 3:D:52:PRO:HD2    | 3:D:85:VAL:HG23   | 1.89                     | 0.53              |
| 3:D:907:GLU:OE1   | 3:D:909:ASN:HB2   | 2.09                     | 0.53              |
| 4:E:54:LEU:CA     | 4:E:58:PRO:HG2    | 2.36                     | 0.53              |
| 1:K:50:GLY:CA     | 1:K:173:PRO:HG3   | 2.38                     | 0.53              |
| 1:K:199:ILE:N     | 1:K:199:ILE:HD12  | 2.23                     | 0.53              |
| 2:M:26:TYR:O      | 2:M:30:LEU:HG     | 2.09                     | 0.53              |
| 2:M:274:ARG:HG3   | 2:M:274:ARG:NH1   | 2.23                     | 0.53              |
| 2:M:302:VAL:O     | 2:M:306:THR:HG23  | 2.09                     | 0.53              |
| 2:M:345:ARG:HA    | 2:M:348:LEU:HB2   | 1.90                     | 0.53              |
| 3:N:133:ILE:HG22  | 3:N:134:VAL:H     | 1.74                     | 0.53              |
| 3:N:708:LEU:HB3   | 3:N:1231:GLU:HB2  | 1.90                     | 0.53              |
| 3:N:767:HIS:NE2   | 4:O:6:ILE:HD13    | 2.23                     | 0.53              |
| 3:N:901:GLN:HG3   | 3:N:901:GLN:O     | 2.09                     | 0.53              |
| 6:H:6:C:C5        | 6:H:7:G:C5        | 2.97                     | 0.53              |
| 1:B:23:PHE:HZ     | 1:B:207:PRO:HB2   | 1.74                     | 0.53              |
| 1:B:59:GLU:HG2    | 1:B:139:ASN:HD22  | 1.73                     | 0.53              |
| 2:C:69:LEU:HD12   | 2:C:97:ARG:CB     | 2.24                     | 0.53              |
| 2:C:532:MET:CG    | 2:C:533:ASP:N     | 2.71                     | 0.53              |
| 2:C:683:ASN:O     | 2:C:872:ASN:CB    | 2.53                     | 0.53              |
| 2:C:850:ALA:HA    | 3:D:632:VAL:CG1   | 2.39                     | 0.53              |
| 2:C:1105:LYS:O    | 2:C:1105:LYS:HD2  | 2.08                     | 0.53              |
| 3:D:799:LYS:HE2   | 3:D:824:ASN:O     | 2.08                     | 0.53              |
| 3:D:875:THR:HG22  | 3:D:876:SER:N     | 2.24                     | 0.53              |
| 3:D:897:TRP:CA    | 3:D:900:ILE:CD1   | 2.81                     | 0.53              |
| 3:D:911:LEU:O     | 3:D:915:VAL:HG23  | 2.09                     | 0.53              |
| 1:K:96:THR:HG23   | 1:K:96:THR:O      | 2.07                     | 0.53              |
| 2:M:6:PHE:HD1     | 2:M:903:SER:HA    | 1.74                     | 0.53              |
| 2:M:129:ILE:CD1   | 2:M:134:ARG:HB2   | 2.36                     | 0.53              |
| 2:M:516:ARG:NH1   | 3:N:1068:LEU:HD22 | 2.23                     | 0.53              |
| 2:M:791:ARG:O     | 2:M:793:PRO:HD3   | 2.09                     | 0.53              |
| 2:M:861:LEU:HD23  | 2:M:862:PRO:CD    | 2.38                     | 0.53              |
| 2:M:976:ASP:OD1   | 2:M:978:ARG:HB2   | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:19:ARG:HH21   | 3:N:516:ALA:CB    | 1.99                     | 0.53              |
| 3:N:470:LEU:HD12  | 3:N:503:LEU:CD2   | 2.39                     | 0.53              |
| 3:N:637:LEU:HD11  | 3:N:641:GLN:C     | 2.34                     | 0.53              |
| 3:N:1068:LEU:O    | 3:N:1072:ILE:HG12 | 2.09                     | 0.53              |
| 3:N:1438:ALA:HA   | 3:N:1446:VAL:HG21 | 1.90                     | 0.53              |
| 2:C:165:LEU:HB3   | 2:C:265:ARG:CZ    | 2.39                     | 0.52              |
| 2:C:211:LEU:HD13  | 2:C:308:ARG:HA    | 1.91                     | 0.52              |
| 2:C:250:ARG:HD3   | 2:C:253:ALA:HB3   | 1.89                     | 0.52              |
| 2:C:403:SER:O     | 2:C:407:LYS:HG3   | 2.09                     | 0.52              |
| 2:C:752:GLY:O     | 3:D:679:ARG:HG2   | 2.08                     | 0.52              |
| 3:D:50:PHE:CD2    | 3:D:521:PRO:HA    | 2.44                     | 0.52              |
| 3:D:553:ARG:O     | 3:D:557:LEU:HG    | 2.09                     | 0.52              |
| 3:D:706:PRO:HG2   | 6:H:15:C:O2       | 2.08                     | 0.52              |
| 3:D:900:ILE:O     | 3:D:902:LEU:HD22  | 2.08                     | 0.52              |
| 3:D:1045:MET:HG2  | 3:D:1073:SER:HA   | 1.91                     | 0.52              |
| 1:K:50:GLY:HA3    | 1:K:171:PHE:O     | 2.09                     | 0.52              |
| 1:L:46:SER:O      | 1:L:148:VAL:HB    | 2.09                     | 0.52              |
| 2:M:83:CYS:HA     | 2:M:88:LEU:HB2    | 1.92                     | 0.52              |
| 2:M:230:ARG:HG2   | 2:M:230:ARG:HH11  | 1.75                     | 0.52              |
| 2:M:405:ARG:NH1   | 2:M:566:THR:HG21  | 2.24                     | 0.52              |
| 2:M:683:ASN:HA    | 2:M:687:ALA:O     | 2.10                     | 0.52              |
| 2:M:684:PHE:HD2   | 3:N:740:PHE:HD1   | 1.57                     | 0.52              |
| 2:M:843:HIS:CE1   | 2:M:887:GLU:OE2   | 2.62                     | 0.52              |
| 3:N:1280:VAL:HB   | 3:N:1316:GLY:O    | 2.09                     | 0.52              |
| 3:N:1395:LEU:HD23 | 3:N:1396:GLU:N    | 2.24                     | 0.52              |
| 6:Y:6:C:N4        | 6:Y:7:G:C6        | 2.77                     | 0.52              |
| 2:C:71:TYR:H      | 2:C:71:TYR:HD2    | 1.54                     | 0.52              |
| 2:C:264:PRO:HB3   | 2:C:289:THR:CB    | 2.39                     | 0.52              |
| 2:C:398:THR:HB    | 2:C:399:ASN:HD22  | 1.73                     | 0.52              |
| 2:C:515:ALA:C     | 2:C:516:ARG:HD3   | 2.34                     | 0.52              |
| 2:C:644:VAL:HG22  | 2:C:647:GLN:OE1   | 2.09                     | 0.52              |
| 2:C:1056:LYS:HD3  | 3:D:623:VAL:CG1   | 2.39                     | 0.52              |
| 3:D:486:ARG:O     | 3:D:490:ALA:HB2   | 2.08                     | 0.52              |
| 3:D:618:LEU:HD12  | 3:D:1467:ILE:HD11 | 1.89                     | 0.52              |
| 3:D:637:LEU:HD21  | 3:D:642:CYS:HA    | 1.91                     | 0.52              |
| 3:D:705:ALA:HB1   | 6:H:14:G:C2       | 2.27                     | 0.52              |
| 3:D:1103:HIS:CD2  | 3:D:1104:GLU:H    | 2.25                     | 0.52              |
| 3:D:1380:GLU:CG   | 3:D:1381:VAL:H    | 2.20                     | 0.52              |
| 1:K:49:PRO:HA     | 1:K:148:VAL:HG22  | 1.91                     | 0.52              |
| 2:M:211:LEU:HD13  | 2:M:308:ARG:CG    | 2.39                     | 0.52              |
| 2:M:340:MET:SD    | 2:M:340:MET:C     | 2.93                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:758:ARG:CZ    | 2:M:788:THR:HB    | 2.39                     | 0.52              |
| 2:M:878:SER:HB3   | 3:N:1029:ARG:HG3  | 1.91                     | 0.52              |
| 3:N:539:ASP:OD2   | 3:N:539:ASP:N     | 2.36                     | 0.52              |
| 2:C:6:PHE:N       | 2:C:6:PHE:CD1     | 2.76                     | 0.52              |
| 2:C:31:GLN:CD     | 2:C:71:TYR:OH     | 2.51                     | 0.52              |
| 2:C:260:LEU:HD12  | 2:C:261:ILE:N     | 2.24                     | 0.52              |
| 2:C:846:LYS:HD3   | 6:H:14:G:OP1      | 2.09                     | 0.52              |
| 2:C:862:PRO:HA    | 2:C:975:TYR:CE1   | 2.45                     | 0.52              |
| 2:C:1038:TRP:O    | 2:C:1041:GLU:HB2  | 2.08                     | 0.52              |
| 3:D:25:GLU:HG3    | 3:D:92:HIS:O      | 2.09                     | 0.52              |
| 3:D:30:GLU:HB3    | 3:D:40:GLU:CB     | 2.39                     | 0.52              |
| 3:D:134:VAL:HG22  | 3:D:455:ARG:O     | 2.08                     | 0.52              |
| 3:D:860:LEU:HB2   | 3:D:861:GLN:OE1   | 2.10                     | 0.52              |
| 3:D:1094:LEU:HD22 | 3:D:1256:LEU:HD11 | 1.90                     | 0.52              |
| 3:D:1388:ARG:H    | 3:D:1388:ARG:CD   | 2.22                     | 0.52              |
| 1:K:189:ARG:HH11  | 1:K:189:ARG:HG3   | 1.74                     | 0.52              |
| 2:M:7:GLY:N       | 2:M:904:PRO:HD2   | 2.13                     | 0.52              |
| 2:M:274:ARG:HG3   | 2:M:285:LEU:HD22  | 1.91                     | 0.52              |
| 2:M:428:ARG:NH1   | 2:M:449:ILE:HG22  | 2.24                     | 0.52              |
| 2:M:1008:ARG:HA   | 3:N:651:GLU:OE2   | 2.09                     | 0.52              |
| 3:N:785:ILE:HD11  | 3:N:939:PHE:CE2   | 2.45                     | 0.52              |
| 3:N:845:ASN:CG    | 3:N:846:PRO:CD    | 2.82                     | 0.52              |
| 4:O:16:LYS:HG2    | 4:O:17:TYR:N      | 2.22                     | 0.52              |
| 4:O:23:VAL:HG22   | 4:O:68:LEU:HD22   | 1.91                     | 0.52              |
| 5:G:7:DA:H2'      | 5:G:8:DC:C6       | 2.44                     | 0.52              |
| 7:I:5:DC:O5'      | 7:I:5:DC:H6       | 1.91                     | 0.52              |
| 2:C:66:LEU:HD12   | 2:C:99:GLN:O      | 2.10                     | 0.52              |
| 2:C:305:PRO:HA    | 2:C:308:ARG:HB2   | 1.92                     | 0.52              |
| 2:C:567:GLN:NE2   | 6:H:12:U:O2'      | 2.41                     | 0.52              |
| 2:C:635:THR:O     | 2:C:705:ILE:HD12  | 2.09                     | 0.52              |
| 2:C:1042:ALA:HB1  | 3:D:710:ARG:HB3   | 1.89                     | 0.52              |
| 3:D:29:PRO:HD3    | 3:D:548:ILE:HG21  | 1.92                     | 0.52              |
| 3:D:30:GLU:HB2    | 3:D:41:ARG:CG     | 2.39                     | 0.52              |
| 3:D:630:VAL:HG12  | 3:D:631:ILE:N     | 2.23                     | 0.52              |
| 3:D:764:LEU:HD11  | 3:D:766:ALA:HB3   | 1.91                     | 0.52              |
| 3:D:1440:PHE:CG   | 3:D:1441:GLN:N    | 2.77                     | 0.52              |
| 3:D:1462:LEU:N    | 3:D:1462:LEU:HD23 | 2.25                     | 0.52              |
| 2:M:6:PHE:CD1     | 2:M:903:SER:HA    | 2.45                     | 0.52              |
| 2:M:12:VAL:HG22   | 2:M:13:ILE:HG23   | 1.90                     | 0.52              |
| 2:M:35:PRO:C      | 2:M:37:GLU:H      | 2.17                     | 0.52              |
| 2:M:77:PRO:HD2    | 2:M:91:GLN:O      | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:163:ILE:HD12  | 2:M:163:ILE:C     | 2.34                     | 0.52              |
| 2:M:395:LYS:HE2   | 2:M:403:SER:CB    | 2.31                     | 0.52              |
| 2:M:436:GLY:HA2   | 2:M:539:VAL:HA    | 1.92                     | 0.52              |
| 2:M:714:ASP:OD1   | 2:M:820:ARG:HD2   | 2.09                     | 0.52              |
| 2:M:1062:GLY:O    | 2:M:1066:ALA:CB   | 2.57                     | 0.52              |
| 3:N:99:ALA:HA     | 3:N:458:ALA:CB    | 2.40                     | 0.52              |
| 3:N:646:LYS:CB    | 3:N:688:TRP:CH2   | 2.93                     | 0.52              |
| 3:N:1128:VAL:C    | 3:N:1129:THR:HG22 | 2.34                     | 0.52              |
| 1:A:161:ARG:NH1   | 1:A:161:ARG:HB2   | 2.25                     | 0.52              |
| 2:C:287:GLY:O     | 2:C:288:ARG:C     | 2.52                     | 0.52              |
| 2:C:1030:GLN:OE1  | 3:D:628:ARG:HD3   | 2.09                     | 0.52              |
| 3:D:613:ARG:HH11  | 3:D:616:GLN:CG    | 2.20                     | 0.52              |
| 3:D:714:GLN:HB3   | 3:D:765:SER:HB3   | 1.91                     | 0.52              |
| 3:D:1084:THR:CA   | 3:D:1087:ARG:HG2  | 2.40                     | 0.52              |
| 3:D:1335:LEU:HD12 | 3:D:1335:LEU:O    | 2.09                     | 0.52              |
| 3:D:1388:ARG:N    | 3:D:1388:ARG:CD   | 2.68                     | 0.52              |
| 1:K:72:LYS:O      | 2:M:608:GLY:CA    | 2.58                     | 0.52              |
| 1:K:206:THR:HG23  | 1:K:209:GLU:H     | 1.73                     | 0.52              |
| 2:M:422:ARG:HB3   | 7:Z:1:DG:N3       | 2.24                     | 0.52              |
| 2:M:433:THR:HG22  | 2:M:437:ARG:NH1   | 2.24                     | 0.52              |
| 2:M:518:LYS:HB3   | 2:M:518:LYS:NZ    | 2.23                     | 0.52              |
| 2:M:524:VAL:HG12  | 2:M:525:SER:H     | 1.74                     | 0.52              |
| 2:M:685:GLU:OE2   | 3:N:783:ARG:NH1   | 2.43                     | 0.52              |
| 2:M:767:PRO:CB    | 2:M:772:ARG:HH21  | 2.22                     | 0.52              |
| 3:N:405:ASP:HB2   | 3:N:423:ASP:OD1   | 2.09                     | 0.52              |
| 3:N:697:GLY:O     | 3:N:699:VAL:HG13  | 2.09                     | 0.52              |
| 3:N:804:LEU:HD12  | 3:N:830:ALA:O     | 2.10                     | 0.52              |
| 3:N:1106:VAL:HG12 | 3:N:1107:VAL:N    | 2.24                     | 0.52              |
| 3:N:1340:GLY:O    | 3:N:1344:VAL:HG22 | 2.10                     | 0.52              |
| 5:G:6:DT:OP1      | 5:G:6:DT:C4'      | 2.54                     | 0.52              |
| 6:Y:6:C:C4        | 6:Y:7:G:C6        | 2.98                     | 0.52              |
| 1:A:35:THR:HG21   | 1:B:43:ILE:HG12   | 1.92                     | 0.52              |
| 2:C:92:ALA:HB2    | 2:C:120:LEU:HD21  | 1.92                     | 0.52              |
| 2:C:439:CYS:SG    | 2:C:541:SER:HB3   | 2.49                     | 0.52              |
| 2:C:957:LYS:CG    | 2:C:961:GLU:HB2   | 2.40                     | 0.52              |
| 2:C:987:ILE:HG12  | 3:D:948:THR:CG2   | 2.39                     | 0.52              |
| 3:D:794:GLN:OE1   | 3:D:905:PRO:HG2   | 2.09                     | 0.52              |
| 2:M:83:CYS:HA     | 2:M:88:LEU:CB     | 2.39                     | 0.52              |
| 2:M:384:GLU:O     | 2:M:388:ARG:HB2   | 2.09                     | 0.52              |
| 2:M:387:SER:OG    | 2:M:388:ARG:HD2   | 2.10                     | 0.52              |
| 2:M:905:ILE:N     | 2:M:905:ILE:HD12  | 2.25                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:1014:SER:O    | 2:M:1017:THR:O   | 2.27                     | 0.52              |
| 2:M:1031:ARG:HA   | 3:N:621:LYS:O    | 2.09                     | 0.52              |
| 3:N:806:PHE:HE1   | 3:N:813:LEU:HB3  | 1.74                     | 0.52              |
| 3:N:820:GLU:HA    | 3:N:825:ALA:O    | 2.09                     | 0.52              |
| 3:N:838:ARG:HH11  | 3:N:838:ARG:HG2  | 1.74                     | 0.52              |
| 3:N:1441:GLN:CG   | 3:N:1442:ASN:N   | 2.73                     | 0.52              |
| 5:X:12:DA:C2      | 5:X:13:DA:C2     | 2.97                     | 0.52              |
| 1:A:54:THR:HB     | 1:A:143:ARG:CG   | 2.39                     | 0.52              |
| 2:C:724:ARG:O     | 2:C:724:ARG:HG2  | 2.09                     | 0.52              |
| 2:C:729:LEU:HD13  | 3:D:675:ARG:HH11 | 1.74                     | 0.52              |
| 2:C:862:PRO:HD2   | 2:C:925:TYR:OH   | 2.09                     | 0.52              |
| 2:C:1037:VAL:CG1  | 2:C:1041:GLU:OE2 | 2.58                     | 0.52              |
| 2:C:1043:TYR:HE1  | 3:D:710:ARG:O    | 1.92                     | 0.52              |
| 3:D:42:ASP:OD2    | 3:D:48:ARG:NH2   | 2.33                     | 0.52              |
| 3:D:530:VAL:O     | 3:D:531:ASP:OD1  | 2.28                     | 0.52              |
| 3:D:640:HIS:NE2   | 3:D:717:GLN:CD   | 2.68                     | 0.52              |
| 3:D:1200:VAL:CG1  | 3:D:1201:CYS:N   | 2.72                     | 0.52              |
| 1:K:206:THR:CG2   | 1:K:209:GLU:H    | 2.22                     | 0.52              |
| 2:M:328:LEU:HD13  | 2:M:328:LEU:H    | 1.74                     | 0.52              |
| 2:M:405:ARG:NH2   | 2:M:566:THR:HG21 | 2.24                     | 0.52              |
| 2:M:577:PRO:HG3   | 2:M:993:PHE:CZ   | 2.45                     | 0.52              |
| 2:M:674:VAL:CG2   | 2:M:869:VAL:HG13 | 2.39                     | 0.52              |
| 3:N:472:ALA:HA    | 3:N:475:LYS:HD3  | 1.91                     | 0.52              |
| 3:N:646:LYS:NZ    | 3:N:688:TRP:CD1  | 2.70                     | 0.52              |
| 3:N:1161:GLU:H    | 3:N:1161:GLU:CD  | 2.17                     | 0.52              |
| 3:N:1479:ASP:CG   | 3:N:1482:ARG:NH2 | 2.67                     | 0.52              |
| 1:A:7:LYS:O       | 1:A:7:LYS:HG2    | 2.08                     | 0.52              |
| 1:A:178:ALA:HB3   | 1:A:198:ARG:HG3  | 1.92                     | 0.52              |
| 1:B:28:LEU:HG     | 1:B:193:ASP:O    | 2.10                     | 0.52              |
| 2:C:553:ASP:OD1   | 2:C:843:HIS:ND1  | 2.41                     | 0.52              |
| 2:C:829:GLN:O     | 2:C:831:ARG:N    | 2.41                     | 0.52              |
| 3:D:50:PHE:O      | 3:D:89:ARG:HD2   | 2.10                     | 0.52              |
| 3:D:699:VAL:HG22  | 3:D:756:GLN:OE1  | 2.09                     | 0.52              |
| 3:D:845:ASN:CG    | 3:D:846:PRO:HD2  | 2.35                     | 0.52              |
| 3:D:1225:ALA:HA   | 3:D:1367:HIS:CE1 | 2.45                     | 0.52              |
| 3:D:1234:THR:O    | 3:D:1235:GLN:C   | 2.51                     | 0.52              |
| 3:D:1435:LEU:HD13 | 3:D:1457:ASP:OD2 | 2.09                     | 0.52              |
| 2:M:10:ARG:HH11   | 2:M:10:ARG:N     | 2.08                     | 0.52              |
| 2:M:328:LEU:CD1   | 2:M:328:LEU:H    | 2.23                     | 0.52              |
| 2:M:749:VAL:C     | 2:M:750:LYS:HD2  | 2.35                     | 0.52              |
| 3:N:107:ASP:OD2   | 3:N:1445:HIS:HA  | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:520:LEU:HD11  | 3:N:524:LEU:CD2   | 2.40                     | 0.52              |
| 3:N:563:PRO:HG3   | 3:N:566:ILE:HD12  | 1.92                     | 0.52              |
| 3:N:821:VAL:HG22  | 3:N:840:LYS:NZ    | 2.25                     | 0.52              |
| 3:N:988:ARG:HD2   | 3:N:988:ARG:C     | 2.35                     | 0.52              |
| 3:N:1087:ARG:HG2  | 3:N:1087:ARG:HH11 | 1.74                     | 0.52              |
| 3:N:1088:THR:HG21 | 5:X:19:DG:C2      | 2.45                     | 0.52              |
| 3:N:1166:LEU:HD12 | 3:N:1171:VAL:HG22 | 1.92                     | 0.52              |
| 3:N:1227:GLN:C    | 3:N:1229:ILE:H    | 2.18                     | 0.52              |
| 5:G:13:DA:H2'     | 5:G:13:DA:O5'     | 2.10                     | 0.52              |
| 5:X:17:DA:H2'     | 5:X:17:DA:O5'     | 2.09                     | 0.52              |
| 6:Y:9:C:HO2'      | 6:Y:10:G:H5'      | 1.74                     | 0.52              |
| 2:C:426:ASP:HA    | 2:C:429:ASP:OD2   | 2.10                     | 0.52              |
| 2:C:578:VAL:HG13  | 2:C:671:ASN:CG    | 2.35                     | 0.52              |
| 2:C:634:GLY:O     | 2:C:705:ILE:HB    | 2.10                     | 0.52              |
| 2:C:729:LEU:CD1   | 3:D:675:ARG:HD2   | 2.40                     | 0.52              |
| 2:C:902:ILE:O     | 2:C:904:PRO:HD3   | 2.10                     | 0.52              |
| 2:C:1003:ASP:CG   | 2:C:1004:LYS:H    | 2.17                     | 0.52              |
| 3:D:17:LYS:HG2    | 3:D:21:TRP:HE1    | 1.75                     | 0.52              |
| 3:D:712:GLY:C     | 3:D:713:ILE:HG13  | 2.35                     | 0.52              |
| 3:D:781:PRO:HG2   | 3:D:911:LEU:HD23  | 1.92                     | 0.52              |
| 3:D:907:GLU:CD    | 3:D:909:ASN:HB2   | 2.35                     | 0.52              |
| 3:D:1153:VAL:HA   | 3:N:561:GLY:HA3   | 1.92                     | 0.52              |
| 1:K:56:VAL:HG12   | 1:K:57:TYR:N      | 2.25                     | 0.52              |
| 2:M:523:ILE:HG23  | 2:M:523:ILE:O     | 2.10                     | 0.52              |
| 2:M:841:ASN:ND2   | 2:M:843:HIS:ND1   | 2.57                     | 0.52              |
| 2:M:1034:GLU:HG2  | 3:N:619:LEU:HD13  | 1.92                     | 0.52              |
| 2:M:1078:GLU:HA   | 2:M:1078:GLU:OE1  | 2.10                     | 0.52              |
| 3:N:445:ARG:HH11  | 3:N:445:ARG:HG2   | 1.74                     | 0.52              |
| 3:N:480:GLU:O     | 3:N:489:ARG:HB2   | 2.10                     | 0.52              |
| 3:N:1189:ARG:HH11 | 3:N:1189:ARG:HG3  | 1.74                     | 0.52              |
| 3:N:1267:ARG:HD3  | 3:N:1268:PRO:O    | 2.09                     | 0.52              |
| 4:O:54:LEU:CG     | 4:O:58:PRO:HG2    | 2.40                     | 0.52              |
| 5:G:10:DA:H2''    | 5:G:11:DC:C6      | 2.45                     | 0.52              |
| 5:G:16:DT:H1'     | 5:G:17:DA:OP1     | 2.09                     | 0.52              |
| 1:A:104:GLU:OE1   | 1:A:137:ARG:HA    | 2.09                     | 0.52              |
| 1:B:43:ILE:HG13   | 1:B:218:LEU:HD13  | 1.91                     | 0.52              |
| 1:B:101:LEU:HD12  | 1:B:114:PHE:N     | 2.25                     | 0.52              |
| 1:B:206:THR:HG23  | 1:B:208:LEU:N     | 2.25                     | 0.52              |
| 2:C:121:MET:HE3   | 2:C:125:GLY:CA    | 2.40                     | 0.52              |
| 2:C:333:ILE:N     | 2:C:333:ILE:HD12  | 2.25                     | 0.52              |
| 2:C:626:ARG:O     | 2:C:638:ASP:HA    | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:855:VAL:HA    | 2:C:858:MET:HG2   | 1.90                     | 0.52              |
| 2:C:957:LYS:CD    | 2:C:961:GLU:HB2   | 2.40                     | 0.52              |
| 3:D:133:ILE:HB    | 3:D:153:LEU:O     | 2.08                     | 0.52              |
| 3:D:608:SER:HA    | 3:D:1443:THR:HG21 | 1.92                     | 0.52              |
| 3:D:644:LEU:C     | 3:D:721:VAL:HG22  | 2.35                     | 0.52              |
| 3:D:834:THR:HG22  | 3:D:838:ARG:NH1   | 2.17                     | 0.52              |
| 3:D:1447:LEU:N    | 3:D:1447:LEU:HD12 | 2.24                     | 0.52              |
| 1:L:62:LEU:CD1    | 1:L:63:HIS:H      | 2.21                     | 0.52              |
| 2:M:142:ARG:HE    | 2:M:325:ILE:HG23  | 1.74                     | 0.52              |
| 2:M:162:ILE:HD12  | 2:M:172:ILE:HB    | 1.92                     | 0.52              |
| 2:M:265:ARG:HG2   | 2:M:267:TYR:HB3   | 1.91                     | 0.52              |
| 2:M:328:LEU:CD1   | 2:M:328:LEU:N     | 2.73                     | 0.52              |
| 2:M:937:ASP:OD2   | 2:M:939:ARG:CG    | 2.58                     | 0.52              |
| 2:M:939:ARG:HG3   | 2:M:975:TYR:CE2   | 2.45                     | 0.52              |
| 3:N:87:ARG:HB2    | 3:N:524:LEU:HD12  | 1.92                     | 0.52              |
| 3:N:123:LEU:O     | 3:N:126:VAL:HB    | 2.10                     | 0.52              |
| 3:N:473:LEU:HA    | 3:N:476:GLU:HB2   | 1.92                     | 0.52              |
| 3:N:626:SER:O     | 3:N:652:LEU:HD11  | 2.10                     | 0.52              |
| 3:N:703:ASN:CA    | 3:N:713:ILE:HG12  | 2.40                     | 0.52              |
| 3:N:838:ARG:N     | 3:N:838:ARG:HD2   | 2.25                     | 0.52              |
| 3:N:899:LEU:HD13  | 3:N:914:LEU:HD23  | 1.92                     | 0.52              |
| 3:N:1011:PHE:HB3  | 3:N:1021:TYR:CG   | 2.45                     | 0.52              |
| 3:N:1229:ILE:HD11 | 3:N:1367:HIS:CB   | 2.40                     | 0.52              |
| 3:N:1445:HIS:CD2  | 3:N:1449:GLU:HB2  | 2.45                     | 0.52              |
| 3:N:1486:VAL:CG2  | 4:O:29:GLN:HE22   | 2.23                     | 0.52              |
| 5:G:3:DC:O5'      | 5:G:3:DC:C6       | 2.63                     | 0.52              |
| 2:C:39:ARG:H      | 2:C:39:ARG:HD2    | 1.75                     | 0.51              |
| 2:C:66:LEU:HD12   | 2:C:99:GLN:C      | 2.35                     | 0.51              |
| 2:C:124:ASP:OD1   | 2:C:125:GLY:N     | 2.43                     | 0.51              |
| 2:C:409:ARG:NH1   | 2:C:444:PRO:CG    | 2.73                     | 0.51              |
| 2:C:460:ARG:HG2   | 2:C:485:TYR:CD2   | 2.45                     | 0.51              |
| 2:C:634:GLY:O     | 2:C:705:ILE:N     | 2.36                     | 0.51              |
| 2:C:1031:ARG:NE   | 3:D:621:LYS:HD2   | 2.25                     | 0.51              |
| 2:C:1038:TRP:HD1  | 2:C:1041:GLU:OE2  | 1.93                     | 0.51              |
| 3:D:696:HIS:CG    | 3:D:697:GLY:N     | 2.79                     | 0.51              |
| 3:D:1105:ILE:HG12 | 3:D:1374:GLN:NE2  | 2.25                     | 0.51              |
| 3:D:1127:GLU:O    | 3:D:1128:VAL:HG23 | 2.10                     | 0.51              |
| 3:D:1347:TYR:CZ   | 3:D:1351:GLU:HG2  | 2.45                     | 0.51              |
| 3:D:1409:ALA:HA   | 2:M:370:ALA:CB    | 2.40                     | 0.51              |
| 3:D:1496:GLU:CD   | 3:D:1500:LYS:HE3  | 2.35                     | 0.51              |
| 4:E:59:ASN:O      | 4:E:63:TRP:CD1    | 2.64                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:442:GLU:OE2   | 2:M:543:ASN:HB3   | 2.09                     | 0.51              |
| 2:M:494:TYR:N     | 2:M:494:TYR:CD1   | 2.77                     | 0.51              |
| 2:M:881:ASN:O     | 2:M:884:GLN:HG3   | 2.10                     | 0.51              |
| 2:M:941:VAL:HA    | 2:M:944:LEU:HD12  | 1.91                     | 0.51              |
| 3:N:29:PRO:HD3    | 3:N:548:ILE:HG21  | 1.92                     | 0.51              |
| 3:N:502:PHE:CZ    | 3:N:1452:ILE:HG13 | 2.45                     | 0.51              |
| 3:N:603:LEU:O     | 3:N:604:THR:C     | 2.53                     | 0.51              |
| 3:N:729:HIS:ND1   | 3:N:730:PRO:HD2   | 2.25                     | 0.51              |
| 7:Z:12:DT:O5'     | 7:Z:12:DT:H6      | 1.93                     | 0.51              |
| 2:C:328:LEU:CB    | 2:C:433:THR:HB    | 2.40                     | 0.51              |
| 2:C:572:ILE:HG13  | 2:C:573:ARG:N     | 2.25                     | 0.51              |
| 2:C:713:ARG:HB3   | 2:C:720:GLU:OE2   | 2.10                     | 0.51              |
| 2:C:964:LYS:O     | 2:C:968:LEU:HG    | 2.11                     | 0.51              |
| 3:D:786:ILE:HA    | 3:D:789:LEU:HD12  | 1.92                     | 0.51              |
| 3:D:796:ARG:NE    | 3:D:828:LYS:HZ3   | 2.07                     | 0.51              |
| 3:D:983:LEU:HG    | 3:D:984:THR:N     | 2.24                     | 0.51              |
| 3:D:1083:ASP:C    | 3:D:1087:ARG:HG2  | 2.35                     | 0.51              |
| 3:D:1227:GLN:C    | 3:D:1229:ILE:N    | 2.67                     | 0.51              |
| 1:K:101:LEU:HB2   | 1:K:114:PHE:HA    | 1.91                     | 0.51              |
| 2:M:455:LEU:HD12  | 2:M:455:LEU:C     | 2.36                     | 0.51              |
| 2:M:905:ILE:CD1   | 2:M:905:ILE:H     | 2.23                     | 0.51              |
| 2:M:988:VAL:HG11  | 3:N:949:ILE:O     | 2.10                     | 0.51              |
| 2:M:1092:LEU:HB3  | 2:M:1099:VAL:CG2  | 2.40                     | 0.51              |
| 2:M:1102:LEU:O    | 3:N:5:VAL:HG12    | 2.10                     | 0.51              |
| 3:N:34:TYR:N      | 3:N:34:TYR:CD2    | 2.78                     | 0.51              |
| 3:N:115:LEU:HD12  | 3:N:498:VAL:HG12  | 1.91                     | 0.51              |
| 3:N:434:ARG:HB3   | 3:N:434:ARG:NH1   | 2.24                     | 0.51              |
| 3:N:782:SER:O     | 3:N:786:ILE:HB    | 2.10                     | 0.51              |
| 3:N:868:TYR:CE1   | 3:N:869:MET:HG3   | 2.45                     | 0.51              |
| 3:N:1292:VAL:HG22 | 3:N:1311:LEU:CD1  | 2.40                     | 0.51              |
| 1:A:33:GLY:O      | 1:A:195:LEU:HD22  | 2.10                     | 0.51              |
| 1:A:42:ARG:HH12   | 1:B:34:VAL:CG1    | 2.23                     | 0.51              |
| 1:B:219:ARG:HA    | 1:B:222:LEU:HD12  | 1.92                     | 0.51              |
| 2:C:21:ILE:HD12   | 2:C:21:ILE:N      | 2.23                     | 0.51              |
| 2:C:214:TYR:HE1   | 2:C:311:PHE:HB3   | 1.75                     | 0.51              |
| 2:C:326:ASP:O     | 2:C:431:HIS:CD2   | 2.62                     | 0.51              |
| 2:C:837:ASP:HA    | 2:C:999:HIS:CE1   | 2.45                     | 0.51              |
| 2:C:1038:TRP:HA   | 2:C:1041:GLU:HB2  | 1.92                     | 0.51              |
| 3:D:629:SER:HB3   | 3:D:726:ILE:CD1   | 2.40                     | 0.51              |
| 3:D:917:GLN:O     | 3:D:920:LEU:HB2   | 2.09                     | 0.51              |
| 3:D:1211:MET:SD   | 3:D:1213:ARG:HG2  | 2.51                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1330:ILE:HD13 | 3:D:1347:TYR:CZ   | 2.46                     | 0.51              |
| 1:L:122:ILE:HG22  | 1:L:124:ASN:H     | 1.76                     | 0.51              |
| 2:M:336:VAL:HA    | 2:M:339:LEU:HD12  | 1.92                     | 0.51              |
| 2:M:1001:VAL:HG21 | 5:X:24:DC:C5'     | 2.39                     | 0.51              |
| 2:M:1075:ASP:HB3  | 4:O:32:ARG:NH2    | 2.25                     | 0.51              |
| 3:N:112:ILE:HD12  | 3:N:116:LEU:HB2   | 1.93                     | 0.51              |
| 3:N:206:ARG:HB2   | 3:N:392:SER:C     | 2.35                     | 0.51              |
| 3:N:529:GLN:HB2   | 3:N:535:PHE:CZ    | 2.46                     | 0.51              |
| 3:N:545:ARG:NH1   | 3:N:545:ARG:HB3   | 2.26                     | 0.51              |
| 3:N:733:CYS:HB3   | 3:N:738:ALA:O     | 2.10                     | 0.51              |
| 3:N:1380:GLU:HB2  | 3:N:1420:LEU:HD11 | 1.92                     | 0.51              |
| 3:N:1466:VAL:O    | 3:N:1469:GLY:N    | 2.42                     | 0.51              |
| 6:H:12:U:C6       | 6:H:12:U:H3'      | 2.45                     | 0.51              |
| 5:X:3:DC:C2'      | 5:X:4:DA:OP2      | 2.53                     | 0.51              |
| 7:Z:17:DA:H8      | 7:Z:17:DA:O5'     | 1.94                     | 0.51              |
| 1:B:9:PRO:HB3     | 1:B:25:LEU:CG     | 2.40                     | 0.51              |
| 2:C:52:PHE:CE2    | 2:C:68:PHE:CB     | 2.72                     | 0.51              |
| 2:C:631:SER:HA    | 2:C:637:LEU:HD11  | 1.93                     | 0.51              |
| 2:C:668:LEU:O     | 2:C:993:PHE:CZ    | 2.64                     | 0.51              |
| 2:C:832:LYS:O     | 2:C:833:LEU:C     | 2.53                     | 0.51              |
| 3:D:800:LYS:HD2   | 3:D:804:LEU:HD22  | 1.92                     | 0.51              |
| 4:E:28:GLN:HB3    | 4:E:32:ARG:NH1    | 2.20                     | 0.51              |
| 1:L:80:LEU:HD12   | 1:L:83:LYS:HZ1    | 1.75                     | 0.51              |
| 2:M:101:ILE:HG22  | 2:M:102:HIS:N     | 2.24                     | 0.51              |
| 2:M:767:PRO:HB3   | 2:M:772:ARG:HH21  | 1.74                     | 0.51              |
| 3:N:114:THR:O     | 3:N:495:ARG:HG3   | 2.10                     | 0.51              |
| 3:N:160:GLU:HB3   | 3:N:165:LYS:HB2   | 1.92                     | 0.51              |
| 3:N:1031:ASN:OD1  | 3:N:1033:GLN:CB   | 2.57                     | 0.51              |
| 3:N:1114:THR:CB   | 3:N:1195:GLN:HB3  | 2.36                     | 0.51              |
| 3:N:1280:VAL:HG12 | 3:N:1318:TYR:N    | 2.26                     | 0.51              |
| 5:G:16:DT:C2'     | 5:G:17:DA:OP1     | 2.58                     | 0.51              |
| 6:H:15:C:OP2      | 6:H:15:C:C6       | 2.56                     | 0.51              |
| 7:I:11:DG:H8      | 7:I:11:DG:P       | 2.34                     | 0.51              |
| 2:C:17:PRO:O      | 2:C:20:GLU:HB3    | 2.10                     | 0.51              |
| 2:C:257:VAL:C     | 2:C:259:GLY:H     | 2.19                     | 0.51              |
| 2:C:334:ARG:HB2   | 2:C:339:LEU:HD21  | 1.93                     | 0.51              |
| 2:C:405:ARG:HG3   | 2:C:442:GLU:OE1   | 2.09                     | 0.51              |
| 2:C:460:ARG:NH1   | 2:C:462:ASP:HA    | 2.25                     | 0.51              |
| 2:C:603:VAL:HB    | 2:C:647:GLN:H     | 1.75                     | 0.51              |
| 2:C:726:ILE:HD13  | 2:C:734:LEU:HG    | 1.92                     | 0.51              |
| 2:C:1115:LEU:HD22 | 3:D:88:TYR:CE1    | 2.46                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:804:LEU:CD1   | 3:D:830:ALA:O    | 2.58                     | 0.51              |
| 3:D:1153:VAL:HG13 | 3:N:561:GLY:CA   | 2.41                     | 0.51              |
| 3:D:1263:PHE:HB3  | 3:D:1424:VAL:CG1 | 2.40                     | 0.51              |
| 3:D:1445:HIS:O    | 3:D:1446:VAL:C   | 2.53                     | 0.51              |
| 1:K:66:SER:O      | 1:K:75:VAL:HG23  | 2.11                     | 0.51              |
| 2:M:35:PRO:C      | 2:M:37:GLU:N     | 2.67                     | 0.51              |
| 2:M:144:PRO:HA    | 2:M:163:ILE:O    | 2.11                     | 0.51              |
| 2:M:257:VAL:C     | 2:M:259:GLY:H    | 2.19                     | 0.51              |
| 2:M:397:GLU:OE2   | 2:M:632:ASN:HB2  | 2.10                     | 0.51              |
| 2:M:516:ARG:CZ    | 3:N:1068:LEU:HB2 | 2.40                     | 0.51              |
| 2:M:927:GLY:CA    | 2:M:930:LYS:HD3  | 2.36                     | 0.51              |
| 3:N:520:LEU:HG    | 3:N:521:PRO:N    | 2.24                     | 0.51              |
| 3:N:715:ALA:HB3   | 3:N:764:LEU:CA   | 2.40                     | 0.51              |
| 3:N:1031:ASN:O    | 3:N:1032:PRO:C   | 2.53                     | 0.51              |
| 7:I:11:DG:H2''    | 7:I:12:DT:C7     | 2.40                     | 0.51              |
| 7:Z:15:DT:C2'     | 7:Z:16:DG:OP2    | 2.57                     | 0.51              |
| 1:A:197:LEU:HD23  | 1:A:197:LEU:N    | 2.26                     | 0.51              |
| 2:C:134:ARG:NH2   | 2:C:392:SER:O    | 2.44                     | 0.51              |
| 2:C:869:VAL:HG22  | 2:C:870:ILE:N    | 2.24                     | 0.51              |
| 3:D:131:LYS:HG3   | 3:D:568:ARG:CG   | 2.41                     | 0.51              |
| 3:D:732:VAL:HG23  | 3:D:736:PHE:HE1  | 1.76                     | 0.51              |
| 3:D:1017:PHE:HA   | 3:D:1022:VAL:CG2 | 2.40                     | 0.51              |
| 3:D:1027:GLY:O    | 3:D:1028:ALA:C   | 2.54                     | 0.51              |
| 4:E:47:LYS:N      | 4:E:54:LEU:HD13  | 2.26                     | 0.51              |
| 1:K:92:PRO:HG3    | 1:K:146:ARG:HH22 | 1.76                     | 0.51              |
| 1:L:71:VAL:HG22   | 1:L:132:LEU:HD12 | 1.93                     | 0.51              |
| 2:M:71:TYR:HA     | 2:M:96:ALA:CB    | 2.41                     | 0.51              |
| 2:M:211:LEU:HD13  | 2:M:308:ARG:HG3  | 1.92                     | 0.51              |
| 2:M:260:LEU:HB3   | 2:M:291:ALA:HB2  | 1.90                     | 0.51              |
| 2:M:265:ARG:HD3   | 2:M:267:TYR:HB3  | 1.92                     | 0.51              |
| 2:M:692:GLU:CD    | 2:M:854:PRO:HA   | 2.36                     | 0.51              |
| 2:M:833:LEU:HD12  | 2:M:996:LYS:HE2  | 1.92                     | 0.51              |
| 3:N:415:VAL:HG12  | 3:N:416:ALA:N    | 2.25                     | 0.51              |
| 3:N:680:GLN:O     | 3:N:683:ILE:HD12 | 2.10                     | 0.51              |
| 3:N:1401:GLU:CD   | 3:N:1401:GLU:C   | 2.79                     | 0.51              |
| 7:Z:2:DT:H2''     | 7:Z:3:DA:OP2     | 2.10                     | 0.51              |
| 1:A:26:GLU:HB2    | 1:A:27:PRO:HA    | 1.91                     | 0.51              |
| 1:A:161:ARG:HB2   | 1:A:161:ARG:CZ   | 2.40                     | 0.51              |
| 2:C:684:PHE:HB3   | 3:D:740:PHE:CE1  | 2.46                     | 0.51              |
| 2:C:854:PRO:HB2   | 2:C:856:GLU:CG   | 2.40                     | 0.51              |
| 2:C:928:LYS:HZ1   | 2:C:932:GLU:HG3  | 1.73                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:925:GLU:HG2  | 3:D:926:LYS:N     | 2.24                     | 0.51              |
| 3:D:1011:PHE:HB3 | 3:D:1021:TYR:CG   | 2.46                     | 0.51              |
| 3:D:1377:LYS:HG3 | 3:D:1377:LYS:O    | 2.10                     | 0.51              |
| 4:E:85:LEU:HD23  | 4:E:85:LEU:C      | 2.36                     | 0.51              |
| 1:K:54:THR:HB    | 1:K:143:ARG:CG    | 2.40                     | 0.51              |
| 2:M:140:ILE:CD1  | 2:M:331:ARG:HH21  | 2.23                     | 0.51              |
| 2:M:430:VAL:HG13 | 2:M:430:VAL:O     | 2.10                     | 0.51              |
| 2:M:435:TYR:O    | 2:M:437:ARG:HD2   | 2.11                     | 0.51              |
| 2:M:691:SER:HB3  | 2:M:868:ASP:O     | 2.10                     | 0.51              |
| 2:M:756:VAL:O    | 2:M:789:SER:HB3   | 2.10                     | 0.51              |
| 2:M:854:PRO:CB   | 2:M:856:GLU:HG3   | 2.41                     | 0.51              |
| 2:M:1102:LEU:HA  | 2:M:1107:ASN:O    | 2.11                     | 0.51              |
| 3:N:136:ASP:OD2  | 3:N:467:GLU:OE1   | 2.29                     | 0.51              |
| 3:N:166:GLN:HA   | 3:N:198:ARG:CG    | 2.40                     | 0.51              |
| 3:N:625:TYR:CE2  | 3:N:652:LEU:O     | 2.64                     | 0.51              |
| 3:N:695:ILE:HD11 | 3:N:718:PRO:CB    | 2.31                     | 0.51              |
| 3:N:704:ARG:HB3  | 3:N:736:PHE:HD2   | 1.76                     | 0.51              |
| 3:N:1227:GLN:C   | 3:N:1229:ILE:N    | 2.66                     | 0.51              |
| 1:A:65:PHE:HE1   | 2:C:799:ILE:HG21  | 1.76                     | 0.51              |
| 1:A:176:ARG:HG3  | 1:A:200:TRP:CE3   | 2.45                     | 0.51              |
| 2:C:274:ARG:O    | 2:C:274:ARG:HD3   | 2.09                     | 0.51              |
| 2:C:295:ASP:C    | 2:C:297:GLU:H     | 2.18                     | 0.51              |
| 2:C:456:ALA:HB1  | 2:C:538:GLN:O     | 2.11                     | 0.51              |
| 2:C:1046:ALA:HB1 | 3:D:1472:ILE:HG12 | 1.91                     | 0.51              |
| 3:D:116:LEU:HD22 | 3:D:118:LEU:HD11  | 1.92                     | 0.51              |
| 3:D:148:GLU:HB3  | 3:D:151:GLN:HB3   | 1.93                     | 0.51              |
| 3:D:924:MET:HB3  | 4:E:6:ILE:CG2     | 2.41                     | 0.51              |
| 3:D:1266:ARG:NH2 | 7:I:4:DG:O3'      | 2.44                     | 0.51              |
| 3:D:1383:ASP:CB  | 3:D:1416:ALA:HB3  | 2.41                     | 0.51              |
| 1:K:56:VAL:CG2   | 1:K:142:VAL:HG12  | 2.38                     | 0.51              |
| 1:K:115:LEU:HD12 | 1:K:116:PRO:HD2   | 1.93                     | 0.51              |
| 1:K:195:LEU:HD12 | 1:K:196:THR:H     | 1.76                     | 0.51              |
| 2:M:61:LYS:O     | 2:M:359:MET:HE1   | 2.11                     | 0.51              |
| 2:M:129:ILE:N    | 2:M:129:ILE:CD1   | 2.73                     | 0.51              |
| 2:M:284:ARG:HG2  | 2:M:301:GLU:CD    | 2.36                     | 0.51              |
| 2:M:287:GLY:O    | 2:M:288:ARG:C     | 2.53                     | 0.51              |
| 2:M:557:ARG:NH1  | 2:M:560:MET:HG3   | 2.26                     | 0.51              |
| 2:M:584:GLU:HB2  | 2:M:666:LEU:N     | 2.24                     | 0.51              |
| 3:N:128:TYR:HB3  | 3:N:129:PHE:CD1   | 2.46                     | 0.51              |
| 3:N:538:SER:O    | 3:N:540:LEU:N     | 2.44                     | 0.51              |
| 3:N:1395:LEU:HA  | 3:N:1398:TRP:HD1  | 1.75                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:1464:GLU:CG  | 3:N:1465:ASN:N   | 2.73                     | 0.51              |
| 5:X:12:DA:N3     | 5:X:13:DA:C5     | 2.78                     | 0.51              |
| 1:A:11:PHE:CA    | 1:A:25:LEU:HD12  | 2.40                     | 0.51              |
| 1:A:140:MET:SD   | 1:A:142:VAL:HG13 | 2.50                     | 0.51              |
| 1:B:83:LYS:HE2   | 1:B:168:ASP:HB2  | 1.92                     | 0.51              |
| 2:C:158:TYR:CD1  | 2:C:313:LEU:HD21 | 2.46                     | 0.51              |
| 2:C:286:SER:HB3  | 2:C:299:LYS:CE   | 2.41                     | 0.51              |
| 2:C:612:VAL:HG22 | 2:C:622:GLU:HA   | 1.92                     | 0.51              |
| 2:C:678:PRO:HG2  | 3:D:947:ILE:HD11 | 1.93                     | 0.51              |
| 2:C:1095:LEU:CG  | 3:D:603:LEU:HD13 | 2.40                     | 0.51              |
| 3:D:127:LEU:HB2  | 3:D:132:TYR:HB2  | 1.92                     | 0.51              |
| 3:D:502:PHE:HB3  | 3:D:509:PRO:HD3  | 1.92                     | 0.51              |
| 3:D:1341:PRO:C   | 3:D:1343:ALA:N   | 2.69                     | 0.51              |
| 3:D:1432:LYS:HB2 | 3:D:1432:LYS:HZ2 | 1.76                     | 0.51              |
| 1:K:226:SER:O    | 1:K:228:PRO:HD3  | 2.10                     | 0.51              |
| 2:M:26:TYR:CD2   | 2:M:121:MET:HB2  | 2.46                     | 0.51              |
| 2:M:350:ARG:HA   | 2:M:353:ARG:NH2  | 2.26                     | 0.51              |
| 2:M:433:THR:C    | 2:M:435:TYR:N    | 2.67                     | 0.51              |
| 2:M:532:MET:HG2  | 2:M:533:ASP:O    | 2.09                     | 0.51              |
| 2:M:553:ASP:HA   | 2:M:881:ASN:HA   | 1.93                     | 0.51              |
| 2:M:575:GLN:C    | 2:M:667:ALA:HB1  | 2.36                     | 0.51              |
| 2:M:1034:GLU:HA  | 2:M:1037:VAL:CG2 | 2.41                     | 0.51              |
| 2:M:1059:ASP:O   | 2:M:1063:ARG:HD3 | 2.11                     | 0.51              |
| 3:N:187:LYS:HG3  | 3:N:198:ARG:C    | 2.35                     | 0.51              |
| 3:N:610:LYS:HA   | 3:N:615:ARG:NE   | 2.25                     | 0.51              |
| 3:N:868:TYR:CD1  | 3:N:869:MET:HG3  | 2.46                     | 0.51              |
| 3:N:1399:ASP:O   | 3:N:1403:LEU:CG  | 2.59                     | 0.51              |
| 5:X:12:DA:N3     | 5:X:13:DA:C4     | 2.78                     | 0.51              |
| 1:A:36:LEU:O     | 1:A:39:PRO:HD2   | 2.10                     | 0.51              |
| 1:B:86:VAL:HG12  | 1:B:124:ASN:HB2  | 1.92                     | 0.51              |
| 2:C:121:MET:HE3  | 2:C:125:GLY:HA2  | 1.92                     | 0.51              |
| 2:C:430:VAL:O    | 2:C:430:VAL:HG13 | 2.10                     | 0.51              |
| 2:C:483:VAL:HG12 | 2:C:484:VAL:N    | 2.25                     | 0.51              |
| 2:C:560:MET:HE2  | 2:C:560:MET:HA   | 1.92                     | 0.51              |
| 2:C:674:VAL:CB   | 2:C:869:VAL:HG13 | 2.41                     | 0.51              |
| 3:D:91:GLY:O     | 3:D:518:PRO:HA   | 2.11                     | 0.51              |
| 3:D:806:PHE:O    | 3:D:808:THR:N    | 2.44                     | 0.51              |
| 1:K:70:GLY:H     | 2:M:607:ASP:CG   | 2.17                     | 0.51              |
| 1:L:33:GLY:O     | 1:L:195:LEU:HD22 | 2.11                     | 0.51              |
| 1:L:179:PHE:N    | 1:L:179:PHE:HD2  | 2.09                     | 0.51              |
| 3:N:82:LYS:HB3   | 3:N:84:ILE:HG23  | 1.93                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:126:VAL:O     | 3:N:130:SER:HB3  | 2.11                     | 0.51              |
| 3:N:473:LEU:HA    | 3:N:476:GLU:OE2  | 2.10                     | 0.51              |
| 3:N:488:ARG:HG2   | 3:N:488:ARG:NH1  | 2.25                     | 0.51              |
| 3:N:609:GLY:C     | 3:N:611:GLN:N    | 2.65                     | 0.51              |
| 3:N:610:LYS:HE3   | 5:X:20:DC:OP2    | 2.11                     | 0.51              |
| 3:N:695:ILE:O     | 3:N:698:LYS:HB2  | 2.11                     | 0.51              |
| 3:N:1274:ILE:HG21 | 3:N:1301:LYS:NZ  | 2.24                     | 0.51              |
| 5:G:2:DT:C2'      | 5:G:3:DC:C6      | 2.94                     | 0.51              |
| 7:I:3:DA:N3       | 7:I:4:DG:O4'     | 2.44                     | 0.51              |
| 5:X:13:DA:C6      | 5:X:14:DG:C6     | 2.99                     | 0.51              |
| 6:Y:8:G:C8        | 6:Y:8:G:C3'      | 2.94                     | 0.51              |
| 2:C:39:ARG:O      | 2:C:41:ASN:N     | 2.43                     | 0.50              |
| 2:C:191:PHE:HB2   | 2:C:241:LEU:CD1  | 2.39                     | 0.50              |
| 2:C:328:LEU:HD12  | 2:C:328:LEU:N    | 2.26                     | 0.50              |
| 2:C:690:ILE:HG22  | 2:C:851:LYS:O    | 2.11                     | 0.50              |
| 2:C:894:GLY:O     | 2:C:898:GLY:N    | 2.43                     | 0.50              |
| 3:D:93:ILE:O      | 3:D:516:ALA:HA   | 2.11                     | 0.50              |
| 3:D:711:LEU:C     | 3:D:713:ILE:N    | 2.69                     | 0.50              |
| 3:D:799:LYS:HD3   | 3:D:826:PRO:HG3  | 1.93                     | 0.50              |
| 3:D:1093:TYR:OH   | 3:D:1440:PHE:HE2 | 1.93                     | 0.50              |
| 1:K:174:VAL:HG22  | 1:K:201:THR:CG2  | 2.41                     | 0.50              |
| 2:M:267:TYR:CZ    | 2:M:273:GLY:HA3  | 2.45                     | 0.50              |
| 2:M:277:ALA:O     | 2:M:278:GLU:C    | 2.54                     | 0.50              |
| 2:M:894:GLY:O     | 2:M:898:GLY:N    | 2.44                     | 0.50              |
| 2:M:1056:LYS:CE   | 3:N:751:LEU:HD11 | 2.21                     | 0.50              |
| 3:N:127:LEU:HB3   | 3:N:132:TYR:HD1  | 1.75                     | 0.50              |
| 3:N:160:GLU:HA    | 3:N:163:TYR:CE1  | 2.46                     | 0.50              |
| 3:N:609:GLY:O     | 3:N:615:ARG:HD3  | 2.11                     | 0.50              |
| 3:N:711:LEU:C     | 3:N:713:ILE:N    | 2.69                     | 0.50              |
| 3:N:754:PHE:HD1   | 4:O:28:GLN:OE1   | 1.93                     | 0.50              |
| 3:N:1122:LEU:HD13 | 3:N:1185:GLU:HA  | 1.94                     | 0.50              |
| 3:N:1168:MET:HG3  | 3:N:1172:HIS:NE2 | 2.25                     | 0.50              |
| 3:N:1348:LEU:HD13 | 3:N:1348:LEU:H   | 1.75                     | 0.50              |
| 4:O:41:GLU:N      | 4:O:42:PRO:CD    | 2.74                     | 0.50              |
| 5:G:5:DC:O5'      | 5:G:5:DC:H6      | 1.94                     | 0.50              |
| 5:X:9:DC:H2''     | 5:X:10:DA:C8     | 2.46                     | 0.50              |
| 7:Z:1:DG:OP3      | 7:Z:1:DG:C3'     | 2.54                     | 0.50              |
| 2:C:22:GLN:C      | 2:C:121:MET:HE1  | 2.37                     | 0.50              |
| 2:C:64:LEU:CD2    | 2:C:359:MET:HG3  | 2.34                     | 0.50              |
| 2:C:394:PHE:CE2   | 5:G:25:DG:H4'    | 2.46                     | 0.50              |
| 2:C:543:ASN:C     | 2:C:543:ASN:OD1  | 2.54                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:2:LYS:HG2     | 3:D:2:LYS:O       | 2.10                     | 0.50              |
| 3:D:33:ASN:ND2    | 3:D:35:ARG:HH12   | 2.08                     | 0.50              |
| 3:D:566:ILE:HA    | 3:D:569:ASN:HB2   | 1.93                     | 0.50              |
| 3:D:728:LEU:HG    | 3:D:729:HIS:O     | 2.11                     | 0.50              |
| 3:D:730:PRO:HG3   | 3:D:939:PHE:HZ    | 1.76                     | 0.50              |
| 3:D:744:GLN:NE2   | 5:G:21:DG:N2      | 2.51                     | 0.50              |
| 3:D:902:LEU:CD2   | 3:D:902:LEU:N     | 2.67                     | 0.50              |
| 3:D:924:MET:N     | 4:E:7:ASP:OD2     | 2.44                     | 0.50              |
| 4:E:40:LEU:CD2    | 4:E:67:GLU:HA     | 2.31                     | 0.50              |
| 1:K:88:ARG:HH12   | 1:K:90:LEU:CD1    | 2.24                     | 0.50              |
| 1:L:76:VAL:O      | 1:L:80:LEU:HB2    | 2.11                     | 0.50              |
| 2:M:685:GLU:HG2   | 3:N:739:ASP:HB2   | 1.93                     | 0.50              |
| 2:M:775:ARG:CZ    | 2:M:782:ALA:HB1   | 2.41                     | 0.50              |
| 2:M:942:GLU:O     | 2:M:946:ARG:HG3   | 2.11                     | 0.50              |
| 3:N:34:TYR:N      | 3:N:34:TYR:HD2    | 2.10                     | 0.50              |
| 3:N:87:ARG:O      | 3:N:524:LEU:HD11  | 2.11                     | 0.50              |
| 3:N:132:TYR:CD2   | 3:N:154:THR:CB    | 2.94                     | 0.50              |
| 3:N:598:ARG:HD3   | 6:Y:8:G:H4'       | 1.92                     | 0.50              |
| 3:N:860:LEU:HA    | 3:N:877:PRO:CB    | 2.33                     | 0.50              |
| 5:G:7:DA:C2'      | 5:G:8:DC:OP2      | 2.59                     | 0.50              |
| 5:X:27:DC:H2'     | 5:X:28:DG:H8      | 1.76                     | 0.50              |
| 7:Z:6:DT:C2'      | 7:Z:7:DT:H72      | 2.41                     | 0.50              |
| 2:C:438:ILE:HD12  | 2:C:438:ILE:N     | 2.26                     | 0.50              |
| 2:C:532:MET:HE3   | 2:C:533:ASP:O     | 2.11                     | 0.50              |
| 2:C:831:ARG:CZ    | 2:C:1004:LYS:NZ   | 2.73                     | 0.50              |
| 2:C:897:LEU:HD21  | 2:C:921:ALA:CA    | 2.42                     | 0.50              |
| 2:C:939:ARG:HB3   | 2:C:982:PRO:CG    | 2.41                     | 0.50              |
| 2:C:1030:GLN:OE1  | 5:G:22:DA:H5''    | 2.11                     | 0.50              |
| 3:D:550:ARG:N     | 3:D:550:ARG:HE    | 2.10                     | 0.50              |
| 3:D:582:LEU:HD23  | 3:D:603:LEU:CD1   | 2.42                     | 0.50              |
| 3:D:704:ARG:HG2   | 3:D:736:PHE:CB    | 2.42                     | 0.50              |
| 3:D:1227:GLN:C    | 3:D:1229:ILE:H    | 2.19                     | 0.50              |
| 3:D:1443:THR:O    | 3:D:1447:LEU:HD22 | 2.11                     | 0.50              |
| 3:D:1468:LEU:HD22 | 3:D:1470:ARG:HB2  | 1.94                     | 0.50              |
| 4:E:36:LYS:HB2    | 4:E:95:VAL:CG2    | 2.41                     | 0.50              |
| 4:E:57:ASP:N      | 4:E:58:PRO:HD3    | 2.26                     | 0.50              |
| 2:M:1012:PRO:HD3  | 2:M:1026:GLN:CG   | 2.40                     | 0.50              |
| 2:M:1038:TRP:HA   | 2:M:1041:GLU:CD   | 2.36                     | 0.50              |
| 3:N:133:ILE:O     | 3:N:152:LEU:HB2   | 2.10                     | 0.50              |
| 3:N:136:ASP:OD2   | 3:N:467:GLU:CD    | 2.54                     | 0.50              |
| 3:N:457:GLY:C     | 3:N:459:GLU:H     | 2.17                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:554:LEU:O     | 3:N:558:LEU:HG    | 2.11                     | 0.50              |
| 3:N:575:GLN:O     | 3:N:578:VAL:HB    | 2.11                     | 0.50              |
| 3:N:587:ARG:C     | 3:N:588:GLY:O     | 2.52                     | 0.50              |
| 3:N:712:GLY:C     | 3:N:713:ILE:HG13  | 2.36                     | 0.50              |
| 3:N:728:LEU:HG    | 3:N:729:HIS:N     | 2.26                     | 0.50              |
| 3:N:807:ALA:HA    | 3:N:833:GLU:CG    | 2.42                     | 0.50              |
| 3:N:1115:THR:CG2  | 3:N:1151:ARG:NH2  | 2.75                     | 0.50              |
| 6:H:12:U:C6       | 6:H:12:U:C3'      | 2.95                     | 0.50              |
| 1:B:56:VAL:HG12   | 1:B:57:TYR:N      | 2.26                     | 0.50              |
| 2:C:182:VAL:CG1   | 2:C:193:LEU:HD13  | 2.41                     | 0.50              |
| 2:C:312:ALA:CB    | 2:C:318:PRO:HG2   | 2.36                     | 0.50              |
| 2:C:405:ARG:C     | 2:C:407:LYS:H     | 2.20                     | 0.50              |
| 2:C:458:TYR:O     | 2:C:459:ALA:C     | 2.54                     | 0.50              |
| 2:C:869:VAL:CG2   | 2:C:870:ILE:N     | 2.74                     | 0.50              |
| 2:C:1016:ILE:CG2  | 3:D:526:PRO:HG3   | 2.42                     | 0.50              |
| 2:C:1081:VAL:CG2  | 2:C:1086:ARG:HH21 | 2.24                     | 0.50              |
| 3:D:820:GLU:HA    | 3:D:825:ALA:O     | 2.12                     | 0.50              |
| 3:D:1128:VAL:O    | 3:D:1129:THR:HG22 | 2.12                     | 0.50              |
| 3:D:1399:ASP:O    | 3:D:1403:LEU:HD12 | 2.11                     | 0.50              |
| 3:D:1433:SER:HB2  | 3:D:1457:ASP:OD2  | 2.11                     | 0.50              |
| 4:E:41:GLU:HG2    | 4:E:42:PRO:CD     | 2.38                     | 0.50              |
| 2:M:1008:ARG:HH21 | 2:M:1012:PRO:N    | 2.10                     | 0.50              |
| 2:M:1053:LEU:HD23 | 2:M:1053:LEU:H    | 1.76                     | 0.50              |
| 3:N:6:ARG:HG2     | 3:N:6:ARG:HH11    | 1.76                     | 0.50              |
| 3:N:420:VAL:HG12  | 3:N:421:LEU:N     | 2.26                     | 0.50              |
| 3:N:1393:GLN:HB2  | 3:N:1398:TRP:HZ2  | 1.76                     | 0.50              |
| 7:Z:14:DG:C2'     | 7:Z:15:DT:OP2     | 2.59                     | 0.50              |
| 1:A:57:TYR:CE1    | 1:A:163:ASN:HB2   | 2.45                     | 0.50              |
| 2:C:431:HIS:HD2   | 2:C:433:THR:H     | 1.58                     | 0.50              |
| 2:C:442:GLU:CD    | 2:C:543:ASN:HD22  | 2.20                     | 0.50              |
| 2:C:502:PRO:O     | 2:C:503:LEU:HG    | 2.12                     | 0.50              |
| 2:C:1046:ALA:CB   | 3:D:1476:THR:H    | 2.25                     | 0.50              |
| 3:D:103:TRP:CD2   | 3:D:1444:THR:HG23 | 2.46                     | 0.50              |
| 3:D:133:ILE:HG12  | 3:D:456:MET:CB    | 2.42                     | 0.50              |
| 3:D:498:VAL:HG12  | 3:D:502:PHE:CE1   | 2.44                     | 0.50              |
| 3:D:966:GLU:O     | 3:D:969:ARG:HG2   | 2.11                     | 0.50              |
| 3:D:1059:SER:CB   | 3:D:1065:LEU:HA   | 2.42                     | 0.50              |
| 3:D:1197:ARG:CG   | 3:D:1198:TYR:H    | 2.25                     | 0.50              |
| 2:M:410:ILE:N     | 2:M:453:THR:O     | 2.40                     | 0.50              |
| 2:M:861:LEU:HD22  | 2:M:863:ASP:CB    | 2.29                     | 0.50              |
| 3:N:15:PRO:O      | 3:N:19:ARG:HG2    | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:28:LYS:CB     | 3:N:41:ARG:HD2    | 2.42                     | 0.50              |
| 3:N:54:LYS:HG3    | 3:N:55:ASP:N      | 2.26                     | 0.50              |
| 3:N:644:LEU:HD12  | 3:N:645:PRO:HD2   | 1.94                     | 0.50              |
| 3:N:713:ILE:C     | 3:N:714:GLN:HG3   | 2.36                     | 0.50              |
| 3:N:761:ILE:O     | 3:N:767:HIS:ND1   | 2.45                     | 0.50              |
| 3:N:840:LYS:HB3   | 3:N:841:TYR:CZ    | 2.47                     | 0.50              |
| 2:C:121:MET:CE    | 2:C:125:GLY:HA2   | 2.42                     | 0.50              |
| 2:C:140:ILE:HG22  | 2:C:333:ILE:HG13  | 1.93                     | 0.50              |
| 2:C:144:PRO:HB2   | 2:C:267:TYR:CE1   | 2.47                     | 0.50              |
| 3:D:550:ARG:O     | 3:D:554:LEU:N     | 2.44                     | 0.50              |
| 3:D:696:HIS:NE2   | 4:E:59:ASN:N      | 2.60                     | 0.50              |
| 3:D:704:ARG:NH1   | 3:D:738:ALA:HB2   | 2.26                     | 0.50              |
| 3:D:704:ARG:CB    | 3:D:745:MET:HE3   | 2.38                     | 0.50              |
| 3:D:704:ARG:HH22  | 6:H:14:G:H2'      | 1.75                     | 0.50              |
| 3:D:953:ASP:O     | 3:D:955:VAL:HG23  | 2.12                     | 0.50              |
| 3:D:1101:VAL:HG13 | 3:D:1428:ALA:CB   | 2.33                     | 0.50              |
| 1:K:58:ILE:CD1    | 1:K:140:MET:HB3   | 2.42                     | 0.50              |
| 1:K:99:LEU:HD12   | 1:K:99:LEU:N      | 2.27                     | 0.50              |
| 1:L:14:ARG:HH21   | 1:L:22:GLU:CD     | 2.19                     | 0.50              |
| 1:L:25:LEU:CD2    | 1:L:195:LEU:HB3   | 2.41                     | 0.50              |
| 2:M:164:PRO:HD2   | 2:M:170:PRO:O     | 2.10                     | 0.50              |
| 2:M:944:LEU:O     | 2:M:948:GLU:HG3   | 2.12                     | 0.50              |
| 2:M:1013:TYR:CG   | 2:M:1063:ARG:NH2  | 2.80                     | 0.50              |
| 3:N:134:VAL:HG22  | 3:N:455:ARG:O     | 2.12                     | 0.50              |
| 3:N:470:LEU:N     | 3:N:470:LEU:HD23  | 2.27                     | 0.50              |
| 3:N:499:VAL:O     | 3:N:500:ARG:C     | 2.54                     | 0.50              |
| 3:N:550:ARG:O     | 3:N:554:LEU:HB2   | 2.11                     | 0.50              |
| 3:N:810:GLU:HA    | 3:N:813:LEU:HD23  | 1.93                     | 0.50              |
| 3:N:1153:VAL:O    | 3:N:1160:LEU:HG   | 2.12                     | 0.50              |
| 3:N:1445:HIS:NE2  | 3:N:1449:GLU:CD   | 2.70                     | 0.50              |
| 4:O:54:LEU:O      | 4:O:58:PRO:HD2    | 2.12                     | 0.50              |
| 5:G:24:DC:C2'     | 5:G:25:DG:C8      | 2.94                     | 0.50              |
| 1:B:50:GLY:O      | 1:B:146:ARG:HA    | 2.12                     | 0.50              |
| 2:C:129:ILE:H     | 2:C:129:ILE:HD13  | 1.76                     | 0.50              |
| 2:C:298:PHE:CD1   | 2:C:298:PHE:N     | 2.77                     | 0.50              |
| 2:C:355:VAL:HG13  | 2:C:356:ARG:N     | 2.27                     | 0.50              |
| 2:C:753:ASP:O     | 2:C:792:VAL:N     | 2.38                     | 0.50              |
| 3:D:470:LEU:HB2   | 3:D:503:LEU:HD21  | 1.93                     | 0.50              |
| 3:D:596:SER:O     | 3:D:598:ARG:N     | 2.43                     | 0.50              |
| 3:D:899:LEU:CD2   | 3:D:917:GLN:HB3   | 2.32                     | 0.50              |
| 3:D:1017:PHE:HA   | 3:D:1022:VAL:HG21 | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1107:VAL:O    | 3:D:1218:GLY:N    | 2.45                     | 0.50              |
| 3:D:1468:LEU:HD22 | 3:D:1470:ARG:CB   | 2.41                     | 0.50              |
| 1:L:57:TYR:HB2    | 1:L:164:ALA:HB2   | 1.93                     | 0.50              |
| 2:M:151:ASP:HB2   | 2:M:157:ARG:O     | 2.12                     | 0.50              |
| 2:M:199:VAL:CG1   | 2:M:235:LEU:HG    | 2.42                     | 0.50              |
| 2:M:200:LEU:HD13  | 2:M:300:ASP:CG    | 2.36                     | 0.50              |
| 2:M:500:ASN:OD1   | 3:N:1067:VAL:HG23 | 2.12                     | 0.50              |
| 2:M:706:GLU:HG2   | 2:M:708:TYR:OH    | 2.12                     | 0.50              |
| 2:M:759:THR:HB    | 2:M:785:VAL:HG11  | 1.94                     | 0.50              |
| 2:M:861:LEU:HD21  | 2:M:925:TYR:CZ    | 2.47                     | 0.50              |
| 2:M:987:ILE:HG12  | 3:N:948:THR:CG2   | 2.42                     | 0.50              |
| 3:N:15:PRO:HA     | 3:N:18:ILE:CG1    | 2.41                     | 0.50              |
| 3:N:850:LEU:HD22  | 3:N:884:ARG:NH2   | 2.27                     | 0.50              |
| 3:N:1389:LEU:HD11 | 3:N:1390:LEU:HG   | 1.94                     | 0.50              |
| 4:O:62:THR:HA     | 4:O:65:MET:SD     | 2.52                     | 0.50              |
| 6:H:15:C:H3'      | 6:H:16:A:C5'      | 2.41                     | 0.50              |
| 6:Y:4:G:O2'       | 6:Y:5:C:H5'       | 2.12                     | 0.50              |
| 1:A:198:ARG:HH22  | 2:C:932:GLU:HB3   | 1.77                     | 0.50              |
| 2:C:86:LYS:HD3    | 2:C:813:VAL:HB    | 1.93                     | 0.50              |
| 2:C:490:GLU:OE1   | 2:C:493:ARG:NH1   | 2.45                     | 0.50              |
| 2:C:1090:LYS:CE   | 3:D:90:MET:HG3    | 2.42                     | 0.50              |
| 3:D:679:ARG:HB2   | 3:D:682:ASP:OD1   | 2.11                     | 0.50              |
| 3:D:741:ASP:C     | 6:H:14:G:H5''     | 2.37                     | 0.50              |
| 3:D:774:SER:HB3   | 3:D:1362:LYS:O    | 2.11                     | 0.50              |
| 3:D:860:LEU:O     | 3:D:876:SER:OG    | 2.30                     | 0.50              |
| 3:D:919:PHE:CZ    | 3:D:1211:MET:HG3  | 2.46                     | 0.50              |
| 3:D:1083:ASP:O    | 3:D:1087:ARG:CD   | 2.59                     | 0.50              |
| 3:D:1264:GLU:O    | 3:D:1265:ALA:C    | 2.53                     | 0.50              |
| 4:E:26:ARG:NH2    | 4:E:37:ASN:O      | 2.44                     | 0.50              |
| 1:K:178:ALA:HB3   | 1:K:198:ARG:HG3   | 1.94                     | 0.50              |
| 1:K:180:GLN:OE1   | 2:M:929:ARG:NE    | 2.44                     | 0.50              |
| 2:M:187:ASN:O     | 2:M:188:LYS:HG3   | 2.11                     | 0.50              |
| 2:M:437:ARG:NH1   | 2:M:491:GLU:OE2   | 2.44                     | 0.50              |
| 2:M:690:ILE:CG1   | 2:M:691:SER:N     | 2.74                     | 0.50              |
| 2:M:1057:SER:HB2  | 3:N:622:ARG:O     | 2.11                     | 0.50              |
| 3:N:394:LEU:HD23  | 3:N:394:LEU:N     | 2.27                     | 0.50              |
| 3:N:568:ARG:O     | 3:N:572:ARG:HG3   | 2.12                     | 0.50              |
| 3:N:757:ALA:O     | 3:N:761:ILE:HG13  | 2.11                     | 0.50              |
| 3:N:877:PRO:O     | 3:N:880:ILE:HG22  | 2.12                     | 0.50              |
| 3:N:1271:LYS:HZ2  | 3:N:1331:ASP:HB2  | 1.75                     | 0.50              |
| 3:N:1275:SER:O    | 3:N:1276:GLU:HB2  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:O:37:ASN:HD22  | 4:O:37:ASN:H      | 1.54                     | 0.50              |
| 1:A:34:VAL:HG13  | 1:B:42:ARG:HE     | 1.77                     | 0.50              |
| 2:C:146:VAL:HG22 | 2:C:162:ILE:HG12  | 1.92                     | 0.50              |
| 2:C:455:LEU:HD12 | 2:C:456:ALA:O     | 2.12                     | 0.50              |
| 2:C:630:ARG:HG2  | 2:C:826:TYR:HE2   | 1.74                     | 0.50              |
| 2:C:768:THR:O    | 2:C:772:ARG:HB2   | 2.10                     | 0.50              |
| 2:C:1093:GLN:HA  | 2:C:1097:LEU:O    | 2.11                     | 0.50              |
| 3:D:502:PHE:CD2  | 3:D:1452:ILE:HG23 | 2.47                     | 0.50              |
| 3:D:827:ILE:HD12 | 3:D:827:ILE:N     | 2.26                     | 0.50              |
| 2:M:119:PRO:HG2  | 2:M:386:PHE:CE2   | 2.47                     | 0.50              |
| 2:M:456:ALA:HB1  | 2:M:538:GLN:O     | 2.12                     | 0.50              |
| 2:M:937:ASP:CB   | 2:M:940:GLU:HG3   | 2.42                     | 0.50              |
| 2:M:1092:LEU:O   | 2:M:1095:LEU:O    | 2.30                     | 0.50              |
| 3:N:81:THR:HG22  | 3:N:82:LYS:H      | 1.75                     | 0.50              |
| 4:O:54:LEU:CD2   | 4:O:63:TRP:NE1    | 2.70                     | 0.50              |
| 1:A:54:THR:HB    | 1:A:143:ARG:HG3   | 1.94                     | 0.49              |
| 1:B:59:GLU:HB2   | 1:B:137:ARG:HH22  | 1.77                     | 0.49              |
| 2:C:66:LEU:HD22  | 2:C:372:LEU:HD23  | 1.93                     | 0.49              |
| 2:C:98:LEU:HD12  | 2:C:98:LEU:H      | 1.77                     | 0.49              |
| 2:C:460:ARG:NH2  | 2:C:468:ARG:NH1   | 2.58                     | 0.49              |
| 2:C:515:ALA:O    | 2:C:516:ARG:HD3   | 2.11                     | 0.49              |
| 2:C:603:VAL:O    | 2:C:646:GLY:HA2   | 2.12                     | 0.49              |
| 3:D:134:VAL:HG12 | 3:D:152:LEU:CB    | 2.42                     | 0.49              |
| 3:D:563:PRO:O    | 3:D:563:PRO:HG2   | 2.12                     | 0.49              |
| 3:D:581:LEU:HD23 | 3:D:581:LEU:H     | 1.77                     | 0.49              |
| 2:M:39:ARG:O     | 2:M:41:ASN:N      | 2.44                     | 0.49              |
| 2:M:73:LEU:HD12  | 2:M:73:LEU:C      | 2.37                     | 0.49              |
| 2:M:129:ILE:CG2  | 2:M:130:ASN:H     | 2.21                     | 0.49              |
| 2:M:640:ARG:NH1  | 2:M:640:ARG:HG2   | 2.26                     | 0.49              |
| 2:M:862:PRO:HD3  | 2:M:973:VAL:O     | 2.12                     | 0.49              |
| 2:M:1104:GLU:OE1 | 3:N:6:ARG:HD3     | 2.11                     | 0.49              |
| 3:N:101:HIS:CE1  | 3:N:103:TRP:HB2   | 2.46                     | 0.49              |
| 3:N:143:ASN:CG   | 3:N:144:GLY:N     | 2.69                     | 0.49              |
| 3:N:564:GLU:HA   | 3:N:567:ILE:HD12  | 1.94                     | 0.49              |
| 3:N:697:GLY:HA2  | 3:N:717:GLN:OE1   | 2.05                     | 0.49              |
| 3:N:714:GLN:HB3  | 3:N:765:SER:HB2   | 1.94                     | 0.49              |
| 3:N:750:PRO:CB   | 3:N:756:GLN:HA    | 2.42                     | 0.49              |
| 3:N:785:ILE:H    | 3:N:785:ILE:CD1   | 2.24                     | 0.49              |
| 3:N:843:PHE:O    | 3:N:866:VAL:HG13  | 2.12                     | 0.49              |
| 3:N:847:ASP:O    | 3:N:848:GLU:C     | 2.54                     | 0.49              |
| 7:Z:11:DG:OP2    | 7:Z:11:DG:C8      | 2.53                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:56:VAL:HG12   | 1:A:57:TYR:N      | 2.27                     | 0.49              |
| 1:B:21:GLY:O      | 1:B:23:PHE:CE2    | 2.64                     | 0.49              |
| 1:B:124:ASN:N     | 1:B:125:PRO:HD3   | 2.26                     | 0.49              |
| 2:C:328:LEU:C     | 2:C:330:ASN:N     | 2.70                     | 0.49              |
| 2:C:328:LEU:HB2   | 2:C:433:THR:CG2   | 2.42                     | 0.49              |
| 2:C:635:THR:C     | 2:C:705:ILE:HD12  | 2.37                     | 0.49              |
| 2:C:748:GLU:HA    | 2:C:799:ILE:HD13  | 1.94                     | 0.49              |
| 2:C:758:ARG:HG2   | 2:C:788:THR:OG1   | 2.12                     | 0.49              |
| 2:C:943:VAL:HG23  | 2:C:985:GLY:N     | 2.25                     | 0.49              |
| 2:C:1013:TYR:CD1  | 2:C:1020:PRO:HG3  | 2.47                     | 0.49              |
| 3:D:50:PHE:CG     | 3:D:522:PRO:HG3   | 2.46                     | 0.49              |
| 3:D:660:LYS:CD    | 3:D:694:VAL:HG22  | 2.32                     | 0.49              |
| 3:D:743:ASP:HA    | 6:H:14:G:C1'      | 2.42                     | 0.49              |
| 3:D:1031:ASN:CB   | 3:D:1034:GLN:CB   | 2.89                     | 0.49              |
| 3:D:1116:ASN:O    | 3:D:1193:THR:CB   | 2.60                     | 0.49              |
| 2:M:113:VAL:CG1   | 2:M:373:VAL:HG11  | 2.41                     | 0.49              |
| 2:M:704:HIS:O     | 2:M:828:ALA:HA    | 2.12                     | 0.49              |
| 2:M:846:LYS:HE3   | 6:Y:14:G:OP1      | 2.12                     | 0.49              |
| 3:N:14:SER:HB2    | 3:N:17:LYS:HB2    | 1.93                     | 0.49              |
| 3:N:97:THR:HG21   | 3:N:459:GLU:HB2   | 1.94                     | 0.49              |
| 3:N:133:ILE:HG22  | 3:N:134:VAL:N     | 2.27                     | 0.49              |
| 3:N:472:ALA:HA    | 3:N:475:LYS:CD    | 2.43                     | 0.49              |
| 3:N:486:ARG:O     | 3:N:490:ALA:CB    | 2.59                     | 0.49              |
| 3:N:610:LYS:CA    | 3:N:615:ARG:HG2   | 2.36                     | 0.49              |
| 3:N:634:GLY:O     | 3:N:637:LEU:HB3   | 2.12                     | 0.49              |
| 3:N:1236:LEU:CD2  | 3:N:1359:GLN:HG3  | 2.42                     | 0.49              |
| 7:I:8:DG:H2''     | 7:I:9:DT:C6       | 2.47                     | 0.49              |
| 5:X:3:DC:O5'      | 5:X:3:DC:C6       | 2.64                     | 0.49              |
| 1:A:74:ASP:O      | 1:A:75:VAL:C      | 2.53                     | 0.49              |
| 1:A:148:VAL:HG12  | 1:A:149:GLY:N     | 2.27                     | 0.49              |
| 2:C:46:ALA:C      | 2:C:48:PHE:N      | 2.70                     | 0.49              |
| 2:C:157:ARG:HD3   | 2:C:314:THR:HG22  | 1.94                     | 0.49              |
| 2:C:324:ASP:O     | 2:C:327:HIS:HB2   | 2.12                     | 0.49              |
| 2:C:938:LYS:HB2   | 2:C:938:LYS:NZ    | 2.26                     | 0.49              |
| 2:C:1016:ILE:HD13 | 2:C:1016:ILE:H    | 1.76                     | 0.49              |
| 3:D:832:ARG:HD2   | 3:D:832:ARG:C     | 2.36                     | 0.49              |
| 3:D:1438:ALA:CB   | 3:D:1447:LEU:HD11 | 2.41                     | 0.49              |
| 3:D:1440:PHE:CE2  | 5:G:17:DA:OP2     | 2.65                     | 0.49              |
| 1:K:29:GLU:HB2    | 1:K:32:PHE:CE1    | 2.48                     | 0.49              |
| 1:L:52:ALA:HB2    | 1:L:170:VAL:O     | 2.12                     | 0.49              |
| 2:M:597:ALA:HB2   | 2:M:655:LEU:HD21  | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:728:HIS:NE2   | 2:M:775:ARG:NH1   | 2.59                     | 0.49              |
| 2:M:832:LYS:O     | 2:M:833:LEU:C     | 2.54                     | 0.49              |
| 2:M:1095:LEU:CD2  | 3:N:603:LEU:CD1   | 2.83                     | 0.49              |
| 3:N:133:ILE:CG1   | 3:N:456:MET:HE2   | 2.41                     | 0.49              |
| 3:N:501:ALA:HB3   | 3:N:1452:ILE:HG22 | 1.92                     | 0.49              |
| 3:N:1341:PRO:C    | 3:N:1343:ALA:H    | 2.19                     | 0.49              |
| 3:N:1372:VAL:CG1  | 3:N:1373:ARG:N    | 2.75                     | 0.49              |
| 3:N:1375:MET:SD   | 3:N:1424:VAL:N    | 2.86                     | 0.49              |
| 3:N:1399:ASP:O    | 3:N:1403:LEU:HD12 | 2.11                     | 0.49              |
| 3:N:1465:ASN:HD21 | 3:N:1470:ARG:NE   | 2.10                     | 0.49              |
| 6:Y:8:G:H2'       | 6:Y:9:C:O5'       | 2.13                     | 0.49              |
| 6:Y:10:G:O2'      | 6:Y:11:C:H5'      | 2.12                     | 0.49              |
| 6:Y:11:C:O2'      | 6:Y:12:U:H5'      | 2.13                     | 0.49              |
| 1:A:2:LEU:O       | 1:A:6:LEU:HB3     | 2.11                     | 0.49              |
| 1:B:62:LEU:H      | 1:B:62:LEU:HD12   | 1.77                     | 0.49              |
| 2:C:261:ILE:CD1   | 2:C:262:ALA:H     | 2.26                     | 0.49              |
| 2:C:926:PHE:HE2   | 2:C:960:GLU:OE1   | 1.96                     | 0.49              |
| 3:D:10:ILE:CD1    | 3:D:1447:LEU:HG   | 2.43                     | 0.49              |
| 3:D:1380:GLU:CG   | 3:D:1381:VAL:N    | 2.75                     | 0.49              |
| 3:D:1435:LEU:CB   | 3:D:1464:GLU:HB3  | 2.42                     | 0.49              |
| 1:L:80:LEU:HD11   | 3:N:842:VAL:HG12  | 1.94                     | 0.49              |
| 1:L:186:LEU:O     | 1:L:188:GLN:N     | 2.45                     | 0.49              |
| 2:M:405:ARG:NH2   | 2:M:409:ARG:NH2   | 2.61                     | 0.49              |
| 2:M:444:PRO:O     | 2:M:449:ILE:HD12  | 2.11                     | 0.49              |
| 2:M:607:ASP:HB3   | 2:M:610:ARG:H     | 1.77                     | 0.49              |
| 2:M:1040:LEU:HD23 | 2:M:1049:LEU:CB   | 2.42                     | 0.49              |
| 2:M:1068:GLU:O    | 2:M:1071:ILE:HB   | 2.13                     | 0.49              |
| 2:M:1098:ASP:CG   | 3:N:17:LYS:HD3    | 2.37                     | 0.49              |
| 3:N:62:LYS:HD2    | 3:N:75:ARG:NH1    | 2.26                     | 0.49              |
| 3:N:95:LEU:HB2    | 3:N:515:GLU:CA    | 2.42                     | 0.49              |
| 3:N:187:LYS:CE    | 3:N:199:LEU:HG    | 2.42                     | 0.49              |
| 3:N:731:LEU:HD22  | 3:N:779:ALA:O     | 2.12                     | 0.49              |
| 3:N:781:PRO:HB2   | 3:N:786:ILE:HG13  | 1.95                     | 0.49              |
| 3:N:813:LEU:C     | 3:N:813:LEU:HD12  | 2.37                     | 0.49              |
| 3:N:880:ILE:O     | 3:N:880:ILE:HD13  | 2.11                     | 0.49              |
| 3:N:883:ALA:O     | 3:N:886:VAL:HB    | 2.13                     | 0.49              |
| 3:N:1115:THR:HG21 | 3:N:1151:ARG:NH2  | 2.27                     | 0.49              |
| 2:C:18:LEU:HD22   | 2:C:590:ASP:HB2   | 1.95                     | 0.49              |
| 2:C:71:TYR:HA     | 2:C:96:ALA:HB2    | 1.94                     | 0.49              |
| 2:C:101:ILE:HG23  | 2:C:107:LEU:HD22  | 1.95                     | 0.49              |
| 2:C:412:ALA:HB3   | 2:C:451:LEU:HB3   | 1.95                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:583:LEU:O     | 2:C:587:VAL:HG23 | 2.11                     | 0.49              |
| 2:C:733:ALA:HB2   | 3:D:679:ARG:NH1  | 2.26                     | 0.49              |
| 2:C:907:ASP:O     | 2:C:907:ASP:CG   | 2.55                     | 0.49              |
| 3:D:131:LYS:HZ2   | 3:D:564:GLU:HB3  | 1.78                     | 0.49              |
| 3:D:916:TYR:O     | 3:D:920:LEU:HG   | 2.13                     | 0.49              |
| 3:D:960:LYS:CE    | 3:D:964:LEU:CD1  | 2.79                     | 0.49              |
| 3:D:1153:VAL:CG1  | 3:N:560:GLN:O    | 2.61                     | 0.49              |
| 3:D:1209:LEU:HD21 | 4:E:16:LYS:HE3   | 1.95                     | 0.49              |
| 3:D:1436:SER:O    | 3:D:1439:SER:OG  | 2.27                     | 0.49              |
| 3:D:1466:VAL:HG12 | 3:D:1467:ILE:N   | 2.27                     | 0.49              |
| 4:E:64:ALA:C      | 4:E:68:LEU:HD22  | 2.37                     | 0.49              |
| 1:K:102:LYS:HA    | 1:K:138:LEU:O    | 2.13                     | 0.49              |
| 1:L:24:VAL:HG22   | 1:L:196:THR:HB   | 1.93                     | 0.49              |
| 1:L:159:LYS:N     | 1:L:159:LYS:HE3  | 2.27                     | 0.49              |
| 2:M:42:VAL:CA     | 2:M:46:ALA:HB2   | 2.41                     | 0.49              |
| 2:M:115:LEU:HB3   | 2:M:375:SER:OG   | 2.12                     | 0.49              |
| 2:M:683:ASN:ND2   | 2:M:683:ASN:C    | 2.68                     | 0.49              |
| 3:N:14:SER:O      | 3:N:15:PRO:C     | 2.54                     | 0.49              |
| 3:N:160:GLU:HG2   | 3:N:165:LYS:CG   | 2.37                     | 0.49              |
| 3:N:1219:GLU:OE1  | 4:O:17:TYR:HE2   | 1.95                     | 0.49              |
| 3:N:1415:VAL:HG23 | 3:N:1415:VAL:O   | 2.11                     | 0.49              |
| 3:N:1468:LEU:HD23 | 3:N:1468:LEU:C   | 2.37                     | 0.49              |
| 3:N:1484:THR:CA   | 4:O:76:GLY:O     | 2.60                     | 0.49              |
| 3:N:1493:LYS:O    | 3:N:1497:GLU:HG2 | 2.13                     | 0.49              |
| 7:Z:12:DT:C2'     | 7:Z:13:DA:C8     | 2.89                     | 0.49              |
| 1:A:28:LEU:O      | 1:A:192:LEU:HD22 | 2.11                     | 0.49              |
| 1:A:48:ILE:HD12   | 1:A:174:VAL:CG2  | 2.42                     | 0.49              |
| 2:C:603:VAL:HB    | 2:C:647:GLN:N    | 2.27                     | 0.49              |
| 2:C:704:HIS:O     | 2:C:828:ALA:HA   | 2.11                     | 0.49              |
| 2:C:1035:MET:CG   | 5:G:20:DC:H5'    | 2.41                     | 0.49              |
| 3:D:4:GLU:HG2     | 3:D:1470:ARG:NE  | 2.28                     | 0.49              |
| 3:D:14:SER:O      | 3:D:15:PRO:C     | 2.55                     | 0.49              |
| 3:D:47:GLU:CD     | 3:D:53:ILE:HB    | 2.37                     | 0.49              |
| 3:D:128:TYR:CE2   | 3:D:458:ALA:CB   | 2.96                     | 0.49              |
| 3:D:615:ARG:HH22  | 3:D:1096:ARG:NH1 | 2.10                     | 0.49              |
| 3:D:705:ALA:CB    | 3:D:706:PRO:CD   | 2.71                     | 0.49              |
| 3:D:1223:ILE:HD11 | 3:D:1462:LEU:CD1 | 2.42                     | 0.49              |
| 1:K:38:ASN:HD21   | 2:M:978:ARG:C    | 2.20                     | 0.49              |
| 1:K:117:VAL:O     | 1:K:120:VAL:HG12 | 2.13                     | 0.49              |
| 2:M:352:ALA:C     | 2:M:355:VAL:HG12 | 2.37                     | 0.49              |
| 2:M:561:GLY:O     | 2:M:565:GLN:HG3  | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:861:LEU:HG    | 2:M:862:PRO:HD2   | 1.93                     | 0.49              |
| 2:M:973:VAL:O     | 2:M:974:LEU:CD1   | 2.50                     | 0.49              |
| 2:M:1043:TYR:CZ   | 3:N:710:ARG:HD3   | 2.48                     | 0.49              |
| 2:M:1053:LEU:CD1  | 3:N:1469:GLY:HA2  | 2.40                     | 0.49              |
| 3:N:764:LEU:HB3   | 3:N:767:HIS:ND1   | 2.28                     | 0.49              |
| 3:N:1160:LEU:N    | 3:N:1160:LEU:HD23 | 2.27                     | 0.49              |
| 3:N:1280:VAL:HG12 | 3:N:1318:TYR:CA   | 2.43                     | 0.49              |
| 3:N:1462:LEU:HD22 | 3:N:1472:ILE:CG2  | 2.42                     | 0.49              |
| 4:O:23:VAL:HG22   | 4:O:68:LEU:CD2    | 2.43                     | 0.49              |
| 5:G:24:DC:H2'     | 5:G:25:DG:C8      | 2.48                     | 0.49              |
| 6:H:11:C:H2'      | 6:H:12:U:C5       | 2.47                     | 0.49              |
| 1:A:9:PRO:HB3     | 1:A:25:LEU:CD2    | 2.43                     | 0.49              |
| 1:A:38:ASN:N      | 1:A:39:PRO:CD     | 2.76                     | 0.49              |
| 1:B:66:SER:O      | 1:B:75:VAL:HG23   | 2.13                     | 0.49              |
| 1:B:79:ILE:HA     | 1:B:82:LEU:CD1    | 2.43                     | 0.49              |
| 2:C:36:PRO:CG     | 2:C:70:GLU:HB3    | 2.37                     | 0.49              |
| 2:C:47:ALA:HB2    | 2:C:345:ARG:HH11  | 1.78                     | 0.49              |
| 2:C:422:ARG:HG2   | 7:I:1:DG:C6       | 2.47                     | 0.49              |
| 2:C:460:ARG:HG3   | 2:C:460:ARG:O     | 2.12                     | 0.49              |
| 2:C:511:GLU:O     | 2:C:526:PRO:HD3   | 2.12                     | 0.49              |
| 2:C:532:MET:HG2   | 2:C:533:ASP:O     | 2.12                     | 0.49              |
| 2:C:941:VAL:HA    | 2:C:944:LEU:HB2   | 1.94                     | 0.49              |
| 2:C:998:TYR:HE2   | 2:C:1000:MET:HG3  | 1.78                     | 0.49              |
| 3:D:155:ASP:O     | 3:D:159:ARG:HB2   | 2.12                     | 0.49              |
| 3:D:683:ILE:HD12  | 3:D:683:ILE:H     | 1.77                     | 0.49              |
| 3:D:895:VAL:HA    | 3:D:898:GLU:CD    | 2.38                     | 0.49              |
| 3:D:916:TYR:CE2   | 3:D:920:LEU:HD11  | 2.47                     | 0.49              |
| 3:D:1112:CYS:SG   | 3:D:1201:CYS:N    | 2.78                     | 0.49              |
| 3:D:1154:GLU:OE2  | 3:N:563:PRO:HA    | 2.12                     | 0.49              |
| 1:K:74:ASP:O      | 1:K:78:ILE:HG13   | 2.12                     | 0.49              |
| 2:M:302:VAL:C     | 2:M:305:PRO:HD2   | 2.38                     | 0.49              |
| 2:M:630:ARG:HD2   | 2:M:631:SER:O     | 2.12                     | 0.49              |
| 3:N:704:ARG:NE    | 3:N:706:PRO:HD2   | 2.25                     | 0.49              |
| 3:N:764:LEU:CD2   | 3:N:767:HIS:CE1   | 2.88                     | 0.49              |
| 3:N:899:LEU:HD22  | 3:N:917:GLN:HB3   | 1.95                     | 0.49              |
| 3:N:1094:LEU:HD12 | 3:N:1097:LYS:CD   | 2.37                     | 0.49              |
| 3:N:1103:HIS:CG   | 3:N:1104:GLU:N    | 2.80                     | 0.49              |
| 3:N:1283:ILE:HD12 | 3:N:1315:ASP:OD2  | 2.13                     | 0.49              |
| 1:A:96:THR:OG1    | 1:A:143:ARG:HD2   | 2.12                     | 0.49              |
| 1:B:102:LYS:HG3   | 1:B:138:LEU:O     | 2.13                     | 0.49              |
| 1:B:140:MET:O     | 1:B:140:MET:HG2   | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:12:VAL:HG13   | 2:C:13:ILE:N      | 2.27                     | 0.49              |
| 2:C:49:ARG:O      | 2:C:53:PRO:HD2    | 2.13                     | 0.49              |
| 2:C:470:PRO:HD3   | 2:C:485:TYR:CZ    | 2.48                     | 0.49              |
| 3:D:503:LEU:O     | 3:D:504:ASP:C     | 2.54                     | 0.49              |
| 3:D:939:PHE:O     | 3:D:943:THR:HG23  | 2.13                     | 0.49              |
| 3:D:1098:LEU:HD23 | 3:D:1226:ALA:CA   | 2.37                     | 0.49              |
| 3:D:1231:GLU:OE1  | 3:D:1232:PRO:HD3  | 2.13                     | 0.49              |
| 3:D:1495:ILE:O    | 3:D:1499:ARG:HG3  | 2.12                     | 0.49              |
| 1:K:11:PHE:HD1    | 1:K:25:LEU:HD13   | 1.77                     | 0.49              |
| 1:K:23:PHE:O      | 1:K:197:LEU:HD23  | 2.13                     | 0.49              |
| 1:L:7:LYS:HZ2     | 1:L:186:LEU:HD13  | 1.78                     | 0.49              |
| 1:L:50:GLY:O      | 1:L:146:ARG:HA    | 2.12                     | 0.49              |
| 2:M:141:HIS:NE2   | 2:M:332:ARG:HB3   | 2.27                     | 0.49              |
| 2:M:162:ILE:CB    | 2:M:172:ILE:HB    | 2.37                     | 0.49              |
| 2:M:555:ALA:O     | 2:M:558:ALA:HB3   | 2.13                     | 0.49              |
| 2:M:636:ALA:O     | 2:M:637:LEU:HD23  | 2.13                     | 0.49              |
| 2:M:969:GLN:HE22  | 3:N:952:ASP:HB3   | 1.78                     | 0.49              |
| 3:N:9:ARG:HG2     | 3:N:9:ARG:HH11    | 1.78                     | 0.49              |
| 3:N:478:LEU:O     | 3:N:1388:ARG:NH2  | 2.45                     | 0.49              |
| 3:N:771:SER:O     | 3:N:774:SER:O     | 2.30                     | 0.49              |
| 3:N:1200:VAL:CG1  | 3:N:1201:CYS:N    | 2.76                     | 0.49              |
| 3:N:1367:HIS:C    | 3:N:1370:ILE:HG12 | 2.38                     | 0.49              |
| 3:N:1481:VAL:HG22 | 4:O:18:ARG:NH2    | 2.28                     | 0.49              |
| 3:N:1485:GLN:NE2  | 4:O:80:VAL:O      | 2.46                     | 0.49              |
| 1:B:186:LEU:O     | 1:B:188:GLN:N     | 2.46                     | 0.49              |
| 2:C:334:ARG:HA    | 2:C:338:GLU:OE2   | 2.12                     | 0.49              |
| 2:C:437:ARG:HG2   | 2:C:467:ILE:O     | 2.13                     | 0.49              |
| 2:C:585:GLU:O     | 2:C:588:VAL:HG22  | 2.13                     | 0.49              |
| 2:C:739:GLU:HG3   | 2:C:742:VAL:CG1   | 2.42                     | 0.49              |
| 3:D:54:LYS:HG3    | 3:D:55:ASP:N      | 2.28                     | 0.49              |
| 3:D:128:TYR:CE2   | 3:D:458:ALA:HA    | 2.41                     | 0.49              |
| 3:D:1225:ALA:HB2  | 3:D:1367:HIS:HD1  | 1.78                     | 0.49              |
| 3:D:1231:GLU:CB   | 3:D:1232:PRO:HD3  | 2.41                     | 0.49              |
| 1:K:67:THR:OG1    | 2:M:609:ASN:ND2   | 2.46                     | 0.49              |
| 2:M:139:GLN:HG2   | 2:M:418:LEU:HD22  | 1.93                     | 0.49              |
| 2:M:468:ARG:CZ    | 2:M:485:TYR:O     | 2.61                     | 0.49              |
| 2:M:583:LEU:N     | 2:M:583:LEU:HD12  | 2.28                     | 0.49              |
| 2:M:603:VAL:HG21  | 2:M:647:GLN:HB3   | 1.93                     | 0.49              |
| 2:M:611:ILE:HG13  | 2:M:625:LEU:HD11  | 1.95                     | 0.49              |
| 2:M:732:ALA:O     | 2:M:735:ARG:HG3   | 2.13                     | 0.49              |
| 2:M:941:VAL:O     | 2:M:944:LEU:HB2   | 2.13                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:1001:VAL:HB  | 5:X:23:DG:O3'     | 2.12                     | 0.49              |
| 3:N:160:GLU:O    | 3:N:161:LEU:C     | 2.56                     | 0.49              |
| 3:N:177:ALA:HB3  | 3:N:205:TYR:OH    | 2.13                     | 0.49              |
| 3:N:795:VAL:HG13 | 3:N:863:VAL:HG22  | 1.95                     | 0.49              |
| 3:N:1176:LYS:O   | 3:N:1179:GLU:HB2  | 2.13                     | 0.49              |
| 3:N:1341:PRO:C   | 3:N:1343:ALA:N    | 2.68                     | 0.49              |
| 3:N:1366:LYS:O   | 3:N:1370:ILE:HG12 | 2.12                     | 0.49              |
| 3:N:1381:VAL:CG1 | 3:N:1382:THR:H    | 2.22                     | 0.49              |
| 4:O:36:LYS:HG2   | 4:O:95:VAL:HG22   | 1.94                     | 0.49              |
| 1:B:59:GLU:HB2   | 1:B:137:ARG:HH12  | 1.78                     | 0.49              |
| 2:C:437:ARG:NH1  | 2:C:488:ALA:HA    | 2.28                     | 0.49              |
| 2:C:685:GLU:OE1  | 3:D:739:ASP:CB    | 2.60                     | 0.49              |
| 2:C:1008:ARG:NH2 | 2:C:1012:PRO:N    | 2.61                     | 0.49              |
| 3:D:133:ILE:O    | 3:D:153:LEU:N     | 2.46                     | 0.49              |
| 3:D:145:VAL:HG13 | 3:D:148:GLU:OE1   | 2.12                     | 0.49              |
| 3:D:531:ASP:C    | 3:D:533:GLY:H     | 2.21                     | 0.49              |
| 3:D:703:ASN:OD1  | 3:D:704:ARG:O     | 2.31                     | 0.49              |
| 2:M:140:ILE:C    | 2:M:140:ILE:HD12  | 2.38                     | 0.49              |
| 2:M:483:VAL:HG12 | 2:M:484:VAL:N     | 2.28                     | 0.49              |
| 2:M:663:ASN:C    | 2:M:665:PHE:H     | 2.21                     | 0.49              |
| 2:M:682:TYR:O    | 2:M:850:ALA:CB    | 2.61                     | 0.49              |
| 2:M:690:ILE:CG2  | 2:M:852:ILE:HA    | 2.42                     | 0.49              |
| 2:M:1037:VAL:O   | 2:M:1041:GLU:HG3  | 2.13                     | 0.49              |
| 3:N:531:ASP:C    | 3:N:533:GLY:H     | 2.20                     | 0.49              |
| 3:N:697:GLY:CA   | 3:N:717:GLN:OE1   | 2.61                     | 0.49              |
| 3:N:701:LEU:HD13 | 3:N:748:HIS:HB2   | 1.95                     | 0.49              |
| 3:N:792:ILE:HG23 | 3:N:793:THR:N     | 2.28                     | 0.49              |
| 3:N:814:ALA:O    | 3:N:818:ARG:HG3   | 2.13                     | 0.49              |
| 3:N:864:VAL:HG12 | 3:N:865:THR:N     | 2.18                     | 0.49              |
| 3:N:986:ARG:HE   | 3:N:1310:ARG:HH12 | 1.60                     | 0.49              |
| 3:N:1084:THR:HA  | 3:N:1087:ARG:NH2  | 2.28                     | 0.49              |
| 3:N:1444:THR:O   | 3:N:1448:THR:OG1  | 2.27                     | 0.49              |
| 3:N:1450:ALA:O   | 3:N:1453:ALA:O    | 2.30                     | 0.49              |
| 5:G:7:DA:H2''    | 5:G:8:DC:H6       | 1.77                     | 0.49              |
| 5:X:19:DG:H2''   | 5:X:20:DC:C5'     | 2.37                     | 0.49              |
| 1:A:9:PRO:HB3    | 1:A:25:LEU:HD21   | 1.93                     | 0.48              |
| 1:A:63:HIS:CE1   | 1:A:65:PHE:O      | 2.66                     | 0.48              |
| 2:C:452:ILE:HD12 | 2:C:452:ILE:N     | 2.27                     | 0.48              |
| 2:C:510:ALA:HB3  | 2:C:513:VAL:CG2   | 2.43                     | 0.48              |
| 2:C:578:VAL:O    | 2:C:900:ARG:HG2   | 2.13                     | 0.48              |
| 2:C:630:ARG:HG2  | 2:C:826:TYR:CE2   | 2.47                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:759:THR:HB    | 2:C:785:VAL:CG1  | 2.43                     | 0.48              |
| 2:C:1014:SER:O    | 2:C:1017:THR:O   | 2.30                     | 0.48              |
| 3:D:739:ASP:H     | 6:H:15:C:C5'     | 2.16                     | 0.48              |
| 3:D:757:ALA:O     | 3:D:761:ILE:HG13 | 2.12                     | 0.48              |
| 3:D:796:ARG:HB2   | 3:D:828:LYS:CD   | 2.36                     | 0.48              |
| 3:D:853:VAL:HG22  | 3:D:858:VAL:HG23 | 1.94                     | 0.48              |
| 3:D:1087:ARG:NE   | 3:D:1236:LEU:CD2 | 2.65                     | 0.48              |
| 1:K:26:GLU:HB2    | 1:K:27:PRO:HA    | 1.94                     | 0.48              |
| 1:L:58:ILE:HG21   | 1:L:61:VAL:HG23  | 1.94                     | 0.48              |
| 2:M:603:VAL:CB    | 2:M:647:GLN:H    | 2.23                     | 0.48              |
| 2:M:753:ASP:C     | 2:M:792:VAL:HG23 | 2.37                     | 0.48              |
| 2:M:1022:GLY:CA   | 2:M:1026:GLN:O   | 2.61                     | 0.48              |
| 3:N:55:ASP:CA     | 3:N:82:LYS:HE2   | 2.43                     | 0.48              |
| 3:N:414:ARG:HD2   | 3:N:414:ARG:N    | 2.28                     | 0.48              |
| 3:N:853:VAL:HG22  | 3:N:858:VAL:HG23 | 1.95                     | 0.48              |
| 3:N:1128:VAL:O    | 3:N:1129:THR:C   | 2.56                     | 0.48              |
| 3:N:1239:ARG:NH1  | 3:N:1239:ARG:CB  | 2.73                     | 0.48              |
| 4:O:37:ASN:N      | 4:O:37:ASN:ND2   | 2.56                     | 0.48              |
| 5:G:3:DC:H1'      | 5:G:4:DA:H5'     | 1.95                     | 0.48              |
| 1:A:110:LYS:C     | 1:A:112:ARG:N    | 2.71                     | 0.48              |
| 2:C:199:VAL:CG1   | 2:C:235:LEU:HG   | 2.40                     | 0.48              |
| 2:C:292:ARG:CD    | 2:C:298:PHE:HA   | 2.43                     | 0.48              |
| 2:C:523:ILE:HG23  | 2:C:523:ILE:O    | 2.13                     | 0.48              |
| 2:C:572:ILE:HG23  | 2:C:703:ILE:CD1  | 2.43                     | 0.48              |
| 2:C:737:LEU:HD21  | 2:C:741:GLY:CA   | 2.43                     | 0.48              |
| 2:C:1031:ARG:HD3  | 5:G:21:DG:OP1    | 2.13                     | 0.48              |
| 2:C:1088:LEU:HD23 | 2:C:1088:LEU:O   | 2.12                     | 0.48              |
| 3:D:39:PRO:O      | 3:D:40:GLU:O     | 2.31                     | 0.48              |
| 3:D:123:LEU:O     | 3:D:124:GLU:C    | 2.54                     | 0.48              |
| 3:D:128:TYR:HE2   | 3:D:458:ALA:CA   | 2.25                     | 0.48              |
| 3:D:134:VAL:O     | 3:D:454:ALA:HA   | 2.13                     | 0.48              |
| 3:D:743:ASP:HA    | 6:H:14:G:H1'     | 1.96                     | 0.48              |
| 3:D:877:PRO:O     | 3:D:880:ILE:HG22 | 2.13                     | 0.48              |
| 3:D:937:TYR:N     | 3:D:937:TYR:CD1  | 2.81                     | 0.48              |
| 3:D:1394:VAL:HB   | 3:D:1397:LYS:HE2 | 1.95                     | 0.48              |
| 1:K:206:THR:HG22  | 1:K:209:GLU:HG3  | 1.95                     | 0.48              |
| 1:L:43:ILE:HG23   | 1:L:47:SER:CB    | 2.43                     | 0.48              |
| 1:L:58:ILE:HG22   | 1:L:61:VAL:H     | 1.77                     | 0.48              |
| 2:M:195:LEU:CG    | 2:M:238:LEU:HG   | 2.43                     | 0.48              |
| 2:M:817:PRO:C     | 2:M:819:VAL:H    | 2.21                     | 0.48              |
| 3:N:28:LYS:O      | 3:N:43:GLY:HA2   | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:159:ARG:HG2   | 3:N:163:TYR:HE2   | 1.78                     | 0.48              |
| 3:N:506:GLY:O     | 3:N:507:ASN:C     | 2.57                     | 0.48              |
| 3:N:584:ASN:HD21  | 3:N:590:PRO:HD2   | 1.78                     | 0.48              |
| 3:N:631:ILE:HD12  | 3:N:740:PHE:CE2   | 2.48                     | 0.48              |
| 3:N:728:LEU:CG    | 3:N:729:HIS:N     | 2.76                     | 0.48              |
| 3:N:813:LEU:HD12  | 3:N:814:ALA:N     | 2.28                     | 0.48              |
| 3:N:1066:THR:HG23 | 3:N:1069:GLU:H    | 1.79                     | 0.48              |
| 3:N:1263:PHE:CE1  | 3:N:1352:ILE:HD13 | 2.48                     | 0.48              |
| 3:N:1281:VAL:HG12 | 3:N:1314:LYS:O    | 2.13                     | 0.48              |
| 2:C:265:ARG:N     | 2:C:289:THR:HG21  | 2.22                     | 0.48              |
| 2:C:272:ALA:O     | 2:C:276:LYS:CE    | 2.60                     | 0.48              |
| 2:C:814:GLU:HG3   | 2:C:814:GLU:O     | 2.13                     | 0.48              |
| 2:C:926:PHE:HD2   | 2:C:960:GLU:OE2   | 1.96                     | 0.48              |
| 3:D:50:PHE:CD2    | 3:D:522:PRO:HD3   | 2.48                     | 0.48              |
| 3:D:676:MET:SD    | 3:D:676:MET:O     | 2.71                     | 0.48              |
| 3:D:1090:ASP:O    | 3:D:1094:LEU:HB2  | 2.13                     | 0.48              |
| 3:D:1378:TYR:CD1  | 3:D:1422:MET:SD   | 3.06                     | 0.48              |
| 1:K:193:ASP:CG    | 2:M:938:LYS:HZ1   | 2.21                     | 0.48              |
| 2:M:31:GLN:HG2    | 2:M:34:VAL:HG23   | 1.94                     | 0.48              |
| 2:M:343:GLN:HG2   | 2:M:385:PHE:CD1   | 2.48                     | 0.48              |
| 2:M:535:SER:N     | 2:M:538:GLN:OE1   | 2.41                     | 0.48              |
| 2:M:551:GLU:OE1   | 2:M:906:PHE:HA    | 2.14                     | 0.48              |
| 2:M:692:GLU:HB2   | 2:M:854:PRO:HA    | 1.96                     | 0.48              |
| 2:M:882:LEU:HD23  | 2:M:885:ILE:HG13  | 1.94                     | 0.48              |
| 2:M:897:LEU:HD21  | 2:M:921:ALA:HA    | 1.96                     | 0.48              |
| 3:N:607:LEU:HD23  | 3:N:613:ARG:CB    | 2.38                     | 0.48              |
| 3:N:693:GLU:HA    | 4:O:48:MET:SD     | 2.53                     | 0.48              |
| 3:N:838:ARG:NH1   | 3:N:838:ARG:HG2   | 2.27                     | 0.48              |
| 3:N:1195:GLN:O    | 3:N:1196:THR:C    | 2.57                     | 0.48              |
| 3:N:1274:ILE:CG2  | 3:N:1301:LYS:HZ1  | 2.14                     | 0.48              |
| 1:A:19:GLU:HA     | 1:A:201:THR:O     | 2.13                     | 0.48              |
| 2:C:193:LEU:HD12  | 2:C:193:LEU:N     | 2.28                     | 0.48              |
| 2:C:643:VAL:HG13  | 2:C:647:GLN:CD    | 2.39                     | 0.48              |
| 2:C:650:ARG:HG2   | 2:C:653:ASP:OD2   | 2.14                     | 0.48              |
| 2:C:838:LYS:HZ3   | 3:D:742:GLY:HA3   | 1.78                     | 0.48              |
| 2:C:1012:PRO:HD3  | 2:C:1026:GLN:CG   | 2.43                     | 0.48              |
| 2:C:1038:TRP:CE2  | 3:D:1099:VAL:HG21 | 2.48                     | 0.48              |
| 3:D:136:ASP:CB    | 3:D:137:PRO:CD    | 2.77                     | 0.48              |
| 3:D:704:ARG:CG    | 3:D:705:ALA:N     | 2.77                     | 0.48              |
| 3:D:1068:LEU:O    | 3:D:1072:ILE:HG12 | 2.14                     | 0.48              |
| 3:D:1102:THR:O    | 3:D:1222:GLY:HA3  | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1154:GLU:N    | 3:N:561:GLY:CA    | 2.76                     | 0.48              |
| 3:D:1209:LEU:HD21 | 4:E:16:LYS:HZ2    | 1.75                     | 0.48              |
| 2:M:324:ASP:O     | 2:M:327:HIS:HB2   | 2.13                     | 0.48              |
| 2:M:571:LEU:HD21  | 2:M:700:TYR:HA    | 1.94                     | 0.48              |
| 2:M:598:GLU:O     | 2:M:651:LYS:HE3   | 2.14                     | 0.48              |
| 2:M:630:ARG:HH11  | 2:M:630:ARG:CG    | 2.26                     | 0.48              |
| 2:M:861:LEU:HD13  | 2:M:865:THR:CG2   | 2.43                     | 0.48              |
| 3:N:109:PRO:O     | 3:N:111:LYS:HD2   | 2.13                     | 0.48              |
| 3:N:806:PHE:O     | 3:N:808:THR:N     | 2.46                     | 0.48              |
| 3:N:1147:ARG:NH2  | 3:N:1369:GLU:OE2  | 2.43                     | 0.48              |
| 3:N:1404:ASN:OD1  | 3:N:1408:ILE:HD12 | 2.14                     | 0.48              |
| 3:N:1442:ASN:OD1  | 3:N:1444:THR:HB   | 2.13                     | 0.48              |
| 4:O:49:GLN:HA     | 4:O:51:LEU:O      | 2.13                     | 0.48              |
| 6:H:4:G:C5        | 6:H:5:C:C4        | 3.02                     | 0.48              |
| 1:A:42:ARG:HH12   | 1:B:34:VAL:CB     | 2.23                     | 0.48              |
| 1:B:79:ILE:HA     | 1:B:82:LEU:HD12   | 1.94                     | 0.48              |
| 2:C:846:LYS:HB3   | 3:D:741:ASP:HB2   | 1.95                     | 0.48              |
| 2:C:1063:ARG:CG   | 2:C:1064:ASN:N    | 2.75                     | 0.48              |
| 3:D:154:THR:O     | 3:D:158:TYR:HB3   | 2.13                     | 0.48              |
| 3:D:715:ALA:HB3   | 3:D:764:LEU:CA    | 2.43                     | 0.48              |
| 3:D:796:ARG:HH21  | 3:D:862:ASP:CG    | 2.20                     | 0.48              |
| 3:D:1264:GLU:CD   | 3:D:1425:THR:HB   | 2.38                     | 0.48              |
| 3:D:1462:LEU:O    | 3:D:1466:VAL:N    | 2.46                     | 0.48              |
| 1:L:26:GLU:CB     | 1:L:27:PRO:HA     | 2.32                     | 0.48              |
| 1:L:101:LEU:HD12  | 1:L:113:ASP:HB3   | 1.92                     | 0.48              |
| 1:L:184:THR:O     | 1:L:192:LEU:HB2   | 2.12                     | 0.48              |
| 2:M:289:THR:O     | 2:M:290:LEU:C     | 2.57                     | 0.48              |
| 2:M:333:ILE:N     | 2:M:333:ILE:CD1   | 2.76                     | 0.48              |
| 2:M:344:PHE:CE2   | 2:M:378:LEU:HD11  | 2.48                     | 0.48              |
| 2:M:350:ARG:HA    | 2:M:353:ARG:HH21  | 1.78                     | 0.48              |
| 3:N:1381:VAL:HB   | 3:N:1389:LEU:O    | 2.13                     | 0.48              |
| 3:N:1395:LEU:O    | 3:N:1398:TRP:HB2  | 2.13                     | 0.48              |
| 5:G:3:DC:H6       | 5:G:3:DC:OP2      | 1.97                     | 0.48              |
| 5:X:20:DC:H2'     | 5:X:21:DG:C8      | 2.48                     | 0.48              |
| 1:A:51:THR:HB     | 1:A:87:VAL:HG23   | 1.94                     | 0.48              |
| 2:C:313:LEU:HG    | 2:C:314:THR:N     | 2.25                     | 0.48              |
| 2:C:861:LEU:HA    | 2:C:974:LEU:HD12  | 1.95                     | 0.48              |
| 2:C:893:ALA:HB1   | 2:C:897:LEU:CD1   | 2.44                     | 0.48              |
| 2:C:922:PHE:CZ    | 2:C:963:LEU:HB3   | 2.49                     | 0.48              |
| 2:C:942:GLU:O     | 2:C:946:ARG:HG3   | 2.13                     | 0.48              |
| 2:C:957:LYS:HD3   | 2:C:961:GLU:CB    | 2.42                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:925:GLU:OE1   | 4:E:5:GLY:CA      | 2.62                     | 0.48              |
| 3:D:949:ILE:HG12  | 3:D:1023:MET:HE1  | 1.95                     | 0.48              |
| 3:D:1468:LEU:HD13 | 3:D:1470:ARG:HD3  | 1.96                     | 0.48              |
| 2:M:49:ARG:HH11   | 2:M:68:PHE:HD2    | 1.61                     | 0.48              |
| 2:M:169:GLY:O     | 2:M:170:PRO:O     | 2.31                     | 0.48              |
| 2:M:211:LEU:CB    | 2:M:308:ARG:HD2   | 2.37                     | 0.48              |
| 2:M:302:VAL:HG13  | 2:M:303:PHE:N     | 2.29                     | 0.48              |
| 2:M:455:LEU:HD12  | 2:M:456:ALA:N     | 2.28                     | 0.48              |
| 2:M:564:MET:HE2   | 2:M:995:MET:HE3   | 1.95                     | 0.48              |
| 2:M:692:GLU:CB    | 2:M:854:PRO:HA    | 2.43                     | 0.48              |
| 2:M:725:ASP:HB3   | 2:M:783:ARG:HH22  | 1.78                     | 0.48              |
| 3:N:552:ASN:O     | 3:N:556:LYS:HG3   | 2.13                     | 0.48              |
| 3:N:1389:LEU:CD1  | 3:N:1390:LEU:N    | 2.76                     | 0.48              |
| 4:O:54:LEU:O      | 4:O:63:TRP:HZ2    | 1.97                     | 0.48              |
| 7:I:2:DT:OP2      | 7:I:2:DT:H2'      | 2.13                     | 0.48              |
| 7:I:2:DT:O4       | 7:I:3:DA:N6       | 2.47                     | 0.48              |
| 7:I:9:DT:H2''     | 7:I:10:DG:OP2     | 2.12                     | 0.48              |
| 1:A:43:ILE:CG2    | 1:A:47:SER:HB2    | 2.34                     | 0.48              |
| 1:B:142:VAL:HG23  | 1:B:142:VAL:O     | 2.14                     | 0.48              |
| 1:B:150:TYR:CE1   | 1:B:170:VAL:HG12  | 2.48                     | 0.48              |
| 2:C:338:GLU:C     | 2:C:341:THR:HG22  | 2.38                     | 0.48              |
| 2:C:1090:LYS:HE3  | 3:D:90:MET:HG3    | 1.96                     | 0.48              |
| 3:D:503:LEU:O     | 3:D:506:GLY:N     | 2.47                     | 0.48              |
| 3:D:637:LEU:HD11  | 3:D:642:CYS:C     | 2.38                     | 0.48              |
| 3:D:695:ILE:O     | 3:D:698:LYS:N     | 2.47                     | 0.48              |
| 1:L:80:LEU:C      | 3:N:844:ALA:HB2   | 2.38                     | 0.48              |
| 2:M:164:PRO:CD    | 2:M:170:PRO:O     | 2.62                     | 0.48              |
| 2:M:236:ILE:HD12  | 2:M:236:ILE:N     | 2.28                     | 0.48              |
| 2:M:265:ARG:HG2   | 2:M:267:TYR:H     | 1.78                     | 0.48              |
| 2:M:292:ARG:HD2   | 2:M:299:LYS:HE2   | 1.94                     | 0.48              |
| 2:M:302:VAL:HG13  | 2:M:303:PHE:H     | 1.77                     | 0.48              |
| 2:M:428:ARG:NH2   | 2:M:451:LEU:HD11  | 2.28                     | 0.48              |
| 2:M:603:VAL:CG2   | 2:M:647:GLN:HB3   | 2.44                     | 0.48              |
| 2:M:724:ARG:O     | 2:M:724:ARG:HG2   | 2.13                     | 0.48              |
| 2:M:726:ILE:HD12  | 2:M:726:ILE:N     | 2.29                     | 0.48              |
| 2:M:1016:ILE:HD13 | 2:M:1016:ILE:N    | 2.18                     | 0.48              |
| 2:M:1045:ALA:HA   | 3:N:758:GLU:CD    | 2.38                     | 0.48              |
| 3:N:525:ARG:HD3   | 3:N:525:ARG:H     | 1.78                     | 0.48              |
| 3:N:618:LEU:HD11  | 3:N:1467:ILE:HD11 | 1.95                     | 0.48              |
| 3:N:631:ILE:HD11  | 3:N:743:ASP:HB2   | 1.94                     | 0.48              |
| 3:N:1350:GLU:OE2  | 3:N:1354:LYS:HE3  | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Y:8:G:C8        | 6:Y:8:G:OP2       | 2.66                     | 0.48              |
| 7:Z:3:DA:H1'      | 7:Z:4:DG:C5'      | 2.24                     | 0.48              |
| 1:A:57:TYR:CE1    | 1:A:161:ARG:HG2   | 2.49                     | 0.48              |
| 1:B:76:VAL:O      | 1:B:80:LEU:HB2    | 2.14                     | 0.48              |
| 2:C:244:PRO:CD    | 2:C:245:GLY:N     | 2.74                     | 0.48              |
| 2:C:722:ILE:O     | 2:C:722:ILE:HG23  | 2.13                     | 0.48              |
| 2:C:730:SER:O     | 2:C:734:LEU:HD13  | 2.13                     | 0.48              |
| 2:C:817:PRO:C     | 2:C:819:VAL:H     | 2.22                     | 0.48              |
| 2:C:1053:LEU:HD13 | 3:D:1469:GLY:HA2  | 1.94                     | 0.48              |
| 2:C:1074:GLU:HG2  | 2:C:1075:ASP:H    | 1.79                     | 0.48              |
| 2:C:1106:ASP:CG   | 3:D:1456:LYS:HD3  | 2.38                     | 0.48              |
| 3:D:104:PHE:CE2   | 3:D:1448:THR:HG23 | 2.49                     | 0.48              |
| 3:D:155:ASP:HA    | 3:D:158:TYR:HD2   | 1.78                     | 0.48              |
| 3:D:615:ARG:NH2   | 3:D:1096:ARG:NH1  | 2.62                     | 0.48              |
| 3:D:618:LEU:CD1   | 3:D:1463:LYS:HG3  | 2.43                     | 0.48              |
| 3:D:794:GLN:OE1   | 3:D:905:PRO:CG    | 2.62                     | 0.48              |
| 3:D:1194:CYS:CB   | 3:D:1204:CYS:SG   | 2.98                     | 0.48              |
| 3:D:1197:ARG:HD3  | 3:D:1198:TYR:N    | 2.27                     | 0.48              |
| 1:L:36:LEU:C      | 1:L:39:PRO:HD2    | 2.38                     | 0.48              |
| 1:L:102:LYS:HD2   | 1:L:139:ASN:HB2   | 1.96                     | 0.48              |
| 1:L:176:ARG:HH22  | 3:N:884:ARG:HG3   | 1.78                     | 0.48              |
| 2:M:375:SER:HB3   | 2:M:379:GLU:OE1   | 2.13                     | 0.48              |
| 2:M:713:ARG:HG2   | 2:M:714:ASP:H     | 1.78                     | 0.48              |
| 2:M:903:SER:O     | 2:M:904:PRO:O     | 2.32                     | 0.48              |
| 3:N:41:ARG:HH11   | 3:N:42:ASP:HB3    | 1.77                     | 0.48              |
| 3:N:57:GLU:HG2    | 3:N:58:CYS:H      | 1.79                     | 0.48              |
| 3:N:95:LEU:HD12   | 3:N:515:GLU:CA    | 2.44                     | 0.48              |
| 3:N:700:VAL:O     | 3:N:715:ALA:HA    | 2.14                     | 0.48              |
| 3:N:1223:ILE:O    | 3:N:1226:ALA:HB3  | 2.13                     | 0.48              |
| 4:O:72:ARG:HB2    | 4:O:73:LEU:HD12   | 1.96                     | 0.48              |
| 7:Z:1:DG:C2'      | 7:Z:2:DT:H71      | 2.43                     | 0.48              |
| 7:Z:6:DT:H2''     | 7:Z:7:DT:C7       | 2.44                     | 0.48              |
| 1:A:30:ARG:NH1    | 1:A:191:ASP:HB2   | 2.29                     | 0.48              |
| 1:A:42:ARG:NH1    | 2:C:978:ARG:HA    | 2.29                     | 0.48              |
| 1:A:63:HIS:ND1    | 1:A:65:PHE:HD1    | 2.11                     | 0.48              |
| 1:A:96:THR:HA     | 1:A:144:VAL:O     | 2.14                     | 0.48              |
| 2:C:182:VAL:HB    | 2:C:193:LEU:HD13  | 1.94                     | 0.48              |
| 2:C:289:THR:O     | 2:C:290:LEU:C     | 2.56                     | 0.48              |
| 2:C:300:ASP:C     | 2:C:302:VAL:N     | 2.71                     | 0.48              |
| 2:C:394:PHE:CE1   | 2:C:632:ASN:HB3   | 2.48                     | 0.48              |
| 2:C:1115:LEU:HD22 | 3:D:88:TYR:CD1    | 2.48                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:554:LEU:HG    | 3:D:558:LEU:HG   | 1.96                     | 0.48              |
| 3:D:1433:SER:HB2  | 3:D:1457:ASP:CG  | 2.38                     | 0.48              |
| 1:K:9:PRO:HB3     | 1:K:25:LEU:CD2   | 2.44                     | 0.48              |
| 2:M:94:LEU:HD12   | 2:M:95:TYR:H     | 1.79                     | 0.48              |
| 2:M:279:GLU:HG3   | 2:M:280:LYS:N    | 2.28                     | 0.48              |
| 2:M:304:LEU:HG    | 2:M:305:PRO:HD3  | 1.95                     | 0.48              |
| 2:M:561:GLY:O     | 2:M:564:MET:HG2  | 2.14                     | 0.48              |
| 2:M:1009:SER:OG   | 2:M:1010:THR:N   | 2.47                     | 0.48              |
| 2:M:1074:GLU:HG2  | 2:M:1075:ASP:N   | 2.23                     | 0.48              |
| 3:N:58:CYS:SG     | 3:N:61:GLY:CA    | 3.02                     | 0.48              |
| 3:N:206:ARG:HG2   | 3:N:394:LEU:CD2  | 2.43                     | 0.48              |
| 3:N:525:ARG:CB    | 3:N:540:LEU:HD12 | 2.42                     | 0.48              |
| 3:N:577:ALA:O     | 3:N:581:LEU:CD2  | 2.61                     | 0.48              |
| 3:N:838:ARG:HD2   | 3:N:838:ARG:H    | 1.78                     | 0.48              |
| 3:N:970:LYS:O     | 3:N:974:ILE:HG13 | 2.13                     | 0.48              |
| 3:N:1283:ILE:HG22 | 3:N:1284:GLU:N   | 2.28                     | 0.48              |
| 4:O:3:GLU:OE1     | 4:O:3:GLU:HA     | 2.13                     | 0.48              |
| 6:Y:4:G:H2'       | 6:Y:5:C:O5'      | 2.14                     | 0.48              |
| 1:B:20:TYR:HE2    | 1:B:198:ARG:HB2  | 1.78                     | 0.48              |
| 2:C:432:ARG:NH1   | 2:C:520:GLU:OE1  | 2.47                     | 0.48              |
| 2:C:460:ARG:HH12  | 2:C:462:ASP:CA   | 2.27                     | 0.48              |
| 2:C:579:VAL:HG13  | 2:C:842:ARG:NH2  | 2.17                     | 0.48              |
| 2:C:596:TYR:C     | 2:C:655:LEU:HD11 | 2.39                     | 0.48              |
| 2:C:862:PRO:HB2   | 2:C:929:ARG:HH12 | 1.78                     | 0.48              |
| 3:D:525:ARG:HG3   | 3:D:541:ASN:OD1  | 2.14                     | 0.48              |
| 3:D:676:MET:SD    | 3:D:684:LYS:HE3  | 2.54                     | 0.48              |
| 3:D:698:LYS:CD    | 4:E:59:ASN:OD1   | 2.62                     | 0.48              |
| 3:D:891:GLU:O     | 3:D:893:GLU:N    | 2.46                     | 0.48              |
| 3:D:892:ASP:OD2   | 3:D:895:VAL:HG23 | 2.14                     | 0.48              |
| 3:D:951:ILE:CG2   | 3:D:952:ASP:N    | 2.77                     | 0.48              |
| 3:D:1102:THR:OG1  | 3:D:1222:GLY:O   | 2.27                     | 0.48              |
| 3:D:1154:GLU:H    | 3:N:561:GLY:CA   | 2.26                     | 0.48              |
| 3:D:1266:ARG:NH2  | 7:I:4:DG:H4'     | 2.29                     | 0.48              |
| 3:D:1442:ASN:CG   | 3:D:1444:THR:HG1 | 2.21                     | 0.48              |
| 1:K:80:LEU:HD23   | 1:K:80:LEU:O     | 2.13                     | 0.48              |
| 2:M:86:LYS:HD3    | 2:M:813:VAL:CB   | 2.32                     | 0.48              |
| 2:M:261:ILE:HD13  | 2:M:262:ALA:H    | 1.78                     | 0.48              |
| 2:M:512:ARG:HB3   | 2:M:523:ILE:HD11 | 1.94                     | 0.48              |
| 2:M:759:THR:HB    | 2:M:785:VAL:CG1  | 2.44                     | 0.48              |
| 2:M:877:PRO:HG3   | 3:N:1023:MET:SD  | 2.54                     | 0.48              |
| 2:M:939:ARG:NE    | 2:M:939:ARG:CA   | 2.64                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:51:GLY:HA3   | 3:N:86:ARG:HA     | 1.95                     | 0.48              |
| 3:N:152:LEU:HD23 | 3:N:152:LEU:N     | 2.26                     | 0.48              |
| 3:N:630:VAL:HG12 | 3:N:631:ILE:N     | 2.27                     | 0.48              |
| 3:N:710:ARG:HH12 | 4:O:16:LYS:HZ3    | 1.62                     | 0.48              |
| 1:B:9:PRO:HB3    | 1:B:25:LEU:HG     | 1.95                     | 0.47              |
| 2:C:589:ARG:HA   | 2:C:596:TYR:CZ    | 2.49                     | 0.47              |
| 3:D:456:MET:O    | 3:D:459:GLU:HB3   | 2.14                     | 0.47              |
| 3:D:651:GLU:O    | 3:D:654:LYS:HB2   | 2.14                     | 0.47              |
| 3:D:730:PRO:O    | 3:D:733:CYS:SG    | 2.72                     | 0.47              |
| 3:D:744:GLN:CG   | 5:G:21:DG:H21     | 2.19                     | 0.47              |
| 3:D:834:THR:HA   | 3:D:838:ARG:NH1   | 2.28                     | 0.47              |
| 3:D:864:VAL:CG1  | 3:D:865:THR:H     | 2.13                     | 0.47              |
| 3:D:1094:LEU:CD2 | 3:D:1256:LEU:HD11 | 2.44                     | 0.47              |
| 1:K:109:VAL:HG23 | 1:K:132:LEU:HD13  | 1.96                     | 0.47              |
| 1:K:193:ASP:HA   | 2:M:938:LYS:NZ    | 2.29                     | 0.47              |
| 1:L:89:PHE:HE2   | 1:L:146:ARG:HB3   | 1.79                     | 0.47              |
| 2:M:837:ASP:HA   | 2:M:999:HIS:CE1   | 2.49                     | 0.47              |
| 2:M:878:SER:OG   | 3:N:1029:ARG:NE   | 2.47                     | 0.47              |
| 2:M:988:VAL:HG11 | 3:N:950:GLY:HA2   | 1.96                     | 0.47              |
| 3:N:486:ARG:HA   | 3:N:489:ARG:CG    | 2.39                     | 0.47              |
| 3:N:710:ARG:HG3  | 3:N:711:LEU:N     | 2.26                     | 0.47              |
| 3:N:808:THR:OG1  | 3:N:809:PRO:HD3   | 2.14                     | 0.47              |
| 3:N:829:VAL:O    | 3:N:835:SER:HB3   | 2.14                     | 0.47              |
| 3:N:871:LYS:HB2  | 3:N:873:LEU:HD21  | 1.94                     | 0.47              |
| 3:N:996:TRP:HA   | 3:N:999:THR:CG2   | 2.42                     | 0.47              |
| 1:B:22:GLU:OE2   | 1:B:198:ARG:HB3   | 2.14                     | 0.47              |
| 1:B:49:PRO:CA    | 1:B:148:VAL:HG12  | 2.42                     | 0.47              |
| 2:C:35:PRO:C     | 2:C:37:GLU:N      | 2.70                     | 0.47              |
| 2:C:265:ARG:C    | 2:C:267:TYR:N     | 2.72                     | 0.47              |
| 2:C:408:ARG:NH2  | 2:C:456:ALA:O     | 2.46                     | 0.47              |
| 2:C:431:HIS:CD2  | 2:C:432:ARG:N     | 2.83                     | 0.47              |
| 2:C:435:TYR:C    | 2:C:437:ARG:H     | 2.22                     | 0.47              |
| 2:C:701:THR:HG21 | 2:C:830:LYS:HD2   | 1.95                     | 0.47              |
| 2:C:926:PHE:HA   | 2:C:929:ARG:HB2   | 1.96                     | 0.47              |
| 3:D:21:TRP:HE3   | 3:D:90:MET:SD     | 2.37                     | 0.47              |
| 3:D:91:GLY:C     | 3:D:519:VAL:HG23  | 2.39                     | 0.47              |
| 3:D:103:TRP:O    | 3:D:107:ASP:HB2   | 2.12                     | 0.47              |
| 3:D:499:VAL:O    | 3:D:500:ARG:C     | 2.57                     | 0.47              |
| 3:D:645:PRO:HB2  | 3:D:648:MET:HG3   | 1.97                     | 0.47              |
| 3:D:897:TRP:CB   | 3:D:900:ILE:CD1   | 2.79                     | 0.47              |
| 3:D:924:MET:HB3  | 4:E:6:ILE:HG23    | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1354:LYS:HA   | 3:D:1357:ARG:HD2  | 1.96                     | 0.47              |
| 1:K:112:ARG:NH1   | 1:K:112:ARG:CG    | 2.77                     | 0.47              |
| 1:L:137:ARG:O     | 1:L:137:ARG:HD3   | 2.14                     | 0.47              |
| 2:M:19:THR:O      | 2:M:19:THR:HG22   | 2.15                     | 0.47              |
| 2:M:502:PRO:HB2   | 2:M:509:ALA:HB3   | 1.96                     | 0.47              |
| 2:M:692:GLU:O     | 2:M:696:LYS:HG3   | 2.14                     | 0.47              |
| 2:M:693:GLU:HG3   | 2:M:697:ARG:HH21  | 1.76                     | 0.47              |
| 2:M:1069:ALA:O    | 2:M:1072:LYS:HB3  | 2.14                     | 0.47              |
| 3:N:8:VAL:HG12    | 3:N:9:ARG:N       | 2.29                     | 0.47              |
| 3:N:131:LYS:C     | 3:N:132:TYR:CG    | 2.92                     | 0.47              |
| 3:N:1100:ASP:HB3  | 3:N:1428:ALA:HB1  | 1.96                     | 0.47              |
| 3:N:1303:TYR:O    | 3:N:1305:LEU:HD23 | 2.13                     | 0.47              |
| 5:X:13:DA:O5'     | 5:X:13:DA:H8      | 1.97                     | 0.47              |
| 1:A:133:GLU:HG2   | 1:A:134:GLU:H     | 1.80                     | 0.47              |
| 3:D:521:PRO:C     | 3:D:525:ARG:NH1   | 2.72                     | 0.47              |
| 3:D:1066:THR:HG22 | 3:D:1069:GLU:HB2  | 1.95                     | 0.47              |
| 3:D:1409:ALA:HA   | 2:M:370:ALA:HB1   | 1.95                     | 0.47              |
| 2:M:90:TYR:HB2    | 2:M:128:ILE:HB    | 1.96                     | 0.47              |
| 2:M:259:GLY:HA2   | 2:M:290:LEU:O     | 2.13                     | 0.47              |
| 2:M:272:ALA:O     | 2:M:276:LYS:NZ    | 2.46                     | 0.47              |
| 2:M:442:GLU:HG2   | 2:M:454:SER:CB    | 2.41                     | 0.47              |
| 2:M:903:SER:O     | 2:M:904:PRO:C     | 2.56                     | 0.47              |
| 2:M:966:LEU:HD21  | 2:M:986:PRO:CG    | 2.39                     | 0.47              |
| 2:M:969:GLN:NE2   | 3:N:952:ASP:CB    | 2.77                     | 0.47              |
| 3:N:480:GLU:O     | 3:N:484:PRO:HD2   | 2.14                     | 0.47              |
| 3:N:1017:PHE:HA   | 3:N:1022:VAL:CG2  | 2.43                     | 0.47              |
| 3:N:1293:PHE:CE1  | 3:N:1302:GLU:HA   | 2.49                     | 0.47              |
| 3:N:1344:VAL:O    | 3:N:1345:GLU:C    | 2.56                     | 0.47              |
| 3:N:1424:VAL:HG13 | 3:N:1425:THR:N    | 2.30                     | 0.47              |
| 4:O:73:LEU:HD12   | 4:O:73:LEU:N      | 2.30                     | 0.47              |
| 5:G:5:DC:O5'      | 5:G:5:DC:C6       | 2.67                     | 0.47              |
| 5:X:2:DT:OP2      | 5:X:2:DT:H4'      | 2.14                     | 0.47              |
| 1:A:24:VAL:HG22   | 1:A:196:THR:HG22  | 1.94                     | 0.47              |
| 1:A:82:LEU:O      | 1:A:85:LEU:HB3    | 2.13                     | 0.47              |
| 1:A:198:ARG:C     | 1:A:199:ILE:HD12  | 2.39                     | 0.47              |
| 2:C:20:GLU:HG2    | 2:C:21:ILE:CD1    | 2.39                     | 0.47              |
| 2:C:160:ALA:HB3   | 2:C:174:LEU:HB2   | 1.97                     | 0.47              |
| 2:C:553:ASP:OD2   | 2:C:883:GLY:HA3   | 2.15                     | 0.47              |
| 2:C:919:ALA:HA    | 2:C:968:LEU:HD21  | 1.96                     | 0.47              |
| 2:C:1047:HIS:HA   | 2:C:1050:GLN:HB3  | 1.97                     | 0.47              |
| 3:D:119:SER:C     | 3:D:121:THR:N     | 2.72                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:947:ILE:HD12  | 3:D:947:ILE:O     | 2.14                     | 0.47              |
| 3:D:1087:ARG:HB3  | 3:D:1236:LEU:HD13 | 1.96                     | 0.47              |
| 3:D:1200:VAL:HG12 | 3:D:1201:CYS:N    | 2.29                     | 0.47              |
| 3:D:1211:MET:SD   | 3:D:1213:ARG:HD3  | 2.55                     | 0.47              |
| 3:D:1437:ALA:C    | 3:D:1446:VAL:HG11 | 2.38                     | 0.47              |
| 1:L:98:THR:HG22   | 1:L:100:LEU:HD21  | 1.96                     | 0.47              |
| 1:L:226:SER:O     | 1:L:228:PRO:HD3   | 2.14                     | 0.47              |
| 2:M:80:GLN:N      | 2:M:90:TYR:HE2    | 2.12                     | 0.47              |
| 2:M:378:LEU:HG    | 2:M:382:ILE:CD1   | 2.43                     | 0.47              |
| 2:M:564:MET:HE1   | 2:M:840:ALA:HB3   | 1.97                     | 0.47              |
| 2:M:582:GLY:C     | 2:M:583:LEU:HD12  | 2.40                     | 0.47              |
| 2:M:720:GLU:HA    | 2:M:759:THR:O     | 2.13                     | 0.47              |
| 2:M:876:VAL:O     | 2:M:879:ARG:O     | 2.32                     | 0.47              |
| 2:M:876:VAL:N     | 2:M:877:PRO:HD2   | 2.29                     | 0.47              |
| 2:M:902:ILE:O     | 2:M:902:ILE:HG22  | 2.13                     | 0.47              |
| 3:N:111:LYS:HZ1   | 3:N:1449:GLU:CG   | 2.27                     | 0.47              |
| 3:N:470:LEU:HD12  | 3:N:503:LEU:HG    | 1.95                     | 0.47              |
| 3:N:549:ASN:O     | 3:N:553:ARG:HB2   | 2.14                     | 0.47              |
| 3:N:585:GLY:C     | 3:N:587:ARG:N     | 2.65                     | 0.47              |
| 3:N:890:VAL:O     | 3:N:890:VAL:HG23  | 2.14                     | 0.47              |
| 3:N:1109:GLU:CB   | 3:N:1201:CYS:HA   | 2.44                     | 0.47              |
| 4:O:13:VAL:HG21   | 4:O:19:LEU:HB2    | 1.96                     | 0.47              |
| 1:A:58:ILE:HD13   | 1:A:140:MET:HB3   | 1.96                     | 0.47              |
| 1:A:102:LYS:CA    | 1:A:138:LEU:O     | 2.61                     | 0.47              |
| 2:C:18:LEU:HD22   | 2:C:590:ASP:CB    | 2.44                     | 0.47              |
| 2:C:77:PRO:HD2    | 2:C:91:GLN:O      | 2.15                     | 0.47              |
| 2:C:151:ASP:HA    | 2:C:159:ILE:HG12  | 1.95                     | 0.47              |
| 2:C:184:MET:SD    | 2:C:191:PHE:HE1   | 2.37                     | 0.47              |
| 2:C:444:PRO:HB3   | 6:H:12:U:P        | 2.54                     | 0.47              |
| 2:C:736:ASP:O     | 2:C:744:ARG:HG2   | 2.15                     | 0.47              |
| 2:C:838:LYS:HZ3   | 3:D:742:GLY:CA    | 2.28                     | 0.47              |
| 2:C:987:ILE:HG12  | 3:D:948:THR:HG23  | 1.96                     | 0.47              |
| 2:C:1020:PRO:HD2  | 3:D:622:ARG:O     | 2.15                     | 0.47              |
| 3:D:543:LEU:HD23  | 3:D:546:ARG:HD2   | 1.97                     | 0.47              |
| 3:D:606:ILE:O     | 3:D:613:ARG:N     | 2.47                     | 0.47              |
| 3:D:783:ARG:HB3   | 3:D:1028:ALA:O    | 2.15                     | 0.47              |
| 3:D:932:ASP:HA    | 3:D:935:LYS:HD3   | 1.96                     | 0.47              |
| 3:D:1112:CYS:CA   | 3:D:1195:GLN:HG2  | 2.42                     | 0.47              |
| 3:D:1369:GLU:O    | 3:D:1370:ILE:C    | 2.57                     | 0.47              |
| 3:D:1377:LYS:HG2  | 3:D:1378:TYR:CD1  | 2.49                     | 0.47              |
| 3:D:1379:VAL:HA   | 3:D:1420:LEU:HB2  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:68:LEU:N      | 4:E:68:LEU:CD1    | 2.77                     | 0.47              |
| 1:K:11:PHE:HA     | 1:K:25:LEU:HD12   | 1.95                     | 0.47              |
| 1:K:165:ILE:O     | 1:K:165:ILE:HG13  | 2.15                     | 0.47              |
| 1:K:220:GLU:O     | 1:K:223:THR:HG22  | 2.14                     | 0.47              |
| 1:L:25:LEU:HD23   | 1:L:195:LEU:HB3   | 1.95                     | 0.47              |
| 1:L:173:PRO:HB2   | 1:L:205:VAL:HG22  | 1.96                     | 0.47              |
| 2:M:15:LEU:H      | 2:M:15:LEU:HD12   | 1.78                     | 0.47              |
| 2:M:334:ARG:HB2   | 2:M:339:LEU:CD2   | 2.41                     | 0.47              |
| 2:M:338:GLU:C     | 2:M:341:THR:HG22  | 2.39                     | 0.47              |
| 2:M:825:VAL:HG12  | 2:M:827:VAL:CG2   | 2.44                     | 0.47              |
| 2:M:902:ILE:O     | 2:M:904:PRO:HD3   | 2.15                     | 0.47              |
| 2:M:971:LYS:CE    | 2:M:988:VAL:HG12  | 2.31                     | 0.47              |
| 3:N:90:MET:CE     | 3:N:520:LEU:HA    | 2.44                     | 0.47              |
| 3:N:545:ARG:CB    | 3:N:545:ARG:CZ    | 2.92                     | 0.47              |
| 3:N:662:GLU:C     | 3:N:664:LYS:O     | 2.58                     | 0.47              |
| 3:N:688:TRP:HA    | 3:N:688:TRP:HE3   | 1.79                     | 0.47              |
| 3:N:1100:ASP:OD2  | 3:N:1440:PHE:CG   | 2.68                     | 0.47              |
| 3:N:1100:ASP:OD2  | 3:N:1440:PHE:HB3  | 2.14                     | 0.47              |
| 3:N:1257:PRO:HA   | 3:N:1260:ILE:HG12 | 1.96                     | 0.47              |
| 3:N:1322:GLY:O    | 3:N:1323:GLN:CB   | 2.59                     | 0.47              |
| 7:I:7:DT:H2''     | 7:I:8:DG:H8       | 1.79                     | 0.47              |
| 1:B:137:ARG:HD3   | 1:B:137:ARG:C     | 2.39                     | 0.47              |
| 2:C:302:VAL:HG13  | 2:C:303:PHE:N     | 2.28                     | 0.47              |
| 2:C:642:ARG:CG    | 2:C:657:ASP:OD2   | 2.63                     | 0.47              |
| 2:C:1090:LYS:O    | 2:C:1094:ALA:N    | 2.47                     | 0.47              |
| 3:D:31:THR:C      | 3:D:32:ILE:HG13   | 2.39                     | 0.47              |
| 3:D:84:ILE:O      | 3:D:87:ARG:HG3    | 2.14                     | 0.47              |
| 3:D:731:LEU:HD21  | 3:D:782:SER:N     | 2.28                     | 0.47              |
| 3:D:738:ALA:HA    | 6:H:15:C:C4'      | 2.40                     | 0.47              |
| 3:D:812:ALA:HB1   | 3:D:816:HIS:CD2   | 2.49                     | 0.47              |
| 3:D:925:GLU:OE2   | 4:E:5:GLY:N       | 2.48                     | 0.47              |
| 3:D:1138:ALA:O    | 3:D:1141:GLU:N    | 2.48                     | 0.47              |
| 3:D:1264:GLU:HA   | 3:D:1423:GLY:HA3  | 1.96                     | 0.47              |
| 3:D:1424:VAL:HG13 | 3:D:1425:THR:H    | 1.78                     | 0.47              |
| 1:K:179:PHE:HB2   | 1:K:195:LEU:HD11  | 1.96                     | 0.47              |
| 2:M:211:LEU:HD13  | 2:M:308:ARG:CD    | 2.44                     | 0.47              |
| 2:M:355:VAL:HG13  | 2:M:356:ARG:N     | 2.28                     | 0.47              |
| 2:M:421:GLU:HG3   | 2:M:421:GLU:O     | 2.14                     | 0.47              |
| 2:M:639:GLN:O     | 2:M:641:PRO:HD3   | 2.15                     | 0.47              |
| 2:M:685:GLU:HG2   | 3:N:739:ASP:CB    | 2.45                     | 0.47              |
| 2:M:1014:SER:CB   | 2:M:1017:THR:O    | 2.59                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:17:LYS:O      | 3:N:20:SER:HB3    | 2.14                     | 0.47              |
| 3:N:117:ASP:HB2   | 3:N:495:ARG:HH22  | 1.80                     | 0.47              |
| 3:N:1114:THR:C    | 3:N:1189:ARG:HH21 | 2.15                     | 0.47              |
| 3:N:1292:VAL:HG11 | 3:N:1313:VAL:CG1  | 2.45                     | 0.47              |
| 3:N:1330:ILE:CD1  | 3:N:1347:TYR:CE1  | 2.97                     | 0.47              |
| 1:A:65:PHE:CE1    | 2:C:799:ILE:CB    | 2.97                     | 0.47              |
| 2:C:31:GLN:HG2    | 2:C:34:VAL:HG23   | 1.97                     | 0.47              |
| 2:C:83:CYS:SG     | 2:C:90:TYR:HD2    | 2.37                     | 0.47              |
| 2:C:128:ILE:HG22  | 2:C:128:ILE:O     | 2.15                     | 0.47              |
| 2:C:206:THR:HG23  | 2:C:207:LEU:N     | 2.30                     | 0.47              |
| 2:C:399:ASN:O     | 2:C:400:PRO:C     | 2.57                     | 0.47              |
| 2:C:607:ASP:HB3   | 2:C:610:ARG:H     | 1.79                     | 0.47              |
| 2:C:786:LYS:HG2   | 2:C:787:ASP:N     | 2.29                     | 0.47              |
| 2:C:861:LEU:HD21  | 2:C:925:TYR:CZ    | 2.49                     | 0.47              |
| 2:C:922:PHE:HB2   | 2:C:967:PHE:CD2   | 2.50                     | 0.47              |
| 2:C:983:ILE:HG23  | 3:D:944:THR:HA    | 1.96                     | 0.47              |
| 2:C:1056:LYS:HE3  | 3:D:751:LEU:HG    | 1.97                     | 0.47              |
| 2:C:1101:THR:OG1  | 2:C:1109:VAL:HB   | 2.13                     | 0.47              |
| 2:C:1112:PHE:CD1  | 2:C:1116:ALA:HB2  | 2.50                     | 0.47              |
| 3:D:133:ILE:CG1   | 3:D:456:MET:HE2   | 2.44                     | 0.47              |
| 3:D:493:ARG:HG3   | 3:D:494:LYS:N     | 2.30                     | 0.47              |
| 3:D:550:ARG:HA    | 3:D:553:ARG:HB3   | 1.97                     | 0.47              |
| 3:D:847:ASP:O     | 3:D:848:GLU:C     | 2.57                     | 0.47              |
| 3:D:907:GLU:CD    | 3:D:909:ASN:H     | 2.21                     | 0.47              |
| 3:D:1255:GLY:CA   | 3:D:1257:PRO:HD2  | 2.45                     | 0.47              |
| 3:D:1263:PHE:CE2  | 3:D:1371:VAL:HG11 | 2.49                     | 0.47              |
| 3:D:1354:LYS:HE3  | 3:D:1357:ARG:NH1  | 2.30                     | 0.47              |
| 3:D:1381:VAL:HG12 | 3:D:1382:THR:N    | 2.29                     | 0.47              |
| 3:D:1468:LEU:HD13 | 3:D:1470:ARG:HB2  | 1.96                     | 0.47              |
| 4:E:48:MET:N      | 4:E:54:LEU:HB2    | 2.29                     | 0.47              |
| 1:K:42:ARG:NH2    | 2:M:857:ASP:HB3   | 2.29                     | 0.47              |
| 1:K:64:GLU:HA     | 1:K:75:VAL:HG11   | 1.95                     | 0.47              |
| 1:K:92:PRO:HA     | 1:K:146:ARG:NH1   | 2.28                     | 0.47              |
| 1:K:92:PRO:N      | 1:K:146:ARG:HH12  | 2.13                     | 0.47              |
| 1:K:193:ASP:CG    | 2:M:938:LYS:NZ    | 2.72                     | 0.47              |
| 2:M:3:ILE:HD13    | 2:M:900:ARG:HB3   | 1.97                     | 0.47              |
| 2:M:146:VAL:HG13  | 2:M:161:SER:O     | 2.15                     | 0.47              |
| 2:M:170:PRO:CG    | 2:M:258:TYR:HE2   | 2.27                     | 0.47              |
| 2:M:185:LYS:HG2   | 2:M:188:LYS:O     | 2.14                     | 0.47              |
| 2:M:269:LEU:CB    | 2:M:288:ARG:HG2   | 2.44                     | 0.47              |
| 2:M:390:GLN:H     | 2:M:390:GLN:HG3   | 1.38                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:433:THR:CG2   | 2:M:488:ALA:HB1   | 2.44                     | 0.47              |
| 2:M:433:THR:HG21  | 2:M:488:ALA:HB1   | 1.97                     | 0.47              |
| 2:M:461:VAL:CG1   | 2:M:465:GLY:HA2   | 2.45                     | 0.47              |
| 2:M:518:LYS:NZ    | 2:M:518:LYS:CB    | 2.77                     | 0.47              |
| 2:M:557:ARG:HD2   | 2:M:557:ARG:HA    | 1.70                     | 0.47              |
| 2:M:620:LEU:HD12  | 2:M:620:LEU:O     | 2.15                     | 0.47              |
| 2:M:629:TYR:HB2   | 2:M:637:LEU:HB2   | 1.97                     | 0.47              |
| 2:M:694:LEU:HD21  | 2:M:868:ASP:HB3   | 1.96                     | 0.47              |
| 2:M:730:SER:O     | 2:M:734:LEU:HD13  | 2.15                     | 0.47              |
| 2:M:757:GLY:HA2   | 2:M:789:SER:OG    | 2.14                     | 0.47              |
| 2:M:910:LYS:O     | 2:M:914:ILE:HG13  | 2.15                     | 0.47              |
| 2:M:937:ASP:O     | 2:M:941:VAL:HG23  | 2.15                     | 0.47              |
| 2:M:969:GLN:NE2   | 3:N:952:ASP:HB3   | 2.29                     | 0.47              |
| 3:N:112:ILE:O     | 3:N:112:ILE:HD12  | 2.15                     | 0.47              |
| 3:N:465:LEU:CD1   | 3:N:510:GLU:HA    | 2.45                     | 0.47              |
| 3:N:641:GLN:HA    | 3:N:717:GLN:H     | 1.80                     | 0.47              |
| 3:N:752:SER:OG    | 3:N:754:PHE:CB    | 2.62                     | 0.47              |
| 3:N:771:SER:HA    | 3:N:778:LEU:HD22  | 1.96                     | 0.47              |
| 3:N:812:ALA:HB1   | 3:N:816:HIS:CD2   | 2.50                     | 0.47              |
| 3:N:850:LEU:HD22  | 3:N:884:ARG:HH21  | 1.80                     | 0.47              |
| 3:N:1031:ASN:C    | 3:N:1033:GLN:N    | 2.69                     | 0.47              |
| 3:N:1126:ASP:HB2  | 3:N:1129:THR:O    | 2.15                     | 0.47              |
| 3:N:1161:GLU:HG2  | 3:N:1164:ARG:HB2  | 1.95                     | 0.47              |
| 3:N:1166:LEU:HD23 | 3:N:1166:LEU:N    | 2.24                     | 0.47              |
| 3:N:1168:MET:HA   | 3:N:1168:MET:HE3  | 1.96                     | 0.47              |
| 3:N:1389:LEU:CD1  | 3:N:1390:LEU:HG   | 2.45                     | 0.47              |
| 3:N:1438:ALA:N    | 3:N:1446:VAL:HG11 | 2.29                     | 0.47              |
| 1:A:28:LEU:HD13   | 1:A:32:PHE:CB     | 2.29                     | 0.47              |
| 1:A:32:PHE:CD1    | 1:B:221:HIS:NE2   | 2.72                     | 0.47              |
| 1:A:48:ILE:CD1    | 1:A:174:VAL:CG2   | 2.92                     | 0.47              |
| 2:C:169:GLY:O     | 2:C:170:PRO:O     | 2.33                     | 0.47              |
| 2:C:292:ARG:HD3   | 2:C:298:PHE:HA    | 1.97                     | 0.47              |
| 2:C:409:ARG:CA    | 2:C:454:SER:HA    | 2.33                     | 0.47              |
| 2:C:967:PHE:HD1   | 2:C:972:VAL:HG12  | 1.80                     | 0.47              |
| 2:C:1034:GLU:O    | 2:C:1037:VAL:N    | 2.48                     | 0.47              |
| 3:D:10:ILE:O      | 3:D:1451:ALA:HA   | 2.14                     | 0.47              |
| 3:D:615:ARG:HD2   | 3:D:615:ARG:HA    | 1.74                     | 0.47              |
| 3:D:1344:VAL:O    | 3:D:1345:GLU:C    | 2.58                     | 0.47              |
| 3:D:1412:LYS:C    | 3:D:1414:PRO:HD3  | 2.40                     | 0.47              |
| 3:D:1459:LEU:HD22 | 3:D:1468:LEU:HD12 | 1.97                     | 0.47              |
| 1:K:55:SER:H      | 1:K:143:ARG:HB3   | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:176:ARG:HG3   | 1:K:200:TRP:HE3   | 1.80                     | 0.47              |
| 1:K:188:GLN:HG3   | 1:K:189:ARG:N     | 2.25                     | 0.47              |
| 2:M:332:ARG:CG    | 2:M:333:ILE:N     | 2.77                     | 0.47              |
| 2:M:663:ASN:C     | 2:M:665:PHE:N     | 2.72                     | 0.47              |
| 2:M:971:LYS:HE3   | 2:M:988:VAL:CG1   | 2.32                     | 0.47              |
| 2:M:971:LYS:HE2   | 2:M:986:PRO:O     | 2.15                     | 0.47              |
| 3:N:658:LEU:HA    | 3:N:661:MET:HG3   | 1.96                     | 0.47              |
| 3:N:699:VAL:HB    | 3:N:716:PHE:O     | 2.15                     | 0.47              |
| 3:N:799:LYS:HE2   | 3:N:824:ASN:O     | 2.15                     | 0.47              |
| 3:N:974:ILE:HG12  | 3:N:991:GLN:OE1   | 2.15                     | 0.47              |
| 3:N:1236:LEU:O    | 3:N:1237:THR:CB   | 2.63                     | 0.47              |
| 3:N:1329:ALA:C    | 3:N:1330:ILE:HG13 | 2.40                     | 0.47              |
| 3:N:1460:ILE:O    | 3:N:1464:GLU:OE2  | 2.33                     | 0.47              |
| 4:O:57:ASP:N      | 4:O:58:PRO:HD3    | 2.29                     | 0.47              |
| 2:C:264:PRO:CB    | 2:C:289:THR:HB    | 2.45                     | 0.47              |
| 2:C:553:ASP:HA    | 2:C:881:ASN:HA    | 1.96                     | 0.47              |
| 2:C:833:LEU:HD12  | 2:C:996:LYS:HE2   | 1.97                     | 0.47              |
| 2:C:994:ILE:HG22  | 2:C:995:MET:N     | 2.30                     | 0.47              |
| 2:C:1012:PRO:CD   | 2:C:1026:GLN:HG2  | 2.45                     | 0.47              |
| 2:C:1111:ILE:HG13 | 2:C:1112:PHE:N    | 2.25                     | 0.47              |
| 3:D:603:LEU:O     | 3:D:607:LEU:HG    | 2.15                     | 0.47              |
| 3:D:813:LEU:O     | 3:D:817:GLU:HB2   | 2.14                     | 0.47              |
| 3:D:1123:PHE:HA   | 3:D:1133:ARG:O    | 2.15                     | 0.47              |
| 1:K:58:ILE:HB     | 1:K:61:VAL:HB     | 1.96                     | 0.47              |
| 2:M:170:PRO:HG2   | 2:M:258:TYR:CD2   | 2.50                     | 0.47              |
| 2:M:393:GLN:HG2   | 6:Y:10:G:O2'      | 2.14                     | 0.47              |
| 2:M:700:TYR:O     | 2:M:833:LEU:HB2   | 2.15                     | 0.47              |
| 2:M:969:GLN:CD    | 3:N:952:ASP:HB2   | 2.39                     | 0.47              |
| 2:M:1032:PHE:O    | 2:M:1036:GLU:CD   | 2.58                     | 0.47              |
| 2:M:1066:ALA:O    | 2:M:1070:ILE:HG13 | 2.15                     | 0.47              |
| 3:N:860:LEU:HD23  | 3:N:877:PRO:CB    | 2.45                     | 0.47              |
| 3:N:1282:ARG:HA   | 3:N:1315:ASP:HA   | 1.97                     | 0.47              |
| 3:N:1304:LYS:C    | 3:N:1305:LEU:HD23 | 2.40                     | 0.47              |
| 3:N:1313:VAL:HG21 | 3:N:1319:VAL:HG11 | 1.97                     | 0.47              |
| 4:O:40:LEU:HD23   | 4:O:72:ARG:HE     | 1.79                     | 0.47              |
| 7:I:1:DG:OP3      | 7:I:1:DG:C3'      | 2.62                     | 0.47              |
| 1:A:216:GLU:O     | 1:A:220:GLU:HB2   | 2.14                     | 0.47              |
| 1:B:47:SER:OG     | 1:B:217:ILE:HG12  | 2.14                     | 0.47              |
| 2:C:12:VAL:CG1    | 2:C:472:ARG:HD3   | 2.45                     | 0.47              |
| 2:C:97:ARG:HD3    | 2:C:109:LYS:HZ3   | 1.80                     | 0.47              |
| 2:C:442:GLU:HG2   | 2:C:454:SER:CB    | 2.44                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:607:ASP:OD2   | 2:C:608:GLY:N     | 2.47                     | 0.47              |
| 2:C:607:ASP:HB2   | 2:C:610:ARG:NH1   | 2.29                     | 0.47              |
| 2:C:863:ASP:C     | 2:C:863:ASP:OD2   | 2.58                     | 0.47              |
| 2:C:863:ASP:CG    | 2:C:865:THR:HG22  | 2.40                     | 0.47              |
| 2:C:903:SER:O     | 2:C:904:PRO:O     | 2.33                     | 0.47              |
| 3:D:127:LEU:C     | 3:D:127:LEU:CD1   | 2.85                     | 0.47              |
| 3:D:128:TYR:HB3   | 3:D:129:PHE:CD1   | 2.50                     | 0.47              |
| 3:D:1093:TYR:HE2  | 3:D:1096:ARG:CZ   | 2.28                     | 0.47              |
| 3:D:1209:LEU:HD23 | 3:D:1211:MET:N    | 2.12                     | 0.47              |
| 3:D:1219:GLU:HB2  | 4:E:17:TYR:HE2    | 1.79                     | 0.47              |
| 3:D:1435:LEU:HB2  | 3:D:1464:GLU:HB3  | 1.95                     | 0.47              |
| 1:K:19:GLU:O      | 1:K:201:THR:N     | 2.40                     | 0.47              |
| 1:L:176:ARG:O     | 1:L:200:TRP:HE3   | 1.98                     | 0.47              |
| 2:M:327:HIS:HE1   | 2:M:489:THR:HA    | 1.80                     | 0.47              |
| 2:M:468:ARG:HA    | 2:M:486:MET:O     | 2.14                     | 0.47              |
| 2:M:603:VAL:HG12  | 2:M:646:GLY:H     | 1.80                     | 0.47              |
| 2:M:1054:THR:O    | 2:M:1056:LYS:N    | 2.48                     | 0.47              |
| 3:N:149:LYS:H     | 3:N:149:LYS:HG3   | 1.41                     | 0.47              |
| 3:N:786:ILE:HD13  | 3:N:1027:GLY:HA3  | 1.97                     | 0.47              |
| 3:N:833:GLU:C     | 3:N:834:THR:HG23  | 2.32                     | 0.47              |
| 3:N:911:LEU:O     | 3:N:915:VAL:HG23  | 2.14                     | 0.47              |
| 3:N:925:GLU:O     | 3:N:928:ALA:HB3   | 2.15                     | 0.47              |
| 3:N:941:PHE:O     | 3:N:945:SER:HB3   | 2.15                     | 0.47              |
| 3:N:1223:ILE:N    | 3:N:1223:ILE:HD12 | 2.30                     | 0.47              |
| 3:N:1466:VAL:C    | 3:N:1469:GLY:H    | 2.23                     | 0.47              |
| 4:O:38:THR:OG1    | 4:O:39:VAL:N      | 2.48                     | 0.47              |
| 5:X:5:DC:H2'      | 5:X:6:DT:O5'      | 2.15                     | 0.47              |
| 1:A:9:PRO:HB3     | 1:A:25:LEU:HG     | 1.96                     | 0.46              |
| 1:B:73:GLU:HB3    | 1:B:77:GLU:CG     | 2.45                     | 0.46              |
| 2:C:7:GLY:HA3     | 2:C:907:ASP:OD2   | 2.14                     | 0.46              |
| 2:C:192:PRO:C     | 2:C:193:LEU:HD12  | 2.40                     | 0.46              |
| 2:C:423:ALA:CB    | 7:I:1:DG:C5'      | 2.78                     | 0.46              |
| 2:C:578:VAL:HG13  | 2:C:671:ASN:CB    | 2.45                     | 0.46              |
| 2:C:627:ARG:O     | 2:C:638:ASP:HB3   | 2.15                     | 0.46              |
| 2:C:1022:GLY:CA   | 2:C:1026:GLN:O    | 2.62                     | 0.46              |
| 3:D:41:ARG:HD3    | 3:D:43:GLY:H      | 1.80                     | 0.46              |
| 3:D:964:LEU:O     | 3:D:968:ASP:HB2   | 2.14                     | 0.46              |
| 3:D:1102:THR:O    | 3:D:1103:HIS:O    | 2.33                     | 0.46              |
| 3:D:1154:GLU:CD   | 3:N:563:PRO:HA    | 2.40                     | 0.46              |
| 1:L:109:VAL:O     | 1:L:129:ILE:HG12  | 2.14                     | 0.46              |
| 1:L:162:ILE:HD11  | 1:L:163:ASN:ND2   | 2.30                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:162:ILE:HD12 | 2:M:172:ILE:CB    | 2.45                     | 0.46              |
| 2:M:295:ASP:C    | 2:M:297:GLU:H     | 2.23                     | 0.46              |
| 2:M:356:ARG:NH1  | 2:M:356:ARG:HB2   | 2.30                     | 0.46              |
| 2:M:472:ARG:HE   | 2:M:532:MET:HE2   | 1.79                     | 0.46              |
| 2:M:580:MET:SD   | 2:M:584:GLU:CG    | 3.00                     | 0.46              |
| 2:M:589:ARG:HA   | 2:M:596:TYR:CE1   | 2.50                     | 0.46              |
| 2:M:1034:GLU:CD  | 2:M:1038:TRP:CZ2  | 2.93                     | 0.46              |
| 3:N:698:LYS:CG   | 4:O:59:ASN:CG     | 2.78                     | 0.46              |
| 3:N:704:ARG:CZ   | 3:N:737:ASN:O     | 2.62                     | 0.46              |
| 3:N:728:LEU:HG   | 3:N:729:HIS:O     | 2.14                     | 0.46              |
| 3:N:736:PHE:CD1  | 3:N:736:PHE:N     | 2.79                     | 0.46              |
| 3:N:1107:VAL:O   | 3:N:1218:GLY:N    | 2.48                     | 0.46              |
| 3:N:1381:VAL:HA  | 3:N:1417:TRP:HA   | 1.96                     | 0.46              |
| 3:N:1443:THR:HA  | 3:N:1446:VAL:HG21 | 1.97                     | 0.46              |
| 4:O:34:GLY:O     | 4:O:37:ASN:ND2    | 2.48                     | 0.46              |
| 5:G:2:DT:OP1     | 5:G:2:DT:H6       | 1.98                     | 0.46              |
| 7:I:7:DT:H2"     | 7:I:8:DG:OP2      | 2.14                     | 0.46              |
| 1:A:127:LEU:HG   | 1:A:129:ILE:HD13  | 1.97                     | 0.46              |
| 1:B:184:THR:O    | 1:B:192:LEU:HD12  | 2.16                     | 0.46              |
| 1:B:185:ARG:HG2  | 1:B:186:LEU:N     | 2.29                     | 0.46              |
| 2:C:139:GLN:OE1  | 2:C:418:LEU:HD22  | 2.14                     | 0.46              |
| 2:C:328:LEU:HB2  | 2:C:433:THR:CB    | 2.44                     | 0.46              |
| 2:C:499:ALA:HA   | 2:C:532:MET:SD    | 2.55                     | 0.46              |
| 2:C:606:VAL:HG21 | 2:C:645:VAL:HG22  | 1.96                     | 0.46              |
| 2:C:724:ARG:NH2  | 2:C:734:LEU:O     | 2.48                     | 0.46              |
| 2:C:737:LEU:HA   | 2:C:743:VAL:HA    | 1.97                     | 0.46              |
| 2:C:1006:HIS:HA  | 2:C:1027:PHE:CD1  | 2.50                     | 0.46              |
| 2:C:1034:GLU:OE1 | 3:D:619:LEU:HD22  | 2.15                     | 0.46              |
| 2:C:1039:ALA:HB2 | 3:D:707:THR:HG22  | 1.96                     | 0.46              |
| 3:D:10:ILE:O     | 3:D:1450:ALA:O    | 2.32                     | 0.46              |
| 3:D:771:SER:O    | 3:D:774:SER:O     | 2.33                     | 0.46              |
| 3:D:800:LYS:HG3  | 3:D:829:VAL:HG12  | 1.98                     | 0.46              |
| 3:D:1389:LEU:O   | 3:D:1390:LEU:C    | 2.58                     | 0.46              |
| 4:E:41:GLU:N     | 4:E:42:PRO:CD     | 2.77                     | 0.46              |
| 1:L:43:ILE:HG23  | 1:L:47:SER:HB3    | 1.97                     | 0.46              |
| 1:L:57:TYR:CE2   | 1:L:161:ARG:HG2   | 2.51                     | 0.46              |
| 2:M:139:GLN:OE1  | 2:M:414:GLY:HA3   | 2.15                     | 0.46              |
| 2:M:402:SER:HB3  | 2:M:566:THR:O     | 2.16                     | 0.46              |
| 2:M:437:ARG:O    | 2:M:438:ILE:HD12  | 2.14                     | 0.46              |
| 2:M:605:LYS:O    | 2:M:611:ILE:HA    | 2.15                     | 0.46              |
| 2:M:884:GLN:O    | 2:M:992:MET:HE1   | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:115:LEU:HD23  | 3:N:115:LEU:O     | 2.15                     | 0.46              |
| 3:N:693:GLU:CA    | 4:O:48:MET:CE     | 2.83                     | 0.46              |
| 3:N:1296:SER:C    | 3:N:1298:GLY:N    | 2.73                     | 0.46              |
| 3:N:1447:LEU:HA   | 3:N:1450:ALA:HB3  | 1.97                     | 0.46              |
| 5:G:23:DG:C2      | 6:H:11:C:O2       | 2.68                     | 0.46              |
| 1:B:65:PHE:CD1    | 1:B:65:PHE:N      | 2.83                     | 0.46              |
| 2:C:304:LEU:N     | 2:C:305:PRO:CD    | 2.78                     | 0.46              |
| 2:C:1093:GLN:O    | 3:D:21:TRP:CZ3    | 2.68                     | 0.46              |
| 2:C:1095:LEU:CB   | 2:C:1097:LEU:HD23 | 2.42                     | 0.46              |
| 2:C:1101:THR:O    | 2:C:1102:LEU:HD12 | 2.16                     | 0.46              |
| 2:C:1114:GLY:C    | 2:C:1115:LEU:HD12 | 2.41                     | 0.46              |
| 3:D:30:GLU:CB     | 3:D:41:ARG:HG3    | 2.45                     | 0.46              |
| 3:D:1109:GLU:HG2  | 3:D:1202:GLN:N    | 2.29                     | 0.46              |
| 3:D:1378:TYR:HH   | 3:D:1431:THR:HA   | 1.79                     | 0.46              |
| 3:D:1433:SER:CA   | 3:D:1457:ASP:OD2  | 2.64                     | 0.46              |
| 4:E:95:VAL:O      | 4:E:96:GLU:HB2    | 2.15                     | 0.46              |
| 1:K:27:PRO:HG2    | 1:K:186:LEU:HD13  | 1.97                     | 0.46              |
| 1:K:213:GLN:O     | 1:K:216:GLU:HB2   | 2.15                     | 0.46              |
| 1:L:101:LEU:C     | 1:L:101:LEU:CD2   | 2.84                     | 0.46              |
| 2:M:5:ARG:HB3     | 2:M:902:ILE:CB    | 2.43                     | 0.46              |
| 2:M:691:SER:HA    | 2:M:858:MET:CE    | 2.44                     | 0.46              |
| 2:M:874:LEU:HD11  | 3:N:783:ARG:HB2   | 1.97                     | 0.46              |
| 3:N:55:ASP:O      | 3:N:81:THR:O      | 2.33                     | 0.46              |
| 3:N:891:GLU:O     | 3:N:893:GLU:N     | 2.49                     | 0.46              |
| 3:N:1122:LEU:HD11 | 3:N:1186:VAL:HG23 | 1.96                     | 0.46              |
| 3:N:1200:VAL:HG12 | 3:N:1201:CYS:O    | 2.14                     | 0.46              |
| 3:N:1292:VAL:HG23 | 3:N:1305:LEU:CG   | 2.37                     | 0.46              |
| 3:N:1438:ALA:CB   | 3:N:1446:VAL:HG11 | 2.45                     | 0.46              |
| 2:C:35:PRO:C      | 2:C:37:GLU:H      | 2.22                     | 0.46              |
| 2:C:39:ARG:O      | 2:C:40:GLU:C      | 2.58                     | 0.46              |
| 2:C:259:GLY:HA2   | 2:C:290:LEU:O     | 2.15                     | 0.46              |
| 2:C:676:ILE:CG2   | 2:C:988:VAL:HG22  | 2.44                     | 0.46              |
| 2:C:724:ARG:HD2   | 2:C:737:LEU:O     | 2.16                     | 0.46              |
| 2:C:1012:PRO:HB2  | 2:C:1021:LEU:O    | 2.16                     | 0.46              |
| 3:D:1042:ARG:NE   | 3:D:1073:SER:HB2  | 2.30                     | 0.46              |
| 4:E:45:ARG:HG2    | 4:E:46:PRO:CD     | 2.45                     | 0.46              |
| 1:L:76:VAL:O      | 1:L:79:ILE:HG12   | 2.15                     | 0.46              |
| 2:M:95:TYR:CD2    | 2:M:114:PHE:HB3   | 2.49                     | 0.46              |
| 2:M:399:ASN:O     | 2:M:400:PRO:C     | 2.57                     | 0.46              |
| 2:M:793:PRO:O     | 2:M:794:PRO:C     | 2.58                     | 0.46              |
| 2:M:853:LEU:HB2   | 2:M:858:MET:CE    | 2.43                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:869:VAL:CG2   | 2:M:870:ILE:N     | 2.78                     | 0.46              |
| 2:M:1053:LEU:HD12 | 3:N:1469:GLY:CA   | 2.44                     | 0.46              |
| 3:N:112:ILE:HD11  | 3:N:116:LEU:CD1   | 2.45                     | 0.46              |
| 3:N:455:ARG:N     | 3:N:455:ARG:HD2   | 2.30                     | 0.46              |
| 3:N:675:ARG:HA    | 3:N:678:GLU:OE2   | 2.16                     | 0.46              |
| 3:N:698:LYS:HE2   | 4:O:59:ASN:OD1    | 2.16                     | 0.46              |
| 3:N:741:ASP:OD2   | 3:N:743:ASP:OD2   | 2.33                     | 0.46              |
| 3:N:774:SER:OG    | 3:N:776:GLU:HB2   | 2.15                     | 0.46              |
| 3:N:840:LYS:HB3   | 3:N:841:TYR:CE2   | 2.51                     | 0.46              |
| 3:N:1129:THR:CB   | 3:N:1320:GLU:OE1  | 2.62                     | 0.46              |
| 3:N:1396:GLU:O    | 3:N:1399:ASP:HB2  | 2.16                     | 0.46              |
| 1:A:34:VAL:HG13   | 1:A:35:THR:N      | 2.30                     | 0.46              |
| 1:B:59:GLU:CB     | 1:B:137:ARG:HH22  | 2.27                     | 0.46              |
| 2:C:130:ASN:HD21  | 2:C:383:ARG:HH21  | 1.64                     | 0.46              |
| 2:C:310:LEU:O     | 2:C:314:THR:HG23  | 2.16                     | 0.46              |
| 2:C:468:ARG:CB    | 2:C:485:TYR:HB3   | 2.45                     | 0.46              |
| 2:C:580:MET:CE    | 2:C:902:ILE:HG12  | 2.46                     | 0.46              |
| 2:C:918:LEU:O     | 2:C:967:PHE:HE2   | 1.99                     | 0.46              |
| 2:C:1091:GLU:O    | 2:C:1094:ALA:HB3  | 2.15                     | 0.46              |
| 2:C:1115:LEU:N    | 2:C:1115:LEU:CD1  | 2.78                     | 0.46              |
| 3:D:949:ILE:HD13  | 3:D:1019:PRO:HB2  | 1.97                     | 0.46              |
| 3:D:1433:SER:HA   | 3:D:1457:ASP:OD2  | 2.16                     | 0.46              |
| 3:D:1468:LEU:O    | 3:D:1468:LEU:HD23 | 2.15                     | 0.46              |
| 1:K:49:PRO:CA     | 1:K:148:VAL:HG22  | 2.46                     | 0.46              |
| 1:L:165:ILE:O     | 1:L:165:ILE:HG13  | 2.16                     | 0.46              |
| 2:M:221:LEU:HG    | 2:M:222:MET:N     | 2.30                     | 0.46              |
| 2:M:291:ALA:O     | 2:M:292:ARG:HB2   | 2.15                     | 0.46              |
| 2:M:437:ARG:CZ    | 2:M:491:GLU:OE2   | 2.64                     | 0.46              |
| 2:M:754:ILE:HA    | 2:M:791:ARG:HA    | 1.98                     | 0.46              |
| 3:N:623:VAL:CG1   | 3:N:624:ASP:N     | 2.79                     | 0.46              |
| 3:N:658:LEU:O     | 3:N:661:MET:HB2   | 2.14                     | 0.46              |
| 3:N:785:ILE:HD12  | 3:N:939:PHE:CE2   | 2.51                     | 0.46              |
| 3:N:1112:CYS:HB2  | 3:N:1195:GLN:HG2  | 1.98                     | 0.46              |
| 3:N:1225:ALA:O    | 3:N:1229:ILE:HG13 | 2.15                     | 0.46              |
| 3:N:1401:GLU:CD   | 3:N:1415:VAL:HG11 | 2.41                     | 0.46              |
| 4:O:23:VAL:O      | 4:O:26:ARG:HB3    | 2.15                     | 0.46              |
| 5:G:10:DA:H2''    | 5:G:11:DC:H6      | 1.80                     | 0.46              |
| 6:H:6:C:C4        | 6:H:7:G:C6        | 3.03                     | 0.46              |
| 6:H:7:G:HO2'      | 6:H:8:G:H5'       | 1.77                     | 0.46              |
| 6:Y:5:C:H2'       | 6:Y:6:C:OP1       | 2.15                     | 0.46              |
| 2:C:73:LEU:CB     | 2:C:93:PRO:O      | 2.61                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:263:ASP:HB2   | 2:C:264:PRO:CD   | 2.39                     | 0.46              |
| 2:C:326:ASP:O     | 2:C:431:HIS:CG   | 2.69                     | 0.46              |
| 2:C:358:ARG:NH1   | 2:C:374:ASN:OD1  | 2.46                     | 0.46              |
| 2:C:966:LEU:HD12  | 2:C:966:LEU:HA   | 1.77                     | 0.46              |
| 3:D:33:ASN:HD21   | 3:D:35:ARG:HH12  | 1.64                     | 0.46              |
| 3:D:758:GLU:CB    | 3:D:762:GLN:HE21 | 2.27                     | 0.46              |
| 3:D:1096:ARG:NH2  | 3:D:1440:PHE:CE2 | 2.84                     | 0.46              |
| 3:D:1127:GLU:O    | 3:D:1128:VAL:CG2 | 2.63                     | 0.46              |
| 3:D:1164:ARG:HG2  | 3:D:1165:TYR:N   | 2.31                     | 0.46              |
| 3:D:1336:LEU:HD12 | 3:D:1340:GLY:HA2 | 1.98                     | 0.46              |
| 1:K:11:PHE:CA     | 1:K:25:LEU:HD12  | 2.46                     | 0.46              |
| 2:M:151:ASP:OD1   | 2:M:152:PRO:HD2  | 2.16                     | 0.46              |
| 2:M:342:ASP:HA    | 2:M:345:ARG:HD3  | 1.97                     | 0.46              |
| 2:M:428:ARG:NE    | 2:M:451:LEU:HD21 | 2.31                     | 0.46              |
| 2:M:680:ASP:HB2   | 2:M:682:TYR:CE2  | 2.51                     | 0.46              |
| 2:M:723:THR:C     | 2:M:725:ASP:H    | 2.24                     | 0.46              |
| 2:M:773:LEU:O     | 2:M:777:ILE:HG13 | 2.15                     | 0.46              |
| 3:N:19:ARG:HE     | 3:N:516:ALA:HB1  | 1.80                     | 0.46              |
| 3:N:160:GLU:CB    | 3:N:165:LYS:HB2  | 2.45                     | 0.46              |
| 3:N:1379:VAL:CG1  | 3:N:1419:PRO:HA  | 2.41                     | 0.46              |
| 4:O:8:LYS:O       | 4:O:12:MET:HG3   | 2.14                     | 0.46              |
| 7:I:17:DA:O5'     | 7:I:17:DA:C8     | 2.66                     | 0.46              |
| 1:B:6:LEU:O       | 1:B:8:ALA:N      | 2.47                     | 0.46              |
| 2:C:157:ARG:NH1   | 2:C:314:THR:O    | 2.46                     | 0.46              |
| 2:C:212:GLY:HA3   | 2:C:218:VAL:CG2  | 2.46                     | 0.46              |
| 2:C:560:MET:O     | 2:C:564:MET:HG2  | 2.15                     | 0.46              |
| 2:C:679:PHE:N     | 2:C:683:ASN:HD21 | 2.07                     | 0.46              |
| 2:C:922:PHE:HB3   | 2:C:964:LYS:HZ1  | 1.75                     | 0.46              |
| 2:C:1035:MET:O    | 3:D:707:THR:HB   | 2.15                     | 0.46              |
| 2:C:1093:GLN:HB3  | 3:D:21:TRP:CZ3   | 2.50                     | 0.46              |
| 3:D:100:ALA:N     | 3:D:128:TYR:OH   | 2.49                     | 0.46              |
| 3:D:500:ARG:O     | 3:D:501:ALA:C    | 2.58                     | 0.46              |
| 3:D:521:PRO:HD2   | 3:D:524:LEU:CD2  | 2.45                     | 0.46              |
| 3:D:982:PHE:C     | 3:D:982:PHE:CD2  | 2.93                     | 0.46              |
| 3:D:1168:MET:HE2  | 3:D:1172:HIS:CE1 | 2.50                     | 0.46              |
| 3:D:1225:ALA:CB   | 3:D:1367:HIS:HD1 | 2.28                     | 0.46              |
| 3:D:1341:PRO:C    | 3:D:1343:ALA:H   | 2.22                     | 0.46              |
| 3:D:1365:ASP:O    | 3:D:1366:LYS:C   | 2.59                     | 0.46              |
| 1:K:94:LEU:HD11   | 1:K:119:ASP:CB   | 2.46                     | 0.46              |
| 1:L:73:GLU:OE1    | 1:L:130:ALA:HA   | 2.16                     | 0.46              |
| 2:M:46:ALA:C      | 2:M:48:PHE:N     | 2.71                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:395:LYS:HG2   | 2:M:397:GLU:HG3   | 1.97                     | 0.46              |
| 2:M:510:ALA:O     | 2:M:513:VAL:HG23  | 2.15                     | 0.46              |
| 2:M:839:LEU:CD2   | 2:M:996:LYS:HA    | 2.46                     | 0.46              |
| 2:M:1021:LEU:HD13 | 6:Y:5:C:O2        | 2.16                     | 0.46              |
| 3:N:821:VAL:HG22  | 3:N:840:LYS:HZ1   | 1.80                     | 0.46              |
| 3:N:1066:THR:HG22 | 3:N:1069:GLU:HB2  | 1.98                     | 0.46              |
| 3:N:1277:ILE:HB   | 3:N:1294:VAL:CG2  | 2.45                     | 0.46              |
| 3:N:1364:HIS:ND1  | 3:N:1365:ASP:N    | 2.64                     | 0.46              |
| 3:N:1399:ASP:O    | 3:N:1403:LEU:HG   | 2.15                     | 0.46              |
| 3:N:1462:LEU:O    | 3:N:1466:VAL:N    | 2.45                     | 0.46              |
| 7:I:10:DG:C2'     | 7:I:11:DG:OP2     | 2.44                     | 0.46              |
| 5:X:23:DG:H2'     | 5:X:24:DC:H6      | 1.78                     | 0.46              |
| 1:B:74:ASP:HB3    | 3:D:872:ARG:NH2   | 2.21                     | 0.46              |
| 2:C:54:ILE:HG12   | 2:C:64:LEU:CD2    | 2.45                     | 0.46              |
| 2:C:101:ILE:CD1   | 2:C:107:LEU:HD22  | 2.46                     | 0.46              |
| 2:C:141:HIS:O     | 2:C:331:ARG:HB3   | 2.15                     | 0.46              |
| 2:C:726:ILE:HD12  | 2:C:726:ILE:N     | 2.31                     | 0.46              |
| 2:C:868:ASP:OD1   | 2:C:868:ASP:N     | 2.49                     | 0.46              |
| 2:C:1010:THR:HG22 | 2:C:1011:GLY:N    | 2.31                     | 0.46              |
| 2:C:1098:ASP:OD1  | 3:D:17:LYS:HD3    | 2.16                     | 0.46              |
| 3:D:133:ILE:HG23  | 3:D:456:MET:HB3   | 1.97                     | 0.46              |
| 3:D:163:TYR:HD1   | 3:D:163:TYR:N     | 2.13                     | 0.46              |
| 3:D:610:LYS:O     | 3:D:615:ARG:CG    | 2.54                     | 0.46              |
| 3:D:1087:ARG:NE   | 3:D:1236:LEU:HD11 | 2.30                     | 0.46              |
| 3:D:1265:ALA:C    | 3:D:1266:ARG:HG3  | 2.40                     | 0.46              |
| 1:K:220:GLU:O     | 1:K:224:TYR:CE2   | 2.69                     | 0.46              |
| 1:L:48:ILE:CD1    | 1:L:210:ALA:HB1   | 2.45                     | 0.46              |
| 1:L:206:THR:HG22  | 1:L:209:GLU:H     | 1.79                     | 0.46              |
| 2:M:39:ARG:O      | 2:M:40:GLU:C      | 2.58                     | 0.46              |
| 2:M:101:ILE:HG23  | 2:M:107:LEU:CD2   | 2.45                     | 0.46              |
| 2:M:549:PHE:CE2   | 2:M:886:LEU:HB3   | 2.51                     | 0.46              |
| 2:M:650:ARG:CG    | 2:M:653:ASP:HB2   | 2.36                     | 0.46              |
| 2:M:874:LEU:HD13  | 3:N:783:ARG:HB2   | 1.98                     | 0.46              |
| 3:N:471:GLU:OE1   | 3:N:471:GLU:N     | 2.33                     | 0.46              |
| 3:N:484:PRO:HB3   | 3:N:488:ARG:CZ    | 2.45                     | 0.46              |
| 3:N:796:ARG:HB2   | 3:N:828:LYS:HD2   | 1.97                     | 0.46              |
| 3:N:1109:GLU:CD   | 3:N:1201:CYS:HA   | 2.41                     | 0.46              |
| 3:N:1117:TYR:HE2  | 3:N:1151:ARG:NH1  | 2.13                     | 0.46              |
| 3:N:1158:VAL:HG12 | 3:N:1159:ARG:N    | 2.31                     | 0.46              |
| 3:N:1281:VAL:CG1  | 3:N:1282:ARG:N    | 2.79                     | 0.46              |
| 4:O:15:SER:O      | 4:O:18:ARG:HB3    | 2.16                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:31:GLY:O     | 1:A:34:VAL:HG13   | 2.15                     | 0.46              |
| 1:B:36:LEU:C     | 1:B:39:PRO:HD2    | 2.41                     | 0.46              |
| 2:C:300:ASP:O    | 2:C:304:LEU:CD2   | 2.64                     | 0.46              |
| 2:C:882:LEU:HD12 | 3:D:1061:PHE:C    | 2.40                     | 0.46              |
| 3:D:127:LEU:HD12 | 3:D:127:LEU:O     | 2.15                     | 0.46              |
| 3:D:554:LEU:HG   | 3:D:558:LEU:HD11  | 1.98                     | 0.46              |
| 3:D:943:THR:OG1  | 3:D:944:THR:N     | 2.48                     | 0.46              |
| 3:D:1197:ARG:NH1 | 3:D:1198:TYR:HD1  | 2.14                     | 0.46              |
| 3:D:1445:HIS:O   | 3:D:1448:THR:HB   | 2.16                     | 0.46              |
| 2:M:94:LEU:HD12  | 2:M:95:TYR:N      | 2.30                     | 0.46              |
| 2:M:140:ILE:HA   | 2:M:332:ARG:O     | 2.15                     | 0.46              |
| 2:M:266:ARG:CA   | 2:M:288:ARG:HD3   | 2.45                     | 0.46              |
| 2:M:313:LEU:HA   | 2:M:321:GLU:OE1   | 2.15                     | 0.46              |
| 2:M:673:LEU:HB3  | 2:M:868:ASP:OD1   | 2.16                     | 0.46              |
| 2:M:737:LEU:HA   | 2:M:743:VAL:HA    | 1.97                     | 0.46              |
| 3:N:917:GLN:O    | 3:N:920:LEU:HB2   | 2.16                     | 0.46              |
| 3:N:950:GLY:N    | 3:N:953:ASP:OD1   | 2.49                     | 0.46              |
| 3:N:1259:VAL:O   | 3:N:1263:PHE:HD1  | 1.98                     | 0.46              |
| 3:N:1394:VAL:O   | 3:N:1397:LYS:HB3  | 2.15                     | 0.46              |
| 3:N:1438:ALA:HB2 | 3:N:1446:VAL:HG11 | 1.98                     | 0.46              |
| 4:O:41:GLU:HG2   | 4:O:42:PRO:HD3    | 1.98                     | 0.46              |
| 4:O:48:MET:N     | 4:O:54:LEU:HB2    | 2.31                     | 0.46              |
| 5:X:17:DA:O5'    | 5:X:17:DA:C2'     | 2.61                     | 0.46              |
| 7:Z:3:DA:H2''    | 7:Z:4:DG:OP2      | 2.16                     | 0.46              |
| 1:A:30:ARG:HH11  | 1:A:191:ASP:HB2   | 1.80                     | 0.46              |
| 1:A:117:VAL:O    | 1:A:120:VAL:HG12  | 2.16                     | 0.46              |
| 2:C:136:ILE:HG21 | 2:C:336:VAL:HG13  | 1.98                     | 0.46              |
| 2:C:141:HIS:HB3  | 2:C:418:LEU:HD23  | 1.98                     | 0.46              |
| 2:C:185:LYS:HG2  | 2:C:188:LYS:O     | 2.16                     | 0.46              |
| 2:C:1008:ARG:NH2 | 2:C:1011:GLY:C    | 2.74                     | 0.46              |
| 2:C:1032:PHE:CE2 | 2:C:1037:VAL:HG22 | 2.51                     | 0.46              |
| 3:D:25:GLU:HB2   | 3:D:92:HIS:CE1    | 2.50                     | 0.46              |
| 3:D:105:VAL:HA   | 3:D:112:ILE:HG21  | 1.98                     | 0.46              |
| 3:D:676:MET:SD   | 3:D:682:ASP:O     | 2.74                     | 0.46              |
| 3:D:925:GLU:OE1  | 4:E:6:ILE:N       | 2.45                     | 0.46              |
| 3:D:1153:VAL:CA  | 3:N:561:GLY:HA3   | 2.45                     | 0.46              |
| 3:D:1450:ALA:O   | 3:D:1453:ALA:O    | 2.33                     | 0.46              |
| 1:L:59:GLU:HB2   | 1:L:137:ARG:NH2   | 2.30                     | 0.46              |
| 2:M:474:VAL:HG23 | 2:M:478:VAL:C     | 2.40                     | 0.46              |
| 2:M:903:SER:C    | 2:M:904:PRO:O     | 2.58                     | 0.46              |
| 3:N:41:ARG:C     | 3:N:43:GLY:N      | 2.72                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:481:MET:CE    | 3:N:1388:ARG:HB2  | 2.46                     | 0.46              |
| 3:N:1209:LEU:HD21 | 4:O:16:LYS:CE     | 2.45                     | 0.46              |
| 3:N:1294:VAL:CG1  | 3:N:1319:VAL:HG21 | 2.27                     | 0.46              |
| 3:N:1365:ASP:O    | 3:N:1366:LYS:C    | 2.59                     | 0.46              |
| 5:X:10:DA:H2''    | 5:X:11:DC:O5'     | 2.16                     | 0.46              |
| 5:X:10:DA:H1'     | 5:X:11:DC:H5'     | 1.97                     | 0.46              |
| 5:X:12:DA:C2      | 5:X:13:DA:C5      | 3.04                     | 0.46              |
| 7:Z:6:DT:H2''     | 7:Z:7:DT:OP2      | 2.16                     | 0.46              |
| 1:A:2:LEU:HA      | 1:A:6:LEU:HD22    | 1.98                     | 0.45              |
| 1:A:80:LEU:HD23   | 1:A:80:LEU:C      | 2.41                     | 0.45              |
| 2:C:2:GLU:C       | 2:C:3:ILE:HD13    | 2.41                     | 0.45              |
| 2:C:136:ILE:CG2   | 2:C:336:VAL:HG22  | 2.46                     | 0.45              |
| 2:C:301:GLU:HA    | 2:C:304:LEU:HD21  | 1.98                     | 0.45              |
| 2:C:307:LEU:HD12  | 2:C:307:LEU:HA    | 1.74                     | 0.45              |
| 2:C:589:ARG:HA    | 2:C:596:TYR:OH    | 2.16                     | 0.45              |
| 2:C:937:ASP:OD2   | 2:C:938:LYS:N     | 2.49                     | 0.45              |
| 3:D:10:ILE:HD11   | 3:D:1434:TRP:HE1  | 1.80                     | 0.45              |
| 3:D:10:ILE:C      | 3:D:1451:ALA:HA   | 2.41                     | 0.45              |
| 3:D:554:LEU:CD1   | 3:D:558:LEU:HD21  | 2.44                     | 0.45              |
| 3:D:629:SER:HB3   | 3:D:726:ILE:HD11  | 1.98                     | 0.45              |
| 3:D:989:TYR:HH    | 3:D:1051:GLU:CG   | 2.12                     | 0.45              |
| 3:D:1031:ASN:HA   | 3:D:1032:PRO:HD3  | 1.51                     | 0.45              |
| 3:D:1131:SER:C    | 3:D:1132:LEU:HD12 | 2.41                     | 0.45              |
| 3:D:1154:GLU:HB2  | 3:N:562:ALA:CA    | 2.47                     | 0.45              |
| 1:K:96:THR:HA     | 1:K:144:VAL:O     | 2.16                     | 0.45              |
| 2:M:66:LEU:HD12   | 2:M:99:GLN:C      | 2.40                     | 0.45              |
| 2:M:313:LEU:CD1   | 2:M:321:GLU:HG2   | 2.36                     | 0.45              |
| 2:M:673:LEU:HD23  | 2:M:674:VAL:N     | 2.31                     | 0.45              |
| 2:M:677:MET:CB    | 3:N:948:THR:CG2   | 2.94                     | 0.45              |
| 2:M:692:GLU:OE1   | 2:M:854:PRO:HA    | 2.16                     | 0.45              |
| 2:M:1060:ILE:HG23 | 2:M:1061:GLU:N    | 2.26                     | 0.45              |
| 3:N:76:CYS:O      | 3:N:76:CYS:SG     | 2.74                     | 0.45              |
| 3:N:116:LEU:O     | 3:N:118:LEU:N     | 2.49                     | 0.45              |
| 3:N:121:THR:OG1   | 7:Z:8:DG:H5''     | 2.16                     | 0.45              |
| 3:N:431:VAL:HG12  | 3:N:432:TYR:N     | 2.30                     | 0.45              |
| 3:N:613:ARG:O     | 3:N:616:GLN:HB3   | 2.16                     | 0.45              |
| 3:N:637:LEU:HD11  | 3:N:642:CYS:HA    | 1.97                     | 0.45              |
| 3:N:762:GLN:HE22  | 4:O:17:TYR:HD1    | 1.65                     | 0.45              |
| 3:N:1094:LEU:O    | 3:N:1097:LYS:HB2  | 2.16                     | 0.45              |
| 3:N:1105:ILE:HB   | 3:N:1222:GLY:HA3  | 1.98                     | 0.45              |
| 3:N:1232:PRO:O    | 3:N:1234:THR:N    | 2.40                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1256:LEU:HB3  | 3:N:1257:PRO:HD3  | 1.98                     | 0.45              |
| 4:O:64:ALA:O      | 4:O:68:LEU:HD13   | 2.16                     | 0.45              |
| 2:C:159:ILE:HG21  | 2:C:175:GLU:OE2   | 2.16                     | 0.45              |
| 2:C:547:ILE:HB    | 2:C:550:LEU:HD13  | 1.96                     | 0.45              |
| 2:C:584:GLU:CD    | 2:C:584:GLU:H     | 2.22                     | 0.45              |
| 2:C:603:VAL:HB    | 2:C:646:GLY:N     | 2.31                     | 0.45              |
| 2:C:1054:THR:O    | 2:C:1056:LYS:N    | 2.49                     | 0.45              |
| 3:D:646:LYS:HD2   | 3:D:688:TRP:CZ2   | 2.51                     | 0.45              |
| 3:D:807:ALA:HA    | 3:D:833:GLU:HB2   | 1.97                     | 0.45              |
| 3:D:935:LYS:HE2   | 3:D:936:TYR:HB2   | 1.98                     | 0.45              |
| 3:D:1058:ARG:HB3  | 3:D:1058:ARG:CZ   | 2.45                     | 0.45              |
| 3:D:1263:PHE:HE2  | 3:D:1371:VAL:HG11 | 1.80                     | 0.45              |
| 3:D:1428:ALA:O    | 3:D:1431:THR:HG22 | 2.16                     | 0.45              |
| 2:M:71:TYR:HA     | 2:M:96:ALA:HB2    | 1.98                     | 0.45              |
| 2:M:84:ARG:HA     | 2:M:131:GLY:HA2   | 1.96                     | 0.45              |
| 2:M:92:ALA:HB2    | 2:M:120:LEU:HD11  | 1.97                     | 0.45              |
| 2:M:142:ARG:HA    | 2:M:331:ARG:HA    | 1.97                     | 0.45              |
| 2:M:265:ARG:C     | 2:M:267:TYR:N     | 2.73                     | 0.45              |
| 3:N:520:LEU:HD12  | 3:N:521:PRO:HD2   | 1.96                     | 0.45              |
| 3:N:796:ARG:NH2   | 3:N:859:ASP:HB2   | 2.32                     | 0.45              |
| 3:N:895:VAL:HG12  | 3:N:895:VAL:O     | 2.16                     | 0.45              |
| 3:N:1172:HIS:HA   | 3:N:1175:ILE:HD12 | 1.97                     | 0.45              |
| 2:C:25:SER:O      | 2:C:29:ALA:HB2    | 2.17                     | 0.45              |
| 2:C:137:VAL:CG2   | 2:C:391:LEU:HG    | 2.46                     | 0.45              |
| 2:C:141:HIS:CD2   | 2:C:332:ARG:O     | 2.70                     | 0.45              |
| 2:C:162:ILE:CG2   | 2:C:172:ILE:HD13  | 2.47                     | 0.45              |
| 2:C:317:VAL:C     | 2:C:319:GLY:N     | 2.68                     | 0.45              |
| 2:C:677:MET:SD    | 2:C:987:ILE:HD13  | 2.55                     | 0.45              |
| 2:C:720:GLU:OE1   | 2:C:758:ARG:HD2   | 2.16                     | 0.45              |
| 2:C:854:PRO:HG2   | 2:C:857:ASP:OD2   | 2.17                     | 0.45              |
| 2:C:889:HIS:NE2   | 2:C:970:GLY:HA3   | 2.31                     | 0.45              |
| 3:D:6:ARG:HD2     | 3:D:1470:ARG:NH1  | 2.27                     | 0.45              |
| 3:D:623:VAL:CG1   | 3:D:624:ASP:N     | 2.79                     | 0.45              |
| 3:D:1115:THR:CG2  | 3:D:1151:ARG:HH21 | 2.30                     | 0.45              |
| 3:D:1144:LEU:HD22 | 3:D:1186:VAL:HG11 | 1.97                     | 0.45              |
| 3:D:1189:ARG:HG3  | 3:D:1189:ARG:NH1  | 2.31                     | 0.45              |
| 3:D:1407:LEU:HD23 | 2:M:361:MET:SD    | 2.56                     | 0.45              |
| 1:K:18:ARG:HD3    | 1:K:123:MET:HE3   | 1.97                     | 0.45              |
| 1:K:38:ASN:O      | 1:K:42:ARG:HG3    | 2.16                     | 0.45              |
| 1:L:58:ILE:HD13   | 1:L:139:ASN:O     | 2.16                     | 0.45              |
| 1:L:179:PHE:HB3   | 1:L:197:LEU:HD12  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:183:ASP:HA    | 1:L:192:LEU:O     | 2.16                     | 0.45              |
| 2:M:92:ALA:CB     | 2:M:120:LEU:HD21  | 2.47                     | 0.45              |
| 2:M:183:SER:CB    | 2:M:190:LYS:HD3   | 2.45                     | 0.45              |
| 2:M:378:LEU:O     | 2:M:382:ILE:HG13  | 2.16                     | 0.45              |
| 2:M:599:GLU:OE2   | 2:M:619:ARG:NH2   | 2.49                     | 0.45              |
| 2:M:601:GLY:HA3   | 2:M:615:TYR:HA    | 1.98                     | 0.45              |
| 2:M:984:GLU:HG3   | 3:N:791:TYR:OH    | 2.16                     | 0.45              |
| 3:N:480:GLU:OE1   | 3:N:488:ARG:CG    | 2.60                     | 0.45              |
| 3:N:703:ASN:ND2   | 3:N:713:ILE:HD11  | 2.32                     | 0.45              |
| 3:N:799:LYS:CB    | 3:N:826:PRO:HG2   | 2.46                     | 0.45              |
| 3:N:827:ILE:HD12  | 3:N:827:ILE:H     | 1.80                     | 0.45              |
| 3:N:1223:ILE:O    | 3:N:1226:ALA:N    | 2.49                     | 0.45              |
| 3:N:1268:PRO:CG   | 3:N:1329:ALA:CB   | 2.93                     | 0.45              |
| 3:N:1369:GLU:O    | 3:N:1370:ILE:C    | 2.58                     | 0.45              |
| 3:N:1481:VAL:O    | 3:N:1483:PHE:N    | 2.50                     | 0.45              |
| 1:A:43:ILE:CD1    | 1:B:32:PHE:HE2    | 2.26                     | 0.45              |
| 1:B:22:GLU:O      | 1:B:23:PHE:CD1    | 2.69                     | 0.45              |
| 1:B:101:LEU:CD1   | 1:B:113:ASP:HB3   | 2.45                     | 0.45              |
| 1:B:105:GLY:O     | 1:B:132:LEU:HB3   | 2.16                     | 0.45              |
| 2:C:129:ILE:HG22  | 2:C:130:ASN:H     | 1.78                     | 0.45              |
| 2:C:267:TYR:CB    | 2:C:272:ALA:HB1   | 2.47                     | 0.45              |
| 2:C:895:TYR:N     | 2:C:991:GLN:NE2   | 2.64                     | 0.45              |
| 2:C:1095:LEU:HD23 | 3:D:582:LEU:HD22  | 1.98                     | 0.45              |
| 3:D:9:ARG:NH1     | 3:D:1454:GLY:HA3  | 2.31                     | 0.45              |
| 3:D:612:GLY:H     | 3:D:615:ARG:CB    | 2.29                     | 0.45              |
| 3:D:625:TYR:HB3   | 3:D:749:VAL:CG2   | 2.46                     | 0.45              |
| 3:D:1041:LEU:HD13 | 3:D:1045:MET:HB2  | 1.98                     | 0.45              |
| 3:D:1093:TYR:CE2  | 3:D:1096:ARG:CZ   | 3.00                     | 0.45              |
| 3:D:1189:ARG:HD3  | 3:D:1189:ARG:HA   | 1.63                     | 0.45              |
| 3:D:1191:PRO:HB3  | 3:D:1200:VAL:HG21 | 1.99                     | 0.45              |
| 1:K:56:VAL:HG13   | 1:K:142:VAL:HG12  | 1.97                     | 0.45              |
| 1:K:111:ALA:O     | 1:K:122:ILE:HD13  | 2.17                     | 0.45              |
| 1:L:196:THR:O     | 1:L:196:THR:OG1   | 2.34                     | 0.45              |
| 2:M:677:MET:HA    | 3:N:948:THR:HG22  | 1.98                     | 0.45              |
| 2:M:691:SER:HA    | 2:M:858:MET:HE1   | 1.99                     | 0.45              |
| 2:M:738:ASP:HB2   | 2:M:744:ARG:HB3   | 1.98                     | 0.45              |
| 2:M:754:ILE:HG12  | 2:M:791:ARG:NH1   | 2.31                     | 0.45              |
| 2:M:881:ASN:OD1   | 2:M:884:GLN:CD    | 2.60                     | 0.45              |
| 2:M:884:GLN:O     | 2:M:992:MET:CE    | 2.65                     | 0.45              |
| 3:N:45:PHE:CE1    | 3:N:522:PRO:HB3   | 2.51                     | 0.45              |
| 3:N:699:VAL:HG21  | 3:N:760:ARG:CB    | 2.44                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:760:ARG:HH11  | 4:O:61:VAL:CG2    | 2.07                     | 0.45              |
| 3:N:1009:LYS:HE3  | 3:N:1013:GLU:OE2  | 2.16                     | 0.45              |
| 3:N:1066:THR:HG22 | 3:N:1069:GLU:CG   | 2.46                     | 0.45              |
| 3:N:1127:GLU:O    | 3:N:1128:VAL:HG23 | 2.17                     | 0.45              |
| 3:N:1189:ARG:HD3  | 3:N:1190:SER:H    | 1.82                     | 0.45              |
| 3:N:1389:LEU:O    | 3:N:1390:LEU:C    | 2.60                     | 0.45              |
| 3:N:1451:ALA:O    | 3:N:1452:ILE:C    | 2.60                     | 0.45              |
| 3:N:1486:VAL:HG21 | 4:O:29:GLN:HE22   | 1.81                     | 0.45              |
| 4:O:56:ASP:C      | 4:O:57:ASP:CG     | 2.84                     | 0.45              |
| 6:H:9:C:H2'       | 6:H:10:G:C8       | 2.52                     | 0.45              |
| 7:I:2:DT:P        | 7:I:2:DT:H3'      | 2.57                     | 0.45              |
| 7:I:5:DC:H1'      | 7:I:6:DT:O5'      | 2.16                     | 0.45              |
| 6:Y:7:G:N3        | 6:Y:7:G:H2'       | 2.32                     | 0.45              |
| 7:Z:6:DT:H2'      | 7:Z:7:DT:H72      | 1.98                     | 0.45              |
| 1:A:35:THR:HG23   | 1:B:42:ARG:HB2    | 1.98                     | 0.45              |
| 2:C:580:MET:HE3   | 2:C:580:MET:HB2   | 1.67                     | 0.45              |
| 2:C:714:ASP:HB2   | 2:C:818:GLY:O     | 2.17                     | 0.45              |
| 2:C:762:LYS:HZ2   | 2:C:786:LYS:HG3   | 1.80                     | 0.45              |
| 2:C:875:GLY:O     | 2:C:879:ARG:HD2   | 2.15                     | 0.45              |
| 2:C:1087:VAL:HG13 | 2:C:1088:LEU:N    | 2.31                     | 0.45              |
| 3:D:109:PRO:O     | 3:D:110:SER:C     | 2.58                     | 0.45              |
| 3:D:485:SER:O     | 3:D:489:ARG:HB3   | 2.17                     | 0.45              |
| 3:D:525:ARG:HB2   | 3:D:538:SER:CB    | 2.44                     | 0.45              |
| 3:D:528:VAL:CG1   | 3:D:529:GLN:H     | 2.28                     | 0.45              |
| 3:D:542:ASP:HB2   | 3:D:600:LEU:CD2   | 2.45                     | 0.45              |
| 3:D:895:VAL:HA    | 3:D:898:GLU:OE1   | 2.15                     | 0.45              |
| 3:D:1115:THR:HG22 | 3:D:1151:ARG:NH2  | 2.32                     | 0.45              |
| 4:E:47:LYS:HA     | 4:E:54:LEU:HB3    | 1.99                     | 0.45              |
| 1:K:34:VAL:HG13   | 1:K:35:THR:H      | 1.82                     | 0.45              |
| 1:L:86:VAL:HG12   | 1:L:124:ASN:HB2   | 1.98                     | 0.45              |
| 2:M:119:PRO:HG2   | 2:M:386:PHE:CD2   | 2.51                     | 0.45              |
| 2:M:691:SER:CB    | 2:M:868:ASP:O     | 2.65                     | 0.45              |
| 2:M:694:LEU:O     | 2:M:699:PHE:HB2   | 2.16                     | 0.45              |
| 2:M:700:TYR:HB2   | 2:M:833:LEU:HD22  | 1.98                     | 0.45              |
| 2:M:832:LYS:O     | 2:M:834:GLN:N     | 2.49                     | 0.45              |
| 2:M:1054:THR:HG1  | 2:M:1055:LEU:N    | 2.15                     | 0.45              |
| 2:M:1098:ASP:HB2  | 3:N:21:TRP:CZ2    | 2.50                     | 0.45              |
| 3:N:143:ASN:HA    | 3:N:161:LEU:CD1   | 2.45                     | 0.45              |
| 3:N:650:LEU:O     | 3:N:654:LYS:CB    | 2.64                     | 0.45              |
| 3:N:860:LEU:HD22  | 3:N:881:LEU:HD23  | 1.97                     | 0.45              |
| 3:N:1109:GLU:OE2  | 3:N:1217:ILE:HG12 | 2.17                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1330:ILE:HB   | 3:N:1347:TYR:OH  | 2.16                     | 0.45              |
| 4:O:54:LEU:CA     | 4:O:58:PRO:HG2   | 2.38                     | 0.45              |
| 5:G:14:DG:H2''    | 5:G:15:DC:OP2    | 2.16                     | 0.45              |
| 7:I:11:DG:OP2     | 7:I:11:DG:H8     | 2.00                     | 0.45              |
| 5:X:7:DA:H4'      | 5:X:7:DA:OP1     | 2.16                     | 0.45              |
| 2:C:399:ASN:CG    | 2:C:402:SER:HB3  | 2.36                     | 0.45              |
| 2:C:459:ALA:HB1   | 2:C:467:ILE:HG21 | 1.98                     | 0.45              |
| 2:C:588:VAL:HG23  | 2:C:596:TYR:OH   | 2.17                     | 0.45              |
| 2:C:783:ARG:NH2   | 2:C:785:VAL:HG11 | 2.32                     | 0.45              |
| 3:D:483:HIS:ND1   | 3:D:483:HIS:N    | 2.65                     | 0.45              |
| 3:D:888:GLU:O     | 3:D:889:ALA:C    | 2.57                     | 0.45              |
| 3:D:1190:SER:C    | 3:D:1204:CYS:SG  | 3.00                     | 0.45              |
| 3:D:1194:CYS:HB2  | 3:D:1204:CYS:CB  | 2.46                     | 0.45              |
| 3:D:1389:LEU:HD12 | 3:D:1390:LEU:H   | 1.81                     | 0.45              |
| 3:D:1442:ASN:HB3  | 3:D:1444:THR:H   | 1.82                     | 0.45              |
| 1:K:49:PRO:HB3    | 1:K:148:VAL:HG22 | 1.97                     | 0.45              |
| 1:L:143:ARG:HD2   | 1:L:160:ASP:OD2  | 2.17                     | 0.45              |
| 2:M:6:PHE:HD1     | 2:M:902:ILE:O    | 2.00                     | 0.45              |
| 2:M:183:SER:OG    | 2:M:190:LYS:NZ   | 2.50                     | 0.45              |
| 2:M:292:ARG:HG2   | 2:M:298:PHE:HA   | 1.97                     | 0.45              |
| 2:M:376:ARG:CB    | 2:M:377:PRO:HD3  | 2.47                     | 0.45              |
| 2:M:458:TYR:O     | 2:M:459:ALA:C    | 2.57                     | 0.45              |
| 2:M:564:MET:CE    | 2:M:840:ALA:HB3  | 2.46                     | 0.45              |
| 2:M:589:ARG:HA    | 2:M:596:TYR:CZ   | 2.52                     | 0.45              |
| 2:M:684:PHE:HD2   | 3:N:740:PHE:CD1  | 2.34                     | 0.45              |
| 2:M:810:ASP:HA    | 2:M:811:PRO:HD3  | 1.81                     | 0.45              |
| 3:N:52:PRO:HG2    | 3:N:85:VAL:HG21  | 1.97                     | 0.45              |
| 3:N:186:VAL:HG12  | 3:N:187:LYS:N    | 2.32                     | 0.45              |
| 3:N:462:GLN:HA    | 3:N:513:ILE:HG21 | 1.98                     | 0.45              |
| 3:N:577:ALA:O     | 3:N:581:LEU:HD23 | 2.17                     | 0.45              |
| 3:N:606:ILE:CG2   | 3:N:607:LEU:N    | 2.80                     | 0.45              |
| 3:N:678:GLU:C     | 3:N:679:ARG:HG3  | 2.41                     | 0.45              |
| 3:N:700:VAL:HG22  | 3:N:718:PRO:HG2  | 1.98                     | 0.45              |
| 3:N:787:LEU:HD12  | 3:N:787:LEU:HA   | 1.73                     | 0.45              |
| 3:N:1216:SER:OG   | 4:O:15:SER:HA    | 2.16                     | 0.45              |
| 3:N:1348:LEU:N    | 3:N:1348:LEU:CD1 | 2.79                     | 0.45              |
| 3:N:1464:GLU:HG3  | 3:N:1465:ASN:N   | 2.31                     | 0.45              |
| 5:X:17:DA:H2''    | 5:X:18:DC:O5'    | 2.16                     | 0.45              |
| 7:Z:5:DC:C2'      | 7:Z:6:DT:H71     | 2.46                     | 0.45              |
| 2:C:21:ILE:H      | 2:C:21:ILE:CD1   | 2.28                     | 0.45              |
| 2:C:144:PRO:HB2   | 2:C:267:TYR:HE1  | 1.81                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:157:ARG:HD3   | 2:C:314:THR:CG2  | 2.46                     | 0.45              |
| 2:C:396:ASP:HA    | 2:C:633:GLN:HE22 | 1.82                     | 0.45              |
| 2:C:431:HIS:CG    | 2:C:432:ARG:H    | 2.34                     | 0.45              |
| 2:C:745:ILE:HD11  | 2:C:803:THR:OG1  | 2.16                     | 0.45              |
| 2:C:905:ILE:HD12  | 2:C:905:ILE:N    | 2.32                     | 0.45              |
| 2:C:1053:LEU:HD13 | 3:D:1466:VAL:O   | 2.16                     | 0.45              |
| 3:D:584:ASN:CG    | 3:D:590:PRO:HD2  | 2.41                     | 0.45              |
| 3:D:631:ILE:HG12  | 3:D:743:ASP:O    | 2.17                     | 0.45              |
| 3:D:634:GLY:HA2   | 3:D:727:GLN:OE1  | 2.16                     | 0.45              |
| 3:D:804:LEU:HD23  | 3:D:804:LEU:H    | 1.81                     | 0.45              |
| 3:D:1435:LEU:HD13 | 3:D:1457:ASP:CG  | 2.41                     | 0.45              |
| 4:E:13:VAL:CG2    | 4:E:19:LEU:HD13  | 2.45                     | 0.45              |
| 1:K:192:LEU:O     | 2:M:938:LYS:NZ   | 2.50                     | 0.45              |
| 1:L:186:LEU:O     | 1:L:186:LEU:HD23 | 2.17                     | 0.45              |
| 2:M:434:HIS:ND1   | 2:M:434:HIS:N    | 2.63                     | 0.45              |
| 2:M:693:GLU:HA    | 2:M:696:LYS:HE3  | 1.98                     | 0.45              |
| 2:M:1012:PRO:HB2  | 2:M:1021:LEU:O   | 2.17                     | 0.45              |
| 2:M:1048:THR:OG1  | 3:N:755:ALA:CB   | 2.64                     | 0.45              |
| 3:N:117:ASP:HB2   | 3:N:495:ARG:NH1  | 2.31                     | 0.45              |
| 3:N:568:ARG:HE    | 3:N:572:ARG:CG   | 2.29                     | 0.45              |
| 3:N:608:SER:O     | 3:N:612:GLY:HA3  | 2.16                     | 0.45              |
| 3:N:771:SER:HB3   | 3:N:778:LEU:CD1  | 2.31                     | 0.45              |
| 3:N:789:LEU:HD13  | 3:N:934:LEU:HD22 | 1.98                     | 0.45              |
| 3:N:1138:ALA:O    | 3:N:1141:GLU:N   | 2.50                     | 0.45              |
| 3:N:1380:GLU:HG3  | 3:N:1381:VAL:N   | 2.30                     | 0.45              |
| 5:G:2:DT:OP2      | 5:G:2:DT:C4'     | 2.64                     | 0.45              |
| 6:H:11:C:O2'      | 6:H:12:U:H5'     | 2.16                     | 0.45              |
| 1:A:134:GLU:C     | 1:A:136:GLY:N    | 2.72                     | 0.45              |
| 1:A:221:HIS:HA    | 1:A:224:TYR:CD2  | 2.51                     | 0.45              |
| 1:B:102:LYS:HG2   | 1:B:104:GLU:OE2  | 2.17                     | 0.45              |
| 2:C:390:GLN:OE1   | 2:C:413:LEU:HD13 | 2.17                     | 0.45              |
| 2:C:438:ILE:O     | 2:C:440:PRO:HD3  | 2.15                     | 0.45              |
| 2:C:473:ARG:HA    | 2:C:531:PHE:CD1  | 2.52                     | 0.45              |
| 2:C:757:GLY:HA2   | 2:C:789:SER:OG   | 2.17                     | 0.45              |
| 2:C:834:GLN:HG2   | 2:C:837:ASP:OD1  | 2.17                     | 0.45              |
| 3:D:11:ALA:HA     | 3:D:1451:ALA:O   | 2.15                     | 0.45              |
| 3:D:30:GLU:O      | 3:D:40:GLU:HB3   | 2.16                     | 0.45              |
| 3:D:465:LEU:HD21  | 3:D:509:PRO:HB2  | 1.98                     | 0.45              |
| 3:D:636:GLN:H     | 3:D:636:GLN:HG2  | 1.47                     | 0.45              |
| 3:D:661:MET:HE2   | 3:D:677:LEU:HD11 | 1.98                     | 0.45              |
| 3:D:675:ARG:O     | 3:D:678:GLU:CD   | 2.59                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:799:LYS:HD3   | 3:D:826:PRO:CG    | 2.47                     | 0.45              |
| 3:D:918:ALA:HA    | 3:D:922:LEU:CD1   | 2.47                     | 0.45              |
| 3:D:977:ALA:O     | 3:D:980:MET:O     | 2.34                     | 0.45              |
| 3:D:1444:THR:O    | 3:D:1448:THR:OG1  | 2.28                     | 0.45              |
| 3:D:1468:LEU:HD22 | 3:D:1470:ARG:CG   | 2.47                     | 0.45              |
| 1:K:36:LEU:C      | 1:K:39:PRO:HD2    | 2.42                     | 0.45              |
| 1:K:42:ARG:NH1    | 1:L:34:VAL:HB     | 2.29                     | 0.45              |
| 1:K:64:GLU:CG     | 1:K:76:VAL:HG22   | 2.47                     | 0.45              |
| 1:K:95:GLN:O      | 1:K:145:ASP:HA    | 2.17                     | 0.45              |
| 1:K:101:LEU:HD13  | 1:K:114:PHE:CZ    | 2.51                     | 0.45              |
| 2:M:18:LEU:H      | 2:M:18:LEU:CD1    | 2.29                     | 0.45              |
| 2:M:191:PHE:CE2   | 2:M:238:LEU:HD21  | 2.52                     | 0.45              |
| 2:M:355:VAL:CG1   | 2:M:356:ARG:N     | 2.80                     | 0.45              |
| 2:M:394:PHE:CZ    | 2:M:632:ASN:CG    | 2.95                     | 0.45              |
| 2:M:616:GLU:OE1   | 2:M:616:GLU:HA    | 2.16                     | 0.45              |
| 2:M:706:GLU:HB3   | 2:M:708:TYR:CE1   | 2.52                     | 0.45              |
| 2:M:808:ARG:NH2   | 2:M:820:ARG:HH21  | 2.00                     | 0.45              |
| 3:N:54:LYS:HG3    | 3:N:55:ASP:H      | 1.82                     | 0.45              |
| 3:N:474:GLU:O     | 3:N:478:LEU:HG    | 2.16                     | 0.45              |
| 3:N:1114:THR:O    | 3:N:1114:THR:HG23 | 2.16                     | 0.45              |
| 5:X:13:DA:OP2     | 5:X:13:DA:H8      | 2.00                     | 0.45              |
| 1:A:42:ARG:HE     | 1:A:42:ARG:HB3    | 1.49                     | 0.45              |
| 1:B:78:ILE:HG23   | 1:B:129:ILE:HG22  | 1.97                     | 0.45              |
| 1:B:210:ALA:O     | 1:B:213:GLN:HB2   | 2.16                     | 0.45              |
| 2:C:64:LEU:CD1    | 2:C:100:LEU:HD11  | 2.44                     | 0.45              |
| 2:C:395:LYS:O     | 2:C:397:GLU:N     | 2.49                     | 0.45              |
| 2:C:587:VAL:HG11  | 2:C:666:LEU:HD22  | 1.99                     | 0.45              |
| 2:C:605:LYS:O     | 2:C:611:ILE:HA    | 2.17                     | 0.45              |
| 2:C:682:TYR:O     | 2:C:850:ALA:CB    | 2.65                     | 0.45              |
| 2:C:720:GLU:HA    | 2:C:759:THR:O     | 2.16                     | 0.45              |
| 2:C:831:ARG:NH2   | 2:C:1004:LYS:HG3  | 2.32                     | 0.45              |
| 2:C:1036:GLU:HA   | 3:D:707:THR:CG2   | 2.31                     | 0.45              |
| 2:C:1084:SER:O    | 2:C:1088:LEU:HB2  | 2.17                     | 0.45              |
| 3:D:16:GLU:CD     | 3:D:16:GLU:N      | 2.75                     | 0.45              |
| 3:D:34:TYR:CG     | 3:D:35:ARG:N      | 2.85                     | 0.45              |
| 3:D:107:ASP:O     | 3:D:110:SER:N     | 2.50                     | 0.45              |
| 3:D:795:VAL:HG13  | 3:D:863:VAL:HG22  | 1.99                     | 0.45              |
| 3:D:804:LEU:HD23  | 3:D:804:LEU:N     | 2.32                     | 0.45              |
| 3:D:1071:PHE:O    | 3:D:1074:SER:HB3  | 2.16                     | 0.45              |
| 4:E:13:VAL:HG12   | 4:E:15:SER:H      | 1.80                     | 0.45              |
| 1:K:117:VAL:HB    | 1:K:120:VAL:CG1   | 2.46                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:124:ASN:N     | 1:L:125:PRO:HD3   | 2.30                     | 0.45              |
| 2:M:136:ILE:HG21  | 2:M:336:VAL:HG13  | 1.98                     | 0.45              |
| 3:N:28:LYS:HD2    | 3:N:41:ARG:CZ     | 2.47                     | 0.45              |
| 3:N:142:LEU:O     | 3:N:161:LEU:HD11  | 2.17                     | 0.45              |
| 3:N:467:GLU:H     | 3:N:467:GLU:HG3   | 1.56                     | 0.45              |
| 3:N:481:MET:O     | 3:N:489:ARG:HD2   | 2.17                     | 0.45              |
| 3:N:666:ILE:CG2   | 3:N:684:LYS:NZ    | 2.79                     | 0.45              |
| 3:N:935:LYS:HE2   | 3:N:935:LYS:HB3   | 1.71                     | 0.45              |
| 3:N:1260:ILE:HD13 | 3:N:1260:ILE:N    | 2.32                     | 0.45              |
| 3:N:1311:LEU:HD23 | 3:N:1311:LEU:N    | 2.31                     | 0.45              |
| 3:N:1485:GLN:N    | 4:O:76:GLY:O      | 2.50                     | 0.45              |
| 5:X:6:DT:H2"      | 5:X:7:DA:H8       | 1.79                     | 0.45              |
| 1:A:61:VAL:HG12   | 1:A:62:LEU:N      | 2.32                     | 0.45              |
| 2:C:221:LEU:C     | 2:C:223:ASP:H     | 2.25                     | 0.45              |
| 2:C:630:ARG:HD3   | 2:C:705:ILE:HG22  | 1.96                     | 0.45              |
| 2:C:1083:GLU:C    | 2:C:1085:PHE:N    | 2.71                     | 0.45              |
| 3:D:8:VAL:HB      | 3:D:1435:LEU:HD11 | 1.99                     | 0.45              |
| 3:D:10:ILE:HD12   | 3:D:1434:TRP:NE1  | 2.31                     | 0.45              |
| 3:D:36:THR:C      | 3:D:38:LYS:N      | 2.73                     | 0.45              |
| 3:D:41:ARG:O      | 3:D:43:GLY:N      | 2.49                     | 0.45              |
| 3:D:493:ARG:HG3   | 3:D:494:LYS:H     | 1.82                     | 0.45              |
| 3:D:796:ARG:HG3   | 3:D:861:GLN:O     | 2.16                     | 0.45              |
| 3:D:914:LEU:HD23  | 3:D:914:LEU:O     | 2.16                     | 0.45              |
| 3:D:1153:VAL:HG12 | 3:D:1160:LEU:HD12 | 1.99                     | 0.45              |
| 3:D:1256:LEU:O    | 3:D:1259:VAL:N    | 2.49                     | 0.45              |
| 3:D:1496:GLU:HA   | 3:D:1499:ARG:HE   | 1.80                     | 0.45              |
| 4:E:36:LYS:HE2    | 4:E:36:LYS:HA     | 1.99                     | 0.45              |
| 1:L:30:ARG:HG2    | 1:L:30:ARG:HH11   | 1.82                     | 0.45              |
| 2:M:310:LEU:HG    | 2:M:311:PHE:HD2   | 1.82                     | 0.45              |
| 2:M:684:PHE:CD1   | 2:M:684:PHE:C     | 2.95                     | 0.45              |
| 2:M:691:SER:C     | 2:M:693:GLU:N     | 2.75                     | 0.45              |
| 2:M:994:ILE:HG22  | 2:M:995:MET:N     | 2.32                     | 0.45              |
| 3:N:42:ASP:O      | 3:N:43:GLY:O      | 2.34                     | 0.45              |
| 3:N:117:ASP:C     | 3:N:118:LEU:HG    | 2.42                     | 0.45              |
| 3:N:401:TYR:O     | 3:N:443:VAL:HG23  | 2.17                     | 0.45              |
| 3:N:470:LEU:HD12  | 3:N:503:LEU:HD21  | 1.98                     | 0.45              |
| 3:N:586:ARG:HD3   | 3:N:586:ARG:HA    | 1.79                     | 0.45              |
| 3:N:827:ILE:HG23  | 3:N:837:GLY:HA2   | 1.99                     | 0.45              |
| 3:N:1151:ARG:HA   | 3:N:1162:GLU:HG2  | 1.99                     | 0.45              |
| 3:N:1279:GLY:O    | 3:N:1318:TYR:HA   | 2.16                     | 0.45              |
| 5:X:2:DT:H2"      | 5:X:3:DC:C6       | 2.53                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:X:17:DA:H1'     | 5:X:18:DC:H5'     | 1.99                     | 0.45              |
| 5:X:26:DC:O2      | 5:X:26:DC:H2'     | 2.17                     | 0.45              |
| 6:Y:8:G:OP2       | 6:Y:8:G:H8        | 2.00                     | 0.45              |
| 6:Y:8:G:H8        | 6:Y:8:G:P         | 2.40                     | 0.45              |
| 1:A:174:VAL:HG22  | 1:A:201:THR:HG22  | 1.99                     | 0.44              |
| 1:B:7:LYS:O       | 1:B:7:LYS:HD3     | 2.16                     | 0.44              |
| 1:B:153:ALA:HA    | 1:B:156:HIS:NE2   | 2.32                     | 0.44              |
| 1:B:173:PRO:HB2   | 1:B:205:VAL:HG22  | 1.99                     | 0.44              |
| 2:C:20:GLU:CG     | 2:C:21:ILE:HD12   | 2.39                     | 0.44              |
| 2:C:79:PRO:CG     | 2:C:82:GLU:HG3    | 2.46                     | 0.44              |
| 2:C:395:LYS:HE3   | 2:C:407:LYS:CD    | 2.40                     | 0.44              |
| 2:C:503:LEU:HD23  | 2:C:507:ARG:C     | 2.42                     | 0.44              |
| 2:C:680:ASP:N     | 3:D:943:THR:HG22  | 2.32                     | 0.44              |
| 2:C:733:ALA:HB2   | 3:D:679:ARG:CZ    | 2.47                     | 0.44              |
| 2:C:762:LYS:HZ2   | 2:C:786:LYS:HA    | 1.81                     | 0.44              |
| 2:C:816:LYS:HB2   | 2:C:819:VAL:HG21  | 1.99                     | 0.44              |
| 2:C:957:LYS:CD    | 2:C:961:GLU:CB    | 2.95                     | 0.44              |
| 2:C:1035:MET:CB   | 2:C:1036:GLU:OE1  | 2.65                     | 0.44              |
| 3:D:531:ASP:O     | 3:D:533:GLY:N     | 2.50                     | 0.44              |
| 3:D:563:PRO:O     | 3:D:564:GLU:C     | 2.59                     | 0.44              |
| 3:D:952:ASP:HA    | 3:D:1062:ARG:HH21 | 1.82                     | 0.44              |
| 3:D:1046:GLN:HG2  | 3:D:1052:THR:CG2  | 2.44                     | 0.44              |
| 3:D:1109:GLU:OE2  | 3:D:1202:GLN:HB2  | 2.17                     | 0.44              |
| 3:D:1366:LYS:O    | 3:D:1370:ILE:HG12 | 2.17                     | 0.44              |
| 3:D:1487:VAL:HG12 | 3:D:1488:ASP:N    | 2.30                     | 0.44              |
| 1:K:48:ILE:HD13   | 1:K:210:ALA:HB1   | 1.99                     | 0.44              |
| 1:K:54:THR:HG22   | 1:K:158:ILE:HG13  | 2.00                     | 0.44              |
| 1:L:59:GLU:CG     | 1:L:137:ARG:HH22  | 2.30                     | 0.44              |
| 1:L:108:GLU:HB3   | 1:L:128:HIS:HE1   | 1.82                     | 0.44              |
| 2:M:21:ILE:H      | 2:M:21:ILE:CD1    | 2.29                     | 0.44              |
| 2:M:553:ASP:OD2   | 2:M:883:GLY:HA3   | 2.17                     | 0.44              |
| 2:M:685:GLU:OE1   | 3:N:739:ASP:HB3   | 2.18                     | 0.44              |
| 2:M:873:PRO:O     | 2:M:877:PRO:CD    | 2.66                     | 0.44              |
| 2:M:893:ALA:HB1   | 2:M:897:LEU:CD1   | 2.45                     | 0.44              |
| 3:N:76:CYS:O      | 3:N:78:VAL:N      | 2.51                     | 0.44              |
| 3:N:524:LEU:HD12  | 3:N:524:LEU:N     | 2.31                     | 0.44              |
| 3:N:820:GLU:CD    | 3:N:820:GLU:C     | 2.84                     | 0.44              |
| 3:N:935:LYS:HG2   | 3:N:936:TYR:N     | 2.28                     | 0.44              |
| 4:O:43:GLU:HG3    | 4:O:44:GLU:N      | 2.25                     | 0.44              |
| 4:O:94:PRO:O      | 4:O:96:GLU:HG3    | 2.17                     | 0.44              |
| 7:Z:5:DC:C2'      | 7:Z:6:DT:OP2      | 2.53                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:76:VAL:O      | 1:A:79:ILE:HG13  | 2.18                     | 0.44              |
| 1:B:24:VAL:HG22   | 1:B:196:THR:CG2  | 2.46                     | 0.44              |
| 2:C:134:ARG:HH11  | 2:C:387:SER:HA   | 1.80                     | 0.44              |
| 2:C:170:PRO:CD    | 2:C:263:ASP:HB3  | 2.47                     | 0.44              |
| 2:C:183:SER:HA    | 2:C:190:LYS:HB3  | 2.00                     | 0.44              |
| 2:C:409:ARG:CB    | 2:C:454:SER:OG   | 2.43                     | 0.44              |
| 2:C:439:CYS:SG    | 2:C:540:PHE:HA   | 2.56                     | 0.44              |
| 2:C:874:LEU:O     | 2:C:877:PRO:HD2  | 2.16                     | 0.44              |
| 2:C:971:LYS:HG2   | 2:C:988:VAL:CB   | 2.48                     | 0.44              |
| 2:C:1054:THR:HG21 | 2:C:1079:PRO:HB3 | 2.00                     | 0.44              |
| 3:D:642:CYS:SG    | 3:D:716:PHE:CB   | 3.03                     | 0.44              |
| 3:D:654:LYS:CB    | 3:D:655:PRO:HD3  | 2.35                     | 0.44              |
| 3:D:658:LEU:O     | 3:D:661:MET:HB2  | 2.18                     | 0.44              |
| 3:D:680:GLN:HA    | 3:D:683:ILE:CD1  | 2.47                     | 0.44              |
| 3:D:696:HIS:CD2   | 4:E:58:PRO:C     | 2.95                     | 0.44              |
| 3:D:739:ASP:OD1   | 6:H:15:C:C5'     | 2.65                     | 0.44              |
| 3:D:1042:ARG:HE   | 3:D:1073:SER:CB  | 2.30                     | 0.44              |
| 3:D:1078:ARG:HA   | 3:D:1078:ARG:HD3 | 1.81                     | 0.44              |
| 1:L:179:PHE:HD2   | 1:L:179:PHE:H    | 1.64                     | 0.44              |
| 2:M:5:ARG:CA      | 2:M:902:ILE:HB   | 2.48                     | 0.44              |
| 2:M:44:ILE:HG21   | 2:M:71:TYR:CD1   | 2.52                     | 0.44              |
| 2:M:212:GLY:HA3   | 2:M:218:VAL:HG21 | 1.99                     | 0.44              |
| 2:M:252:LYS:HB3   | 2:M:298:PHE:CZ   | 2.53                     | 0.44              |
| 2:M:317:VAL:C     | 2:M:319:GLY:N    | 2.68                     | 0.44              |
| 2:M:586:ARG:NH1   | 2:M:590:ASP:OD2  | 2.49                     | 0.44              |
| 2:M:838:LYS:HG3   | 2:M:997:LEU:HB2  | 1.99                     | 0.44              |
| 2:M:1040:LEU:HD12 | 2:M:1040:LEU:HA  | 1.84                     | 0.44              |
| 2:M:1049:LEU:O    | 2:M:1053:LEU:HG  | 2.17                     | 0.44              |
| 3:N:84:ILE:O      | 3:N:87:ARG:N     | 2.48                     | 0.44              |
| 3:N:134:VAL:HG22  | 3:N:460:ALA:HB1  | 1.99                     | 0.44              |
| 3:N:564:GLU:O     | 3:N:565:ILE:C    | 2.59                     | 0.44              |
| 3:N:587:ARG:O     | 3:N:588:GLY:O    | 2.34                     | 0.44              |
| 3:N:885:ILE:O     | 3:N:888:GLU:HB2  | 2.16                     | 0.44              |
| 3:N:899:LEU:HD22  | 3:N:917:GLN:CB   | 2.47                     | 0.44              |
| 3:N:900:ILE:CD1   | 3:N:902:LEU:HD22 | 2.47                     | 0.44              |
| 3:N:1293:PHE:HB3  | 3:N:1295:GLU:CG  | 2.44                     | 0.44              |
| 4:O:4:PRO:O       | 4:O:5:GLY:C      | 2.60                     | 0.44              |
| 2:C:101:ILE:HG23  | 2:C:107:LEU:CD2  | 2.48                     | 0.44              |
| 2:C:166:PRO:O     | 2:C:167:LYS:C    | 2.59                     | 0.44              |
| 2:C:326:ASP:CB    | 2:C:431:HIS:ND1  | 2.73                     | 0.44              |
| 2:C:334:ARG:HB2   | 2:C:339:LEU:CD2  | 2.47                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:355:VAL:CG1   | 2:C:356:ARG:N    | 2.80                     | 0.44              |
| 2:C:541:SER:OG    | 2:C:543:ASN:HB3  | 2.16                     | 0.44              |
| 2:C:1081:VAL:HB   | 2:C:1086:ARG:NH2 | 2.33                     | 0.44              |
| 3:D:84:ILE:HA     | 3:D:87:ARG:HG2   | 1.99                     | 0.44              |
| 3:D:128:TYR:HB3   | 3:D:129:PHE:HD1  | 1.83                     | 0.44              |
| 3:D:660:LYS:O     | 3:D:663:GLU:HB2  | 2.18                     | 0.44              |
| 3:D:696:HIS:HD2   | 4:E:59:ASN:CB    | 2.26                     | 0.44              |
| 3:D:930:LEU:O     | 3:D:933:ALA:HB3  | 2.18                     | 0.44              |
| 3:D:941:PHE:O     | 3:D:945:SER:HB3  | 2.17                     | 0.44              |
| 3:D:1111:ASP:O    | 3:D:1112:CYS:C   | 2.60                     | 0.44              |
| 3:D:1146:GLY:HA3  | 3:D:1207:TYR:CB  | 2.45                     | 0.44              |
| 3:D:1395:LEU:O    | 3:D:1398:TRP:HB2 | 2.18                     | 0.44              |
| 3:D:1461:GLY:O    | 3:D:1465:ASN:HB2 | 2.16                     | 0.44              |
| 4:E:4:PRO:O       | 4:E:5:GLY:C      | 2.60                     | 0.44              |
| 4:E:27:ALA:HB1    | 4:E:60:ALA:CB    | 2.46                     | 0.44              |
| 1:L:58:ILE:HD13   | 1:L:58:ILE:HA    | 1.91                     | 0.44              |
| 1:L:138:LEU:HD23  | 1:L:138:LEU:C    | 2.42                     | 0.44              |
| 1:L:195:LEU:HD12  | 1:L:195:LEU:C    | 2.42                     | 0.44              |
| 2:M:661:SER:HA    | 2:M:665:PHE:O    | 2.18                     | 0.44              |
| 2:M:676:ILE:O     | 3:N:948:THR:HB   | 2.18                     | 0.44              |
| 2:M:685:GLU:O     | 2:M:686:ASP:OD2  | 2.35                     | 0.44              |
| 2:M:884:GLN:CB    | 2:M:992:MET:HE1  | 2.47                     | 0.44              |
| 2:M:1084:SER:O    | 2:M:1088:LEU:HB2 | 2.17                     | 0.44              |
| 2:M:1095:LEU:HD21 | 3:N:603:LEU:HD12 | 1.98                     | 0.44              |
| 3:N:400:VAL:CG2   | 3:N:443:VAL:HG21 | 2.47                     | 0.44              |
| 3:N:480:GLU:OE1   | 3:N:488:ARG:C    | 2.60                     | 0.44              |
| 3:N:833:GLU:OE1   | 3:N:833:GLU:HA   | 2.17                     | 0.44              |
| 3:N:1164:ARG:HG2  | 3:N:1165:TYR:N   | 2.33                     | 0.44              |
| 3:N:1484:THR:CG2  | 4:O:76:GLY:O     | 2.65                     | 0.44              |
| 5:G:14:DG:C2'     | 5:G:15:DC:OP2    | 2.65                     | 0.44              |
| 6:H:6:C:OP2       | 6:H:6:C:H5       | 2.00                     | 0.44              |
| 7:I:5:DC:C6       | 7:I:5:DC:O5'     | 2.69                     | 0.44              |
| 7:I:10:DG:C2      | 7:I:11:DG:C4     | 3.06                     | 0.44              |
| 7:I:11:DG:C4      | 7:I:12:DT:C4     | 3.05                     | 0.44              |
| 5:X:2:DT:C2'      | 5:X:3:DC:C5      | 3.00                     | 0.44              |
| 5:X:8:DC:H2''     | 5:X:9:DC:C5      | 2.52                     | 0.44              |
| 5:X:13:DA:O5'     | 5:X:13:DA:C8     | 2.70                     | 0.44              |
| 1:A:175:ARG:HE    | 1:A:176:ARG:HB3  | 1.83                     | 0.44              |
| 1:B:206:THR:HG22  | 1:B:209:GLU:CD   | 2.42                     | 0.44              |
| 2:C:45:GLN:HA     | 2:C:48:PHE:HD2   | 1.82                     | 0.44              |
| 2:C:468:ARG:HB2   | 2:C:485:TYR:HD2  | 1.82                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:831:ARG:NH1   | 2:C:1004:LYS:CG  | 2.76                     | 0.44              |
| 2:C:876:VAL:H     | 2:C:877:PRO:HD2  | 1.81                     | 0.44              |
| 2:C:959:PRO:HA    | 2:C:962:GLN:HG3  | 1.98                     | 0.44              |
| 3:D:30:GLU:CB     | 3:D:40:GLU:HG2   | 2.46                     | 0.44              |
| 3:D:1124:GLN:HA   | 3:D:1125:PRO:HD3 | 1.78                     | 0.44              |
| 3:D:1132:LEU:HD12 | 3:D:1132:LEU:N   | 2.32                     | 0.44              |
| 3:D:1255:GLY:HA3  | 3:D:1257:PRO:HD2 | 1.98                     | 0.44              |
| 2:M:163:ILE:C     | 2:M:163:ILE:CD1  | 2.91                     | 0.44              |
| 2:M:275:TYR:OH    | 2:M:489:THR:HG21 | 2.17                     | 0.44              |
| 2:M:333:ILE:HD13  | 2:M:465:GLY:O    | 2.18                     | 0.44              |
| 2:M:351:LEU:HD13  | 2:M:374:ASN:O    | 2.18                     | 0.44              |
| 2:M:1094:ALA:CA   | 3:N:90:MET:HE1   | 2.48                     | 0.44              |
| 3:N:104:PHE:HD2   | 3:N:1448:THR:CG2 | 2.28                     | 0.44              |
| 3:N:183:GLU:CG    | 3:N:184:GLU:N    | 2.76                     | 0.44              |
| 3:N:551:ASN:O     | 3:N:555:LYS:HG3  | 2.18                     | 0.44              |
| 3:N:567:ILE:HG22  | 3:N:571:LYS:HE3  | 2.00                     | 0.44              |
| 3:N:703:ASN:HB2   | 3:N:713:ILE:HG12 | 1.99                     | 0.44              |
| 3:N:868:TYR:HB2   | 3:N:873:LEU:HD12 | 1.97                     | 0.44              |
| 3:N:1192:LEU:HD13 | 3:N:1345:GLU:CG  | 2.48                     | 0.44              |
| 3:N:1281:VAL:HG11 | 3:N:1313:VAL:CG1 | 2.36                     | 0.44              |
| 1:A:20:TYR:HE2    | 1:A:198:ARG:HB2  | 1.82                     | 0.44              |
| 1:A:133:GLU:HG2   | 1:A:134:GLU:N    | 2.32                     | 0.44              |
| 1:B:62:LEU:HD12   | 1:B:63:HIS:H     | 1.82                     | 0.44              |
| 1:B:80:LEU:C      | 1:B:82:LEU:N     | 2.74                     | 0.44              |
| 1:B:179:PHE:HB3   | 1:B:197:LEU:HD12 | 1.99                     | 0.44              |
| 2:C:48:PHE:O      | 2:C:52:PHE:CA    | 2.64                     | 0.44              |
| 2:C:101:ILE:HG22  | 2:C:102:HIS:N    | 2.32                     | 0.44              |
| 2:C:405:ARG:NH2   | 2:C:409:ARG:CZ   | 2.80                     | 0.44              |
| 2:C:897:LEU:CD2   | 2:C:920:GLN:HE22 | 2.30                     | 0.44              |
| 2:C:903:SER:C     | 2:C:904:PRO:O    | 2.61                     | 0.44              |
| 2:C:1074:GLU:CG   | 2:C:1075:ASP:H   | 2.31                     | 0.44              |
| 3:D:28:LYS:HB3    | 3:D:41:ARG:NH1   | 2.32                     | 0.44              |
| 3:D:45:PHE:O      | 3:D:46:ASP:C     | 2.61                     | 0.44              |
| 3:D:473:LEU:HA    | 3:D:476:GLU:HB2  | 2.00                     | 0.44              |
| 3:D:631:ILE:O     | 3:D:632:VAL:HG23 | 2.17                     | 0.44              |
| 3:D:698:LYS:HE3   | 3:D:698:LYS:HB3  | 1.66                     | 0.44              |
| 3:D:853:VAL:HG11  | 3:D:860:LEU:HD21 | 1.98                     | 0.44              |
| 3:D:928:ALA:C     | 3:D:930:LEU:N    | 2.73                     | 0.44              |
| 3:D:1434:TRP:HZ3  | 3:D:1455:LYS:HB3 | 1.73                     | 0.44              |
| 4:E:54:LEU:O      | 4:E:63:TRP:HZ2   | 2.01                     | 0.44              |
| 1:K:123:MET:O     | 1:K:125:PRO:HD3  | 2.16                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:50:GLY:HA3   | 1:L:171:PHE:O    | 2.17                     | 0.44              |
| 1:L:90:LEU:HG    | 1:L:91:ASN:HD22  | 1.82                     | 0.44              |
| 1:L:101:LEU:HG   | 1:L:102:LYS:N    | 2.33                     | 0.44              |
| 1:L:137:ARG:HD3  | 1:L:137:ARG:C    | 2.43                     | 0.44              |
| 1:L:170:VAL:HG11 | 3:N:848:GLU:OE2  | 2.18                     | 0.44              |
| 2:M:5:ARG:HA     | 2:M:902:ILE:HB   | 2.00                     | 0.44              |
| 2:M:18:LEU:HD12  | 2:M:18:LEU:N     | 2.31                     | 0.44              |
| 2:M:79:PRO:HG2   | 2:M:82:GLU:CB    | 2.38                     | 0.44              |
| 2:M:141:HIS:O    | 2:M:331:ARG:CB   | 2.66                     | 0.44              |
| 2:M:393:GLN:NE2  | 6:Y:10:G:H4'     | 2.31                     | 0.44              |
| 2:M:768:THR:HB   | 2:M:771:GLU:CB   | 2.32                     | 0.44              |
| 2:M:946:ARG:NH1  | 2:M:984:GLU:HB2  | 2.33                     | 0.44              |
| 3:N:111:LYS:HE3  | 3:N:1449:GLU:N   | 2.32                     | 0.44              |
| 3:N:115:LEU:HB2  | 3:N:498:VAL:HG11 | 2.00                     | 0.44              |
| 3:N:154:THR:CG2  | 3:N:157:GLU:CD   | 2.91                     | 0.44              |
| 3:N:792:ILE:HG12 | 3:N:878:GLY:HA2  | 1.98                     | 0.44              |
| 3:N:1209:LEU:CD2 | 4:O:16:LYS:HE3   | 2.47                     | 0.44              |
| 3:N:1236:LEU:CD1 | 3:N:1256:LEU:HB2 | 2.38                     | 0.44              |
| 7:I:11:DG:H2''   | 7:I:12:DT:H6     | 1.82                     | 0.44              |
| 5:X:22:DA:H2     | 6:Y:12:U:O2      | 2.00                     | 0.44              |
| 7:Z:1:DG:C3'     | 7:Z:1:DG:OP1     | 2.65                     | 0.44              |
| 1:A:9:PRO:HD2    | 1:B:224:TYR:CE1  | 2.53                     | 0.44              |
| 2:C:87:ASP:O     | 2:C:814:GLU:CD   | 2.61                     | 0.44              |
| 2:C:943:VAL:CG2  | 2:C:986:PRO:HD3  | 2.48                     | 0.44              |
| 2:C:1008:ARG:NH2 | 2:C:1012:PRO:O   | 2.51                     | 0.44              |
| 2:C:1032:PHE:O   | 2:C:1036:GLU:CB  | 2.61                     | 0.44              |
| 2:C:1046:ALA:HB1 | 3:D:1472:ILE:CG1 | 2.48                     | 0.44              |
| 3:D:26:VAL:HG11  | 3:D:44:LEU:CD2   | 2.36                     | 0.44              |
| 3:D:85:VAL:HG23  | 3:D:86:ARG:N     | 2.32                     | 0.44              |
| 3:D:565:ILE:H    | 3:D:565:ILE:CD1  | 1.97                     | 0.44              |
| 3:D:631:ILE:HD13 | 3:D:743:ASP:HB2  | 1.93                     | 0.44              |
| 3:D:851:LEU:N    | 3:D:851:LEU:HD23 | 2.31                     | 0.44              |
| 3:D:1481:VAL:O   | 3:D:1483:PHE:N   | 2.50                     | 0.44              |
| 1:L:62:LEU:HD12  | 1:L:62:LEU:H     | 1.83                     | 0.44              |
| 2:M:31:GLN:HE21  | 2:M:38:LYS:HB2   | 1.82                     | 0.44              |
| 2:M:114:PHE:CG   | 2:M:114:PHE:O    | 2.70                     | 0.44              |
| 2:M:186:VAL:HG23 | 2:M:187:ASN:N    | 2.22                     | 0.44              |
| 2:M:468:ARG:HB2  | 2:M:485:TYR:HB3  | 1.99                     | 0.44              |
| 2:M:676:ILE:HG22 | 2:M:988:VAL:HG22 | 2.00                     | 0.44              |
| 2:M:752:GLY:N    | 2:M:792:VAL:HB   | 2.31                     | 0.44              |
| 2:M:762:LYS:HD2  | 2:M:786:LYS:CG   | 2.48                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:875:GLY:HA2  | 3:N:1029:ARG:HH22 | 1.75                     | 0.44              |
| 3:N:101:HIS:O    | 3:N:105:VAL:HG23  | 2.18                     | 0.44              |
| 3:N:646:LYS:HE2  | 3:N:722:GLU:CD    | 2.42                     | 0.44              |
| 3:N:1102:THR:O   | 3:N:1222:GLY:HA3  | 2.18                     | 0.44              |
| 3:N:1481:VAL:C   | 3:N:1483:PHE:N    | 2.76                     | 0.44              |
| 4:O:51:LEU:HG    | 4:O:53:GLY:H      | 1.83                     | 0.44              |
| 5:G:9:DC:H2''    | 5:G:10:DA:C8      | 2.53                     | 0.44              |
| 7:Z:3:DA:H2'     | 7:Z:3:DA:O5'      | 2.18                     | 0.44              |
| 1:A:3:ASP:CG     | 1:A:4:SER:N       | 2.75                     | 0.44              |
| 2:C:64:LEU:HD13  | 2:C:359:MET:HG3   | 1.98                     | 0.44              |
| 2:C:110:GLU:HG3  | 2:C:369:PRO:CG    | 2.45                     | 0.44              |
| 2:C:144:PRO:O    | 2:C:267:TYR:HE1   | 2.01                     | 0.44              |
| 2:C:414:GLY:C    | 2:C:416:GLY:N     | 2.75                     | 0.44              |
| 2:C:497:ALA:HA   | 2:C:515:ALA:HA    | 1.99                     | 0.44              |
| 2:C:691:SER:C    | 2:C:693:GLU:N     | 2.75                     | 0.44              |
| 2:C:860:HIS:CE1  | 2:C:975:TYR:HB2   | 2.53                     | 0.44              |
| 2:C:971:LYS:HG2  | 2:C:988:VAL:HG12  | 1.99                     | 0.44              |
| 2:C:1035:MET:HB2 | 2:C:1036:GLU:OE1  | 2.17                     | 0.44              |
| 3:D:506:GLY:O    | 3:D:508:ARG:N     | 2.50                     | 0.44              |
| 3:D:562:ALA:C    | 3:D:567:ILE:HD11  | 2.43                     | 0.44              |
| 3:D:776:GLU:OE1  | 3:D:912:LYS:HE2   | 2.18                     | 0.44              |
| 3:D:785:ILE:HG23 | 3:D:938:GLY:CA    | 2.47                     | 0.44              |
| 3:D:895:VAL:O    | 3:D:895:VAL:HG12  | 2.16                     | 0.44              |
| 3:D:896:ALA:O    | 3:D:900:ILE:HG23  | 2.17                     | 0.44              |
| 3:D:918:ALA:HA   | 3:D:922:LEU:HD12  | 2.00                     | 0.44              |
| 3:D:1351:GLU:HA  | 3:D:1351:GLU:OE1  | 2.18                     | 0.44              |
| 3:D:1399:ASP:O   | 3:D:1403:LEU:HB2  | 2.18                     | 0.44              |
| 4:E:3:GLU:HA     | 4:E:3:GLU:OE1     | 2.18                     | 0.44              |
| 1:K:62:LEU:HD12  | 1:K:62:LEU:N      | 2.33                     | 0.44              |
| 1:K:217:ILE:HG22 | 1:K:221:HIS:HE2   | 1.83                     | 0.44              |
| 1:L:104:GLU:HA   | 1:L:136:GLY:O     | 2.18                     | 0.44              |
| 2:M:321:GLU:H    | 2:M:321:GLU:CD    | 2.26                     | 0.44              |
| 2:M:342:ASP:O    | 2:M:345:ARG:HG2   | 2.17                     | 0.44              |
| 2:M:395:LYS:O    | 2:M:633:GLN:OE1   | 2.35                     | 0.44              |
| 2:M:643:VAL:CG1  | 2:M:644:VAL:N     | 2.80                     | 0.44              |
| 2:M:983:ILE:HG22 | 3:N:946:GLY:CA    | 2.48                     | 0.44              |
| 3:N:66:GLN:O     | 3:N:68:PHE:N      | 2.51                     | 0.44              |
| 3:N:157:GLU:CA   | 3:N:160:GLU:CD    | 2.77                     | 0.44              |
| 3:N:185:VAL:HG13 | 3:N:189:GLN:OE1   | 2.18                     | 0.44              |
| 3:N:204:LEU:O    | 3:N:393:ILE:HG23  | 2.18                     | 0.44              |
| 3:N:868:TYR:HB2  | 3:N:873:LEU:CD1   | 2.47                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:925:GLU:N    | 4:O:7:ASP:OD2     | 2.51                     | 0.44              |
| 3:N:1108:ARG:O   | 3:N:1109:GLU:HB3  | 2.17                     | 0.44              |
| 3:N:1109:GLU:OE2 | 3:N:1202:GLN:HB2  | 2.18                     | 0.44              |
| 3:N:1239:ARG:CB  | 3:N:1239:ARG:CZ   | 2.96                     | 0.44              |
| 3:N:1341:PRO:O   | 3:N:1343:ALA:N    | 2.51                     | 0.44              |
| 4:O:3:GLU:OE2    | 4:O:65:MET:HE1    | 2.18                     | 0.44              |
| 4:O:37:ASN:HA    | 4:O:93:TYR:CD2    | 2.53                     | 0.44              |
| 5:G:3:DC:C6      | 5:G:3:DC:OP2      | 2.71                     | 0.44              |
| 7:I:1:DG:H3'     | 7:I:1:DG:OP1      | 2.17                     | 0.44              |
| 1:A:20:TYR:CE2   | 1:A:198:ARG:HB2   | 2.52                     | 0.44              |
| 1:A:176:ARG:HH11 | 2:C:865:THR:CB    | 2.25                     | 0.44              |
| 1:B:101:LEU:HD13 | 1:B:114:PHE:CD1   | 2.52                     | 0.44              |
| 1:B:138:LEU:HD23 | 1:B:138:LEU:C     | 2.43                     | 0.44              |
| 2:C:15:LEU:HA    | 2:C:458:TYR:CE2   | 2.53                     | 0.44              |
| 2:C:71:TYR:HA    | 2:C:96:ALA:CB     | 2.47                     | 0.44              |
| 2:C:612:VAL:HG13 | 2:C:621:VAL:O     | 2.18                     | 0.44              |
| 2:C:918:LEU:HD23 | 2:C:968:LEU:CA    | 2.39                     | 0.44              |
| 3:D:502:PHE:CE2  | 3:D:1452:ILE:HG13 | 2.53                     | 0.44              |
| 3:D:554:LEU:HG   | 3:D:558:LEU:CG    | 2.47                     | 0.44              |
| 3:D:644:LEU:HD12 | 3:D:645:PRO:CD    | 2.48                     | 0.44              |
| 3:D:1412:LYS:HB2 | 2:M:376:ARG:CZ    | 2.48                     | 0.44              |
| 1:K:64:GLU:O     | 1:K:76:VAL:HG23   | 2.18                     | 0.44              |
| 1:K:222:LEU:HD23 | 1:L:219:ARG:CA    | 2.48                     | 0.44              |
| 2:M:16:PRO:O     | 2:M:18:LEU:N      | 2.50                     | 0.44              |
| 2:M:721:ARG:HH11 | 2:M:721:ARG:HG3   | 1.82                     | 0.44              |
| 2:M:969:GLN:CD   | 3:N:952:ASP:CB    | 2.91                     | 0.44              |
| 3:N:9:ARG:NH1    | 3:N:11:ALA:HB2    | 2.32                     | 0.44              |
| 3:N:55:ASP:HA    | 3:N:82:LYS:HE2    | 2.00                     | 0.44              |
| 3:N:87:ARG:HA    | 3:N:521:PRO:HB3   | 1.98                     | 0.44              |
| 3:N:127:LEU:HD12 | 3:N:128:TYR:N     | 2.33                     | 0.44              |
| 3:N:400:VAL:HG13 | 3:N:400:VAL:O     | 2.17                     | 0.44              |
| 3:N:639:LEU:N    | 3:N:729:HIS:NE2   | 2.66                     | 0.44              |
| 3:N:794:GLN:HG2  | 3:N:1017:PHE:CE2  | 2.53                     | 0.44              |
| 3:N:1128:VAL:O   | 3:N:1129:THR:HG22 | 2.18                     | 0.44              |
| 5:G:19:DG:H2''   | 5:G:20:DC:C5'     | 2.48                     | 0.44              |
| 1:B:76:VAL:HA    | 1:B:79:ILE:CD1    | 2.48                     | 0.44              |
| 2:C:16:PRO:O     | 2:C:18:LEU:N      | 2.51                     | 0.44              |
| 2:C:22:GLN:NE2   | 2:C:136:ILE:O     | 2.51                     | 0.44              |
| 2:C:195:LEU:HD21 | 2:C:238:LEU:HG    | 2.00                     | 0.44              |
| 2:C:242:LEU:HD23 | 2:C:242:LEU:HA    | 1.89                     | 0.44              |
| 2:C:402:SER:HB2  | 2:C:566:THR:O     | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:723:THR:C     | 2:C:725:ASP:H     | 2.26                     | 0.44              |
| 2:C:752:GLY:H     | 2:C:792:VAL:HB    | 1.83                     | 0.44              |
| 2:C:876:VAL:O     | 2:C:879:ARG:O     | 2.35                     | 0.44              |
| 2:C:926:PHE:HE2   | 2:C:960:GLU:CD    | 2.24                     | 0.44              |
| 2:C:1034:GLU:C    | 2:C:1036:GLU:N    | 2.74                     | 0.44              |
| 3:D:14:SER:O      | 3:D:17:LYS:N      | 2.50                     | 0.44              |
| 3:D:15:PRO:O      | 3:D:18:ILE:HB     | 2.18                     | 0.44              |
| 3:D:714:GLN:HE21  | 3:D:765:SER:HB2   | 1.80                     | 0.44              |
| 3:D:1197:ARG:CZ   | 3:D:1198:TYR:CD1  | 3.01                     | 0.44              |
| 1:K:71:VAL:O      | 2:M:608:GLY:N     | 2.51                     | 0.44              |
| 1:K:78:ILE:O      | 1:K:81:ASN:N      | 2.51                     | 0.44              |
| 1:L:42:ARG:HG2    | 1:L:42:ARG:HH11   | 1.83                     | 0.44              |
| 1:L:83:LYS:HE2    | 1:L:168:ASP:OD2   | 2.18                     | 0.44              |
| 2:M:15:LEU:HA     | 2:M:458:TYR:CE2   | 2.53                     | 0.44              |
| 2:M:166:PRO:O     | 2:M:167:LYS:C     | 2.60                     | 0.44              |
| 2:M:431:HIS:CB    | 2:M:434:HIS:CE1   | 2.81                     | 0.44              |
| 2:M:435:TYR:C     | 2:M:437:ARG:H     | 2.24                     | 0.44              |
| 2:M:478:VAL:HA    | 2:M:506:ASN:O     | 2.18                     | 0.44              |
| 2:M:493:ARG:HB2   | 2:M:494:TYR:CD1   | 2.53                     | 0.44              |
| 2:M:580:MET:SD    | 2:M:584:GLU:CD    | 3.01                     | 0.44              |
| 2:M:707:ARG:HD2   | 2:M:826:TYR:OH    | 2.18                     | 0.44              |
| 2:M:922:PHE:CB    | 2:M:964:LYS:NZ    | 2.79                     | 0.44              |
| 2:M:1094:ALA:HA   | 3:N:90:MET:HE1    | 1.99                     | 0.44              |
| 3:N:115:LEU:C     | 3:N:115:LEU:CD2   | 2.90                     | 0.44              |
| 3:N:396:VAL:HB    | 3:N:447:VAL:HG12  | 1.99                     | 0.44              |
| 3:N:401:TYR:C     | 3:N:443:VAL:HG23  | 2.43                     | 0.44              |
| 3:N:1313:VAL:HG21 | 3:N:1319:VAL:CG1  | 2.48                     | 0.44              |
| 3:N:1432:LYS:O    | 3:N:1455:LYS:NZ   | 2.48                     | 0.44              |
| 6:H:6:C:N4        | 6:H:7:G:O6        | 2.51                     | 0.44              |
| 1:B:29:GLU:HB3    | 1:B:30:ARG:H      | 1.72                     | 0.43              |
| 1:B:100:LEU:HB2   | 1:B:115:LEU:HD21  | 2.00                     | 0.43              |
| 2:C:130:ASN:OD1   | 2:C:383:ARG:NH2   | 2.51                     | 0.43              |
| 2:C:260:LEU:HD21  | 2:C:293:PHE:CE2   | 2.52                     | 0.43              |
| 2:C:410:ILE:N     | 2:C:453:THR:O     | 2.42                     | 0.43              |
| 2:C:433:THR:C     | 2:C:435:TYR:N     | 2.66                     | 0.43              |
| 2:C:468:ARG:HA    | 2:C:486:MET:O     | 2.17                     | 0.43              |
| 2:C:473:ARG:HA    | 2:C:531:PHE:CE1   | 2.53                     | 0.43              |
| 2:C:793:PRO:O     | 2:C:794:PRO:C     | 2.59                     | 0.43              |
| 3:D:8:VAL:HG23    | 3:D:1459:LEU:CD1  | 2.48                     | 0.43              |
| 3:D:608:SER:HB3   | 3:D:1443:THR:HG23 | 1.99                     | 0.43              |
| 3:D:850:LEU:HD12  | 3:D:850:LEU:N     | 2.31                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:1087:ARG:HE   | 3:D:1236:LEU:CD1 | 2.29                     | 0.43              |
| 3:D:1119:SER:O    | 3:D:1121:PRO:HD3 | 2.17                     | 0.43              |
| 3:D:1242:HIS:O    | 3:D:1251:ASP:N   | 2.42                     | 0.43              |
| 3:D:1364:HIS:CE1  | 3:D:1366:LYS:HG3 | 2.53                     | 0.43              |
| 1:K:218:LEU:O     | 1:K:222:LEU:HD13 | 2.18                     | 0.43              |
| 1:L:28:LEU:HD11   | 1:L:195:LEU:H    | 1.83                     | 0.43              |
| 2:M:157:ARG:HG3   | 2:M:158:TYR:H    | 1.83                     | 0.43              |
| 2:M:191:PHE:CD2   | 2:M:241:LEU:HD13 | 2.53                     | 0.43              |
| 2:M:286:SER:HB3   | 2:M:299:LYS:CE   | 2.47                     | 0.43              |
| 2:M:456:ALA:HB3   | 2:M:459:ALA:HB2  | 1.99                     | 0.43              |
| 3:N:52:PRO:HG2    | 3:N:82:LYS:O     | 2.18                     | 0.43              |
| 3:N:98:PRO:CG     | 3:N:462:GLN:CD   | 2.79                     | 0.43              |
| 3:N:539:ASP:C     | 3:N:541:ASN:N    | 2.76                     | 0.43              |
| 3:N:795:VAL:HG23  | 3:N:879:ARG:NH1  | 2.33                     | 0.43              |
| 3:N:1209:LEU:C    | 3:N:1211:MET:N   | 2.73                     | 0.43              |
| 3:N:1273:VAL:HG23 | 3:N:1274:ILE:N   | 2.33                     | 0.43              |
| 3:N:1281:VAL:HG23 | 3:N:1319:VAL:CG2 | 2.47                     | 0.43              |
| 3:N:1354:LYS:HA   | 3:N:1357:ARG:HD2 | 1.99                     | 0.43              |
| 3:N:1483:PHE:O    | 4:O:77:GLU:HA    | 2.18                     | 0.43              |
| 6:Y:4:G:H2'       | 6:Y:5:C:C6       | 2.49                     | 0.43              |
| 1:A:9:PRO:HB3     | 1:A:25:LEU:CG    | 2.48                     | 0.43              |
| 1:A:18:ARG:HB2    | 1:A:203:GLY:HA2  | 2.00                     | 0.43              |
| 1:A:90:LEU:HD13   | 1:A:119:ASP:O    | 2.19                     | 0.43              |
| 2:C:553:ASP:OD2   | 2:C:553:ASP:N    | 2.51                     | 0.43              |
| 2:C:663:ASN:C     | 2:C:665:PHE:H    | 2.24                     | 0.43              |
| 2:C:706:GLU:HG2   | 2:C:708:TYR:CZ   | 2.53                     | 0.43              |
| 2:C:721:ARG:HG3   | 2:C:721:ARG:HH11 | 1.83                     | 0.43              |
| 2:C:953:VAL:O     | 2:C:955:PRO:HD3  | 2.18                     | 0.43              |
| 2:C:1040:LEU:HD12 | 2:C:1040:LEU:HA  | 1.71                     | 0.43              |
| 2:C:1040:LEU:CG   | 2:C:1045:ALA:HB3 | 2.44                     | 0.43              |
| 3:D:30:GLU:HA     | 3:D:30:GLU:OE1   | 2.18                     | 0.43              |
| 3:D:100:ALA:CB    | 3:D:128:TYR:OH   | 2.65                     | 0.43              |
| 3:D:521:PRO:CD    | 3:D:524:LEU:HD22 | 2.46                     | 0.43              |
| 3:D:620:GLY:O     | 3:D:621:LYS:HD3  | 2.18                     | 0.43              |
| 3:D:758:GLU:CB    | 3:D:762:GLN:NE2  | 2.81                     | 0.43              |
| 3:D:847:ASP:O     | 3:D:851:LEU:CG   | 2.63                     | 0.43              |
| 3:D:983:LEU:HD23  | 3:D:983:LEU:C    | 2.43                     | 0.43              |
| 3:D:1041:LEU:CD1  | 3:D:1045:MET:HB2 | 2.47                     | 0.43              |
| 3:D:1209:LEU:HD11 | 4:E:16:LYS:HD2   | 2.00                     | 0.43              |
| 3:D:1225:ALA:CA   | 3:D:1367:HIS:ND1 | 2.77                     | 0.43              |
| 3:D:1268:PRO:HB2  | 3:D:1329:ALA:HB3 | 1.99                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:E:40:LEU:HD21   | 4:E:67:GLU:CA    | 2.36                     | 0.43              |
| 2:M:183:SER:HG    | 2:M:190:LYS:HZ3  | 1.64                     | 0.43              |
| 2:M:392:SER:O     | 2:M:393:GLN:HG3  | 2.19                     | 0.43              |
| 2:M:397:GLU:H     | 2:M:633:GLN:CD   | 2.25                     | 0.43              |
| 2:M:762:LYS:HD2   | 2:M:786:LYS:HG3  | 1.99                     | 0.43              |
| 2:M:785:VAL:HG13  | 2:M:786:LYS:N    | 2.33                     | 0.43              |
| 3:N:33:ASN:HD22   | 3:N:40:GLU:CD    | 2.24                     | 0.43              |
| 3:N:470:LEU:HD23  | 3:N:470:LEU:H    | 1.82                     | 0.43              |
| 3:N:539:ASP:O     | 3:N:540:LEU:C    | 2.61                     | 0.43              |
| 3:N:563:PRO:O     | 3:N:564:GLU:C    | 2.61                     | 0.43              |
| 3:N:691:LEU:C     | 3:N:693:GLU:N    | 2.75                     | 0.43              |
| 3:N:736:PHE:H     | 3:N:736:PHE:HD1  | 1.62                     | 0.43              |
| 3:N:761:ILE:HD12  | 4:O:20:THR:HA    | 2.01                     | 0.43              |
| 3:N:928:ALA:C     | 3:N:930:LEU:N    | 2.72                     | 0.43              |
| 3:N:1311:LEU:HD23 | 3:N:1311:LEU:H   | 1.82                     | 0.43              |
| 1:A:109:VAL:HG23  | 1:A:132:LEU:HD13 | 2.00                     | 0.43              |
| 1:A:217:ILE:HG22  | 1:A:221:HIS:NE2  | 2.33                     | 0.43              |
| 1:B:43:ILE:HG23   | 1:B:47:SER:CB    | 2.47                     | 0.43              |
| 1:B:152:PRO:HB2   | 1:B:155:LYS:HB2  | 2.00                     | 0.43              |
| 2:C:90:TYR:CD1    | 2:C:120:LEU:HB2  | 2.54                     | 0.43              |
| 2:C:203:ASP:HB2   | 2:C:205:GLU:OE2  | 2.18                     | 0.43              |
| 2:C:334:ARG:HG2   | 2:C:338:GLU:OE1  | 2.19                     | 0.43              |
| 2:C:479:VAL:CG2   | 2:C:506:ASN:HA   | 2.44                     | 0.43              |
| 2:C:708:TYR:HE2   | 2:C:793:PRO:HG2  | 1.83                     | 0.43              |
| 2:C:903:SER:O     | 2:C:904:PRO:C    | 2.62                     | 0.43              |
| 3:D:85:VAL:O      | 3:D:88:TYR:HB2   | 2.18                     | 0.43              |
| 3:D:128:TYR:CZ    | 3:D:458:ALA:HB2  | 2.54                     | 0.43              |
| 3:D:731:LEU:HA    | 3:D:731:LEU:HD23 | 1.70                     | 0.43              |
| 3:D:787:LEU:HD21  | 3:D:947:ILE:HD11 | 2.00                     | 0.43              |
| 3:D:884:ARG:HD2   | 3:D:884:ARG:C    | 2.43                     | 0.43              |
| 3:D:1100:ASP:CA   | 3:D:1463:LYS:HZ1 | 2.30                     | 0.43              |
| 3:D:1137:ARG:O    | 3:D:1141:GLU:HG3 | 2.18                     | 0.43              |
| 3:D:1138:ALA:O    | 3:D:1139:ASP:C   | 2.61                     | 0.43              |
| 3:D:1189:ARG:HD2  | 3:D:1190:SER:H   | 1.84                     | 0.43              |
| 1:K:45:LEU:N      | 1:K:45:LEU:HD12  | 2.33                     | 0.43              |
| 1:K:186:LEU:O     | 1:K:188:GLN:N    | 2.50                     | 0.43              |
| 1:L:159:LYS:HE3   | 1:L:159:LYS:H    | 1.83                     | 0.43              |
| 1:L:175:ARG:HB3   | 3:N:847:ASP:OD2  | 2.19                     | 0.43              |
| 2:M:76:PRO:HG3    | 2:M:120:LEU:HD11 | 2.01                     | 0.43              |
| 2:M:101:ILE:CD1   | 2:M:107:LEU:HD22 | 2.48                     | 0.43              |
| 2:M:157:ARG:HG3   | 2:M:158:TYR:N    | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:221:LEU:C    | 2:M:223:ASP:H    | 2.25                     | 0.43              |
| 2:M:304:LEU:O    | 2:M:308:ARG:HB2  | 2.19                     | 0.43              |
| 2:M:414:GLY:C    | 2:M:416:GLY:N    | 2.75                     | 0.43              |
| 2:M:486:MET:HG3  | 2:M:487:THR:N    | 2.32                     | 0.43              |
| 2:M:564:MET:HE1  | 2:M:840:ALA:O    | 2.17                     | 0.43              |
| 2:M:657:ASP:C    | 2:M:658:GLY:O    | 2.62                     | 0.43              |
| 2:M:780:GLU:C    | 2:M:782:ALA:H    | 2.25                     | 0.43              |
| 2:M:987:ILE:HG12 | 3:N:948:THR:HG23 | 2.00                     | 0.43              |
| 3:N:136:ASP:HB3  | 3:N:453:ASP:HB2  | 2.00                     | 0.43              |
| 3:N:145:VAL:HG22 | 3:N:146:PRO:HD2  | 2.00                     | 0.43              |
| 3:N:812:ALA:O    | 3:N:816:HIS:HB2  | 2.18                     | 0.43              |
| 3:N:960:LYS:O    | 3:N:964:LEU:HB2  | 2.19                     | 0.43              |
| 3:N:966:GLU:O    | 3:N:969:ARG:HG2  | 2.18                     | 0.43              |
| 4:O:9:LEU:HD23   | 4:O:12:MET:SD    | 2.57                     | 0.43              |
| 4:O:54:LEU:HD22  | 4:O:63:TRP:HE1   | 1.78                     | 0.43              |
| 7:Z:4:DG:C2      | 7:Z:5:DC:C2      | 3.07                     | 0.43              |
| 1:A:28:LEU:CD2   | 1:A:32:PHE:CD1   | 2.59                     | 0.43              |
| 1:A:117:VAL:HB   | 1:A:120:VAL:HG11 | 1.99                     | 0.43              |
| 1:B:11:PHE:HB2   | 1:B:25:LEU:HD12  | 2.01                     | 0.43              |
| 2:C:275:TYR:OH   | 2:C:329:GLY:O    | 2.36                     | 0.43              |
| 2:C:686:ASP:HB3  | 2:C:846:LYS:O    | 2.18                     | 0.43              |
| 2:C:836:GLY:HA2  | 3:D:725:SER:CB   | 2.45                     | 0.43              |
| 2:C:1016:ILE:CG2 | 3:D:524:LEU:O    | 2.66                     | 0.43              |
| 2:C:1035:MET:HE1 | 5:G:19:DG:H4'    | 1.99                     | 0.43              |
| 2:C:1072:LYS:HB3 | 2:C:1072:LYS:HE2 | 1.81                     | 0.43              |
| 3:D:10:ILE:CD1   | 3:D:1434:TRP:HE1 | 2.31                     | 0.43              |
| 3:D:23:TYR:CZ    | 3:D:89:ARG:HG2   | 2.53                     | 0.43              |
| 3:D:543:LEU:HD11 | 3:D:600:LEU:HB2  | 2.00                     | 0.43              |
| 3:D:698:LYS:NZ   | 3:D:756:GLN:HG2  | 2.33                     | 0.43              |
| 3:D:732:VAL:CG2  | 3:D:736:PHE:HE1  | 2.30                     | 0.43              |
| 3:D:812:ALA:O    | 3:D:816:HIS:HB2  | 2.19                     | 0.43              |
| 3:D:1189:ARG:CZ  | 3:D:1204:CYS:SG  | 3.05                     | 0.43              |
| 3:D:1258:ARG:NH1 | 3:D:1329:ALA:CB  | 2.71                     | 0.43              |
| 1:K:134:GLU:C    | 1:K:136:GLY:N    | 2.74                     | 0.43              |
| 1:L:18:ARG:O     | 1:L:207:PRO:HD3  | 2.18                     | 0.43              |
| 1:L:56:VAL:CG1   | 1:L:57:TYR:N     | 2.81                     | 0.43              |
| 1:L:65:PHE:CE1   | 3:N:813:LEU:HD13 | 2.53                     | 0.43              |
| 2:M:44:ILE:HG21  | 2:M:71:TYR:CE1   | 2.53                     | 0.43              |
| 2:M:129:ILE:CD1  | 2:M:129:ILE:H    | 2.30                     | 0.43              |
| 2:M:265:ARG:CD   | 2:M:267:TYR:HB3  | 2.49                     | 0.43              |
| 2:M:430:VAL:HG13 | 3:N:1075:HIS:ND1 | 2.33                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:498:GLN:HG3   | 2:M:516:ARG:HH21  | 1.81                     | 0.43              |
| 2:M:604:ALA:O     | 2:M:645:VAL:HG12  | 2.18                     | 0.43              |
| 2:M:1000:MET:HE1  | 6:Y:12:U:O2'      | 2.18                     | 0.43              |
| 2:M:1008:ARG:O    | 3:N:624:ASP:O     | 2.36                     | 0.43              |
| 3:N:87:ARG:C      | 3:N:88:TYR:HD2    | 2.26                     | 0.43              |
| 3:N:104:PHE:HA    | 3:N:1448:THR:HG23 | 2.01                     | 0.43              |
| 3:N:502:PHE:CD1   | 3:N:509:PRO:HB3   | 2.53                     | 0.43              |
| 3:N:563:PRO:HG2   | 3:N:566:ILE:HD12  | 2.01                     | 0.43              |
| 3:N:771:SER:CB    | 3:N:778:LEU:HD13  | 2.31                     | 0.43              |
| 3:N:1182:GLU:C    | 3:N:1183:ILE:HG13 | 2.43                     | 0.43              |
| 3:N:1205:TYR:CE2  | 3:N:1215:VAL:HG21 | 2.53                     | 0.43              |
| 3:N:1255:GLY:C    | 3:N:1257:PRO:HD2  | 2.43                     | 0.43              |
| 3:N:1395:LEU:HD23 | 3:N:1395:LEU:C    | 2.43                     | 0.43              |
| 3:N:1462:LEU:O    | 3:N:1463:LYS:C    | 2.59                     | 0.43              |
| 3:N:1491:THR:O    | 3:N:1494:ALA:HB3  | 2.18                     | 0.43              |
| 4:O:36:LYS:HG2    | 4:O:95:VAL:HG21   | 1.99                     | 0.43              |
| 5:X:19:DG:C2'     | 5:X:20:DC:C5'     | 2.96                     | 0.43              |
| 7:Z:4:DG:C5       | 7:Z:5:DC:C4       | 3.06                     | 0.43              |
| 1:A:139:ASN:HD22  | 1:A:140:MET:N     | 2.17                     | 0.43              |
| 2:C:146:VAL:HG13  | 2:C:161:SER:O     | 2.18                     | 0.43              |
| 2:C:460:ARG:HG3   | 2:C:460:ARG:NH1   | 2.33                     | 0.43              |
| 2:C:663:ASN:C     | 2:C:665:PHE:N     | 2.75                     | 0.43              |
| 2:C:861:LEU:CG    | 2:C:862:PRO:HD2   | 2.34                     | 0.43              |
| 2:C:1090:LYS:HE2  | 2:C:1112:PHE:HE1  | 1.81                     | 0.43              |
| 3:D:8:VAL:O       | 3:D:1434:TRP:HH2  | 2.02                     | 0.43              |
| 3:D:148:GLU:HB3   | 3:D:151:GLN:HB2   | 1.99                     | 0.43              |
| 3:D:731:LEU:HD21  | 3:D:785:ILE:HD13  | 1.99                     | 0.43              |
| 3:D:924:MET:SD    | 4:E:6:ILE:HG12    | 2.59                     | 0.43              |
| 1:K:26:GLU:CB     | 1:K:27:PRO:HA     | 2.49                     | 0.43              |
| 1:K:170:VAL:HG23  | 1:K:170:VAL:O     | 2.18                     | 0.43              |
| 1:L:100:LEU:HD22  | 1:L:141:GLU:HB3   | 2.00                     | 0.43              |
| 2:M:31:GLN:OE1    | 2:M:31:GLN:O      | 2.37                     | 0.43              |
| 2:M:116:GLY:C     | 2:M:117:HIS:HD1   | 2.26                     | 0.43              |
| 2:M:252:LYS:NZ    | 2:M:296:GLY:HA3   | 2.34                     | 0.43              |
| 2:M:375:SER:O     | 2:M:379:GLU:OE1   | 2.37                     | 0.43              |
| 2:M:431:HIS:HB3   | 2:M:434:HIS:CD2   | 2.52                     | 0.43              |
| 2:M:581:THR:OG1   | 2:M:583:LEU:HD13  | 2.19                     | 0.43              |
| 2:M:878:SER:OG    | 3:N:1029:ARG:CZ   | 2.67                     | 0.43              |
| 2:M:1102:LEU:HB2  | 3:N:7:LYS:O       | 2.19                     | 0.43              |
| 3:N:95:LEU:HB2    | 3:N:515:GLU:C     | 2.44                     | 0.43              |
| 3:N:620:GLY:O     | 3:N:621:LYS:HD3   | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:885:ILE:H     | 3:N:885:ILE:HG13  | 1.70                     | 0.43              |
| 3:N:888:GLU:O     | 3:N:889:ALA:C     | 2.59                     | 0.43              |
| 3:N:973:GLN:O     | 3:N:977:ALA:HB2   | 2.18                     | 0.43              |
| 3:N:1009:LYS:O    | 3:N:1012:GLU:HB3  | 2.19                     | 0.43              |
| 6:H:7:G:C2'       | 6:H:8:G:C5'       | 2.96                     | 0.43              |
| 7:Z:1:DG:C4       | 7:Z:2:DT:C7       | 3.02                     | 0.43              |
| 1:A:78:ILE:O      | 1:A:82:LEU:HG     | 2.17                     | 0.43              |
| 1:A:206:THR:HG22  | 1:A:209:GLU:H     | 1.82                     | 0.43              |
| 1:A:213:GLN:O     | 1:A:217:ILE:HG13  | 2.18                     | 0.43              |
| 1:B:64:GLU:O      | 1:B:64:GLU:HG2    | 2.19                     | 0.43              |
| 2:C:92:ALA:CB     | 2:C:120:LEU:HD21  | 2.49                     | 0.43              |
| 2:C:143:SER:HB2   | 2:C:276:LYS:CE    | 2.44                     | 0.43              |
| 2:C:344:PHE:CZ    | 2:C:348:LEU:HD11  | 2.53                     | 0.43              |
| 2:C:349:ALA:O     | 2:C:353:ARG:HB2   | 2.19                     | 0.43              |
| 2:C:462:ASP:HB3   | 2:C:468:ARG:CZ    | 2.48                     | 0.43              |
| 2:C:943:VAL:HG22  | 2:C:986:PRO:HD3   | 2.00                     | 0.43              |
| 2:C:1038:TRP:CH2  | 3:D:1096:ARG:HA   | 2.53                     | 0.43              |
| 2:C:1046:ALA:HA   | 3:D:1472:ILE:HG13 | 2.01                     | 0.43              |
| 2:C:1096:ALA:HB2  | 3:D:101:His:CD2   | 2.53                     | 0.43              |
| 3:D:119:SER:C     | 3:D:121:THR:H     | 2.27                     | 0.43              |
| 3:D:530:VAL:O     | 6:H:4:G:C5'       | 2.59                     | 0.43              |
| 3:D:686:GLU:HA    | 3:D:689:ASP:OD2   | 2.18                     | 0.43              |
| 3:D:925:GLU:O     | 3:D:928:ALA:HB3   | 2.18                     | 0.43              |
| 3:D:1223:ILE:O    | 3:D:1226:ALA:N    | 2.52                     | 0.43              |
| 3:D:1468:LEU:CD2  | 3:D:1470:ARG:HG3  | 2.48                     | 0.43              |
| 4:E:85:LEU:HD23   | 4:E:85:LEU:O      | 2.19                     | 0.43              |
| 1:K:180:GLN:HA    | 2:M:937:ASP:OD1   | 2.19                     | 0.43              |
| 1:K:195:LEU:HD12  | 1:K:196:THR:N     | 2.34                     | 0.43              |
| 1:K:198:ARG:HD3   | 1:K:200:TRP:CH2   | 2.54                     | 0.43              |
| 1:L:123:MET:HE2   | 1:L:204:SER:HA    | 2.00                     | 0.43              |
| 2:M:56:GLU:OE2    | 2:M:59:LYS:HD2    | 2.18                     | 0.43              |
| 2:M:537:LYS:HG3   | 2:M:905:ILE:HG12  | 2.01                     | 0.43              |
| 2:M:677:MET:HB3   | 2:M:987:ILE:CG2   | 2.47                     | 0.43              |
| 2:M:996:LYS:C     | 2:M:997:LEU:HD22  | 2.43                     | 0.43              |
| 3:N:17:LYS:HG2    | 3:N:21:TRP:CE2    | 2.53                     | 0.43              |
| 3:N:118:LEU:O     | 3:N:120:ALA:N     | 2.51                     | 0.43              |
| 3:N:163:TYR:HE1   | 3:N:165:LYS:HA    | 1.81                     | 0.43              |
| 3:N:806:PHE:O     | 3:N:807:ALA:C     | 2.62                     | 0.43              |
| 3:N:1256:LEU:N    | 3:N:1257:PRO:CD   | 2.82                     | 0.43              |
| 3:N:1394:VAL:HG12 | 3:N:1397:LYS:H    | 1.83                     | 0.43              |
| 1:A:86:VAL:HG13   | 1:A:86:VAL:O      | 2.19                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:42:ARG:HG2   | 1:B:42:ARG:HH11   | 1.84                     | 0.43              |
| 1:B:73:GLU:HB3   | 1:B:77:GLU:HG3    | 2.00                     | 0.43              |
| 1:B:124:ASN:ND2  | 1:B:127:LEU:HB2   | 2.34                     | 0.43              |
| 1:B:173:PRO:HB3  | 1:B:204:SER:HB3   | 2.00                     | 0.43              |
| 1:B:198:ARG:NH2  | 3:D:888:GLU:OE2   | 2.52                     | 0.43              |
| 2:C:399:ASN:O    | 2:C:399:ASN:CG    | 2.61                     | 0.43              |
| 2:C:404:LEU:HD13 | 2:C:591:SER:HB2   | 2.00                     | 0.43              |
| 2:C:725:ASP:HB3  | 2:C:783:ARG:NH2   | 2.34                     | 0.43              |
| 2:C:878:SER:HB3  | 3:D:1029:ARG:HD2  | 2.00                     | 0.43              |
| 2:C:1034:GLU:O   | 2:C:1035:MET:C    | 2.62                     | 0.43              |
| 2:C:1040:LEU:HB3 | 2:C:1049:LEU:HD13 | 2.00                     | 0.43              |
| 3:D:8:VAL:O      | 3:D:1457:ASP:N    | 2.35                     | 0.43              |
| 3:D:522:PRO:N    | 3:D:525:ARG:NH1   | 2.67                     | 0.43              |
| 3:D:671:LYS:HE2  | 3:D:671:LYS:HB3   | 1.59                     | 0.43              |
| 3:D:749:VAL:HA   | 3:D:750:PRO:HD3   | 1.87                     | 0.43              |
| 3:D:1000:THR:O   | 3:D:1003:VAL:HG12 | 2.19                     | 0.43              |
| 3:D:1336:LEU:HB2 | 3:D:1344:VAL:HG21 | 2.01                     | 0.43              |
| 4:E:54:LEU:CD2   | 4:E:63:TRP:HE1    | 2.24                     | 0.43              |
| 1:L:149:GLY:O    | 1:L:171:PHE:HB2   | 2.19                     | 0.43              |
| 2:M:115:LEU:HD22 | 2:M:373:VAL:CG1   | 2.49                     | 0.43              |
| 2:M:710:ILE:HB   | 2:M:790:LEU:HD22  | 2.01                     | 0.43              |
| 2:M:843:HIS:ND1  | 2:M:884:GLN:HB3   | 2.32                     | 0.43              |
| 2:M:906:PHE:CE2  | 3:N:1067:VAL:HA   | 2.54                     | 0.43              |
| 3:N:15:PRO:CA    | 3:N:18:ILE:HG12   | 2.47                     | 0.43              |
| 3:N:111:LYS:HZ1  | 3:N:1449:GLU:HG3  | 1.82                     | 0.43              |
| 3:N:554:LEU:O    | 3:N:555:LYS:C     | 2.61                     | 0.43              |
| 3:N:754:PHE:CG   | 4:O:24:ALA:HB1    | 2.54                     | 0.43              |
| 3:N:1166:LEU:H   | 3:N:1166:LEU:CD2  | 2.18                     | 0.43              |
| 6:Y:6:C:N4       | 6:Y:7:G:O6        | 2.51                     | 0.43              |
| 1:A:13:VAL:CG1   | 1:A:14:ARG:H      | 2.30                     | 0.43              |
| 1:A:46:SER:HB3   | 2:C:856:GLU:CD    | 2.43                     | 0.43              |
| 1:A:48:ILE:CG2   | 1:A:173:PRO:HD2   | 2.48                     | 0.43              |
| 1:A:135:GLY:O    | 1:A:137:ARG:HG3   | 2.19                     | 0.43              |
| 1:A:152:PRO:CB   | 1:A:154:GLU:OE1   | 2.61                     | 0.43              |
| 1:A:186:LEU:O    | 1:A:188:GLN:N     | 2.52                     | 0.43              |
| 1:A:223:THR:C    | 1:A:225:PHE:N     | 2.76                     | 0.43              |
| 2:C:68:PHE:O     | 2:C:69:LEU:HD23   | 2.19                     | 0.43              |
| 2:C:358:ARG:NE   | 2:C:371:LYS:O     | 2.52                     | 0.43              |
| 2:C:583:LEU:HD12 | 2:C:583:LEU:N     | 2.34                     | 0.43              |
| 2:C:661:SER:HA   | 2:C:665:PHE:O     | 2.19                     | 0.43              |
| 2:C:976:ASP:C    | 2:C:978:ARG:H     | 2.26                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:7:LYS:HE2     | 3:D:1458:GLU:OE2 | 2.18                     | 0.43              |
| 3:D:760:ARG:NH1   | 4:E:62:THR:HG23  | 2.34                     | 0.43              |
| 3:D:949:ILE:HD11  | 3:D:1023:MET:CE  | 2.48                     | 0.43              |
| 3:D:1109:GLU:HG2  | 3:D:1201:CYS:C   | 2.44                     | 0.43              |
| 1:K:55:SER:N      | 1:K:143:ARG:HB3  | 2.34                     | 0.43              |
| 1:L:39:PRO:O      | 1:L:40:LEU:C     | 2.61                     | 0.43              |
| 1:L:73:GLU:H      | 1:L:73:GLU:HG2   | 1.52                     | 0.43              |
| 1:L:221:HIS:HA    | 1:L:224:TYR:CD2  | 2.53                     | 0.43              |
| 2:M:68:PHE:O      | 2:M:69:LEU:HD23  | 2.17                     | 0.43              |
| 2:M:326:ASP:HB3   | 2:M:431:HIS:CG   | 2.52                     | 0.43              |
| 2:M:349:ALA:O     | 2:M:353:ARG:HB2  | 2.18                     | 0.43              |
| 2:M:395:LYS:CG    | 2:M:397:GLU:HG3  | 2.49                     | 0.43              |
| 2:M:436:GLY:O     | 2:M:456:ALA:HB3  | 2.18                     | 0.43              |
| 2:M:524:VAL:CG1   | 2:M:525:SER:N    | 2.80                     | 0.43              |
| 2:M:686:ASP:HB3   | 2:M:846:LYS:O    | 2.19                     | 0.43              |
| 2:M:723:THR:CG2   | 2:M:725:ASP:HB2  | 2.48                     | 0.43              |
| 2:M:939:ARG:HG3   | 2:M:975:TYR:HE2  | 1.84                     | 0.43              |
| 3:N:55:ASP:HB3    | 3:N:82:LYS:HE2   | 2.01                     | 0.43              |
| 3:N:87:ARG:HB3    | 3:N:523:ASP:CB   | 2.48                     | 0.43              |
| 3:N:520:LEU:HG    | 3:N:521:PRO:CD   | 2.48                     | 0.43              |
| 3:N:789:LEU:CD1   | 3:N:934:LEU:HD22 | 2.49                     | 0.43              |
| 3:N:953:ASP:OD1   | 3:N:1019:PRO:HG2 | 2.19                     | 0.43              |
| 3:N:1019:PRO:O    | 3:N:1023:MET:HE3 | 2.19                     | 0.43              |
| 3:N:1191:PRO:HA   | 3:N:1194:CYS:HB2 | 2.00                     | 0.43              |
| 3:N:1200:VAL:HG13 | 3:N:1204:CYS:CB  | 2.41                     | 0.43              |
| 3:N:1205:TYR:CE1  | 3:N:1366:LYS:HD3 | 2.54                     | 0.43              |
| 3:N:1382:THR:CG2  | 3:N:1418:LYS:HE3 | 2.47                     | 0.43              |
| 4:O:33:HIS:CE1    | 4:O:89:MET:HG2   | 2.53                     | 0.43              |
| 5:G:3:DC:H6       | 5:G:3:DC:P       | 2.42                     | 0.43              |
| 5:G:7:DA:H8       | 5:G:7:DA:P       | 2.42                     | 0.43              |
| 7:I:17:DA:H8      | 7:I:17:DA:P      | 2.42                     | 0.43              |
| 1:A:78:ILE:C      | 1:A:80:LEU:N     | 2.75                     | 0.43              |
| 1:B:172:SER:HA    | 1:B:173:PRO:HD3  | 1.74                     | 0.43              |
| 2:C:205:GLU:H     | 2:C:205:GLU:HG3  | 1.60                     | 0.43              |
| 2:C:250:ARG:O     | 2:C:251:ASP:C    | 2.61                     | 0.43              |
| 2:C:398:THR:HB    | 2:C:399:ASN:ND2  | 2.33                     | 0.43              |
| 2:C:409:ARG:HA    | 2:C:454:SER:CA   | 2.33                     | 0.43              |
| 2:C:749:VAL:HG23  | 2:C:749:VAL:O    | 2.19                     | 0.43              |
| 2:C:1092:LEU:O    | 2:C:1095:LEU:O   | 2.37                     | 0.43              |
| 2:C:1098:ASP:HB2  | 3:D:21:TRP:HZ2   | 1.83                     | 0.43              |
| 3:D:513:ILE:HD12  | 3:D:513:ILE:O    | 2.18                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:630:VAL:O     | 3:D:726:ILE:N    | 2.46                     | 0.43              |
| 3:D:630:VAL:CG1   | 3:D:631:ILE:N    | 2.82                     | 0.43              |
| 3:D:705:ALA:HB2   | 6:H:14:G:H21     | 1.61                     | 0.43              |
| 3:D:709:HIS:HA    | 3:D:1227:GLN:CB  | 2.48                     | 0.43              |
| 3:D:731:LEU:HD22  | 3:D:780:LYS:O    | 2.19                     | 0.43              |
| 3:D:970:LYS:O     | 3:D:974:ILE:HG13 | 2.19                     | 0.43              |
| 3:D:1031:ASN:HB2  | 3:D:1034:GLN:HB3 | 2.01                     | 0.43              |
| 3:D:1191:PRO:C    | 3:D:1193:THR:N   | 2.75                     | 0.43              |
| 3:D:1200:VAL:HG22 | 3:D:1373:ARG:NH1 | 2.31                     | 0.43              |
| 3:D:1363:LEU:HD23 | 3:D:1363:LEU:H   | 1.82                     | 0.43              |
| 1:L:76:VAL:HA     | 1:L:79:ILE:HG12  | 2.01                     | 0.43              |
| 2:M:113:VAL:CG1   | 2:M:115:LEU:HD23 | 2.49                     | 0.43              |
| 2:M:195:LEU:O     | 2:M:199:VAL:HG23 | 2.19                     | 0.43              |
| 2:M:677:MET:HE3   | 2:M:678:PRO:C    | 2.44                     | 0.43              |
| 2:M:677:MET:HE2   | 2:M:870:ILE:HG21 | 2.00                     | 0.43              |
| 2:M:718:GLY:HA3   | 2:M:761:PHE:CE1  | 2.54                     | 0.43              |
| 2:M:724:ARG:NH2   | 2:M:734:LEU:O    | 2.52                     | 0.43              |
| 2:M:987:ILE:HA    | 3:N:948:THR:OG1  | 2.18                     | 0.43              |
| 2:M:1054:THR:C    | 2:M:1056:LYS:N   | 2.76                     | 0.43              |
| 3:N:155:ASP:O     | 3:N:159:ARG:HB2  | 2.19                     | 0.43              |
| 3:N:434:ARG:HH12  | 3:N:436:GLU:HG3  | 1.84                     | 0.43              |
| 3:N:581:LEU:O     | 3:N:603:LEU:HG   | 2.19                     | 0.43              |
| 3:N:610:LYS:HA    | 3:N:615:ARG:CD   | 2.49                     | 0.43              |
| 3:N:618:LEU:C     | 3:N:619:LEU:HD23 | 2.44                     | 0.43              |
| 3:N:645:PRO:HB3   | 3:N:723:GLY:O    | 2.19                     | 0.43              |
| 3:N:657:LEU:HD13  | 3:N:691:LEU:HD13 | 2.01                     | 0.43              |
| 3:N:699:VAL:HG22  | 3:N:760:ARG:HB3  | 1.99                     | 0.43              |
| 3:N:704:ARG:HG3   | 3:N:705:ALA:N    | 2.34                     | 0.43              |
| 3:N:811:GLU:O     | 3:N:815:ALA:HB3  | 2.19                     | 0.43              |
| 3:N:950:GLY:H     | 3:N:953:ASP:HB2  | 1.82                     | 0.43              |
| 3:N:1107:VAL:HG23 | 3:N:1219:GLU:O   | 2.17                     | 0.43              |
| 3:N:1280:VAL:O    | 3:N:1294:VAL:HA  | 2.19                     | 0.43              |
| 3:N:1348:LEU:HD13 | 3:N:1348:LEU:N   | 2.34                     | 0.43              |
| 3:N:1472:ILE:C    | 3:N:1474:ALA:H   | 2.27                     | 0.43              |
| 4:O:32:ARG:HB2    | 4:O:32:ARG:CZ    | 2.49                     | 0.43              |
| 1:A:57:TYR:CZ     | 1:A:161:ARG:HD2  | 2.52                     | 0.43              |
| 2:C:115:LEU:H     | 2:C:115:LEU:HG   | 1.60                     | 0.43              |
| 2:C:288:ARG:HG3   | 2:C:288:ARG:NH1  | 2.33                     | 0.43              |
| 2:C:341:THR:O     | 2:C:345:ARG:HG2  | 2.19                     | 0.43              |
| 2:C:444:PRO:CB    | 6:H:12:U:OP1     | 2.64                     | 0.43              |
| 2:C:1038:TRP:O    | 2:C:1042:ALA:N   | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:7:LYS:HE2     | 3:D:1458:GLU:CD   | 2.44                     | 0.43              |
| 3:D:465:LEU:HD22  | 3:D:510:GLU:HA    | 1.99                     | 0.43              |
| 3:D:615:ARG:NH1   | 3:D:1096:ARG:NE   | 2.52                     | 0.43              |
| 3:D:771:SER:HA    | 3:D:772:PRO:HD3   | 1.90                     | 0.43              |
| 3:D:1084:THR:HA   | 3:D:1087:ARG:CG   | 2.48                     | 0.43              |
| 3:D:1106:VAL:C    | 3:D:1108:ARG:HD3  | 2.43                     | 0.43              |
| 3:D:1379:VAL:C    | 3:D:1420:LEU:HD12 | 2.44                     | 0.43              |
| 3:D:1442:ASN:O    | 3:D:1443:THR:OG1  | 2.33                     | 0.43              |
| 3:D:1442:ASN:O    | 3:D:1443:THR:CB   | 2.66                     | 0.43              |
| 4:E:36:LYS:HB2    | 4:E:95:VAL:HG22   | 2.01                     | 0.43              |
| 2:M:6:PHE:CD1     | 2:M:6:PHE:N       | 2.86                     | 0.43              |
| 2:M:217:LEU:HD11  | 2:M:314:THR:OG1   | 2.19                     | 0.43              |
| 2:M:537:LYS:CD    | 2:M:905:ILE:HD13  | 2.38                     | 0.43              |
| 2:M:610:ARG:HH11  | 2:M:610:ARG:HG3   | 1.82                     | 0.43              |
| 2:M:762:LYS:HG3   | 2:M:786:LYS:CE    | 2.49                     | 0.43              |
| 2:M:966:LEU:HD12  | 2:M:966:LEU:HA    | 1.84                     | 0.43              |
| 2:M:1055:LEU:HD23 | 2:M:1062:GLY:HA3  | 2.01                     | 0.43              |
| 2:M:1118:LYS:O    | 2:M:1119:ARG:O    | 2.37                     | 0.43              |
| 3:N:581:LEU:HD23  | 3:N:581:LEU:N     | 2.22                     | 0.43              |
| 3:N:1149:LEU:HD13 | 3:N:1151:ARG:O    | 2.19                     | 0.43              |
| 3:N:1330:ILE:HB   | 3:N:1347:TYR:CZ   | 2.53                     | 0.43              |
| 1:A:9:PRO:HG2     | 1:B:224:TYR:CG    | 2.54                     | 0.42              |
| 1:A:81:ASN:O      | 1:A:84:GLU:HB3    | 2.19                     | 0.42              |
| 2:C:48:PHE:CB     | 2:C:52:PHE:HD2    | 2.31                     | 0.42              |
| 2:C:207:LEU:HD23  | 2:C:207:LEU:C     | 2.44                     | 0.42              |
| 2:C:408:ARG:NH1   | 2:C:542:VAL:HG23  | 2.34                     | 0.42              |
| 2:C:606:VAL:CG2   | 2:C:645:VAL:HG22  | 2.49                     | 0.42              |
| 2:C:1031:ARG:HA   | 3:D:621:LYS:O     | 2.19                     | 0.42              |
| 2:C:1102:LEU:HA   | 2:C:1107:ASN:O    | 2.18                     | 0.42              |
| 3:D:122:GLU:HG2   | 3:D:126:VAL:HG23  | 2.01                     | 0.42              |
| 3:D:133:ILE:HG13  | 3:D:456:MET:HE2   | 1.99                     | 0.42              |
| 3:D:502:PHE:CD2   | 3:D:509:PRO:HD3   | 2.54                     | 0.42              |
| 3:D:582:LEU:HD23  | 3:D:603:LEU:HD12  | 1.99                     | 0.42              |
| 3:D:1100:ASP:CG   | 3:D:1463:LYS:HZ2  | 2.27                     | 0.42              |
| 3:D:1155:VAL:HB   | 3:D:1156:LEU:H    | 1.62                     | 0.42              |
| 3:D:1393:GLN:CB   | 3:D:1398:TRP:HZ2  | 2.32                     | 0.42              |
| 3:D:1479:ASP:OD2  | 3:D:1482:ARG:NH2  | 2.52                     | 0.42              |
| 1:K:191:ASP:CG    | 1:K:191:ASP:O     | 2.61                     | 0.42              |
| 1:L:80:LEU:C      | 1:L:82:LEU:N      | 2.75                     | 0.42              |
| 2:M:520:GLU:OE2   | 2:M:521:PRO:HD2   | 2.19                     | 0.42              |
| 2:M:578:VAL:HG13  | 2:M:671:ASN:CB    | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:1038:TRP:HA   | 2:M:1041:GLU:HG3  | 2.00                     | 0.42              |
| 3:N:104:PHE:HA    | 3:N:1448:THR:CG2  | 2.48                     | 0.42              |
| 3:N:104:PHE:CG    | 3:N:512:MET:SD    | 3.12                     | 0.42              |
| 3:N:521:PRO:HA    | 3:N:522:PRO:HD3   | 1.86                     | 0.42              |
| 3:N:625:TYR:HE2   | 3:N:655:PRO:CD    | 2.32                     | 0.42              |
| 3:N:638:LYS:HB2   | 3:N:641:GLN:CD    | 2.44                     | 0.42              |
| 3:N:639:LEU:HG    | 3:N:932:ASP:OD1   | 2.18                     | 0.42              |
| 3:N:774:SER:O     | 3:N:776:GLU:N     | 2.52                     | 0.42              |
| 3:N:972:LEU:HA    | 3:N:975:GLU:HB2   | 2.00                     | 0.42              |
| 3:N:1094:LEU:HD12 | 3:N:1094:LEU:HA   | 1.87                     | 0.42              |
| 3:N:1271:LYS:HZ3  | 3:N:1331:ASP:HB2  | 1.80                     | 0.42              |
| 4:O:25:LYS:HA     | 4:O:28:GLN:HE21   | 1.81                     | 0.42              |
| 1:A:66:SER:O      | 1:A:75:VAL:HG23   | 2.18                     | 0.42              |
| 1:A:99:LEU:HB3    | 1:A:114:PHE:CD2   | 2.54                     | 0.42              |
| 2:C:79:PRO:O      | 2:C:83:CYS:SG     | 2.67                     | 0.42              |
| 2:C:328:LEU:HD13  | 2:C:433:THR:CA    | 2.49                     | 0.42              |
| 2:C:345:ARG:CA    | 2:C:348:LEU:HD22  | 2.45                     | 0.42              |
| 2:C:368:THR:HB    | 2:C:369:PRO:CD    | 2.43                     | 0.42              |
| 2:C:422:ARG:HB3   | 7:I:1:DG:C6       | 2.54                     | 0.42              |
| 2:C:460:ARG:HH12  | 2:C:462:ASP:HA    | 1.84                     | 0.42              |
| 2:C:697:ARG:O     | 2:C:697:ARG:HG3   | 2.18                     | 0.42              |
| 2:C:796:GLU:CB    | 2:C:1004:LYS:NZ   | 2.75                     | 0.42              |
| 2:C:1046:ALA:HB3  | 3:D:1476:THR:OG1  | 2.19                     | 0.42              |
| 3:D:549:ASN:CB    | 3:D:550:ARG:HH21  | 2.31                     | 0.42              |
| 3:D:618:LEU:HD13  | 3:D:1439:SER:CB   | 2.43                     | 0.42              |
| 3:D:904:VAL:HA    | 3:D:905:PRO:HD3   | 1.89                     | 0.42              |
| 3:D:916:TYR:OH    | 3:D:1145:TYR:HE2  | 2.02                     | 0.42              |
| 3:D:1026:SER:C    | 3:D:1028:ALA:N    | 2.75                     | 0.42              |
| 3:D:1129:THR:HG23 | 3:D:1130:ARG:H    | 1.81                     | 0.42              |
| 3:D:1396:GLU:O    | 3:D:1399:ASP:HB2  | 2.19                     | 0.42              |
| 1:L:83:LYS:O      | 1:L:170:VAL:HG21  | 2.19                     | 0.42              |
| 1:L:108:GLU:HB3   | 1:L:128:HIS:CE1   | 2.54                     | 0.42              |
| 1:L:206:THR:HG23  | 1:L:208:LEU:N     | 2.33                     | 0.42              |
| 2:M:25:SER:OG     | 2:M:335:THR:HB    | 2.19                     | 0.42              |
| 2:M:141:HIS:O     | 2:M:331:ARG:CA    | 2.66                     | 0.42              |
| 2:M:459:ALA:HB1   | 2:M:467:ILE:CG2   | 2.49                     | 0.42              |
| 2:M:493:ARG:CZ    | 2:M:494:TYR:OH    | 2.68                     | 0.42              |
| 2:M:520:GLU:O     | 2:M:522:VAL:HG23  | 2.18                     | 0.42              |
| 2:M:775:ARG:O     | 2:M:779:GLY:C     | 2.62                     | 0.42              |
| 2:M:1101:THR:O    | 2:M:1102:LEU:HD12 | 2.18                     | 0.42              |
| 3:N:66:GLN:O      | 3:N:69:GLU:N      | 2.51                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:525:ARG:H     | 3:N:525:ARG:CD    | 2.31                     | 0.42              |
| 3:N:697:GLY:O     | 3:N:698:LYS:C     | 2.62                     | 0.42              |
| 3:N:764:LEU:HB3   | 3:N:767:HIS:CE1   | 2.54                     | 0.42              |
| 3:N:864:VAL:CG1   | 3:N:865:THR:H     | 2.21                     | 0.42              |
| 3:N:1082:ALA:O    | 3:N:1085:ALA:HB3  | 2.19                     | 0.42              |
| 3:N:1472:ILE:C    | 3:N:1474:ALA:N    | 2.75                     | 0.42              |
| 6:Y:8:G:H3'       | 6:Y:8:G:H8        | 1.80                     | 0.42              |
| 1:B:101:LEU:HB2   | 1:B:114:PHE:CG    | 2.53                     | 0.42              |
| 2:C:72:ARG:NE     | 2:C:95:TYR:HE1    | 2.17                     | 0.42              |
| 2:C:701:THR:HG21  | 2:C:830:LYS:CD    | 2.49                     | 0.42              |
| 3:D:54:LYS:CG     | 3:D:57:GLU:HB3    | 2.49                     | 0.42              |
| 3:D:520:LEU:O     | 3:D:521:PRO:C     | 2.60                     | 0.42              |
| 3:D:662:GLU:HA    | 3:D:667:ALA:O     | 2.19                     | 0.42              |
| 3:D:731:LEU:CD2   | 3:D:782:SER:N     | 2.83                     | 0.42              |
| 3:D:924:MET:CG    | 4:E:6:ILE:HG21    | 2.50                     | 0.42              |
| 3:D:1103:HIS:O    | 3:D:1105:ILE:N    | 2.52                     | 0.42              |
| 3:D:1106:VAL:HG12 | 3:D:1107:VAL:H    | 1.83                     | 0.42              |
| 3:D:1191:PRO:O    | 3:D:1193:THR:N    | 2.52                     | 0.42              |
| 3:D:1225:ALA:O    | 3:D:1229:ILE:HG13 | 2.19                     | 0.42              |
| 3:D:1381:VAL:HB   | 3:D:1389:LEU:C    | 2.43                     | 0.42              |
| 3:D:1442:ASN:O    | 3:D:1443:THR:CG2  | 2.67                     | 0.42              |
| 4:E:68:LEU:HD13   | 4:E:68:LEU:N      | 2.34                     | 0.42              |
| 1:K:35:THR:HG23   | 1:L:42:ARG:HB2    | 2.01                     | 0.42              |
| 1:K:78:ILE:C      | 1:K:80:LEU:N      | 2.76                     | 0.42              |
| 1:K:117:VAL:HB    | 1:K:120:VAL:HG12  | 2.01                     | 0.42              |
| 1:L:75:VAL:O      | 1:L:79:ILE:HG23   | 2.19                     | 0.42              |
| 2:M:15:LEU:HD12   | 2:M:15:LEU:N      | 2.34                     | 0.42              |
| 2:M:56:GLU:HB3    | 2:M:359:MET:SD    | 2.59                     | 0.42              |
| 2:M:72:ARG:HD2    | 2:M:72:ARG:C      | 2.44                     | 0.42              |
| 2:M:369:PRO:O     | 2:M:373:VAL:HG23  | 2.19                     | 0.42              |
| 2:M:737:LEU:HD21  | 2:M:741:GLY:C     | 2.44                     | 0.42              |
| 2:M:922:PHE:HB3   | 2:M:964:LYS:HZ2   | 1.82                     | 0.42              |
| 2:M:973:VAL:C     | 2:M:974:LEU:HD12  | 2.42                     | 0.42              |
| 2:M:1090:LYS:HA   | 2:M:1090:LYS:HD3  | 1.84                     | 0.42              |
| 3:N:204:LEU:HB2   | 3:N:394:LEU:CD2   | 2.48                     | 0.42              |
| 3:N:564:GLU:OE2   | 3:N:567:ILE:HD12  | 2.19                     | 0.42              |
| 3:N:736:PHE:O     | 3:N:738:ALA:N     | 2.53                     | 0.42              |
| 3:N:829:VAL:O     | 3:N:831:GLY:N     | 2.48                     | 0.42              |
| 3:N:960:LYS:O     | 3:N:960:LYS:HG2   | 2.20                     | 0.42              |
| 3:N:1442:ASN:O    | 3:N:1446:VAL:HG21 | 2.13                     | 0.42              |
| 1:A:88:ARG:HH11   | 1:A:88:ARG:CG     | 2.30                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:91:ASN:HA    | 1:A:92:PRO:HD3   | 1.92                     | 0.42              |
| 1:B:24:VAL:HG12  | 1:B:26:GLU:OE2   | 2.19                     | 0.42              |
| 2:C:185:LYS:HB3  | 2:C:188:LYS:O    | 2.19                     | 0.42              |
| 2:C:198:ARG:HD2  | 2:C:204:GLN:OE1  | 2.19                     | 0.42              |
| 2:C:293:PHE:CD1  | 2:C:293:PHE:C    | 2.95                     | 0.42              |
| 2:C:412:ALA:CB   | 2:C:451:LEU:HB3  | 2.50                     | 0.42              |
| 2:C:437:ARG:NH1  | 2:C:491:GLU:OE2  | 2.53                     | 0.42              |
| 2:C:459:ALA:HB1  | 2:C:467:ILE:HG23 | 1.98                     | 0.42              |
| 2:C:581:THR:C    | 2:C:902:ILE:HG23 | 2.44                     | 0.42              |
| 2:C:674:VAL:HG11 | 2:C:992:MET:HB3  | 2.02                     | 0.42              |
| 2:C:683:ASN:CA   | 2:C:687:ALA:HB3  | 2.48                     | 0.42              |
| 2:C:1056:LYS:HZ2 | 3:D:749:VAL:H    | 1.67                     | 0.42              |
| 3:D:500:ARG:HD2  | 3:D:500:ARG:HA   | 1.87                     | 0.42              |
| 3:D:520:LEU:HD21 | 3:D:524:LEU:HB3  | 2.01                     | 0.42              |
| 3:D:800:LYS:HG3  | 3:D:829:VAL:CG1  | 2.49                     | 0.42              |
| 3:D:950:GLY:H    | 3:D:953:ASP:CG   | 2.28                     | 0.42              |
| 3:D:1011:PHE:CG  | 3:D:1021:TYR:HB2 | 2.54                     | 0.42              |
| 1:K:64:GLU:O     | 1:K:75:VAL:HB    | 2.18                     | 0.42              |
| 1:L:73:GLU:HG3   | 1:L:130:ALA:HB2  | 2.00                     | 0.42              |
| 1:L:90:LEU:HG    | 1:L:91:ASN:ND2   | 2.34                     | 0.42              |
| 1:L:176:ARG:HG3  | 1:L:200:TRP:CE3  | 2.55                     | 0.42              |
| 2:M:43:GLY:O     | 2:M:47:ALA:N     | 2.37                     | 0.42              |
| 2:M:185:LYS:HB3  | 2:M:188:LYS:O    | 2.19                     | 0.42              |
| 2:M:269:LEU:HG   | 2:M:288:ARG:CA   | 2.47                     | 0.42              |
| 2:M:400:PRO:O    | 2:M:403:SER:OG   | 2.30                     | 0.42              |
| 2:M:603:VAL:HG11 | 2:M:645:VAL:HA   | 2.01                     | 0.42              |
| 2:M:931:GLY:C    | 2:M:933:GLY:H    | 2.28                     | 0.42              |
| 2:M:1081:VAL:CG1 | 2:M:1086:ARG:HG2 | 2.50                     | 0.42              |
| 3:N:28:LYS:HB2   | 3:N:41:ARG:CD    | 2.48                     | 0.42              |
| 3:N:50:PHE:CD2   | 3:N:522:PRO:HD3  | 2.54                     | 0.42              |
| 3:N:396:VAL:O    | 3:N:398:ALA:N    | 2.52                     | 0.42              |
| 3:N:676:MET:O    | 3:N:676:MET:SD   | 2.77                     | 0.42              |
| 3:N:732:VAL:O    | 3:N:736:PHE:HD1  | 2.01                     | 0.42              |
| 3:N:972:LEU:HG   | 3:N:976:GLN:OE1  | 2.20                     | 0.42              |
| 3:N:1112:CYS:O   | 3:N:1189:ARG:NH2 | 2.51                     | 0.42              |
| 3:N:1380:GLU:HB2 | 3:N:1420:LEU:CD1 | 2.50                     | 0.42              |
| 7:Z:5:DC:H2"     | 7:Z:6:DT:H71     | 2.01                     | 0.42              |
| 1:A:26:GLU:CB    | 1:A:27:PRO:HA    | 2.49                     | 0.42              |
| 1:B:3:ASP:HB3    | 1:B:4:SER:H      | 1.67                     | 0.42              |
| 1:B:39:PRO:O     | 1:B:40:LEU:C     | 2.62                     | 0.42              |
| 2:C:22:GLN:O     | 2:C:121:MET:HE1  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:394:PHE:O    | 2:C:406:HIS:CE1   | 2.72                     | 0.42              |
| 2:C:601:GLY:HA3  | 2:C:615:TYR:HA    | 2.01                     | 0.42              |
| 2:C:630:ARG:HD3  | 2:C:705:ILE:HG21  | 1.98                     | 0.42              |
| 2:C:686:ASP:HB2  | 3:D:740:PHE:C     | 2.45                     | 0.42              |
| 2:C:700:TYR:O    | 2:C:833:LEU:HB2   | 2.19                     | 0.42              |
| 2:C:841:ASN:HD22 | 2:C:841:ASN:N     | 2.17                     | 0.42              |
| 2:C:1081:VAL:CB  | 2:C:1086:ARG:HH21 | 2.32                     | 0.42              |
| 2:C:1089:VAL:O   | 2:C:1092:LEU:CB   | 2.67                     | 0.42              |
| 3:D:84:ILE:CG1   | 3:D:85:VAL:N      | 2.81                     | 0.42              |
| 3:D:105:VAL:HA   | 3:D:112:ILE:HG22  | 1.99                     | 0.42              |
| 3:D:549:ASN:O    | 3:D:553:ARG:CB    | 2.68                     | 0.42              |
| 3:D:618:LEU:HD11 | 3:D:1463:LYS:HE2  | 2.01                     | 0.42              |
| 3:D:657:LEU:O    | 3:D:661:MET:HG2   | 2.19                     | 0.42              |
| 3:D:770:LEU:HA   | 3:D:777:PRO:HA    | 2.00                     | 0.42              |
| 4:E:9:LEU:HD21   | 4:E:69:LEU:HD12   | 2.00                     | 0.42              |
| 4:E:27:ALA:HB1   | 4:E:60:ALA:HB1    | 2.01                     | 0.42              |
| 4:E:92:LEU:O     | 4:E:94:PRO:HD3    | 2.19                     | 0.42              |
| 1:K:38:ASN:N     | 1:K:39:PRO:CD     | 2.83                     | 0.42              |
| 1:K:54:THR:HB    | 1:K:143:ARG:HG2   | 2.00                     | 0.42              |
| 1:K:99:LEU:N     | 1:K:99:LEU:CD1    | 2.82                     | 0.42              |
| 1:L:52:ALA:HB1   | 1:L:170:VAL:N     | 2.27                     | 0.42              |
| 2:M:118:ILE:HA   | 2:M:119:PRO:HD3   | 1.90                     | 0.42              |
| 2:M:191:PHE:CE2  | 2:M:238:LEU:HD11  | 2.54                     | 0.42              |
| 2:M:394:PHE:CE1  | 2:M:632:ASN:OD1   | 2.73                     | 0.42              |
| 2:M:606:VAL:HG21 | 2:M:645:VAL:HG22  | 2.01                     | 0.42              |
| 2:M:677:MET:O    | 2:M:870:ILE:HG22  | 2.19                     | 0.42              |
| 2:M:987:ILE:HG23 | 3:N:948:THR:CG2   | 2.38                     | 0.42              |
| 3:N:52:PRO:CG    | 3:N:80:VAL:HG13   | 2.50                     | 0.42              |
| 3:N:484:PRO:HB3  | 3:N:488:ARG:HH21  | 1.80                     | 0.42              |
| 3:N:521:PRO:O    | 3:N:524:LEU:HB2   | 2.19                     | 0.42              |
| 3:N:1196:THR:O   | 3:N:1197:ARG:C    | 2.62                     | 0.42              |
| 3:N:1351:GLU:OE1 | 3:N:1351:GLU:HA   | 2.20                     | 0.42              |
| 5:X:27:DC:H3'    | 5:X:27:DC:OP1     | 2.19                     | 0.42              |
| 6:Y:11:C:H2'     | 6:Y:12:U:O4'      | 2.20                     | 0.42              |
| 1:A:58:ILE:HB    | 1:A:61:VAL:HB     | 2.00                     | 0.42              |
| 1:B:9:PRO:HB2    | 1:B:25:LEU:HD11   | 2.00                     | 0.42              |
| 1:B:52:ALA:CB    | 1:B:170:VAL:C     | 2.89                     | 0.42              |
| 1:B:154:GLU:O    | 1:B:154:GLU:HG2   | 2.19                     | 0.42              |
| 2:C:49:ARG:O     | 2:C:53:PRO:CD     | 2.68                     | 0.42              |
| 2:C:182:VAL:HG11 | 2:C:193:LEU:HD22  | 2.02                     | 0.42              |
| 2:C:202:TYR:CZ   | 2:C:304:LEU:HD13  | 2.54                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:359:MET:HE2  | 2:C:359:MET:O     | 2.19                     | 0.42              |
| 2:C:408:ARG:NH1  | 2:C:542:VAL:CG2   | 2.82                     | 0.42              |
| 2:C:658:GLY:N    | 2:C:661:SER:OG    | 2.52                     | 0.42              |
| 2:C:739:GLU:O    | 2:C:742:VAL:N     | 2.52                     | 0.42              |
| 2:C:830:LYS:O    | 2:C:831:ARG:C     | 2.61                     | 0.42              |
| 2:C:832:LYS:O    | 2:C:834:GLN:N     | 2.53                     | 0.42              |
| 2:C:1001:VAL:O   | 2:C:1001:VAL:HG12 | 2.18                     | 0.42              |
| 2:C:1035:MET:HE2 | 5:G:19:DG:H2"     | 2.01                     | 0.42              |
| 3:D:51:GLY:N     | 3:D:86:ARG:HG3    | 2.34                     | 0.42              |
| 3:D:454:ALA:O    | 3:D:455:ARG:HG3   | 2.19                     | 0.42              |
| 3:D:774:SER:O    | 3:D:776:GLU:N     | 2.53                     | 0.42              |
| 3:D:879:ARG:HH12 | 3:D:905:PRO:CD    | 2.32                     | 0.42              |
| 3:D:1095:THR:O   | 3:D:1098:LEU:HB2  | 2.19                     | 0.42              |
| 3:D:1135:ARG:HB3 | 3:D:1140:ILE:CG1  | 2.49                     | 0.42              |
| 3:D:1259:VAL:O   | 3:D:1263:PHE:HD1  | 2.02                     | 0.42              |
| 3:D:1260:ILE:C   | 3:D:1262:LEU:N    | 2.77                     | 0.42              |
| 4:E:49:GLN:HA    | 4:E:51:LEU:O      | 2.19                     | 0.42              |
| 1:K:38:ASN:HB3   | 1:K:39:PRO:HD3    | 2.00                     | 0.42              |
| 1:K:152:PRO:C    | 1:K:154:GLU:N     | 2.76                     | 0.42              |
| 1:L:94:LEU:HD11  | 1:L:119:ASP:HB2   | 2.00                     | 0.42              |
| 2:M:6:PHE:CD2    | 2:M:909:ALA:HB2   | 2.55                     | 0.42              |
| 2:M:63:GLY:O     | 2:M:65:VAL:HG23   | 2.19                     | 0.42              |
| 2:M:75:GLU:O     | 2:M:93:PRO:CD     | 2.68                     | 0.42              |
| 2:M:122:THR:C    | 2:M:124:ASP:N     | 2.76                     | 0.42              |
| 2:M:170:PRO:HG2  | 2:M:258:TYR:HE2   | 1.84                     | 0.42              |
| 2:M:518:LYS:HB3  | 2:M:518:LYS:HZ3   | 1.83                     | 0.42              |
| 2:M:553:ASP:OD1  | 2:M:843:HIS:HD2   | 2.02                     | 0.42              |
| 2:M:887:GLU:HB3  | 2:M:992:MET:CE    | 2.49                     | 0.42              |
| 2:M:1056:LYS:CD  | 3:N:623:VAL:HG13  | 2.49                     | 0.42              |
| 2:M:1105:LYS:O   | 2:M:1107:ASN:N    | 2.53                     | 0.42              |
| 3:N:540:LEU:HA   | 3:N:543:LEU:HD12  | 2.00                     | 0.42              |
| 3:N:1257:PRO:C   | 3:N:1260:ILE:HG12 | 2.44                     | 0.42              |
| 3:N:1341:PRO:HA  | 3:N:1344:VAL:HG23 | 2.01                     | 0.42              |
| 4:O:46:PRO:C     | 4:O:54:LEU:HD13   | 2.45                     | 0.42              |
| 7:Z:7:DT:H2"     | 7:Z:8:DG:OP2      | 2.18                     | 0.42              |
| 1:A:111:ALA:O    | 1:A:114:PHE:HD1   | 2.02                     | 0.42              |
| 2:C:165:LEU:HA   | 2:C:166:PRO:C     | 2.45                     | 0.42              |
| 2:C:328:LEU:CD1  | 2:C:328:LEU:H     | 2.32                     | 0.42              |
| 2:C:579:VAL:CG1  | 2:C:842:ARG:HH22  | 2.20                     | 0.42              |
| 2:C:1009:SER:HB3 | 3:D:651:GLU:O     | 2.19                     | 0.42              |
| 2:C:1033:GLY:O   | 2:C:1037:VAL:HG23 | 2.19                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:1105:LYS:O   | 2:C:1107:ASN:N    | 2.53                     | 0.42              |
| 3:D:763:MET:O    | 3:D:764:LEU:C     | 2.63                     | 0.42              |
| 3:D:771:SER:HB3  | 3:D:778:LEU:HD22  | 2.01                     | 0.42              |
| 3:D:1176:LYS:O   | 3:D:1179:GLU:HB2  | 2.19                     | 0.42              |
| 3:D:1266:ARG:O   | 3:D:1268:PRO:HD3  | 2.20                     | 0.42              |
| 3:D:1336:LEU:O   | 3:D:1340:GLY:N    | 2.50                     | 0.42              |
| 3:D:1401:GLU:OE2 | 3:D:1415:VAL:HG11 | 2.19                     | 0.42              |
| 4:E:24:ALA:O     | 4:E:28:GLN:HG3    | 2.19                     | 0.42              |
| 1:K:79:ILE:C     | 1:K:79:ILE:HD12   | 2.44                     | 0.42              |
| 1:K:80:LEU:HD23  | 1:K:80:LEU:C      | 2.45                     | 0.42              |
| 1:K:158:ILE:H    | 1:K:166:PRO:CG    | 2.32                     | 0.42              |
| 1:K:178:ALA:HB2  | 2:M:864:GLY:CA    | 2.48                     | 0.42              |
| 1:L:25:LEU:HG    | 1:L:28:LEU:HD21   | 2.01                     | 0.42              |
| 1:L:31:GLY:O     | 1:L:35:THR:OG1    | 2.36                     | 0.42              |
| 2:M:13:ILE:HA    | 2:M:14:PRO:HD3    | 1.86                     | 0.42              |
| 2:M:197:LEU:HD22 | 2:M:202:TYR:CD2   | 2.55                     | 0.42              |
| 2:M:250:ARG:O    | 2:M:251:ASP:C     | 2.62                     | 0.42              |
| 2:M:259:GLY:O    | 2:M:290:LEU:O     | 2.37                     | 0.42              |
| 2:M:408:ARG:HH21 | 2:M:455:LEU:CD1   | 2.33                     | 0.42              |
| 2:M:575:GLN:N    | 2:M:670:GLN:OE1   | 2.53                     | 0.42              |
| 2:M:683:ASN:O    | 2:M:872:ASN:CB    | 2.63                     | 0.42              |
| 2:M:853:LEU:CB   | 2:M:858:MET:HE3   | 2.50                     | 0.42              |
| 2:M:854:PRO:CB   | 2:M:856:GLU:CD    | 2.93                     | 0.42              |
| 2:M:983:ILE:O    | 2:M:984:GLU:C     | 2.62                     | 0.42              |
| 2:M:994:ILE:C    | 2:M:995:MET:HG3   | 2.45                     | 0.42              |
| 2:M:1052:MET:SD  | 2:M:1056:LYS:HD2  | 2.59                     | 0.42              |
| 2:M:1088:LEU:O   | 2:M:1091:GLU:HB2  | 2.20                     | 0.42              |
| 3:N:108:VAL:HB   | 3:N:109:PRO:CD    | 2.37                     | 0.42              |
| 3:N:689:ASP:O    | 3:N:692:GLU:HB3   | 2.19                     | 0.42              |
| 3:N:1168:MET:HG3 | 3:N:1172:HIS:CE1  | 2.54                     | 0.42              |
| 3:N:1258:ARG:NE  | 3:N:1262:LEU:HD11 | 2.33                     | 0.42              |
| 3:N:1417:TRP:CD1 | 3:N:1417:TRP:C    | 2.97                     | 0.42              |
| 3:N:1417:TRP:CD1 | 3:N:1418:LYS:N    | 2.88                     | 0.42              |
| 4:O:59:ASN:HB3   | 4:O:62:THR:OG1    | 2.20                     | 0.42              |
| 7:Z:4:DG:C4      | 7:Z:5:DC:C5       | 3.07                     | 0.42              |
| 1:A:78:ILE:O     | 1:A:81:ASN:N      | 2.52                     | 0.42              |
| 1:B:76:VAL:HA    | 1:B:79:ILE:HD11   | 2.02                     | 0.42              |
| 1:B:115:LEU:HD12 | 1:B:115:LEU:C     | 2.45                     | 0.42              |
| 2:C:260:LEU:HD21 | 2:C:293:PHE:CZ    | 2.54                     | 0.42              |
| 2:C:473:ARG:HG3  | 2:C:474:VAL:N     | 2.34                     | 0.42              |
| 2:C:693:GLU:HG2  | 2:C:697:ARG:NH2   | 2.26                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:922:PHE:HD2  | 2:C:964:LYS:HZ2   | 1.66                     | 0.42              |
| 2:C:1046:ALA:HA  | 3:D:1472:ILE:HD11 | 2.01                     | 0.42              |
| 3:D:33:ASN:O     | 3:D:36:THR:O      | 2.37                     | 0.42              |
| 3:D:107:ASP:OD2  | 3:D:1445:HIS:CD2  | 2.72                     | 0.42              |
| 3:D:117:ASP:HB2  | 3:D:495:ARG:HH12  | 1.80                     | 0.42              |
| 3:D:612:GLY:H    | 3:D:615:ARG:HB2   | 1.84                     | 0.42              |
| 3:D:644:LEU:HD12 | 3:D:645:PRO:HD2   | 2.02                     | 0.42              |
| 3:D:880:ILE:O    | 3:D:883:ALA:HB3   | 2.19                     | 0.42              |
| 3:D:951:ILE:HD12 | 3:D:1062:ARG:NE   | 2.22                     | 0.42              |
| 3:D:1377:LYS:HE2 | 3:D:1378:TYR:OH   | 2.20                     | 0.42              |
| 4:E:31:LEU:HB2   | 4:E:32:ARG:H      | 1.69                     | 0.42              |
| 2:M:172:ILE:HG23 | 2:M:184:MET:HE3   | 2.00                     | 0.42              |
| 2:M:863:ASP:OD2  | 2:M:863:ASP:C     | 2.63                     | 0.42              |
| 2:M:941:VAL:CA   | 2:M:944:LEU:HB2   | 2.48                     | 0.42              |
| 3:N:603:LEU:HA   | 3:N:603:LEU:HD23  | 1.83                     | 0.42              |
| 3:N:764:LEU:HD12 | 3:N:765:SER:H     | 1.83                     | 0.42              |
| 3:N:1231:GLU:HB3 | 3:N:1232:PRO:HD3  | 2.02                     | 0.42              |
| 5:G:12:DA:C2'    | 5:G:13:DA:OP2     | 2.67                     | 0.42              |
| 1:A:65:PHE:HE1   | 2:C:799:ILE:CG2   | 2.32                     | 0.42              |
| 1:B:104:GLU:HA   | 1:B:136:GLY:O     | 2.19                     | 0.42              |
| 2:C:50:GLU:HA    | 2:C:266:ARG:NE    | 2.27                     | 0.42              |
| 2:C:520:GLU:HA   | 2:C:521:PRO:HD3   | 1.86                     | 0.42              |
| 2:C:733:ALA:C    | 2:C:734:LEU:HD12  | 2.45                     | 0.42              |
| 2:C:768:THR:HG22 | 2:C:771:GLU:H     | 1.84                     | 0.42              |
| 2:C:768:THR:HA   | 2:C:769:PRO:HD3   | 1.88                     | 0.42              |
| 2:C:878:SER:HB3  | 3:D:1029:ARG:NH1  | 2.35                     | 0.42              |
| 2:C:1098:ASP:HB2 | 3:D:13:ALA:HB2    | 2.01                     | 0.42              |
| 3:D:528:VAL:O    | 3:D:535:PHE:CD2   | 2.72                     | 0.42              |
| 3:D:613:ARG:HA   | 3:D:613:ARG:HD3   | 1.74                     | 0.42              |
| 3:D:743:ASP:OD2  | 3:D:743:ASP:N     | 2.53                     | 0.42              |
| 3:D:1071:PHE:O   | 3:D:1071:PHE:CD1  | 2.73                     | 0.42              |
| 4:E:27:ALA:HA    | 4:E:30:LEU:CD1    | 2.48                     | 0.42              |
| 2:M:31:GLN:O     | 2:M:31:GLN:CG     | 2.68                     | 0.42              |
| 2:M:247:PRO:HA   | 2:M:248:PRO:HD3   | 1.88                     | 0.42              |
| 2:M:252:LYS:HB3  | 2:M:298:PHE:HZ    | 1.83                     | 0.42              |
| 2:M:431:HIS:CD2  | 2:M:434:HIS:CE1   | 3.08                     | 0.42              |
| 2:M:711:GLU:HG2  | 2:M:822:VAL:HG12  | 2.02                     | 0.42              |
| 2:M:1047:HIS:CE1 | 3:N:754:PHE:CE1   | 3.07                     | 0.42              |
| 3:N:484:PRO:O    | 3:N:489:ARG:CD    | 2.68                     | 0.42              |
| 3:N:538:SER:O    | 3:N:539:ASP:C     | 2.61                     | 0.42              |
| 3:N:625:TYR:HD2  | 3:N:652:LEU:O     | 1.99                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:644:LEU:O    | 3:N:720:LEU:HA    | 2.20                     | 0.42              |
| 3:N:806:PHE:C    | 3:N:808:THR:N     | 2.78                     | 0.42              |
| 3:N:1284:GLU:HG3 | 3:N:1286:THR:H    | 1.84                     | 0.42              |
| 3:N:1383:ASP:HB2 | 3:N:1416:ALA:CB   | 2.42                     | 0.42              |
| 3:N:1432:LYS:HB2 | 3:N:1432:LYS:NZ   | 2.34                     | 0.42              |
| 3:N:1492:LEU:C   | 3:N:1492:LEU:HD13 | 2.44                     | 0.42              |
| 6:H:5:C:O2       | 6:H:5:C:H2'       | 2.14                     | 0.42              |
| 5:X:13:DA:C4     | 5:X:14:DG:N7      | 2.88                     | 0.42              |
| 1:A:112:ARG:NH2  | 1:A:125:PRO:HB2   | 2.24                     | 0.42              |
| 1:A:218:LEU:HD23 | 1:B:222:LEU:HD22  | 2.01                     | 0.42              |
| 1:B:76:VAL:O     | 1:B:79:ILE:HG12   | 2.20                     | 0.42              |
| 1:B:150:TYR:CE2  | 1:B:168:ASP:HB3   | 2.52                     | 0.42              |
| 2:C:64:LEU:HD13  | 2:C:359:MET:CG    | 2.50                     | 0.42              |
| 2:C:269:LEU:HB2  | 2:C:288:ARG:HG3   | 2.02                     | 0.42              |
| 2:C:430:VAL:HG13 | 3:D:1075:HIS:ND1  | 2.35                     | 0.42              |
| 2:C:583:LEU:N    | 2:C:583:LEU:CD1   | 2.83                     | 0.42              |
| 2:C:675:ALA:HB2  | 2:C:867:VAL:HG11  | 2.01                     | 0.42              |
| 2:C:688:ILE:HD13 | 2:C:847:GLY:CA    | 2.43                     | 0.42              |
| 2:C:738:ASP:HB2  | 2:C:744:ARG:HB3   | 2.01                     | 0.42              |
| 2:C:926:PHE:CE2  | 2:C:960:GLU:CD    | 2.98                     | 0.42              |
| 2:C:974:LEU:HD12 | 2:C:974:LEU:HA    | 1.92                     | 0.42              |
| 3:D:62:LYS:HB2   | 3:D:73:CYS:SG     | 2.60                     | 0.42              |
| 3:D:646:LYS:O    | 3:D:649:ALA:HB3   | 2.20                     | 0.42              |
| 3:D:824:ASN:ND2  | 3:D:824:ASN:C     | 2.78                     | 0.42              |
| 3:D:1093:TYR:OH  | 5:G:17:DA:H1'     | 2.20                     | 0.42              |
| 3:D:1112:CYS:O   | 3:D:1189:ARG:NH2  | 2.50                     | 0.42              |
| 3:D:1223:ILE:CD1 | 3:D:1462:LEU:HD11 | 2.49                     | 0.42              |
| 3:D:1336:LEU:HA  | 3:D:1344:VAL:HG22 | 2.02                     | 0.42              |
| 3:D:1447:LEU:O   | 3:D:1450:ALA:N    | 2.53                     | 0.42              |
| 1:K:109:VAL:HG21 | 1:K:138:LEU:HD23  | 2.02                     | 0.42              |
| 2:M:437:ARG:HH22 | 2:M:488:ALA:HA    | 1.81                     | 0.42              |
| 2:M:455:LEU:HD12 | 2:M:456:ALA:C     | 2.37                     | 0.42              |
| 2:M:677:MET:HB2  | 2:M:987:ILE:HD13  | 2.00                     | 0.42              |
| 2:M:700:TYR:CB   | 2:M:833:LEU:HD22  | 2.49                     | 0.42              |
| 2:M:751:PRO:HA   | 2:M:792:VAL:HG12  | 2.02                     | 0.42              |
| 3:N:109:PRO:O    | 3:N:111:LYS:N     | 2.52                     | 0.42              |
| 3:N:149:LYS:HE3  | 3:N:150:ARG:N     | 2.26                     | 0.42              |
| 3:N:520:LEU:HG   | 3:N:521:PRO:HD2   | 2.01                     | 0.42              |
| 3:N:640:HIS:CD2  | 3:N:641:GLN:HG3   | 2.55                     | 0.42              |
| 3:N:739:ASP:OD1  | 3:N:739:ASP:N     | 2.53                     | 0.42              |
| 3:N:777:PRO:O    | 3:N:780:LYS:HE2   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:1129:THR:CB  | 3:N:1320:GLU:CD   | 2.76                     | 0.42              |
| 3:N:1257:PRO:O   | 3:N:1260:ILE:HG12 | 2.19                     | 0.42              |
| 3:N:1271:LYS:NZ  | 3:N:1331:ASP:CB   | 2.68                     | 0.42              |
| 7:I:1:DG:P       | 7:I:1:DG:C3'      | 3.06                     | 0.42              |
| 7:Z:14:DG:C5     | 7:Z:15:DT:H73     | 2.54                     | 0.42              |
| 1:B:102:LYS:CE   | 1:B:139:ASN:HB2   | 2.44                     | 0.41              |
| 2:C:187:ASN:OD1  | 2:C:188:LYS:HE2   | 2.19                     | 0.41              |
| 2:C:191:PHE:O    | 2:C:193:LEU:HD12  | 2.20                     | 0.41              |
| 2:C:275:TYR:OH   | 2:C:489:THR:HG21  | 2.19                     | 0.41              |
| 2:C:328:LEU:CD1  | 2:C:328:LEU:N     | 2.83                     | 0.41              |
| 2:C:404:LEU:O    | 2:C:407:LYS:HB2   | 2.20                     | 0.41              |
| 2:C:630:ARG:HD2  | 2:C:634:GLY:CA    | 2.21                     | 0.41              |
| 2:C:670:GLN:NE2  | 2:C:699:PHE:HD2   | 2.18                     | 0.41              |
| 2:C:861:LEU:HD21 | 2:C:925:TYR:HE2   | 1.79                     | 0.41              |
| 2:C:926:PHE:CE2  | 2:C:930:LYS:HD2   | 2.55                     | 0.41              |
| 2:C:1105:LYS:NZ  | 2:C:1107:ASN:HB2  | 2.34                     | 0.41              |
| 3:D:92:HIS:HA    | 3:D:517:VAL:O     | 2.20                     | 0.41              |
| 3:D:97:THR:HG23  | 3:D:98:PRO:HD2    | 2.01                     | 0.41              |
| 3:D:100:ALA:HB2  | 3:D:513:ILE:HG22  | 2.02                     | 0.41              |
| 3:D:486:ARG:O    | 3:D:490:ALA:CB    | 2.68                     | 0.41              |
| 3:D:1189:ARG:CD  | 3:D:1204:CYS:SG   | 3.00                     | 0.41              |
| 1:K:211:LEU:O    | 1:K:215:VAL:HG23  | 2.20                     | 0.41              |
| 1:L:201:THR:CG2  | 1:L:205:VAL:HG23  | 2.50                     | 0.41              |
| 2:M:676:ILE:HD13 | 3:N:949:ILE:O     | 2.19                     | 0.41              |
| 2:M:715:THR:C    | 2:M:717:LEU:H     | 2.27                     | 0.41              |
| 2:M:817:PRO:O    | 3:N:532:GLY:CA    | 2.67                     | 0.41              |
| 2:M:926:PHE:HA   | 2:M:929:ARG:HB2   | 2.01                     | 0.41              |
| 3:N:181:ASP:HB2  | 3:N:441:ARG:HD3   | 1.94                     | 0.41              |
| 3:N:187:LYS:HE2  | 3:N:199:LEU:HG    | 2.01                     | 0.41              |
| 3:N:204:LEU:HD12 | 3:N:394:LEU:HG    | 2.02                     | 0.41              |
| 3:N:413:ASP:O    | 3:N:435:VAL:HG23  | 2.20                     | 0.41              |
| 3:N:654:LYS:N    | 3:N:655:PRO:CD    | 2.82                     | 0.41              |
| 3:N:1209:LEU:O   | 3:N:1210:SER:C    | 2.63                     | 0.41              |
| 3:N:1323:GLN:N   | 3:N:1324:PRO:HD3  | 2.34                     | 0.41              |
| 3:N:1331:ASP:HA  | 3:N:1332:PRO:HD3  | 1.76                     | 0.41              |
| 3:N:1447:LEU:O   | 3:N:1450:ALA:N    | 2.53                     | 0.41              |
| 3:N:1483:PHE:O   | 4:O:77:GLU:O      | 2.38                     | 0.41              |
| 7:Z:2:DT:C1'     | 7:Z:3:DA:H5'      | 2.41                     | 0.41              |
| 1:A:123:MET:O    | 1:A:125:PRO:HD3   | 2.21                     | 0.41              |
| 2:C:267:TYR:CE2  | 2:C:289:THR:HG23  | 2.55                     | 0.41              |
| 2:C:279:GLU:C    | 2:C:279:GLU:CD    | 2.87                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:600:ASP:C     | 2:C:616:GLU:HG2  | 2.45                     | 0.41              |
| 2:C:634:GLY:O     | 2:C:705:ILE:CB   | 2.68                     | 0.41              |
| 2:C:668:LEU:HD12  | 2:C:668:LEU:H    | 1.84                     | 0.41              |
| 3:D:40:GLU:OE1    | 3:D:40:GLU:HA    | 2.18                     | 0.41              |
| 3:D:550:ARG:HA    | 3:D:550:ARG:HD3  | 1.71                     | 0.41              |
| 3:D:706:PRO:HG3   | 5:G:19:DG:N2     | 2.35                     | 0.41              |
| 3:D:759:ALA:HA    | 3:D:763:MET:HB2  | 2.02                     | 0.41              |
| 3:D:1237:THR:HG22 | 3:D:1238:MET:HG3 | 2.01                     | 0.41              |
| 4:E:8:LYS:O       | 4:E:12:MET:HG3   | 2.19                     | 0.41              |
| 1:L:59:GLU:CB     | 1:L:137:ARG:HH22 | 2.33                     | 0.41              |
| 2:M:140:ILE:HD13  | 2:M:331:ARG:NH2  | 2.31                     | 0.41              |
| 2:M:288:ARG:HH11  | 2:M:288:ARG:HG3  | 1.83                     | 0.41              |
| 2:M:368:THR:N     | 2:M:369:PRO:CD   | 2.83                     | 0.41              |
| 2:M:1090:LYS:O    | 2:M:1094:ALA:N   | 2.47                     | 0.41              |
| 3:N:30:GLU:HB2    | 3:N:41:ARG:HG3   | 2.01                     | 0.41              |
| 3:N:131:LYS:O     | 3:N:132:TYR:CD2  | 2.73                     | 0.41              |
| 3:N:147:VAL:HG13  | 3:N:147:VAL:O    | 2.20                     | 0.41              |
| 3:N:539:ASP:O     | 3:N:541:ASN:N    | 2.53                     | 0.41              |
| 3:N:587:ARG:HG2   | 3:N:587:ARG:HH11 | 1.85                     | 0.41              |
| 3:N:609:GLY:O     | 3:N:615:ARG:CG   | 2.68                     | 0.41              |
| 3:N:633:VAL:HG22  | 3:N:634:GLY:N    | 2.35                     | 0.41              |
| 3:N:698:LYS:CE    | 4:O:59:ASN:OD1   | 2.68                     | 0.41              |
| 3:N:704:ARG:N     | 3:N:745:MET:HE3  | 2.34                     | 0.41              |
| 3:N:783:ARG:O     | 3:N:787:LEU:HB2  | 2.19                     | 0.41              |
| 3:N:847:ASP:HA    | 3:N:850:LEU:HD13 | 2.02                     | 0.41              |
| 3:N:1123:PHE:HA   | 3:N:1133:ARG:O   | 2.20                     | 0.41              |
| 3:N:1195:GLN:HG3  | 3:N:1196:THR:N   | 2.35                     | 0.41              |
| 1:A:109:VAL:C     | 1:A:110:LYS:HD3  | 2.45                     | 0.41              |
| 2:C:140:ILE:HD12  | 2:C:140:ILE:O    | 2.21                     | 0.41              |
| 2:C:584:GLU:HB2   | 2:C:666:LEU:H    | 1.84                     | 0.41              |
| 2:C:694:LEU:O     | 2:C:697:ARG:O    | 2.38                     | 0.41              |
| 3:D:7:LYS:HG2     | 3:D:1458:GLU:CA  | 2.44                     | 0.41              |
| 3:D:17:LYS:C      | 3:D:20:SER:HB3   | 2.43                     | 0.41              |
| 3:D:18:ILE:HG23   | 3:D:518:PRO:HG3  | 2.02                     | 0.41              |
| 3:D:99:ALA:HA     | 3:D:458:ALA:CB   | 2.50                     | 0.41              |
| 3:D:493:ARG:CG    | 3:D:494:LYS:N    | 2.83                     | 0.41              |
| 3:D:764:LEU:HD12  | 3:D:765:SER:N    | 2.35                     | 0.41              |
| 3:D:924:MET:HG2   | 4:E:6:ILE:HG21   | 2.01                     | 0.41              |
| 3:D:983:LEU:CG    | 3:D:984:THR:N    | 2.82                     | 0.41              |
| 3:D:1114:THR:CG2  | 3:D:1195:GLN:HB3 | 2.46                     | 0.41              |
| 3:D:1264:GLU:OE2  | 3:D:1425:THR:HB  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1371:VAL:HG12 | 3:D:1375:MET:HE2  | 2.02                     | 0.41              |
| 1:K:38:ASN:HB2    | 2:M:980:GLY:HA3   | 2.03                     | 0.41              |
| 1:L:123:MET:H     | 1:L:123:MET:HG2   | 1.55                     | 0.41              |
| 1:L:186:LEU:O     | 1:L:187:GLY:C     | 2.63                     | 0.41              |
| 2:M:141:HIS:CD2   | 2:M:332:ARG:O     | 2.71                     | 0.41              |
| 2:M:170:PRO:CG    | 2:M:258:TYR:CE2   | 3.03                     | 0.41              |
| 2:M:264:PRO:CB    | 2:M:289:THR:CB    | 2.96                     | 0.41              |
| 2:M:285:LEU:HD11  | 2:M:288:ARG:O     | 2.21                     | 0.41              |
| 2:M:393:GLN:HG2   | 6:Y:10:G:C4'      | 2.45                     | 0.41              |
| 2:M:677:MET:HA    | 2:M:678:PRO:HD3   | 1.88                     | 0.41              |
| 2:M:1051:GLU:OE2  | 3:N:752:SER:N     | 2.53                     | 0.41              |
| 2:M:1112:PHE:N    | 2:M:1112:PHE:CD2  | 2.85                     | 0.41              |
| 3:N:51:GLY:HA3    | 3:N:86:ARG:CA     | 2.50                     | 0.41              |
| 3:N:407:VAL:HG12  | 3:N:408:GLU:N     | 2.35                     | 0.41              |
| 3:N:596:SER:C     | 3:N:598:ARG:H     | 2.27                     | 0.41              |
| 3:N:606:ILE:O     | 3:N:613:ARG:HB2   | 2.20                     | 0.41              |
| 3:N:845:ASN:N     | 3:N:848:GLU:HG3   | 2.36                     | 0.41              |
| 3:N:1129:THR:CG2  | 3:N:1130:ARG:H    | 2.01                     | 0.41              |
| 3:N:1138:ALA:O    | 3:N:1139:ASP:C    | 2.63                     | 0.41              |
| 5:G:24:DC:H2''    | 5:G:25:DG:C8      | 2.55                     | 0.41              |
| 5:X:26:DC:O2      | 5:X:26:DC:C2'     | 2.65                     | 0.41              |
| 7:Z:10:DG:C2      | 7:Z:11:DG:C4      | 3.08                     | 0.41              |
| 1:B:58:ILE:HD13   | 1:B:58:ILE:HA     | 1.89                     | 0.41              |
| 2:C:13:ILE:HA     | 2:C:14:PRO:HD3    | 1.89                     | 0.41              |
| 2:C:23:VAL:HA     | 2:C:121:MET:HE2   | 2.02                     | 0.41              |
| 2:C:140:ILE:HA    | 2:C:332:ARG:O     | 2.20                     | 0.41              |
| 2:C:189:ARG:NE    | 2:C:189:ARG:HA    | 2.34                     | 0.41              |
| 2:C:208:ALA:HB1   | 2:C:218:VAL:HG11  | 2.02                     | 0.41              |
| 2:C:532:MET:CE    | 2:C:533:ASP:O     | 2.68                     | 0.41              |
| 2:C:905:ILE:N     | 2:C:905:ILE:CD1   | 2.84                     | 0.41              |
| 2:C:946:ARG:HH11  | 2:C:946:ARG:CB    | 2.31                     | 0.41              |
| 3:D:609:GLY:O     | 3:D:615:ARG:HD3   | 2.20                     | 0.41              |
| 3:D:618:LEU:C     | 3:D:619:LEU:HD23  | 2.44                     | 0.41              |
| 3:D:649:ALA:O     | 3:D:650:LEU:C     | 2.64                     | 0.41              |
| 3:D:741:ASP:O     | 6:H:14:G:H5'      | 2.20                     | 0.41              |
| 3:D:794:GLN:CD    | 3:D:905:PRO:HG2   | 2.46                     | 0.41              |
| 3:D:1094:LEU:CD1  | 3:D:1260:ILE:HD12 | 2.49                     | 0.41              |
| 3:D:1154:GLU:HB2  | 3:N:562:ALA:H     | 1.82                     | 0.41              |
| 3:D:1158:VAL:HG12 | 3:D:1159:ARG:N    | 2.35                     | 0.41              |
| 3:D:1239:ARG:C    | 3:D:1239:ARG:HD3  | 2.46                     | 0.41              |
| 3:D:1344:VAL:HG12 | 3:D:1348:LEU:CD1  | 2.51                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:E:5:GLY:HA3     | 4:E:8:LYS:HD2    | 2.02                     | 0.41              |
| 4:E:7:ASP:O       | 4:E:8:LYS:C      | 2.63                     | 0.41              |
| 1:K:20:TYR:HD2    | 1:K:199:ILE:O    | 2.03                     | 0.41              |
| 1:K:23:PHE:HB2    | 1:K:197:LEU:HG   | 2.01                     | 0.41              |
| 1:K:94:LEU:HD11   | 1:K:119:ASP:HB3  | 2.02                     | 0.41              |
| 1:K:201:THR:C     | 1:K:203:GLY:N    | 2.78                     | 0.41              |
| 1:L:201:THR:HG22  | 1:L:203:GLY:H    | 1.85                     | 0.41              |
| 2:M:88:LEU:HD13   | 2:M:88:LEU:HA    | 1.82                     | 0.41              |
| 2:M:89:THR:O      | 2:M:91:GLN:HG3   | 2.19                     | 0.41              |
| 2:M:403:SER:OG    | 2:M:404:LEU:N    | 2.53                     | 0.41              |
| 2:M:461:VAL:HG13  | 2:M:465:GLY:HA2  | 2.01                     | 0.41              |
| 2:M:535:SER:O     | 2:M:538:GLN:OE1  | 2.38                     | 0.41              |
| 2:M:557:ARG:NH1   | 2:M:844:GLY:O    | 2.53                     | 0.41              |
| 2:M:714:ASP:OD1   | 2:M:719:PRO:HB3  | 2.19                     | 0.41              |
| 2:M:737:LEU:O     | 2:M:737:LEU:HD23 | 2.19                     | 0.41              |
| 2:M:959:PRO:CA    | 2:M:962:GLN:HG3  | 2.44                     | 0.41              |
| 2:M:1040:LEU:HD23 | 2:M:1049:LEU:HB2 | 2.02                     | 0.41              |
| 2:M:1081:VAL:O    | 2:M:1086:ARG:NE  | 2.54                     | 0.41              |
| 2:M:1096:ALA:O    | 2:M:1097:LEU:C   | 2.63                     | 0.41              |
| 3:N:401:TYR:OH    | 3:N:430:ASP:OD2  | 2.37                     | 0.41              |
| 3:N:586:ARG:NH2   | 5:X:16:DT:OP1    | 2.53                     | 0.41              |
| 3:N:753:SER:HB3   | 4:O:27:ALA:HB3   | 2.02                     | 0.41              |
| 3:N:784:ASP:HB3   | 3:N:939:PHE:CE2  | 2.48                     | 0.41              |
| 3:N:835:SER:N     | 3:N:838:ARG:HD3  | 2.35                     | 0.41              |
| 3:N:1103:HIS:O    | 3:N:1105:ILE:N   | 2.53                     | 0.41              |
| 4:O:7:ASP:O       | 4:O:8:LYS:C      | 2.62                     | 0.41              |
| 7:Z:8:DG:H2"      | 7:Z:9:DT:OP2     | 2.19                     | 0.41              |
| 1:A:137:ARG:HG3   | 1:A:137:ARG:HH11 | 1.85                     | 0.41              |
| 2:C:31:GLN:OE1    | 2:C:31:GLN:O     | 2.39                     | 0.41              |
| 2:C:199:VAL:HG22  | 2:C:234:ALA:C    | 2.46                     | 0.41              |
| 2:C:267:TYR:HE2   | 2:C:289:THR:HG23 | 1.86                     | 0.41              |
| 2:C:272:ALA:O     | 2:C:276:LYS:NZ   | 2.51                     | 0.41              |
| 2:C:766:GLU:HA    | 2:C:767:PRO:HD3  | 1.87                     | 0.41              |
| 2:C:862:PRO:HD3   | 2:C:973:VAL:O    | 2.21                     | 0.41              |
| 2:C:890:LEU:HD21  | 2:C:901:TYR:CD1  | 2.55                     | 0.41              |
| 2:C:976:ASP:HB2   | 2:C:981:GLU:O    | 2.20                     | 0.41              |
| 3:D:97:THR:CB     | 3:D:571:LYS:HE2  | 2.45                     | 0.41              |
| 3:D:652:LEU:C     | 3:D:654:LYS:H    | 2.28                     | 0.41              |
| 3:D:741:ASP:OD1   | 6:H:15:C:OP1     | 2.37                     | 0.41              |
| 3:D:785:ILE:HG22  | 3:D:938:GLY:HA3  | 2.02                     | 0.41              |
| 3:D:806:PHE:C     | 3:D:808:THR:N    | 2.78                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:910:SER:OG    | 3:D:911:LEU:HD12 | 2.20                     | 0.41              |
| 3:D:918:ALA:HB3   | 3:D:927:THR:HG23 | 2.01                     | 0.41              |
| 3:D:1041:LEU:HD13 | 3:D:1045:MET:CB  | 2.50                     | 0.41              |
| 4:E:4:PRO:HG2     | 4:E:66:LYS:HZ2   | 1.85                     | 0.41              |
| 1:K:178:ALA:HB3   | 1:K:198:ARG:CG   | 2.50                     | 0.41              |
| 1:L:201:THR:CG2   | 1:L:205:VAL:O    | 2.61                     | 0.41              |
| 2:M:6:PHE:HD1     | 2:M:902:ILE:C    | 2.28                     | 0.41              |
| 2:M:265:ARG:CG    | 2:M:267:TYR:HB3  | 2.51                     | 0.41              |
| 2:M:267:TYR:CB    | 2:M:272:ALA:HB1  | 2.49                     | 0.41              |
| 2:M:612:VAL:HG22  | 2:M:622:GLU:HA   | 2.02                     | 0.41              |
| 2:M:631:SER:C     | 2:M:633:GLN:N    | 2.76                     | 0.41              |
| 2:M:650:ARG:HD2   | 2:M:653:ASP:OD2  | 2.20                     | 0.41              |
| 2:M:976:ASP:CG    | 2:M:979:THR:HG22 | 2.45                     | 0.41              |
| 2:M:1066:ALA:O    | 2:M:1069:ALA:HB3 | 2.21                     | 0.41              |
| 3:N:117:ASP:CB    | 3:N:495:ARG:HH22 | 2.33                     | 0.41              |
| 3:N:171:LEU:CG    | 3:N:195:VAL:CG2  | 2.89                     | 0.41              |
| 3:N:564:GLU:HA    | 3:N:567:ILE:CD1  | 2.50                     | 0.41              |
| 3:N:607:LEU:C     | 3:N:613:ARG:H    | 2.27                     | 0.41              |
| 3:N:778:LEU:HA    | 3:N:778:LEU:HD12 | 1.79                     | 0.41              |
| 3:N:949:ILE:HD13  | 3:N:1019:PRO:HB2 | 2.01                     | 0.41              |
| 3:N:1447:LEU:N    | 3:N:1447:LEU:CD1 | 2.83                     | 0.41              |
| 5:G:8:DC:C2'      | 5:G:9:DC:OP2     | 2.55                     | 0.41              |
| 7:I:8:DG:C2'      | 7:I:8:DG:O5'     | 2.68                     | 0.41              |
| 1:B:106:PRO:HG3   | 1:B:133:GLU:O    | 2.20                     | 0.41              |
| 2:C:9:ILE:O       | 2:C:9:ILE:CD1    | 2.69                     | 0.41              |
| 2:C:72:ARG:CZ     | 2:C:95:TYR:HE1   | 2.33                     | 0.41              |
| 2:C:75:GLU:O      | 2:C:93:PRO:CD    | 2.68                     | 0.41              |
| 2:C:115:LEU:HD12  | 2:C:115:LEU:O    | 2.20                     | 0.41              |
| 2:C:176:VAL:HG12  | 2:C:182:VAL:HG13 | 2.01                     | 0.41              |
| 2:C:634:GLY:CA    | 2:C:705:ILE:O    | 2.67                     | 0.41              |
| 2:C:754:ILE:HA    | 2:C:791:ARG:HA   | 2.02                     | 0.41              |
| 2:C:759:THR:HB    | 2:C:785:VAL:HG13 | 2.02                     | 0.41              |
| 2:C:878:SER:HB2   | 3:D:1029:ARG:NH1 | 2.36                     | 0.41              |
| 3:D:153:LEU:O     | 3:D:153:LEU:HD12 | 2.21                     | 0.41              |
| 3:D:163:TYR:N     | 3:D:163:TYR:CD1  | 2.82                     | 0.41              |
| 3:D:487:ALA:HB2   | 5:G:8:DC:OP2     | 2.20                     | 0.41              |
| 3:D:549:ASN:O     | 3:D:553:ARG:N    | 2.46                     | 0.41              |
| 3:D:750:PRO:HB3   | 3:D:756:GLN:HA   | 2.03                     | 0.41              |
| 3:D:770:LEU:HD23  | 3:D:777:PRO:HA   | 2.02                     | 0.41              |
| 3:D:1046:GLN:HG2  | 3:D:1052:THR:CA  | 2.49                     | 0.41              |
| 3:D:1074:SER:O    | 3:D:1078:ARG:HB2 | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1147:ARG:NH1  | 3:D:1189:ARG:O    | 2.53                     | 0.41              |
| 3:D:1154:GLU:CA   | 3:N:562:ALA:H     | 2.34                     | 0.41              |
| 3:D:1209:LEU:O    | 3:D:1210:SER:C    | 2.62                     | 0.41              |
| 3:D:1481:VAL:C    | 3:D:1483:PHE:N    | 2.77                     | 0.41              |
| 1:K:39:PRO:O      | 1:K:43:ILE:HG12   | 2.20                     | 0.41              |
| 1:K:101:LEU:HD23  | 1:K:101:LEU:O     | 2.20                     | 0.41              |
| 1:L:80:LEU:O      | 3:N:844:ALA:CB    | 2.65                     | 0.41              |
| 1:L:80:LEU:C      | 1:L:82:LEU:H      | 2.28                     | 0.41              |
| 1:L:90:LEU:H      | 1:L:94:LEU:HD12   | 1.86                     | 0.41              |
| 1:L:126:ASP:O     | 1:L:127:LEU:C     | 2.63                     | 0.41              |
| 1:L:176:ARG:NH2   | 3:N:884:ARG:HG3   | 2.36                     | 0.41              |
| 2:M:402:SER:HB2   | 2:M:566:THR:HG22  | 2.02                     | 0.41              |
| 2:M:430:VAL:O     | 2:M:430:VAL:HG22  | 2.21                     | 0.41              |
| 2:M:571:LEU:O     | 2:M:572:ILE:C     | 2.63                     | 0.41              |
| 2:M:630:ARG:CG    | 2:M:630:ARG:NH1   | 2.81                     | 0.41              |
| 2:M:754:ILE:CD1   | 2:M:791:ARG:CZ    | 2.98                     | 0.41              |
| 2:M:799:ILE:O     | 2:M:827:VAL:HG13  | 2.20                     | 0.41              |
| 2:M:937:ASP:H     | 2:M:940:GLU:HG3   | 1.86                     | 0.41              |
| 2:M:1008:ARG:HH21 | 2:M:1012:PRO:CD   | 2.33                     | 0.41              |
| 2:M:1039:ALA:O    | 2:M:1042:ALA:HB3  | 2.21                     | 0.41              |
| 3:N:62:LYS:HD2    | 3:N:75:ARG:HH11   | 1.86                     | 0.41              |
| 3:N:80:VAL:HG12   | 3:N:81:THR:N      | 2.36                     | 0.41              |
| 3:N:107:ASP:OD2   | 3:N:109:PRO:HD2   | 2.20                     | 0.41              |
| 3:N:477:LEU:HD22  | 3:N:492:ALA:CB    | 2.48                     | 0.41              |
| 3:N:648:MET:HE2   | 3:N:648:MET:HB3   | 1.88                     | 0.41              |
| 3:N:704:ARG:HE    | 3:N:706:PRO:CD    | 2.25                     | 0.41              |
| 3:N:861:GLN:CD    | 3:N:861:GLN:H     | 2.28                     | 0.41              |
| 3:N:881:LEU:O     | 3:N:885:ILE:HG13  | 2.21                     | 0.41              |
| 3:N:1267:ARG:HG2  | 3:N:1268:PRO:HD2  | 2.02                     | 0.41              |
| 3:N:1394:VAL:CB   | 3:N:1397:LYS:HE2  | 2.48                     | 0.41              |
| 3:N:1404:ASN:CG   | 3:N:1408:ILE:HD12 | 2.46                     | 0.41              |
| 3:N:1465:ASN:HD22 | 3:N:1465:ASN:HA   | 1.58                     | 0.41              |
| 7:I:4:DG:O5'      | 7:I:4:DG:H2'      | 2.21                     | 0.41              |
| 6:Y:5:C:C2'       | 6:Y:6:C:OP1       | 2.69                     | 0.41              |
| 1:A:101:LEU:O     | 1:A:101:LEU:HD23  | 2.20                     | 0.41              |
| 1:A:110:LYS:HB2   | 1:A:112:ARG:HG2   | 2.02                     | 0.41              |
| 1:A:163:ASN:CG    | 2:C:744:ARG:NH2   | 2.79                     | 0.41              |
| 1:B:186:LEU:O     | 1:B:187:GLY:C     | 2.64                     | 0.41              |
| 2:C:75:GLU:O      | 2:C:93:PRO:HD3    | 2.20                     | 0.41              |
| 2:C:122:THR:C     | 2:C:124:ASP:N     | 2.77                     | 0.41              |
| 2:C:264:PRO:CB    | 2:C:289:THR:CB    | 2.98                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:573:ARG:HB2   | 2:C:670:GLN:HE22  | 1.86                     | 0.41              |
| 2:C:668:LEU:HD12  | 2:C:668:LEU:N     | 2.36                     | 0.41              |
| 2:C:1030:GLN:HE22 | 3:D:628:ARG:HG2   | 1.85                     | 0.41              |
| 3:D:100:ALA:HB3   | 3:D:128:TYR:OH    | 2.20                     | 0.41              |
| 3:D:147:VAL:HG13  | 3:D:147:VAL:O     | 2.20                     | 0.41              |
| 3:D:662:GLU:HG3   | 3:D:668:PRO:O     | 2.20                     | 0.41              |
| 3:D:820:GLU:C     | 3:D:820:GLU:CD    | 2.88                     | 0.41              |
| 1:L:101:LEU:HD13  | 1:L:114:PHE:CD1   | 2.56                     | 0.41              |
| 1:L:158:ILE:CG2   | 1:L:159:LYS:N     | 2.83                     | 0.41              |
| 2:M:141:HIS:O     | 2:M:331:ARG:HB3   | 2.21                     | 0.41              |
| 2:M:364:GLU:HB3   | 2:M:365:ASP:H     | 1.77                     | 0.41              |
| 2:M:412:ALA:HB1   | 2:M:419:THR:HG21  | 2.03                     | 0.41              |
| 2:M:449:ILE:C     | 2:M:451:LEU:H     | 2.29                     | 0.41              |
| 2:M:843:HIS:NE2   | 2:M:883:GLY:C     | 2.79                     | 0.41              |
| 2:M:1111:ILE:H    | 2:M:1111:ILE:HG12 | 1.46                     | 0.41              |
| 3:N:25:GLU:HG3    | 3:N:92:HIS:O      | 2.21                     | 0.41              |
| 3:N:52:PRO:HG3    | 3:N:80:VAL:HG13   | 2.02                     | 0.41              |
| 3:N:55:ASP:CB     | 3:N:82:LYS:HE2    | 2.50                     | 0.41              |
| 3:N:653:PHE:HZ    | 3:N:749:VAL:HG13  | 1.83                     | 0.41              |
| 3:N:704:ARG:HD3   | 3:N:738:ALA:HB2   | 2.03                     | 0.41              |
| 3:N:829:VAL:HG12  | 3:N:830:ALA:N     | 2.35                     | 0.41              |
| 3:N:871:LYS:HE2   | 3:N:871:LYS:HB3   | 1.83                     | 0.41              |
| 3:N:912:LYS:NZ    | 3:N:1362:LYS:NZ   | 2.68                     | 0.41              |
| 3:N:962:GLN:O     | 3:N:965:GLU:HB3   | 2.21                     | 0.41              |
| 3:N:1276:GLU:CD   | 3:N:1303:TYR:OH   | 2.64                     | 0.41              |
| 1:A:56:VAL:HG22   | 1:A:142:VAL:HG12  | 2.03                     | 0.41              |
| 1:A:102:LYS:CB    | 1:A:139:ASN:CG    | 2.88                     | 0.41              |
| 2:C:160:ALA:CB    | 2:C:174:LEU:HD12  | 2.50                     | 0.41              |
| 2:C:186:VAL:HG23  | 2:C:187:ASN:N     | 2.22                     | 0.41              |
| 2:C:352:ALA:HA    | 2:C:355:VAL:CG1   | 2.51                     | 0.41              |
| 2:C:518:LYS:NZ    | 2:C:518:LYS:CB    | 2.83                     | 0.41              |
| 2:C:524:VAL:CG1   | 2:C:525:SER:H     | 2.32                     | 0.41              |
| 2:C:754:ILE:HG12  | 2:C:791:ARG:NH1   | 2.36                     | 0.41              |
| 3:D:481:MET:O     | 3:D:489:ARG:HB2   | 2.20                     | 0.41              |
| 3:D:792:ILE:HD12  | 3:D:941:PHE:CZ    | 2.56                     | 0.41              |
| 3:D:880:ILE:CG2   | 3:D:881:LEU:N     | 2.84                     | 0.41              |
| 3:D:907:GLU:OE2   | 3:D:909:ASN:HB2   | 2.21                     | 0.41              |
| 3:D:988:ARG:O     | 3:D:992:ILE:HG13  | 2.20                     | 0.41              |
| 3:D:1046:GLN:HG2  | 3:D:1052:THR:CB   | 2.51                     | 0.41              |
| 3:D:1086:LEU:HD12 | 3:D:1086:LEU:N    | 2.35                     | 0.41              |
| 3:D:1153:VAL:HG22 | 3:N:560:GLN:C     | 2.45                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1225:ALA:HA  | 3:D:1367:HIS:CG   | 2.56                     | 0.41              |
| 3:D:1264:GLU:HB3 | 3:D:1266:ARG:CD   | 2.50                     | 0.41              |
| 3:D:1489:GLN:H   | 3:D:1489:GLN:HG2  | 1.56                     | 0.41              |
| 1:K:45:LEU:N     | 1:K:45:LEU:CD1    | 2.84                     | 0.41              |
| 1:K:198:ARG:C    | 1:K:199:ILE:HD12  | 2.46                     | 0.41              |
| 2:M:683:ASN:CA   | 2:M:687:ALA:HB3   | 2.51                     | 0.41              |
| 2:M:822:VAL:C    | 2:M:823:VAL:HG23  | 2.46                     | 0.41              |
| 2:M:882:LEU:HD12 | 3:N:1061:PHE:C    | 2.46                     | 0.41              |
| 2:M:905:ILE:HG22 | 2:M:906:PHE:CD1   | 2.56                     | 0.41              |
| 2:M:1002:GLU:CA  | 5:X:23:DG:H5"     | 2.46                     | 0.41              |
| 3:N:117:ASP:HB2  | 3:N:495:ARG:NH2   | 2.36                     | 0.41              |
| 3:N:455:ARG:HB3  | 3:N:459:GLU:HG2   | 2.02                     | 0.41              |
| 3:N:522:PRO:CA   | 3:N:525:ARG:NH1   | 2.72                     | 0.41              |
| 3:N:549:ASN:O    | 3:N:553:ARG:CB    | 2.69                     | 0.41              |
| 3:N:918:ALA:HB3  | 3:N:927:THR:HG23  | 2.01                     | 0.41              |
| 3:N:1033:GLN:O   | 3:N:1036:ARG:HB3  | 2.21                     | 0.41              |
| 3:N:1150:ALA:C   | 3:N:1151:ARG:HG2  | 2.44                     | 0.41              |
| 3:N:1294:VAL:O   | 3:N:1300:SER:HA   | 2.20                     | 0.41              |
| 4:O:13:VAL:HG12  | 4:O:14:ASP:N      | 2.34                     | 0.41              |
| 4:O:21:VAL:O     | 4:O:24:ALA:HB3    | 2.21                     | 0.41              |
| 5:G:2:DT:OP1     | 5:G:2:DT:O4'      | 2.39                     | 0.41              |
| 5:X:3:DC:O5'     | 5:X:3:DC:H2'      | 2.21                     | 0.41              |
| 7:Z:2:DT:H1'     | 7:Z:3:DA:C5'      | 2.43                     | 0.41              |
| 7:Z:3:DA:O5'     | 7:Z:3:DA:C2'      | 2.69                     | 0.41              |
| 1:A:32:PHE:O     | 1:A:36:LEU:HG     | 2.21                     | 0.41              |
| 1:A:101:LEU:HB2  | 1:A:114:PHE:HA    | 2.03                     | 0.41              |
| 1:A:222:LEU:HD23 | 1:B:219:ARG:CG    | 2.50                     | 0.41              |
| 1:B:59:GLU:CG    | 1:B:137:ARG:HH22  | 2.33                     | 0.41              |
| 2:C:18:LEU:CD1   | 2:C:18:LEU:N      | 2.76                     | 0.41              |
| 2:C:20:GLU:CG    | 2:C:21:ILE:N      | 2.84                     | 0.41              |
| 2:C:35:PRO:HA    | 2:C:36:PRO:HD3    | 1.92                     | 0.41              |
| 2:C:93:PRO:HA    | 2:C:117:HIS:CE1   | 2.56                     | 0.41              |
| 2:C:293:PHE:CD1  | 2:C:293:PHE:N     | 2.89                     | 0.41              |
| 2:C:329:GLY:O    | 2:C:330:ASN:ND2   | 2.39                     | 0.41              |
| 2:C:578:VAL:HG13 | 2:C:671:ASN:HB3   | 2.02                     | 0.41              |
| 2:C:650:ARG:HG3  | 2:C:653:ASP:HB2   | 2.03                     | 0.41              |
| 2:C:983:ILE:O    | 2:C:984:GLU:C     | 2.63                     | 0.41              |
| 2:C:1014:SER:N   | 2:C:1019:GLN:O    | 2.53                     | 0.41              |
| 2:C:1042:ALA:N   | 3:D:1223:ILE:HG21 | 2.36                     | 0.41              |
| 2:C:1046:ALA:HA  | 3:D:1472:ILE:CD1  | 2.51                     | 0.41              |
| 2:C:1098:ASP:CG  | 3:D:17:LYS:HD3    | 2.46                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:1115:LEU:CD2  | 3:D:88:TYR:CD1   | 3.04                     | 0.41              |
| 3:D:15:PRO:HB2    | 3:D:16:GLU:OE2   | 2.20                     | 0.41              |
| 3:D:145:VAL:HG23  | 3:D:146:PRO:HD2  | 2.03                     | 0.41              |
| 3:D:528:VAL:CG1   | 3:D:529:GLN:N    | 2.76                     | 0.41              |
| 3:D:696:HIS:CD2   | 4:E:59:ASN:CA    | 3.04                     | 0.41              |
| 3:D:706:PRO:HG2   | 5:G:19:DG:N2     | 2.35                     | 0.41              |
| 3:D:708:LEU:O     | 3:D:1227:GLN:HG2 | 2.21                     | 0.41              |
| 3:D:781:PRO:O     | 3:D:786:ILE:HD11 | 2.21                     | 0.41              |
| 3:D:807:ALA:HA    | 3:D:833:GLU:CB   | 2.51                     | 0.41              |
| 3:D:875:THR:HG22  | 3:D:876:SER:H    | 1.86                     | 0.41              |
| 3:D:899:LEU:HD22  | 3:D:917:GLN:HG2  | 1.93                     | 0.41              |
| 3:D:900:ILE:O     | 3:D:900:ILE:HD12 | 2.21                     | 0.41              |
| 3:D:918:ALA:O     | 3:D:919:PHE:C    | 2.63                     | 0.41              |
| 3:D:924:MET:H     | 4:E:7:ASP:CG     | 2.27                     | 0.41              |
| 3:D:932:ASP:O     | 3:D:935:LYS:CE   | 2.69                     | 0.41              |
| 3:D:998:GLU:HG3   | 3:D:1247:ALA:HB2 | 2.02                     | 0.41              |
| 3:D:1046:GLN:HG2  | 3:D:1052:THR:HA  | 2.03                     | 0.41              |
| 3:D:1096:ARG:NH1  | 5:G:18:DC:OP1    | 2.54                     | 0.41              |
| 3:D:1348:LEU:O    | 3:D:1349:VAL:C   | 2.63                     | 0.41              |
| 3:D:1408:ILE:HG23 | 2:M:371:LYS:CA   | 2.51                     | 0.41              |
| 1:K:42:ARG:HH12   | 1:L:34:VAL:HG12  | 1.86                     | 0.41              |
| 1:K:82:LEU:C      | 1:K:84:GLU:N     | 2.77                     | 0.41              |
| 1:K:91:ASN:C      | 1:K:146:ARG:HH12 | 2.28                     | 0.41              |
| 1:K:112:ARG:NH2   | 1:K:125:PRO:HB2  | 2.36                     | 0.41              |
| 1:K:124:ASN:OD1   | 1:K:127:LEU:HB2  | 2.21                     | 0.41              |
| 1:K:179:PHE:CD1   | 1:K:179:PHE:C    | 2.96                     | 0.41              |
| 1:L:141:GLU:H     | 1:L:141:GLU:HG2  | 1.73                     | 0.41              |
| 1:L:199:ILE:HG22  | 1:L:200:TRP:N    | 2.35                     | 0.41              |
| 2:M:31:GLN:NE2    | 2:M:35:PRO:O     | 2.54                     | 0.41              |
| 2:M:163:ILE:O     | 2:M:163:ILE:HG13 | 2.21                     | 0.41              |
| 2:M:408:ARG:NH2   | 2:M:455:LEU:CD1  | 2.84                     | 0.41              |
| 2:M:437:ARG:NH2   | 2:M:491:GLU:OE2  | 2.54                     | 0.41              |
| 2:M:952:LEU:HD13  | 2:M:952:LEU:HA   | 1.97                     | 0.41              |
| 2:M:1004:LYS:HD3  | 2:M:1004:LYS:HA  | 1.77                     | 0.41              |
| 2:M:1005:MET:HE3  | 3:N:648:MET:HG3  | 2.03                     | 0.41              |
| 2:M:1034:GLU:HB2  | 2:M:1038:TRP:CE2 | 2.56                     | 0.41              |
| 2:M:1105:LYS:H    | 2:M:1105:LYS:HG3 | 1.68                     | 0.41              |
| 2:M:1111:ILE:HG13 | 2:M:1112:PHE:N   | 2.33                     | 0.41              |
| 3:N:87:ARG:HB3    | 3:N:523:ASP:CG   | 2.46                     | 0.41              |
| 3:N:95:LEU:HA     | 3:N:95:LEU:HD23  | 1.83                     | 0.41              |
| 3:N:129:PHE:O     | 3:N:572:ARG:HG2  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:143:ASN:OD1   | 3:N:145:VAL:N     | 2.50                     | 0.41              |
| 3:N:401:TYR:HB3   | 3:N:427:VAL:HG13  | 2.02                     | 0.41              |
| 3:N:452:ILE:HG23  | 3:N:452:ILE:O     | 2.20                     | 0.41              |
| 3:N:552:ASN:O     | 3:N:555:LYS:HB2   | 2.20                     | 0.41              |
| 3:N:646:LYS:CG    | 3:N:688:TRP:CZ2   | 3.03                     | 0.41              |
| 3:N:649:ALA:O     | 3:N:650:LEU:C     | 2.63                     | 0.41              |
| 3:N:693:GLU:C     | 4:O:48:MET:HE1    | 2.43                     | 0.41              |
| 3:N:875:THR:CG2   | 3:N:879:ARG:HB2   | 2.51                     | 0.41              |
| 3:N:880:ILE:CG2   | 3:N:881:LEU:N     | 2.83                     | 0.41              |
| 3:N:1108:ARG:HD3  | 3:N:1108:ARG:N    | 2.36                     | 0.41              |
| 3:N:1122:LEU:HD13 | 3:N:1184:GLN:C    | 2.46                     | 0.41              |
| 3:N:1200:VAL:HG12 | 3:N:1201:CYS:N    | 2.36                     | 0.41              |
| 3:N:1257:PRO:O    | 3:N:1261:GLU:HG3  | 2.21                     | 0.41              |
| 3:N:1340:GLY:O    | 3:N:1343:ALA:HB3  | 2.20                     | 0.41              |
| 3:N:1364:HIS:CE1  | 3:N:1366:LYS:HG3  | 2.55                     | 0.41              |
| 3:N:1428:ALA:O    | 3:N:1429:LEU:C    | 2.64                     | 0.41              |
| 5:G:13:DA:O5'     | 5:G:13:DA:C2'     | 2.67                     | 0.41              |
| 7:I:8:DG:C2'      | 7:I:9:DT:OP2      | 2.65                     | 0.41              |
| 5:X:4:DA:O5'      | 5:X:4:DA:H2'      | 2.21                     | 0.41              |
| 6:Y:7:G:H2'       | 6:Y:8:G:O5'       | 2.21                     | 0.41              |
| 7:Z:5:DC:O5'      | 7:Z:5:DC:H2'      | 2.21                     | 0.41              |
| 1:A:42:ARG:CD     | 1:B:35:THR:HA     | 2.39                     | 0.41              |
| 1:A:82:LEU:C      | 1:A:84:GLU:N      | 2.76                     | 0.41              |
| 1:A:208:LEU:HD23  | 1:A:208:LEU:C     | 2.45                     | 0.41              |
| 1:B:76:VAL:HA     | 1:B:79:ILE:HG12   | 2.03                     | 0.41              |
| 2:C:468:ARG:HB2   | 2:C:485:TYR:HB3   | 2.02                     | 0.41              |
| 2:C:764:GLU:OE2   | 6:H:2:C:H4'       | 2.21                     | 0.41              |
| 3:D:22:SER:HB2    | 3:D:92:HIS:HB3    | 2.03                     | 0.41              |
| 3:D:502:PHE:CE2   | 3:D:1452:ILE:HG23 | 2.56                     | 0.41              |
| 3:D:550:ARG:HD3   | 3:D:553:ARG:HD2   | 2.03                     | 0.41              |
| 3:D:551:ASN:OD1   | 3:D:555:LYS:HE3   | 2.21                     | 0.41              |
| 3:D:576:GLU:O     | 3:D:576:GLU:OE2   | 2.39                     | 0.41              |
| 3:D:625:TYR:OH    | 3:D:655:PRO:HG2   | 2.20                     | 0.41              |
| 3:D:1239:ARG:O    | 3:D:1239:ARG:HD3  | 2.21                     | 0.41              |
| 3:D:1383:ASP:HB3  | 3:D:1416:ALA:HB3  | 2.02                     | 0.41              |
| 3:D:1491:THR:O    | 3:D:1495:ILE:HD13 | 2.21                     | 0.41              |
| 1:K:223:THR:C     | 1:K:225:PHE:N     | 2.77                     | 0.41              |
| 1:L:66:SER:O      | 1:L:75:VAL:HG23   | 2.21                     | 0.41              |
| 2:M:310:LEU:HD12  | 2:M:314:THR:CG2   | 2.51                     | 0.41              |
| 2:M:428:ARG:HH11  | 2:M:449:ILE:HG22  | 1.85                     | 0.41              |
| 2:M:762:LYS:CE    | 2:M:786:LYS:HG3   | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:861:LEU:HD23  | 2:M:862:PRO:HD2   | 2.02                     | 0.41              |
| 2:M:880:MET:C     | 2:M:881:ASN:HD22  | 2.27                     | 0.41              |
| 2:M:1089:VAL:HG13 | 2:M:1099:VAL:HB   | 2.03                     | 0.41              |
| 2:M:1091:GLU:O    | 2:M:1094:ALA:HB3  | 2.21                     | 0.41              |
| 3:N:112:ILE:CD1   | 3:N:116:LEU:HD12  | 2.49                     | 0.41              |
| 3:N:159:ARG:O     | 3:N:162:ARG:HB3   | 2.21                     | 0.41              |
| 3:N:481:MET:O     | 3:N:489:ARG:CD    | 2.69                     | 0.41              |
| 3:N:502:PHE:O     | 3:N:503:LEU:C     | 2.63                     | 0.41              |
| 3:N:648:MET:O     | 3:N:649:ALA:C     | 2.64                     | 0.41              |
| 3:N:653:PHE:O     | 3:N:657:LEU:N     | 2.45                     | 0.41              |
| 3:N:1031:ASN:C    | 3:N:1033:GLN:H    | 2.29                     | 0.41              |
| 3:N:1350:GLU:OE2  | 3:N:1357:ARG:CZ   | 2.69                     | 0.41              |
| 3:N:1405:GLU:O    | 3:N:1405:GLU:HG3  | 2.20                     | 0.41              |
| 3:N:1412:LYS:HE2  | 3:N:1414:PRO:HG3  | 2.03                     | 0.41              |
| 3:N:1465:ASN:CB   | 3:N:1473:PRO:HD3  | 2.50                     | 0.41              |
| 4:O:22:VAL:O      | 4:O:23:VAL:C      | 2.64                     | 0.41              |
| 5:G:7:DA:C5       | 5:G:8:DC:C4       | 3.09                     | 0.41              |
| 1:B:40:LEU:O      | 1:B:44:LEU:HG     | 2.21                     | 0.40              |
| 2:C:19:THR:HG22   | 2:C:19:THR:O      | 2.20                     | 0.40              |
| 2:C:101:ILE:HD12  | 2:C:107:LEU:HD22  | 2.02                     | 0.40              |
| 2:C:165:LEU:HB3   | 2:C:265:ARG:HH12  | 1.84                     | 0.40              |
| 2:C:165:LEU:O     | 2:C:265:ARG:NE    | 2.54                     | 0.40              |
| 2:C:499:ALA:HA    | 2:C:532:MET:CE    | 2.50                     | 0.40              |
| 2:C:516:ARG:HD2   | 3:D:1068:LEU:HD22 | 2.02                     | 0.40              |
| 2:C:557:ARG:HH11  | 2:C:560:MET:HG3   | 1.85                     | 0.40              |
| 2:C:677:MET:HA    | 2:C:678:PRO:HD3   | 1.86                     | 0.40              |
| 2:C:931:GLY:C     | 2:C:933:GLY:H     | 2.29                     | 0.40              |
| 2:C:994:ILE:HG22  | 2:C:995:MET:H     | 1.86                     | 0.40              |
| 2:C:1035:MET:SD   | 5:G:20:DC:C5'     | 3.04                     | 0.40              |
| 3:D:701:LEU:C     | 3:D:702:LEU:HD12  | 2.46                     | 0.40              |
| 3:D:800:LYS:HD2   | 3:D:804:LEU:HD13  | 2.03                     | 0.40              |
| 3:D:978:TYR:HA    | 3:D:983:LEU:HD21  | 2.03                     | 0.40              |
| 3:D:983:LEU:H     | 3:D:983:LEU:HD23  | 1.85                     | 0.40              |
| 3:D:1488:ASP:OD2  | 3:D:1491:THR:OG1  | 2.36                     | 0.40              |
| 1:K:221:HIS:HA    | 1:K:224:TYR:CE2   | 2.56                     | 0.40              |
| 1:L:227:ASN:HA    | 1:L:228:PRO:HD3   | 1.71                     | 0.40              |
| 2:M:12:VAL:HG13   | 2:M:13:ILE:N      | 2.36                     | 0.40              |
| 2:M:88:LEU:HD22   | 2:M:814:GLU:HG2   | 2.03                     | 0.40              |
| 2:M:334:ARG:HH22  | 2:M:342:ASP:CB    | 2.33                     | 0.40              |
| 2:M:572:ILE:H     | 2:M:572:ILE:HG13  | 1.57                     | 0.40              |
| 2:M:985:GLY:HA2   | 2:M:986:PRO:HD3   | 1.91                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:131:LYS:O    | 3:N:132:TYR:CG    | 2.75                     | 0.40              |
| 3:N:133:ILE:O    | 3:N:153:LEU:N     | 2.49                     | 0.40              |
| 3:N:494:LYS:O    | 3:N:494:LYS:HG2   | 2.21                     | 0.40              |
| 3:N:565:ILE:H    | 3:N:565:ILE:CD1   | 2.29                     | 0.40              |
| 3:N:1059:SER:HB2 | 3:N:1065:LEU:HA   | 2.01                     | 0.40              |
| 3:N:1209:LEU:HG  | 3:N:1219:GLU:OE2  | 2.21                     | 0.40              |
| 7:I:8:DG:O5'     | 7:I:8:DG:H2'      | 2.21                     | 0.40              |
| 1:A:178:ALA:HB3  | 1:A:198:ARG:CG    | 2.51                     | 0.40              |
| 1:B:75:VAL:O     | 1:B:79:ILE:HG23   | 2.21                     | 0.40              |
| 1:B:79:ILE:HA    | 1:B:82:LEU:HG     | 2.02                     | 0.40              |
| 1:B:126:ASP:O    | 1:B:127:LEU:C     | 2.65                     | 0.40              |
| 2:C:1004:LYS:HD3 | 2:C:1004:LYS:HA   | 1.72                     | 0.40              |
| 2:C:1046:ALA:CB  | 3:D:1472:ILE:CG1  | 2.99                     | 0.40              |
| 2:C:1071:ILE:O   | 3:D:659:LYS:HD3   | 2.21                     | 0.40              |
| 2:C:1090:LYS:HD2 | 3:D:90:MET:HG2    | 2.03                     | 0.40              |
| 3:D:519:VAL:HA   | 3:D:544:TYR:OH    | 2.21                     | 0.40              |
| 3:D:1038:LEU:CD1 | 3:D:1042:ARG:HH11 | 2.34                     | 0.40              |
| 3:D:1089:ALA:O   | 3:D:1093:TYR:HB2  | 2.20                     | 0.40              |
| 3:D:1139:ASP:CG  | 3:D:1357:ARG:CZ   | 2.94                     | 0.40              |
| 3:D:1225:ALA:CB  | 3:D:1367:HIS:ND1  | 2.84                     | 0.40              |
| 4:E:22:VAL:O     | 4:E:23:VAL:C      | 2.63                     | 0.40              |
| 1:K:56:VAL:HG13  | 1:K:142:VAL:CG1   | 2.51                     | 0.40              |
| 1:K:76:VAL:HA    | 1:K:79:ILE:HG12   | 2.03                     | 0.40              |
| 1:K:222:LEU:HD23 | 1:L:219:ARG:HA    | 2.03                     | 0.40              |
| 1:L:86:VAL:CG1   | 1:L:124:ASN:HB2   | 2.52                     | 0.40              |
| 1:L:213:GLN:O    | 1:L:217:ILE:HD13  | 2.22                     | 0.40              |
| 2:M:17:PRO:O     | 2:M:18:LEU:C      | 2.64                     | 0.40              |
| 2:M:221:LEU:HG   | 2:M:222:MET:H     | 1.86                     | 0.40              |
| 2:M:306:THR:OG1  | 2:M:307:LEU:N     | 2.55                     | 0.40              |
| 2:M:411:SER:OG   | 2:M:412:ALA:N     | 2.53                     | 0.40              |
| 2:M:452:ILE:N    | 2:M:452:ILE:CD1   | 2.84                     | 0.40              |
| 2:M:540:PHE:HB3  | 2:M:544:THR:CG2   | 2.50                     | 0.40              |
| 2:M:863:ASP:O    | 2:M:865:THR:N     | 2.53                     | 0.40              |
| 2:M:1096:ALA:O   | 3:N:13:ALA:HB2    | 2.22                     | 0.40              |
| 3:N:160:GLU:O    | 3:N:162:ARG:N     | 2.55                     | 0.40              |
| 3:N:473:LEU:HD12 | 3:N:473:LEU:N     | 2.36                     | 0.40              |
| 3:N:475:LYS:HA   | 3:N:478:LEU:HD12  | 2.02                     | 0.40              |
| 3:N:1112:CYS:HB2 | 3:N:1195:GLN:CG   | 2.52                     | 0.40              |
| 3:N:1213:ARG:NH2 | 4:O:14:ASP:CA     | 2.83                     | 0.40              |
| 3:N:1219:GLU:OE1 | 4:O:17:TYR:CE2    | 2.73                     | 0.40              |
| 3:N:1227:GLN:O   | 3:N:1229:ILE:N    | 2.53                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1422:MET:HE1  | 3:N:1430:SER:OG   | 2.21                     | 0.40              |
| 5:G:22:DA:H2      | 6:H:12:U:O2       | 2.04                     | 0.40              |
| 1:A:11:PHE:HB3    | 1:B:227:ASN:O     | 2.21                     | 0.40              |
| 1:A:107:LYS:NZ    | 1:A:113:ASP:OD2   | 2.49                     | 0.40              |
| 1:A:152:PRO:C     | 1:A:154:GLU:N     | 2.78                     | 0.40              |
| 2:C:26:TYR:HD2    | 2:C:121:MET:HB2   | 1.85                     | 0.40              |
| 2:C:31:GLN:HG2    | 2:C:34:VAL:CG2    | 2.51                     | 0.40              |
| 2:C:243:ARG:HG3   | 2:C:243:ARG:NH1   | 2.35                     | 0.40              |
| 2:C:292:ARG:CB    | 2:C:299:LYS:HG2   | 2.45                     | 0.40              |
| 2:C:684:PHE:HB3   | 3:D:740:PHE:HE1   | 1.84                     | 0.40              |
| 2:C:979:THR:C     | 2:C:981:GLU:H     | 2.28                     | 0.40              |
| 2:C:1014:SER:CB   | 2:C:1017:THR:O    | 2.62                     | 0.40              |
| 2:C:1086:ARG:HH22 | 2:C:1113:GLU:HG2  | 1.86                     | 0.40              |
| 2:C:1088:LEU:HD23 | 2:C:1088:LEU:C    | 2.47                     | 0.40              |
| 3:D:19:ARG:HG3    | 3:D:19:ARG:NH1    | 2.36                     | 0.40              |
| 3:D:87:ARG:N      | 3:D:523:ASP:OD2   | 2.55                     | 0.40              |
| 3:D:660:LYS:NZ    | 3:D:660:LYS:HB2   | 2.35                     | 0.40              |
| 3:D:757:ALA:O     | 3:D:758:GLU:C     | 2.64                     | 0.40              |
| 1:K:11:PHE:CD1    | 1:K:25:LEU:HD13   | 2.55                     | 0.40              |
| 1:K:20:TYR:C      | 1:K:207:PRO:HG2   | 2.46                     | 0.40              |
| 1:K:29:GLU:HB3    | 1:K:30:ARG:H      | 1.69                     | 0.40              |
| 1:L:195:LEU:HD12  | 1:L:196:THR:H     | 1.83                     | 0.40              |
| 2:M:175:GLU:O     | 2:M:183:SER:HB3   | 2.21                     | 0.40              |
| 2:M:473:ARG:NH1   | 2:M:473:ARG:HG2   | 2.36                     | 0.40              |
| 2:M:517:ARG:HB3   | 2:M:518:LYS:H     | 1.66                     | 0.40              |
| 2:M:640:ARG:CG    | 2:M:640:ARG:HH11  | 2.35                     | 0.40              |
| 2:M:663:ASN:HB2   | 2:M:665:PHE:CE1   | 2.57                     | 0.40              |
| 2:M:707:ARG:CD    | 2:M:824:ARG:CD    | 2.99                     | 0.40              |
| 2:M:816:LYS:O     | 2:M:819:VAL:HB    | 2.21                     | 0.40              |
| 2:M:826:TYR:N     | 2:M:826:TYR:CD1   | 2.89                     | 0.40              |
| 2:M:874:LEU:C     | 2:M:876:VAL:H     | 2.29                     | 0.40              |
| 2:M:937:ASP:N     | 2:M:940:GLU:OE2   | 2.52                     | 0.40              |
| 2:M:1084:SER:HA   | 2:M:1087:VAL:HG12 | 2.03                     | 0.40              |
| 2:M:1118:LYS:C    | 2:M:1119:ARG:O    | 2.64                     | 0.40              |
| 3:N:30:GLU:OE1    | 3:N:30:GLU:HA     | 2.21                     | 0.40              |
| 3:N:160:GLU:C     | 3:N:162:ARG:N     | 2.78                     | 0.40              |
| 3:N:646:LYS:O     | 3:N:649:ALA:HB3   | 2.22                     | 0.40              |
| 3:N:753:SER:HB3   | 4:O:27:ALA:CB     | 2.51                     | 0.40              |
| 3:N:763:MET:O     | 3:N:764:LEU:C     | 2.62                     | 0.40              |
| 3:N:951:ILE:CG2   | 3:N:952:ASP:N     | 2.83                     | 0.40              |
| 3:N:1014:ASN:C    | 3:N:1016:PRO:HD3  | 2.46                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1271:LYS:HD3  | 3:N:1273:VAL:CG1 | 2.51                     | 0.40              |
| 3:N:1294:VAL:HG23 | 3:N:1301:LYS:HB3 | 2.01                     | 0.40              |
| 3:N:1305:LEU:HD12 | 3:N:1311:LEU:HB3 | 2.03                     | 0.40              |
| 3:N:1463:LYS:HB2  | 3:N:1463:LYS:HE3 | 1.84                     | 0.40              |
| 1:A:20:TYR:HD2    | 1:A:199:ILE:O    | 2.05                     | 0.40              |
| 1:A:219:ARG:HA    | 1:A:222:LEU:HD13 | 2.04                     | 0.40              |
| 2:C:214:TYR:OH    | 2:C:308:ARG:O    | 2.38                     | 0.40              |
| 2:C:328:LEU:CG    | 2:C:433:THR:HB   | 2.50                     | 0.40              |
| 2:C:470:PRO:HB2   | 2:C:534:VAL:HG21 | 2.04                     | 0.40              |
| 2:C:480:THR:C     | 2:C:482:GLU:H    | 2.29                     | 0.40              |
| 2:C:657:ASP:C     | 2:C:658:GLY:O    | 2.63                     | 0.40              |
| 2:C:863:ASP:O     | 2:C:865:THR:N    | 2.54                     | 0.40              |
| 2:C:874:LEU:C     | 2:C:876:VAL:H    | 2.28                     | 0.40              |
| 3:D:619:LEU:CD1   | 3:D:621:LYS:HZ1  | 2.31                     | 0.40              |
| 3:D:648:MET:O     | 3:D:649:ALA:C    | 2.63                     | 0.40              |
| 3:D:783:ARG:HB3   | 3:D:1028:ALA:C   | 2.47                     | 0.40              |
| 3:D:788:GLY:O     | 3:D:792:ILE:HG22 | 2.21                     | 0.40              |
| 3:D:796:ARG:NH2   | 3:D:859:ASP:HB2  | 2.36                     | 0.40              |
| 3:D:925:GLU:OE1   | 4:E:5:GLY:N      | 2.54                     | 0.40              |
| 3:D:1042:ARG:HE   | 3:D:1073:SER:HB2 | 1.86                     | 0.40              |
| 3:D:1156:LEU:HD12 | 3:D:1177:ALA:HB2 | 2.04                     | 0.40              |
| 3:D:1339:LYS:HG2  | 3:D:1343:ALA:HB2 | 2.03                     | 0.40              |
| 3:D:1408:ILE:HG23 | 2:M:371:LYS:N    | 2.37                     | 0.40              |
| 4:E:29:GLN:OE1    | 4:E:89:MET:HE2   | 2.22                     | 0.40              |
| 4:E:54:LEU:HD21   | 4:E:63:TRP:NE1   | 2.28                     | 0.40              |
| 4:E:68:LEU:CD1    | 4:E:73:LEU:HD13  | 2.46                     | 0.40              |
| 2:M:172:ILE:HG22  | 2:M:173:ASP:N    | 2.36                     | 0.40              |
| 2:M:269:LEU:HG    | 2:M:288:ARG:CG   | 2.48                     | 0.40              |
| 2:M:397:GLU:O     | 2:M:398:THR:C    | 2.63                     | 0.40              |
| 2:M:567:GLN:HE22  | 6:Y:13:C:H5'     | 1.86                     | 0.40              |
| 2:M:650:ARG:CD    | 2:M:653:ASP:OD2  | 2.70                     | 0.40              |
| 2:M:692:GLU:OE1   | 2:M:854:PRO:CB   | 2.68                     | 0.40              |
| 2:M:970:GLY:O     | 2:M:988:VAL:HB   | 2.21                     | 0.40              |
| 3:N:111:LYS:HE3   | 3:N:1449:GLU:CA  | 2.52                     | 0.40              |
| 3:N:480:GLU:OE2   | 3:N:484:PRO:HG2  | 2.21                     | 0.40              |
| 3:N:568:ARG:HH21  | 3:N:572:ARG:HA   | 1.87                     | 0.40              |
| 3:N:812:ALA:O     | 3:N:816:HIS:CG   | 2.75                     | 0.40              |
| 3:N:1401:GLU:OE2  | 3:N:1402:ALA:N   | 2.54                     | 0.40              |
| 4:O:41:GLU:OE1    | 4:O:42:PRO:HD3   | 2.21                     | 0.40              |
| 4:O:47:LYS:N      | 4:O:54:LEU:CD1   | 2.83                     | 0.40              |
| 5:G:13:DA:C2'     | 5:G:14:DG:OP2    | 2.43                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:Z:9:DT:C2'      | 7:Z:10:DG:OP2    | 2.61                     | 0.40              |
| 1:B:80:LEU:C      | 1:B:82:LEU:H     | 2.30                     | 0.40              |
| 1:B:99:LEU:HB2    | 1:B:142:VAL:CG2  | 2.51                     | 0.40              |
| 2:C:31:GLN:NE2    | 2:C:38:LYS:CB    | 2.84                     | 0.40              |
| 2:C:137:VAL:O     | 2:C:391:LEU:HD21 | 2.21                     | 0.40              |
| 2:C:243:ARG:N     | 2:C:244:PRO:HD3  | 2.36                     | 0.40              |
| 2:C:251:ASP:HB3   | 2:C:252:LYS:HG3  | 2.03                     | 0.40              |
| 2:C:256:TYR:CE1   | 2:C:293:PHE:HB2  | 2.57                     | 0.40              |
| 2:C:260:LEU:HB3   | 2:C:291:ALA:HB2  | 1.98                     | 0.40              |
| 2:C:409:ARG:HB3   | 2:C:454:SER:CB   | 2.45                     | 0.40              |
| 2:C:498:GLN:O     | 2:C:532:MET:SD   | 2.80                     | 0.40              |
| 2:C:793:PRO:C     | 2:C:794:PRO:O    | 2.65                     | 0.40              |
| 2:C:1040:LEU:HD23 | 2:C:1049:LEU:HB2 | 2.02                     | 0.40              |
| 2:C:1092:LEU:HB3  | 2:C:1099:VAL:CG2 | 2.52                     | 0.40              |
| 3:D:481:MET:HE1   | 3:D:496:LEU:HD23 | 2.02                     | 0.40              |
| 3:D:691:LEU:C     | 3:D:693:GLU:N    | 2.76                     | 0.40              |
| 3:D:901:GLN:H     | 3:D:901:GLN:HG2  | 1.71                     | 0.40              |
| 3:D:1093:TYR:CE2  | 3:D:1096:ARG:NH1 | 2.90                     | 0.40              |
| 3:D:1094:LEU:HD11 | 3:D:1260:ILE:CD1 | 2.49                     | 0.40              |
| 3:D:1135:ARG:HD3  | 3:D:1139:ASP:CB  | 2.51                     | 0.40              |
| 3:D:1195:GLN:O    | 3:D:1196:THR:C   | 2.64                     | 0.40              |
| 4:E:28:GLN:HA     | 4:E:31:LEU:HD12  | 2.03                     | 0.40              |
| 4:E:36:LYS:NZ     | 4:E:45:ARG:HH22  | 2.18                     | 0.40              |
| 1:K:210:ALA:HA    | 1:K:213:GLN:OE1  | 2.21                     | 0.40              |
| 1:L:52:ALA:CB     | 1:L:170:VAL:C    | 2.90                     | 0.40              |
| 2:M:69:LEU:HD12   | 2:M:97:ARG:CB    | 2.48                     | 0.40              |
| 2:M:162:ILE:CG2   | 2:M:172:ILE:HD13 | 2.51                     | 0.40              |
| 2:M:423:ALA:HB2   | 7:Z:1:DG:C1'     | 2.51                     | 0.40              |
| 2:M:497:ALA:HA    | 2:M:515:ALA:HA   | 2.04                     | 0.40              |
| 2:M:694:LEU:HD22  | 2:M:699:PHE:CD1  | 2.57                     | 0.40              |
| 2:M:1014:SER:C    | 2:M:1017:THR:O   | 2.64                     | 0.40              |
| 3:N:704:ARG:CA    | 3:N:745:MET:HE3  | 2.52                     | 0.40              |
| 3:N:827:ILE:O     | 3:N:827:ILE:HG22 | 2.21                     | 0.40              |
| 3:N:1443:THR:HA   | 3:N:1446:VAL:CG2 | 2.52                     | 0.40              |
| 4:O:41:GLU:O      | 4:O:42:PRO:O     | 2.39                     | 0.40              |
| 5:G:6:DT:H2''     | 5:G:7:DA:C8      | 2.57                     | 0.40              |
| 5:X:11:DC:O5'     | 5:X:11:DC:H2'    | 2.22                     | 0.40              |
| 5:X:25:DG:H2'     | 5:X:26:DC:C6     | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)    | 194 (86%)  | 24 (11%)  | 9 (4%)   | 2           | 18 |
| 1   | B     | 227/315 (72%)    | 195 (86%)  | 23 (10%)  | 9 (4%)   | 2           | 18 |
| 1   | K     | 227/315 (72%)    | 193 (85%)  | 26 (12%)  | 8 (4%)   | 3           | 20 |
| 1   | L     | 227/315 (72%)    | 201 (88%)  | 17 (8%)   | 9 (4%)   | 2           | 18 |
| 2   | C     | 1117/1119 (100%) | 893 (80%)  | 151 (14%) | 73 (6%)  | 1           | 13 |
| 2   | M     | 1117/1119 (100%) | 889 (80%)  | 153 (14%) | 75 (7%)  | 1           | 12 |
| 3   | D     | 1143/1524 (75%)  | 903 (79%)  | 167 (15%) | 73 (6%)  | 1           | 13 |
| 3   | N     | 1280/1524 (84%)  | 1011 (79%) | 190 (15%) | 79 (6%)  | 1           | 13 |
| 4   | E     | 93/99 (94%)      | 67 (72%)   | 15 (16%)  | 11 (12%) | 0           | 4  |
| 4   | O     | 93/99 (94%)      | 69 (74%)   | 13 (14%)  | 11 (12%) | 0           | 4  |
| All | All   | 5751/6744 (85%)  | 4615 (80%) | 779 (14%) | 357 (6%) | 1           | 13 |

All (357) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | ASP  |
| 1   | A     | 29  | GLU  |
| 1   | A     | 118 | ALA  |
| 1   | A     | 133 | GLU  |
| 1   | A     | 187 | GLY  |
| 1   | B     | 187 | GLY  |
| 2   | C     | 59  | LYS  |
| 2   | C     | 87  | ASP  |
| 2   | C     | 129 | ILE  |
| 2   | C     | 164 | PRO  |
| 2   | C     | 170 | PRO  |
| 2   | C     | 223 | ASP  |
| 2   | C     | 231 | PRO  |
| 2   | C     | 244 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 253  | ALA  |
| 2   | C     | 262  | ALA  |
| 2   | C     | 288  | ARG  |
| 2   | C     | 290  | LEU  |
| 2   | C     | 292  | ARG  |
| 2   | C     | 369  | PRO  |
| 2   | C     | 434  | HIS  |
| 2   | C     | 457  | ALA  |
| 2   | C     | 517  | ARG  |
| 2   | C     | 627  | ARG  |
| 2   | C     | 680  | ASP  |
| 2   | C     | 684  | PHE  |
| 2   | C     | 698  | ASP  |
| 2   | C     | 727  | PRO  |
| 2   | C     | 1005 | MET  |
| 2   | C     | 1033 | GLY  |
| 2   | C     | 1106 | ASP  |
| 3   | D     | 40   | GLU  |
| 3   | D     | 55   | ASP  |
| 3   | D     | 120  | ALA  |
| 3   | D     | 136  | ASP  |
| 3   | D     | 705  | ALA  |
| 3   | D     | 725  | SER  |
| 3   | D     | 735  | ALA  |
| 3   | D     | 1028 | ALA  |
| 3   | D     | 1032 | PRO  |
| 3   | D     | 1237 | THR  |
| 3   | D     | 1389 | LEU  |
| 3   | D     | 1446 | VAL  |
| 4   | E     | 22   | VAL  |
| 4   | E     | 42   | PRO  |
| 4   | E     | 43   | GLU  |
| 4   | E     | 58   | PRO  |
| 4   | E     | 95   | VAL  |
| 1   | K     | 3    | ASP  |
| 1   | K     | 29   | GLU  |
| 1   | K     | 118  | ALA  |
| 1   | K     | 133  | GLU  |
| 1   | K     | 187  | GLY  |
| 1   | L     | 187  | GLY  |
| 2   | M     | 44   | ILE  |
| 2   | M     | 87   | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 129  | ILE  |
| 2   | M     | 164  | PRO  |
| 2   | M     | 170  | PRO  |
| 2   | M     | 223  | ASP  |
| 2   | M     | 231  | PRO  |
| 2   | M     | 244  | PRO  |
| 2   | M     | 253  | ALA  |
| 2   | M     | 262  | ALA  |
| 2   | M     | 288  | ARG  |
| 2   | M     | 290  | LEU  |
| 2   | M     | 369  | PRO  |
| 2   | M     | 457  | ALA  |
| 2   | M     | 517  | ARG  |
| 2   | M     | 680  | ASP  |
| 2   | M     | 684  | PHE  |
| 2   | M     | 698  | ASP  |
| 2   | M     | 727  | PRO  |
| 2   | M     | 905  | ILE  |
| 2   | M     | 1005 | MET  |
| 2   | M     | 1033 | GLY  |
| 2   | M     | 1096 | ALA  |
| 2   | M     | 1106 | ASP  |
| 2   | M     | 1113 | GLU  |
| 3   | N     | 40   | GLU  |
| 3   | N     | 43   | GLY  |
| 3   | N     | 55   | ASP  |
| 3   | N     | 136  | ASP  |
| 3   | N     | 167  | GLU  |
| 3   | N     | 539  | ASP  |
| 3   | N     | 1265 | ALA  |
| 3   | N     | 1323 | GLN  |
| 3   | N     | 1389 | LEU  |
| 3   | N     | 1408 | ILE  |
| 3   | N     | 1446 | VAL  |
| 4   | O     | 22   | VAL  |
| 4   | O     | 42   | PRO  |
| 4   | O     | 43   | GLU  |
| 4   | O     | 58   | PRO  |
| 2   | C     | 40   | GLU  |
| 2   | C     | 80   | GLN  |
| 2   | C     | 138  | SER  |
| 2   | C     | 144  | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 152  | PRO  |
| 2   | C     | 156  | GLY  |
| 2   | C     | 178  | PRO  |
| 2   | C     | 205  | GLU  |
| 2   | C     | 251  | ASP  |
| 2   | C     | 261  | ILE  |
| 2   | C     | 264  | PRO  |
| 2   | C     | 268  | ASP  |
| 2   | C     | 325  | ILE  |
| 2   | C     | 366  | SER  |
| 2   | C     | 465  | GLY  |
| 2   | C     | 548  | PRO  |
| 2   | C     | 593  | ALA  |
| 2   | C     | 762  | LYS  |
| 2   | C     | 765  | SER  |
| 2   | C     | 831  | ARG  |
| 2   | C     | 864  | GLY  |
| 2   | C     | 905  | ILE  |
| 2   | C     | 908  | GLY  |
| 2   | C     | 1055 | LEU  |
| 3   | D     | 43   | GLY  |
| 3   | D     | 98   | PRO  |
| 3   | D     | 530  | VAL  |
| 3   | D     | 532  | GLY  |
| 3   | D     | 564  | GLU  |
| 3   | D     | 620  | GLY  |
| 3   | D     | 652  | LEU  |
| 3   | D     | 803  | GLY  |
| 3   | D     | 807  | ALA  |
| 3   | D     | 822  | ALA  |
| 3   | D     | 924  | MET  |
| 3   | D     | 1045 | MET  |
| 3   | D     | 1104 | GLU  |
| 3   | D     | 1161 | GLU  |
| 3   | D     | 1197 | ARG  |
| 3   | D     | 1408 | ILE  |
| 3   | D     | 1410 | GLU  |
| 3   | D     | 1441 | GLN  |
| 3   | D     | 1454 | GLY  |
| 1   | L     | 125  | PRO  |
| 2   | M     | 40   | GLU  |
| 2   | M     | 80   | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 138  | SER  |
| 2   | M     | 144  | PRO  |
| 2   | M     | 152  | PRO  |
| 2   | M     | 156  | GLY  |
| 2   | M     | 178  | PRO  |
| 2   | M     | 261  | ILE  |
| 2   | M     | 264  | PRO  |
| 2   | M     | 292  | ARG  |
| 2   | M     | 325  | ILE  |
| 2   | M     | 434  | HIS  |
| 2   | M     | 465  | GLY  |
| 2   | M     | 593  | ALA  |
| 2   | M     | 627  | ARG  |
| 2   | M     | 740  | GLU  |
| 2   | M     | 864  | GLY  |
| 2   | M     | 908  | GLY  |
| 2   | M     | 984  | GLU  |
| 2   | M     | 1055 | LEU  |
| 3   | N     | 31   | THR  |
| 3   | N     | 59   | ALA  |
| 3   | N     | 67   | ARG  |
| 3   | N     | 77   | GLY  |
| 3   | N     | 110  | SER  |
| 3   | N     | 117  | ASP  |
| 3   | N     | 120  | ALA  |
| 3   | N     | 486  | ARG  |
| 3   | N     | 620  | GLY  |
| 3   | N     | 735  | ALA  |
| 3   | N     | 803  | GLY  |
| 3   | N     | 807  | ALA  |
| 3   | N     | 844  | ALA  |
| 3   | N     | 1104 | GLU  |
| 3   | N     | 1306 | PRO  |
| 3   | N     | 1332 | PRO  |
| 3   | N     | 1385 | GLY  |
| 3   | N     | 1410 | GLU  |
| 3   | N     | 1454 | GLY  |
| 3   | N     | 1482 | ARG  |
| 1   | A     | 157  | GLY  |
| 1   | B     | 29   | GLU  |
| 1   | B     | 118  | ALA  |
| 1   | B     | 125  | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 188  | LYS  |
| 2   | C     | 278  | GLU  |
| 2   | C     | 646  | GLY  |
| 2   | C     | 738  | ASP  |
| 2   | C     | 740  | GLU  |
| 2   | C     | 904  | PRO  |
| 2   | C     | 984  | GLU  |
| 2   | C     | 1114 | GLY  |
| 3   | D     | 3    | LYS  |
| 3   | D     | 31   | THR  |
| 3   | D     | 119  | SER  |
| 3   | D     | 137  | PRO  |
| 3   | D     | 140  | ALA  |
| 3   | D     | 507  | ASN  |
| 3   | D     | 522  | PRO  |
| 3   | D     | 594  | PRO  |
| 3   | D     | 834  | THR  |
| 3   | D     | 844  | ALA  |
| 3   | D     | 869  | MET  |
| 3   | D     | 1111 | ASP  |
| 3   | D     | 1125 | PRO  |
| 3   | D     | 1138 | ALA  |
| 3   | D     | 1196 | THR  |
| 3   | D     | 1208 | ASP  |
| 3   | D     | 1385 | GLY  |
| 3   | D     | 1407 | LEU  |
| 4   | E     | 5    | GLY  |
| 4   | E     | 82   | GLU  |
| 1   | L     | 3    | ASP  |
| 1   | L     | 29   | GLU  |
| 1   | L     | 191  | ASP  |
| 2   | M     | 10   | ARG  |
| 2   | M     | 251  | ASP  |
| 2   | M     | 268  | ASP  |
| 2   | M     | 363  | SER  |
| 2   | M     | 366  | SER  |
| 2   | M     | 462  | ASP  |
| 2   | M     | 548  | PRO  |
| 2   | M     | 762  | LYS  |
| 2   | M     | 767  | PRO  |
| 3   | N     | 34   | TYR  |
| 3   | N     | 37   | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 96   | ALA  |
| 3   | N     | 98   | PRO  |
| 3   | N     | 137  | PRO  |
| 3   | N     | 160  | GLU  |
| 3   | N     | 564  | GLU  |
| 3   | N     | 594  | PRO  |
| 3   | N     | 696  | HIS  |
| 3   | N     | 822  | ALA  |
| 3   | N     | 834  | THR  |
| 3   | N     | 869  | MET  |
| 3   | N     | 1067 | VAL  |
| 3   | N     | 1111 | ASP  |
| 3   | N     | 1125 | PRO  |
| 3   | N     | 1161 | GLU  |
| 3   | N     | 1197 | ARG  |
| 3   | N     | 1237 | THR  |
| 3   | N     | 1315 | ASP  |
| 3   | N     | 1390 | LEU  |
| 3   | N     | 1407 | LEU  |
| 4   | O     | 40   | LEU  |
| 1   | B     | 73   | GLU  |
| 2   | C     | 18   | LEU  |
| 2   | C     | 111  | ASP  |
| 2   | C     | 462  | ASP  |
| 2   | C     | 1000 | MET  |
| 2   | C     | 1079 | PRO  |
| 3   | D     | 37   | LEU  |
| 3   | D     | 42   | ASP  |
| 3   | D     | 503  | LEU  |
| 3   | D     | 808  | THR  |
| 3   | D     | 1103 | HIS  |
| 3   | D     | 1207 | TYR  |
| 3   | D     | 1240 | THR  |
| 3   | D     | 1348 | LEU  |
| 3   | D     | 1390 | LEU  |
| 3   | D     | 1482 | ARG  |
| 4   | E     | 32   | ARG  |
| 4   | E     | 40   | LEU  |
| 4   | E     | 55   | PHE  |
| 1   | K     | 157  | GLY  |
| 1   | L     | 118  | ALA  |
| 2   | M     | 53   | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 111  | ASP  |
| 2   | M     | 188  | LYS  |
| 2   | M     | 205  | GLU  |
| 2   | M     | 326  | ASP  |
| 2   | M     | 646  | GLY  |
| 2   | M     | 904  | PRO  |
| 2   | M     | 1079 | PRO  |
| 2   | M     | 1114 | GLY  |
| 3   | N     | 119  | SER  |
| 3   | N     | 397  | LYS  |
| 3   | N     | 504  | ASP  |
| 3   | N     | 530  | VAL  |
| 3   | N     | 751  | LEU  |
| 3   | N     | 808  | THR  |
| 3   | N     | 924  | MET  |
| 3   | N     | 1276 | GLU  |
| 3   | N     | 1457 | ASP  |
| 4   | O     | 55   | PHE  |
| 4   | O     | 82   | GLU  |
| 1   | B     | 3    | ASP  |
| 1   | B     | 9    | PRO  |
| 1   | B     | 47   | SER  |
| 2   | C     | 39   | ARG  |
| 2   | C     | 74   | GLY  |
| 3   | D     | 124  | GLU  |
| 1   | K     | 224  | TYR  |
| 1   | L     | 9    | PRO  |
| 1   | L     | 126  | ASP  |
| 2   | M     | 18   | LEU  |
| 2   | M     | 39   | ARG  |
| 2   | M     | 74   | GLY  |
| 2   | M     | 141  | HIS  |
| 2   | M     | 467  | ILE  |
| 2   | M     | 1027 | PHE  |
| 3   | N     | 507  | ASN  |
| 3   | N     | 540  | LEU  |
| 3   | N     | 705  | ALA  |
| 3   | N     | 757  | ALA  |
| 3   | N     | 1138 | ALA  |
| 3   | N     | 1155 | VAL  |
| 3   | N     | 1341 | PRO  |
| 3   | N     | 1355 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | O     | 5    | GLY  |
| 1   | A     | 9    | PRO  |
| 1   | A     | 224  | TYR  |
| 2   | C     | 1024 | LYS  |
| 3   | D     | 108  | VAL  |
| 3   | D     | 523  | ASP  |
| 3   | D     | 751  | LEU  |
| 3   | D     | 920  | LEU  |
| 3   | D     | 1155 | VAL  |
| 3   | D     | 1205 | TYR  |
| 4   | E     | 57   | ASP  |
| 2   | M     | 377  | PRO  |
| 2   | M     | 400  | PRO  |
| 2   | M     | 765  | SER  |
| 3   | N     | 503  | LEU  |
| 3   | N     | 522  | PRO  |
| 3   | N     | 604  | THR  |
| 3   | N     | 668  | PRO  |
| 3   | N     | 1327 | ARG  |
| 4   | O     | 16   | LYS  |
| 4   | O     | 57   | ASP  |
| 1   | B     | 10   | VAL  |
| 2   | C     | 377  | PRO  |
| 2   | C     | 400  | PRO  |
| 2   | C     | 812  | GLY  |
| 3   | D     | 1341 | PRO  |
| 3   | D     | 1370 | ILE  |
| 1   | K     | 125  | PRO  |
| 2   | M     | 812  | GLY  |
| 3   | N     | 1128 | VAL  |
| 3   | N     | 1349 | VAL  |
| 2   | C     | 467  | ILE  |
| 3   | D     | 146  | PRO  |
| 3   | D     | 499  | VAL  |
| 3   | N     | 588  | GLY  |
| 2   | C     | 263  | ASP  |
| 3   | D     | 1050 | GLY  |
| 1   | L     | 10   | VAL  |
| 2   | M     | 113  | VAL  |
| 3   | N     | 548  | ILE  |
| 1   | A     | 125  | PRO  |
| 2   | C     | 113  | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 128  | ILE  |
| 2   | C     | 424  | GLY  |
| 3   | D     | 1349 | VAL  |
| 2   | M     | 424  | GLY  |
| 3   | N     | 499  | VAL  |
| 4   | O     | 81   | PRO  |
| 3   | D     | 668  | 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%)   | 181 (90%)  | 21 (10%)  | 7           | 23 |
| 1   | B     | 202/273 (74%)   | 180 (89%)  | 22 (11%)  | 6           | 22 |
| 1   | K     | 202/273 (74%)   | 183 (91%)  | 19 (9%)   | 8           | 27 |
| 1   | L     | 202/273 (74%)   | 177 (88%)  | 25 (12%)  | 4           | 18 |
| 2   | C     | 941/941 (100%)  | 775 (82%)  | 166 (18%) | 2           | 11 |
| 2   | M     | 941/941 (100%)  | 783 (83%)  | 158 (17%) | 2           | 12 |
| 3   | D     | 968/1279 (76%)  | 803 (83%)  | 165 (17%) | 2           | 12 |
| 3   | N     | 1088/1279 (85%) | 913 (84%)  | 175 (16%) | 2           | 13 |
| 4   | E     | 84/88 (96%)     | 66 (79%)   | 18 (21%)  | 1           | 6  |
| 4   | O     | 84/88 (96%)     | 69 (82%)   | 15 (18%)  | 2           | 11 |
| All | All   | 4914/5708 (86%) | 4130 (84%) | 784 (16%) | 2           | 13 |

All (784) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 25  | LEU  |
| 1   | A     | 26  | GLU  |
| 1   | A     | 54  | THR  |
| 1   | A     | 65  | PHE  |
| 1   | A     | 69  | PRO  |
| 1   | A     | 73  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 96  | THR  |
| 1   | A     | 100 | LEU  |
| 1   | A     | 101 | LEU  |
| 1   | A     | 104 | GLU  |
| 1   | A     | 126 | ASP  |
| 1   | A     | 139 | ASN  |
| 1   | A     | 141 | GLU  |
| 1   | A     | 154 | GLU  |
| 1   | A     | 168 | ASP  |
| 1   | A     | 175 | ARG  |
| 1   | A     | 189 | ARG  |
| 1   | A     | 197 | LEU  |
| 1   | A     | 206 | THR  |
| 1   | A     | 219 | ARG  |
| 1   | A     | 226 | SER  |
| 1   | B     | 3   | ASP  |
| 1   | B     | 34  | VAL  |
| 1   | B     | 62  | LEU  |
| 1   | B     | 73  | GLU  |
| 1   | B     | 81  | ASN  |
| 1   | B     | 83  | LYS  |
| 1   | B     | 96  | THR  |
| 1   | B     | 123 | MET  |
| 1   | B     | 124 | ASN  |
| 1   | B     | 140 | MET  |
| 1   | B     | 141 | GLU  |
| 1   | B     | 159 | LYS  |
| 1   | B     | 163 | ASN  |
| 1   | B     | 176 | ARG  |
| 1   | B     | 179 | PHE  |
| 1   | B     | 189 | ARG  |
| 1   | B     | 201 | THR  |
| 1   | B     | 206 | THR  |
| 1   | B     | 213 | GLN  |
| 1   | B     | 215 | VAL  |
| 1   | B     | 218 | LEU  |
| 1   | B     | 226 | SER  |
| 2   | C     | 5   | ARG  |
| 2   | C     | 9   | ILE  |
| 2   | C     | 30  | LEU  |
| 2   | C     | 33  | ASP  |
| 2   | C     | 34  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 48  | PHE  |
| 2   | C     | 51  | THR  |
| 2   | C     | 67  | ASP  |
| 2   | C     | 71  | TYR  |
| 2   | C     | 72  | ARG  |
| 2   | C     | 75  | GLU  |
| 2   | C     | 88  | LEU  |
| 2   | C     | 91  | GLN  |
| 2   | C     | 94  | LEU  |
| 2   | C     | 95  | TYR  |
| 2   | C     | 98  | LEU  |
| 2   | C     | 103 | LYS  |
| 2   | C     | 104 | ASP  |
| 2   | C     | 113 | VAL  |
| 2   | C     | 115 | LEU  |
| 2   | C     | 117 | HIS  |
| 2   | C     | 121 | MET  |
| 2   | C     | 129 | ILE  |
| 2   | C     | 133 | ASP  |
| 2   | C     | 141 | HIS  |
| 2   | C     | 142 | ARG  |
| 2   | C     | 158 | TYR  |
| 2   | C     | 170 | PRO  |
| 2   | C     | 173 | ASP  |
| 2   | C     | 179 | ASN  |
| 2   | C     | 186 | VAL  |
| 2   | C     | 188 | LYS  |
| 2   | C     | 190 | LYS  |
| 2   | C     | 194 | VAL  |
| 2   | C     | 196 | LEU  |
| 2   | C     | 198 | ARG  |
| 2   | C     | 205 | GLU  |
| 2   | C     | 209 | ARG  |
| 2   | C     | 210 | GLU  |
| 2   | C     | 211 | LEU  |
| 2   | C     | 224 | GLU  |
| 2   | C     | 237 | ARG  |
| 2   | C     | 238 | LEU  |
| 2   | C     | 239 | PHE  |
| 2   | C     | 243 | ARG  |
| 2   | C     | 252 | LYS  |
| 2   | C     | 261 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 266 | ARG  |
| 2   | C     | 267 | TYR  |
| 2   | C     | 268 | ASP  |
| 2   | C     | 274 | ARG  |
| 2   | C     | 275 | TYR  |
| 2   | C     | 281 | LEU  |
| 2   | C     | 285 | LEU  |
| 2   | C     | 289 | THR  |
| 2   | C     | 290 | LEU  |
| 2   | C     | 292 | ARG  |
| 2   | C     | 293 | PHE  |
| 2   | C     | 297 | GLU  |
| 2   | C     | 298 | PHE  |
| 2   | C     | 302 | VAL  |
| 2   | C     | 306 | THR  |
| 2   | C     | 308 | ARG  |
| 2   | C     | 309 | TYR  |
| 2   | C     | 313 | LEU  |
| 2   | C     | 321 | GLU  |
| 2   | C     | 322 | VAL  |
| 2   | C     | 327 | HIS  |
| 2   | C     | 330 | ASN  |
| 2   | C     | 345 | ARG  |
| 2   | C     | 358 | ARG  |
| 2   | C     | 359 | MET  |
| 2   | C     | 365 | ASP  |
| 2   | C     | 367 | LEU  |
| 2   | C     | 376 | ARG  |
| 2   | C     | 392 | SER  |
| 2   | C     | 398 | THR  |
| 2   | C     | 400 | PRO  |
| 2   | C     | 404 | LEU  |
| 2   | C     | 419 | THR  |
| 2   | C     | 422 | ARG  |
| 2   | C     | 433 | THR  |
| 2   | C     | 443 | THR  |
| 2   | C     | 453 | THR  |
| 2   | C     | 464 | LEU  |
| 2   | C     | 469 | THR  |
| 2   | C     | 474 | VAL  |
| 2   | C     | 486 | MET  |
| 2   | C     | 489 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 498 | GLN  |
| 2   | C     | 500 | ASN  |
| 2   | C     | 503 | LEU  |
| 2   | C     | 506 | ASN  |
| 2   | C     | 518 | LYS  |
| 2   | C     | 537 | LYS  |
| 2   | C     | 541 | SER  |
| 2   | C     | 548 | PRO  |
| 2   | C     | 557 | ARG  |
| 2   | C     | 571 | LEU  |
| 2   | C     | 578 | VAL  |
| 2   | C     | 584 | GLU  |
| 2   | C     | 599 | GLU  |
| 2   | C     | 602 | GLU  |
| 2   | C     | 606 | VAL  |
| 2   | C     | 617 | ASP  |
| 2   | C     | 620 | LEU  |
| 2   | C     | 621 | VAL  |
| 2   | C     | 632 | ASN  |
| 2   | C     | 635 | THR  |
| 2   | C     | 640 | ARG  |
| 2   | C     | 645 | VAL  |
| 2   | C     | 668 | LEU  |
| 2   | C     | 680 | ASP  |
| 2   | C     | 690 | ILE  |
| 2   | C     | 695 | LEU  |
| 2   | C     | 699 | PHE  |
| 2   | C     | 701 | THR  |
| 2   | C     | 714 | ASP  |
| 2   | C     | 727 | PRO  |
| 2   | C     | 728 | HIS  |
| 2   | C     | 738 | ASP  |
| 2   | C     | 739 | GLU  |
| 2   | C     | 751 | PRO  |
| 2   | C     | 766 | GLU  |
| 2   | C     | 780 | GLU  |
| 2   | C     | 784 | ASP  |
| 2   | C     | 785 | VAL  |
| 2   | C     | 796 | GLU  |
| 2   | C     | 805 | ARG  |
| 2   | C     | 815 | LEU  |
| 2   | C     | 830 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 839  | LEU  |
| 2   | C     | 841  | ASN  |
| 2   | C     | 856  | GLU  |
| 2   | C     | 858  | MET  |
| 2   | C     | 862  | PRO  |
| 2   | C     | 863  | ASP  |
| 2   | C     | 884  | GLN  |
| 2   | C     | 886  | LEU  |
| 2   | C     | 907  | ASP  |
| 2   | C     | 918  | LEU  |
| 2   | C     | 930  | LYS  |
| 2   | C     | 938  | LYS  |
| 2   | C     | 950  | LEU  |
| 2   | C     | 958  | THR  |
| 2   | C     | 963  | LEU  |
| 2   | C     | 984  | GLU  |
| 2   | C     | 986  | PRO  |
| 2   | C     | 988  | VAL  |
| 2   | C     | 999  | HIS  |
| 2   | C     | 1002 | GLU  |
| 2   | C     | 1003 | ASP  |
| 2   | C     | 1005 | MET  |
| 2   | C     | 1016 | ILE  |
| 2   | C     | 1018 | GLN  |
| 2   | C     | 1021 | LEU  |
| 2   | C     | 1026 | GLN  |
| 2   | C     | 1035 | MET  |
| 2   | C     | 1050 | GLN  |
| 2   | C     | 1074 | GLU  |
| 2   | C     | 1079 | PRO  |
| 2   | C     | 1090 | LYS  |
| 2   | C     | 1095 | LEU  |
| 2   | C     | 1105 | LYS  |
| 2   | C     | 1111 | ILE  |
| 2   | C     | 1115 | LEU  |
| 3   | D     | 4    | GLU  |
| 3   | D     | 6    | ARG  |
| 3   | D     | 21   | TRP  |
| 3   | D     | 29   | PRO  |
| 3   | D     | 41   | ARG  |
| 3   | D     | 47   | GLU  |
| 3   | D     | 60   | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 64  | LYS  |
| 3   | D     | 72  | VAL  |
| 3   | D     | 74  | GLU  |
| 3   | D     | 75  | ARG  |
| 3   | D     | 80  | VAL  |
| 3   | D     | 87  | ARG  |
| 3   | D     | 95  | LEU  |
| 3   | D     | 101 | HIS  |
| 3   | D     | 108 | VAL  |
| 3   | D     | 116 | LEU  |
| 3   | D     | 123 | LEU  |
| 3   | D     | 124 | GLU  |
| 3   | D     | 127 | LEU  |
| 3   | D     | 130 | SER  |
| 3   | D     | 135 | LEU  |
| 3   | D     | 142 | LEU  |
| 3   | D     | 157 | GLU  |
| 3   | D     | 162 | ARG  |
| 3   | D     | 163 | TYR  |
| 3   | D     | 456 | MET  |
| 3   | D     | 465 | LEU  |
| 3   | D     | 470 | LEU  |
| 3   | D     | 485 | SER  |
| 3   | D     | 493 | ARG  |
| 3   | D     | 512 | MET  |
| 3   | D     | 525 | ARG  |
| 3   | D     | 531 | ASP  |
| 3   | D     | 537 | THR  |
| 3   | D     | 538 | SER  |
| 3   | D     | 544 | TYR  |
| 3   | D     | 550 | ARG  |
| 3   | D     | 565 | ILE  |
| 3   | D     | 594 | PRO  |
| 3   | D     | 600 | LEU  |
| 3   | D     | 619 | LEU  |
| 3   | D     | 624 | ASP  |
| 3   | D     | 633 | VAL  |
| 3   | D     | 636 | GLN  |
| 3   | D     | 639 | LEU  |
| 3   | D     | 641 | GLN  |
| 3   | D     | 644 | LEU  |
| 3   | D     | 651 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 652 | LEU  |
| 3   | D     | 660 | LYS  |
| 3   | D     | 670 | VAL  |
| 3   | D     | 686 | GLU  |
| 3   | D     | 688 | TRP  |
| 3   | D     | 694 | VAL  |
| 3   | D     | 701 | LEU  |
| 3   | D     | 709 | HIS  |
| 3   | D     | 734 | GLU  |
| 3   | D     | 736 | PHE  |
| 3   | D     | 749 | VAL  |
| 3   | D     | 758 | GLU  |
| 3   | D     | 763 | MET  |
| 3   | D     | 764 | LEU  |
| 3   | D     | 783 | ARG  |
| 3   | D     | 784 | ASP  |
| 3   | D     | 792 | ILE  |
| 3   | D     | 805 | GLU  |
| 3   | D     | 813 | LEU  |
| 3   | D     | 835 | SER  |
| 3   | D     | 842 | VAL  |
| 3   | D     | 863 | VAL  |
| 3   | D     | 865 | THR  |
| 3   | D     | 879 | ARG  |
| 3   | D     | 880 | ILE  |
| 3   | D     | 888 | GLU  |
| 3   | D     | 892 | ASP  |
| 3   | D     | 897 | TRP  |
| 3   | D     | 899 | LEU  |
| 3   | D     | 900 | ILE  |
| 3   | D     | 902 | LEU  |
| 3   | D     | 907 | GLU  |
| 3   | D     | 917 | GLN  |
| 3   | D     | 922 | LEU  |
| 3   | D     | 925 | GLU  |
| 3   | D     | 935 | LYS  |
| 3   | D     | 937 | TYR  |
| 3   | D     | 940 | THR  |
| 3   | D     | 941 | PHE  |
| 3   | D     | 942 | SER  |
| 3   | D     | 951 | ILE  |
| 3   | D     | 959 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 964  | LEU  |
| 3   | D     | 983  | LEU  |
| 3   | D     | 985  | ASP  |
| 3   | D     | 988  | ARG  |
| 3   | D     | 991  | GLN  |
| 3   | D     | 1001 | GLU  |
| 3   | D     | 1008 | PHE  |
| 3   | D     | 1019 | PRO  |
| 3   | D     | 1023 | MET  |
| 3   | D     | 1026 | SER  |
| 3   | D     | 1036 | ARG  |
| 3   | D     | 1038 | LEU  |
| 3   | D     | 1039 | CYS  |
| 3   | D     | 1041 | LEU  |
| 3   | D     | 1042 | ARG  |
| 3   | D     | 1044 | LEU  |
| 3   | D     | 1052 | THR  |
| 3   | D     | 1062 | ARG  |
| 3   | D     | 1068 | LEU  |
| 3   | D     | 1087 | ARG  |
| 3   | D     | 1088 | THR  |
| 3   | D     | 1094 | LEU  |
| 3   | D     | 1095 | THR  |
| 3   | D     | 1100 | ASP  |
| 3   | D     | 1108 | ARG  |
| 3   | D     | 1112 | CYS  |
| 3   | D     | 1119 | SER  |
| 3   | D     | 1130 | ARG  |
| 3   | D     | 1133 | ARG  |
| 3   | D     | 1149 | LEU  |
| 3   | D     | 1151 | ARG  |
| 3   | D     | 1153 | VAL  |
| 3   | D     | 1161 | GLU  |
| 3   | D     | 1166 | LEU  |
| 3   | D     | 1169 | ASP  |
| 3   | D     | 1179 | GLU  |
| 3   | D     | 1183 | ILE  |
| 3   | D     | 1189 | ARG  |
| 3   | D     | 1196 | THR  |
| 3   | D     | 1197 | ARG  |
| 3   | D     | 1204 | CYS  |
| 3   | D     | 1207 | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1209 | LEU  |
| 3   | D     | 1223 | ILE  |
| 3   | D     | 1231 | GLU  |
| 3   | D     | 1237 | THR  |
| 3   | D     | 1238 | MET  |
| 3   | D     | 1240 | THR  |
| 3   | D     | 1253 | THR  |
| 3   | D     | 1344 | VAL  |
| 3   | D     | 1382 | THR  |
| 3   | D     | 1389 | LEU  |
| 3   | D     | 1391 | GLU  |
| 3   | D     | 1396 | GLU  |
| 3   | D     | 1399 | ASP  |
| 3   | D     | 1412 | LYS  |
| 3   | D     | 1424 | VAL  |
| 3   | D     | 1431 | THR  |
| 3   | D     | 1432 | LYS  |
| 3   | D     | 1436 | SER  |
| 3   | D     | 1439 | SER  |
| 3   | D     | 1441 | GLN  |
| 3   | D     | 1442 | ASN  |
| 3   | D     | 1447 | LEU  |
| 3   | D     | 1462 | LEU  |
| 3   | D     | 1464 | GLU  |
| 3   | D     | 1465 | ASN  |
| 3   | D     | 1466 | VAL  |
| 3   | D     | 1472 | ILE  |
| 3   | D     | 1485 | GLN  |
| 3   | D     | 1488 | ASP  |
| 3   | D     | 1489 | GLN  |
| 3   | D     | 1496 | GLU  |
| 3   | D     | 1501 | GLU  |
| 4   | E     | 10   | PHE  |
| 4   | E     | 14   | ASP  |
| 4   | E     | 31   | LEU  |
| 4   | E     | 33   | HIS  |
| 4   | E     | 42   | PRO  |
| 4   | E     | 43   | GLU  |
| 4   | E     | 44   | GLU  |
| 4   | E     | 46   | PRO  |
| 4   | E     | 51   | LEU  |
| 4   | E     | 57   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | E     | 62  | THR  |
| 4   | E     | 68  | LEU  |
| 4   | E     | 69  | LEU  |
| 4   | E     | 70  | THR  |
| 4   | E     | 77  | GLU  |
| 4   | E     | 78  | ASN  |
| 4   | E     | 83  | ASP  |
| 4   | E     | 95  | VAL  |
| 1   | K     | 5   | LYS  |
| 1   | K     | 18  | ARG  |
| 1   | K     | 22  | GLU  |
| 1   | K     | 26  | GLU  |
| 1   | K     | 54  | THR  |
| 1   | K     | 60  | ASP  |
| 1   | K     | 65  | PHE  |
| 1   | K     | 73  | GLU  |
| 1   | K     | 86  | VAL  |
| 1   | K     | 101 | LEU  |
| 1   | K     | 123 | MET  |
| 1   | K     | 141 | GLU  |
| 1   | K     | 155 | LYS  |
| 1   | K     | 168 | ASP  |
| 1   | K     | 175 | ARG  |
| 1   | K     | 180 | GLN  |
| 1   | K     | 189 | ARG  |
| 1   | K     | 208 | LEU  |
| 1   | K     | 219 | ARG  |
| 1   | L     | 2   | LEU  |
| 1   | L     | 5   | LYS  |
| 1   | L     | 25  | LEU  |
| 1   | L     | 36  | LEU  |
| 1   | L     | 58  | ILE  |
| 1   | L     | 62  | LEU  |
| 1   | L     | 73  | GLU  |
| 1   | L     | 101 | LEU  |
| 1   | L     | 119 | ASP  |
| 1   | L     | 123 | MET  |
| 1   | L     | 124 | ASN  |
| 1   | L     | 126 | ASP  |
| 1   | L     | 129 | ILE  |
| 1   | L     | 141 | GLU  |
| 1   | L     | 145 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 159 | LYS  |
| 1   | L     | 162 | ILE  |
| 1   | L     | 163 | ASN  |
| 1   | L     | 176 | ARG  |
| 1   | L     | 179 | PHE  |
| 1   | L     | 184 | THR  |
| 1   | L     | 186 | LEU  |
| 1   | L     | 206 | THR  |
| 1   | L     | 213 | GLN  |
| 1   | L     | 215 | VAL  |
| 2   | M     | 9   | ILE  |
| 2   | M     | 10  | ARG  |
| 2   | M     | 30  | LEU  |
| 2   | M     | 34  | VAL  |
| 2   | M     | 44  | ILE  |
| 2   | M     | 49  | ARG  |
| 2   | M     | 75  | GLU  |
| 2   | M     | 88  | LEU  |
| 2   | M     | 89  | THR  |
| 2   | M     | 91  | GLN  |
| 2   | M     | 95  | TYR  |
| 2   | M     | 98  | LEU  |
| 2   | M     | 104 | ASP  |
| 2   | M     | 110 | GLU  |
| 2   | M     | 112 | GLU  |
| 2   | M     | 115 | LEU  |
| 2   | M     | 129 | ILE  |
| 2   | M     | 130 | ASN  |
| 2   | M     | 133 | ASP  |
| 2   | M     | 142 | ARG  |
| 2   | M     | 144 | PRO  |
| 2   | M     | 158 | TYR  |
| 2   | M     | 163 | ILE  |
| 2   | M     | 170 | PRO  |
| 2   | M     | 173 | ASP  |
| 2   | M     | 177 | GLU  |
| 2   | M     | 178 | PRO  |
| 2   | M     | 186 | VAL  |
| 2   | M     | 190 | LYS  |
| 2   | M     | 198 | ARG  |
| 2   | M     | 205 | GLU  |
| 2   | M     | 210 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 211 | LEU  |
| 2   | M     | 216 | GLU  |
| 2   | M     | 218 | VAL  |
| 2   | M     | 221 | LEU  |
| 2   | M     | 226 | VAL  |
| 2   | M     | 237 | ARG  |
| 2   | M     | 238 | LEU  |
| 2   | M     | 252 | LYS  |
| 2   | M     | 261 | ILE  |
| 2   | M     | 267 | TYR  |
| 2   | M     | 271 | GLU  |
| 2   | M     | 274 | ARG  |
| 2   | M     | 285 | LEU  |
| 2   | M     | 286 | SER  |
| 2   | M     | 289 | THR  |
| 2   | M     | 293 | PHE  |
| 2   | M     | 297 | GLU  |
| 2   | M     | 307 | LEU  |
| 2   | M     | 308 | ARG  |
| 2   | M     | 309 | TYR  |
| 2   | M     | 310 | LEU  |
| 2   | M     | 321 | GLU  |
| 2   | M     | 328 | LEU  |
| 2   | M     | 358 | ARG  |
| 2   | M     | 359 | MET  |
| 2   | M     | 360 | LEU  |
| 2   | M     | 367 | LEU  |
| 2   | M     | 376 | ARG  |
| 2   | M     | 379 | GLU  |
| 2   | M     | 383 | ARG  |
| 2   | M     | 390 | GLN  |
| 2   | M     | 396 | ASP  |
| 2   | M     | 404 | LEU  |
| 2   | M     | 410 | ILE  |
| 2   | M     | 421 | GLU  |
| 2   | M     | 433 | THR  |
| 2   | M     | 434 | HIS  |
| 2   | M     | 449 | ILE  |
| 2   | M     | 455 | LEU  |
| 2   | M     | 490 | GLU  |
| 2   | M     | 491 | GLU  |
| 2   | M     | 498 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 503 | LEU  |
| 2   | M     | 508 | ILE  |
| 2   | M     | 517 | ARG  |
| 2   | M     | 518 | LYS  |
| 2   | M     | 528 | GLU  |
| 2   | M     | 554 | ASP  |
| 2   | M     | 557 | ARG  |
| 2   | M     | 572 | ILE  |
| 2   | M     | 578 | VAL  |
| 2   | M     | 579 | VAL  |
| 2   | M     | 584 | GLU  |
| 2   | M     | 585 | GLU  |
| 2   | M     | 586 | ARG  |
| 2   | M     | 588 | VAL  |
| 2   | M     | 595 | LEU  |
| 2   | M     | 620 | LEU  |
| 2   | M     | 630 | ARG  |
| 2   | M     | 632 | ASN  |
| 2   | M     | 633 | GLN  |
| 2   | M     | 635 | THR  |
| 2   | M     | 640 | ARG  |
| 2   | M     | 644 | VAL  |
| 2   | M     | 645 | VAL  |
| 2   | M     | 668 | LEU  |
| 2   | M     | 677 | MET  |
| 2   | M     | 683 | ASN  |
| 2   | M     | 685 | GLU  |
| 2   | M     | 688 | ILE  |
| 2   | M     | 689 | VAL  |
| 2   | M     | 693 | GLU  |
| 2   | M     | 699 | PHE  |
| 2   | M     | 703 | ILE  |
| 2   | M     | 719 | PRO  |
| 2   | M     | 727 | PRO  |
| 2   | M     | 730 | SER  |
| 2   | M     | 738 | ASP  |
| 2   | M     | 748 | GLU  |
| 2   | M     | 749 | VAL  |
| 2   | M     | 780 | GLU  |
| 2   | M     | 784 | ASP  |
| 2   | M     | 785 | VAL  |
| 2   | M     | 787 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | M     | 791  | ARG  |
| 2   | M     | 805  | ARG  |
| 2   | M     | 824  | ARG  |
| 2   | M     | 834  | GLN  |
| 2   | M     | 856  | GLU  |
| 2   | M     | 862  | PRO  |
| 2   | M     | 863  | ASP  |
| 2   | M     | 878  | SER  |
| 2   | M     | 881  | ASN  |
| 2   | M     | 884  | GLN  |
| 2   | M     | 904  | PRO  |
| 2   | M     | 916  | GLU  |
| 2   | M     | 918  | LEU  |
| 2   | M     | 923  | GLU  |
| 2   | M     | 929  | ARG  |
| 2   | M     | 937  | ASP  |
| 2   | M     | 938  | LYS  |
| 2   | M     | 939  | ARG  |
| 2   | M     | 942  | GLU  |
| 2   | M     | 950  | LEU  |
| 2   | M     | 958  | THR  |
| 2   | M     | 960  | GLU  |
| 2   | M     | 963  | LEU  |
| 2   | M     | 981  | GLU  |
| 2   | M     | 988  | VAL  |
| 2   | M     | 999  | HIS  |
| 2   | M     | 1003 | ASP  |
| 2   | M     | 1004 | LYS  |
| 2   | M     | 1005 | MET  |
| 2   | M     | 1006 | HIS  |
| 2   | M     | 1016 | ILE  |
| 2   | M     | 1021 | LEU  |
| 2   | M     | 1030 | GLN  |
| 2   | M     | 1035 | MET  |
| 2   | M     | 1053 | LEU  |
| 2   | M     | 1070 | ILE  |
| 2   | M     | 1079 | PRO  |
| 2   | M     | 1104 | GLU  |
| 2   | M     | 1105 | LYS  |
| 2   | M     | 1107 | ASN  |
| 2   | M     | 1111 | ILE  |
| 2   | M     | 1115 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | N     | 5   | VAL  |
| 3   | N     | 12  | LEU  |
| 3   | N     | 21  | TRP  |
| 3   | N     | 34  | TYR  |
| 3   | N     | 41  | ARG  |
| 3   | N     | 56  | TYR  |
| 3   | N     | 60  | CYS  |
| 3   | N     | 64  | LYS  |
| 3   | N     | 69  | GLU  |
| 3   | N     | 74  | GLU  |
| 3   | N     | 76  | CYS  |
| 3   | N     | 80  | VAL  |
| 3   | N     | 82  | LYS  |
| 3   | N     | 85  | VAL  |
| 3   | N     | 87  | ARG  |
| 3   | N     | 90  | MET  |
| 3   | N     | 103 | TRP  |
| 3   | N     | 112 | ILE  |
| 3   | N     | 116 | LEU  |
| 3   | N     | 118 | LEU  |
| 3   | N     | 124 | GLU  |
| 3   | N     | 127 | LEU  |
| 3   | N     | 128 | TYR  |
| 3   | N     | 135 | LEU  |
| 3   | N     | 145 | VAL  |
| 3   | N     | 148 | GLU  |
| 3   | N     | 149 | LYS  |
| 3   | N     | 150 | ARG  |
| 3   | N     | 153 | LEU  |
| 3   | N     | 156 | GLU  |
| 3   | N     | 157 | GLU  |
| 3   | N     | 161 | LEU  |
| 3   | N     | 179 | VAL  |
| 3   | N     | 197 | SER  |
| 3   | N     | 199 | LEU  |
| 3   | N     | 410 | SER  |
| 3   | N     | 434 | ARG  |
| 3   | N     | 438 | ASP  |
| 3   | N     | 441 | ARG  |
| 3   | N     | 453 | ASP  |
| 3   | N     | 455 | ARG  |
| 3   | N     | 456 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | N     | 465 | LEU  |
| 3   | N     | 467 | GLU  |
| 3   | N     | 470 | LEU  |
| 3   | N     | 476 | GLU  |
| 3   | N     | 481 | MET  |
| 3   | N     | 493 | ARG  |
| 3   | N     | 512 | MET  |
| 3   | N     | 525 | ARG  |
| 3   | N     | 537 | THR  |
| 3   | N     | 539 | ASP  |
| 3   | N     | 547 | LEU  |
| 3   | N     | 550 | ARG  |
| 3   | N     | 565 | ILE  |
| 3   | N     | 576 | GLU  |
| 3   | N     | 581 | LEU  |
| 3   | N     | 594 | PRO  |
| 3   | N     | 600 | LEU  |
| 3   | N     | 611 | GLN  |
| 3   | N     | 619 | LEU  |
| 3   | N     | 639 | LEU  |
| 3   | N     | 641 | GLN  |
| 3   | N     | 651 | GLU  |
| 3   | N     | 652 | LEU  |
| 3   | N     | 660 | LYS  |
| 3   | N     | 666 | ILE  |
| 3   | N     | 670 | VAL  |
| 3   | N     | 688 | TRP  |
| 3   | N     | 701 | LEU  |
| 3   | N     | 707 | THR  |
| 3   | N     | 709 | HIS  |
| 3   | N     | 710 | ARG  |
| 3   | N     | 727 | GLN  |
| 3   | N     | 736 | PHE  |
| 3   | N     | 749 | VAL  |
| 3   | N     | 758 | GLU  |
| 3   | N     | 763 | MET  |
| 3   | N     | 764 | LEU  |
| 3   | N     | 772 | PRO  |
| 3   | N     | 778 | LEU  |
| 3   | N     | 792 | ILE  |
| 3   | N     | 805 | GLU  |
| 3   | N     | 808 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 816  | HIS  |
| 3   | N     | 817  | GLU  |
| 3   | N     | 855  | HIS  |
| 3   | N     | 863  | VAL  |
| 3   | N     | 864  | VAL  |
| 3   | N     | 873  | LEU  |
| 3   | N     | 876  | SER  |
| 3   | N     | 880  | ILE  |
| 3   | N     | 881  | LEU  |
| 3   | N     | 891  | GLU  |
| 3   | N     | 892  | ASP  |
| 3   | N     | 897  | TRP  |
| 3   | N     | 902  | LEU  |
| 3   | N     | 914  | LEU  |
| 3   | N     | 922  | LEU  |
| 3   | N     | 925  | GLU  |
| 3   | N     | 939  | PHE  |
| 3   | N     | 941  | PHE  |
| 3   | N     | 951  | ILE  |
| 3   | N     | 959  | GLU  |
| 3   | N     | 965  | GLU  |
| 3   | N     | 975  | GLU  |
| 3   | N     | 982  | PHE  |
| 3   | N     | 990  | ASP  |
| 3   | N     | 991  | GLN  |
| 3   | N     | 994  | GLN  |
| 3   | N     | 1023 | MET  |
| 3   | N     | 1029 | ARG  |
| 3   | N     | 1062 | ARG  |
| 3   | N     | 1087 | ARG  |
| 3   | N     | 1101 | VAL  |
| 3   | N     | 1108 | ARG  |
| 3   | N     | 1114 | THR  |
| 3   | N     | 1115 | THR  |
| 3   | N     | 1124 | GLN  |
| 3   | N     | 1135 | ARG  |
| 3   | N     | 1149 | LEU  |
| 3   | N     | 1151 | ARG  |
| 3   | N     | 1159 | ARG  |
| 3   | N     | 1160 | LEU  |
| 3   | N     | 1161 | GLU  |
| 3   | N     | 1166 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 1183 | ILE  |
| 3   | N     | 1189 | ARG  |
| 3   | N     | 1193 | THR  |
| 3   | N     | 1207 | TYR  |
| 3   | N     | 1210 | SER  |
| 3   | N     | 1237 | THR  |
| 3   | N     | 1238 | MET  |
| 3   | N     | 1260 | ILE  |
| 3   | N     | 1262 | LEU  |
| 3   | N     | 1267 | ARG  |
| 3   | N     | 1274 | ILE  |
| 3   | N     | 1275 | SER  |
| 3   | N     | 1282 | ARG  |
| 3   | N     | 1285 | GLU  |
| 3   | N     | 1287 | GLU  |
| 3   | N     | 1288 | GLU  |
| 3   | N     | 1291 | SER  |
| 3   | N     | 1294 | VAL  |
| 3   | N     | 1297 | GLU  |
| 3   | N     | 1299 | PHE  |
| 3   | N     | 1300 | SER  |
| 3   | N     | 1305 | LEU  |
| 3   | N     | 1311 | LEU  |
| 3   | N     | 1317 | ASP  |
| 3   | N     | 1319 | VAL  |
| 3   | N     | 1320 | GLU  |
| 3   | N     | 1326 | THR  |
| 3   | N     | 1330 | ILE  |
| 3   | N     | 1336 | LEU  |
| 3   | N     | 1337 | GLU  |
| 3   | N     | 1344 | VAL  |
| 3   | N     | 1348 | LEU  |
| 3   | N     | 1375 | MET  |
| 3   | N     | 1376 | MET  |
| 3   | N     | 1383 | ASP  |
| 3   | N     | 1389 | LEU  |
| 3   | N     | 1391 | GLU  |
| 3   | N     | 1412 | LYS  |
| 3   | N     | 1422 | MET  |
| 3   | N     | 1431 | THR  |
| 3   | N     | 1432 | LYS  |
| 3   | N     | 1435 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | N     | 1441 | GLN  |
| 3   | N     | 1455 | LYS  |
| 3   | N     | 1465 | ASN  |
| 3   | N     | 1472 | ILE  |
| 3   | N     | 1485 | GLN  |
| 3   | N     | 1488 | ASP  |
| 3   | N     | 1496 | GLU  |
| 4   | O     | 23   | VAL  |
| 4   | O     | 37   | ASN  |
| 4   | O     | 38   | THR  |
| 4   | O     | 46   | PRO  |
| 4   | O     | 48   | MET  |
| 4   | O     | 51   | LEU  |
| 4   | O     | 54   | LEU  |
| 4   | O     | 56   | ASP  |
| 4   | O     | 57   | ASP  |
| 4   | O     | 58   | PRO  |
| 4   | O     | 70   | THR  |
| 4   | O     | 72   | ARG  |
| 4   | O     | 77   | GLU  |
| 4   | O     | 81   | PRO  |
| 4   | O     | 83   | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 38   | ASN  |
| 2   | C     | 91   | GLN  |
| 2   | C     | 860  | HIS  |
| 2   | C     | 884  | GLN  |
| 2   | C     | 1019 | GLN  |
| 2   | C     | 1047 | HIS  |
| 3   | D     | 748  | HIS  |
| 3   | D     | 816  | HIS  |
| 3   | D     | 976  | GLN  |
| 3   | D     | 1014 | ASN  |
| 3   | D     | 1103 | HIS  |
| 3   | D     | 1124 | GLN  |
| 3   | D     | 1172 | HIS  |
| 3   | D     | 1227 | GLN  |
| 3   | D     | 1235 | GLN  |
| 1   | L     | 91   | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L     | 212  | ASN  |
| 1   | L     | 213  | GLN  |
| 2   | M     | 179  | ASN  |
| 2   | M     | 393  | GLN  |
| 2   | M     | 406  | HIS  |
| 2   | M     | 434  | HIS  |
| 2   | M     | 567  | GLN  |
| 2   | M     | 632  | ASN  |
| 2   | M     | 841  | ASN  |
| 2   | M     | 845  | ASN  |
| 2   | M     | 889  | HIS  |
| 3   | N     | 151  | GLN  |
| 3   | N     | 669  | ASN  |
| 3   | N     | 744  | GLN  |
| 3   | N     | 748  | HIS  |
| 3   | N     | 861  | GLN  |
| 3   | N     | 1010 | ASN  |
| 3   | N     | 1031 | ASN  |
| 3   | N     | 1033 | GLN  |
| 3   | N     | 1034 | GLN  |
| 3   | N     | 1116 | ASN  |
| 4   | O     | 29   | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 6   | H     | 15/16 (93%) | 5 (33%)           | 1 (6%)          |
| 6   | Y     | 14/16 (87%) | 3 (21%)           | 1 (7%)          |
| All | All   | 29/32 (90%) | 8 (27%)           | 2 (6%)          |

All (8) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | H     | 4   | G    |
| 6   | H     | 5   | C    |
| 6   | H     | 6   | C    |
| 6   | H     | 15  | C    |
| 6   | H     | 16  | A    |
| 6   | Y     | 3   | A    |
| 6   | Y     | 4   | G    |
| 6   | Y     | 6   | C    |

All (2) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | H     | 5   | C    |
| 6   | Y     | 5   | C    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 1   | A     | 229/315 (72%)    | -0.94  | 0 100 100     | 154, 243, 347, 432    | 0     |
| 1   | B     | 229/315 (72%)    | -0.81  | 0 100 100     | 202, 343, 460, 525    | 0     |
| 1   | K     | 229/315 (72%)    | -0.86  | 1 (0%) 88 77  | 157, 255, 375, 500    | 0     |
| 1   | L     | 229/315 (72%)    | -0.79  | 0 100 100     | 193, 363, 452, 538    | 0     |
| 2   | C     | 1119/1119 (100%) | -0.90  | 2 (0%) 91 83  | 12, 213, 336, 454     | 0     |
| 2   | M     | 1119/1119 (100%) | -0.90  | 3 (0%) 90 80  | 60, 238, 426, 549     | 0     |
| 3   | D     | 1151/1524 (75%)  | -0.93  | 4 (0%) 90 80  | 8, 205, 382, 548      | 0     |
| 3   | N     | 1288/1524 (84%)  | -0.94  | 2 (0%) 91 83  | 81, 249, 452, 545     | 0     |
| 4   | E     | 95/99 (95%)      | -0.97  | 0 100 100     | 156, 217, 337, 395    | 0     |
| 4   | O     | 95/99 (95%)      | -0.87  | 1 (1%) 78 62  | 205, 297, 426, 451    | 0     |
| 5   | G     | 27/28 (96%)      | -0.72  | 0 100 100     | 152, 210, 372, 381    | 0     |
| 5   | X     | 27/28 (96%)      | -0.63  | 0 100 100     | 238, 279, 353, 374    | 0     |
| 6   | H     | 16/16 (100%)     | -0.82  | 0 100 100     | 97, 189, 363, 385     | 0     |
| 6   | Y     | 15/16 (93%)      | -0.90  | 0 100 100     | 208, 249, 351, 378    | 0     |
| 7   | I     | 17/21 (80%)      | -0.64  | 0 100 100     | 215, 276, 418, 428    | 0     |
| 7   | Z     | 17/21 (80%)      | -0.72  | 0 100 100     | 264, 305, 348, 352    | 0     |
| All | All   | 5902/6874 (85%)  | -0.90  | 13 (0%) 91 83 | 8, 240, 416, 549      | 0     |

All (13) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | D     | 626  | SER  | 4.6  |
| 2   | M     | 416  | GLY  | 4.1  |
| 3   | D     | 146  | PRO  | 4.0  |
| 3   | N     | 801  | GLY  | 3.2  |
| 2   | C     | 1024 | LYS  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | D     | 625  | TYR  | 2.5  |
| 2   | M     | 1024 | LYS  | 2.5  |
| 2   | M     | 193  | LEU  | 2.3  |
| 3   | N     | 802  | ALA  | 2.2  |
| 3   | D     | 801  | GLY  | 2.2  |
| 1   | K     | 66   | SER  | 2.1  |
| 4   | O     | 2    | ALA  | 2.1  |
| 2   | C     | 570  | PRO  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 8   | ZN   | D     | 1601 | 1/1   | 1.00 | 0.06 | 72,72,72,72                | 0     |
| 8   | ZN   | D     | 1602 | 1/1   | 1.00 | 0.01 | 72,72,72,72                | 0     |
| 8   | ZN   | N     | 1601 | 1/1   | 1.00 | 0.01 | 72,72,72,72                | 0     |
| 8   | ZN   | N     | 1602 | 1/1   | 1.00 | 0.00 | 72,72,72,72                | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.