



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:50 AM UTC

PDB ID : 2O5J / pdb\_00002o5j  
Title : Crystal structure of the T. thermophilus RNAP polymerase elongation complex with the NTP substrate analog  
Authors : Vassilyev, D.G.; Vassilyeva, M.N.  
Deposited on : 2006-12-06  
Resolution : 3.00 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                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| 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                                                             |

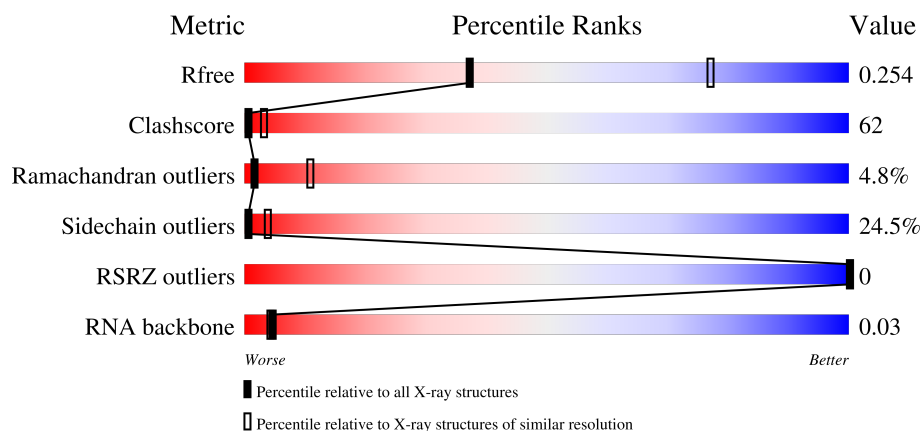
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



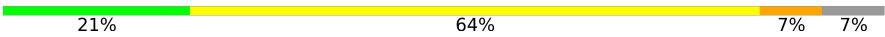
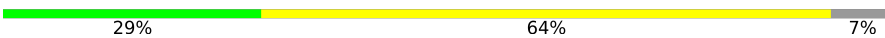
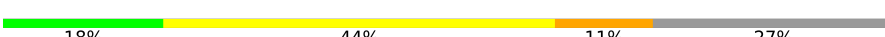
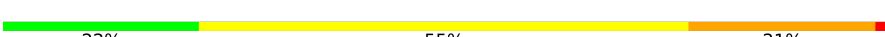
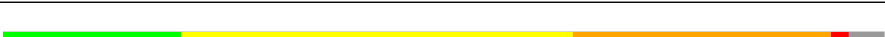
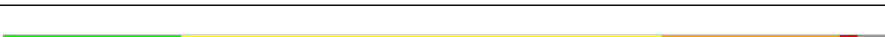
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2672 (3.00-3.00)                                      |
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |
| RSRZ outliers         | 180081                      | 2671 (3.00-3.00)                                      |
| RNA backbone          | 3983                        | 1109 (3.20-2.80)                                      |

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   | G     | 23     | <div> <div>22%</div> <div>43%</div> <div>30%</div> <div>.</div> </div> |
| 1   | X     | 23     | <div> <div>22%</div> <div>48%</div> <div>26%</div> <div>.</div> </div> |
| 2   | H     | 16     | <div> <div>12%</div> <div>25%</div> <div>62%</div> </div>              |
| 2   | Y     | 16     | <div> <div>19%</div> <div>44%</div> <div>38%</div> </div>              |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 3   | I     | 14     |  |
| 3   | Z     | 14     |  |
| 4   | A     | 315    |  |
| 4   | B     | 315    |  |
| 4   | K     | 315    |  |
| 4   | L     | 315    |  |
| 5   | C     | 1119   |  |
| 5   | M     | 1119   |  |
| 6   | D     | 1524   |  |
| 6   | N     | 1524   |  |
| 7   | E     | 99     |  |
| 7   | O     | 99     |  |

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 51213 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 DNA chain called 5'-D(P\*CP\*CP\*CP\*TP\*GP\*TP\*CP\*TP\*GP\*GP\*CP\*GP\*TP\*TP\*CP\*GP\*CP\*GP\*CP\*GP\*CP\*GP\*CP\*G)-3'.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 1   | G     | 23       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 467   | 220 | 80 | 144 | 23 |         |         |       |
| 1   | X     | 23       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 467   | 220 | 80 | 144 | 23 |         |         |       |

- Molecule 2 is a RNA chain called 5'-R(P\*GP\*AP\*GP\*UP\*CP\*UP\*GP\*CP\*GP\*GP\*CP\*GP\*CP\*GP\*CP\*G)-3'.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 2   | H     | 16       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 347   | 153 | 64 | 114 | 16 |         |         |       |
| 2   | Y     | 16       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 347   | 153 | 64 | 114 | 16 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 3   | I     | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 270   | 126 | 57 | 74 | 13 |         |         |       |
| 3   | Z     | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 270   | 126 | 57 | 74 | 13 |         |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase alpha chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | A     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1806  | 1153 | 313 | 337 | 3 |         |         |       |
| 4   | B     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1806  | 1153 | 313 | 337 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | K     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1806  | 1153 | 313 | 337 | 3 |         |         |       |
| 4   | L     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1806  | 1153 | 313 | 337 | 3 |         |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerase beta chain.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 5   | C     | 1119     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8829  | 5581 | 1577 | 1647 | 24 |         |         |       |
| 5   | M     | 1119     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8829  | 5581 | 1577 | 1647 | 24 |         |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerase beta' chain.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 6   | D     | 1264     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9960  | 6302 | 1773 | 1852 | 33 |         |         |       |
| 6   | N     | 1264     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9960  | 6302 | 1773 | 1852 | 33 |         |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerase omega chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | E     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 770   | 491 | 133 | 142 | 4 |         |         |       |
| 7   | O     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 770   | 491 | 133 | 142 | 4 |         |         |       |

- 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  |         |         |

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

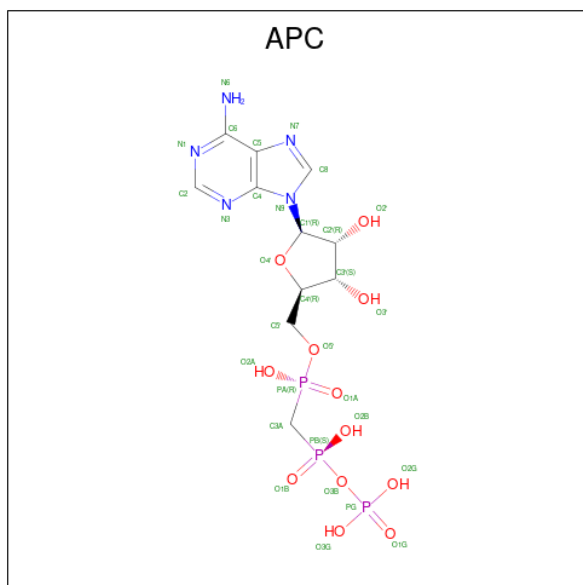
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | D     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | N     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 10 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 10  | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 11 | 5 | 12 | 3 |         |         |
| 10  | N     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 11 | 5 | 12 | 3 |         |         |

- Molecule 11 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 11  | G     | 32       | Total | O  | 0       | 0       |
|     |       |          | 32    | 32 |         |         |
| 11  | H     | 37       | Total | O  | 0       | 0       |
|     |       |          | 37    | 37 |         |         |
| 11  | I     | 22       | Total | O  | 0       | 0       |
|     |       |          | 22    | 22 |         |         |
| 11  | X     | 43       | Total | O  | 0       | 0       |
|     |       |          | 43    | 43 |         |         |
| 11  | Y     | 30       | Total | O  | 0       | 0       |
|     |       |          | 30    | 30 |         |         |
| 11  | Z     | 30       | Total | O  | 0       | 0       |
|     |       |          | 30    | 30 |         |         |

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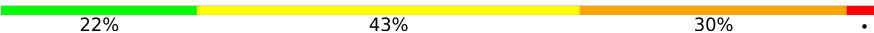
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 11  | A     | 106      | Total<br>106 | O<br>106 | 0       | 0       |
| 11  | B     | 82       | Total<br>82  | O<br>82  | 0       | 0       |
| 11  | C     | 482      | Total<br>482 | O<br>482 | 0       | 0       |
| 11  | D     | 506      | Total<br>506 | O<br>506 | 0       | 0       |
| 11  | E     | 60       | Total<br>60  | O<br>60  | 0       | 0       |
| 11  | K     | 86       | Total<br>86  | O<br>86  | 0       | 0       |
| 11  | L     | 104      | Total<br>104 | O<br>104 | 0       | 0       |
| 11  | M     | 483      | Total<br>483 | O<br>483 | 0       | 0       |
| 11  | N     | 491      | Total<br>491 | O<br>491 | 0       | 0       |
| 11  | O     | 39       | Total<br>39  | O<br>39  | 0       | 0       |

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

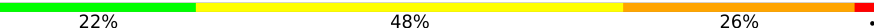
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5'-D(P\*CP\*CP\*CP\*TP\*GP\*TP\*CP\*TP\*GP\*GP\*CP\*GP\*TP\*TP\*CP\*GP\*CP\*GP\*CP\*GP\*CP\*CP\*G)-3'

Chain G: 



- Molecule 1: 5'-D(P\*CP\*CP\*CP\*TP\*GP\*TP\*CP\*TP\*GP\*GP\*CP\*GP\*TP\*TP\*CP\*GP\*CP\*GP\*CP\*GP\*CP\*CP\*G)-3'

Chain X: 



- Molecule 2: 5'-R(P\*GP\*AP\*GP\*UP\*CP\*UP\*GP\*CP\*GP\*GP\*CP\*GP\*CP\*GP\*CP\*G)-3',

Chain H: 



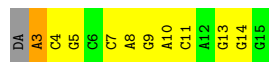
- Molecule 2: 5'-R(P\*GP\*AP\*GP\*UP\*CP\*UP\*GP\*CP\*GP\*GP\*CP\*GP\*CP\*GP\*CP\*G)-3',

Chain Y: 



- Molecule 3: 5'-D(\*AP\*AP\*CP\*GP\*CP\*CP\*AP\*GP\*AP\*CP\*AP\*GP\*GP\*G)-3'

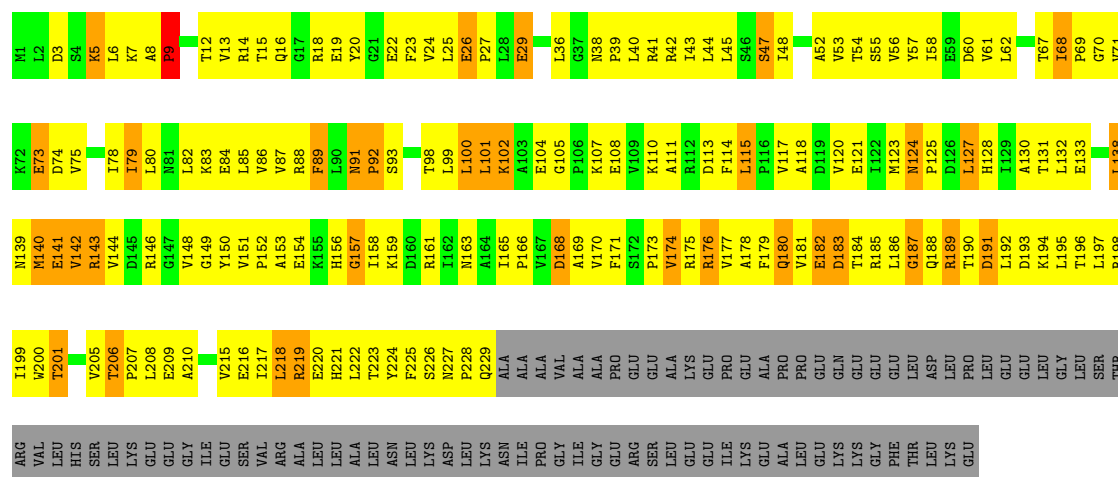
Chain I: 



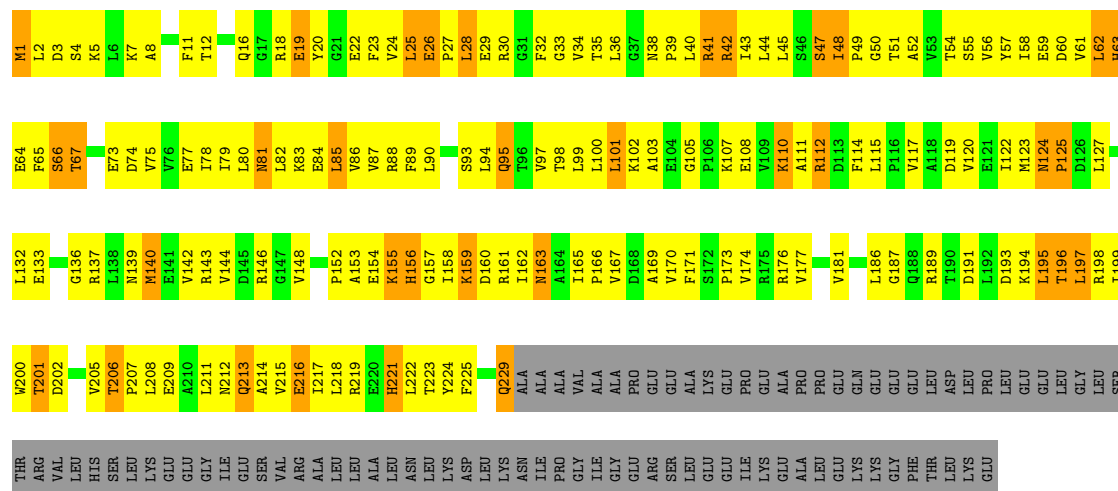
- Molecule 3: 5'-D(\*AP\*AP\*CP\*GP\*CP\*CP\*AP\*GP\*AP\*CP\*AP\*GP\*GP\*G)-3'



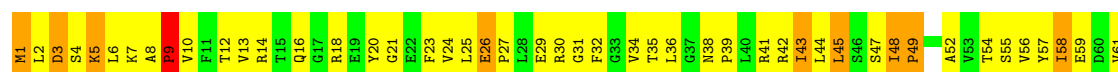
Chain A:  19% 42% 11% 27%

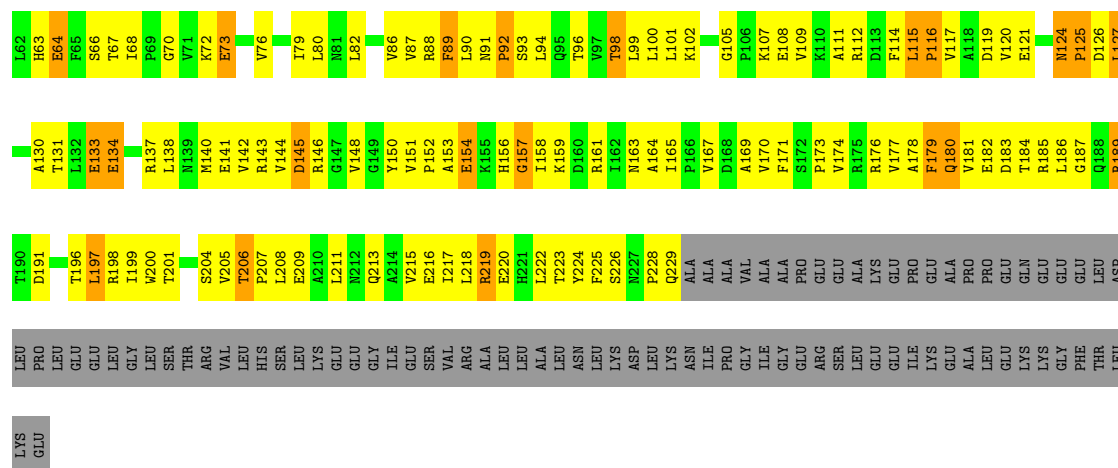


Chain B:  20% 42% 11% 27%

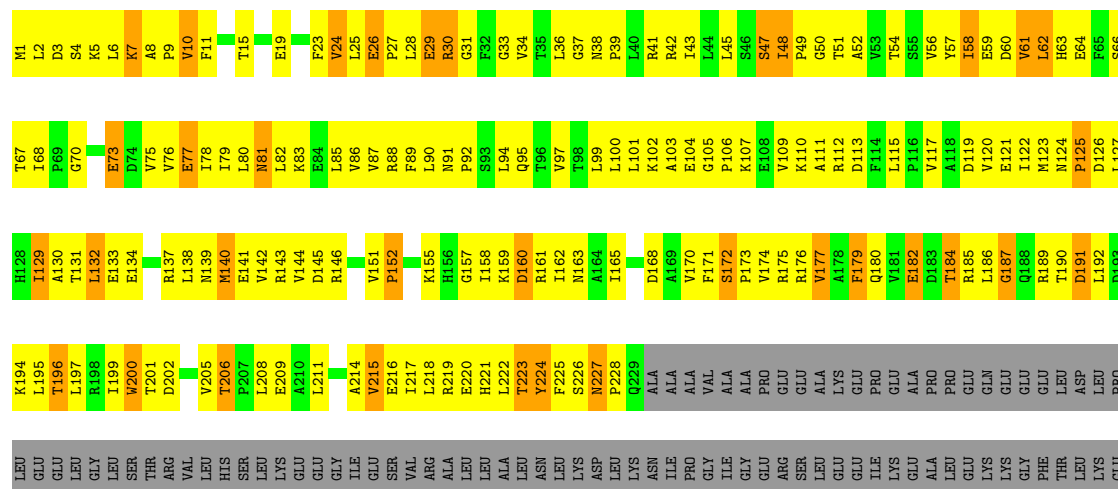
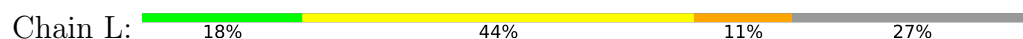


Chain K:  20% 43% 10% 27%

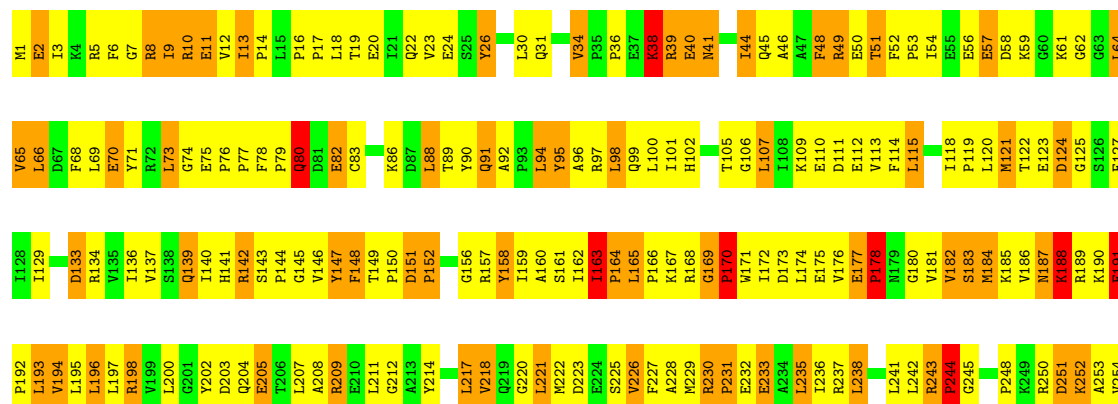




• Molecule 4: DNA-directed RNA polymerase alpha chain



• Molecule 5: DNA-directed RNA polymerase beta chain



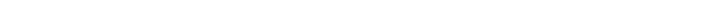


|       |      |      |      |      |      |       |      |      |      |      |      |      |      |      |      |      |
|-------|------|------|------|------|------|-------|------|------|------|------|------|------|------|------|------|------|
| Q1030 | Q969 | L968 | Q899 | G988 | G836 | L773  | G644 | V579 | A515 | T403 | L378 | V317 | A253 | V186 | G125 | G63  |
| R1031 | Q970 | G970 | R900 | G989 | D837 | L774  | V645 | M580 | R516 | P444 | A381 | P318 | V254 | M187 | S126 | L64  |
| F1032 | R971 | R775 | R839 | T581 | G582 | E711  | G646 | T581 | R517 | G451 | R189 | G319 | A255 | K188 | F127 | V65  |
| G1033 | R972 | S776 | A840 | G583 | L583 | A712  | Q647 | G582 | R518 | L451 | R382 | H320 | V256 | R189 | L128 | L66  |
| E1034 | S973 | T777 | V649 | E584 | E520 | D714  | V649 | E584 | E520 | T453 | R383 | E321 | V257 | K190 | I129 | D67  |
| L1035 | R974 | G779 | R650 | E585 | P521 | T715  | R650 | E585 | P521 | S454 | F385 | D323 | G259 | F191 | N130 | F68  |
| E1036 | P906 | E780 | G651 | R586 | F522 | K716  | G651 | R586 | F522 | L455 | F386 | D324 | L260 | P192 | G131 | L69  |
| V1037 | F906 | K781 | G652 | V587 | V523 | L717  | G652 | V587 | V523 | A456 | S387 | I325 | I261 | V194 | A132 | E70  |
| W1038 | G977 | A782 | R719 | V588 | V524 | G718  | L654 | V588 | V524 | A457 | R388 | I326 | A262 | L196 | D133 | R72  |
| A1039 | R978 | R783 | F719 | R589 | S525 | F719  | L654 | R589 | S525 | Y458 | G327 | H327 | D263 | L195 | V135 | L73  |
| L1040 | G980 | D784 | E720 | R593 | P526 | E720  | L655 | R593 | P526 | A459 | S392 | L328 | P264 | L197 | L136 | G74  |
| Y1043 | E911 | V785 | R721 | A593 | E527 | R721  | L656 | A593 | E527 | R460 | Q393 | G329 | R265 | R198 | W137 | E75  |
| G1044 | P912 | K786 | D657 | A594 | E528 | L722  | D657 | A594 | E528 | V461 | F394 | N330 | R266 | V199 | P76  | P76  |
| A1045 | E913 | T788 | G658 | L596 | V529 | I726  | G658 | L596 | V529 | D462 | K395 | R331 | Y267 | G331 | S138 | P77  |
| H1046 | R983 | F788 | P659 | E530 | E530 | F727  | P659 | E530 | E530 | D463 | K396 | R332 | D268 | L200 | I140 | F78  |
| H1047 | E984 | S789 | A660 | A597 | F531 | H728  | A660 | A597 | F531 | L464 | E397 | I333 | L269 | G204 | H141 | F79  |
| T1048 | R985 | L790 | S661 | E598 | M532 | R729  | S661 | E598 | M532 | G465 | T398 | R334 | G270 | Q204 | R142 | Q80  |
| L1049 | P854 | R791 | E662 | E599 | D533 | L729  | E662 | E599 | D533 | F466 | N399 | T335 | E271 | E205 | S143 | D81  |
| L1050 | R855 | V792 | N633 | D600 | V534 | S730  | N633 | D600 | V534 | L467 | P400 | V336 | A272 | T206 | P144 | E82  |
| Q1051 | E856 | F793 | G664 | G601 | S535 | E731  | G664 | G601 | S535 | R468 | L401 | G337 | G273 | L207 | G145 | C83  |
| E1052 | R857 | P794 | F665 | E602 | P536 | A732  | F665 | E602 | P536 | T469 | S402 | E338 | R274 | A208 | V146 | R84  |
| L1053 | P859 | G798 | L666 | V603 | K537 | A733  | L666 | V603 | K537 | P470 | S403 | L339 | Y275 | R209 | Y147 | E85  |
| T1054 | R860 | I799 | A667 | A604 | Q538 | L734  | A667 | A604 | Q538 | Y471 | L404 | M340 | K276 | E210 | F148 | K86  |
| L1055 | F926 | R735 | L668 | K605 | V539 | R735  | L668 | K605 | V539 | R472 | R405 | T341 | G212 | L211 | T149 | D87  |
| G1056 | G927 | D736 | G689 | V606 | F540 | D736  | G689 | V606 | F540 | R473 | H406 | D842 | K280 | G212 | P150 | L88  |
| S1057 | R928 | L737 | Q670 | D607 | S541 | L737  | Q670 | D607 | S541 | Y474 | K407 | Q343 | L281 | E216 | D151 | T89  |
| L1058 | R929 | D738 | N671 | G608 | V542 | E739  | N671 | G608 | V542 | V478 | R408 | F344 | G282 | P152 | Y90  | Y90  |
| D1059 | G931 | E740 | L673 | R610 | N543 | E740  | L673 | R610 | N543 | V479 | R409 | I283 | R284 | A153 | R154 | Q91  |
| Y1060 | E932 | G741 | V674 | L611 | L546 | G741  | V674 | L611 | L546 | T480 | S411 | V346 | R284 | V218 | A154 | G91  |
| E1061 | R806 | V742 | A675 | V612 | T547 | V742  | A675 | V612 | T547 | V483 | A412 | L348 | S286 | L221 | P155 | L94  |
| G1062 | D807 | F743 | L676 | V613 | F549 | F743  | L676 | V613 | F549 | V484 | A413 | A349 | G287 | M222 | G156 | Y85  |
| R1063 | R808 | R744 | N677 | R614 | F549 | R744  | N677 | R614 | F549 | Y485 | G414 | R350 | R288 | R157 | A96  | A96  |
| A1065 | G809 | L745 | P678 | V615 | L550 | L745  | P678 | V615 | L550 | M486 | G416 | R351 | T289 | D223 | Y158 | R97  |
| A1066 | P811 | E748 | F679 | E616 | E551 | E748  | F679 | E616 | E551 | T487 | G417 | A352 | L290 | E224 | I159 | L98  |
| W1067 | G812 | G812 | D680 | D617 | D552 | G812  | D680 | D617 | D552 | A488 | L418 | R353 | A291 | S225 | A160 | Q99  |
| I1070 | E813 | E813 | F684 | R619 | D564 | E813  | F684 | R619 | D564 | T489 | T419 | G354 | R292 | V226 | S161 | L100 |
| R1008 | E814 | E814 | E686 | L620 | R557 | E814  | E686 | L620 | R557 | E490 | R422 | R358 | D295 | R230 | I163 | I101 |
| S1009 | R816 | R816 | D686 | V621 | G561 | R816  | D686 | V621 | G561 | Y494 | A423 | M359 | G296 | P231 | P164 | H102 |
| T1010 | R817 | R817 | A687 | E622 | M560 | R817  | A687 | E622 | M560 | T495 | G424 | L360 | K299 | E232 | L165 | K103 |
| G1073 | P817 | P817 | L688 | V623 | G561 | P817  | L688 | V623 | G561 | T496 | G425 | M361 | D300 | E233 | P166 | G106 |
| E1074 | R819 | R819 | L690 | P624 | M564 | R819  | L690 | P624 | M564 | T496 | D426 | G362 | E301 | E234 | G169 | L107 |
| D1075 | R820 | R820 | S691 | R626 | T566 | R820  | S691 | R626 | T566 | A497 | V427 | E364 | D300 | E235 | P170 | L108 |
| G1076 | R821 | R821 | E692 | R627 | T566 | R821  | E692 | R627 | T566 | Q498 | V430 | D365 | E301 | L235 | W171 | K109 |
| E1077 | R822 | R822 | E693 | F628 | Q567 | R822  | E693 | F628 | Q567 | P502 | H431 | L241 | F303 | G239 | D172 | E110 |
| P1079 | R823 | R823 | L694 | V629 | Q567 | R823  | L694 | V629 | Q567 | L503 | R432 | L242 | L304 | F239 | D173 | D111 |
| S1080 | R824 | R824 | L695 | R630 | A568 | R824  | L695 | R630 | A568 | L503 | R432 | L242 | L304 | G239 | D174 | E112 |
| Q1018 | R886 | R886 | K696 | S631 | V569 | Q1018 | K696 | S631 | V569 | M506 | T433 | T368 | T306 | E244 | E177 | F114 |
| E1081 | E887 | E887 | R697 | N632 | P570 | E887  | R697 | N632 | P570 | H434 | R432 | T368 | L307 | R243 | G116 | G116 |
| P1082 | R888 | R888 | D698 | Q633 | L571 | P1082 | D698 | Q633 | L571 | Y435 | A370 | R369 | L307 | P244 | P178 | H117 |
| S1084 | H889 | H889 | F699 | Q633 | L571 | S1084 | F699 | Q633 | L571 | T508 | G436 | R371 | Y309 | G246 | N179 | I118 |
| R1085 | E961 | E961 | Y700 | L637 | I572 | R1085 | Y700 | L637 | I572 | A509 | R437 | L372 | F311 | D247 | G180 | P119 |
| G1023 | R831 | R831 | T768 | T701 | A574 | G1023 | T768 | T701 | A574 | R573 | L372 | V373 | F311 | P248 | V181 | L120 |
| K1024 | R832 | R832 | P769 | S702 | Q575 | K1024 | P769 | S702 | Q575 | B511 | C439 | N374 | A312 | K249 | V182 | M121 |
| A1025 | R833 | R833 | E770 | I703 | A576 | A1025 | E770 | I703 | A576 | B512 | P440 | S375 | L313 | R250 | S183 | L122 |
| V1089 | Q834 | Q834 | E771 | H704 | P577 | V1089 | Q834 | E771 | H704 | V513 | V441 | R376 | T314 | K252 | M184 | E123 |
| F1027 | V835 | V835 | R772 | I705 | V578 | F1027 | V835 | R772 | I705 | V514 | E442 | P377 | G252 | K185 | K185 | D124 |

Chain D:  20% 46% 16% • 17%





Chain N:  20% 47% 15% • 17%



|       |       |       |       |      |      |      |      |      |      |      |     |     |      |
|-------|-------|-------|-------|------|------|------|------|------|------|------|-----|-----|------|
| D1139 | H1075 | I947  | I880  | A814 | L751 | A690 | S626 | F502 | R441 | PRO  | MET | ALA | L191 |
| I1140 |       | T948  | L881  | A815 |      | L691 | S627 | L503 | N442 | GLU  | PRO | GLU | A192 |
| E1141 | R1078 | I949  | F882  | H816 | F754 | E692 | R628 |      | V443 | GLU  | ARG | GLU | P193 |
| A1142 | K1079 | G950  | A883  | E817 | A755 | E693 | S629 | G506 | V444 | GLN  | ARG | GLU | G194 |
| G1143 | G1080 | I951  | R884  | R818 | Q756 | V694 | V630 | R507 | R445 | VAL  | VAL | GLY | V195 |
| L1144 | G1081 | D952  | T885  | G819 | A757 | V695 | V631 | R508 | V446 | ILE  | ARG | VAL | R198 |
| V1145 | A1082 | D953  | V886  | E820 | E758 | H696 | V632 | P509 | V447 | ALA  | ALA | VAL | L199 |
| G1146 | D1083 | D954  | A887  | V821 | A759 |      | V633 | E510 | E448 | GLU  | ALA | GLU |      |
| R1147 | V955  | A954  | A888  | V822 | R760 | V699 | G634 | M511 | S449 | ALA  | GLN | LEU | V202 |
| L1148 | A1085 | V956  | A889  | L823 | L761 | V700 | P635 | M512 | V450 | VAL  | VAL | GLY | A203 |
| L1149 | L1086 | P957  | V890  | R824 | Q762 | L701 | Q636 | I513 | D451 | GLY  | GLU | GLU | L204 |
| A1150 | R1087 | E958  |       | A825 | V763 | L702 | L637 | L514 | I452 | VAL  | ALA | LEU | Y205 |
| R1151 | E959  | G959  | E893  | P826 | M764 | R703 | R638 | E515 | D453 | VAL  | GLU | GLU | R206 |
| E1152 | K960  | K960  | F894  | I827 | S765 | R704 | L639 | A516 | A454 | HIS  | GLU | GLU | P207 |
| V1153 | K961  | R828  | R895  | R828 |      |      | H640 | V517 | R455 | LEU  | GLU | GLY |      |
| E1154 | Q962  | V829  | A896  | R829 | M768 | P706 | H641 | P518 | M456 | HIS  | GLY | ALA |      |
| V1155 | R897  | A830  | R897  | A830 | L769 | T707 | C642 | V519 | C457 | GLU  | GLU | PHE |      |
| L1156 | L964  | P963  | E898  | G831 | L770 | L708 | G643 | L520 | A458 | THR  | THR | VAL |      |
| G1157 | L965  | E965  | L899  | R832 | S771 | H709 | L644 | P521 | E459 | VAL  | VAL | VAL |      |
| V1158 | E966  | E966  | I900  | E833 | P772 | R710 | P645 | P522 | A460 | A391 | TYR | ARG |      |
| R1159 | A967  | A967  | Q901  | E834 | A773 | L711 | R646 | D523 | I393 | S392 | LEU | ARG |      |
| K1097 | D968  | R968  | L902  | S835 | S774 | G712 | R647 | D531 | L394 | I393 | THR | ARG |      |
| E1161 | L1098 | R969  | D903  | V836 | G775 | L713 | R648 | C532 | Q462 | V395 | LEU | GLU |      |
| G1162 | E1099 | K970  | V904  | C837 | V776 | Q714 |      | P526 | L464 | V396 | PHE | ASP |      |
| E1163 | D1100 | L971  | P905  | R838 | P777 | A715 | E651 | M527 | L465 | K397 | LEU | GLU |      |
| R1164 | V1101 | L972  | Q906  | L839 | L778 | F716 | L652 | V528 | K466 | A398 | GLU | PRO |      |
| V1165 | H1102 | Q973  | E907  | R840 | A779 | Q717 | F653 | Q529 | E467 | R399 | THR | VAL |      |
| L1166 | L1103 | R1042 | K908  | Y841 | K780 | L786 | R654 | V530 | L468 | V400 | THR | VAL |      |
| S1167 | E1104 | G1043 |       |      | P781 | V719 | P655 | D531 | D469 | Y401 | GLU | THR |      |
| M1168 | I1105 | L1044 | L911  | A844 | S782 | L720 | F656 | C532 | L470 | P402 | PRO | THR |      |
| D1169 | V1106 | M1045 | K912  | N845 | R783 | V721 | L657 | G533 | E471 | F403 | LYS | PHE |      |
| D1170 | V1107 | Q1046 | D913  | P846 | D784 | E722 | L658 | R534 | A472 | S404 | ASP | LEU |      |
| V1171 | R1108 | L1047 | L914  | R847 | L785 | G723 | K659 |      | L473 | D405 | TYR | PRO |      |
|       | E1109 | P1048 | V915  | E848 | L786 | Q724 | K660 | T537 | E474 | D406 | ARG | VAL |      |
| L1174 | A1110 | S1049 | Y916  | L851 | L787 | S725 | M661 | S638 | K475 | V407 | VAL | GLY |      |
|       | D1111 | G1050 | Q917  |      | G788 | I726 |      | D539 | E476 | E408 | GLN | MET |      |
| G1112 | G1112 | E1051 | A918  | A852 | L789 | Q727 |      | L540 | L477 | V409 | PRO | THR |      |
| G1113 | G1113 | T1052 | F919  | V853 | V790 | L728 |      | N541 | L478 |      | HIS | PRO |      |
| T1114 | T1114 | F1053 | I920  |      | Y791 | H729 |      | D542 | D413 |      | NET | LEU |      |
| Q1184 | T1115 | E1054 | R921  | T857 | I792 | P730 |      | L543 | E479 | D413 | ASN | VAL |      |
| E1185 | N1116 | P1055 | L922  | V858 | T793 | L731 |      | Y544 | M481 | R414 | VAL | VAL |      |
| V1186 | Y1117 | P1056 | Q923  | D859 | Q794 | V732 |      | R545 | K482 | V415 | VAL | HIS |      |
| P1187 | I1118 | P1057 | N924  | L860 | V795 | G733 |      | R546 | H483 | A416 | VAL | GLY |      |
| V1188 | S1119 | R1058 | F925  | O861 | R796 | E734 |      | I547 | P484 | L421 | PRO | GLU |      |
| R1189 | V1120 | S1059 | K926  | D862 | K797 | A735 |      | I548 | S485 | A422 | GLU | ILE |      |
| S1190 | P1121 | S1060 |       | V863 | E798 | V736 |      | N549 | R486 |      | GLY | VAL |      |
| P1191 | L1122 | F1061 | R929  | V864 | K799 | A738 |      | N551 | K426 | V427 | ARG | GLY |      |
| L1192 | F1123 | E1062 | I930  |      | K800 | D739 |      | N552 | R489 |      | VAL | VAL |      |
| T1193 | Q1124 | R1063 | L934  | Y868 | G803 | F740 |      | R553 | K490 | D430 | GLU | GLN |      |
| C1194 | P1125 | G1064 | K935  | H869 | L804 | D741 |      | R554 | K491 | V431 | ALA | PRO |      |
| Q1195 |       | L1065 | T1000 | G870 | E805 | G742 |      |      | R492 | Y432 | GLY | LEU |      |
| T1196 | V1128 | T1066 | E1001 | R871 | F806 | D682 |      |      | K493 | G433 | ASP | ALA |      |
| R1197 | T1129 | V1067 | K1002 | H872 | A807 | D743 |      |      | R494 | R434 | LYS | GLU |      |
|       | R1130 | V1003 | V1003 | L873 | A807 | Q744 |      |      | R495 | V435 | ILE | ALA |      |
|       |       |       |       | T808 | T808 | V745 |      |      | L496 | V435 | VAL | LYS |      |
| V1200 | L1134 | V1007 |       | T875 | P809 | K746 |      |      | E497 | V437 | VAL | GLY |      |
| C1201 | R1135 | F1068 | T943  | S876 | E810 | V747 |      |      | V498 | V437 | ALA | TYR |      |
| Q1202 | K1136 | K1009 | T944  | P877 | E811 | H748 |      |      | V499 | D438 | ALA | LEU |      |
| L1203 | R1137 | N1010 | S945  | R877 | A812 | V749 |      |      | P663 | L438 | ILE | PHE |      |
| C1204 | A1138 | F1011 | G946  | R879 | L813 | P750 |      |      | A501 | V440 | ASP | ARG |      |



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 41                                                        | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 152.34Å 152.34Å 524.57Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 40.00 – 3.00<br>40.00 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 89.3 (40.00-3.00)<br>83.5 (40.00-3.00)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | 0.08                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.51 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.225 , 0.257<br>0.229 , 0.254                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 11219 reflections (5.70%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 64.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.049                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 142.7                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$ | Xtriage          |
| Estimated twinning fraction                                             | 0.146 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 51213                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 61.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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, APC, MG

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | G     | 0.56         | 0/520           | 1.09        | 4/798 (0.5%)     |
| 1   | X     | 0.62         | 0/520           | 1.10        | 4/798 (0.5%)     |
| 2   | H     | 1.12         | 1/387 (0.3%)    | 2.04        | 19/601 (3.2%)    |
| 2   | Y     | 1.04         | 1/387 (0.3%)    | 2.05        | 13/601 (2.2%)    |
| 3   | I     | 0.43         | 0/304           | 0.78        | 0/467            |
| 3   | Z     | 0.43         | 0/304           | 0.76        | 0/467            |
| 4   | A     | 0.77         | 0/1838          | 1.07        | 6/2498 (0.2%)    |
| 4   | B     | 0.84         | 1/1838 (0.1%)   | 1.05        | 5/2498 (0.2%)    |
| 4   | K     | 0.83         | 1/1838 (0.1%)   | 1.12        | 7/2498 (0.3%)    |
| 4   | L     | 0.86         | 1/1838 (0.1%)   | 1.09        | 2/2498 (0.1%)    |
| 5   | C     | 0.90         | 6/8997 (0.1%)   | 1.26        | 58/12164 (0.5%)  |
| 5   | M     | 0.90         | 7/8997 (0.1%)   | 1.24        | 65/12164 (0.5%)  |
| 6   | D     | 0.91         | 7/10128 (0.1%)  | 1.25        | 74/13681 (0.5%)  |
| 6   | N     | 0.90         | 11/10128 (0.1%) | 1.23        | 68/13681 (0.5%)  |
| 7   | E     | 1.01         | 6/784 (0.8%)    | 1.51        | 17/1057 (1.6%)   |
| 7   | O     | 0.97         | 3/784 (0.4%)    | 1.62        | 16/1057 (1.5%)   |
| All | All   | 0.89         | 45/49592 (0.1%) | 1.25        | 358/67528 (0.5%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | G     | 0                   | 6                   |
| 1   | X     | 0                   | 5                   |
| 2   | H     | 0                   | 2                   |
| 2   | Y     | 0                   | 1                   |
| 3   | I     | 0                   | 1                   |
| All | All   | 0                   | 15                  |

All (45) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | H     | 1    | G    | OP3-P | 12.69 | 1.73        | 1.48     |
| 5   | M     | 163  | ILE  | CA-CB | 9.89  | 1.64        | 1.53     |
| 2   | Y     | 1    | G    | OP3-P | 9.61  | 1.67        | 1.48     |
| 5   | C     | 163  | ILE  | CA-CB | 9.01  | 1.63        | 1.53     |
| 7   | E     | 94   | PRO  | N-CA  | 7.96  | 1.58        | 1.47     |
| 7   | O     | 94   | PRO  | N-CA  | 7.61  | 1.57        | 1.47     |
| 6   | D     | 1114 | THR  | CA-CB | 7.37  | 1.62        | 1.53     |
| 5   | M     | 423  | ALA  | CA-C  | 7.15  | 1.60        | 1.52     |
| 6   | N     | 90   | MET  | SD-CE | -6.92 | 1.62        | 1.79     |
| 6   | D     | 396  | VAL  | N-CA  | -6.89 | 1.38        | 1.46     |
| 5   | C     | 995  | MET  | SD-CE | -6.68 | 1.62        | 1.79     |
| 6   | N     | 145  | VAL  | CA-C  | 6.66  | 1.58        | 1.52     |
| 5   | M     | 425  | PHE  | N-CA  | 6.62  | 1.54        | 1.46     |
| 7   | E     | 93   | TYR  | CA-C  | 6.59  | 1.60        | 1.52     |
| 6   | N     | 1416 | ALA  | CA-CB | -6.53 | 1.44        | 1.53     |
| 6   | N     | 1114 | THR  | CA-CB | 6.33  | 1.60        | 1.52     |
| 6   | N     | 427  | VAL  | CA-CB | 6.27  | 1.60        | 1.53     |
| 5   | M     | 988  | VAL  | CA-CB | 6.16  | 1.61        | 1.54     |
| 6   | N     | 147  | VAL  | CA-CB | 6.12  | 1.61        | 1.54     |
| 4   | L     | 165  | ILE  | CA-CB | 5.84  | 1.59        | 1.54     |
| 7   | E     | 24   | ALA  | CA-CB | -5.70 | 1.44        | 1.53     |
| 7   | O     | 93   | TYR  | CA-C  | 5.68  | 1.59        | 1.52     |
| 7   | E     | 93   | TYR  | C-N   | 5.65  | 1.41        | 1.33     |
| 6   | N     | 136  | ASP  | CA-C  | 5.64  | 1.59        | 1.52     |
| 5   | M     | 474  | VAL  | CA-CB | 5.59  | 1.62        | 1.54     |
| 6   | D     | 1375 | MET  | SD-CE | -5.52 | 1.65        | 1.79     |
| 7   | E     | 94   | PRO  | C-N   | -5.50 | 1.27        | 1.34     |
| 5   | C     | 488  | ALA  | CA-CB | -5.50 | 1.44        | 1.53     |
| 7   | O     | 93   | TYR  | C-N   | 5.36  | 1.40        | 1.33     |
| 5   | C     | 988  | VAL  | CA-CB | 5.35  | 1.60        | 1.54     |
| 6   | D     | 1330 | ILE  | CA-C  | 5.33  | 1.59        | 1.52     |
| 5   | C     | 1001 | VAL  | CA-CB | 5.32  | 1.60        | 1.54     |
| 6   | N     | 481  | MET  | SD-CE | 5.30  | 1.92        | 1.79     |
| 4   | K     | 98   | THR  | CA-CB | 5.30  | 1.60        | 1.53     |
| 6   | N     | 1379 | VAL  | CA-CB | 5.27  | 1.61        | 1.54     |
| 6   | D     | 1095 | THR  | CA-CB | 5.25  | 1.61        | 1.53     |
| 6   | N     | 131  | LYS  | CA-C  | 5.18  | 1.58        | 1.53     |
| 6   | D     | 416  | ALA  | CA-C  | 5.15  | 1.57        | 1.52     |
| 7   | E     | 42   | PRO  | CA-C  | 5.09  | 1.59        | 1.52     |
| 6   | D     | 1237 | THR  | CA-CB | -5.07 | 1.44        | 1.53     |
| 5   | M     | 424  | GLY  | CA-C  | 5.07  | 1.59        | 1.51     |
| 6   | N     | 1379 | VAL  | CA-C  | 5.07  | 1.59        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 5   | M     | 1001 | VAL  | CA-CB | 5.05 | 1.60        | 1.54     |
| 4   | B     | 98   | THR  | CA-CB | 5.04 | 1.59        | 1.53     |
| 5   | C     | 474  | VAL  | CA-CB | 5.03 | 1.61        | 1.54     |

All (358) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 7   | O     | 94   | PRO  | N-CA-C      | 17.16  | 136.15      | 113.84   |
| 7   | E     | 94   | PRO  | N-CA-C      | 16.23  | 135.55      | 113.65   |
| 7   | O     | 93   | TYR  | CA-C-N      | 15.96  | 135.84      | 119.56   |
| 7   | O     | 93   | TYR  | C-N-CA      | 15.96  | 135.84      | 119.56   |
| 5   | C     | 191  | PHE  | CA-C-N      | -15.65 | 100.27      | 119.84   |
| 5   | C     | 191  | PHE  | C-N-CA      | -15.65 | 100.27      | 119.84   |
| 5   | C     | 177  | GLU  | CA-C-N      | 15.56  | 139.29      | 119.84   |
| 5   | C     | 177  | GLU  | C-N-CA      | 15.56  | 139.29      | 119.84   |
| 5   | M     | 177  | GLU  | CA-C-N      | 15.18  | 138.81      | 119.84   |
| 5   | M     | 177  | GLU  | C-N-CA      | 15.18  | 138.81      | 119.84   |
| 2   | Y     | 2    | A    | N9-C1'-C2'  | -14.35 | 90.48       | 112.00   |
| 6   | D     | 1124 | GLN  | CA-C-N      | 13.23  | 136.38      | 119.84   |
| 6   | D     | 1124 | GLN  | C-N-CA      | 13.23  | 136.38      | 119.84   |
| 6   | N     | 1124 | GLN  | CA-C-N      | 13.07  | 136.18      | 119.84   |
| 6   | N     | 1124 | GLN  | C-N-CA      | 13.07  | 136.18      | 119.84   |
| 6   | D     | 1331 | ASP  | CA-C-N      | 12.91  | 132.67      | 119.24   |
| 6   | D     | 1331 | ASP  | C-N-CA      | 12.91  | 132.67      | 119.24   |
| 6   | D     | 525  | ARG  | CA-C-N      | 12.90  | 135.96      | 119.84   |
| 6   | D     | 525  | ARG  | C-N-CA      | 12.90  | 135.96      | 119.84   |
| 5   | M     | 726  | ILE  | CA-C-N      | 12.69  | 135.70      | 119.84   |
| 5   | M     | 726  | ILE  | C-N-CA      | 12.69  | 135.70      | 119.84   |
| 5   | C     | 726  | ILE  | CA-C-N      | 12.50  | 135.46      | 119.84   |
| 5   | C     | 726  | ILE  | C-N-CA      | 12.50  | 135.46      | 119.84   |
| 7   | E     | 94   | PRO  | CA-N-CD     | -11.64 | 95.71       | 112.00   |
| 5   | C     | 243  | ARG  | CA-C-N      | 11.61  | 134.35      | 119.84   |
| 5   | C     | 243  | ARG  | C-N-CA      | 11.61  | 134.35      | 119.84   |
| 7   | O     | 94   | PRO  | CA-N-CD     | -11.49 | 95.92       | 112.00   |
| 2   | Y     | 1    | G    | C2'-C3'-O3' | -10.84 | 97.45       | 113.70   |
| 7   | E     | 93   | TYR  | CA-C-N      | 10.74  | 131.09      | 119.28   |
| 7   | E     | 93   | TYR  | C-N-CA      | 10.74  | 131.09      | 119.28   |
| 5   | M     | 243  | ARG  | CA-C-N      | 10.57  | 133.05      | 119.84   |
| 5   | M     | 243  | ARG  | C-N-CA      | 10.57  | 133.05      | 119.84   |
| 6   | D     | 609  | GLY  | N-CA-C      | 9.91   | 122.09      | 112.08   |
| 6   | N     | 525  | ARG  | CA-C-N      | 9.82   | 132.12      | 119.84   |
| 6   | N     | 525  | ARG  | C-N-CA      | 9.82   | 132.12      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | D     | 1340 | GLY  | CA-C-N      | 9.78  | 132.07      | 119.84   |
| 6   | D     | 1340 | GLY  | C-N-CA      | 9.78  | 132.07      | 119.84   |
| 2   | H     | 1    | G    | N9-C1'-C2'  | 9.71  | 128.56      | 114.00   |
| 6   | D     | 508  | ARG  | CA-C-N      | 9.43  | 130.58      | 120.12   |
| 6   | D     | 508  | ARG  | C-N-CA      | 9.43  | 130.58      | 120.12   |
| 6   | N     | 705  | ALA  | CA-C-N      | -9.40 | 106.65      | 120.46   |
| 6   | N     | 705  | ALA  | C-N-CA      | -9.40 | 106.65      | 120.46   |
| 2   | Y     | 7    | G    | N9-C1'-C2'  | -9.32 | 98.02       | 112.00   |
| 2   | Y     | 2    | A    | C4'-C3'-O3' | -9.31 | 99.03       | 113.00   |
| 6   | D     | 133  | ILE  | CA-C-N      | 9.28  | 138.68      | 121.97   |
| 6   | D     | 133  | ILE  | C-N-CA      | 9.28  | 138.68      | 121.97   |
| 6   | N     | 634  | GLY  | CA-C-N      | 9.27  | 131.43      | 119.84   |
| 6   | N     | 634  | GLY  | C-N-CA      | 9.27  | 131.43      | 119.84   |
| 6   | D     | 634  | GLY  | CA-C-N      | 9.13  | 131.25      | 119.84   |
| 6   | D     | 634  | GLY  | C-N-CA      | 9.13  | 131.25      | 119.84   |
| 6   | N     | 508  | ARG  | CA-C-N      | 9.02  | 130.13      | 120.12   |
| 6   | N     | 508  | ARG  | C-N-CA      | 9.02  | 130.13      | 120.12   |
| 6   | D     | 705  | ALA  | CA-C-N      | -8.97 | 108.62      | 119.84   |
| 6   | D     | 705  | ALA  | C-N-CA      | -8.97 | 108.62      | 119.84   |
| 6   | N     | 1331 | ASP  | CA-C-N      | 8.80  | 130.84      | 119.84   |
| 6   | N     | 1331 | ASP  | C-N-CA      | 8.80  | 130.84      | 119.84   |
| 7   | O     | 93   | TYR  | CB-CA-C     | 8.71  | 119.84      | 110.17   |
| 6   | N     | 621  | LYS  | CA-C-N      | -8.56 | 110.03      | 122.44   |
| 6   | N     | 621  | LYS  | C-N-CA      | -8.56 | 110.03      | 122.44   |
| 6   | D     | 621  | LYS  | CA-C-N      | -8.44 | 110.20      | 122.44   |
| 6   | D     | 621  | LYS  | C-N-CA      | -8.44 | 110.20      | 122.44   |
| 5   | M     | 230  | ARG  | CA-C-N      | 8.40  | 130.35      | 119.84   |
| 5   | M     | 230  | ARG  | C-N-CA      | 8.40  | 130.35      | 119.84   |
| 5   | C     | 810  | ASP  | CA-C-N      | 8.36  | 130.28      | 119.84   |
| 5   | C     | 810  | ASP  | C-N-CA      | 8.36  | 130.28      | 119.84   |
| 6   | D     | 1109 | GLU  | CA-C-N      | 8.28  | 135.96      | 122.29   |
| 6   | D     | 1109 | GLU  | C-N-CA      | 8.28  | 135.96      | 122.29   |
| 5   | M     | 264  | PRO  | CA-C-N      | -8.25 | 109.76      | 122.62   |
| 5   | M     | 264  | PRO  | C-N-CA      | -8.25 | 109.76      | 122.62   |
| 6   | N     | 1477 | GLY  | N-CA-C      | -8.23 | 105.62      | 114.67   |
| 2   | H     | 7    | G    | N9-C1'-C2'  | -8.20 | 99.70       | 112.00   |
| 4   | A     | 105  | GLY  | CA-C-N      | 8.18  | 130.06      | 119.84   |
| 4   | A     | 105  | GLY  | C-N-CA      | 8.18  | 130.06      | 119.84   |
| 2   | H     | 7    | G    | C4'-C3'-O3' | 8.18  | 125.26      | 113.00   |
| 4   | K     | 105  | GLY  | CA-C-N      | 8.11  | 129.97      | 119.84   |
| 4   | K     | 105  | GLY  | C-N-CA      | 8.11  | 129.97      | 119.84   |
| 5   | C     | 230  | ARG  | CA-C-N      | 8.00  | 129.84      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | C     | 230  | ARG  | C-N-CA      | 8.00  | 129.84      | 119.84   |
| 6   | N     | 1109 | GLU  | CA-C-N      | 7.94  | 135.39      | 122.29   |
| 6   | N     | 1109 | GLU  | C-N-CA      | 7.94  | 135.39      | 122.29   |
| 2   | Y     | 7    | G    | C4'-C3'-O3' | 7.87  | 124.81      | 113.00   |
| 1   | G     | 18   | DG   | N9-C1'-C2'  | -7.86 | 101.72      | 113.50   |
| 5   | C     | 38   | LYS  | CA-C-N      | 7.85  | 130.79      | 120.28   |
| 5   | C     | 38   | LYS  | C-N-CA      | 7.85  | 130.79      | 120.28   |
| 4   | B     | 105  | GLY  | CA-C-N      | 7.78  | 129.56      | 119.84   |
| 4   | B     | 105  | GLY  | C-N-CA      | 7.78  | 129.56      | 119.84   |
| 2   | H     | 2    | A    | P-O3'-C3'   | -7.76 | 108.56      | 120.20   |
| 5   | M     | 810  | ASP  | CA-C-N      | 7.67  | 129.43      | 119.84   |
| 5   | M     | 810  | ASP  | C-N-CA      | 7.67  | 129.43      | 119.84   |
| 5   | C     | 58   | ASP  | CA-C-N      | 7.62  | 136.09      | 121.54   |
| 5   | C     | 58   | ASP  | C-N-CA      | 7.62  | 136.09      | 121.54   |
| 5   | M     | 169  | GLY  | CA-C-N      | 7.62  | 129.36      | 119.84   |
| 5   | M     | 169  | GLY  | C-N-CA      | 7.62  | 129.36      | 119.84   |
| 5   | C     | 264  | PRO  | CA-C-N      | -7.59 | 110.77      | 122.62   |
| 5   | C     | 264  | PRO  | C-N-CA      | -7.59 | 110.77      | 122.62   |
| 5   | M     | 58   | ASP  | CA-C-N      | 7.59  | 136.04      | 121.54   |
| 5   | M     | 58   | ASP  | C-N-CA      | 7.59  | 136.04      | 121.54   |
| 6   | N     | 1101 | VAL  | CB-CA-C     | -7.59 | 104.38      | 111.06   |
| 6   | N     | 1244 | GLY  | N-CA-C      | 7.51  | 130.97      | 113.18   |
| 6   | D     | 1244 | GLY  | N-CA-C      | 7.50  | 130.96      | 113.18   |
| 4   | L     | 105  | GLY  | CA-C-N      | 7.41  | 129.10      | 119.84   |
| 4   | L     | 105  | GLY  | C-N-CA      | 7.41  | 129.10      | 119.84   |
| 6   | D     | 1101 | VAL  | CB-CA-C     | -7.39 | 101.23      | 111.65   |
| 1   | X     | 18   | DG   | N9-C1'-C2'  | -7.39 | 102.42      | 113.50   |
| 5   | M     | 1078 | GLU  | CA-C-N      | 7.38  | 129.07      | 119.84   |
| 5   | M     | 1078 | GLU  | C-N-CA      | 7.38  | 129.07      | 119.84   |
| 7   | O     | 95   | VAL  | N-CA-C      | 7.33  | 122.69      | 112.35   |
| 7   | E     | 95   | VAL  | N-CA-C      | 7.33  | 122.44      | 111.89   |
| 6   | D     | 454  | ALA  | CA-C-N      | -7.30 | 111.50      | 122.74   |
| 6   | D     | 454  | ALA  | C-N-CA      | -7.30 | 111.50      | 122.74   |
| 2   | H     | 1    | G    | C2'-C3'-O3' | -7.18 | 98.73       | 109.50   |
| 2   | H     | 2    | A    | N9-C1'-C2'  | -7.14 | 101.29      | 112.00   |
| 5   | M     | 317  | VAL  | CA-C-N      | -7.08 | 111.49      | 119.28   |
| 5   | M     | 317  | VAL  | C-N-CA      | -7.08 | 111.49      | 119.28   |
| 5   | M     | 38   | LYS  | CA-C-N      | 7.08  | 129.76      | 120.28   |
| 5   | M     | 38   | LYS  | C-N-CA      | 7.08  | 129.76      | 120.28   |
| 4   | K     | 48   | ILE  | CA-C-N      | 6.94  | 128.22      | 120.66   |
| 4   | K     | 48   | ILE  | C-N-CA      | 6.94  | 128.22      | 120.66   |
| 5   | C     | 318  | PRO  | CA-C-N      | 6.93  | 131.50      | 121.03   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | C     | 318  | PRO  | C-N-CA      | 6.93  | 131.50      | 121.03   |
| 5   | C     | 165  | LEU  | CA-C-N      | 6.90  | 143.56      | 127.00   |
| 5   | C     | 165  | LEU  | C-N-CA      | 6.90  | 143.56      | 127.00   |
| 6   | N     | 450  | TYR  | CA-C-N      | 6.88  | 132.29      | 121.56   |
| 6   | N     | 450  | TYR  | C-N-CA      | 6.88  | 132.29      | 121.56   |
| 5   | C     | 169  | GLY  | CA-C-N      | 6.88  | 128.44      | 119.84   |
| 5   | C     | 169  | GLY  | C-N-CA      | 6.88  | 128.44      | 119.84   |
| 5   | M     | 1109 | VAL  | CA-C-N      | -6.87 | 113.31      | 122.99   |
| 5   | M     | 1109 | VAL  | C-N-CA      | -6.87 | 113.31      | 122.99   |
| 6   | N     | 79   | GLU  | CA-C-N      | -6.83 | 112.88      | 122.71   |
| 6   | N     | 79   | GLU  | C-N-CA      | -6.83 | 112.88      | 122.71   |
| 2   | Y     | 9    | G    | C5'-C4'-O4' | -6.76 | 99.66       | 109.80   |
| 5   | M     | 728  | HIS  | CA-C-N      | -6.73 | 108.69      | 121.54   |
| 5   | M     | 728  | HIS  | C-N-CA      | -6.73 | 108.69      | 121.54   |
| 6   | N     | 1209 | LEU  | CA-C-O      | -6.72 | 113.68      | 121.82   |
| 6   | D     | 561  | GLY  | CA-C-N      | -6.70 | 113.80      | 122.98   |
| 6   | D     | 561  | GLY  | C-N-CA      | -6.70 | 113.80      | 122.98   |
| 5   | C     | 1078 | GLU  | CA-C-N      | 6.70  | 128.21      | 119.84   |
| 5   | C     | 1078 | GLU  | C-N-CA      | 6.70  | 128.21      | 119.84   |
| 5   | M     | 318  | PRO  | CA-C-N      | 6.69  | 131.13      | 121.03   |
| 5   | M     | 318  | PRO  | C-N-CA      | 6.69  | 131.13      | 121.03   |
| 2   | H     | 9    | G    | C5'-C4'-O4' | -6.68 | 99.79       | 109.80   |
| 1   | G     | 12   | DG   | C2'-C3'-O3' | 6.65  | 121.48      | 111.50   |
| 5   | C     | 317  | VAL  | CA-C-N      | -6.65 | 111.96      | 119.28   |
| 5   | C     | 317  | VAL  | C-N-CA      | -6.65 | 111.96      | 119.28   |
| 6   | D     | 593  | ASN  | CA-C-N      | 6.58  | 128.07      | 119.84   |
| 6   | D     | 593  | ASN  | C-N-CA      | 6.58  | 128.07      | 119.84   |
| 6   | N     | 609  | GLY  | N-CA-C      | 6.57  | 118.74      | 112.04   |
| 6   | N     | 561  | GLY  | CA-C-N      | -6.56 | 113.99      | 122.98   |
| 6   | N     | 561  | GLY  | C-N-CA      | -6.56 | 113.99      | 122.98   |
| 1   | X     | 12   | DG   | C2'-C3'-O3' | 6.56  | 121.34      | 111.50   |
| 6   | D     | 79   | GLU  | CA-C-N      | -6.54 | 113.26      | 122.75   |
| 6   | D     | 79   | GLU  | C-N-CA      | -6.54 | 113.26      | 122.75   |
| 5   | C     | 728  | HIS  | CA-C-N      | -6.53 | 109.07      | 121.54   |
| 5   | C     | 728  | HIS  | C-N-CA      | -6.53 | 109.07      | 121.54   |
| 6   | N     | 1383 | ASP  | CA-C-N      | 6.51  | 127.41      | 120.11   |
| 6   | N     | 1383 | ASP  | C-N-CA      | 6.51  | 127.41      | 120.11   |
| 7   | E     | 50   | THR  | CA-C-N      | 6.48  | 134.56      | 122.84   |
| 7   | E     | 50   | THR  | C-N-CA      | 6.48  | 134.56      | 122.84   |
| 6   | N     | 145  | VAL  | N-CA-CB     | -6.47 | 107.37      | 111.83   |
| 5   | C     | 1108 | PRO  | CA-C-N      | 6.44  | 131.50      | 122.23   |
| 5   | C     | 1108 | PRO  | C-N-CA      | 6.44  | 131.50      | 122.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | E     | 41   | GLU  | CA-C-N      | 6.42  | 127.86      | 119.84   |
| 7   | E     | 41   | GLU  | C-N-CA      | 6.42  | 127.86      | 119.84   |
| 7   | O     | 50   | THR  | CA-C-N      | 6.41  | 134.43      | 122.84   |
| 7   | O     | 50   | THR  | C-N-CA      | 6.41  | 134.43      | 122.84   |
| 5   | M     | 409  | ARG  | NE-CZ-NH1   | 6.35  | 127.85      | 121.50   |
| 6   | N     | 593  | ASN  | CA-C-N      | 6.33  | 127.75      | 119.84   |
| 6   | N     | 593  | ASN  | C-N-CA      | 6.33  | 127.75      | 119.84   |
| 5   | C     | 761  | PHE  | CA-C-N      | 6.29  | 129.53      | 120.79   |
| 5   | C     | 761  | PHE  | C-N-CA      | 6.29  | 129.53      | 120.79   |
| 6   | D     | 133  | ILE  | O-C-N       | 6.28  | 130.42      | 122.57   |
| 7   | O     | 41   | GLU  | CA-C-N      | 6.22  | 127.62      | 119.84   |
| 7   | O     | 41   | GLU  | C-N-CA      | 6.22  | 127.62      | 119.84   |
| 6   | N     | 1043 | GLY  | CA-C-N      | -6.21 | 114.25      | 123.00   |
| 6   | N     | 1043 | GLY  | C-N-CA      | -6.21 | 114.25      | 123.00   |
| 6   | D     | 450  | TYR  | CA-CB-CG    | -6.20 | 102.75      | 113.90   |
| 2   | H     | 2    | A    | C4'-C3'-C2' | 6.17  | 108.77      | 102.60   |
| 6   | D     | 1209 | LEU  | CA-C-O      | -6.17 | 113.79      | 121.50   |
| 5   | M     | 191  | PHE  | CA-C-N      | -6.14 | 112.16      | 119.84   |
| 5   | M     | 191  | PHE  | C-N-CA      | -6.14 | 112.16      | 119.84   |
| 5   | C     | 981  | GLU  | CA-C-N      | -6.13 | 114.42      | 120.98   |
| 5   | C     | 981  | GLU  | C-N-CA      | -6.13 | 114.42      | 120.98   |
| 6   | N     | 450  | TYR  | CA-CB-CG    | -6.12 | 102.88      | 113.90   |
| 6   | N     | 1243 | THR  | CA-C-N      | -6.11 | 109.44      | 121.41   |
| 6   | N     | 1243 | THR  | C-N-CA      | -6.11 | 109.44      | 121.41   |
| 6   | D     | 22   | SER  | CA-C-N      | 6.09  | 131.48      | 121.86   |
| 6   | D     | 22   | SER  | C-N-CA      | 6.09  | 131.48      | 121.86   |
| 5   | M     | 1108 | PRO  | CA-C-N      | 6.06  | 131.77      | 122.25   |
| 5   | M     | 1108 | PRO  | C-N-CA      | 6.06  | 131.77      | 122.25   |
| 5   | M     | 727  | PRO  | CA-C-N      | -6.03 | 112.00      | 122.36   |
| 5   | M     | 727  | PRO  | C-N-CA      | -6.03 | 112.00      | 122.36   |
| 1   | X     | 12   | DG   | C4'-C3'-O3' | 5.99  | 118.99      | 110.00   |
| 5   | C     | 1109 | VAL  | CA-C-N      | -5.99 | 114.56      | 123.00   |
| 5   | C     | 1109 | VAL  | C-N-CA      | -5.99 | 114.56      | 123.00   |
| 2   | H     | 1    | G    | O4'-C4'-C3' | -5.98 | 100.12      | 106.10   |
| 2   | Y     | 14   | G    | N9-C1'-C2'  | -5.98 | 103.03      | 112.00   |
| 5   | M     | 981  | GLU  | CA-C-N      | -5.93 | 114.65      | 120.52   |
| 5   | M     | 981  | GLU  | C-N-CA      | -5.93 | 114.65      | 120.52   |
| 6   | D     | 397  | LYS  | CA-C-N      | 5.92  | 132.32      | 122.73   |
| 6   | D     | 397  | LYS  | C-N-CA      | 5.92  | 132.32      | 122.73   |
| 5   | M     | 165  | LEU  | CA-C-N      | 5.90  | 141.16      | 127.00   |
| 5   | M     | 165  | LEU  | C-N-CA      | 5.90  | 141.16      | 127.00   |
| 5   | M     | 728  | HIS  | CA-C-O      | -5.89 | 112.59      | 119.24   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | D     | 1043 | GLY  | CA-C-N      | -5.88 | 114.72      | 123.00   |
| 6   | D     | 1043 | GLY  | C-N-CA      | -5.88 | 114.72      | 123.00   |
| 6   | N     | 1109 | GLU  | CA-C-O      | 5.87  | 127.21      | 121.05   |
| 2   | H     | 2    | A    | P-O5'-C5'   | -5.84 | 112.13      | 120.90   |
| 5   | M     | 424  | GLY  | N-CA-C      | 5.80  | 126.93      | 113.18   |
| 6   | D     | 131  | LYS  | CA-C-N      | -5.78 | 110.51      | 121.54   |
| 6   | D     | 131  | LYS  | C-N-CA      | -5.78 | 110.51      | 121.54   |
| 2   | H     | 13   | C    | N1-C1'-C2'  | -5.76 | 103.36      | 112.00   |
| 5   | C     | 728  | HIS  | CA-C-O      | -5.76 | 112.73      | 119.24   |
| 6   | D     | 1243 | THR  | CA-C-N      | -5.75 | 110.14      | 121.41   |
| 6   | D     | 1243 | THR  | C-N-CA      | -5.75 | 110.14      | 121.41   |
| 6   | D     | 694  | VAL  | CB-CA-C     | -5.74 | 104.30      | 112.22   |
| 4   | K     | 124  | ASN  | CA-C-N      | 5.73  | 127.00      | 119.84   |
| 4   | K     | 124  | ASN  | C-N-CA      | 5.73  | 127.00      | 119.84   |
| 6   | D     | 740  | PHE  | CA-C-N      | 5.73  | 131.85      | 121.89   |
| 6   | D     | 740  | PHE  | C-N-CA      | 5.73  | 131.85      | 121.89   |
| 5   | C     | 319  | GLY  | CA-C-O      | -5.72 | 116.01      | 121.62   |
| 6   | D     | 1383 | ASP  | CA-C-N      | 5.71  | 126.50      | 120.11   |
| 6   | D     | 1383 | ASP  | C-N-CA      | 5.71  | 126.50      | 120.11   |
| 7   | O     | 51   | LEU  | CA-C-O      | -5.71 | 115.00      | 120.94   |
| 5   | C     | 727  | PRO  | CA-C-N      | -5.69 | 112.58      | 122.36   |
| 5   | C     | 727  | PRO  | C-N-CA      | -5.69 | 112.58      | 122.36   |
| 7   | E     | 80   | VAL  | CA-C-N      | 5.68  | 126.94      | 119.84   |
| 7   | E     | 80   | VAL  | C-N-CA      | 5.68  | 126.94      | 119.84   |
| 7   | E     | 57   | ASP  | CA-C-N      | -5.63 | 112.80      | 119.84   |
| 7   | E     | 57   | ASP  | C-N-CA      | -5.63 | 112.80      | 119.84   |
| 2   | Y     | 9    | G    | N9-C1'-C2'  | -5.63 | 103.56      | 112.00   |
| 6   | N     | 1244 | GLY  | CA-C-O      | -5.63 | 110.78      | 120.57   |
| 6   | D     | 108  | VAL  | CA-C-N      | -5.62 | 113.49      | 120.79   |
| 6   | D     | 108  | VAL  | C-N-CA      | -5.62 | 113.49      | 120.79   |
| 6   | D     | 1243 | THR  | CA-C-O      | -5.62 | 112.69      | 119.03   |
| 6   | D     | 450  | TYR  | CA-C-N      | 5.61  | 128.81      | 120.90   |
| 6   | D     | 450  | TYR  | C-N-CA      | 5.61  | 128.81      | 120.90   |
| 1   | X     | 11   | DC   | C4'-C3'-O3' | 5.60  | 118.40      | 110.00   |
| 5   | C     | 149  | THR  | CA-C-N      | 5.58  | 125.53      | 119.78   |
| 5   | C     | 149  | THR  | C-N-CA      | 5.58  | 125.53      | 119.78   |
| 2   | H     | 1    | G    | C4'-C3'-C2' | 5.57  | 108.17      | 102.60   |
| 6   | D     | 133  | ILE  | CA-C-O      | 5.57  | 127.74      | 120.78   |
| 6   | N     | 1243 | THR  | CA-C-O      | -5.56 | 112.75      | 119.03   |
| 5   | C     | 244  | PRO  | CA-N-CD     | -5.54 | 104.24      | 112.00   |
| 5   | M     | 729  | LEU  | CA-C-N      | -5.53 | 112.18      | 121.75   |
| 5   | M     | 729  | LEU  | C-N-CA      | -5.53 | 112.18      | 121.75   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | C     | 57   | GLU  | CA-C-N      | -5.53 | 114.22      | 122.74   |
| 5   | C     | 57   | GLU  | C-N-CA      | -5.53 | 114.22      | 122.74   |
| 5   | M     | 443  | THR  | CA-C-N      | 5.53  | 125.45      | 119.76   |
| 5   | M     | 443  | THR  | C-N-CA      | 5.53  | 125.45      | 119.76   |
| 2   | H     | 14   | G    | N9-C1'-C2'  | -5.51 | 103.73      | 112.00   |
| 6   | D     | 1109 | GLU  | CA-C-O      | 5.50  | 126.83      | 121.05   |
| 6   | N     | 1242 | HIS  | CA-C-N      | -5.50 | 113.40      | 121.99   |
| 6   | N     | 1242 | HIS  | C-N-CA      | -5.50 | 113.40      | 121.99   |
| 5   | C     | 416  | GLY  | N-CA-C      | -5.49 | 107.11      | 114.25   |
| 6   | N     | 621  | LYS  | CA-C-O      | -5.47 | 113.20      | 119.60   |
| 6   | N     | 1368 | ILE  | CB-CA-C     | -5.47 | 104.88      | 112.04   |
| 4   | A     | 124  | ASN  | CA-C-N      | 5.47  | 126.67      | 119.84   |
| 4   | A     | 124  | ASN  | C-N-CA      | 5.47  | 126.67      | 119.84   |
| 5   | M     | 761  | PHE  | CA-C-N      | 5.46  | 128.38      | 120.79   |
| 5   | M     | 761  | PHE  | C-N-CA      | 5.46  | 128.38      | 120.79   |
| 5   | C     | 243  | ARG  | C-N-CD      | -5.45 | 102.66      | 125.00   |
| 6   | N     | 80   | VAL  | CA-C-N      | 5.45  | 131.94      | 121.54   |
| 6   | N     | 80   | VAL  | C-N-CA      | 5.45  | 131.94      | 121.54   |
| 5   | C     | 165  | LEU  | C-N-CD      | -5.44 | 108.63      | 120.60   |
| 5   | M     | 409  | ARG  | CA-CB-CG    | 5.42  | 124.94      | 114.10   |
| 6   | N     | 132  | TYR  | CA-C-N      | -5.42 | 115.00      | 122.69   |
| 6   | N     | 132  | TYR  | C-N-CA      | -5.42 | 115.00      | 122.69   |
| 5   | M     | 165  | LEU  | C-N-CD      | -5.38 | 108.75      | 120.60   |
| 7   | E     | 51   | LEU  | CA-C-O      | -5.38 | 115.35      | 120.94   |
| 4   | B     | 124  | ASN  | CA-C-N      | 5.37  | 126.56      | 119.84   |
| 4   | B     | 124  | ASN  | C-N-CA      | 5.37  | 126.56      | 119.84   |
| 2   | H     | 5    | C    | C4'-C3'-O3' | 5.35  | 121.02      | 113.00   |
| 6   | N     | 1209 | LEU  | CA-C-N      | -5.35 | 112.58      | 120.28   |
| 6   | N     | 1209 | LEU  | C-N-CA      | -5.35 | 112.58      | 120.28   |
| 5   | M     | 319  | GLY  | CA-C-O      | -5.33 | 116.39      | 121.62   |
| 2   | H     | 9    | G    | N9-C1'-C2'  | -5.32 | 104.01      | 112.00   |
| 7   | O     | 57   | ASP  | CA-C-N      | -5.32 | 113.19      | 119.84   |
| 7   | O     | 57   | ASP  | C-N-CA      | -5.32 | 113.19      | 119.84   |
| 6   | D     | 18   | ILE  | CB-CA-C     | -5.32 | 104.89      | 111.70   |
| 5   | C     | 489  | THR  | CB-CA-C     | -5.31 | 102.52      | 110.90   |
| 5   | C     | 858  | MET  | CB-CG-SD    | -5.30 | 96.81       | 112.70   |
| 7   | E     | 94   | PRO  | CB-CA-C     | -5.29 | 103.96      | 112.21   |
| 6   | N     | 885  | ILE  | CB-CA-C     | -5.29 | 105.11      | 111.88   |
| 6   | D     | 28   | LYS  | CA-C-N      | 5.29  | 126.45      | 119.84   |
| 6   | D     | 28   | LYS  | C-N-CA      | 5.29  | 126.45      | 119.84   |
| 5   | C     | 547  | ILE  | CA-C-N      | 5.28  | 126.44      | 119.84   |
| 5   | C     | 547  | ILE  | C-N-CA      | 5.28  | 126.44      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | N     | 1389 | LEU  | CA-CB-CG    | 5.27  | 134.74      | 116.30   |
| 6   | N     | 740  | PHE  | CA-C-N      | 5.26  | 130.18      | 121.86   |
| 6   | N     | 740  | PHE  | C-N-CA      | 5.26  | 130.18      | 121.86   |
| 6   | N     | 450  | TYR  | CA-C-O      | 5.26  | 127.57      | 120.47   |
| 2   | H     | 6    | U    | C4'-C3'-O3' | 5.26  | 120.89      | 113.00   |
| 6   | D     | 80   | VAL  | N-CA-C      | 5.25  | 115.83      | 108.17   |
| 2   | Y     | 5    | C    | C4'-C3'-O3' | 5.24  | 120.86      | 113.00   |
| 6   | D     | 81   | THR  | CA-C-O      | -5.24 | 114.49      | 121.46   |
| 5   | C     | 163  | ILE  | N-CA-C      | 5.24  | 113.20      | 107.60   |
| 6   | N     | 28   | LYS  | CA-C-N      | 5.24  | 126.39      | 119.84   |
| 6   | N     | 28   | LYS  | C-N-CA      | 5.24  | 126.39      | 119.84   |
| 6   | N     | 1209 | LEU  | N-CA-C      | -5.23 | 102.25      | 110.36   |
| 6   | D     | 1120 | VAL  | CA-C-N      | 5.23  | 124.99      | 119.76   |
| 6   | D     | 1120 | VAL  | C-N-CA      | 5.23  | 124.99      | 119.76   |
| 6   | D     | 1109 | GLU  | O-C-N       | 5.22  | 128.72      | 122.72   |
| 5   | M     | 416  | GLY  | N-CA-C      | -5.22 | 107.47      | 114.25   |
| 2   | Y     | 2    | A    | C1'-C2'-O2' | 5.21  | 116.21      | 108.40   |
| 6   | D     | 1128 | VAL  | CA-C-O      | -5.20 | 114.96      | 120.48   |
| 6   | D     | 1244 | GLY  | CA-C-O      | -5.20 | 111.52      | 120.57   |
| 7   | E     | 81   | PRO  | CA-C-N      | 5.20  | 131.47      | 121.54   |
| 7   | E     | 81   | PRO  | C-N-CA      | 5.20  | 131.47      | 121.54   |
| 6   | D     | 1209 | LEU  | CA-C-N      | -5.17 | 112.83      | 120.38   |
| 6   | D     | 1209 | LEU  | C-N-CA      | -5.17 | 112.83      | 120.38   |
| 5   | M     | 1110 | ASP  | CA-C-N      | 5.16  | 127.02      | 120.72   |
| 5   | M     | 1110 | ASP  | C-N-CA      | 5.16  | 127.02      | 120.72   |
| 5   | M     | 296  | GLY  | N-CA-C      | -5.15 | 108.95      | 115.08   |
| 4   | A     | 91   | ASN  | CA-C-N      | 5.15  | 126.28      | 119.84   |
| 4   | A     | 91   | ASN  | C-N-CA      | 5.15  | 126.28      | 119.84   |
| 5   | M     | 163  | ILE  | N-CA-C      | 5.14  | 113.10      | 107.60   |
| 5   | M     | 1019 | GLN  | CA-C-N      | 5.14  | 125.05      | 119.76   |
| 5   | M     | 1019 | GLN  | C-N-CA      | 5.14  | 125.05      | 119.76   |
| 2   | H     | 8    | C    | C1'-C2'-O2' | -5.13 | 100.70      | 108.40   |
| 6   | D     | 118  | LEU  | CA-C-O      | -5.13 | 115.62      | 121.58   |
| 6   | N     | 622  | ARG  | CA-C-N      | 5.12  | 127.47      | 120.35   |
| 6   | N     | 622  | ARG  | C-N-CA      | 5.12  | 127.47      | 120.35   |
| 5   | C     | 669  | GLY  | CA-C-O      | -5.11 | 118.77      | 122.45   |
| 7   | O     | 80   | VAL  | CA-C-N      | 5.10  | 126.21      | 119.84   |
| 7   | O     | 80   | VAL  | C-N-CA      | 5.10  | 126.21      | 119.84   |
| 2   | Y     | 16   | G    | C4'-C3'-O3' | 5.10  | 120.64      | 113.00   |
| 2   | H     | 12   | G    | C4'-C3'-C2' | 5.09  | 107.69      | 102.60   |
| 6   | N     | 51   | GLY  | CA-C-N      | 5.09  | 126.21      | 119.84   |
| 6   | N     | 51   | GLY  | C-N-CA      | 5.09  | 126.21      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | O     | 94   | PRO  | N-CA-CB     | -5.09 | 98.39       | 103.48   |
| 5   | C     | 591  | SER  | CA-C-O      | -5.08 | 116.10      | 121.94   |
| 1   | G     | 12   | DG   | C4'-C3'-O3' | 5.08  | 117.62      | 110.00   |
| 4   | K     | 197  | LEU  | CA-CB-CG    | 5.08  | 134.07      | 116.30   |
| 5   | C     | 795  | GLY  | N-CA-C      | -5.08 | 101.15      | 113.18   |
| 4   | B     | 108  | GLU  | CA-CB-CG    | 5.07  | 124.24      | 114.10   |
| 5   | M     | 244  | PRO  | CA-N-CD     | -5.07 | 104.91      | 112.00   |
| 5   | M     | 608  | GLY  | N-CA-C      | -5.06 | 107.76      | 115.66   |
| 6   | D     | 1109 | GLU  | N-CA-C      | 5.06  | 114.92      | 108.24   |
| 5   | M     | 1017 | THR  | CA-C-N      | -5.06 | 115.04      | 122.83   |
| 5   | M     | 1017 | THR  | C-N-CA      | -5.06 | 115.04      | 122.83   |
| 2   | Y     | 12   | G    | C4'-C3'-C2' | 5.06  | 107.66      | 102.60   |
| 5   | M     | 1110 | ASP  | CA-C-O      | 5.06  | 125.82      | 120.36   |
| 6   | D     | 98   | PRO  | CA-C-N      | 5.04  | 130.66      | 122.39   |
| 6   | D     | 98   | PRO  | C-N-CA      | 5.04  | 130.66      | 122.39   |
| 5   | M     | 143  | SER  | CA-C-N      | 5.04  | 126.14      | 119.84   |
| 5   | M     | 143  | SER  | C-N-CA      | 5.04  | 126.14      | 119.84   |
| 6   | N     | 99   | ALA  | CA-C-N      | -5.04 | 114.05      | 122.21   |
| 6   | N     | 99   | ALA  | C-N-CA      | -5.04 | 114.05      | 122.21   |
| 2   | H     | 16   | G    | C2'-C3'-O3' | 5.03  | 121.24      | 113.70   |
| 5   | M     | 243  | ARG  | C-N-CD      | -5.02 | 104.41      | 125.00   |
| 1   | G     | 11   | DC   | C4'-C3'-O3' | 5.02  | 117.53      | 110.00   |
| 2   | Y     | 12   | G    | N9-C1'-C2'  | -5.02 | 104.48      | 112.00   |
| 6   | D     | 459  | GLU  | CA-C-N      | 5.01  | 127.76      | 120.79   |
| 6   | D     | 459  | GLU  | C-N-CA      | 5.01  | 127.76      | 120.79   |
| 6   | N     | 68   | PHE  | CA-C-N      | 5.01  | 126.99      | 120.28   |
| 6   | N     | 68   | PHE  | C-N-CA      | 5.01  | 126.99      | 120.28   |
| 6   | N     | 459  | GLU  | CA-C-N      | 5.00  | 126.95      | 120.44   |
| 6   | N     | 459  | GLU  | C-N-CA      | 5.00  | 126.95      | 120.44   |

There are no chirality outliers.

All (15) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | G     | 13  | DT   | Sidechain |
| 1   | G     | 15  | DC   | Sidechain |
| 1   | G     | 16  | DG   | Sidechain |
| 1   | G     | 17  | DC   | Sidechain |
| 1   | G     | 18  | DG   | Sidechain |
| 1   | G     | 19  | DC   | Sidechain |
| 2   | H     | 14  | G    | Sidechain |
| 2   | H     | 16  | G    | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | I     | 3   | DA   | Sidechain |
| 1   | X     | 13  | DT   | Sidechain |
| 1   | X     | 15  | DC   | Sidechain |
| 1   | X     | 16  | DG   | Sidechain |
| 1   | X     | 17  | DC   | Sidechain |
| 1   | X     | 18  | DG   | Sidechain |
| 2   | Y     | 14  | G    | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | G     | 467   | 0        | 259      | 43      | 0            |
| 1   | X     | 467   | 0        | 259      | 43      | 0            |
| 2   | H     | 347   | 0        | 174      | 58      | 0            |
| 2   | Y     | 347   | 0        | 174      | 82      | 0            |
| 3   | I     | 270   | 0        | 144      | 14      | 0            |
| 3   | Z     | 270   | 0        | 144      | 12      | 0            |
| 4   | A     | 1806  | 0        | 1861     | 177     | 0            |
| 4   | B     | 1806  | 0        | 1861     | 177     | 0            |
| 4   | K     | 1806  | 0        | 1861     | 187     | 0            |
| 4   | L     | 1806  | 0        | 1861     | 199     | 0            |
| 5   | C     | 8829  | 0        | 8933     | 1236    | 0            |
| 5   | M     | 8829  | 0        | 8933     | 1220    | 0            |
| 6   | D     | 9960  | 0        | 10183    | 1417    | 0            |
| 6   | N     | 9960  | 0        | 10183    | 1390    | 0            |
| 7   | E     | 770   | 0        | 784      | 112     | 0            |
| 7   | O     | 770   | 0        | 784      | 104     | 0            |
| 8   | D     | 2     | 0        | 0        | 0       | 0            |
| 8   | N     | 2     | 0        | 0        | 0       | 0            |
| 9   | D     | 2     | 0        | 0        | 0       | 0            |
| 9   | N     | 2     | 0        | 0        | 0       | 0            |
| 10  | D     | 31    | 0        | 14       | 2       | 0            |
| 10  | N     | 31    | 0        | 14       | 2       | 0            |
| 11  | A     | 106   | 0        | 0        | 16      | 0            |
| 11  | B     | 82    | 0        | 0        | 21      | 0            |
| 11  | C     | 482   | 0        | 0        | 120     | 0            |
| 11  | D     | 506   | 0        | 0        | 139     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | E     | 60    | 0        | 0        | 6       | 0            |
| 11  | G     | 32    | 0        | 0        | 3       | 0            |
| 11  | H     | 37    | 0        | 0        | 3       | 0            |
| 11  | I     | 22    | 0        | 0        | 3       | 0            |
| 11  | K     | 86    | 0        | 0        | 19      | 0            |
| 11  | L     | 104   | 0        | 0        | 23      | 0            |
| 11  | M     | 483   | 0        | 0        | 132     | 0            |
| 11  | N     | 491   | 0        | 0        | 114     | 0            |
| 11  | O     | 39    | 0        | 0        | 6       | 0            |
| 11  | X     | 43    | 0        | 0        | 4       | 0            |
| 11  | Y     | 30    | 0        | 0        | 6       | 0            |
| 11  | Z     | 30    | 0        | 0        | 4       | 0            |
| All | All   | 51213 | 0        | 48426    | 6009    | 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 62.

All (6009) 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:Y:7:G:N1        | 5:M:1014:SER:HA   | 1.62                     | 1.13              |
| 2:Y:16:G:H21      | 6:N:705:ALA:HB1   | 1.11                     | 1.12              |
| 6:N:18:ILE:HG23   | 6:N:518:PRO:HG3   | 1.33                     | 1.10              |
| 5:C:409:ARG:HA    | 5:C:454:SER:HA    | 1.27                     | 1.10              |
| 6:N:1189:ARG:HB3  | 6:N:1204:CYS:HA   | 1.34                     | 1.09              |
| 6:D:695:ILE:HD11  | 6:D:718:PRO:HB2   | 1.31                     | 1.08              |
| 4:K:112:ARG:HE    | 4:K:125:PRO:HB2   | 1.15                     | 1.07              |
| 5:M:1005:MET:HB2  | 6:N:648:MET:HE3   | 1.37                     | 1.05              |
| 6:D:908:LYS:HB2   | 6:D:1027:GLY:HA3  | 1.39                     | 1.04              |
| 4:B:59:GLU:HB2    | 4:B:137:ARG:HH12  | 1.20                     | 1.04              |
| 6:N:1220:ALA:HB1  | 6:N:1223:ILE:HD13 | 1.39                     | 1.03              |
| 6:D:783:ARG:HA    | 6:D:1028:ALA:HA   | 1.40                     | 1.03              |
| 6:N:1335:LEU:HD23 | 6:N:1344:VAL:HG22 | 1.39                     | 1.03              |
| 6:D:161:LEU:HD21  | 6:D:452:ILE:HG21  | 1.38                     | 1.02              |
| 5:C:305:PRO:HG3   | 5:C:308:ARG:HH22  | 1.22                     | 1.02              |
| 5:M:536:PRO:HD2   | 5:M:537:LYS:HZ2   | 1.25                     | 1.02              |
| 5:C:752:GLY:H     | 5:C:792:VAL:HB    | 1.25                     | 1.01              |
| 6:D:798:GLU:HB2   | 6:D:828:LYS:HE3   | 1.43                     | 1.01              |
| 5:M:695:LEU:HD21  | 5:M:832:LYS:HD3   | 1.43                     | 1.01              |
| 5:C:433:THR:HG21  | 5:C:488:ALA:HB1   | 1.42                     | 1.01              |
| 5:M:946:ARG:HB3   | 5:M:946:ARG:HH11  | 1.22                     | 1.01              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:180:LYS:HG2   | 6:N:183:GLU:HB2   | 1.42                     | 1.01              |
| 2:Y:2:A:C8        | 2:Y:2:A:H3'       | 1.94                     | 1.00              |
| 5:M:905:ILE:H     | 5:M:905:ILE:HD12  | 1.27                     | 1.00              |
| 6:N:633:VAL:HG22  | 6:N:635:PRO:HD3   | 1.43                     | 1.00              |
| 4:L:179:PHE:HB3   | 4:L:197:LEU:HD12  | 1.44                     | 0.99              |
| 2:Y:7:G:H1        | 5:M:1014:SER:HA   | 0.85                     | 0.99              |
| 6:D:637:LEU:HD21  | 6:D:642:CYS:HA    | 1.45                     | 0.99              |
| 6:N:783:ARG:HA    | 6:N:1028:ALA:HA   | 1.41                     | 0.98              |
| 2:Y:7:G:H21       | 5:M:1021:LEU:HB2  | 1.27                     | 0.98              |
| 6:N:1379:VAL:HG12 | 6:N:1419:PRO:HA   | 1.40                     | 0.98              |
| 6:N:95:LEU:HD11   | 6:N:517:VAL:HG23  | 1.46                     | 0.97              |
| 5:C:578:VAL:HG13  | 5:C:671:ASN:HB3   | 1.46                     | 0.97              |
| 6:N:1042:ARG:HH21 | 6:N:1073:SER:HB3  | 1.28                     | 0.97              |
| 6:D:1183:ILE:HG22 | 6:N:561:GLY:HA2   | 1.47                     | 0.97              |
| 2:Y:7:G:H1        | 5:M:1014:SER:CA   | 1.79                     | 0.96              |
| 4:A:85:LEU:HA     | 4:A:124:ASN:HD22  | 1.28                     | 0.96              |
| 6:D:1109:GLU:HG2  | 6:D:1201:CYS:HA   | 1.44                     | 0.96              |
| 6:D:1112:CYS:HB2  | 6:D:1195:GLN:HG2  | 1.45                     | 0.96              |
| 5:M:333:ILE:H     | 5:M:465:GLY:HA3   | 1.31                     | 0.96              |
| 5:C:579:VAL:HG11  | 5:C:887:GLU:HG3   | 1.47                     | 0.96              |
| 6:N:996:TRP:HA    | 6:N:999:THR:HG22  | 1.46                     | 0.96              |
| 7:O:45:ARG:HG2    | 7:O:46:PRO:HD2    | 1.47                     | 0.96              |
| 6:D:455:ARG:HB2   | 6:D:460:ALA:HA    | 1.47                     | 0.95              |
| 5:M:110:GLU:HG3   | 5:M:369:PRO:HB3   | 1.44                     | 0.95              |
| 6:N:543:LEU:HD22  | 6:N:580:ALA:HB1   | 1.47                     | 0.95              |
| 6:N:921:ARG:HB3   | 6:N:921:ARG:HH11  | 1.29                     | 0.95              |
| 6:N:972:LEU:HG    | 6:N:976:GLN:HE22  | 1.31                     | 0.95              |
| 5:C:636:ALA:HB3   | 5:C:703:ILE:HD13  | 1.46                     | 0.95              |
| 4:L:89:PHE:HB3    | 4:L:94:LEU:HD13   | 1.47                     | 0.94              |
| 5:M:292:ARG:HD2   | 5:M:299:LYS:HZ3   | 1.31                     | 0.94              |
| 6:N:1144:LEU:HD12 | 6:N:1171:VAL:HG13 | 1.48                     | 0.94              |
| 5:M:478:VAL:HG13  | 5:M:506:ASN:HB3   | 1.48                     | 0.94              |
| 5:M:120:LEU:HD22  | 5:M:121:MET:H     | 1.32                     | 0.94              |
| 4:B:64:GLU:HB2    | 4:B:165:ILE:HG21  | 1.48                     | 0.94              |
| 6:N:1109:GLU:HG2  | 6:N:1201:CYS:HA   | 1.48                     | 0.94              |
| 5:M:157:ARG:HD3   | 5:M:314:THR:HB    | 1.49                     | 0.93              |
| 6:N:793:THR:HB    | 6:N:879:ARG:HD3   | 1.49                     | 0.93              |
| 6:D:136:ASP:HB3   | 6:D:137:PRO:HD3   | 1.51                     | 0.93              |
| 5:M:304:LEU:HD23  | 5:M:305:PRO:HD3   | 1.47                     | 0.93              |
| 5:C:39:ARG:H      | 5:C:39:ARG:HD2    | 1.31                     | 0.93              |
| 5:M:183:SER:HB2   | 5:M:190:LYS:HG2   | 1.48                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:939:ARG:HB3   | 5:M:982:PRO:HG3   | 1.47                     | 0.93              |
| 2:Y:12:G:H8       | 2:Y:12:G:H5'      | 1.32                     | 0.93              |
| 6:N:1487:VAL:HG11 | 6:N:1492:LEU:HD23 | 1.50                     | 0.93              |
| 5:C:36:PRO:HG2    | 5:C:70:GLU:HB3    | 1.50                     | 0.93              |
| 5:M:395:LYS:HE2   | 5:M:403:SER:HB2   | 1.49                     | 0.93              |
| 5:M:857:ASP:HB2   | 5:M:978:ARG:HG2   | 1.49                     | 0.93              |
| 2:Y:2:A:H5''      | 6:N:671:LYS:HZ1   | 1.31                     | 0.92              |
| 1:X:18:DG:H2''    | 1:X:19:DC:H5'     | 1.51                     | 0.92              |
| 6:D:1223:ILE:HG22 | 6:D:1227:GLN:HE21 | 1.33                     | 0.92              |
| 5:M:121:MET:HE3   | 5:M:125:GLY:HA2   | 1.49                     | 0.92              |
| 5:M:313:LEU:HD13  | 5:M:321:GLU:HB2   | 1.50                     | 0.92              |
| 1:X:14:DT:H5''    | 6:N:1089:ALA:HA   | 1.48                     | 0.92              |
| 4:B:97:VAL:HG11   | 4:B:120:VAL:HG21  | 1.52                     | 0.92              |
| 6:D:143:ASN:HD21  | 6:D:145:VAL:HG12  | 1.32                     | 0.92              |
| 6:N:133:ILE:HD12  | 6:N:153:LEU:HD13  | 1.50                     | 0.91              |
| 5:M:1097:LEU:H    | 5:M:1097:LEU:HD22 | 1.33                     | 0.91              |
| 5:M:197:LEU:HD13  | 5:M:207:LEU:HD11  | 1.52                     | 0.91              |
| 5:C:313:LEU:HB2   | 11:C:1168:HOH:O   | 1.70                     | 0.91              |
| 11:B:374:HOH:O    | 6:D:847:ASP:HB3   | 1.69                     | 0.91              |
| 5:C:673:LEU:HD22  | 5:C:867:VAL:HA    | 1.52                     | 0.91              |
| 2:H:6:U:H2'       | 2:H:7:G:C8        | 2.06                     | 0.90              |
| 2:Y:2:A:C8        | 2:Y:2:A:C3'       | 2.51                     | 0.90              |
| 2:Y:8:C:O2'       | 2:Y:9:G:H5'       | 1.71                     | 0.90              |
| 6:D:785:ILE:H     | 6:D:785:ILE:HD12  | 1.34                     | 0.90              |
| 2:H:13:C:H4'      | 5:C:409:ARG:HH22  | 1.37                     | 0.90              |
| 6:D:141:ILE:HD11  | 6:D:165:LYS:HZ2   | 1.36                     | 0.90              |
| 6:D:1253:THR:O    | 6:D:1257:PRO:HD2  | 1.71                     | 0.90              |
| 6:D:145:VAL:HG22  | 6:D:146:PRO:HD2   | 1.53                     | 0.90              |
| 6:N:52:PRO:HD2    | 6:N:85:VAL:HG21   | 1.52                     | 0.90              |
| 6:N:890:VAL:HG12  | 6:N:926:LYS:HD2   | 1.54                     | 0.90              |
| 2:H:12:G:H5'      | 2:H:12:G:H8       | 1.38                     | 0.89              |
| 2:Y:6:U:H2'       | 2:Y:7:G:C8        | 2.07                     | 0.89              |
| 5:M:170:PRO:HB3   | 5:M:186:VAL:HG12  | 1.52                     | 0.89              |
| 4:L:87:VAL:HG21   | 4:L:144:VAL:HG11  | 1.53                     | 0.89              |
| 5:C:853:LEU:HB2   | 5:C:858:MET:HE3   | 1.53                     | 0.89              |
| 6:N:507:ASN:HD22  | 6:N:507:ASN:H     | 1.16                     | 0.89              |
| 6:D:785:ILE:HG22  | 6:D:789:LEU:HD11  | 1.53                     | 0.89              |
| 5:C:1049:LEU:HD23 | 6:D:1472:ILE:HD12 | 1.55                     | 0.89              |
| 5:C:176:VAL:HG12  | 5:C:182:VAL:HG13  | 1.54                     | 0.89              |
| 5:C:260:LEU:HB2   | 5:C:291:ALA:HB1   | 1.55                     | 0.89              |
| 6:N:206:ARG:HG2   | 6:N:394:LEU:HD22  | 1.55                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:613:ARG:NH1   | 6:D:616:GLN:HG2   | 1.88                     | 0.88              |
| 5:M:755:LEU:HD21  | 5:M:792:VAL:HG22  | 1.52                     | 0.88              |
| 5:C:305:PRO:HG3   | 5:C:308:ARG:NH2   | 1.88                     | 0.88              |
| 6:D:206:ARG:HG2   | 6:D:394:LEU:HD22  | 1.52                     | 0.88              |
| 5:M:578:VAL:HG11  | 5:M:991:GLN:HB3   | 1.56                     | 0.88              |
| 2:Y:14:G:O2'      | 2:Y:15:C:H5'      | 1.73                     | 0.88              |
| 6:D:1468:LEU:HD22 | 6:D:1470:ARG:HB2  | 1.52                     | 0.88              |
| 5:M:39:ARG:H      | 5:M:39:ARG:HD2    | 1.34                     | 0.88              |
| 2:H:14:G:O2'      | 2:H:15:C:H5'      | 1.72                     | 0.88              |
| 5:M:739:GLU:HG3   | 5:M:742:VAL:HB    | 1.52                     | 0.88              |
| 6:N:1121:PRO:HD2  | 6:N:1346:ARG:HH21 | 1.35                     | 0.88              |
| 5:C:148:PHE:HE2   | 5:C:281:LEU:HD13  | 1.39                     | 0.88              |
| 6:D:204:LEU:HD21  | 6:D:400:VAL:HB    | 1.53                     | 0.88              |
| 5:C:759:THR:HB    | 5:C:785:VAL:HG11  | 1.56                     | 0.88              |
| 2:H:8:C:O2'       | 2:H:9:G:H5'       | 1.71                     | 0.88              |
| 5:M:537:LYS:H     | 5:M:537:LYS:HD2   | 1.38                     | 0.88              |
| 6:N:1253:THR:O    | 6:N:1257:PRO:HD2  | 1.74                     | 0.88              |
| 1:X:15:DC:H4'     | 5:M:1035:MET:SD   | 2.13                     | 0.87              |
| 6:N:394:LEU:HD11  | 6:N:445:ARG:NH1   | 1.90                     | 0.87              |
| 6:N:786:ILE:HG21  | 6:N:1027:GLY:H    | 1.37                     | 0.87              |
| 6:D:708:LEU:HB3   | 6:D:1231:GLU:HB2  | 1.55                     | 0.87              |
| 6:N:1258:ARG:HH12 | 6:N:1268:PRO:HB3  | 1.40                     | 0.87              |
| 6:D:786:ILE:HG22  | 6:D:1026:SER:HB3  | 1.55                     | 0.87              |
| 4:L:59:GLU:HB2    | 4:L:137:ARG:HH12  | 1.39                     | 0.87              |
| 5:C:1055:LEU:HD22 | 5:C:1066:ALA:HB2  | 1.54                     | 0.87              |
| 5:M:64:LEU:HB2    | 5:M:359:MET:SD    | 2.14                     | 0.87              |
| 4:K:117:VAL:HB    | 4:K:120:VAL:HG12  | 1.57                     | 0.87              |
| 4:B:82:LEU:HA     | 4:B:85:LEU:HD12   | 1.57                     | 0.87              |
| 5:C:342:ASP:HA    | 5:C:345:ARG:HD2   | 1.55                     | 0.87              |
| 1:G:18:DG:H2''    | 1:G:19:DC:H5'     | 1.57                     | 0.86              |
| 5:M:700:TYR:HB3   | 5:M:833:LEU:HD13  | 1.55                     | 0.86              |
| 6:N:87:ARG:HB3    | 6:N:523:ASP:HB3   | 1.57                     | 0.86              |
| 6:N:1124:GLN:HE21 | 6:N:1135:ARG:HA   | 1.37                     | 0.86              |
| 5:C:578:VAL:HG11  | 5:C:991:GLN:HB3   | 1.57                     | 0.86              |
| 4:B:56:VAL:HG13   | 4:B:142:VAL:HG12  | 1.55                     | 0.86              |
| 1:G:22:DC:H4'     | 5:C:388:ARG:HD2   | 1.56                     | 0.86              |
| 2:Y:7:G:H21       | 5:M:1021:LEU:CB   | 1.87                     | 0.86              |
| 5:C:721:ARG:HG2   | 5:C:820:ARG:HH22  | 1.41                     | 0.86              |
| 6:N:501:ALA:HB1   | 6:N:1453:ALA:HB2  | 1.58                     | 0.86              |
| 5:C:573:ARG:HB2   | 5:C:573:ARG:HH11  | 1.39                     | 0.86              |
| 6:N:1492:LEU:HB3  | 6:N:1493:LYS:HE2  | 1.57                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:178:ALA:HB3   | 4:A:198:ARG:HG3   | 1.58                     | 0.86              |
| 5:C:192:PRO:HD2   | 5:C:195:LEU:HB2   | 1.55                     | 0.86              |
| 4:L:102:LYS:NZ    | 4:L:137:ARG:HG2   | 1.91                     | 0.86              |
| 4:B:103:ALA:HB1   | 4:B:107:LYS:HD3   | 1.57                     | 0.86              |
| 6:D:484:PRO:HB3   | 6:D:488:ARG:HE    | 1.38                     | 0.85              |
| 4:A:54:THR:HG22   | 4:A:158:ILE:HG13  | 1.56                     | 0.85              |
| 6:D:1144:LEU:HD11 | 6:D:1186:VAL:HG21 | 1.56                     | 0.85              |
| 2:Y:12:G:H5'      | 2:Y:12:G:C8       | 2.11                     | 0.85              |
| 5:M:345:ARG:HA    | 5:M:348:LEU:HD12  | 1.57                     | 0.85              |
| 5:M:810:ASP:HB3   | 5:M:813:VAL:HG12  | 1.57                     | 0.85              |
| 2:Y:16:G:N2       | 6:N:705:ALA:HB1   | 1.90                     | 0.85              |
| 5:C:478:VAL:HG13  | 5:C:506:ASN:HB3   | 1.56                     | 0.85              |
| 6:D:462:GLN:HG3   | 6:D:513:ILE:HD13  | 1.59                     | 0.85              |
| 6:N:1036:ARG:NH2  | 6:N:1042:ARG:HA   | 1.92                     | 0.85              |
| 6:N:1223:ILE:H    | 6:N:1223:ILE:HD12 | 1.41                     | 0.85              |
| 2:Y:13:C:H4'      | 5:M:409:ARG:HH22  | 1.41                     | 0.85              |
| 5:C:174:LEU:HD22  | 5:C:307:LEU:HB2   | 1.57                     | 0.85              |
| 6:N:897:TRP:HA    | 6:N:900:ILE:HG12  | 1.58                     | 0.85              |
| 5:C:587:VAL:HG11  | 5:C:666:LEU:HD22  | 1.56                     | 0.85              |
| 6:D:526:PRO:O     | 6:D:537:THR:HA    | 1.77                     | 0.85              |
| 2:Y:2:A:H5''      | 6:N:671:LYS:NZ    | 1.90                     | 0.84              |
| 4:B:87:VAL:HG21   | 4:B:144:VAL:HG11  | 1.59                     | 0.84              |
| 5:C:144:PRO:HG2   | 5:C:265:ARG:HH21  | 1.41                     | 0.84              |
| 5:C:197:LEU:HD13  | 5:C:207:LEU:HD11  | 1.57                     | 0.84              |
| 5:M:675:ALA:HB2   | 5:M:867:VAL:HG11  | 1.55                     | 0.84              |
| 5:M:953:VAL:HG13  | 5:M:966:LEU:HD13  | 1.58                     | 0.84              |
| 6:D:24:GLY:HA3    | 6:D:49:ILE:HG12   | 1.57                     | 0.84              |
| 5:M:36:PRO:HG2    | 5:M:70:GLU:HB3    | 1.60                     | 0.84              |
| 6:N:1259:VAL:HG11 | 6:N:1356:TYR:OH   | 1.77                     | 0.84              |
| 5:C:409:ARG:HA    | 5:C:454:SER:CA    | 2.07                     | 0.84              |
| 5:M:141:HIS:HB3   | 5:M:418:LEU:HD23  | 1.57                     | 0.84              |
| 5:M:5:ARG:HE      | 5:M:8:ARG:HH22    | 1.24                     | 0.84              |
| 5:C:857:ASP:HB3   | 5:C:978:ARG:HG2   | 1.60                     | 0.84              |
| 5:C:687:ALA:HB2   | 6:D:740:PHE:HB2   | 1.59                     | 0.84              |
| 6:D:1271:LYS:NZ   | 6:D:1331:ASP:HB3  | 1.92                     | 0.84              |
| 6:N:86:ARG:O      | 6:N:522:PRO:HD2   | 1.77                     | 0.84              |
| 4:L:1:MET:HG2     | 4:L:5:LYS:HB3     | 1.58                     | 0.84              |
| 5:M:160:ALA:HB2   | 11:M:1183:HOH:O   | 1.78                     | 0.84              |
| 5:M:467:ILE:HA    | 11:M:1287:HOH:O   | 1.76                     | 0.84              |
| 5:M:675:ALA:HA    | 5:M:989:VAL:HG12  | 1.58                     | 0.84              |
| 6:D:1393:GLN:CD   | 6:D:1394:VAL:H    | 1.85                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:486:ARG:HA    | 6:D:489:ARG:HD3   | 1.60                     | 0.83              |
| 4:K:34:VAL:HB     | 5:M:939:ARG:NH1   | 1.93                     | 0.83              |
| 5:C:1031:ARG:HA   | 6:D:621:LYS:O     | 1.76                     | 0.83              |
| 5:M:595:LEU:HG    | 5:M:655:LEU:HD12  | 1.59                     | 0.83              |
| 4:B:94:LEU:HD11   | 4:B:119:ASP:HB2   | 1.59                     | 0.83              |
| 6:D:853:VAL:HG22  | 6:D:858:VAL:HG23  | 1.60                     | 0.83              |
| 6:D:1144:LEU:HB3  | 6:D:1166:LEU:HD11 | 1.58                     | 0.83              |
| 5:M:436:GLY:HA2   | 5:M:538:GLN:O     | 1.79                     | 0.83              |
| 4:L:102:LYS:HD3   | 4:L:139:ASN:HB2   | 1.59                     | 0.83              |
| 5:C:326:ASP:HB3   | 5:C:431:HIS:HB2   | 1.60                     | 0.83              |
| 6:D:8:VAL:HG23    | 6:D:1457:ASP:HB3  | 1.59                     | 0.83              |
| 6:D:28:LYS:HB2    | 6:D:41:ARG:HH11   | 1.43                     | 0.83              |
| 2:H:14:G:H4'      | 5:C:567:GLN:HE22  | 1.44                     | 0.83              |
| 5:C:987:ILE:HG23  | 6:D:948:THR:HG21  | 1.60                     | 0.83              |
| 6:N:111:LYS:HE2   | 6:N:1452:ILE:HD13 | 1.60                     | 0.83              |
| 4:B:18:ARG:HH12   | 4:B:123:MET:HE1   | 1.43                     | 0.83              |
| 5:M:1065:ALA:HB1  | 5:M:1077:PRO:HG2  | 1.59                     | 0.83              |
| 2:Y:5:C:H2'       | 2:Y:6:U:C6        | 2.13                     | 0.83              |
| 5:C:751:PRO:HG3   | 5:C:796:GLU:HA    | 1.58                     | 0.83              |
| 6:D:396:VAL:HG12  | 6:D:447:VAL:HA    | 1.61                     | 0.83              |
| 6:N:1205:TYR:HD2  | 6:N:1215:VAL:HG21 | 1.43                     | 0.83              |
| 6:D:1228:SER:O    | 6:D:1232:PRO:HD2  | 1.78                     | 0.83              |
| 5:C:478:VAL:HA    | 5:C:506:ASN:O     | 1.79                     | 0.82              |
| 5:M:12:VAL:HG12   | 5:M:534:VAL:HG13  | 1.61                     | 0.82              |
| 6:D:521:PRO:HG2   | 6:D:524:LEU:HD22  | 1.59                     | 0.82              |
| 6:N:119:SER:H     | 6:N:123:LEU:HD22  | 1.44                     | 0.82              |
| 6:D:1389:LEU:HG   | 6:D:1390:LEU:H    | 1.44                     | 0.82              |
| 5:C:34:VAL:HB     | 5:C:38:LYS:HG3    | 1.60                     | 0.82              |
| 6:D:1481:VAL:HG11 | 7:E:18:ARG:HA     | 1.59                     | 0.82              |
| 6:N:172:PRO:HG3   | 11:N:9050:HOH:O   | 1.79                     | 0.82              |
| 5:C:512:ARG:HB3   | 5:C:523:ILE:HD11  | 1.61                     | 0.82              |
| 6:D:455:ARG:CB    | 6:D:460:ALA:HA    | 2.09                     | 0.82              |
| 6:D:1046:GLN:HA   | 6:D:1052:THR:HA   | 1.61                     | 0.82              |
| 7:O:41:GLU:HA     | 7:O:45:ARG:HG3    | 1.62                     | 0.82              |
| 5:M:732:ALA:HA    | 5:M:735:ARG:HH21  | 1.45                     | 0.82              |
| 6:D:119:SER:H     | 6:D:123:LEU:HD22  | 1.42                     | 0.82              |
| 6:D:434:ARG:H     | 6:D:447:VAL:HG22  | 1.42                     | 0.82              |
| 6:D:1449:GLU:HA   | 6:D:1452:ILE:HD12 | 1.60                     | 0.82              |
| 5:C:953:VAL:HG13  | 5:C:966:LEU:HD13  | 1.60                     | 0.82              |
| 6:D:123:LEU:HD11  | 6:D:152:LEU:HD22  | 1.61                     | 0.82              |
| 4:L:25:LEU:HD23   | 4:L:28:LEU:HD21   | 1.62                     | 0.82              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:M:715:THR:HB   | 5:M:717:LEU:HG    | 1.60                     | 0.82              |
| 5:M:405:ARG:HH22 | 5:M:566:THR:HG21  | 1.45                     | 0.82              |
| 5:M:701:THR:HG22 | 5:M:832:LYS:HG2   | 1.62                     | 0.82              |
| 6:N:540:LEU:H    | 6:N:540:LEU:HD12  | 1.44                     | 0.82              |
| 2:H:12:G:H5'     | 2:H:12:G:C8       | 2.14                     | 0.81              |
| 4:A:117:VAL:HB   | 4:A:120:VAL:HG12  | 1.59                     | 0.81              |
| 5:C:146:VAL:HG11 | 5:C:306:THR:HB    | 1.62                     | 0.81              |
| 7:O:18:ARG:HD3   | 7:O:75:PHE:HE1    | 1.44                     | 0.81              |
| 4:B:85:LEU:HG    | 4:B:127:LEU:HD23  | 1.62                     | 0.81              |
| 6:D:81:THR:HG22  | 6:D:82:LYS:H      | 1.45                     | 0.81              |
| 6:D:1464:GLU:HB3 | 11:D:8024:HOH:O   | 1.80                     | 0.81              |
| 6:N:543:LEU:HD13 | 6:N:581:LEU:HA    | 1.59                     | 0.81              |
| 6:N:1045:MET:HE2 | 6:N:1073:SER:HB3  | 1.61                     | 0.81              |
| 2:H:5:C:H2'      | 2:H:6:U:C6        | 2.14                     | 0.81              |
| 5:C:343:GLN:HA   | 5:C:343:GLN:HE21  | 1.45                     | 0.81              |
| 6:D:616:GLN:HE22 | 6:D:621:LYS:HG2   | 1.44                     | 0.81              |
| 6:D:618:LEU:HD11 | 6:D:1463:LYS:HE2  | 1.62                     | 0.81              |
| 5:M:435:TYR:HE1  | 5:M:539:VAL:HG22  | 1.44                     | 0.81              |
| 6:N:1046:GLN:HA  | 6:N:1052:THR:HA   | 1.62                     | 0.81              |
| 6:N:1108:ARG:HB2 | 6:N:1108:ARG:HH11 | 1.45                     | 0.81              |
| 4:B:59:GLU:HG3   | 4:B:139:ASN:ND2   | 1.94                     | 0.81              |
| 6:D:799:LYS:HB3  | 6:D:826:PRO:HG2   | 1.63                     | 0.81              |
| 6:D:1376:MET:SD  | 6:D:1421:LEU:HD13 | 2.20                     | 0.81              |
| 4:A:111:ALA:HB2  | 4:A:127:LEU:HD23  | 1.63                     | 0.81              |
| 5:C:408:ARG:HG3  | 5:C:455:LEU:HG    | 1.62                     | 0.81              |
| 5:C:708:TYR:HB2  | 5:C:825:VAL:HG23  | 1.62                     | 0.81              |
| 5:M:139:GLN:O    | 5:M:333:ILE:HA    | 1.81                     | 0.81              |
| 6:N:119:SER:HB2  | 6:N:123:LEU:HB2   | 1.62                     | 0.81              |
| 4:A:58:ILE:HB    | 4:A:61:VAL:HB     | 1.63                     | 0.81              |
| 5:M:110:GLU:H    | 5:M:368:THR:HG21  | 1.45                     | 0.81              |
| 5:M:442:GLU:HG2  | 5:M:454:SER:HB2   | 1.63                     | 0.81              |
| 5:M:938:LYS:HB2  | 5:M:938:LYS:HZ2   | 1.46                     | 0.81              |
| 6:N:400:VAL:HG22 | 6:N:443:VAL:HG21  | 1.61                     | 0.81              |
| 5:C:121:MET:HE3  | 5:C:125:GLY:HA2   | 1.61                     | 0.81              |
| 6:D:793:THR:HG21 | 6:D:906:GLN:HG2   | 1.63                     | 0.81              |
| 5:M:239:PHE:HE1  | 5:M:254:VAL:HB    | 1.44                     | 0.81              |
| 5:M:478:VAL:HA   | 5:M:506:ASN:O     | 1.81                     | 0.81              |
| 1:X:13:DT:H5''   | 6:N:1093:TYR:CE2  | 2.15                     | 0.81              |
| 6:D:1205:TYR:HD2 | 6:D:1215:VAL:HG21 | 1.44                     | 0.81              |
| 7:E:47:LYS:HB2   | 7:E:52:GLU:OE2    | 1.79                     | 0.81              |
| 2:H:13:C:H4'     | 5:C:409:ARG:NH2   | 1.96                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:1262:LEU:HD21 | 6:D:1351:GLU:HG3  | 1.63                     | 0.80              |
| 6:D:772:PRO:HB3   | 6:D:1224:VAL:HG13 | 1.61                     | 0.80              |
| 5:M:585:GLU:HG2   | 5:M:589:ARG:HH12  | 1.47                     | 0.80              |
| 6:N:73:CYS:HB3    | 6:N:76:CYS:O      | 1.82                     | 0.80              |
| 6:N:133:ILE:HG12  | 6:N:456:MET:HE2   | 1.60                     | 0.80              |
| 5:C:5:ARG:HE      | 5:C:8:ARG:HH12    | 1.30                     | 0.80              |
| 6:D:616:GLN:NE2   | 6:D:621:LYS:HG2   | 1.96                     | 0.80              |
| 6:D:1220:ALA:HB1  | 6:D:1223:ILE:HD12 | 1.63                     | 0.80              |
| 6:N:610:LYS:O     | 6:N:615:ARG:HD3   | 1.81                     | 0.80              |
| 4:L:97:VAL:HG11   | 4:L:120:VAL:HG21  | 1.62                     | 0.80              |
| 7:O:40:LEU:HB3    | 7:O:72:ARG:HH21   | 1.45                     | 0.80              |
| 5:C:703:ILE:HD12  | 5:C:703:ILE:H     | 1.46                     | 0.80              |
| 6:N:785:ILE:HG12  | 6:N:935:LYS:HA    | 1.62                     | 0.80              |
| 7:E:13:VAL:HG21   | 7:E:19:LEU:HB2    | 1.63                     | 0.80              |
| 5:M:736:ASP:HA    | 5:M:744:ARG:NH1   | 1.96                     | 0.80              |
| 6:N:156:GLU:O     | 6:N:159:ARG:HG2   | 1.82                     | 0.80              |
| 5:C:677:MET:SD    | 5:C:987:ILE:HG21  | 2.22                     | 0.80              |
| 5:C:949:LYS:HD3   | 6:D:796:ARG:HH22  | 1.44                     | 0.80              |
| 5:M:1056:LYS:O    | 6:N:624:ASP:HB2   | 1.81                     | 0.80              |
| 6:N:520:LEU:HD12  | 6:N:521:PRO:HD2   | 1.64                     | 0.80              |
| 4:A:206:THR:HG22  | 4:A:209:GLU:HG3   | 1.62                     | 0.79              |
| 2:Y:7:G:N2        | 5:M:1021:LEU:HB2  | 1.96                     | 0.79              |
| 6:D:740:PHE:HB3   | 11:D:8291:HOH:O   | 1.82                     | 0.79              |
| 6:D:1153:VAL:HG13 | 6:N:561:GLY:HA3   | 1.63                     | 0.79              |
| 6:D:1196:THR:HG23 | 11:D:8314:HOH:O   | 1.82                     | 0.79              |
| 6:N:481:MET:SD    | 6:N:1388:ARG:HB3  | 2.22                     | 0.79              |
| 1:G:17:DC:H2''    | 1:G:18:DG:H5'     | 1.62                     | 0.79              |
| 5:M:65:VAL:HB     | 5:M:101:ILE:HB    | 1.63                     | 0.79              |
| 5:M:854:PRO:HB2   | 5:M:856:GLU:HG3   | 1.64                     | 0.79              |
| 5:M:915:LYS:HA    | 11:M:1454:HOH:O   | 1.83                     | 0.79              |
| 5:M:1055:LEU:HD22 | 5:M:1066:ALA:HB2  | 1.64                     | 0.79              |
| 5:M:1109:VAL:HG22 | 6:N:3:LYS:HE3     | 1.62                     | 0.79              |
| 6:N:96:ALA:HB3    | 6:N:554:LEU:HD23  | 1.64                     | 0.79              |
| 5:C:1017:THR:OG1  | 5:C:1019:GLN:HG2  | 1.83                     | 0.79              |
| 5:C:139:GLN:HG2   | 5:C:334:ARG:HB2   | 1.65                     | 0.79              |
| 6:D:899:LEU:HD13  | 6:D:914:LEU:HD21  | 1.62                     | 0.79              |
| 5:M:260:LEU:HB2   | 5:M:291:ALA:HB1   | 1.64                     | 0.79              |
| 5:M:462:ASP:HB3   | 5:M:468:ARG:HD2   | 1.65                     | 0.79              |
| 5:M:762:LYS:HD2   | 5:M:786:LYS:HG3   | 1.65                     | 0.79              |
| 4:B:1:MET:HG2     | 4:B:5:LYS:HB3     | 1.65                     | 0.79              |
| 5:C:710:ILE:HB    | 5:C:790:LEU:HD22  | 1.65                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:597:ALA:HB2   | 5:M:655:LEU:HD21  | 1.63                     | 0.79              |
| 5:M:732:ALA:HB2   | 11:M:1476:HOH:O   | 1.82                     | 0.79              |
| 4:L:62:LEU:HD12   | 4:L:62:LEU:H      | 1.45                     | 0.79              |
| 6:D:1003:VAL:O    | 6:D:1007:VAL:HG23 | 1.83                     | 0.79              |
| 6:D:1495:ILE:HG12 | 7:E:80:VAL:HG11   | 1.63                     | 0.79              |
| 6:N:1168:MET:HE3  | 6:N:1171:VAL:HB   | 1.62                     | 0.79              |
| 4:K:31:GLY:HA3    | 4:L:42:ARG:HH21   | 1.49                     | 0.78              |
| 6:N:1459:LEU:HB3  | 6:N:1465:ASN:HD21 | 1.47                     | 0.78              |
| 5:C:140:ILE:HG22  | 5:C:333:ILE:HG13  | 1.64                     | 0.78              |
| 5:C:356:ARG:HA    | 11:C:1191:HOH:O   | 1.82                     | 0.78              |
| 6:D:550:ARG:HA    | 6:D:550:ARG:HE    | 1.45                     | 0.78              |
| 6:N:796:ARG:HE    | 6:N:828:LYS:HZ3   | 1.30                     | 0.78              |
| 6:N:887:ALA:HB1   | 6:N:893:GLU:HG3   | 1.66                     | 0.78              |
| 5:M:66:LEU:HD22   | 5:M:372:LEU:HD23  | 1.66                     | 0.78              |
| 5:M:141:HIS:O     | 5:M:331:ARG:HA    | 1.84                     | 0.78              |
| 5:M:1034:GLU:HB3  | 6:N:619:LEU:HD22  | 1.65                     | 0.78              |
| 5:C:2:GLU:HG3     | 5:C:899:GLN:HB3   | 1.64                     | 0.78              |
| 6:D:771:SER:HB3   | 6:D:778:LEU:HD13  | 1.65                     | 0.78              |
| 6:D:782:SER:H     | 6:D:785:ILE:HD13  | 1.48                     | 0.78              |
| 4:K:87:VAL:HG21   | 4:K:144:VAL:HG11  | 1.66                     | 0.78              |
| 5:M:360:LEU:HD23  | 11:M:1129:HOH:O   | 1.84                     | 0.78              |
| 5:M:769:PRO:HD2   | 6:N:65:ARG:CZ     | 2.12                     | 0.78              |
| 6:N:810:GLU:O     | 6:N:813:LEU:HG    | 1.84                     | 0.78              |
| 6:N:1204:CYS:HB3  | 11:N:9238:HOH:O   | 1.82                     | 0.78              |
| 2:Y:9:G:H2'       | 2:Y:10:G:C8       | 2.17                     | 0.78              |
| 2:Y:16:G:H21      | 6:N:705:ALA:CB    | 1.95                     | 0.78              |
| 5:M:671:ASN:HD22  | 5:M:671:ASN:N     | 1.81                     | 0.78              |
| 6:N:1036:ARG:HH21 | 6:N:1042:ARG:HA   | 1.48                     | 0.78              |
| 4:L:85:LEU:HA     | 4:L:124:ASN:HD22  | 1.48                     | 0.78              |
| 5:M:151:ASP:HB2   | 5:M:157:ARG:O     | 1.83                     | 0.78              |
| 5:C:625:LEU:HA    | 5:C:639:GLN:HE21  | 1.47                     | 0.78              |
| 5:C:748:GLU:HB2   | 5:C:799:ILE:HD12  | 1.64                     | 0.78              |
| 6:D:127:LEU:HD12  | 6:D:128:TYR:H     | 1.49                     | 0.78              |
| 5:M:1090:LYS:HD2  | 6:N:90:MET:HG3    | 1.66                     | 0.78              |
| 4:A:87:VAL:HG21   | 4:A:144:VAL:HG11  | 1.65                     | 0.78              |
| 5:C:198:ARG:HD2   | 5:C:204:GLN:HE21  | 1.47                     | 0.78              |
| 5:C:752:GLY:N     | 5:C:792:VAL:HB    | 1.99                     | 0.77              |
| 6:D:1099:VAL:HA   | 11:D:8257:HOH:O   | 1.84                     | 0.77              |
| 5:M:12:VAL:HB     | 5:M:472:ARG:CZ    | 2.15                     | 0.77              |
| 5:M:468:ARG:HH21  | 5:M:487:THR:H     | 1.32                     | 0.77              |
| 5:M:1050:GLN:HE22 | 6:N:1471:LEU:N    | 1.82                     | 0.77              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:N:774:SER:HB3  | 6:N:1362:LYS:O    | 1.84                     | 0.77              |
| 2:Y:12:G:H2'     | 2:Y:13:C:C6       | 2.20                     | 0.77              |
| 4:A:43:ILE:HG13  | 4:A:218:LEU:HD12  | 1.65                     | 0.77              |
| 5:C:10:ARG:HA    | 5:C:10:ARG:HH11   | 1.47                     | 0.77              |
| 5:C:308:ARG:HG2  | 11:C:1224:HOH:O   | 1.84                     | 0.77              |
| 5:C:577:PRO:HD2  | 5:C:580:MET:SD    | 2.24                     | 0.77              |
| 5:C:684:PHE:H    | 5:C:687:ALA:HB3   | 1.49                     | 0.77              |
| 4:L:179:PHE:HB2  | 4:L:195:LEU:HD11  | 1.66                     | 0.77              |
| 5:M:413:LEU:H    | 5:M:413:LEU:HD12  | 1.48                     | 0.77              |
| 5:M:684:PHE:H    | 5:M:687:ALA:HB3   | 1.48                     | 0.77              |
| 4:L:24:VAL:HG13  | 4:L:196:THR:HG22  | 1.66                     | 0.77              |
| 5:M:516:ARG:HD2  | 5:M:521:PRO:HA    | 1.66                     | 0.77              |
| 6:N:394:LEU:HD21 | 6:N:445:ARG:NH2   | 1.99                     | 0.77              |
| 5:C:979:THR:HG23 | 5:C:981:GLU:H     | 1.48                     | 0.77              |
| 6:D:1231:GLU:CD  | 6:D:1232:PRO:HD3  | 2.09                     | 0.77              |
| 6:D:1271:LYS:HZ2 | 6:D:1331:ASP:HB3  | 1.47                     | 0.77              |
| 5:C:687:ALA:HB1  | 11:C:1474:HOH:O   | 1.83                     | 0.77              |
| 5:C:1082:PRO:HG2 | 6:D:1469:GLY:HA3  | 1.66                     | 0.77              |
| 5:M:905:ILE:H    | 5:M:905:ILE:CD1   | 1.96                     | 0.77              |
| 5:C:958:THR:HG23 | 5:C:961:GLU:HB2   | 1.67                     | 0.77              |
| 5:M:64:LEU:HD22  | 5:M:359:MET:HG3   | 1.66                     | 0.77              |
| 6:N:684:LYS:HB2  | 6:N:686:GLU:HG3   | 1.66                     | 0.77              |
| 6:N:1266:ARG:HG2 | 6:N:1267:ARG:H    | 1.50                     | 0.77              |
| 5:C:328:LEU:HB2  | 5:C:433:THR:HB    | 1.66                     | 0.77              |
| 6:D:699:VAL:H    | 6:D:756:GLN:NE2   | 1.83                     | 0.77              |
| 6:N:1426:LYS:HA  | 6:N:1429:LEU:HD13 | 1.66                     | 0.77              |
| 5:C:139:GLN:HE21 | 5:C:334:ARG:HD3   | 1.49                     | 0.77              |
| 5:C:433:THR:HG22 | 5:C:437:ARG:NH1   | 1.99                     | 0.77              |
| 6:D:774:SER:HB3  | 6:D:1362:LYS:O    | 1.84                     | 0.77              |
| 6:D:785:ILE:HG13 | 6:D:939:PHE:CE2   | 2.19                     | 0.77              |
| 5:M:516:ARG:NE   | 6:N:1068:LEU:HD13 | 1.99                     | 0.77              |
| 6:N:397:LYS:O    | 6:N:448:GLU:HB2   | 1.84                     | 0.77              |
| 5:M:511:GLU:O    | 5:M:526:PRO:HD3   | 1.84                     | 0.77              |
| 5:M:758:ARG:CZ   | 5:M:788:THR:HB    | 2.14                     | 0.77              |
| 6:D:9:ARG:HA     | 6:D:1455:LYS:O    | 1.84                     | 0.77              |
| 6:D:136:ASP:CB   | 6:D:455:ARG:HE    | 1.99                     | 0.77              |
| 6:D:897:TRP:HA   | 6:D:900:ILE:HG12  | 1.65                     | 0.77              |
| 6:N:554:LEU:HD13 | 6:N:570:GLU:HG2   | 1.67                     | 0.76              |
| 5:C:1083:GLU:HG2 | 5:C:1086:ARG:HH21 | 1.48                     | 0.76              |
| 6:N:1459:LEU:HB3 | 6:N:1465:ASN:ND2  | 2.00                     | 0.76              |
| 5:C:431:HIS:CD2  | 5:C:433:THR:H     | 2.03                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:908:LYS:CB    | 6:D:1027:GLY:HA3  | 2.15                     | 0.76              |
| 6:N:1003:VAL:O    | 6:N:1007:VAL:HG23 | 1.85                     | 0.76              |
| 5:C:874:LEU:O     | 5:C:877:PRO:HD2   | 1.86                     | 0.76              |
| 6:D:202:VAL:HB    | 6:D:398:ALA:O     | 1.86                     | 0.76              |
| 6:D:710:ARG:HG2   | 6:D:772:PRO:HG2   | 1.68                     | 0.76              |
| 6:D:1087:ARG:HG3  | 6:D:1237:THR:HG21 | 1.67                     | 0.76              |
| 5:M:608:GLY:C     | 5:M:609:ASN:HD22  | 1.94                     | 0.76              |
| 5:M:1032:PHE:O    | 5:M:1036:GLU:HB2  | 1.86                     | 0.76              |
| 6:N:895:VAL:HG11  | 6:N:922:LEU:HD21  | 1.65                     | 0.76              |
| 6:D:28:LYS:HG3    | 6:D:29:PRO:HD2    | 1.68                     | 0.76              |
| 5:M:5:ARG:NE      | 5:M:8:ARG:HH12    | 1.83                     | 0.76              |
| 5:M:244:PRO:HD2   | 5:M:245:GLY:H     | 1.50                     | 0.76              |
| 11:M:1524:HOH:O   | 6:N:616:GLN:HA    | 1.84                     | 0.76              |
| 6:N:1390:LEU:HD21 | 11:N:9287:HOH:O   | 1.86                     | 0.76              |
| 5:C:1032:PHE:O    | 5:C:1036:GLU:HB2  | 1.85                     | 0.76              |
| 5:M:998:TYR:HE2   | 5:M:1000:MET:HG3  | 1.49                     | 0.76              |
| 6:N:486:ARG:HA    | 6:N:489:ARG:HG2   | 1.68                     | 0.76              |
| 6:N:1481:VAL:HG11 | 7:O:18:ARG:HA     | 1.68                     | 0.76              |
| 5:C:614:ARG:HG3   | 5:C:620:LEU:HD22  | 1.68                     | 0.76              |
| 6:N:1108:ARG:HB2  | 6:N:1108:ARG:NH1  | 2.01                     | 0.76              |
| 6:N:1394:VAL:HB   | 6:N:1397:LYS:HB2  | 1.68                     | 0.76              |
| 4:A:75:VAL:HA     | 4:A:78:ILE:HD12   | 1.68                     | 0.75              |
| 4:A:222:LEU:HD21  | 4:B:218:LEU:HB3   | 1.68                     | 0.75              |
| 6:D:25:GLU:HG3    | 6:D:93:ILE:HA     | 1.66                     | 0.75              |
| 6:D:53:ILE:HD12   | 6:D:86:ARG:HH22   | 1.51                     | 0.75              |
| 6:D:131:LYS:HG3   | 6:D:568:ARG:HG2   | 1.68                     | 0.75              |
| 6:D:554:LEU:HD21  | 6:D:571:LYS:HE2   | 1.66                     | 0.75              |
| 5:M:584:GLU:CD    | 5:M:584:GLU:H     | 1.95                     | 0.75              |
| 6:D:73:CYS:HB3    | 6:D:76:CYS:O      | 1.87                     | 0.75              |
| 6:D:455:ARG:O     | 6:D:460:ALA:HB2   | 1.87                     | 0.75              |
| 6:N:47:GLU:HA     | 11:N:9490:HOH:O   | 1.85                     | 0.75              |
| 6:N:122:GLU:O     | 6:N:126:VAL:HG23  | 1.84                     | 0.75              |
| 6:N:399:ARG:HB2   | 6:N:401:TYR:CZ    | 2.21                     | 0.75              |
| 5:C:1016:ILE:HD13 | 5:C:1016:ILE:H    | 1.50                     | 0.75              |
| 5:M:312:ALA:HB1   | 5:M:318:PRO:HG2   | 1.67                     | 0.75              |
| 4:B:52:ALA:HB2    | 4:B:170:VAL:O     | 1.86                     | 0.75              |
| 6:D:1103:HIS:CD2  | 6:D:1463:LYS:H    | 2.05                     | 0.75              |
| 5:M:997:LEU:HD21  | 11:M:1517:HOH:O   | 1.87                     | 0.75              |
| 6:N:136:ASP:HB3   | 6:N:137:PRO:HD3   | 1.67                     | 0.75              |
| 1:X:17:DC:H2''    | 1:X:18:DG:H5'     | 1.66                     | 0.75              |
| 5:C:1031:ARG:HE   | 6:D:621:LYS:HB3   | 1.50                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:626:ARG:HH12  | 5:M:637:LEU:HB2   | 1.51                     | 0.75              |
| 5:M:331:ARG:HH21  | 5:M:427:VAL:HG13  | 1.51                     | 0.75              |
| 5:M:378:LEU:HG    | 5:M:382:ILE:HD11  | 1.69                     | 0.75              |
| 5:M:758:ARG:HB3   | 5:M:788:THR:O     | 1.87                     | 0.75              |
| 6:N:603:LEU:O     | 6:N:606:ILE:HG22  | 1.87                     | 0.75              |
| 5:C:650:ARG:HG3   | 5:C:653:ASP:HB2   | 1.67                     | 0.75              |
| 4:L:162:ILE:HA    | 11:L:316:HOH:O    | 1.86                     | 0.75              |
| 5:M:150:PRO:HA    | 5:M:158:TYR:HB3   | 1.69                     | 0.75              |
| 6:N:496:LEU:HD12  | 6:N:500:ARG:HG2   | 1.69                     | 0.75              |
| 6:N:764:LEU:HD12  | 6:N:765:SER:H     | 1.52                     | 0.75              |
| 4:B:152:PRO:HB2   | 4:B:155:LYS:HD2   | 1.69                     | 0.75              |
| 6:D:139:GLY:O     | 6:D:147:VAL:HB    | 1.87                     | 0.75              |
| 5:C:677:MET:HE1   | 5:C:974:LEU:HD23  | 1.69                     | 0.75              |
| 6:D:148:GLU:HB3   | 6:D:151:GLN:HB2   | 1.69                     | 0.75              |
| 6:D:651:GLU:HA    | 6:D:654:LYS:NZ    | 2.02                     | 0.75              |
| 6:D:1149:LEU:HD12 | 6:D:1161:GLU:O    | 1.87                     | 0.75              |
| 6:N:29:PRO:HD3    | 6:N:548:ILE:HG21  | 1.68                     | 0.75              |
| 2:H:12:G:H2'      | 2:H:13:C:C6       | 2.22                     | 0.74              |
| 4:B:211:LEU:O     | 4:B:215:VAL:HG13  | 1.86                     | 0.74              |
| 5:C:169:GLY:HA3   | 5:C:263:ASP:HB3   | 1.69                     | 0.74              |
| 6:N:853:VAL:HG22  | 6:N:858:VAL:HG23  | 1.69                     | 0.74              |
| 1:X:13:DT:H5''    | 6:N:1093:TYR:HE2  | 1.51                     | 0.74              |
| 4:B:41:ARG:HD2    | 4:B:177:VAL:HG23  | 1.69                     | 0.74              |
| 6:N:1155:VAL:HA   | 11:N:9051:HOH:O   | 1.88                     | 0.74              |
| 6:N:1448:THR:O    | 6:N:1452:ILE:HD12 | 1.87                     | 0.74              |
| 2:Y:2:A:H3'       | 2:Y:2:A:H8        | 1.48                     | 0.74              |
| 5:C:141:HIS:HB3   | 5:C:418:LEU:HD23  | 1.67                     | 0.74              |
| 5:C:904:PRO:HD2   | 5:C:908:GLY:HA2   | 1.67                     | 0.74              |
| 4:A:57:TYR:HB3    | 4:A:141:GLU:HG3   | 1.67                     | 0.74              |
| 6:D:1195:GLN:HG3  | 6:D:1196:THR:N    | 2.02                     | 0.74              |
| 5:M:1092:LEU:HA   | 5:M:1095:LEU:HD12 | 1.68                     | 0.74              |
| 6:N:139:GLY:O     | 6:N:147:VAL:HB    | 1.86                     | 0.74              |
| 6:N:1228:SER:O    | 6:N:1232:PRO:HD2  | 1.88                     | 0.74              |
| 2:H:9:G:H2'       | 2:H:10:G:C8       | 2.21                     | 0.74              |
| 2:Y:10:G:H1'      | 11:Y:1398:HOH:O   | 1.86                     | 0.74              |
| 2:Y:10:G:H2'      | 2:Y:11:C:C6       | 2.23                     | 0.74              |
| 5:C:186:VAL:HG23  | 5:C:187:ASN:H     | 1.51                     | 0.74              |
| 5:C:1034:GLU:HB3  | 6:D:619:LEU:HD22  | 1.67                     | 0.74              |
| 5:M:443:THR:HG21  | 6:N:1078:ARG:HE   | 1.52                     | 0.74              |
| 5:C:943:VAL:HG11  | 5:C:973:VAL:HG21  | 1.70                     | 0.74              |
| 5:M:5:ARG:HB2     | 5:M:8:ARG:HH22    | 1.51                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:433:THR:HG21  | 5:M:488:ALA:HB1   | 1.70                     | 0.74              |
| 5:M:807:ARG:H     | 5:M:807:ARG:HE    | 1.36                     | 0.74              |
| 6:N:1424:VAL:HG13 | 6:N:1425:THR:H    | 1.50                     | 0.74              |
| 5:C:328:LEU:H     | 5:C:433:THR:CB    | 1.99                     | 0.74              |
| 5:C:437:ARG:HE    | 5:C:469:THR:HB    | 1.52                     | 0.74              |
| 5:C:872:ASN:HD21  | 5:C:874:LEU:HD13  | 1.51                     | 0.74              |
| 6:D:581:LEU:HG    | 6:D:582:LEU:HG    | 1.68                     | 0.74              |
| 5:M:781:LYS:HD3   | 5:M:781:LYS:H     | 1.51                     | 0.74              |
| 6:N:409:VAL:HG21  | 6:N:421:LEU:HD23  | 1.67                     | 0.74              |
| 5:M:673:LEU:HD22  | 5:M:867:VAL:HA    | 1.69                     | 0.74              |
| 5:C:959:PRO:HB2   | 11:C:1203:HOH:O   | 1.85                     | 0.74              |
| 6:N:972:LEU:HG    | 6:N:976:GLN:NE2   | 2.03                     | 0.74              |
| 4:B:59:GLU:HB2    | 4:B:137:ARG:NH1   | 1.99                     | 0.74              |
| 6:D:65:ARG:HG3    | 6:D:66:GLN:H      | 1.53                     | 0.74              |
| 6:D:806:PHE:CE1   | 6:D:813:LEU:HB3   | 2.23                     | 0.74              |
| 5:M:68:PHE:HZ     | 5:M:71:TYR:HD2    | 1.36                     | 0.74              |
| 6:N:204:LEU:HD13  | 6:N:445:ARG:NE    | 2.03                     | 0.74              |
| 6:N:786:ILE:HG21  | 6:N:1027:GLY:N    | 2.01                     | 0.74              |
| 4:K:39:PRO:HG3    | 11:L:348:HOH:O    | 1.86                     | 0.73              |
| 5:M:1034:GLU:N    | 6:N:619:LEU:HB3   | 2.03                     | 0.73              |
| 6:N:1093:TYR:O    | 6:N:1097:LYS:HG2  | 1.88                     | 0.73              |
| 5:C:1042:ALA:HA   | 6:D:1220:ALA:HB3  | 1.68                     | 0.73              |
| 6:D:1098:LEU:HD23 | 6:D:1226:ALA:HA   | 1.70                     | 0.73              |
| 6:N:166:GLN:HG3   | 6:N:447:VAL:HB    | 1.71                     | 0.73              |
| 4:A:194:LYS:HG3   | 11:A:338:HOH:O    | 1.86                     | 0.73              |
| 6:D:603:LEU:O     | 6:D:606:ILE:HG22  | 1.88                     | 0.73              |
| 11:D:8449:HOH:O   | 7:E:28:GLN:HG3    | 1.88                     | 0.73              |
| 5:M:546:LEU:HD12  | 5:M:565:GLN:HE22  | 1.50                     | 0.73              |
| 6:N:1166:LEU:H    | 6:N:1166:LEU:HD23 | 1.53                     | 0.73              |
| 4:A:82:LEU:HD22   | 4:A:142:VAL:HG11  | 1.69                     | 0.73              |
| 11:A:325:HOH:O    | 4:B:215:VAL:HG21  | 1.89                     | 0.73              |
| 7:E:54:LEU:HG     | 7:E:58:PRO:HG2    | 1.71                     | 0.73              |
| 5:C:172:ILE:HG23  | 5:C:184:MET:HE3   | 1.70                     | 0.73              |
| 5:C:668:LEU:HD13  | 5:C:995:MET:SD    | 2.29                     | 0.73              |
| 5:C:722:ILE:HD12  | 5:C:823:VAL:HG21  | 1.69                     | 0.73              |
| 6:D:483:HIS:HB2   | 6:D:484:PRO:HD3   | 1.68                     | 0.73              |
| 6:N:959:GLU:HB2   | 6:N:963:TYR:CE1   | 2.24                     | 0.73              |
| 6:N:1481:VAL:HG13 | 7:O:18:ARG:HE     | 1.53                     | 0.73              |
| 5:C:810:ASP:HB3   | 5:C:813:VAL:HG12  | 1.70                     | 0.73              |
| 6:D:171:LEU:HD21  | 6:D:192:ALA:CB    | 2.18                     | 0.73              |
| 6:D:1105:ILE:HD12 | 6:D:1373:ARG:HH21 | 1.52                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:L:59:GLU:HB2    | 4:L:137:ARG:NH1   | 2.03                     | 0.73              |
| 5:M:671:ASN:HA    | 11:M:1511:HOH:O   | 1.88                     | 0.73              |
| 5:C:516:ARG:NE    | 6:D:1068:LEU:HD13 | 2.03                     | 0.73              |
| 5:C:881:ASN:O     | 5:C:884:GLN:HG3   | 1.89                     | 0.73              |
| 5:C:946:ARG:HB3   | 5:C:946:ARG:HH11  | 1.52                     | 0.73              |
| 5:M:52:PHE:CD2    | 5:M:68:PHE:HB2    | 2.24                     | 0.73              |
| 5:M:290:LEU:HD22  | 5:M:302:VAL:HG11  | 1.70                     | 0.73              |
| 6:N:541:ASN:O     | 6:N:545:ARG:HG3   | 1.89                     | 0.73              |
| 5:C:263:ASP:HB2   | 5:C:264:PRO:HD3   | 1.69                     | 0.73              |
| 5:C:837:ASP:HA    | 5:C:999:HIS:HE1   | 1.52                     | 0.73              |
| 5:C:1035:MET:HA   | 5:C:1038:TRP:CE3  | 2.24                     | 0.73              |
| 6:D:171:LEU:HD23  | 6:D:172:PRO:HD2   | 1.69                     | 0.73              |
| 6:D:1462:LEU:HD21 | 6:D:1474:ALA:HB3  | 1.71                     | 0.73              |
| 5:M:758:ARG:NH2   | 5:M:788:THR:HB    | 2.04                     | 0.73              |
| 6:N:989:TYR:O     | 6:N:993:LEU:HG    | 1.87                     | 0.73              |
| 6:D:834:THR:HG22  | 6:D:838:ARG:HH11  | 1.53                     | 0.73              |
| 5:M:132:ALA:HB1   | 5:M:632:ASN:HD21  | 1.54                     | 0.73              |
| 5:C:479:VAL:HG11  | 5:C:503:LEU:HD11  | 1.71                     | 0.73              |
| 6:D:1083:ASP:O    | 6:D:1087:ARG:HG2  | 1.89                     | 0.73              |
| 4:K:42:ARG:HH11   | 5:M:978:ARG:HA    | 1.53                     | 0.73              |
| 4:K:189:ARG:HH12  | 4:L:155:LYS:HE3   | 1.54                     | 0.73              |
| 4:L:218:LEU:O     | 4:L:222:LEU:HG    | 1.88                     | 0.73              |
| 5:M:313:LEU:HD23  | 11:M:1189:HOH:O   | 1.89                     | 0.73              |
| 6:N:1166:LEU:HD12 | 6:N:1171:VAL:HG22 | 1.71                     | 0.73              |
| 7:O:48:MET:HB2    | 7:O:54:LEU:HB2    | 1.70                     | 0.73              |
| 7:E:76:GLY:HA3    | 7:E:79:LEU:HD13   | 1.69                     | 0.72              |
| 5:M:554:ASP:CB    | 5:M:880:MET:HB2   | 2.19                     | 0.72              |
| 5:M:872:ASN:HD21  | 5:M:874:LEU:HB2   | 1.53                     | 0.72              |
| 6:N:1111:ASP:CG   | 6:N:1203:LYS:HG3  | 2.14                     | 0.72              |
| 2:Y:6:U:H2'       | 2:Y:7:G:N7        | 2.03                     | 0.72              |
| 5:C:1095:LEU:HD23 | 6:D:582:LEU:HD22  | 1.71                     | 0.72              |
| 5:M:756:VAL:O     | 5:M:789:SER:HB3   | 1.89                     | 0.72              |
| 6:N:643:GLY:HA3   | 6:N:727:GLN:HB2   | 1.70                     | 0.72              |
| 5:C:768:THR:HB    | 5:C:771:GLU:HB3   | 1.72                     | 0.72              |
| 5:M:578:VAL:HG23  | 5:M:579:VAL:HG12  | 1.71                     | 0.72              |
| 2:H:10:G:H2'      | 2:H:11:C:C6       | 2.25                     | 0.72              |
| 2:Y:13:C:H4'      | 5:M:409:ARG:NH2   | 2.05                     | 0.72              |
| 5:C:312:ALA:HB1   | 5:C:318:PRO:HG2   | 1.70                     | 0.72              |
| 5:C:710:ILE:HD12  | 5:C:790:LEU:HB2   | 1.70                     | 0.72              |
| 5:C:850:ALA:HB2   | 11:C:1474:HOH:O   | 1.88                     | 0.72              |
| 6:D:486:ARG:HA    | 6:D:489:ARG:CD    | 2.19                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:25:GLU:HA     | 6:D:92:HIS:O      | 1.89                     | 0.72              |
| 6:D:68:PHE:HB2    | 11:D:8148:HOH:O   | 1.89                     | 0.72              |
| 6:D:153:LEU:HD11  | 6:D:158:TYR:HB2   | 1.72                     | 0.72              |
| 6:D:394:LEU:O     | 6:D:396:VAL:HG23  | 1.88                     | 0.72              |
| 5:M:495:THR:H     | 5:M:530:GLU:CD    | 1.96                     | 0.72              |
| 5:M:1005:MET:HE1  | 6:N:724:GLN:HA    | 1.72                     | 0.72              |
| 6:N:95:LEU:HD12   | 6:N:95:LEU:H      | 1.54                     | 0.72              |
| 6:N:929:ARG:NH1   | 6:N:929:ARG:HB2   | 2.05                     | 0.72              |
| 4:B:79:ILE:HA     | 4:B:82:LEU:HD12   | 1.70                     | 0.72              |
| 5:C:677:MET:HB3   | 5:C:987:ILE:HD13  | 1.71                     | 0.72              |
| 6:D:1465:ASN:HD21 | 6:D:1470:ARG:HE   | 1.36                     | 0.72              |
| 5:M:412:ALA:HB1   | 5:M:419:THR:HG21  | 1.71                     | 0.72              |
| 5:M:1005:MET:HB2  | 6:N:648:MET:CE    | 2.18                     | 0.72              |
| 6:N:116:LEU:HD13  | 6:N:118:LEU:HD11  | 1.71                     | 0.72              |
| 4:A:226:SER:O     | 4:A:228:PRO:HD3   | 1.90                     | 0.72              |
| 4:B:218:LEU:O     | 4:B:222:LEU:HG    | 1.89                     | 0.72              |
| 5:C:464:LEU:HD21  | 11:C:1308:HOH:O   | 1.89                     | 0.72              |
| 6:N:637:LEU:HD11  | 6:N:641:GLN:C     | 2.15                     | 0.72              |
| 6:N:951:ILE:HG23  | 6:N:1062:ARG:HE   | 1.55                     | 0.72              |
| 7:O:46:PRO:HG3    | 7:O:66:LYS:HD3    | 1.70                     | 0.72              |
| 7:O:54:LEU:O      | 7:O:54:LEU:HD23   | 1.90                     | 0.72              |
| 4:B:186:LEU:HD21  | 11:B:367:HOH:O    | 1.87                     | 0.72              |
| 6:D:53:ILE:HD12   | 6:D:86:ARG:NH2    | 2.04                     | 0.72              |
| 4:K:189:ARG:NH1   | 4:L:155:LYS:HE3   | 2.04                     | 0.72              |
| 6:N:493:ARG:HG2   | 6:N:1390:LEU:HB2  | 1.71                     | 0.72              |
| 6:D:30:GLU:HB3    | 6:D:40:GLU:HG2    | 1.71                     | 0.72              |
| 5:C:689:VAL:HB    | 5:C:870:ILE:HG13  | 1.71                     | 0.72              |
| 6:D:122:GLU:O     | 6:D:126:VAL:HG23  | 1.90                     | 0.72              |
| 6:D:810:GLU:O     | 6:D:813:LEU:HG    | 1.89                     | 0.72              |
| 4:K:38:ASN:HB2    | 5:M:980:GLY:HA3   | 1.71                     | 0.72              |
| 6:N:179:VAL:HG13  | 6:N:183:GLU:HB3   | 1.72                     | 0.72              |
| 6:N:1205:TYR:CD2  | 6:N:1215:VAL:HG21 | 2.25                     | 0.72              |
| 4:A:61:VAL:HG23   | 11:A:319:HOH:O    | 1.90                     | 0.71              |
| 6:D:677:LEU:HD23  | 6:D:683:ILE:HG13  | 1.72                     | 0.71              |
| 4:K:89:PHE:HD1    | 4:K:120:VAL:HG23  | 1.54                     | 0.71              |
| 5:M:1060:ILE:HG22 | 11:M:1405:HOH:O   | 1.90                     | 0.71              |
| 6:N:421:LEU:HD22  | 6:N:444:VAL:HG11  | 1.69                     | 0.71              |
| 5:C:158:TYR:HD1   | 5:C:314:THR:HG22  | 1.54                     | 0.71              |
| 5:C:409:ARG:CA    | 5:C:454:SER:HA    | 2.16                     | 0.71              |
| 5:C:861:LEU:HA    | 5:C:974:LEU:HD12  | 1.72                     | 0.71              |
| 6:N:133:ILE:HG21  | 6:N:454:ALA:HB1   | 1.71                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:179:PHE:HB2   | 4:A:195:LEU:HD11  | 1.71                     | 0.71              |
| 5:C:129:ILE:HD13  | 5:C:134:ARG:HB2   | 1.73                     | 0.71              |
| 5:C:436:GLY:O     | 5:C:459:ALA:HB2   | 1.90                     | 0.71              |
| 5:C:675:ALA:HB2   | 5:C:867:VAL:HG11  | 1.71                     | 0.71              |
| 5:C:872:ASN:HD22  | 5:C:872:ASN:C     | 1.99                     | 0.71              |
| 6:D:409:VAL:HG23  | 6:D:421:LEU:HA    | 1.71                     | 0.71              |
| 6:D:646:LYS:HG3   | 6:D:720:LEU:HD23  | 1.70                     | 0.71              |
| 4:K:153:ALA:HA    | 4:K:156:HIS:CE1   | 2.26                     | 0.71              |
| 5:M:270:GLY:O     | 5:M:274:ARG:HB3   | 1.89                     | 0.71              |
| 5:M:704:HIS:O     | 5:M:828:ALA:HA    | 1.90                     | 0.71              |
| 5:M:874:LEU:HA    | 6:N:1023:MET:SD   | 2.31                     | 0.71              |
| 5:C:1031:ARG:NE   | 6:D:621:LYS:HB3   | 2.06                     | 0.71              |
| 4:K:56:VAL:HG22   | 4:K:142:VAL:HG12  | 1.70                     | 0.71              |
| 5:M:34:VAL:HB     | 5:M:38:LYS:HG3    | 1.71                     | 0.71              |
| 5:M:677:MET:HE1   | 5:M:679:PHE:HD1   | 1.54                     | 0.71              |
| 5:M:1090:LYS:HE3  | 5:M:1112:PHE:HE1  | 1.55                     | 0.71              |
| 5:M:1101:THR:HG21 | 5:M:1111:ILE:HG23 | 1.71                     | 0.71              |
| 6:N:1042:ARG:NH2  | 6:N:1073:SER:HB3  | 2.05                     | 0.71              |
| 6:N:1136:LYS:HB2  | 6:N:1139:ASP:OD2  | 1.90                     | 0.71              |
| 5:C:355:VAL:HA    | 5:C:358:ARG:HD3   | 1.72                     | 0.71              |
| 5:C:950:LEU:HB3   | 5:C:952:LEU:HD23  | 1.72                     | 0.71              |
| 6:D:119:SER:HB2   | 6:D:123:LEU:HB2   | 1.72                     | 0.71              |
| 5:M:554:ASP:HB2   | 5:M:880:MET:HB2   | 1.71                     | 0.71              |
| 6:N:145:VAL:HG22  | 6:N:146:PRO:HD2   | 1.71                     | 0.71              |
| 6:N:661:MET:HE2   | 6:N:677:LEU:HD11  | 1.72                     | 0.71              |
| 6:N:792:ILE:HD11  | 6:N:878:GLY:O     | 1.91                     | 0.71              |
| 6:N:921:ARG:HB3   | 6:N:921:ARG:NH1   | 2.05                     | 0.71              |
| 5:C:142:ARG:HB3   | 5:C:142:ARG:HH11  | 1.55                     | 0.71              |
| 5:C:675:ALA:HA    | 5:C:989:VAL:HG13  | 1.71                     | 0.71              |
| 5:C:804:VAL:HG11  | 5:C:824:ARG:HH21  | 1.56                     | 0.71              |
| 6:D:185:VAL:HG11  | 6:D:191:LEU:HD21  | 1.72                     | 0.71              |
| 6:D:421:LEU:HB2   | 6:D:427:VAL:HG12  | 1.72                     | 0.71              |
| 6:D:1037:GLN:HG2  | 6:D:1042:ARG:HB3  | 1.73                     | 0.71              |
| 11:M:1216:HOH:O   | 6:N:950:GLY:HA3   | 1.91                     | 0.71              |
| 6:N:521:PRO:HG2   | 6:N:524:LEU:HD22  | 1.72                     | 0.71              |
| 5:C:675:ALA:HB1   | 5:C:677:MET:SD    | 2.31                     | 0.71              |
| 5:C:837:ASP:HA    | 5:C:999:HIS:CE1   | 2.25                     | 0.71              |
| 6:D:615:ARG:NH2   | 6:D:1096:ARG:NH1  | 2.39                     | 0.71              |
| 5:M:376:ARG:HG2   | 11:M:1395:HOH:O   | 1.90                     | 0.71              |
| 5:M:546:LEU:HD21  | 11:M:1376:HOH:O   | 1.90                     | 0.71              |
| 5:M:1115:LEU:HG   | 6:N:85:VAL:HG12   | 1.72                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:83:SER:O      | 6:D:86:ARG:HB3    | 1.90                     | 0.71              |
| 4:K:178:ALA:HB2   | 5:M:864:GLY:H     | 1.55                     | 0.71              |
| 5:M:325:ILE:HD11  | 11:M:1567:HOH:O   | 1.91                     | 0.71              |
| 5:M:1019:GLN:NE2  | 6:N:616:GLN:HE22  | 1.88                     | 0.71              |
| 6:N:50:PHE:CG     | 6:N:522:PRO:HD3   | 2.26                     | 0.71              |
| 6:N:1146:GLY:HA3  | 6:N:1207:TYR:HB2  | 1.71                     | 0.71              |
| 6:D:486:ARG:HA    | 6:D:489:ARG:HG2   | 1.73                     | 0.71              |
| 6:D:1160:LEU:HD11 | 6:D:1174:LEU:HD21 | 1.71                     | 0.71              |
| 6:D:1332:PRO:HG3  | 6:D:1347:TYR:HE2  | 1.54                     | 0.71              |
| 4:K:178:ALA:HB3   | 4:K:198:ARG:HG3   | 1.72                     | 0.71              |
| 4:L:89:PHE:HB3    | 4:L:94:LEU:CD1    | 2.21                     | 0.71              |
| 6:D:1087:ARG:HH21 | 6:D:1253:THR:HG22 | 1.56                     | 0.70              |
| 6:D:1383:ASP:HB2  | 6:D:1416:ALA:HB3  | 1.71                     | 0.70              |
| 6:D:1481:VAL:HG22 | 7:E:18:ARG:HE     | 1.56                     | 0.70              |
| 5:M:609:ASN:HD22  | 5:M:609:ASN:N     | 1.86                     | 0.70              |
| 6:N:502:PHE:CE1   | 6:N:509:PRO:HB3   | 2.26                     | 0.70              |
| 6:N:1033:GLN:HE21 | 6:N:1036:ARG:NH1  | 1.88                     | 0.70              |
| 6:N:1094:LEU:HB2  | 6:N:1260:ILE:HD11 | 1.72                     | 0.70              |
| 2:H:12:G:H1'      | 5:C:393:GLN:HG2   | 1.73                     | 0.70              |
| 5:C:1046:ALA:HA   | 6:D:1472:ILE:HG13 | 1.72                     | 0.70              |
| 6:D:1093:TYR:O    | 6:D:1097:LYS:HG2  | 1.91                     | 0.70              |
| 4:K:220:GLU:O     | 4:K:223:THR:HG22  | 1.89                     | 0.70              |
| 5:M:1:MET:HE1     | 11:M:1332:HOH:O   | 1.91                     | 0.70              |
| 6:N:1406:ARG:HG3  | 6:N:1412:LYS:HG2  | 1.72                     | 0.70              |
| 1:G:13:DT:H5''    | 6:D:1093:TYR:CE2  | 2.26                     | 0.70              |
| 5:C:884:GLN:HB3   | 5:C:992:MET:HE1   | 1.73                     | 0.70              |
| 4:L:102:LYS:HE3   | 4:L:104:GLU:HG3   | 1.73                     | 0.70              |
| 5:M:1031:ARG:HA   | 6:N:621:LYS:O     | 1.92                     | 0.70              |
| 5:C:502:PRO:HB2   | 5:C:509:ALA:HB3   | 1.73                     | 0.70              |
| 5:C:1007:ALA:HB1  | 6:D:652:LEU:HD13  | 1.72                     | 0.70              |
| 6:N:78:VAL:HG12   | 6:N:80:VAL:HG22   | 1.74                     | 0.70              |
| 6:N:507:ASN:H     | 6:N:507:ASN:ND2   | 1.90                     | 0.70              |
| 2:H:6:U:H2'       | 2:H:7:G:N7        | 2.05                     | 0.70              |
| 5:C:1017:THR:HB   | 6:D:613:ARG:HH22  | 1.56                     | 0.70              |
| 6:D:403:PHE:HB2   | 6:D:423:ASP:OD1   | 1.91                     | 0.70              |
| 5:M:108:ILE:HB    | 5:M:368:THR:OG1   | 1.91                     | 0.70              |
| 5:M:200:LEU:HD13  | 5:M:300:ASP:CG    | 2.16                     | 0.70              |
| 2:Y:2:A:OP2       | 6:N:671:LYS:NZ    | 2.25                     | 0.70              |
| 5:C:608:GLY:C     | 5:C:609:ASN:HD22  | 1.99                     | 0.70              |
| 5:C:1085:PHE:O    | 5:C:1089:VAL:HG23 | 1.91                     | 0.70              |
| 6:D:150:ARG:HH22  | 6:D:473:LEU:HD21  | 1.57                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:177:ALA:HB3   | 6:D:205:TYR:OH    | 1.90                     | 0.70              |
| 5:M:433:THR:HG22  | 5:M:437:ARG:HH11  | 1.56                     | 0.70              |
| 6:N:434:ARG:NH1   | 6:N:434:ARG:HB3   | 2.07                     | 0.70              |
| 6:N:786:ILE:HG22  | 6:N:1026:SER:HB3  | 1.73                     | 0.70              |
| 5:C:244:PRO:HB3   | 11:C:1256:HOH:O   | 1.92                     | 0.70              |
| 6:D:179:VAL:HG13  | 6:D:183:GLU:HB3   | 1.74                     | 0.70              |
| 6:D:1090:ASP:HA   | 6:D:1093:TYR:HB2  | 1.72                     | 0.70              |
| 6:D:1098:LEU:HD21 | 6:D:1229:ILE:HD12 | 1.73                     | 0.70              |
| 4:K:48:ILE:HB     | 11:K:973:HOH:O    | 1.90                     | 0.70              |
| 5:M:745:ILE:HD12  | 5:M:745:ILE:H     | 1.57                     | 0.70              |
| 5:C:144:PRO:HG2   | 5:C:265:ARG:NH2   | 2.06                     | 0.70              |
| 5:C:673:LEU:HB3   | 5:C:868:ASP:OD1   | 1.92                     | 0.70              |
| 6:D:117:ASP:H     | 6:D:150:ARG:NH1   | 1.90                     | 0.70              |
| 6:D:117:ASP:HB2   | 6:D:495:ARG:NH2   | 2.07                     | 0.70              |
| 6:D:1209:LEU:HD23 | 6:D:1210:SER:N    | 2.06                     | 0.70              |
| 6:D:1496:GLU:HA   | 6:D:1499:ARG:NE   | 2.06                     | 0.70              |
| 4:K:88:ARG:O      | 4:K:121:GLU:HG2   | 1.91                     | 0.70              |
| 5:M:806:LEU:HD11  | 5:M:824:ARG:NH2   | 2.06                     | 0.70              |
| 6:N:565:ILE:H     | 6:N:565:ILE:HD12  | 1.56                     | 0.70              |
| 2:Y:9:G:H2'       | 2:Y:10:G:H8       | 1.56                     | 0.70              |
| 4:A:227:ASN:O     | 4:B:11:PHE:HB3    | 1.91                     | 0.70              |
| 5:C:762:LYS:HD3   | 5:C:784:ASP:O     | 1.90                     | 0.70              |
| 6:D:496:LEU:O     | 6:D:500:ARG:HG2   | 1.92                     | 0.70              |
| 6:D:584:ASN:OD1   | 6:D:590:PRO:HD2   | 1.91                     | 0.70              |
| 6:D:759:ALA:HA    | 6:D:763:MET:HE2   | 1.74                     | 0.70              |
| 6:D:1005:GLN:HA   | 6:D:1005:GLN:HE21 | 1.57                     | 0.70              |
| 5:M:39:ARG:HD2    | 5:M:39:ARG:N      | 2.05                     | 0.70              |
| 6:N:1042:ARG:O    | 6:N:1057:VAL:HB   | 1.92                     | 0.70              |
| 4:B:38:ASN:HB3    | 4:B:39:PRO:HD3    | 1.74                     | 0.70              |
| 6:D:119:SER:HB2   | 6:D:123:LEU:H     | 1.57                     | 0.70              |
| 6:D:1086:LEU:HD12 | 11:D:8404:HOH:O   | 1.91                     | 0.70              |
| 4:L:110:LYS:HD3   | 4:L:126:ASP:HA    | 1.74                     | 0.70              |
| 6:N:871:LYS:HB3   | 6:N:873:LEU:HD21  | 1.74                     | 0.70              |
| 5:C:874:LEU:H     | 5:C:874:LEU:HD12  | 1.56                     | 0.69              |
| 6:D:1231:GLU:HG2  | 6:D:1235:GLN:CD   | 2.16                     | 0.69              |
| 6:N:462:GLN:HB2   | 6:N:513:ILE:HD13  | 1.74                     | 0.69              |
| 7:O:54:LEU:HA     | 7:O:58:PRO:HG2    | 1.74                     | 0.69              |
| 4:B:89:PHE:HB3    | 4:B:94:LEU:HD12   | 1.74                     | 0.69              |
| 5:C:841:ASN:HD22  | 5:C:841:ASN:H     | 1.38                     | 0.69              |
| 6:D:105:VAL:HG21  | 6:D:128:TYR:HE1   | 1.57                     | 0.69              |
| 6:N:760:ARG:HH11  | 7:O:61:VAL:HG23   | 1.57                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:56:VAL:HG22   | 4:A:142:VAL:HG13  | 1.73                     | 0.69              |
| 5:C:547:ILE:HG21  | 5:C:550:LEU:HD13  | 1.74                     | 0.69              |
| 5:C:886:LEU:HD13  | 6:D:951:ILE:HG13  | 1.73                     | 0.69              |
| 6:D:546:ARG:HA    | 11:D:8178:HOH:O   | 1.91                     | 0.69              |
| 6:D:684:LYS:HB3   | 6:D:686:GLU:HG3   | 1.72                     | 0.69              |
| 5:M:242:LEU:HD13  | 11:M:1532:HOH:O   | 1.92                     | 0.69              |
| 5:C:159:ILE:HG13  | 11:C:1362:HOH:O   | 1.93                     | 0.69              |
| 5:C:689:VAL:HG12  | 5:C:690:ILE:H     | 1.56                     | 0.69              |
| 6:D:38:LYS:HG2    | 6:D:39:PRO:HD2    | 1.73                     | 0.69              |
| 6:D:786:ILE:HD13  | 6:D:908:LYS:HB2   | 1.75                     | 0.69              |
| 5:M:872:ASN:ND2   | 5:M:874:LEU:HB2   | 2.06                     | 0.69              |
| 6:D:136:ASP:HB2   | 6:D:455:ARG:HE    | 1.57                     | 0.69              |
| 6:D:141:ILE:HD11  | 6:D:165:LYS:NZ    | 2.08                     | 0.69              |
| 6:D:756:GLN:HG3   | 6:D:760:ARG:HH11  | 1.57                     | 0.69              |
| 6:D:1147:ARG:HB3  | 6:D:1188:VAL:HG21 | 1.73                     | 0.69              |
| 6:D:1192:LEU:HB3  | 6:D:1345:GLU:OE2  | 1.92                     | 0.69              |
| 6:D:1395:LEU:HD23 | 6:D:1396:GLU:N    | 2.08                     | 0.69              |
| 5:M:333:ILE:N     | 5:M:465:GLY:HA3   | 2.05                     | 0.69              |
| 5:M:462:ASP:CG    | 5:M:463:GLU:H     | 2.01                     | 0.69              |
| 5:M:877:PRO:HG2   | 6:N:1023:MET:SD   | 2.31                     | 0.69              |
| 6:N:41:ARG:HD3    | 6:N:42:ASP:H      | 1.57                     | 0.69              |
| 6:N:554:LEU:HD21  | 6:N:571:LYS:HD3   | 1.75                     | 0.69              |
| 7:O:31:LEU:HD21   | 7:O:60:ALA:HB2    | 1.73                     | 0.69              |
| 5:C:69:LEU:HB2    | 5:C:97:ARG:HB2    | 1.73                     | 0.69              |
| 5:C:265:ARG:HH11  | 5:C:267:TYR:HB3   | 1.55                     | 0.69              |
| 5:C:341:THR:HA    | 11:C:1289:HOH:O   | 1.91                     | 0.69              |
| 5:C:457:ALA:HB3   | 5:C:538:GLN:HA    | 1.74                     | 0.69              |
| 5:C:872:ASN:HD21  | 5:C:874:LEU:CD1   | 2.04                     | 0.69              |
| 5:C:1100:GLN:HA   | 5:C:1100:GLN:HE21 | 1.57                     | 0.69              |
| 6:D:741:ASP:O     | 6:D:743:ASP:N     | 2.25                     | 0.69              |
| 6:D:957:PRO:HA    | 11:D:8083:HOH:O   | 1.91                     | 0.69              |
| 6:D:1059:SER:HA   | 11:D:8349:HOH:O   | 1.93                     | 0.69              |
| 5:M:838:LYS:HG2   | 11:M:1491:HOH:O   | 1.93                     | 0.69              |
| 5:M:853:LEU:HD23  | 5:M:858:MET:HB3   | 1.74                     | 0.69              |
| 6:N:130:SER:HB3   | 6:N:132:TYR:HE1   | 1.57                     | 0.69              |
| 4:A:197:LEU:HG    | 4:A:199:ILE:HD11  | 1.75                     | 0.69              |
| 5:C:134:ARG:HH21  | 5:C:392:SER:HB2   | 1.56                     | 0.69              |
| 5:C:431:HIS:HD2   | 5:C:433:THR:H     | 1.41                     | 0.69              |
| 5:C:511:GLU:O     | 5:C:526:PRO:HD3   | 1.93                     | 0.69              |
| 5:C:578:VAL:HG23  | 5:C:579:VAL:HG12  | 1.74                     | 0.69              |
| 6:D:95:LEU:HD21   | 6:D:574:LEU:HD21  | 1.73                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:399:ARG:HH11  | 6:D:430:ASP:HB2   | 1.57                     | 0.69              |
| 6:D:656:PHE:HB3   | 6:D:694:VAL:HG11  | 1.73                     | 0.69              |
| 7:E:41:GLU:OE1    | 7:E:42:PRO:HD3    | 1.93                     | 0.69              |
| 4:L:52:ALA:HB2    | 4:L:170:VAL:O     | 1.92                     | 0.69              |
| 5:M:689:VAL:HG12  | 5:M:690:ILE:H     | 1.57                     | 0.69              |
| 6:N:54:LYS:HD2    | 6:N:55:ASP:H      | 1.58                     | 0.69              |
| 6:N:586:ARG:NH2   | 6:N:1444:THR:HG21 | 2.07                     | 0.69              |
| 6:N:889:ALA:HB3   | 6:N:930:LEU:HD12  | 1.74                     | 0.69              |
| 6:N:1124:GLN:HB3  | 6:N:1135:ARG:HD3  | 1.74                     | 0.69              |
| 2:H:8:C:H5''      | 11:H:37:HOH:O     | 1.93                     | 0.69              |
| 4:B:64:GLU:HA     | 4:B:165:ILE:HD13  | 1.75                     | 0.69              |
| 5:C:1034:GLU:H    | 6:D:619:LEU:HD13  | 1.58                     | 0.69              |
| 6:D:644:LEU:HD23  | 6:D:718:PRO:HB3   | 1.73                     | 0.69              |
| 6:D:1403:LEU:HD23 | 6:D:1407:LEU:HD13 | 1.74                     | 0.69              |
| 5:M:580:MET:SD    | 5:M:584:GLU:HG3   | 2.33                     | 0.69              |
| 5:M:881:ASN:O     | 5:M:884:GLN:HG3   | 1.91                     | 0.69              |
| 1:X:17:DC:H5''    | 5:M:1030:GLN:HE21 | 1.58                     | 0.69              |
| 11:B:374:HOH:O    | 6:D:851:LEU:HD21  | 1.93                     | 0.69              |
| 5:C:31:GLN:HB3    | 5:C:71:TYR:OH     | 1.92                     | 0.69              |
| 5:C:411:SER:HA    | 5:C:451:LEU:O     | 1.93                     | 0.69              |
| 6:D:554:LEU:HD11  | 6:D:571:LYS:HD3   | 1.75                     | 0.69              |
| 5:M:331:ARG:NH2   | 5:M:427:VAL:HG13  | 2.07                     | 0.69              |
| 5:M:405:ARG:HH22  | 5:M:566:THR:CG2   | 2.05                     | 0.69              |
| 5:C:182:VAL:HG21  | 5:C:220:GLY:O     | 1.93                     | 0.68              |
| 6:D:10:ILE:HB     | 6:D:1451:ALA:HA   | 1.73                     | 0.68              |
| 6:D:634:GLY:HA2   | 6:D:727:GLN:HE21  | 1.57                     | 0.68              |
| 6:D:781:PRO:HG2   | 6:D:911:LEU:HD23  | 1.75                     | 0.68              |
| 6:D:1046:GLN:HG2  | 6:D:1052:THR:HG22 | 1.74                     | 0.68              |
| 5:M:361:MET:HE3   | 5:M:371:LYS:HE3   | 1.75                     | 0.68              |
| 5:M:904:PRO:HD2   | 5:M:908:GLY:HA2   | 1.75                     | 0.68              |
| 6:N:489:ARG:NH2   | 6:N:1389:LEU:HD21 | 2.07                     | 0.68              |
| 6:N:834:THR:HG22  | 6:N:838:ARG:HH11  | 1.58                     | 0.68              |
| 5:C:405:ARG:HG3   | 5:C:442:GLU:OE1   | 1.93                     | 0.68              |
| 5:C:946:ARG:HH22  | 6:D:861:GLN:HE22  | 1.40                     | 0.68              |
| 4:K:94:LEU:HD21   | 4:K:119:ASP:HB3   | 1.74                     | 0.68              |
| 5:M:148:PHE:HZ    | 5:M:281:LEU:HD13  | 1.57                     | 0.68              |
| 5:M:252:LYS:NZ    | 5:M:296:GLY:HA3   | 2.08                     | 0.68              |
| 5:M:479:VAL:HG11  | 5:M:503:LEU:HD11  | 1.75                     | 0.68              |
| 1:G:14:DT:H6      | 1:G:14:DT:H5'     | 1.59                     | 0.68              |
| 4:B:197:LEU:HD21  | 4:B:199:ILE:HD11  | 1.74                     | 0.68              |
| 6:D:524:LEU:O     | 6:D:526:PRO:HD3   | 1.92                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:1399:ASP:O    | 6:D:1403:LEU:HB2  | 1.93                     | 0.68              |
| 4:L:61:VAL:HG21   | 4:L:75:VAL:HG21   | 1.75                     | 0.68              |
| 5:M:333:ILE:H     | 5:M:465:GLY:CA    | 2.05                     | 0.68              |
| 6:N:807:ALA:HB2   | 6:N:833:GLU:OE1   | 1.93                     | 0.68              |
| 6:N:1042:ARG:HH21 | 6:N:1045:MET:HE2  | 1.59                     | 0.68              |
| 6:N:1492:LEU:HD12 | 6:N:1493:LYS:NZ   | 2.09                     | 0.68              |
| 4:B:59:GLU:CB     | 4:B:137:ARG:HH12  | 2.03                     | 0.68              |
| 5:C:158:TYR:O     | 5:C:310:LEU:HD11  | 1.93                     | 0.68              |
| 6:D:136:ASP:CG    | 6:D:463:GLN:HB3   | 2.18                     | 0.68              |
| 6:D:868:TYR:HB2   | 6:D:873:LEU:HD12  | 1.76                     | 0.68              |
| 6:D:1109:GLU:HG2  | 6:D:1201:CYS:CA   | 2.20                     | 0.68              |
| 6:D:1196:THR:HG22 | 11:D:8501:HOH:O   | 1.94                     | 0.68              |
| 6:D:1380:GLU:HG3  | 6:D:1420:LEU:HD12 | 1.74                     | 0.68              |
| 5:M:343:GLN:HG2   | 5:M:385:PHE:HB2   | 1.75                     | 0.68              |
| 5:C:5:ARG:CZ      | 5:C:8:ARG:HH22    | 2.06                     | 0.68              |
| 6:D:98:PRO:HB3    | 11:D:8058:HOH:O   | 1.93                     | 0.68              |
| 6:D:409:VAL:CG2   | 6:D:421:LEU:HA    | 2.24                     | 0.68              |
| 6:D:526:PRO:HA    | 11:D:8171:HOH:O   | 1.93                     | 0.68              |
| 6:D:701:LEU:HD21  | 6:D:763:MET:HE3   | 1.75                     | 0.68              |
| 6:D:800:LYS:HE3   | 6:D:804:LEU:HD22  | 1.74                     | 0.68              |
| 6:D:964:LEU:HD21  | 6:D:1058:ARG:HE   | 1.57                     | 0.68              |
| 5:M:305:PRO:HG3   | 5:M:308:ARG:HH22  | 1.59                     | 0.68              |
| 6:N:1161:GLU:HG2  | 6:N:1164:ARG:HB2  | 1.74                     | 0.68              |
| 6:D:22:SER:HB2    | 6:D:92:HIS:HB3    | 1.76                     | 0.68              |
| 6:D:988:ARG:O     | 6:D:992:ILE:HG13  | 1.94                     | 0.68              |
| 4:K:58:ILE:HG21   | 4:K:68:ILE:HD11   | 1.75                     | 0.68              |
| 6:N:1191:PRO:HG2  | 6:N:1370:ILE:HD13 | 1.74                     | 0.68              |
| 5:C:435:TYR:HE1   | 5:C:539:VAL:HG22  | 1.58                     | 0.68              |
| 6:D:650:LEU:HD23  | 6:D:691:LEU:HD23  | 1.75                     | 0.68              |
| 6:D:1197:ARG:HB3  | 6:D:1396:GLU:HG3  | 1.74                     | 0.68              |
| 6:D:1223:ILE:CG2  | 6:D:1227:GLN:HE21 | 2.06                     | 0.68              |
| 6:D:1252:ILE:HG13 | 6:D:1253:THR:H    | 1.59                     | 0.68              |
| 5:M:874:LEU:O     | 5:M:877:PRO:HD2   | 1.93                     | 0.68              |
| 6:N:119:SER:HB2   | 6:N:123:LEU:H     | 1.59                     | 0.68              |
| 6:N:394:LEU:O     | 6:N:396:VAL:HG23  | 1.94                     | 0.68              |
| 6:N:879:ARG:HH21  | 6:N:904:VAL:N     | 1.90                     | 0.68              |
| 6:D:455:ARG:HB3   | 6:D:459:GLU:HG2   | 1.76                     | 0.68              |
| 6:D:984:THR:HG22  | 6:D:987:GLU:HG3   | 1.76                     | 0.68              |
| 5:M:244:PRO:HG2   | 5:M:246:ASP:OD2   | 1.94                     | 0.68              |
| 5:M:510:ALA:HB3   | 5:M:513:VAL:HG23  | 1.76                     | 0.68              |
| 4:B:85:LEU:HA     | 4:B:124:ASN:HD22  | 1.57                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:123:MET:C     | 4:B:125:PRO:HD3   | 2.19                     | 0.68              |
| 5:C:408:ARG:HG2   | 5:C:454:SER:HB3   | 1.74                     | 0.68              |
| 6:D:1032:PRO:HB2  | 11:D:8254:HOH:O   | 1.93                     | 0.68              |
| 6:N:526:PRO:O     | 6:N:537:THR:HA    | 1.94                     | 0.68              |
| 5:M:292:ARG:HD2   | 5:M:299:LYS:NZ    | 2.08                     | 0.68              |
| 5:M:516:ARG:NH1   | 5:M:521:PRO:HB3   | 2.09                     | 0.68              |
| 5:M:691:SER:HA    | 5:M:858:MET:HE1   | 1.75                     | 0.68              |
| 7:O:51:LEU:HD23   | 7:O:52:GLU:H      | 1.59                     | 0.68              |
| 5:C:709:GLU:HG3   | 5:C:824:ARG:HG2   | 1.76                     | 0.67              |
| 5:M:768:THR:HB    | 5:M:771:GLU:HB3   | 1.75                     | 0.67              |
| 6:N:546:ARG:NH1   | 6:N:546:ARG:HB3   | 2.08                     | 0.67              |
| 2:H:8:C:HO2'      | 2:H:9:G:H5'       | 1.58                     | 0.67              |
| 5:C:106:GLY:O     | 5:C:107:LEU:HD23  | 1.94                     | 0.67              |
| 5:C:610:ARG:HD3   | 5:C:622:GLU:OE2   | 1.94                     | 0.67              |
| 6:D:29:PRO:CG     | 6:D:549:ASN:HD21  | 2.07                     | 0.67              |
| 6:D:97:THR:HG21   | 6:D:571:LYS:HZ3   | 1.58                     | 0.67              |
| 6:D:782:SER:N     | 6:D:785:ILE:HD13  | 2.08                     | 0.67              |
| 6:D:1252:ILE:HG13 | 6:D:1253:THR:N    | 2.09                     | 0.67              |
| 4:L:206:THR:HG22  | 4:L:209:GLU:H     | 1.59                     | 0.67              |
| 5:M:432:ARG:HH22  | 6:N:1047:LYS:HD3  | 1.59                     | 0.67              |
| 5:M:438:ILE:HD11  | 5:M:467:ILE:HD12  | 1.75                     | 0.67              |
| 5:M:762:LYS:HD3   | 5:M:784:ASP:O     | 1.94                     | 0.67              |
| 5:M:1111:ILE:HG13 | 5:M:1112:PHE:H    | 1.57                     | 0.67              |
| 6:N:90:MET:HE1    | 6:N:518:PRO:HB2   | 1.76                     | 0.67              |
| 6:N:402:PRO:HG2   | 11:N:9030:HOH:O   | 1.93                     | 0.67              |
| 2:Y:11:C:H2'      | 2:Y:12:G:C8       | 2.30                     | 0.67              |
| 5:C:1:MET:HG2     | 5:C:900:ARG:HH22  | 1.60                     | 0.67              |
| 5:C:762:LYS:HD2   | 5:C:786:LYS:HB2   | 1.75                     | 0.67              |
| 5:M:1034:GLU:HB3  | 6:N:619:LEU:HD13  | 1.75                     | 0.67              |
| 6:N:1412:LYS:O    | 6:N:1414:PRO:HD3  | 1.93                     | 0.67              |
| 5:C:185:LYS:HE2   | 5:C:190:LYS:HZ3   | 1.60                     | 0.67              |
| 5:C:433:THR:HG22  | 5:C:437:ARG:HH11  | 1.58                     | 0.67              |
| 5:C:630:ARG:HA    | 5:C:705:ILE:HD13  | 1.77                     | 0.67              |
| 5:C:1050:GLN:HE22 | 6:D:1471:LEU:HB2  | 1.59                     | 0.67              |
| 6:D:761:ILE:HG12  | 7:E:65:MET:HE3    | 1.77                     | 0.67              |
| 6:D:786:ILE:HG21  | 6:D:1027:GLY:H    | 1.58                     | 0.67              |
| 6:D:952:ASP:HA    | 6:D:1062:ARG:HH21 | 1.60                     | 0.67              |
| 6:D:1101:VAL:CG2  | 6:D:1424:VAL:HG23 | 2.23                     | 0.67              |
| 6:N:524:LEU:O     | 6:N:526:PRO:HD3   | 1.95                     | 0.67              |
| 6:N:814:ALA:O     | 6:N:818:ARG:HG3   | 1.95                     | 0.67              |
| 6:N:1124:GLN:NE2  | 6:N:1135:ARG:HA   | 2.10                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:1434:TRP:CZ3  | 6:N:1457:ASP:HB2  | 2.29                     | 0.67              |
| 5:C:909:ALA:HB1   | 5:C:914:ILE:HD11  | 1.76                     | 0.67              |
| 6:D:455:ARG:HB2   | 6:D:460:ALA:CA    | 2.25                     | 0.67              |
| 6:D:610:LYS:O     | 6:D:615:ARG:HD3   | 1.93                     | 0.67              |
| 6:D:654:LYS:HB3   | 6:D:655:PRO:HD3   | 1.77                     | 0.67              |
| 5:M:549:PHE:CD1   | 5:M:886:LEU:HD23  | 2.30                     | 0.67              |
| 6:N:483:HIS:HB2   | 6:N:484:PRO:HD3   | 1.76                     | 0.67              |
| 4:B:58:ILE:HB     | 4:B:61:VAL:HB     | 1.76                     | 0.67              |
| 5:C:235:LEU:HD21  | 11:C:1313:HOH:O   | 1.93                     | 0.67              |
| 5:C:898:GLY:HA2   | 11:C:1408:HOH:O   | 1.94                     | 0.67              |
| 5:M:805:ARG:HD3   | 5:M:823:VAL:HG22  | 1.75                     | 0.67              |
| 6:N:131:LYS:HD3   | 6:N:456:MET:SD    | 2.35                     | 0.67              |
| 6:N:520:LEU:HD21  | 6:N:524:LEU:HD23  | 1.76                     | 0.67              |
| 5:M:252:LYS:HA    | 11:M:1276:HOH:O   | 1.95                     | 0.67              |
| 6:N:394:LEU:HD21  | 6:N:445:ARG:HH22  | 1.58                     | 0.67              |
| 6:N:1201:CYS:SG   | 6:N:1204:CYS:HB2  | 2.35                     | 0.67              |
| 4:B:206:THR:HG22  | 4:B:209:GLU:H     | 1.59                     | 0.67              |
| 5:C:443:THR:HG22  | 5:C:453:THR:HB    | 1.77                     | 0.67              |
| 6:D:134:VAL:HB    | 6:D:464:LEU:HD11  | 1.75                     | 0.67              |
| 6:D:396:VAL:O     | 6:D:398:ALA:N     | 2.25                     | 0.67              |
| 6:D:396:VAL:C     | 6:D:398:ALA:H     | 2.03                     | 0.67              |
| 6:D:715:ALA:HB3   | 6:D:764:LEU:HA    | 1.76                     | 0.67              |
| 6:D:1393:GLN:OE1  | 6:D:1394:VAL:HG23 | 1.95                     | 0.67              |
| 5:M:1115:LEU:HB3  | 6:N:89:ARG:NH1    | 2.10                     | 0.67              |
| 6:N:908:LYS:HB2   | 6:N:1027:GLY:HA3  | 1.76                     | 0.67              |
| 6:N:971:LEU:O     | 6:N:975:GLU:HG2   | 1.94                     | 0.67              |
| 6:D:101:HIS:HD1   | 6:D:103:TRP:HB2   | 1.59                     | 0.67              |
| 6:D:1498:ALA:HB2  | 7:E:88:GLU:OE1    | 1.95                     | 0.67              |
| 4:K:1:MET:SD      | 4:K:5:LYS:HB3     | 2.35                     | 0.67              |
| 5:M:971:LYS:HA    | 5:M:988:VAL:HA    | 1.76                     | 0.67              |
| 6:N:1340:GLY:O    | 6:N:1344:VAL:HG23 | 1.94                     | 0.67              |
| 6:N:1480:PHE:HB2  | 11:N:9408:HOH:O   | 1.94                     | 0.67              |
| 1:G:17:DC:H4'     | 6:D:628:ARG:CZ    | 2.25                     | 0.67              |
| 6:D:963:TYR:CE2   | 6:D:1002:LYS:HB3  | 2.29                     | 0.67              |
| 6:D:1465:ASN:ND2  | 6:D:1470:ARG:HB3  | 2.09                     | 0.67              |
| 6:D:1485:GLN:HE21 | 7:E:78:ASN:HA     | 1.60                     | 0.67              |
| 5:M:399:ASN:OD1   | 5:M:401:LEU:HB3   | 1.95                     | 0.67              |
| 5:M:552:HIS:CD2   | 5:M:886:LEU:HD22  | 2.30                     | 0.67              |
| 6:N:1267:ARG:HG3  | 6:N:1271:LYS:HZ3  | 1.59                     | 0.67              |
| 1:G:18:DG:O3'     | 5:C:1001:VAL:HB   | 1.94                     | 0.66              |
| 2:H:11:C:H2'      | 2:H:12:G:C8       | 2.29                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:5:ARG:NE     | 5:C:8:ARG:HH22    | 1.93                     | 0.66              |
| 5:C:244:PRO:HG3  | 11:C:1490:HOH:O   | 1.95                     | 0.66              |
| 5:C:518:LYS:O    | 5:C:520:GLU:HG2   | 1.95                     | 0.66              |
| 6:D:38:LYS:NZ    | 6:D:59:ALA:HB1    | 2.09                     | 0.66              |
| 6:D:127:LEU:HD12 | 6:D:128:TYR:N     | 2.10                     | 0.66              |
| 6:D:396:VAL:HG12 | 6:D:398:ALA:HB2   | 1.77                     | 0.66              |
| 6:D:434:ARG:N    | 6:D:447:VAL:HG22  | 2.09                     | 0.66              |
| 6:D:584:ASN:HB2  | 6:D:602:SER:HB3   | 1.78                     | 0.66              |
| 6:D:786:ILE:HG21 | 6:D:1027:GLY:N    | 2.10                     | 0.66              |
| 6:D:1252:ILE:O   | 6:D:1256:LEU:HD12 | 1.95                     | 0.66              |
| 5:M:473:ARG:HA   | 5:M:531:PHE:HD1   | 1.60                     | 0.66              |
| 6:N:1346:ARG:HD3 | 11:N:9293:HOH:O   | 1.95                     | 0.66              |
| 1:G:14:DT:H2''   | 1:G:15:DC:H5'     | 1.76                     | 0.66              |
| 4:A:79:ILE:HA    | 4:A:82:LEU:HD12   | 1.77                     | 0.66              |
| 5:C:270:GLY:O    | 5:C:274:ARG:HB3   | 1.96                     | 0.66              |
| 6:D:716:PHE:CE1  | 6:D:765:SER:HB3   | 2.30                     | 0.66              |
| 6:D:977:ALA:HB1  | 6:D:983:LEU:HD21  | 1.77                     | 0.66              |
| 4:K:150:TYR:HE2  | 4:K:152:PRO:HG3   | 1.60                     | 0.66              |
| 5:M:45:GLN:HB2   | 5:M:71:TYR:CE2    | 2.31                     | 0.66              |
| 5:M:433:THR:HG22 | 5:M:437:ARG:NH1   | 2.10                     | 0.66              |
| 5:M:561:GLY:O    | 5:M:564:MET:HG3   | 1.95                     | 0.66              |
| 5:M:764:GLU:HB2  | 6:N:54:LYS:HD3    | 1.77                     | 0.66              |
| 6:N:1121:PRO:HD2 | 6:N:1346:ARG:NH2  | 2.09                     | 0.66              |
| 5:C:435:TYR:CE1  | 5:C:539:VAL:HG22  | 2.31                     | 0.66              |
| 5:C:494:TYR:HB3  | 11:C:1172:HOH:O   | 1.96                     | 0.66              |
| 6:D:480:GLU:O    | 6:D:484:PRO:HD2   | 1.96                     | 0.66              |
| 5:M:251:ASP:HB3  | 5:M:252:LYS:HD2   | 1.78                     | 0.66              |
| 5:M:953:VAL:HB   | 5:M:962:GLN:NE2   | 2.10                     | 0.66              |
| 6:N:119:SER:H    | 6:N:123:LEU:CD2   | 2.07                     | 0.66              |
| 6:N:1000:THR:O   | 6:N:1003:VAL:HG12 | 1.95                     | 0.66              |
| 5:C:313:LEU:HB2  | 5:C:321:GLU:HG3   | 1.76                     | 0.66              |
| 5:C:315:ALA:HB3  | 11:C:1454:HOH:O   | 1.94                     | 0.66              |
| 5:M:102:HIS:HB2  | 5:M:106:GLY:O     | 1.95                     | 0.66              |
| 5:M:288:ARG:HG3  | 11:M:1542:HOH:O   | 1.94                     | 0.66              |
| 5:M:841:ASN:ND2  | 5:M:844:GLY:H     | 1.93                     | 0.66              |
| 6:N:800:LYS:NZ   | 6:N:804:LEU:HD13  | 2.11                     | 0.66              |
| 6:N:813:LEU:O    | 6:N:817:GLU:HB2   | 1.96                     | 0.66              |
| 6:N:1266:ARG:HG2 | 6:N:1267:ARG:N    | 2.10                     | 0.66              |
| 5:C:516:ARG:HD2  | 5:C:521:PRO:HA    | 1.76                     | 0.66              |
| 6:D:52:PRO:HG2   | 6:D:80:VAL:HG13   | 1.76                     | 0.66              |
| 6:N:900:ILE:HG22 | 6:N:914:LEU:HD11  | 1.75                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:1111:ASP:HB2  | 6:N:1203:LYS:HZ1  | 1.60                     | 0.66              |
| 5:C:7:GLY:C       | 5:C:8:ARG:HD2     | 2.20                     | 0.66              |
| 5:C:151:ASP:HB2   | 5:C:157:ARG:O     | 1.95                     | 0.66              |
| 5:C:987:ILE:HG13  | 11:C:1149:HOH:O   | 1.94                     | 0.66              |
| 5:C:1118:LYS:HA   | 6:D:23:TYR:OH     | 1.95                     | 0.66              |
| 4:K:31:GLY:HA3    | 4:L:42:ARG:NH2    | 2.09                     | 0.66              |
| 4:L:56:VAL:HG13   | 4:L:142:VAL:HG12  | 1.78                     | 0.66              |
| 5:M:129:ILE:HG12  | 5:M:386:PHE:O     | 1.95                     | 0.66              |
| 5:M:861:LEU:HD13  | 5:M:865:THR:CG2   | 2.25                     | 0.66              |
| 6:N:796:ARG:NE    | 6:N:828:LYS:HZ3   | 1.94                     | 0.66              |
| 6:N:1106:VAL:HG11 | 6:N:1474:ALA:HB1  | 1.78                     | 0.66              |
| 4:A:14:ARG:HH22   | 4:A:24:VAL:HG23   | 1.61                     | 0.66              |
| 4:B:125:PRO:HD2   | 11:B:346:HOH:O    | 1.94                     | 0.66              |
| 5:C:629:TYR:HA    | 11:C:1337:HOH:O   | 1.96                     | 0.66              |
| 5:C:1091:GLU:OE1  | 6:D:613:ARG:HG2   | 1.96                     | 0.66              |
| 6:D:691:LEU:O     | 6:D:695:ILE:HG22  | 1.95                     | 0.66              |
| 6:D:1462:LEU:HD22 | 6:D:1472:ILE:HG22 | 1.77                     | 0.66              |
| 5:M:443:THR:HG21  | 6:N:1078:ARG:NE   | 2.10                     | 0.66              |
| 5:M:689:VAL:HG12  | 5:M:690:ILE:N     | 2.11                     | 0.66              |
| 6:N:1111:ASP:HB2  | 6:N:1203:LYS:NZ   | 2.11                     | 0.66              |
| 5:C:236:ILE:HG13  | 11:C:1121:HOH:O   | 1.96                     | 0.66              |
| 5:C:244:PRO:HD2   | 5:C:245:GLY:H     | 1.60                     | 0.66              |
| 5:C:678:PRO:HD2   | 11:D:8199:HOH:O   | 1.95                     | 0.66              |
| 5:C:1103:ASP:HB3  | 5:C:1105:LYS:HZ1  | 1.60                     | 0.66              |
| 6:D:879:ARG:HH21  | 6:D:903:ASP:HA    | 1.60                     | 0.66              |
| 4:K:124:ASN:HD22  | 4:K:127:LEU:HD22  | 1.60                     | 0.66              |
| 5:M:473:ARG:HA    | 5:M:531:PHE:CD1   | 2.30                     | 0.66              |
| 5:M:810:ASP:OD2   | 5:M:815:LEU:HD22  | 1.96                     | 0.66              |
| 6:N:396:VAL:HG12  | 6:N:447:VAL:HA    | 1.76                     | 0.66              |
| 6:N:542:ASP:HA    | 6:N:545:ARG:HE    | 1.60                     | 0.66              |
| 7:O:45:ARG:HG2    | 7:O:46:PRO:CD     | 2.24                     | 0.66              |
| 2:H:6:U:H5'       | 11:H:45:HOH:O     | 1.94                     | 0.66              |
| 5:C:516:ARG:HE    | 6:D:1068:LEU:HD13 | 1.60                     | 0.66              |
| 5:C:597:ALA:HB2   | 5:C:655:LEU:HD21  | 1.78                     | 0.66              |
| 5:C:755:LEU:HD21  | 5:C:792:VAL:HG22  | 1.75                     | 0.66              |
| 5:C:838:LYS:HG3   | 5:C:997:LEU:HB2   | 1.78                     | 0.66              |
| 6:D:466:LYS:HA    | 11:D:8320:HOH:O   | 1.95                     | 0.66              |
| 6:D:568:ARG:O     | 6:D:572:ARG:HG3   | 1.96                     | 0.66              |
| 6:D:1252:ILE:HA   | 11:D:8219:HOH:O   | 1.96                     | 0.66              |
| 6:D:1396:GLU:HA   | 6:D:1399:ASP:OD2  | 1.96                     | 0.66              |
| 4:L:221:HIS:HB3   | 11:L:365:HOH:O    | 1.96                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:267:TYR:HB2   | 5:M:272:ALA:HB1   | 1.78                     | 0.66              |
| 5:M:979:THR:HG23  | 5:M:981:GLU:H     | 1.60                     | 0.66              |
| 6:N:1044:LEU:HD22 | 6:N:1052:THR:HG22 | 1.76                     | 0.66              |
| 4:A:117:VAL:HB    | 4:A:120:VAL:CG1   | 2.26                     | 0.66              |
| 5:C:12:VAL:HG13   | 5:C:13:ILE:HG12   | 1.78                     | 0.66              |
| 5:C:69:LEU:HD13   | 5:C:109:LYS:HE3   | 1.78                     | 0.66              |
| 6:D:1089:ALA:HB3  | 11:D:8250:HOH:O   | 1.95                     | 0.66              |
| 6:D:1189:ARG:HB3  | 6:D:1204:CYS:HA   | 1.78                     | 0.66              |
| 5:M:553:ASP:HA    | 5:M:881:ASN:HA    | 1.78                     | 0.66              |
| 5:M:861:LEU:HD23  | 5:M:863:ASP:H     | 1.61                     | 0.66              |
| 5:M:928:LYS:NZ    | 5:M:932:GLU:HG3   | 2.10                     | 0.66              |
| 6:N:468:LEU:HB3   | 11:N:9068:HOH:O   | 1.96                     | 0.66              |
| 6:N:618:LEU:HB3   | 6:N:619:LEU:HD23  | 1.78                     | 0.66              |
| 6:N:1151:ARG:HG2  | 6:N:1187:PRO:HB2  | 1.77                     | 0.66              |
| 5:C:83:CYS:HA     | 5:C:88:LEU:HB2    | 1.78                     | 0.65              |
| 6:D:890:VAL:HG11  | 6:D:922:LEU:HD13  | 1.78                     | 0.65              |
| 6:D:1329:ALA:O    | 6:D:1330:ILE:HD12 | 1.96                     | 0.65              |
| 4:K:198:ARG:HH22  | 5:M:932:GLU:HB3   | 1.61                     | 0.65              |
| 5:M:502:PRO:HB2   | 5:M:509:ALA:HB3   | 1.77                     | 0.65              |
| 5:M:690:ILE:CD1   | 5:M:833:LEU:HD23  | 2.26                     | 0.65              |
| 6:N:413:ASP:O     | 6:N:435:VAL:HG23  | 1.96                     | 0.65              |
| 6:N:553:ARG:O     | 6:N:557:LEU:HG    | 1.96                     | 0.65              |
| 7:O:27:ALA:HB2    | 7:O:61:VAL:HG12   | 1.77                     | 0.65              |
| 5:C:676:ILE:CG2   | 5:C:988:VAL:HG13  | 2.27                     | 0.65              |
| 6:D:761:ILE:HG23  | 7:E:6:ILE:HD11    | 1.78                     | 0.65              |
| 5:M:98:LEU:HD13   | 5:M:110:GLU:O     | 1.95                     | 0.65              |
| 6:N:769:LEU:HD12  | 6:N:770:LEU:HG    | 1.77                     | 0.65              |
| 6:N:917:GLN:O     | 6:N:921:ARG:HG2   | 1.96                     | 0.65              |
| 6:N:1148:VAL:HB   | 6:N:1203:LYS:O    | 1.96                     | 0.65              |
| 6:N:1342:GLU:HA   | 11:N:9208:HOH:O   | 1.96                     | 0.65              |
| 5:C:52:PHE:CD2    | 5:C:68:PHE:HB2    | 2.31                     | 0.65              |
| 5:C:194:VAL:HA    | 5:C:197:LEU:HD12  | 1.78                     | 0.65              |
| 5:C:937:ASP:HB2   | 5:C:940:GLU:HG3   | 1.78                     | 0.65              |
| 5:C:1067:TYR:O    | 5:C:1071:ILE:HG12 | 1.96                     | 0.65              |
| 6:D:796:ARG:HH21  | 6:D:828:LYS:HE2   | 1.61                     | 0.65              |
| 5:M:689:VAL:HB    | 5:M:870:ILE:HG13  | 1.78                     | 0.65              |
| 5:M:911:GLU:O     | 5:M:915:LYS:HG2   | 1.96                     | 0.65              |
| 6:N:788:GLY:O     | 6:N:792:ILE:HG22  | 1.95                     | 0.65              |
| 1:G:17:DC:O3'     | 6:D:628:ARG:NH2   | 2.29                     | 0.65              |
| 4:B:213:GLN:O     | 4:B:217:ILE:HD13  | 1.96                     | 0.65              |
| 6:D:879:ARG:HH11  | 6:D:879:ARG:HG3   | 1.60                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:1476:THR:HG23 | 7:E:21:VAL:HG22   | 1.77                     | 0.65              |
| 5:M:129:ILE:HD13  | 5:M:134:ARG:HB2   | 1.78                     | 0.65              |
| 11:M:1409:HOH:O   | 7:O:31:LEU:HD13   | 1.96                     | 0.65              |
| 6:N:150:ARG:HG3   | 11:N:9044:HOH:O   | 1.96                     | 0.65              |
| 6:N:960:LYS:HB3   | 11:N:9374:HOH:O   | 1.96                     | 0.65              |
| 5:C:22:GLN:HE22   | 5:C:407:LYS:HG2   | 1.59                     | 0.65              |
| 4:L:102:LYS:HB2   | 4:L:139:ASN:OD1   | 1.96                     | 0.65              |
| 6:N:660:LYS:HD2   | 6:N:694:VAL:HG22  | 1.78                     | 0.65              |
| 6:N:1112:CYS:HB2  | 6:N:1195:GLN:HG2  | 1.78                     | 0.65              |
| 6:N:1437:ALA:O    | 6:N:1446:VAL:HG21 | 1.95                     | 0.65              |
| 6:N:1490:LYS:HE2  | 7:O:93:TYR:OH     | 1.96                     | 0.65              |
| 6:N:778:LEU:HA    | 6:N:780:LYS:HE2   | 1.78                     | 0.65              |
| 6:N:1174:LEU:HD22 | 6:N:1183:ILE:HD13 | 1.79                     | 0.65              |
| 2:Y:10:G:O2'      | 2:Y:11:C:H5'      | 1.96                     | 0.65              |
| 4:A:197:LEU:HD23  | 4:A:197:LEU:H     | 1.62                     | 0.65              |
| 5:C:274:ARG:HG3   | 5:C:285:LEU:HD22  | 1.79                     | 0.65              |
| 5:C:837:ASP:O     | 5:C:848:VAL:HG13  | 1.96                     | 0.65              |
| 5:C:841:ASN:HD22  | 5:C:841:ASN:N     | 1.91                     | 0.65              |
| 5:C:971:LYS:HA    | 5:C:988:VAL:HA    | 1.79                     | 0.65              |
| 4:K:112:ARG:NE    | 4:K:125:PRO:HB2   | 2.00                     | 0.65              |
| 5:M:305:PRO:HG3   | 5:M:308:ARG:NH2   | 2.12                     | 0.65              |
| 5:M:705:ILE:HA    | 5:M:827:VAL:O     | 1.97                     | 0.65              |
| 5:M:716:LYS:HZ1   | 6:N:36:THR:HA     | 1.61                     | 0.65              |
| 5:M:808:ARG:NH2   | 5:M:820:ARG:HH21  | 1.95                     | 0.65              |
| 6:N:132:TYR:HA    | 11:N:9432:HOH:O   | 1.96                     | 0.65              |
| 6:N:421:LEU:HB2   | 6:N:427:VAL:HG12  | 1.79                     | 0.65              |
| 6:N:661:MET:HA    | 6:N:666:ILE:HD12  | 1.79                     | 0.65              |
| 2:H:12:G:O2'      | 2:H:13:C:H5'      | 1.97                     | 0.65              |
| 4:B:137:ARG:NH1   | 4:B:139:ASN:HB3   | 2.11                     | 0.65              |
| 5:C:17:PRO:HB2    | 5:C:20:GLU:HB2    | 1.77                     | 0.65              |
| 5:C:328:LEU:H     | 5:C:433:THR:HB    | 1.61                     | 0.65              |
| 6:D:131:LYS:HA    | 6:D:456:MET:HB2   | 1.77                     | 0.65              |
| 6:D:133:ILE:O     | 6:D:152:LEU:HB2   | 1.97                     | 0.65              |
| 6:D:996:TRP:O     | 6:D:1000:THR:HG22 | 1.96                     | 0.65              |
| 5:M:435:TYR:CE1   | 5:M:539:VAL:HG22  | 2.29                     | 0.65              |
| 5:M:937:ASP:HB3   | 5:M:940:GLU:H     | 1.62                     | 0.65              |
| 6:N:637:LEU:HD21  | 6:N:642:CYS:HA    | 1.79                     | 0.65              |
| 6:N:754:PHE:CE2   | 6:N:1476:THR:HG21 | 2.32                     | 0.65              |
| 4:B:54:THR:HG22   | 4:B:158:ILE:HG13  | 1.78                     | 0.65              |
| 5:C:1060:ILE:HG23 | 5:C:1061:GLU:H    | 1.62                     | 0.65              |
| 6:D:50:PHE:HB3    | 6:D:522:PRO:HG3   | 1.79                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:K:27:PRO:HG2    | 4:K:186:LEU:HD13  | 1.77                     | 0.65              |
| 6:N:74:GLU:HB3    | 6:N:75:ARG:NH2    | 2.12                     | 0.65              |
| 6:N:876:SER:O     | 6:N:880:ILE:HG12  | 1.97                     | 0.65              |
| 6:N:1109:GLU:CD   | 6:N:1202:GLN:H    | 2.03                     | 0.65              |
| 7:O:28:GLN:HB3    | 7:O:32:ARG:HH22   | 1.61                     | 0.65              |
| 1:G:16:DG:OP1     | 5:C:1031:ARG:HD3  | 1.95                     | 0.65              |
| 5:C:290:LEU:HD22  | 5:C:302:VAL:HG11  | 1.79                     | 0.65              |
| 6:D:822:ALA:HB1   | 11:D:8089:HOH:O   | 1.97                     | 0.65              |
| 6:D:1084:THR:OG1  | 6:D:1238:MET:HA   | 1.96                     | 0.65              |
| 7:E:27:ALA:HB2    | 7:E:61:VAL:HG12   | 1.79                     | 0.65              |
| 5:M:1056:LYS:HB3  | 6:N:624:ASP:H     | 1.60                     | 0.65              |
| 6:N:131:LYS:HG2   | 6:N:568:ARG:HG2   | 1.79                     | 0.65              |
| 6:N:948:THR:HB    | 11:N:9020:HOH:O   | 1.97                     | 0.65              |
| 7:O:3:GLU:OE1     | 7:O:65:MET:HE1    | 1.96                     | 0.65              |
| 6:D:882:PHE:HA    | 6:D:885:ILE:HD12  | 1.79                     | 0.64              |
| 6:D:895:VAL:O     | 6:D:899:LEU:HG    | 1.97                     | 0.64              |
| 5:M:442:GLU:HG2   | 5:M:454:SER:CB    | 2.26                     | 0.64              |
| 6:N:1147:ARG:HB3  | 6:N:1188:VAL:HG21 | 1.79                     | 0.64              |
| 5:C:343:GLN:HA    | 5:C:343:GLN:NE2   | 2.11                     | 0.64              |
| 5:C:689:VAL:HG12  | 5:C:690:ILE:N     | 2.12                     | 0.64              |
| 5:M:158:TYR:CE1   | 5:M:313:LEU:HG    | 2.33                     | 0.64              |
| 5:M:166:PRO:HG3   | 11:M:1337:HOH:O   | 1.97                     | 0.64              |
| 2:H:10:G:O2'      | 2:H:11:C:H5'      | 1.97                     | 0.64              |
| 4:B:25:LEU:O      | 4:B:28:LEU:HD21   | 1.97                     | 0.64              |
| 5:C:158:TYR:CD1   | 5:C:313:LEU:HG    | 2.32                     | 0.64              |
| 5:C:470:PRO:HB2   | 5:C:534:VAL:HG21  | 1.78                     | 0.64              |
| 5:C:525:SER:HB2   | 5:C:527:GLU:HG3   | 1.79                     | 0.64              |
| 6:D:141:ILE:HD13  | 6:D:450:TYR:HB3   | 1.79                     | 0.64              |
| 6:D:484:PRO:CB    | 6:D:488:ARG:HE    | 2.07                     | 0.64              |
| 6:D:1101:VAL:HG21 | 6:D:1424:VAL:HG23 | 1.78                     | 0.64              |
| 6:D:1376:MET:HE3  | 6:D:1421:LEU:HB2  | 1.78                     | 0.64              |
| 7:E:48:MET:HB2    | 7:E:54:LEU:HD12   | 1.80                     | 0.64              |
| 4:K:52:ALA:HA     | 11:K:1094:HOH:O   | 1.96                     | 0.64              |
| 5:M:771:GLU:HG3   | 11:M:1181:HOH:O   | 1.96                     | 0.64              |
| 6:N:762:GLN:HA    | 11:N:9032:HOH:O   | 1.97                     | 0.64              |
| 6:N:793:THR:HB    | 6:N:879:ARG:CD    | 2.25                     | 0.64              |
| 6:N:996:TRP:O     | 6:N:1000:THR:HG22 | 1.96                     | 0.64              |
| 6:N:1087:ARG:HB3  | 6:N:1256:LEU:HD22 | 1.79                     | 0.64              |
| 4:A:48:ILE:HD12   | 4:A:174:VAL:HG21  | 1.78                     | 0.64              |
| 5:C:146:VAL:HG22  | 5:C:162:ILE:HG23  | 1.77                     | 0.64              |
| 5:C:609:ASN:HD22  | 5:C:609:ASN:N     | 1.94                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:119:SER:OG    | 6:D:123:LEU:HD13  | 1.96                     | 0.64              |
| 6:D:402:PRO:HA    | 6:D:443:VAL:HG23  | 1.80                     | 0.64              |
| 6:D:792:ILE:HG23  | 6:D:793:THR:HG23  | 1.79                     | 0.64              |
| 6:D:804:LEU:HB2   | 6:D:830:ALA:O     | 1.98                     | 0.64              |
| 6:D:1209:LEU:HD21 | 7:E:16:LYS:NZ     | 2.12                     | 0.64              |
| 4:K:30:ARG:HH22   | 5:M:938:LYS:HD2   | 1.63                     | 0.64              |
| 5:M:140:ILE:HA    | 5:M:332:ARG:O     | 1.97                     | 0.64              |
| 5:M:143:SER:C     | 5:M:276:LYS:HZ3   | 2.05                     | 0.64              |
| 5:M:542:VAL:HG23  | 11:M:1602:HOH:O   | 1.96                     | 0.64              |
| 3:Z:8:DA:H1'      | 3:Z:9:DG:H5'      | 1.79                     | 0.64              |
| 4:A:12:THR:OG1    | 4:A:24:VAL:HB     | 1.97                     | 0.64              |
| 4:A:36:LEU:O      | 4:A:40:LEU:HG     | 1.97                     | 0.64              |
| 4:A:71:VAL:HG22   | 4:A:132:LEU:HG    | 1.78                     | 0.64              |
| 4:B:59:GLU:HG3    | 4:B:139:ASN:HD22  | 1.61                     | 0.64              |
| 6:D:436:GLU:CD    | 6:D:445:ARG:HG3   | 2.22                     | 0.64              |
| 4:L:138:LEU:HD12  | 11:L:362:HOH:O    | 1.98                     | 0.64              |
| 4:L:177:VAL:HG12  | 4:L:199:ILE:HG12  | 1.79                     | 0.64              |
| 5:M:29:ALA:O      | 5:M:44:ILE:HG12   | 1.96                     | 0.64              |
| 5:M:362:GLY:HA3   | 5:M:367:LEU:HD23  | 1.78                     | 0.64              |
| 5:M:836:GLY:HA3   | 6:N:724:GLN:NE2   | 2.12                     | 0.64              |
| 6:N:15:PRO:HA     | 6:N:18:ILE:HG12   | 1.79                     | 0.64              |
| 6:N:396:VAL:HG12  | 6:N:398:ALA:HB2   | 1.80                     | 0.64              |
| 6:N:786:ILE:HD13  | 6:N:1027:GLY:HA3  | 1.78                     | 0.64              |
| 2:H:9:G:O2'       | 2:H:10:G:H5'      | 1.97                     | 0.64              |
| 11:A:362:HOH:O    | 5:C:832:LYS:HD2   | 1.98                     | 0.64              |
| 4:B:212:ASN:O     | 4:B:215:VAL:HG22  | 1.97                     | 0.64              |
| 5:C:124:ASP:OD2   | 5:C:592:LEU:HB2   | 1.97                     | 0.64              |
| 5:C:204:GLN:OE1   | 5:C:221:LEU:HD12  | 1.97                     | 0.64              |
| 6:D:104:PHE:HB3   | 6:D:512:MET:SD    | 2.38                     | 0.64              |
| 6:D:613:ARG:HH12  | 6:D:616:GLN:HG2   | 1.62                     | 0.64              |
| 6:D:813:LEU:HD21  | 11:D:8233:HOH:O   | 1.97                     | 0.64              |
| 6:D:823:LEU:HD23  | 6:D:823:LEU:O     | 1.98                     | 0.64              |
| 5:M:684:PHE:CD2   | 5:M:685:GLU:HG2   | 2.33                     | 0.64              |
| 6:N:1422:MET:SD   | 6:N:1426:LYS:HB3  | 2.37                     | 0.64              |
| 7:O:47:LYS:HA     | 7:O:54:LEU:HB3    | 1.80                     | 0.64              |
| 5:C:839:LEU:HD22  | 5:C:996:LYS:HA    | 1.80                     | 0.64              |
| 5:C:1105:LYS:NZ   | 5:C:1107:ASN:HD22 | 1.96                     | 0.64              |
| 6:D:71:LYS:HB2    | 6:D:71:LYS:NZ     | 2.12                     | 0.64              |
| 6:D:973:GLN:HB3   | 11:D:8398:HOH:O   | 1.96                     | 0.64              |
| 4:L:59:GLU:HG3    | 4:L:137:ARG:HH22  | 1.63                     | 0.64              |
| 5:M:265:ARG:NH2   | 5:M:332:ARG:HH22  | 1.95                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:536:PRO:HD2   | 5:M:537:LYS:NZ    | 2.08                     | 0.64              |
| 6:N:91:GLY:O      | 6:N:519:VAL:N     | 2.21                     | 0.64              |
| 6:N:554:LEU:O     | 6:N:558:LEU:HG    | 1.96                     | 0.64              |
| 6:D:860:LEU:HD23  | 6:D:877:PRO:HB2   | 1.79                     | 0.64              |
| 6:D:1087:ARG:HD2  | 6:D:1256:LEU:HD13 | 1.78                     | 0.64              |
| 6:D:1471:LEU:HD23 | 11:D:8477:HOH:O   | 1.98                     | 0.64              |
| 6:D:1485:GLN:NE2  | 7:E:79:LEU:H      | 1.96                     | 0.64              |
| 5:M:100:LEU:HD23  | 5:M:368:THR:HA    | 1.80                     | 0.64              |
| 6:N:17:LYS:HA     | 6:N:20:SER:HB3    | 1.80                     | 0.64              |
| 6:N:41:ARG:HD3    | 6:N:42:ASP:N      | 2.13                     | 0.64              |
| 6:N:679:ARG:HB2   | 6:N:682:ASP:OD2   | 1.98                     | 0.64              |
| 6:N:1415:VAL:HB   | 11:N:9268:HOH:O   | 1.96                     | 0.64              |
| 5:C:18:LEU:H      | 5:C:18:LEU:HD12   | 1.61                     | 0.64              |
| 5:C:194:VAL:HG21  | 5:C:221:LEU:O     | 1.97                     | 0.64              |
| 5:C:872:ASN:HD22  | 5:C:873:PRO:N     | 1.95                     | 0.64              |
| 6:D:18:ILE:HG23   | 6:D:518:PRO:HG3   | 1.80                     | 0.64              |
| 6:D:496:LEU:HD21  | 6:D:1388:ARG:HG3  | 1.79                     | 0.64              |
| 6:D:1044:LEU:HD21 | 6:D:1053:PHE:O    | 1.98                     | 0.64              |
| 5:M:9:ILE:HG21    | 11:M:1490:HOH:O   | 1.98                     | 0.64              |
| 5:M:170:PRO:HG2   | 11:M:1194:HOH:O   | 1.98                     | 0.64              |
| 5:M:410:ILE:HD11  | 5:M:455:LEU:HB3   | 1.79                     | 0.64              |
| 6:N:29:PRO:HG3    | 6:N:549:ASN:HD21  | 1.61                     | 0.64              |
| 5:C:9:ILE:HG13    | 5:C:907:ASP:OD2   | 1.98                     | 0.64              |
| 5:C:143:SER:HB2   | 5:C:276:LYS:HZ3   | 1.62                     | 0.64              |
| 6:D:486:ARG:HA    | 6:D:489:ARG:CG    | 2.28                     | 0.64              |
| 5:M:314:THR:HG21  | 11:M:1381:HOH:O   | 1.97                     | 0.64              |
| 5:M:342:ASP:O     | 5:M:345:ARG:HG2   | 1.98                     | 0.64              |
| 5:M:906:PHE:CD1   | 6:N:1067:VAL:HG22 | 2.33                     | 0.64              |
| 6:N:800:LYS:HZ2   | 6:N:804:LEU:HD13  | 1.63                     | 0.64              |
| 6:N:1353:GLN:HB3  | 6:N:1357:ARG:NE   | 2.12                     | 0.64              |
| 2:H:11:C:H2'      | 2:H:12:G:H8       | 1.63                     | 0.63              |
| 4:A:206:THR:HG22  | 4:A:209:GLU:H     | 1.63                     | 0.63              |
| 5:C:688:ILE:HG21  | 5:C:871:LEU:HD23  | 1.80                     | 0.63              |
| 6:D:637:LEU:HB2   | 11:D:8105:HOH:O   | 1.98                     | 0.63              |
| 4:K:117:VAL:HB    | 4:K:120:VAL:CG1   | 2.26                     | 0.63              |
| 4:K:226:SER:O     | 4:K:228:PRO:HD3   | 1.97                     | 0.63              |
| 4:L:175:ARG:O     | 6:N:851:LEU:HD11  | 1.98                     | 0.63              |
| 5:M:598:GLU:O     | 5:M:651:LYS:HG3   | 1.98                     | 0.63              |
| 6:N:792:ILE:HD13  | 6:N:793:THR:HG22  | 1.80                     | 0.63              |
| 6:N:1491:THR:O    | 6:N:1495:ILE:HD13 | 1.98                     | 0.63              |
| 4:B:42:ARG:NH1    | 4:B:42:ARG:HA     | 2.13                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:694:LEU:HD21  | 5:C:868:ASP:HB3   | 1.80                     | 0.63              |
| 6:D:440:VAL:HB    | 6:D:441:ARG:HH21  | 1.61                     | 0.63              |
| 6:D:1169:ASP:O    | 6:D:1173:LEU:HD13 | 1.98                     | 0.63              |
| 5:M:83:CYS:HA     | 5:M:88:LEU:HB2    | 1.78                     | 0.63              |
| 6:N:887:ALA:HB1   | 6:N:893:GLU:CG    | 2.27                     | 0.63              |
| 6:N:970:LYS:HA    | 6:N:973:GLN:CD    | 2.23                     | 0.63              |
| 6:N:971:LEU:HA    | 6:N:974:ILE:HD12  | 1.80                     | 0.63              |
| 6:N:1462:LEU:HD22 | 6:N:1472:ILE:HG22 | 1.79                     | 0.63              |
| 5:C:174:LEU:HB3   | 5:C:307:LEU:HD13  | 1.79                     | 0.63              |
| 5:C:265:ARG:HB3   | 5:C:267:TYR:CD2   | 2.34                     | 0.63              |
| 5:C:492:ASP:CG    | 5:C:518:LYS:HB3   | 2.24                     | 0.63              |
| 5:C:1031:ARG:NH2  | 6:D:621:LYS:HG3   | 2.13                     | 0.63              |
| 6:D:1119:SER:HA   | 6:D:1186:VAL:O    | 1.99                     | 0.63              |
| 4:K:156:HIS:CD2   | 4:K:158:ILE:HG12  | 2.34                     | 0.63              |
| 5:M:861:LEU:HD13  | 5:M:865:THR:HG23  | 1.79                     | 0.63              |
| 6:N:474:GLU:O     | 6:N:478:LEU:HG    | 1.98                     | 0.63              |
| 6:N:760:ARG:HH11  | 7:O:61:VAL:CG2    | 2.11                     | 0.63              |
| 7:O:41:GLU:HB2    | 7:O:45:ARG:CZ     | 2.27                     | 0.63              |
| 5:C:284:ARG:HG3   | 5:C:285:LEU:H     | 1.64                     | 0.63              |
| 5:C:631:SER:HB3   | 5:C:637:LEU:HD11  | 1.79                     | 0.63              |
| 6:D:610:LYS:HA    | 6:D:615:ARG:HD3   | 1.80                     | 0.63              |
| 6:D:632:VAL:HG22  | 11:D:8291:HOH:O   | 1.99                     | 0.63              |
| 6:D:705:ALA:HB3   | 6:D:706:PRO:HD3   | 1.80                     | 0.63              |
| 6:D:1412:LYS:O    | 6:D:1414:PRO:HD3  | 1.99                     | 0.63              |
| 5:M:395:LYS:HD3   | 5:M:397:GLU:OE2   | 1.99                     | 0.63              |
| 5:M:549:PHE:CD2   | 5:M:886:LEU:HB3   | 2.33                     | 0.63              |
| 6:N:799:LYS:O     | 6:N:826:PRO:HD2   | 1.98                     | 0.63              |
| 6:N:806:PHE:CE1   | 6:N:813:LEU:HB3   | 2.34                     | 0.63              |
| 1:X:17:DC:H5''    | 5:M:1030:GLN:NE2  | 2.14                     | 0.63              |
| 2:Y:7:G:H2'       | 2:Y:7:G:N3        | 2.12                     | 0.63              |
| 2:Y:12:G:H2'      | 2:Y:13:C:H6       | 1.64                     | 0.63              |
| 2:Y:12:G:O2'      | 2:Y:13:C:H5'      | 1.98                     | 0.63              |
| 5:C:874:LEU:HG    | 6:D:1023:MET:SD   | 2.39                     | 0.63              |
| 6:D:1185:GLU:HG2  | 6:N:559:ALA:HB1   | 1.80                     | 0.63              |
| 5:M:352:ALA:HA    | 5:M:355:VAL:HG12  | 1.80                     | 0.63              |
| 5:M:729:LEU:HD13  | 6:N:675:ARG:CZ    | 2.29                     | 0.63              |
| 6:N:98:PRO:HA     | 11:N:9070:HOH:O   | 1.97                     | 0.63              |
| 6:N:654:LYS:O     | 6:N:658:LEU:HG    | 1.98                     | 0.63              |
| 6:N:1109:GLU:OE1  | 6:N:1201:CYS:HB2  | 1.98                     | 0.63              |
| 6:N:1402:ALA:HA   | 11:N:9043:HOH:O   | 1.98                     | 0.63              |
| 5:C:100:LEU:HD22  | 5:C:372:LEU:HD22  | 1.81                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:C:410:ILE:HG21 | 5:C:438:ILE:HD11 | 1.79                     | 0.63              |
| 5:C:437:ARG:HB3  | 5:C:467:ILE:HB   | 1.80                     | 0.63              |
| 5:C:805:ARG:HD3  | 5:C:807:ARG:HG3  | 1.81                     | 0.63              |
| 6:D:82:LYS:HB3   | 6:D:84:ILE:HG12  | 1.79                     | 0.63              |
| 6:D:657:LEU:HD22 | 6:D:691:LEU:HD23 | 1.81                     | 0.63              |
| 6:D:1047:LYS:HG2 | 6:D:1053:PHE:CZ  | 2.33                     | 0.63              |
| 5:M:146:VAL:HG12 | 5:M:162:ILE:HG12 | 1.81                     | 0.63              |
| 5:M:759:THR:HB   | 5:M:785:VAL:CG1  | 2.28                     | 0.63              |
| 5:C:157:ARG:HG3  | 5:C:314:THR:CG2  | 2.29                     | 0.63              |
| 5:C:408:ARG:HG3  | 5:C:455:LEU:H    | 1.64                     | 0.63              |
| 5:C:600:ASP:OD1  | 5:C:651:LYS:N    | 2.32                     | 0.63              |
| 5:C:906:PHE:CE1  | 6:D:1067:VAL:HA  | 2.34                     | 0.63              |
| 6:D:119:SER:H    | 6:D:123:LEU:CD2  | 2.11                     | 0.63              |
| 6:D:704:ARG:HD3  | 6:D:738:ALA:HB2  | 1.79                     | 0.63              |
| 7:E:37:ASN:HD22  | 7:E:89:MET:HE2   | 1.64                     | 0.63              |
| 7:E:54:LEU:HG    | 7:E:58:PRO:CG    | 2.28                     | 0.63              |
| 5:M:432:ARG:HG3  | 11:M:1314:HOH:O  | 1.99                     | 0.63              |
| 5:M:650:ARG:HG3  | 5:M:653:ASP:HB2  | 1.81                     | 0.63              |
| 4:A:220:GLU:O    | 4:A:223:THR:HG22 | 1.99                     | 0.63              |
| 5:C:276:LYS:HG2  | 5:C:280:LYS:NZ   | 2.14                     | 0.63              |
| 5:C:279:GLU:HG3  | 5:C:280:LYS:HG3  | 1.79                     | 0.63              |
| 5:C:670:GLN:NE2  | 5:C:699:PHE:O    | 2.30                     | 0.63              |
| 5:C:672:VAL:HG12 | 5:C:699:PHE:CE1  | 2.34                     | 0.63              |
| 5:C:690:ILE:CD1  | 5:C:833:LEU:HD23 | 2.29                     | 0.63              |
| 6:D:614:PHE:CZ   | 6:D:1438:ALA:HB1 | 2.34                     | 0.63              |
| 4:K:12:THR:OG1   | 4:K:24:VAL:HB    | 1.99                     | 0.63              |
| 5:M:176:VAL:HG12 | 5:M:182:VAL:HG12 | 1.80                     | 0.63              |
| 5:M:693:GLU:HA   | 5:M:696:LYS:HD2  | 1.80                     | 0.63              |
| 6:N:675:ARG:HA   | 6:N:678:GLU:HG2  | 1.80                     | 0.63              |
| 6:N:696:HIS:HD2  | 7:O:59:ASN:HB2   | 1.64                     | 0.63              |
| 6:N:1049:SER:O   | 6:N:1079:LYS:HE3 | 1.98                     | 0.63              |
| 5:C:327:HIS:HA   | 5:C:433:THR:OG1  | 1.98                     | 0.63              |
| 5:C:410:ILE:HD12 | 5:C:438:ILE:CG1  | 2.29                     | 0.63              |
| 5:C:441:VAL:HG13 | 5:C:559:LEU:HA   | 1.81                     | 0.63              |
| 6:D:753:SER:HB2  | 11:D:8449:HOH:O  | 1.98                     | 0.63              |
| 6:D:793:THR:O    | 6:D:879:ARG:HD3  | 1.99                     | 0.63              |
| 7:E:48:MET:N     | 7:E:54:LEU:HB2   | 2.14                     | 0.63              |
| 5:M:290:LEU:HD23 | 5:M:290:LEU:H    | 1.64                     | 0.63              |
| 6:N:1380:GLU:HG3 | 6:N:1381:VAL:N   | 2.13                     | 0.63              |
| 2:H:4:U:H2'      | 2:H:5:C:C6       | 2.34                     | 0.62              |
| 3:I:8:DA:H1'     | 3:I:9:DG:H5'     | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:10:ARG:HA     | 5:C:10:ARG:NH1    | 2.12                     | 0.62              |
| 5:C:98:LEU:O      | 5:C:109:LYS:HD2   | 1.99                     | 0.62              |
| 5:C:1033:GLY:O    | 5:C:1037:VAL:HG23 | 1.97                     | 0.62              |
| 5:M:580:MET:HB3   | 5:M:584:GLU:OE1   | 1.99                     | 0.62              |
| 6:N:131:LYS:HE2   | 6:N:564:GLU:OE1   | 1.98                     | 0.62              |
| 6:N:1440:PHE:HB3  | 11:N:9289:HOH:O   | 1.99                     | 0.62              |
| 2:H:6:U:C2'       | 2:H:7:G:C8        | 2.82                     | 0.62              |
| 1:X:14:DT:H3'     | 6:N:610:LYS:NZ    | 2.14                     | 0.62              |
| 5:C:218:VAL:HA    | 5:C:221:LEU:HD23  | 1.81                     | 0.62              |
| 5:C:710:ILE:HD12  | 5:C:790:LEU:HD13  | 1.81                     | 0.62              |
| 5:C:882:LEU:HD23  | 5:C:885:ILE:HB    | 1.81                     | 0.62              |
| 6:D:455:ARG:CZ    | 6:D:463:GLN:HG3   | 2.29                     | 0.62              |
| 6:D:891:GLU:HB2   | 11:D:8407:HOH:O   | 1.98                     | 0.62              |
| 6:D:1267:ARG:HB2  | 6:D:1267:ARG:HH11 | 1.64                     | 0.62              |
| 6:D:1364:HIS:ND1  | 6:D:1366:LYS:HG3  | 2.14                     | 0.62              |
| 7:E:70:THR:HB     | 7:E:72:ARG:HG2    | 1.81                     | 0.62              |
| 5:M:304:LEU:HG    | 5:M:308:ARG:HH21  | 1.64                     | 0.62              |
| 6:N:165:LYS:HA    | 6:N:199:LEU:HD22  | 1.81                     | 0.62              |
| 4:B:20:TYR:OH     | 4:B:198:ARG:HD2   | 1.98                     | 0.62              |
| 5:C:750:LYS:HD3   | 6:D:681:ARG:HD3   | 1.81                     | 0.62              |
| 5:C:775:ARG:HD2   | 5:C:782:ALA:HB3   | 1.80                     | 0.62              |
| 5:C:840:ALA:HB2   | 5:C:846:LYS:HG3   | 1.79                     | 0.62              |
| 5:C:1037:VAL:O    | 5:C:1041:GLU:HG3  | 1.99                     | 0.62              |
| 6:D:143:ASN:ND2   | 6:D:145:VAL:HG12  | 2.10                     | 0.62              |
| 6:D:175:VAL:HG11  | 11:D:8081:HOH:O   | 1.99                     | 0.62              |
| 6:D:396:VAL:C     | 6:D:398:ALA:N     | 2.56                     | 0.62              |
| 6:D:1029:ARG:HH22 | 10:D:3999:APC:PG  | 2.22                     | 0.62              |
| 6:D:1437:ALA:O    | 6:D:1446:VAL:HG21 | 1.99                     | 0.62              |
| 4:K:180:GLN:HE22  | 5:M:937:ASP:HA    | 1.65                     | 0.62              |
| 5:M:44:ILE:HG23   | 5:M:344:PHE:HE1   | 1.64                     | 0.62              |
| 5:M:576:ALA:HB3   | 5:M:900:ARG:NH1   | 2.13                     | 0.62              |
| 5:M:841:ASN:C     | 5:M:841:ASN:HD22  | 2.07                     | 0.62              |
| 5:M:906:PHE:CE1   | 6:N:1067:VAL:HA   | 2.35                     | 0.62              |
| 6:N:95:LEU:HB2    | 11:N:9070:HOH:O   | 1.99                     | 0.62              |
| 6:N:1219:GLU:HG2  | 6:N:1221:VAL:HG23 | 1.81                     | 0.62              |
| 2:H:9:G:H2'       | 2:H:10:G:H8       | 1.63                     | 0.62              |
| 5:C:358:ARG:HH22  | 5:C:373:VAL:C     | 2.06                     | 0.62              |
| 5:C:720:GLU:HG2   | 5:C:760:SER:HB3   | 1.82                     | 0.62              |
| 6:D:574:LEU:O     | 6:D:578:VAL:HG23  | 1.98                     | 0.62              |
| 6:D:1000:THR:O    | 6:D:1003:VAL:HG12 | 1.99                     | 0.62              |
| 7:E:54:LEU:HD23   | 7:E:54:LEU:O      | 2.00                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:L:211:LEU:O     | 4:L:215:VAL:HG13  | 2.00                     | 0.62              |
| 5:M:307:LEU:HG    | 5:M:311:PHE:CE2   | 2.34                     | 0.62              |
| 5:M:468:ARG:HE    | 5:M:487:THR:N     | 1.98                     | 0.62              |
| 5:M:807:ARG:H     | 5:M:807:ARG:NE    | 1.96                     | 0.62              |
| 5:M:1098:ASP:HB2  | 6:N:21:TRP:HZ2    | 1.64                     | 0.62              |
| 6:N:895:VAL:O     | 6:N:899:LEU:HG    | 2.00                     | 0.62              |
| 6:N:1051:GLU:HG3  | 6:N:1051:GLU:O    | 2.00                     | 0.62              |
| 5:C:144:PRO:HA    | 5:C:163:ILE:HD11  | 1.81                     | 0.62              |
| 6:D:138:LYS:HD3   | 11:D:8147:HOH:O   | 2.00                     | 0.62              |
| 6:D:660:LYS:HD2   | 6:D:694:VAL:HG22  | 1.80                     | 0.62              |
| 6:D:853:VAL:HG11  | 6:D:860:LEU:HG    | 1.81                     | 0.62              |
| 6:D:1083:ASP:OD1  | 6:D:1252:ILE:HD12 | 2.00                     | 0.62              |
| 5:M:135:VAL:HG11  | 5:M:407:LYS:HA    | 1.81                     | 0.62              |
| 5:M:537:LYS:HE3   | 5:M:905:ILE:HD13  | 1.81                     | 0.62              |
| 5:M:759:THR:HA    | 5:M:786:LYS:O     | 2.00                     | 0.62              |
| 6:N:172:PRO:HG2   | 6:N:175:VAL:HG21  | 1.82                     | 0.62              |
| 6:N:1125:PRO:HB3  | 6:N:1130:ARG:HH22 | 1.64                     | 0.62              |
| 1:X:20:DG:H3'     | 11:X:610:HOH:O    | 2.00                     | 0.62              |
| 2:Y:6:U:C2'       | 2:Y:7:G:C8        | 2.82                     | 0.62              |
| 5:C:573:ARG:HB2   | 5:C:573:ARG:NH1   | 2.13                     | 0.62              |
| 5:C:798:GLY:H     | 5:C:827:VAL:CG1   | 2.13                     | 0.62              |
| 6:D:398:ALA:HB1   | 6:D:446:VAL:H     | 1.64                     | 0.62              |
| 6:D:959:GLU:H     | 6:D:959:GLU:CD    | 2.04                     | 0.62              |
| 6:D:1495:ILE:HG21 | 7:E:80:VAL:HG13   | 1.82                     | 0.62              |
| 4:K:42:ARG:HH21   | 4:L:31:GLY:C      | 2.08                     | 0.62              |
| 4:L:58:ILE:CG2    | 4:L:61:VAL:HB     | 2.29                     | 0.62              |
| 5:M:1090:LYS:HG2  | 5:M:1112:PHE:HZ   | 1.65                     | 0.62              |
| 6:N:130:SER:HB3   | 6:N:132:TYR:CE1   | 2.34                     | 0.62              |
| 6:N:166:GLN:CG    | 6:N:396:VAL:HG13  | 2.29                     | 0.62              |
| 6:N:764:LEU:HD12  | 6:N:765:SER:N     | 2.14                     | 0.62              |
| 6:N:1424:VAL:HG13 | 6:N:1425:THR:N    | 2.14                     | 0.62              |
| 7:O:41:GLU:HG2    | 7:O:42:PRO:HD3    | 1.82                     | 0.62              |
| 1:X:14:DT:H2''    | 1:X:15:DC:H5'     | 1.80                     | 0.62              |
| 2:Y:1:G:O6        | 5:M:773:LEU:HD12  | 2.00                     | 0.62              |
| 5:C:162:ILE:HD11  | 5:C:306:THR:HG21  | 1.82                     | 0.62              |
| 5:C:329:GLY:N     | 5:C:488:ALA:HB3   | 2.13                     | 0.62              |
| 5:C:410:ILE:O     | 5:C:452:ILE:HA    | 1.99                     | 0.62              |
| 5:C:436:GLY:HA2   | 5:C:538:GLN:O     | 1.99                     | 0.62              |
| 6:D:792:ILE:O     | 6:D:878:GLY:HA3   | 1.99                     | 0.62              |
| 5:M:120:LEU:HD22  | 5:M:121:MET:N     | 2.11                     | 0.62              |
| 5:M:273:GLY:HA2   | 5:M:276:LYS:HE3   | 1.80                     | 0.62              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:M:457:ALA:HB3   | 5:M:538:GLN:HA   | 1.80                     | 0.62              |
| 5:M:587:VAL:HG12  | 5:M:588:VAL:N    | 2.13                     | 0.62              |
| 5:M:1087:VAL:HG23 | 6:N:524:LEU:HD11 | 1.80                     | 0.62              |
| 6:N:1146:GLY:O    | 6:N:1207:TYR:HB2 | 2.00                     | 0.62              |
| 5:C:554:ASP:HB2   | 6:D:1061:PHE:HE2 | 1.65                     | 0.62              |
| 5:C:674:VAL:HG23  | 5:C:869:VAL:HG13 | 1.82                     | 0.62              |
| 5:M:113:VAL:HG11  | 5:M:373:VAL:CG1  | 2.30                     | 0.62              |
| 5:M:194:VAL:HA    | 5:M:197:LEU:HD12 | 1.82                     | 0.62              |
| 5:M:194:VAL:HG11  | 5:M:221:LEU:O    | 2.00                     | 0.62              |
| 6:N:741:ASP:O     | 6:N:743:ASP:N    | 2.29                     | 0.62              |
| 2:Y:7:G:C2        | 5:M:1014:SER:HA  | 2.33                     | 0.62              |
| 5:C:862:PRO:HD2   | 5:C:925:TYR:OH   | 2.00                     | 0.62              |
| 6:D:81:THR:HG22   | 6:D:82:LYS:N     | 2.14                     | 0.62              |
| 6:N:471:GLU:O     | 6:N:474:GLU:HB3  | 2.00                     | 0.62              |
| 6:N:490:ALA:O     | 6:N:493:ARG:HG3  | 1.99                     | 0.62              |
| 6:N:583:ASP:CG    | 6:N:586:ARG:HG3  | 2.25                     | 0.62              |
| 6:N:639:LEU:HB3   | 11:N:9466:HOH:O  | 1.98                     | 0.62              |
| 11:N:9137:HOH:O   | 7:O:17:TYR:HB2   | 1.99                     | 0.62              |
| 7:O:86:GLN:O      | 7:O:90:GLU:HG3   | 2.00                     | 0.62              |
| 2:Y:10:G:H2'      | 2:Y:11:C:H6      | 1.64                     | 0.62              |
| 5:C:830:LYS:HD3   | 5:C:832:LYS:HE2  | 1.82                     | 0.62              |
| 4:L:102:LYS:HZ1   | 4:L:137:ARG:HG2  | 1.64                     | 0.62              |
| 5:M:91:GLN:CD     | 5:M:383:ARG:HH22 | 2.08                     | 0.62              |
| 5:M:629:TYR:HB3   | 11:M:1373:HOH:O  | 1.99                     | 0.62              |
| 6:N:1121:PRO:HD3  | 6:N:1346:ARG:HE  | 1.63                     | 0.62              |
| 4:B:78:ILE:O      | 4:B:82:LEU:HG    | 2.00                     | 0.61              |
| 5:C:101:ILE:HG23  | 5:C:107:LEU:HD22 | 1.82                     | 0.61              |
| 6:D:550:ARG:HE    | 6:D:550:ARG:CA   | 2.11                     | 0.61              |
| 4:K:58:ILE:HB     | 4:K:61:VAL:HB    | 1.82                     | 0.61              |
| 5:M:265:ARG:HB3   | 5:M:267:TYR:CE2  | 2.35                     | 0.61              |
| 6:N:41:ARG:HD3    | 6:N:42:ASP:HB2   | 1.80                     | 0.61              |
| 6:N:626:SER:HB2   | 6:N:748:HIS:CE1  | 2.34                     | 0.61              |
| 6:N:902:LEU:HD23  | 6:N:902:LEU:H    | 1.65                     | 0.61              |
| 4:B:102:LYS:NZ    | 4:B:139:ASN:HB2  | 2.14                     | 0.61              |
| 5:C:343:GLN:HB2   | 5:C:385:PHE:CE2  | 2.34                     | 0.61              |
| 6:D:455:ARG:C     | 6:D:460:ALA:HB2  | 2.25                     | 0.61              |
| 5:M:198:ARG:NH1   | 5:M:231:PRO:HG3  | 2.15                     | 0.61              |
| 5:M:1030:GLN:NE2  | 6:N:628:ARG:HD3  | 2.15                     | 0.61              |
| 6:N:583:ASP:OD2   | 6:N:604:THR:HG21 | 1.99                     | 0.61              |
| 6:N:1036:ARG:NH1  | 6:N:1036:ARG:HB3 | 2.15                     | 0.61              |
| 5:C:456:ALA:HB1   | 5:C:538:GLN:O    | 1.99                     | 0.61              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:D:440:VAL:HB    | 6:D:441:ARG:HE   | 1.63                     | 0.61              |
| 6:D:544:TYR:O     | 6:D:548:ILE:HG12 | 2.00                     | 0.61              |
| 6:D:762:GLN:HB2   | 7:E:16:LYS:HE2   | 1.82                     | 0.61              |
| 4:A:41:ARG:O      | 4:A:45:LEU:HD13  | 2.00                     | 0.61              |
| 5:C:436:GLY:HA3   | 5:C:538:GLN:OE1  | 2.01                     | 0.61              |
| 6:D:101:HIS:ND1   | 6:D:103:TRP:HB2  | 2.15                     | 0.61              |
| 6:D:559:ALA:HB2   | 11:D:8141:HOH:O  | 1.98                     | 0.61              |
| 6:D:707:THR:HG23  | 6:D:712:GLY:HA3  | 1.81                     | 0.61              |
| 5:M:30:LEU:HA     | 5:M:44:ILE:HG12  | 1.80                     | 0.61              |
| 11:M:1524:HOH:O   | 6:N:621:LYS:HE3  | 2.00                     | 0.61              |
| 2:H:13:C:H2'      | 2:H:14:G:H8      | 1.65                     | 0.61              |
| 4:B:47:SER:OG     | 4:B:48:ILE:HD12  | 1.99                     | 0.61              |
| 5:C:400:PRO:HG2   | 5:C:593:ALA:HB2  | 1.82                     | 0.61              |
| 5:C:672:VAL:HG12  | 5:C:699:PHE:HE1  | 1.65                     | 0.61              |
| 5:C:1076:VAL:HG21 | 11:D:8371:HOH:O  | 1.99                     | 0.61              |
| 6:D:135:LEU:HA    | 6:D:453:ASP:O    | 2.01                     | 0.61              |
| 6:D:677:LEU:HD21  | 6:D:687:VAL:HG11 | 1.81                     | 0.61              |
| 6:D:1101:VAL:HG13 | 6:D:1427:SER:OG  | 2.00                     | 0.61              |
| 6:D:1219:GLU:HA   | 7:E:17:TYR:HE2   | 1.65                     | 0.61              |
| 6:D:1267:ARG:HH11 | 6:D:1267:ARG:CB  | 2.13                     | 0.61              |
| 5:M:909:ALA:HB1   | 5:M:914:ILE:HD11 | 1.81                     | 0.61              |
| 6:N:824:ASN:C     | 6:N:824:ASN:HD22 | 2.09                     | 0.61              |
| 4:A:181:VAL:HG11  | 11:A:382:HOH:O   | 2.01                     | 0.61              |
| 4:A:182:GLU:O     | 4:A:194:LYS:HB3  | 2.00                     | 0.61              |
| 5:C:79:PRO:HG2    | 5:C:82:GLU:HB2   | 1.80                     | 0.61              |
| 5:C:464:LEU:O     | 5:C:466:PHE:N    | 2.34                     | 0.61              |
| 6:D:10:ILE:HD12   | 6:D:1450:ALA:HB3 | 1.82                     | 0.61              |
| 6:D:1493:LYS:O    | 6:D:1497:GLU:HG2 | 2.01                     | 0.61              |
| 4:K:90:LEU:HB2    | 4:K:119:ASP:OD2  | 2.01                     | 0.61              |
| 5:M:759:THR:HB    | 5:M:785:VAL:CG2  | 2.31                     | 0.61              |
| 6:N:36:THR:C      | 6:N:38:LYS:H     | 2.07                     | 0.61              |
| 6:N:584:ASN:ND2   | 6:N:590:PRO:HD2  | 2.16                     | 0.61              |
| 2:Y:4:U:H2'       | 2:Y:5:C:C6       | 2.36                     | 0.61              |
| 4:B:133:GLU:OE1   | 4:B:133:GLU:HA   | 2.00                     | 0.61              |
| 5:C:99:GLN:HB3    | 5:C:109:LYS:HD3  | 1.81                     | 0.61              |
| 5:C:857:ASP:CB    | 5:C:978:ARG:HG2  | 2.31                     | 0.61              |
| 6:D:724:GLN:HG3   | 6:D:725:SER:N    | 2.14                     | 0.61              |
| 6:D:955:VAL:HG11  | 6:D:1015:TYR:HE2 | 1.66                     | 0.61              |
| 4:L:78:ILE:O      | 4:L:82:LEU:HG    | 2.00                     | 0.61              |
| 5:M:110:GLU:N     | 5:M:368:THR:HG21 | 2.14                     | 0.61              |
| 5:C:198:ARG:HD2   | 5:C:204:GLN:NE2  | 2.15                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:398:THR:HG21  | 5:C:567:GLN:HA    | 1.83                     | 0.61              |
| 6:D:36:THR:C      | 6:D:38:LYS:H      | 2.09                     | 0.61              |
| 6:D:123:LEU:HG    | 6:D:152:LEU:HD13  | 1.82                     | 0.61              |
| 6:D:1346:ARG:HH12 | 6:D:1349:VAL:HG11 | 1.66                     | 0.61              |
| 4:L:123:MET:C     | 4:L:125:PRO:HD3   | 2.24                     | 0.61              |
| 5:M:172:ILE:HG23  | 5:M:184:MET:HE3   | 1.82                     | 0.61              |
| 5:M:408:ARG:NE    | 5:M:455:LEU:HD11  | 2.15                     | 0.61              |
| 5:M:694:LEU:HD21  | 5:M:868:ASP:HB3   | 1.83                     | 0.61              |
| 6:N:50:PHE:CD2    | 6:N:522:PRO:HD3   | 2.36                     | 0.61              |
| 11:N:9036:HOH:O   | 7:O:89:MET:HE1    | 1.99                     | 0.61              |
| 5:C:318:PRO:HD2   | 5:C:321:GLU:OE1   | 2.01                     | 0.61              |
| 5:C:431:HIS:CG    | 5:C:432:ARG:N     | 2.69                     | 0.61              |
| 5:C:988:VAL:HG23  | 11:C:1330:HOH:O   | 2.00                     | 0.61              |
| 5:C:1060:ILE:HG22 | 5:C:1086:ARG:NH2  | 2.15                     | 0.61              |
| 6:D:393:ILE:HD13  | 11:D:8118:HOH:O   | 2.01                     | 0.61              |
| 6:D:615:ARG:HH22  | 6:D:1096:ARG:HD2  | 1.64                     | 0.61              |
| 6:D:633:VAL:HB    | 6:D:740:PHE:CE1   | 2.36                     | 0.61              |
| 5:M:113:VAL:HG11  | 5:M:373:VAL:HG11  | 1.81                     | 0.61              |
| 5:M:232:GLU:HB3   | 11:M:1516:HOH:O   | 1.99                     | 0.61              |
| 5:M:524:VAL:CG1   | 5:M:528:GLU:HB2   | 2.31                     | 0.61              |
| 5:M:676:ILE:CG2   | 5:M:988:VAL:HG13  | 2.31                     | 0.61              |
| 6:N:135:LEU:HA    | 6:N:453:ASP:O     | 2.01                     | 0.61              |
| 6:N:507:ASN:HD22  | 6:N:507:ASN:N     | 1.90                     | 0.61              |
| 6:N:1105:ILE:HD11 | 6:N:1374:GLN:OE1  | 2.01                     | 0.61              |
| 2:H:12:G:H2'      | 2:H:13:C:H6       | 1.66                     | 0.61              |
| 4:A:39:PRO:O      | 4:A:43:ILE:HG12   | 1.99                     | 0.61              |
| 5:C:252:LYS:HB3   | 5:C:298:PHE:HZ    | 1.65                     | 0.61              |
| 5:C:267:TYR:HB2   | 5:C:272:ALA:HB1   | 1.82                     | 0.61              |
| 5:C:578:VAL:HG21  | 5:C:991:GLN:O     | 2.01                     | 0.61              |
| 5:C:911:GLU:O     | 5:C:915:LYS:HG2   | 2.00                     | 0.61              |
| 6:D:19:ARG:HH21   | 6:D:516:ALA:HB2   | 1.64                     | 0.61              |
| 4:K:41:ARG:HH21   | 5:M:977:GLY:HA2   | 1.65                     | 0.61              |
| 5:M:554:ASP:HB3   | 5:M:880:MET:O     | 2.01                     | 0.61              |
| 5:M:816:LYS:HB2   | 5:M:819:VAL:HG21  | 1.83                     | 0.61              |
| 5:M:983:ILE:HG21  | 5:M:987:ILE:HD12  | 1.80                     | 0.61              |
| 7:O:30:LEU:O      | 7:O:35:PHE:HA     | 2.01                     | 0.61              |
| 4:A:124:ASN:ND2   | 4:A:127:LEU:HD22  | 2.16                     | 0.60              |
| 4:A:225:PHE:CE1   | 4:B:40:LEU:HD11   | 2.35                     | 0.60              |
| 6:D:8:VAL:HB      | 6:D:1434:TRP:CH2  | 2.36                     | 0.60              |
| 6:D:153:LEU:CD1   | 6:D:158:TYR:HB2   | 2.31                     | 0.60              |
| 6:D:1141:GLU:CD   | 6:D:1168:MET:HE2  | 2.26                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:464:LEU:O     | 5:M:466:PHE:N     | 2.33                     | 0.60              |
| 6:N:619:LEU:HD12  | 6:N:621:LYS:HZ3   | 1.66                     | 0.60              |
| 6:N:780:LYS:HD3   | 6:N:912:LYS:HE3   | 1.82                     | 0.60              |
| 4:B:115:LEU:HB3   | 11:B:371:HOH:O    | 2.01                     | 0.60              |
| 5:C:451:LEU:C     | 5:C:452:ILE:HD12  | 2.26                     | 0.60              |
| 5:C:584:GLU:H     | 5:C:584:GLU:CD    | 2.07                     | 0.60              |
| 5:C:597:ALA:HA    | 5:C:655:LEU:HD11  | 1.83                     | 0.60              |
| 5:C:626:ARG:H     | 5:C:639:GLN:NE2   | 1.98                     | 0.60              |
| 6:D:873:LEU:HD11  | 11:D:8072:HOH:O   | 2.01                     | 0.60              |
| 6:D:1166:LEU:HD23 | 6:D:1166:LEU:H    | 1.65                     | 0.60              |
| 6:N:489:ARG:CZ    | 6:N:1389:LEU:HD21 | 2.31                     | 0.60              |
| 6:N:699:VAL:HG22  | 6:N:756:GLN:HE22  | 1.64                     | 0.60              |
| 6:N:1045:MET:HG3  | 6:N:1073:SER:OG   | 2.00                     | 0.60              |
| 6:N:1145:TYR:O    | 6:N:1147:ARG:HG2  | 2.01                     | 0.60              |
| 6:N:1243:THR:HG22 | 11:N:9395:HOH:O   | 2.01                     | 0.60              |
| 6:N:1350:GLU:O    | 6:N:1354:LYS:HG2  | 2.02                     | 0.60              |
| 7:O:46:PRO:C      | 7:O:47:LYS:HG2    | 2.25                     | 0.60              |
| 2:H:1:G:N2        | 5:C:770:GLU:HB3   | 2.17                     | 0.60              |
| 2:Y:13:C:H2'      | 2:Y:14:G:H8       | 1.64                     | 0.60              |
| 5:C:136:ILE:HG21  | 5:C:336:VAL:HG13  | 1.81                     | 0.60              |
| 5:C:798:GLY:H     | 5:C:827:VAL:HG11  | 1.66                     | 0.60              |
| 5:C:806:LEU:HD13  | 5:C:813:VAL:HG21  | 1.83                     | 0.60              |
| 5:C:881:ASN:HD22  | 5:C:881:ASN:N     | 1.99                     | 0.60              |
| 6:D:136:ASP:CB    | 6:D:137:PRO:HD3   | 2.30                     | 0.60              |
| 6:D:137:PRO:HD2   | 6:D:453:ASP:CG    | 2.27                     | 0.60              |
| 6:D:592:THR:N     | 6:D:600:LEU:HD11  | 2.16                     | 0.60              |
| 4:K:111:ALA:HB2   | 4:K:127:LEU:HD23  | 1.82                     | 0.60              |
| 4:K:209:GLU:HB3   | 11:K:1765:HOH:O   | 2.00                     | 0.60              |
| 5:M:537:LYS:HD2   | 5:M:537:LYS:N     | 2.12                     | 0.60              |
| 6:N:804:LEU:HB2   | 6:N:830:ALA:O     | 2.02                     | 0.60              |
| 6:N:1007:VAL:HG12 | 6:N:1011:PHE:CE2  | 2.35                     | 0.60              |
| 6:N:1109:GLU:HG2  | 6:N:1201:CYS:CA   | 2.29                     | 0.60              |
| 6:N:1268:PRO:HD2  | 6:N:1271:LYS:NZ   | 2.15                     | 0.60              |
| 4:A:85:LEU:HA     | 4:A:124:ASN:ND2   | 2.08                     | 0.60              |
| 5:C:56:GLU:HB3    | 5:C:64:LEU:HD23   | 1.82                     | 0.60              |
| 5:C:564:MET:SD    | 5:C:995:MET:HE3   | 2.41                     | 0.60              |
| 5:C:575:GLN:HB2   | 5:C:670:GLN:OE1   | 2.02                     | 0.60              |
| 6:D:754:PHE:CD1   | 7:E:24:ALA:HB1    | 2.36                     | 0.60              |
| 6:D:1216:SER:HB3  | 7:E:16:LYS:H      | 1.67                     | 0.60              |
| 4:K:42:ARG:NH2    | 4:L:34:VAL:HB     | 2.15                     | 0.60              |
| 5:M:1050:GLN:HE22 | 6:N:1470:ARG:C    | 2.09                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:118:LEU:HD13  | 6:N:124:GLU:OE2   | 2.01                     | 0.60              |
| 11:N:9248:HOH:O   | 7:O:16:LYS:HB2    | 2.02                     | 0.60              |
| 5:C:86:LYS:HB3    | 11:C:1560:HOH:O   | 2.02                     | 0.60              |
| 5:C:627:ARG:O     | 5:C:638:ASP:HB2   | 2.00                     | 0.60              |
| 5:C:764:GLU:HG3   | 6:D:54:LYS:NZ     | 2.15                     | 0.60              |
| 6:D:853:VAL:HG13  | 6:D:858:VAL:O     | 2.01                     | 0.60              |
| 4:K:94:LEU:HD11   | 4:K:119:ASP:CG    | 2.25                     | 0.60              |
| 4:K:112:ARG:HE    | 4:K:125:PRO:CB    | 2.03                     | 0.60              |
| 5:M:110:GLU:H     | 5:M:368:THR:CG2   | 2.12                     | 0.60              |
| 5:M:751:PRO:HA    | 5:M:792:VAL:HB    | 1.83                     | 0.60              |
| 5:M:805:ARG:HG2   | 5:M:823:VAL:HG13  | 1.84                     | 0.60              |
| 5:M:1007:ALA:HB1  | 6:N:652:LEU:HD13  | 1.84                     | 0.60              |
| 6:N:929:ARG:HB2   | 6:N:929:ARG:HH11  | 1.65                     | 0.60              |
| 6:N:1228:SER:HB2  | 11:N:9308:HOH:O   | 2.00                     | 0.60              |
| 6:D:28:LYS:HA     | 11:D:8201:HOH:O   | 2.01                     | 0.60              |
| 6:D:480:GLU:HB2   | 11:D:8139:HOH:O   | 2.00                     | 0.60              |
| 6:D:764:LEU:HD11  | 6:D:766:ALA:HB3   | 1.84                     | 0.60              |
| 6:D:829:VAL:HA    | 11:D:8279:HOH:O   | 2.01                     | 0.60              |
| 6:D:1371:VAL:HG12 | 6:D:1375:MET:CE   | 2.32                     | 0.60              |
| 7:E:54:LEU:HA     | 7:E:58:PRO:HG2    | 1.83                     | 0.60              |
| 6:N:1438:ALA:N    | 6:N:1446:VAL:HG11 | 2.16                     | 0.60              |
| 5:C:65:VAL:HG23   | 5:C:101:ILE:HB    | 1.83                     | 0.60              |
| 5:C:326:ASP:HB2   | 5:C:431:HIS:ND1   | 2.17                     | 0.60              |
| 5:C:499:ALA:HA    | 5:C:532:MET:HE3   | 1.83                     | 0.60              |
| 5:C:660:ALA:HB1   | 5:C:667:ALA:O     | 2.02                     | 0.60              |
| 6:D:762:GLN:HE22  | 7:E:20:THR:CG2    | 2.15                     | 0.60              |
| 6:D:952:ASP:HA    | 6:D:1062:ARG:NH2  | 2.16                     | 0.60              |
| 6:D:1042:ARG:HH21 | 6:D:1061:PHE:HZ   | 1.50                     | 0.60              |
| 6:D:1263:PHE:HB3  | 6:D:1424:VAL:HG11 | 1.83                     | 0.60              |
| 6:D:1336:LEU:HD11 | 6:D:1341:PRO:HG3  | 1.82                     | 0.60              |
| 5:M:759:THR:HG21  | 5:M:783:ARG:HH21  | 1.67                     | 0.60              |
| 6:N:399:ARG:HE    | 6:N:431:VAL:HG23  | 1.65                     | 0.60              |
| 6:N:1438:ALA:O    | 6:N:1443:THR:HG22 | 2.01                     | 0.60              |
| 4:B:154:GLU:CD    | 4:B:155:LYS:HZ1   | 2.10                     | 0.60              |
| 5:C:19:THR:O      | 5:C:23:VAL:HG23   | 2.01                     | 0.60              |
| 5:C:573:ARG:CG    | 5:C:670:GLN:HE22  | 2.14                     | 0.60              |
| 5:C:859:PRO:HB3   | 5:C:974:LEU:HD23  | 1.83                     | 0.60              |
| 5:C:910:LYS:HB2   | 11:C:1325:HOH:O   | 2.01                     | 0.60              |
| 5:C:943:VAL:HG11  | 5:C:973:VAL:CG2   | 2.31                     | 0.60              |
| 6:D:54:LYS:HD2    | 6:D:55:ASP:H      | 1.66                     | 0.60              |
| 6:D:109:PRO:O     | 6:D:111:LYS:HD3   | 2.01                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:127:LEU:HD22  | 6:D:460:ALA:CB    | 2.32                     | 0.60              |
| 6:D:896:ALA:HB2   | 11:D:8341:HOH:O   | 2.02                     | 0.60              |
| 5:M:52:PHE:CG     | 5:M:68:PHE:HB2    | 2.36                     | 0.60              |
| 5:M:637:LEU:HD22  | 5:M:659:PRO:HG2   | 1.83                     | 0.60              |
| 5:M:1033:GLY:O    | 5:M:1037:VAL:HG23 | 2.02                     | 0.60              |
| 6:N:29:PRO:HD3    | 6:N:548:ILE:CG2   | 2.32                     | 0.60              |
| 6:N:522:PRO:O     | 6:N:525:ARG:HD3   | 2.02                     | 0.60              |
| 1:G:18:DG:H2''    | 1:G:19:DC:C5'     | 2.32                     | 0.60              |
| 5:C:843:HIS:HA    | 11:C:1257:HOH:O   | 2.01                     | 0.60              |
| 6:D:8:VAL:HB      | 6:D:1434:TRP:HH2  | 1.67                     | 0.60              |
| 6:D:119:SER:CB    | 6:D:123:LEU:HD13  | 2.31                     | 0.60              |
| 6:D:963:TYR:CD2   | 6:D:1002:LYS:HB3  | 2.37                     | 0.60              |
| 6:D:1495:ILE:HG22 | 6:D:1499:ARG:HH21 | 1.66                     | 0.60              |
| 5:M:267:TYR:HB2   | 5:M:272:ALA:CB    | 2.32                     | 0.60              |
| 6:N:398:ALA:HB2   | 6:N:447:VAL:HA    | 1.82                     | 0.60              |
| 6:N:610:LYS:HA    | 11:N:9272:HOH:O   | 2.01                     | 0.60              |
| 5:C:1099:VAL:HA   | 6:D:9:ARG:O       | 2.02                     | 0.60              |
| 6:D:521:PRO:CG    | 6:D:524:LEU:HD22  | 2.29                     | 0.60              |
| 6:D:1205:TYR:CD2  | 6:D:1215:VAL:HG21 | 2.31                     | 0.60              |
| 6:D:1255:GLY:O    | 6:D:1259:VAL:HG23 | 2.02                     | 0.60              |
| 5:M:144:PRO:HG3   | 5:M:265:ARG:NH1   | 2.16                     | 0.60              |
| 5:M:176:VAL:C     | 5:M:178:PRO:HD3   | 2.27                     | 0.60              |
| 6:N:76:CYS:HB3    | 11:N:9086:HOH:O   | 2.01                     | 0.60              |
| 6:N:633:VAL:HG22  | 6:N:635:PRO:CD    | 2.25                     | 0.60              |
| 6:N:1267:ARG:HG3  | 6:N:1271:LYS:NZ   | 2.17                     | 0.60              |
| 4:A:83:LYS:NZ     | 4:A:168:ASP:HB2   | 2.17                     | 0.59              |
| 5:C:45:GLN:HG2    | 5:C:49:ARG:CZ     | 2.32                     | 0.59              |
| 5:C:461:VAL:HG12  | 11:C:1351:HOH:O   | 2.02                     | 0.59              |
| 5:C:721:ARG:HG3   | 5:C:820:ARG:HH12  | 1.66                     | 0.59              |
| 6:D:116:LEU:CD2   | 6:D:150:ARG:HD3   | 2.32                     | 0.59              |
| 6:D:1259:VAL:HG11 | 6:D:1356:TYR:OH   | 2.02                     | 0.59              |
| 6:D:1485:GLN:NE2  | 7:E:78:ASN:HA     | 2.17                     | 0.59              |
| 4:K:151:VAL:HB    | 4:K:169:ALA:HB3   | 1.84                     | 0.59              |
| 5:M:127:PHE:HB3   | 11:M:1483:HOH:O   | 2.01                     | 0.59              |
| 5:M:409:ARG:HA    | 5:M:454:SER:HA    | 1.84                     | 0.59              |
| 5:M:1005:MET:CE   | 6:N:724:GLN:HA    | 2.32                     | 0.59              |
| 6:N:185:VAL:HG21  | 6:N:203:ALA:HB2   | 1.84                     | 0.59              |
| 6:N:1192:LEU:HD13 | 6:N:1345:GLU:HG2  | 1.83                     | 0.59              |
| 4:A:159:LYS:NZ    | 4:A:166:PRO:HD3   | 2.17                     | 0.59              |
| 5:C:148:PHE:CE2   | 5:C:281:LEU:HD13  | 2.28                     | 0.59              |
| 5:C:218:VAL:HG22  | 5:C:221:LEU:HD21  | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:456:MET:HG2   | 6:D:459:GLU:OE1   | 2.02                     | 0.59              |
| 6:D:970:LYS:HD3   | 6:D:995:LEU:HD13  | 1.84                     | 0.59              |
| 6:N:477:LEU:HD11  | 6:N:495:ARG:HD3   | 1.84                     | 0.59              |
| 6:N:478:LEU:HD23  | 6:N:496:LEU:HD21  | 1.84                     | 0.59              |
| 6:N:495:ARG:O     | 6:N:499:VAL:HG23  | 2.02                     | 0.59              |
| 6:N:761:ILE:HB    | 7:O:20:THR:HG23   | 1.83                     | 0.59              |
| 6:N:1106:VAL:HG11 | 6:N:1474:ALA:CB   | 2.31                     | 0.59              |
| 2:H:7:G:N3        | 2:H:7:G:H2'       | 2.17                     | 0.59              |
| 4:A:8:ALA:HB1     | 4:B:224:TYR:HE1   | 1.65                     | 0.59              |
| 5:C:26:TYR:HD2    | 5:C:121:MET:HB2   | 1.66                     | 0.59              |
| 6:D:99:ALA:O      | 6:D:514:LEU:N     | 2.33                     | 0.59              |
| 6:D:1080:GLY:O    | 6:D:1083:ASP:HB3  | 2.02                     | 0.59              |
| 6:D:1231:GLU:O    | 6:D:1235:GLN:HG3  | 2.02                     | 0.59              |
| 6:D:1335:LEU:HD23 | 6:D:1344:VAL:HG22 | 1.84                     | 0.59              |
| 4:K:89:PHE:HB3    | 4:K:94:LEU:HD13   | 1.84                     | 0.59              |
| 5:M:876:VAL:HG13  | 5:M:881:ASN:ND2   | 2.16                     | 0.59              |
| 6:N:98:PRO:C      | 6:N:458:ALA:HB3   | 2.27                     | 0.59              |
| 6:N:480:GLU:O     | 6:N:484:PRO:HD2   | 2.02                     | 0.59              |
| 6:N:1268:PRO:HD2  | 6:N:1271:LYS:HZ2  | 1.67                     | 0.59              |
| 5:C:252:LYS:HB3   | 5:C:298:PHE:CZ    | 2.38                     | 0.59              |
| 5:C:583:LEU:HB3   | 11:C:1190:HOH:O   | 2.01                     | 0.59              |
| 6:D:675:ARG:HA    | 6:D:678:GLU:CD    | 2.27                     | 0.59              |
| 6:D:1438:ALA:N    | 6:D:1446:VAL:HG11 | 2.17                     | 0.59              |
| 4:K:67:THR:CG2    | 5:M:609:ASN:HD21  | 2.15                     | 0.59              |
| 4:K:133:GLU:OE1   | 5:M:605:LYS:HB3   | 2.02                     | 0.59              |
| 5:M:18:LEU:H      | 5:M:18:LEU:HD12   | 1.67                     | 0.59              |
| 5:M:149:THR:HG21  | 11:M:1567:HOH:O   | 2.01                     | 0.59              |
| 5:M:1051:GLU:OE1  | 5:M:1056:LYS:HE2  | 2.03                     | 0.59              |
| 5:M:1056:LYS:HD3  | 6:N:625:TYR:HD1   | 1.67                     | 0.59              |
| 6:N:23:TYR:O      | 6:N:49:ILE:HG23   | 2.01                     | 0.59              |
| 6:N:161:LEU:O     | 6:N:161:LEU:HD23  | 2.03                     | 0.59              |
| 6:N:794:GLN:HG2   | 6:N:1017:PHE:CZ   | 2.38                     | 0.59              |
| 6:N:966:GLU:HA    | 6:N:969:ARG:NH2   | 2.18                     | 0.59              |
| 6:N:983:LEU:HD13  | 6:N:991:GLN:OE1   | 2.02                     | 0.59              |
| 6:N:1375:MET:HB3  | 6:N:1422:MET:O    | 2.02                     | 0.59              |
| 2:Y:6:U:H1'       | 11:Y:2617:HOH:O   | 2.03                     | 0.59              |
| 4:A:38:ASN:HB3    | 4:A:39:PRO:HD3    | 1.85                     | 0.59              |
| 4:A:89:PHE:CZ     | 4:A:146:ARG:HB2   | 2.37                     | 0.59              |
| 5:C:73:LEU:HD22   | 5:C:94:LEU:HD13   | 1.84                     | 0.59              |
| 5:C:318:PRO:HG3   | 11:C:1342:HOH:O   | 2.01                     | 0.59              |
| 5:C:352:ALA:HA    | 5:C:355:VAL:HG12  | 1.85                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:135:LEU:H     | 6:D:135:LEU:HD12  | 1.67                     | 0.59              |
| 6:D:172:PRO:HG2   | 6:D:175:VAL:HG21  | 1.84                     | 0.59              |
| 6:D:769:LEU:HD12  | 6:D:919:PHE:HE1   | 1.68                     | 0.59              |
| 6:D:803:GLY:HA3   | 11:D:8427:HOH:O   | 2.00                     | 0.59              |
| 4:K:31:GLY:CA     | 4:L:42:ARG:HH21   | 2.15                     | 0.59              |
| 4:K:209:GLU:O     | 4:K:213:GLN:HG3   | 2.02                     | 0.59              |
| 4:L:68:ILE:HD13   | 11:L:362:HOH:O    | 2.01                     | 0.59              |
| 6:N:584:ASN:CG    | 6:N:590:PRO:HD2   | 2.27                     | 0.59              |
| 6:N:615:ARG:HG3   | 6:N:619:LEU:HD21  | 1.84                     | 0.59              |
| 6:N:1125:PRO:C    | 6:N:1130:ARG:HH12 | 2.11                     | 0.59              |
| 6:N:1209:LEU:HD23 | 6:N:1210:SER:H    | 1.66                     | 0.59              |
| 6:N:1412:LYS:HD2  | 6:N:1414:PRO:HG3  | 1.83                     | 0.59              |
| 4:A:91:ASN:OD1    | 4:A:92:PRO:HD2    | 2.03                     | 0.59              |
| 6:D:32:ILE:HB     | 6:D:527:MET:HE3   | 1.85                     | 0.59              |
| 6:D:1209:LEU:HD23 | 6:D:1210:SER:H    | 1.65                     | 0.59              |
| 4:K:79:ILE:HA     | 4:K:82:LEU:HD12   | 1.84                     | 0.59              |
| 5:M:468:ARG:HH21  | 5:M:487:THR:N     | 2.00                     | 0.59              |
| 5:M:854:PRO:HB2   | 5:M:856:GLU:CG    | 2.32                     | 0.59              |
| 6:N:156:GLU:HB2   | 6:N:157:GLU:OE1   | 2.02                     | 0.59              |
| 6:N:1389:LEU:HG   | 6:N:1390:LEU:HG   | 1.84                     | 0.59              |
| 4:A:54:THR:HB     | 4:A:143:ARG:HG2   | 1.85                     | 0.59              |
| 5:C:260:LEU:HD22  | 11:C:1406:HOH:O   | 2.00                     | 0.59              |
| 5:C:274:ARG:HB2   | 5:C:285:LEU:HD13  | 1.85                     | 0.59              |
| 5:C:516:ARG:NH1   | 5:C:521:PRO:HB3   | 2.17                     | 0.59              |
| 5:C:627:ARG:HG3   | 5:C:628:PHE:H     | 1.67                     | 0.59              |
| 5:C:835:VAL:HG12  | 11:C:1129:HOH:O   | 2.03                     | 0.59              |
| 6:D:106:LYS:HG2   | 11:D:8237:HOH:O   | 2.01                     | 0.59              |
| 6:D:165:LYS:HD3   | 6:D:448:GLU:CD    | 2.27                     | 0.59              |
| 6:N:1009:LYS:HG2  | 11:N:9338:HOH:O   | 2.03                     | 0.59              |
| 6:N:1059:SER:OG   | 6:N:1065:LEU:HD12 | 2.03                     | 0.59              |
| 5:C:193:LEU:HD21  | 11:C:1142:HOH:O   | 2.02                     | 0.59              |
| 5:C:200:LEU:HD13  | 5:C:300:ASP:CG    | 2.27                     | 0.59              |
| 5:C:692:GLU:HG2   | 5:C:696:LYS:HE2   | 1.83                     | 0.59              |
| 6:D:1465:ASN:HD21 | 6:D:1470:ARG:HB3  | 1.68                     | 0.59              |
| 4:K:5:LYS:HA      | 4:K:5:LYS:HE3     | 1.85                     | 0.59              |
| 5:M:119:PRO:HG2   | 5:M:386:PHE:CG    | 2.37                     | 0.59              |
| 5:M:575:GLN:HB2   | 5:M:670:GLN:HG2   | 1.85                     | 0.59              |
| 5:M:1055:LEU:CD2  | 5:M:1066:ALA:HB2  | 2.31                     | 0.59              |
| 6:N:422:ALA:HA    | 11:N:9357:HOH:O   | 2.01                     | 0.59              |
| 6:N:455:ARG:HB3   | 6:N:460:ALA:HA    | 1.83                     | 0.59              |
| 6:N:481:MET:CE    | 6:N:493:ARG:HA    | 2.32                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:584:ASN:OD1   | 6:N:590:PRO:HD2   | 2.03                     | 0.59              |
| 6:N:787:LEU:HD13  | 6:N:1023:MET:HA   | 1.84                     | 0.59              |
| 6:D:93:ILE:HG13   | 6:D:519:VAL:HG22  | 1.85                     | 0.59              |
| 6:D:161:LEU:CD2   | 6:D:452:ILE:HD13  | 2.33                     | 0.59              |
| 6:D:462:GLN:O     | 6:D:466:LYS:HE3   | 2.03                     | 0.59              |
| 6:D:1440:PHE:CG   | 6:D:1441:GLN:N    | 2.71                     | 0.59              |
| 7:E:17:TYR:O      | 7:E:21:VAL:HG23   | 2.03                     | 0.59              |
| 4:A:225:PHE:HE1   | 4:B:40:LEU:HD11   | 1.68                     | 0.59              |
| 4:B:94:LEU:HD11   | 4:B:119:ASP:CB    | 2.32                     | 0.59              |
| 5:C:182:VAL:HG21  | 5:C:220:GLY:C     | 2.28                     | 0.59              |
| 5:C:833:LEU:HD21  | 5:C:839:LEU:HD11  | 1.84                     | 0.59              |
| 4:K:224:TYR:HB3   | 4:L:9:PRO:HB2     | 1.83                     | 0.59              |
| 4:L:94:LEU:HD11   | 4:L:119:ASP:CB    | 2.33                     | 0.59              |
| 5:M:140:ILE:HB    | 5:M:331:ARG:HG2   | 1.83                     | 0.59              |
| 5:M:498:GLN:HA    | 5:M:533:ASP:OD2   | 2.03                     | 0.59              |
| 5:M:1000:MET:HB3  | 5:M:1002:GLU:HG2  | 1.84                     | 0.59              |
| 5:M:1081:VAL:HG23 | 5:M:1086:ARG:HH21 | 1.67                     | 0.59              |
| 6:N:86:ARG:HD3    | 6:N:523:ASP:OD2   | 2.02                     | 0.59              |
| 6:N:396:VAL:O     | 6:N:398:ALA:N     | 2.31                     | 0.59              |
| 6:N:860:LEU:HD23  | 6:N:877:PRO:HB2   | 1.85                     | 0.59              |
| 1:G:2:DC:H2'      | 1:G:3:DC:C6       | 2.38                     | 0.58              |
| 2:Y:11:C:O2'      | 2:Y:12:G:H5'      | 2.02                     | 0.58              |
| 5:C:48:PHE:O      | 5:C:52:PHE:HB2    | 2.02                     | 0.58              |
| 5:C:218:VAL:HG22  | 5:C:221:LEU:CD2   | 2.33                     | 0.58              |
| 5:C:342:ASP:O     | 5:C:346:VAL:HG23  | 2.03                     | 0.58              |
| 5:C:488:ALA:HA    | 11:C:1287:HOH:O   | 2.02                     | 0.58              |
| 6:D:401:TYR:CZ    | 6:D:429:SER:HA    | 2.38                     | 0.58              |
| 6:D:582:LEU:HA    | 6:D:603:LEU:HD12  | 1.85                     | 0.58              |
| 6:D:799:LYS:O     | 6:D:826:PRO:HD2   | 2.02                     | 0.58              |
| 4:L:173:PRO:HB2   | 11:L:366:HOH:O    | 2.02                     | 0.58              |
| 5:M:755:LEU:HD12  | 5:M:790:LEU:HG    | 1.85                     | 0.58              |
| 6:N:191:LEU:HB3   | 6:N:393:ILE:HD12  | 1.85                     | 0.58              |
| 2:H:9:G:H5'       | 2:H:9:G:C8        | 2.38                     | 0.58              |
| 1:X:18:DG:H5'     | 1:X:18:DG:H8      | 1.68                     | 0.58              |
| 4:A:5:LYS:HA      | 4:A:5:LYS:HE3     | 1.84                     | 0.58              |
| 4:A:54:THR:CG2    | 4:A:158:ILE:HG13  | 2.30                     | 0.58              |
| 4:B:20:TYR:HE2    | 4:B:198:ARG:HB3   | 1.68                     | 0.58              |
| 5:C:913:GLU:O     | 5:C:917:LEU:HG    | 2.03                     | 0.58              |
| 5:C:983:ILE:HG21  | 5:C:987:ILE:HD11  | 1.85                     | 0.58              |
| 5:C:1009:SER:HB2  | 6:D:651:GLU:O     | 2.03                     | 0.58              |
| 6:D:481:MET:HE2   | 6:D:493:ARG:HB2   | 1.84                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:D:693:GLU:HA   | 11:D:8294:HOH:O   | 2.03                     | 0.58              |
| 6:D:918:ALA:O    | 6:D:922:LEU:HG    | 2.02                     | 0.58              |
| 4:L:174:VAL:HG23 | 11:L:366:HOH:O    | 2.02                     | 0.58              |
| 5:M:701:THR:HG21 | 5:M:830:LYS:HE2   | 1.84                     | 0.58              |
| 5:M:946:ARG:HH11 | 5:M:946:ARG:CB    | 2.08                     | 0.58              |
| 6:N:464:LEU:O    | 6:N:468:LEU:HG    | 2.02                     | 0.58              |
| 6:N:567:ILE:O    | 6:N:571:LYS:HG2   | 2.03                     | 0.58              |
| 6:N:728:LEU:HD21 | 6:N:733:CYS:SG    | 2.43                     | 0.58              |
| 7:O:18:ARG:HD3   | 7:O:75:PHE:CE1    | 2.33                     | 0.58              |
| 2:Y:8:C:HO2'     | 2:Y:9:G:H5'       | 1.66                     | 0.58              |
| 4:B:99:LEU:HB3   | 4:B:114:PHE:CD2   | 2.38                     | 0.58              |
| 5:C:398:THR:HA   | 11:C:1367:HOH:O   | 2.03                     | 0.58              |
| 6:D:752:SER:HB2  | 11:D:8371:HOH:O   | 2.03                     | 0.58              |
| 6:D:835:SER:N    | 6:D:838:ARG:HD3   | 2.18                     | 0.58              |
| 6:D:1236:LEU:CD1 | 6:D:1359:GLN:HB3  | 2.33                     | 0.58              |
| 5:M:861:LEU:HA   | 5:M:974:LEU:HD12  | 1.85                     | 0.58              |
| 6:N:15:PRO:O     | 6:N:18:ILE:HB     | 2.03                     | 0.58              |
| 6:N:815:ALA:HA   | 6:N:818:ARG:HD2   | 1.84                     | 0.58              |
| 7:O:40:LEU:CB    | 7:O:72:ARG:HH21   | 2.15                     | 0.58              |
| 7:O:48:MET:N     | 7:O:54:LEU:HB2    | 2.18                     | 0.58              |
| 2:Y:13:C:C4'     | 5:M:409:ARG:HH22  | 2.13                     | 0.58              |
| 4:A:44:LEU:O     | 4:A:174:VAL:HG21  | 2.04                     | 0.58              |
| 6:D:124:GLU:O    | 6:D:127:LEU:HD12  | 2.02                     | 0.58              |
| 6:D:1084:THR:HB  | 6:D:1241:PHE:CD2  | 2.38                     | 0.58              |
| 6:D:1238:MET:HG3 | 11:D:8018:HOH:O   | 2.03                     | 0.58              |
| 5:M:102:HIS:NE2  | 5:M:365:ASP:HA    | 2.18                     | 0.58              |
| 5:M:252:LYS:HZ3  | 5:M:296:GLY:HA3   | 1.69                     | 0.58              |
| 6:N:522:PRO:HG2  | 6:N:523:ASP:H     | 1.68                     | 0.58              |
| 6:N:695:ILE:HD11 | 6:N:718:PRO:HB2   | 1.84                     | 0.58              |
| 6:N:1146:GLY:CA  | 6:N:1207:TYR:HB2  | 2.33                     | 0.58              |
| 4:A:9:PRO:HB3    | 4:A:25:LEU:HG     | 1.84                     | 0.58              |
| 6:D:23:TYR:O     | 6:D:49:ILE:HG23   | 2.03                     | 0.58              |
| 6:D:101:HIS:O    | 6:D:105:VAL:HG23  | 2.02                     | 0.58              |
| 6:D:957:PRO:HG2  | 6:D:1007:VAL:HG22 | 1.85                     | 0.58              |
| 4:L:59:GLU:CB    | 4:L:137:ARG:HH22  | 2.16                     | 0.58              |
| 4:L:137:ARG:C    | 4:L:137:ARG:HD3   | 2.28                     | 0.58              |
| 5:M:497:ALA:HA   | 5:M:515:ALA:HA    | 1.85                     | 0.58              |
| 6:N:711:LEU:HD21 | 6:N:768:ASN:CB    | 2.33                     | 0.58              |
| 6:N:962:GLN:HG2  | 6:N:966:GLU:OE1   | 2.03                     | 0.58              |
| 6:N:989:TYR:HA   | 6:N:992:ILE:HD12  | 1.83                     | 0.58              |
| 6:N:1112:CYS:HB2 | 6:N:1195:GLN:CG   | 2.34                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:1100:GLN:HA   | 5:C:1100:GLN:NE2  | 2.18                     | 0.58              |
| 6:D:50:PHE:CD2    | 6:D:522:PRO:HD3   | 2.38                     | 0.58              |
| 6:D:426:LYS:HE3   | 6:D:427:VAL:HG23  | 1.85                     | 0.58              |
| 7:E:48:MET:HG2    | 7:E:49:GLN:H      | 1.69                     | 0.58              |
| 5:M:99:GLN:HG2    | 5:M:109:LYS:HG3   | 1.85                     | 0.58              |
| 6:N:136:ASP:CB    | 6:N:137:PRO:HD3   | 2.33                     | 0.58              |
| 1:G:6:DT:H2''     | 1:G:7:DC:C6       | 2.39                     | 0.58              |
| 4:B:177:VAL:HG12  | 4:B:199:ILE:HG23  | 1.86                     | 0.58              |
| 5:C:211:LEU:CD1   | 5:C:308:ARG:HA    | 2.34                     | 0.58              |
| 5:C:548:PRO:HD3   | 5:C:842:ARG:HD2   | 1.86                     | 0.58              |
| 5:C:580:MET:SD    | 5:C:584:GLU:HG3   | 2.44                     | 0.58              |
| 5:C:712:ALA:O     | 5:C:820:ARG:HB3   | 2.04                     | 0.58              |
| 5:C:841:ASN:H     | 5:C:841:ASN:ND2   | 2.02                     | 0.58              |
| 5:C:1014:SER:HB2  | 5:C:1017:THR:HG23 | 1.85                     | 0.58              |
| 5:M:347:GLY:HA2   | 11:M:1457:HOH:O   | 2.02                     | 0.58              |
| 5:M:831:ARG:HA    | 11:M:1437:HOH:O   | 2.04                     | 0.58              |
| 5:M:841:ASN:HD21  | 5:M:844:GLY:H     | 1.51                     | 0.58              |
| 6:N:95:LEU:HD13   | 6:N:515:GLU:C     | 2.28                     | 0.58              |
| 6:N:584:ASN:HD21  | 6:N:589:ALA:HA    | 1.67                     | 0.58              |
| 6:N:1486:VAL:HG23 | 11:N:9307:HOH:O   | 2.03                     | 0.58              |
| 5:C:573:ARG:HB3   | 11:C:1209:HOH:O   | 2.03                     | 0.58              |
| 5:C:693:GLU:OE1   | 5:C:696:LYS:HD2   | 2.03                     | 0.58              |
| 6:D:871:LYS:HE2   | 6:D:873:LEU:HD21  | 1.86                     | 0.58              |
| 7:E:26:ARG:O      | 7:E:30:LEU:HD12   | 2.04                     | 0.58              |
| 5:M:34:VAL:HG12   | 11:M:1176:HOH:O   | 2.04                     | 0.58              |
| 5:M:54:ILE:CG2    | 5:M:66:LEU:HB3    | 2.34                     | 0.58              |
| 5:M:549:PHE:HB3   | 5:M:552:HIS:HD2   | 1.67                     | 0.58              |
| 5:M:564:MET:HE1   | 5:M:995:MET:SD    | 2.44                     | 0.58              |
| 5:M:701:THR:CG2   | 5:M:832:LYS:HG2   | 2.32                     | 0.58              |
| 6:N:996:TRP:HA    | 6:N:999:THR:CG2   | 2.25                     | 0.58              |
| 2:Y:13:C:H2'      | 2:Y:14:G:C8       | 2.39                     | 0.58              |
| 4:B:54:THR:CG2    | 4:B:158:ILE:HG13  | 2.33                     | 0.58              |
| 6:D:206:ARG:HB3   | 6:D:206:ARG:HH11  | 1.68                     | 0.58              |
| 6:D:465:LEU:HD22  | 6:D:510:GLU:HA    | 1.86                     | 0.58              |
| 6:D:796:ARG:NE    | 6:D:828:LYS:HZ3   | 2.01                     | 0.58              |
| 6:D:1017:PHE:HE1  | 11:D:8095:HOH:O   | 1.87                     | 0.58              |
| 6:D:1373:ARG:HE   | 6:D:1374:GLN:NE2  | 2.02                     | 0.58              |
| 4:K:211:LEU:O     | 4:K:215:VAL:HG23  | 2.04                     | 0.58              |
| 5:M:431:HIS:H     | 5:M:434:HIS:CE1   | 2.22                     | 0.58              |
| 5:M:444:PRO:HD2   | 5:M:452:ILE:O     | 2.04                     | 0.58              |
| 5:M:874:LEU:H     | 5:M:874:LEU:HD12  | 1.69                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:M:1056:LYS:HD3 | 6:N:751:LEU:HD11  | 1.86                     | 0.58              |
| 6:N:134:VAL:HG12 | 6:N:152:LEU:HD22  | 1.86                     | 0.58              |
| 6:N:966:GLU:HA   | 6:N:969:ARG:HH22  | 1.67                     | 0.58              |
| 6:N:1081:GLY:O   | 6:N:1084:THR:HG22 | 2.04                     | 0.58              |
| 6:N:1119:SER:O   | 6:N:1121:PRO:HD3  | 2.04                     | 0.58              |
| 3:I:7:DC:H5"     | 6:D:1264:GLU:OE2  | 2.04                     | 0.58              |
| 4:B:99:LEU:HG    | 11:B:336:HOH:O    | 2.03                     | 0.58              |
| 5:C:775:ARG:NH1  | 5:C:782:ALA:HB1   | 2.18                     | 0.58              |
| 6:D:116:LEU:HD22 | 6:D:118:LEU:HD21  | 1.86                     | 0.58              |
| 6:D:132:TYR:C    | 6:D:133:ILE:HD13  | 2.29                     | 0.58              |
| 6:D:182:GLY:HA3  | 6:D:400:VAL:HG11  | 1.85                     | 0.58              |
| 6:D:616:GLN:HG3  | 11:D:8092:HOH:O   | 2.03                     | 0.58              |
| 6:D:786:ILE:HD11 | 6:D:908:LYS:HD3   | 1.85                     | 0.58              |
| 5:M:310:LEU:HB2  | 11:M:1183:HOH:O   | 2.03                     | 0.58              |
| 5:M:452:ILE:H    | 5:M:452:ILE:HD12  | 1.69                     | 0.58              |
| 5:M:464:LEU:HB2  | 11:M:1525:HOH:O   | 2.03                     | 0.58              |
| 5:M:549:PHE:HB3  | 5:M:552:HIS:CD2   | 2.39                     | 0.58              |
| 6:N:161:LEU:HD21 | 11:N:9092:HOH:O   | 2.02                     | 0.58              |
| 6:N:679:ARG:HB2  | 6:N:682:ASP:CG    | 2.29                     | 0.58              |
| 6:N:930:LEU:O    | 6:N:934:LEU:HG    | 2.04                     | 0.58              |
| 6:N:970:LYS:HG3  | 6:N:973:GLN:OE1   | 2.04                     | 0.58              |
| 1:G:6:DT:H73     | 11:G:2394:HOH:O   | 2.04                     | 0.57              |
| 1:X:6:DT:H2"     | 1:X:7:DC:C6       | 2.39                     | 0.57              |
| 5:C:211:LEU:HD11 | 5:C:308:ARG:HA    | 1.86                     | 0.57              |
| 5:C:495:THR:HG23 | 11:C:1226:HOH:O   | 2.03                     | 0.57              |
| 5:C:626:ARG:H    | 5:C:639:GLN:HE21  | 1.50                     | 0.57              |
| 5:C:959:PRO:HG2  | 11:C:1413:HOH:O   | 2.03                     | 0.57              |
| 5:C:1101:THR:OG1 | 6:D:5:VAL:HG12    | 2.03                     | 0.57              |
| 6:D:810:GLU:HB3  | 11:D:8233:HOH:O   | 2.03                     | 0.57              |
| 6:D:890:VAL:HG23 | 11:D:8341:HOH:O   | 2.03                     | 0.57              |
| 6:D:1171:VAL:O   | 6:D:1175:ILE:HG13 | 2.04                     | 0.57              |
| 5:M:134:ARG:HH11 | 5:M:392:SER:CB    | 2.17                     | 0.57              |
| 5:M:470:PRO:HD3  | 5:M:485:TYR:CE2   | 2.39                     | 0.57              |
| 5:M:546:LEU:CD1  | 5:M:565:GLN:HE22  | 2.17                     | 0.57              |
| 5:M:715:THR:HG21 | 11:M:1222:HOH:O   | 2.03                     | 0.57              |
| 5:M:875:GLY:O    | 5:M:879:ARG:HD2   | 2.03                     | 0.57              |
| 5:M:1030:GLN:HB2 | 6:N:626:SER:OG    | 2.04                     | 0.57              |
| 5:M:1032:PHE:O   | 5:M:1033:GLY:O    | 2.21                     | 0.57              |
| 6:N:1397:LYS:HE3 | 6:N:1432:LYS:HD2  | 1.85                     | 0.57              |
| 5:C:573:ARG:HB3  | 5:C:670:GLN:HE22  | 1.69                     | 0.57              |
| 6:D:30:GLU:HB3   | 6:D:40:GLU:CB     | 2.34                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:D:400:VAL:HG22 | 6:D:443:VAL:HG21 | 1.85                     | 0.57              |
| 5:M:535:SER:HB3  | 5:M:537:LYS:NZ   | 2.19                     | 0.57              |
| 6:N:62:LYS:HG3   | 6:N:75:ARG:NH1   | 2.19                     | 0.57              |
| 6:N:149:LYS:HD2  | 6:N:150:ARG:H    | 1.69                     | 0.57              |
| 6:N:677:LEU:HD23 | 6:N:683:ILE:HG13 | 1.86                     | 0.57              |
| 7:O:32:ARG:CZ    | 7:O:32:ARG:HB2   | 2.34                     | 0.57              |
| 2:H:10:G:H2'     | 2:H:11:C:H6      | 1.66                     | 0.57              |
| 2:H:13:C:H2'     | 2:H:14:G:C8      | 2.39                     | 0.57              |
| 2:Y:14:G:H4'     | 11:Y:1734:HOH:O  | 2.03                     | 0.57              |
| 11:Y:1707:HOH:O  | 5:M:777:ILE:HG21 | 2.03                     | 0.57              |
| 5:C:99:GLN:HB3   | 5:C:109:LYS:CD   | 2.34                     | 0.57              |
| 5:C:264:PRO:HG3  | 11:C:1383:HOH:O  | 2.04                     | 0.57              |
| 5:C:577:PRO:HB3  | 5:C:842:ARG:NH2  | 2.18                     | 0.57              |
| 5:C:679:PHE:C    | 6:D:943:THR:HG22 | 2.29                     | 0.57              |
| 6:D:30:GLU:HB3   | 6:D:40:GLU:CG    | 2.34                     | 0.57              |
| 6:D:444:VAL:HB   | 11:D:8164:HOH:O  | 2.04                     | 0.57              |
| 6:D:614:PHE:CE2  | 6:D:1438:ALA:HB1 | 2.39                     | 0.57              |
| 6:D:1418:LYS:HD3 | 6:D:1419:PRO:HD2 | 1.85                     | 0.57              |
| 4:K:49:PRO:HB3   | 4:K:148:VAL:HG22 | 1.86                     | 0.57              |
| 4:K:145:ASP:HB3  | 11:K:1799:HOH:O  | 2.03                     | 0.57              |
| 5:M:79:PRO:HG2   | 5:M:82:GLU:HB2   | 1.85                     | 0.57              |
| 5:M:205:GLU:HA   | 5:M:209:ARG:NH1  | 2.20                     | 0.57              |
| 6:N:399:ARG:HE   | 6:N:431:VAL:CG2  | 2.18                     | 0.57              |
| 6:N:510:GLU:HB2  | 6:N:511:TRP:CZ3  | 2.39                     | 0.57              |
| 6:N:637:LEU:HD11 | 6:N:641:GLN:HB2  | 1.86                     | 0.57              |
| 6:N:1128:VAL:O   | 6:N:1129:THR:C   | 2.47                     | 0.57              |
| 7:O:33:HIS:HB2   | 7:O:37:ASN:ND2   | 2.18                     | 0.57              |
| 5:C:1030:GLN:NE2 | 6:D:628:ARG:HD3  | 2.20                     | 0.57              |
| 6:D:155:ASP:O    | 6:D:159:ARG:HG3  | 2.04                     | 0.57              |
| 6:D:793:THR:HG21 | 6:D:906:GLN:CG   | 2.33                     | 0.57              |
| 4:L:58:ILE:HG21  | 4:L:68:ILE:HD11  | 1.85                     | 0.57              |
| 5:M:1031:ARG:HG3 | 6:N:621:LYS:HB3  | 1.86                     | 0.57              |
| 6:N:394:LEU:HG   | 6:N:396:VAL:HG23 | 1.85                     | 0.57              |
| 2:Y:9:G:O2'      | 2:Y:10:G:H5'     | 2.04                     | 0.57              |
| 4:B:170:VAL:HG11 | 6:D:848:GLU:OE1  | 2.04                     | 0.57              |
| 5:C:468:ARG:HE   | 5:C:487:THR:N    | 2.02                     | 0.57              |
| 6:D:501:ALA:HB1  | 6:D:1453:ALA:HB2 | 1.87                     | 0.57              |
| 6:D:525:ARG:HB2  | 6:D:538:SER:HB3  | 1.86                     | 0.57              |
| 6:D:879:ARG:HG3  | 6:D:879:ARG:NH1  | 2.17                     | 0.57              |
| 4:K:181:VAL:HG21 | 5:M:939:ARG:HH11 | 1.70                     | 0.57              |
| 5:M:166:PRO:HB3  | 11:M:1157:HOH:O  | 2.03                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:452:ILE:HD12  | 5:M:452:ILE:N     | 2.19                     | 0.57              |
| 5:M:975:TYR:HE1   | 11:M:1220:HOH:O   | 1.86                     | 0.57              |
| 6:N:28:LYS:HG3    | 6:N:29:PRO:HD2    | 1.87                     | 0.57              |
| 1:G:20:DG:H4'     | 5:C:394:PHE:CE1   | 2.39                     | 0.57              |
| 4:A:43:ILE:HG13   | 4:A:218:LEU:CD1   | 2.33                     | 0.57              |
| 6:D:772:PRO:HB3   | 6:D:1224:VAL:CG1  | 2.34                     | 0.57              |
| 4:K:70:GLY:H      | 5:M:607:ASP:CG    | 2.12                     | 0.57              |
| 5:M:205:GLU:HA    | 5:M:209:ARG:CZ    | 2.34                     | 0.57              |
| 6:N:758:GLU:HA    | 7:O:20:THR:HG21   | 1.86                     | 0.57              |
| 6:N:1083:ASP:O    | 6:N:1087:ARG:HG2  | 2.05                     | 0.57              |
| 6:N:1191:PRO:HG3  | 11:N:9238:HOH:O   | 2.03                     | 0.57              |
| 6:N:1336:LEU:HA   | 6:N:1344:VAL:CG2  | 2.34                     | 0.57              |
| 1:G:13:DT:H5''    | 6:D:1093:TYR:HE2  | 1.68                     | 0.57              |
| 2:Y:11:C:H2'      | 2:Y:12:G:H8       | 1.66                     | 0.57              |
| 4:A:100:LEU:HD22  | 4:A:102:LYS:HE2   | 1.87                     | 0.57              |
| 4:A:221:HIS:HB3   | 4:B:36:LEU:HD21   | 1.86                     | 0.57              |
| 4:B:85:LEU:HG     | 4:B:127:LEU:CD2   | 2.32                     | 0.57              |
| 5:C:971:LYS:HD2   | 5:C:986:PRO:HG2   | 1.87                     | 0.57              |
| 6:D:1020:LEU:HD21 | 6:D:1038:LEU:HD12 | 1.86                     | 0.57              |
| 6:D:1103:HIS:CD2  | 6:D:1463:LYS:HB2  | 2.40                     | 0.57              |
| 6:D:1168:MET:HA   | 6:D:1168:MET:HE3  | 1.87                     | 0.57              |
| 6:D:1263:PHE:HE2  | 6:D:1371:VAL:HG11 | 1.69                     | 0.57              |
| 4:L:214:ALA:O     | 4:L:217:ILE:HG22  | 2.04                     | 0.57              |
| 5:M:567:GLN:O     | 5:M:997:LEU:HD12  | 2.05                     | 0.57              |
| 6:N:139:GLY:HA2   | 6:N:451:ASP:O     | 2.05                     | 0.57              |
| 6:N:1129:THR:HG23 | 6:N:1130:ARG:H    | 1.69                     | 0.57              |
| 4:A:68:ILE:H      | 4:A:68:ILE:HD12   | 1.69                     | 0.57              |
| 5:C:188:LYS:HD3   | 11:C:1301:HOH:O   | 2.03                     | 0.57              |
| 5:C:834:GLN:HB2   | 11:C:1129:HOH:O   | 2.04                     | 0.57              |
| 6:D:1216:SER:CB   | 7:E:16:LYS:H      | 2.18                     | 0.57              |
| 6:D:1224:VAL:HA   | 6:D:1227:GLN:OE1  | 2.05                     | 0.57              |
| 6:D:1332:PRO:HG3  | 6:D:1347:TYR:CE2  | 2.37                     | 0.57              |
| 6:D:1335:LEU:HD22 | 6:D:1344:VAL:HG13 | 1.86                     | 0.57              |
| 6:D:1485:GLN:HE21 | 7:E:79:LEU:H      | 1.51                     | 0.57              |
| 4:K:138:LEU:HD11  | 4:K:140:MET:SD    | 2.44                     | 0.57              |
| 4:L:124:ASN:OD1   | 4:L:127:LEU:HB2   | 2.05                     | 0.57              |
| 5:M:208:ALA:HB3   | 5:M:209:ARG:HH21  | 1.70                     | 0.57              |
| 5:M:498:GLN:OE1   | 6:N:1067:VAL:HB   | 2.05                     | 0.57              |
| 5:M:693:GLU:HA    | 5:M:696:LYS:CD    | 2.34                     | 0.57              |
| 5:M:1046:ALA:HB2  | 11:N:9022:HOH:O   | 2.03                     | 0.57              |
| 6:N:1023:MET:O    | 6:N:1028:ALA:HB3  | 2.05                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:1153:VAL:HG12 | 6:N:1155:VAL:HG13 | 1.86                     | 0.57              |
| 1:X:19:DC:H5''    | 5:M:1001:VAL:HB   | 1.87                     | 0.57              |
| 5:C:144:PRO:CG    | 5:C:265:ARG:HH21  | 2.13                     | 0.57              |
| 5:C:192:PRO:HD2   | 5:C:195:LEU:CB    | 2.32                     | 0.57              |
| 5:C:472:ARG:HG3   | 5:C:534:VAL:HG22  | 1.85                     | 0.57              |
| 5:C:1049:LEU:HD11 | 5:C:1053:LEU:HD11 | 1.87                     | 0.57              |
| 5:C:1103:ASP:OD1  | 6:D:3:LYS:HD3     | 2.05                     | 0.57              |
| 6:D:1271:LYS:HZ1  | 6:D:1331:ASP:HB3  | 1.70                     | 0.57              |
| 5:M:162:ILE:O     | 5:M:164:PRO:HD3   | 2.05                     | 0.57              |
| 5:M:691:SER:OG    | 5:M:694:LEU:HG    | 2.04                     | 0.57              |
| 6:N:434:ARG:HB3   | 6:N:434:ARG:HH11  | 1.70                     | 0.57              |
| 2:Y:7:G:C8        | 2:Y:7:G:C5'       | 2.88                     | 0.57              |
| 4:B:88:ARG:HG3    | 11:B:365:HOH:O    | 2.04                     | 0.57              |
| 5:C:51:THR:OG1    | 5:C:348:LEU:HG    | 2.05                     | 0.57              |
| 5:C:531:PHE:HB2   | 11:C:1172:HOH:O   | 2.05                     | 0.57              |
| 5:C:975:TYR:HA    | 5:C:982:PRO:HA    | 1.86                     | 0.57              |
| 6:D:65:ARG:CG     | 6:D:66:GLN:H      | 2.18                     | 0.57              |
| 6:D:657:LEU:HD22  | 6:D:691:LEU:CD2   | 2.35                     | 0.57              |
| 6:D:1406:ARG:HD2  | 6:D:1412:LYS:HZ3  | 1.70                     | 0.57              |
| 4:K:42:ARG:CZ     | 4:L:34:VAL:HB     | 2.35                     | 0.57              |
| 4:L:79:ILE:HA     | 4:L:82:LEU:HD12   | 1.87                     | 0.57              |
| 5:M:174:LEU:HD22  | 5:M:307:LEU:HD13  | 1.87                     | 0.57              |
| 5:M:400:PRO:HG2   | 5:M:593:ALA:HB2   | 1.87                     | 0.57              |
| 5:M:1085:PHE:O    | 5:M:1089:VAL:HG23 | 2.05                     | 0.57              |
| 6:N:54:LYS:CD     | 6:N:55:ASP:H      | 2.17                     | 0.57              |
| 6:N:161:LEU:HD13  | 6:N:452:ILE:HD13  | 1.87                     | 0.57              |
| 6:N:1025:GLN:NE2  | 6:N:1025:GLN:HA   | 2.20                     | 0.57              |
| 7:O:17:TYR:O      | 7:O:21:VAL:HG23   | 2.05                     | 0.57              |
| 5:C:949:LYS:HA    | 11:C:1221:HOH:O   | 2.05                     | 0.56              |
| 4:K:73:GLU:CD     | 4:K:130:ALA:HA    | 2.30                     | 0.56              |
| 5:M:286:SER:HB3   | 11:M:1441:HOH:O   | 2.05                     | 0.56              |
| 5:M:578:VAL:CG2   | 5:M:579:VAL:HG12  | 2.34                     | 0.56              |
| 5:M:871:LEU:HD11  | 5:M:992:MET:SD    | 2.44                     | 0.56              |
| 5:M:1050:GLN:OE1  | 6:N:1471:LEU:HA   | 2.04                     | 0.56              |
| 6:N:1045:MET:HB3  | 6:N:1073:SER:HA   | 1.87                     | 0.56              |
| 6:N:1057:VAL:HG13 | 6:N:1069:GLU:HB3  | 1.87                     | 0.56              |
| 7:O:41:GLU:HB2    | 7:O:45:ARG:NE     | 2.19                     | 0.56              |
| 1:G:22:DC:H4'     | 5:C:388:ARG:CD    | 2.33                     | 0.56              |
| 2:Y:8:C:H5'       | 11:Y:1683:HOH:O   | 2.04                     | 0.56              |
| 4:A:52:ALA:HB2    | 4:A:170:VAL:O     | 2.04                     | 0.56              |
| 4:A:225:PHE:HB2   | 11:A:325:HOH:O    | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:338:GLU:O     | 5:C:341:THR:HG22  | 2.05                     | 0.56              |
| 5:C:957:LYS:HD3   | 5:C:961:GLU:CD    | 2.30                     | 0.56              |
| 6:D:1436:SER:HB3  | 11:D:8024:HOH:O   | 2.05                     | 0.56              |
| 7:E:19:LEU:O      | 7:E:23:VAL:HG23   | 2.05                     | 0.56              |
| 4:L:43:ILE:O      | 4:L:47:SER:HB3    | 2.05                     | 0.56              |
| 5:M:292:ARG:HH11  | 5:M:299:LYS:HD3   | 1.70                     | 0.56              |
| 5:M:805:ARG:HB3   | 5:M:805:ARG:HH11  | 1.70                     | 0.56              |
| 6:N:714:GLN:NE2   | 6:N:765:SER:HA    | 2.20                     | 0.56              |
| 6:N:1091:SER:OG   | 6:N:1234:THR:HG23 | 2.04                     | 0.56              |
| 1:X:2:DC:H2"      | 1:X:3:DC:C6       | 2.40                     | 0.56              |
| 4:B:201:THR:HG21  | 4:B:205:VAL:HG23  | 1.87                     | 0.56              |
| 5:C:148:PHE:CZ    | 5:C:281:LEU:HB3   | 2.39                     | 0.56              |
| 5:C:159:ILE:HD13  | 11:C:1523:HOH:O   | 2.06                     | 0.56              |
| 5:C:186:VAL:HG11  | 11:C:1130:HOH:O   | 2.05                     | 0.56              |
| 5:C:412:ALA:HB1   | 5:C:419:THR:HG21  | 1.87                     | 0.56              |
| 5:C:676:ILE:HD13  | 6:D:948:THR:HB    | 1.88                     | 0.56              |
| 5:C:943:VAL:HG23  | 5:C:985:GLY:H     | 1.70                     | 0.56              |
| 5:C:1018:GLN:C    | 5:C:1019:GLN:HE21 | 2.14                     | 0.56              |
| 6:D:136:ASP:HB3   | 6:D:455:ARG:HE    | 1.70                     | 0.56              |
| 6:D:696:HIS:NE2   | 7:E:54:LEU:HD11   | 2.20                     | 0.56              |
| 6:D:703:ASN:ND2   | 6:D:704:ARG:H     | 2.03                     | 0.56              |
| 6:D:758:GLU:HA    | 6:D:762:GLN:NE2   | 2.20                     | 0.56              |
| 6:D:1042:ARG:O    | 6:D:1057:VAL:HB   | 2.04                     | 0.56              |
| 6:D:1226:ALA:HB2  | 11:D:8257:HOH:O   | 2.05                     | 0.56              |
| 6:D:1236:LEU:HD11 | 6:D:1361:VAL:HG23 | 1.88                     | 0.56              |
| 7:E:41:GLU:HG2    | 7:E:42:PRO:HD3    | 1.87                     | 0.56              |
| 7:E:59:ASN:HD22   | 7:E:59:ASN:N      | 2.02                     | 0.56              |
| 7:E:80:VAL:HG22   | 11:E:151:HOH:O    | 2.06                     | 0.56              |
| 4:L:92:PRO:HA     | 4:L:146:ARG:NH2   | 2.20                     | 0.56              |
| 4:L:92:PRO:HA     | 4:L:146:ARG:CZ    | 2.35                     | 0.56              |
| 5:M:39:ARG:HH11   | 5:M:39:ARG:HG3    | 1.68                     | 0.56              |
| 5:M:257:VAL:HA    | 11:M:1334:HOH:O   | 2.04                     | 0.56              |
| 5:M:546:LEU:HD12  | 5:M:565:GLN:NE2   | 2.18                     | 0.56              |
| 5:M:886:LEU:HD12  | 6:N:951:ILE:HG13  | 1.87                     | 0.56              |
| 5:M:1054:THR:HG21 | 5:M:1079:PRO:HB3  | 1.87                     | 0.56              |
| 6:N:80:VAL:HG12   | 6:N:81:THR:O      | 2.05                     | 0.56              |
| 6:N:794:GLN:HG3   | 6:N:795:VAL:N     | 2.20                     | 0.56              |
| 6:N:799:LYS:HE2   | 6:N:824:ASN:O     | 2.04                     | 0.56              |
| 6:N:806:PHE:HE1   | 6:N:813:LEU:HB3   | 1.69                     | 0.56              |
| 6:N:828:LYS:HG2   | 6:N:863:VAL:HG22  | 1.86                     | 0.56              |
| 6:N:1189:ARG:HD2  | 6:N:1204:CYS:SG   | 2.46                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:N:1238:MET:HA  | 6:N:1241:PHE:CE2  | 2.40                     | 0.56              |
| 6:N:1493:LYS:O   | 6:N:1496:GLU:HG2  | 2.04                     | 0.56              |
| 7:O:13:VAL:HG21  | 7:O:19:LEU:HB2    | 1.88                     | 0.56              |
| 7:O:84:ARG:HD3   | 11:O:1385:HOH:O   | 2.05                     | 0.56              |
| 4:A:42:ARG:NH2   | 4:B:34:VAL:HB     | 2.20                     | 0.56              |
| 4:B:160:ASP:HB3  | 11:B:345:HOH:O    | 2.05                     | 0.56              |
| 5:C:333:ILE:HD13 | 5:C:467:ILE:HG13  | 1.86                     | 0.56              |
| 5:C:577:PRO:HA   | 5:C:671:ASN:ND2   | 2.20                     | 0.56              |
| 5:C:838:LYS:O    | 5:C:839:LEU:HD23  | 2.06                     | 0.56              |
| 6:D:65:ARG:H     | 6:D:68:PHE:HE1    | 1.51                     | 0.56              |
| 6:D:116:LEU:HD11 | 6:D:464:LEU:HB3   | 1.86                     | 0.56              |
| 6:D:117:ASP:N    | 6:D:150:ARG:NH1   | 2.53                     | 0.56              |
| 6:D:700:VAL:HG22 | 6:D:718:PRO:HG3   | 1.87                     | 0.56              |
| 6:D:754:PHE:HE1  | 7:E:28:GLN:HE22   | 1.53                     | 0.56              |
| 6:D:847:ASP:O    | 6:D:851:LEU:HG    | 2.06                     | 0.56              |
| 4:L:187:GLY:HA3  | 11:L:397:HOH:O    | 2.05                     | 0.56              |
| 5:M:48:PHE:O     | 5:M:52:PHE:HB2    | 2.05                     | 0.56              |
| 5:M:532:MET:HB3  | 11:M:1310:HOH:O   | 2.04                     | 0.56              |
| 5:M:611:ILE:HG13 | 5:M:625:LEU:HD21  | 1.87                     | 0.56              |
| 5:M:668:LEU:HD13 | 5:M:995:MET:HE2   | 1.87                     | 0.56              |
| 5:M:928:LYS:HZ2  | 5:M:932:GLU:HG3   | 1.71                     | 0.56              |
| 6:N:47:GLU:OE1   | 6:N:53:ILE:HB     | 2.06                     | 0.56              |
| 6:N:704:ARG:HD3  | 6:N:738:ALA:HB2   | 1.87                     | 0.56              |
| 6:N:988:ARG:O    | 6:N:992:ILE:HG13  | 2.05                     | 0.56              |
| 6:N:1271:LYS:NZ  | 6:N:1331:ASP:HB2  | 2.20                     | 0.56              |
| 1:G:16:DG:H5''   | 5:C:1031:ARG:HB3  | 1.88                     | 0.56              |
| 4:A:54:THR:HB    | 4:A:143:ARG:CG    | 2.35                     | 0.56              |
| 4:B:16:GLN:HG3   | 11:B:397:HOH:O    | 2.05                     | 0.56              |
| 5:C:284:ARG:HG3  | 5:C:285:LEU:N     | 2.19                     | 0.56              |
| 6:D:29:PRO:HG3   | 6:D:549:ASN:HD21  | 1.69                     | 0.56              |
| 6:D:117:ASP:HB2  | 6:D:495:ARG:HH21  | 1.69                     | 0.56              |
| 6:D:1267:ARG:O   | 6:D:1267:ARG:HG2  | 2.05                     | 0.56              |
| 5:M:457:ALA:N    | 5:M:540:PHE:O     | 2.36                     | 0.56              |
| 5:M:577:PRO:HG3  | 5:M:993:PHE:CE1   | 2.41                     | 0.56              |
| 6:N:119:SER:HB2  | 6:N:123:LEU:CB    | 2.33                     | 0.56              |
| 6:N:792:ILE:O    | 6:N:878:GLY:HA3   | 2.04                     | 0.56              |
| 6:N:1336:LEU:HA  | 6:N:1344:VAL:HG21 | 1.86                     | 0.56              |
| 2:H:11:C:O2'     | 2:H:12:G:H5''     | 2.05                     | 0.56              |
| 1:X:14:DT:H6     | 1:X:14:DT:H5'     | 1.70                     | 0.56              |
| 2:Y:14:G:HO2'    | 2:Y:15:C:H5'      | 1.69                     | 0.56              |
| 4:B:117:VAL:HG22 | 11:B:392:HOH:O    | 2.06                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:12:VAL:HG13   | 5:C:13:ILE:CG1    | 2.36                     | 0.56              |
| 5:C:141:HIS:C     | 5:C:331:ARG:HG2   | 2.31                     | 0.56              |
| 5:C:232:GLU:O     | 5:C:235:LEU:HB3   | 2.05                     | 0.56              |
| 5:C:437:ARG:HA    | 5:C:467:ILE:HG21  | 1.86                     | 0.56              |
| 5:C:693:GLU:HA    | 5:C:696:LYS:HG3   | 1.88                     | 0.56              |
| 5:C:697:ARG:O     | 5:C:699:PHE:N     | 2.39                     | 0.56              |
| 5:C:804:VAL:HG11  | 5:C:824:ARG:NH2   | 2.19                     | 0.56              |
| 6:D:964:LEU:HD22  | 6:D:1058:ARG:HH21 | 1.70                     | 0.56              |
| 4:K:92:PRO:HD3    | 11:K:1047:HOH:O   | 2.05                     | 0.56              |
| 4:K:178:ALA:HB2   | 5:M:864:GLY:N     | 2.21                     | 0.56              |
| 4:K:206:THR:HG23  | 4:K:207:PRO:HD2   | 1.88                     | 0.56              |
| 5:M:307:LEU:HD12  | 5:M:310:LEU:HD23  | 1.87                     | 0.56              |
| 5:M:600:ASP:OD1   | 5:M:651:LYS:HB2   | 2.05                     | 0.56              |
| 5:M:626:ARG:HH22  | 5:M:637:LEU:HD13  | 1.70                     | 0.56              |
| 11:M:1366:HOH:O   | 6:N:6:ARG:HB2     | 2.04                     | 0.56              |
| 6:N:180:LYS:H     | 6:N:180:LYS:HD2   | 1.69                     | 0.56              |
| 6:N:853:VAL:HG11  | 6:N:860:LEU:HG    | 1.88                     | 0.56              |
| 6:N:960:LYS:NZ    | 6:N:1041:LEU:HD13 | 2.21                     | 0.56              |
| 5:C:265:ARG:NH1   | 5:C:267:TYR:HB3   | 2.20                     | 0.56              |
| 5:C:1105:LYS:HZ3  | 5:C:1107:ASN:HB2  | 1.70                     | 0.56              |
| 6:D:1124:GLN:HG2  | 6:D:1133:ARG:HG3  | 1.88                     | 0.56              |
| 5:M:516:ARG:HE    | 6:N:1068:LEU:HD13 | 1.69                     | 0.56              |
| 5:M:516:ARG:HH21  | 6:N:1068:LEU:HB3  | 1.71                     | 0.56              |
| 5:M:1070:ILE:HG21 | 6:N:655:PRO:HB2   | 1.88                     | 0.56              |
| 6:N:24:GLY:HA3    | 6:N:49:ILE:HG12   | 1.87                     | 0.56              |
| 5:C:162:ILE:HD12  | 5:C:172:ILE:HB    | 1.86                     | 0.56              |
| 5:C:265:ARG:HD2   | 5:C:267:TYR:HB3   | 1.88                     | 0.56              |
| 5:C:334:ARG:HG2   | 5:C:338:GLU:CD    | 2.31                     | 0.56              |
| 5:C:654:LEU:HD13  | 5:C:664:GLY:N     | 2.21                     | 0.56              |
| 5:C:842:ARG:HG3   | 5:C:995:MET:HE2   | 1.87                     | 0.56              |
| 6:D:116:LEU:HD13  | 6:D:118:LEU:HD11  | 1.87                     | 0.56              |
| 6:D:703:ASN:HD22  | 6:D:704:ARG:H     | 1.53                     | 0.56              |
| 6:D:906:GLN:HB3   | 6:D:911:LEU:HD11  | 1.88                     | 0.56              |
| 6:D:1091:SER:HB3  | 6:D:1234:THR:OG1  | 2.05                     | 0.56              |
| 6:D:1102:THR:HB   | 11:D:8257:HOH:O   | 2.04                     | 0.56              |
| 7:E:30:LEU:O      | 7:E:35:PHE:HA     | 2.06                     | 0.56              |
| 4:L:101:LEU:HA    | 11:L:368:HOH:O    | 2.06                     | 0.56              |
| 5:M:260:LEU:HB2   | 11:M:1400:HOH:O   | 2.05                     | 0.56              |
| 5:M:695:LEU:HD11  | 11:M:1250:HOH:O   | 2.05                     | 0.56              |
| 6:N:883:ALA:HB2   | 11:N:9040:HOH:O   | 2.04                     | 0.56              |
| 3:I:3:DA:H3'      | 11:I:500:HOH:O    | 2.05                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:B:124:ASN:ND2   | 4:B:127:LEU:HD22 | 2.21                     | 0.56              |
| 5:C:410:ILE:HD12  | 5:C:438:ILE:HG13 | 1.88                     | 0.56              |
| 5:C:439:CYS:HB2   | 5:C:541:SER:HB2  | 1.87                     | 0.56              |
| 5:C:897:LEU:HD23  | 5:C:924:VAL:HG21 | 1.88                     | 0.56              |
| 6:D:28:LYS:HB2    | 6:D:41:ARG:NH1   | 2.19                     | 0.56              |
| 6:D:714:GLN:NE2   | 6:D:765:SER:HA   | 2.20                     | 0.56              |
| 7:E:27:ALA:CB     | 7:E:61:VAL:HG12  | 2.35                     | 0.56              |
| 7:E:40:LEU:HB3    | 7:E:72:ARG:HH21  | 1.68                     | 0.56              |
| 7:E:58:PRO:C      | 7:E:59:ASN:HD22  | 2.13                     | 0.56              |
| 4:L:197:LEU:HD23  | 4:L:199:ILE:HG13 | 1.87                     | 0.56              |
| 5:M:290:LEU:HB3   | 5:M:302:VAL:HG12 | 1.88                     | 0.56              |
| 5:M:1034:GLU:H    | 6:N:619:LEU:HD13 | 1.71                     | 0.56              |
| 6:N:150:ARG:HD3   | 6:N:464:LEU:HD21 | 1.88                     | 0.56              |
| 6:N:482:LYS:HE2   | 6:N:1384:PRO:HG2 | 1.88                     | 0.56              |
| 6:N:879:ARG:HH21  | 6:N:903:ASP:C    | 2.13                     | 0.56              |
| 6:N:1353:GLN:HB3  | 6:N:1357:ARG:HE  | 1.70                     | 0.56              |
| 2:Y:8:C:H6        | 2:Y:8:C:O5'      | 1.89                     | 0.56              |
| 5:C:233:GLU:HB3   | 11:C:1182:HOH:O  | 2.06                     | 0.56              |
| 5:C:358:ARG:HA    | 5:C:361:MET:HG2  | 1.87                     | 0.56              |
| 5:C:474:VAL:HG12  | 5:C:531:PHE:HA   | 1.88                     | 0.56              |
| 5:C:578:VAL:HG13  | 5:C:671:ASN:CB   | 2.29                     | 0.56              |
| 5:C:680:ASP:HB2   | 5:C:682:TYR:CE2  | 2.40                     | 0.56              |
| 6:D:129:PHE:C     | 6:D:568:ARG:HH21 | 2.14                     | 0.56              |
| 6:D:1222:GLY:O    | 6:D:1225:ALA:HB3 | 2.06                     | 0.56              |
| 5:M:569:VAL:HG12  | 5:M:996:LYS:O    | 2.07                     | 0.56              |
| 5:M:1057:SER:HB2  | 6:N:622:ARG:O    | 2.05                     | 0.56              |
| 6:N:783:ARG:CA    | 6:N:1028:ALA:HA  | 2.26                     | 0.56              |
| 7:O:13:VAL:HG13   | 7:O:75:PHE:CZ    | 2.41                     | 0.56              |
| 7:O:27:ALA:CB     | 7:O:61:VAL:HG12  | 2.35                     | 0.56              |
| 7:O:54:LEU:HG     | 7:O:58:PRO:HG2   | 1.88                     | 0.56              |
| 5:C:150:PRO:HA    | 5:C:158:TYR:HB3  | 1.89                     | 0.55              |
| 5:C:166:PRO:HD2   | 5:C:263:ASP:O    | 2.06                     | 0.55              |
| 6:D:710:ARG:CG    | 6:D:772:PRO:HG2  | 2.34                     | 0.55              |
| 6:D:957:PRO:CG    | 6:D:1007:VAL:HA  | 2.36                     | 0.55              |
| 6:D:1197:ARG:HB3  | 6:D:1396:GLU:CG  | 2.36                     | 0.55              |
| 6:D:1209:LEU:HD11 | 7:E:16:LYS:HD2   | 1.88                     | 0.55              |
| 6:D:1336:LEU:HD22 | 6:D:1421:LEU:HB2 | 1.87                     | 0.55              |
| 7:E:31:LEU:HD21   | 7:E:60:ALA:HB2   | 1.88                     | 0.55              |
| 4:K:32:PHE:O      | 4:K:36:LEU:HG    | 2.05                     | 0.55              |
| 4:L:59:GLU:CG     | 4:L:137:ARG:HH22 | 2.18                     | 0.55              |
| 4:L:101:LEU:HD11  | 4:L:113:ASP:HB3  | 1.89                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:M:102:HIS:HE2  | 5:M:365:ASP:HA    | 1.71                     | 0.55              |
| 5:M:697:ARG:O    | 5:M:699:PHE:N     | 2.38                     | 0.55              |
| 6:N:165:LYS:HG2  | 6:N:448:GLU:OE2   | 2.06                     | 0.55              |
| 6:N:1121:PRO:CD  | 6:N:1346:ARG:HH21 | 2.14                     | 0.55              |
| 2:Y:9:G:H5'      | 2:Y:9:G:C8        | 2.41                     | 0.55              |
| 5:C:267:TYR:HB2  | 5:C:272:ALA:CB    | 2.37                     | 0.55              |
| 5:C:328:LEU:C    | 5:C:488:ALA:HB3   | 2.30                     | 0.55              |
| 5:C:676:ILE:HG21 | 5:C:988:VAL:HG13  | 1.88                     | 0.55              |
| 5:C:850:ALA:HA   | 6:D:632:VAL:HG11  | 1.87                     | 0.55              |
| 5:C:965:GLU:O    | 5:C:969:GLN:HG2   | 2.05                     | 0.55              |
| 5:C:1016:ILE:H   | 5:C:1016:ILE:CD1  | 2.16                     | 0.55              |
| 5:C:1020:PRO:O   | 5:C:1021:LEU:HD12 | 2.07                     | 0.55              |
| 6:D:114:THR:HG22 | 6:D:495:ARG:HA    | 1.87                     | 0.55              |
| 6:D:462:GLN:HG2  | 6:D:466:LYS:NZ    | 2.21                     | 0.55              |
| 6:D:700:VAL:HG12 | 6:D:749:VAL:HG12  | 1.88                     | 0.55              |
| 6:D:804:LEU:HD23 | 6:D:804:LEU:H     | 1.71                     | 0.55              |
| 4:K:112:ARG:HG2  | 4:K:125:PRO:CB    | 2.37                     | 0.55              |
| 5:M:946:ARG:HB3  | 5:M:946:ARG:NH1   | 2.07                     | 0.55              |
| 6:N:120:ALA:HB2  | 11:N:9298:HOH:O   | 2.07                     | 0.55              |
| 6:N:834:THR:HG22 | 6:N:838:ARG:NH1   | 2.21                     | 0.55              |
| 6:N:1016:PRO:HB3 | 11:N:9351:HOH:O   | 2.04                     | 0.55              |
| 6:N:1258:ARG:NH1 | 6:N:1268:PRO:HB3  | 2.16                     | 0.55              |
| 4:B:30:ARG:HH22  | 5:C:854:PRO:CG    | 2.20                     | 0.55              |
| 4:B:48:ILE:HG13  | 11:B:331:HOH:O    | 2.07                     | 0.55              |
| 5:C:92:ALA:HB2   | 5:C:120:LEU:HD11  | 1.87                     | 0.55              |
| 5:C:472:ARG:HG2  | 5:C:483:VAL:HG22  | 1.88                     | 0.55              |
| 5:C:759:THR:HB   | 5:C:785:VAL:CG1   | 2.33                     | 0.55              |
| 6:D:473:LEU:O    | 6:D:477:LEU:HG    | 2.06                     | 0.55              |
| 6:D:808:THR:OG1  | 6:D:809:PRO:HD3   | 2.07                     | 0.55              |
| 4:L:58:ILE:HG22  | 4:L:61:VAL:H      | 1.71                     | 0.55              |
| 5:M:134:ARG:HD3  | 5:M:392:SER:HB3   | 1.86                     | 0.55              |
| 5:M:173:ASP:HB2  | 5:M:185:LYS:NZ    | 2.22                     | 0.55              |
| 5:M:943:VAL:HG23 | 5:M:985:GLY:H     | 1.72                     | 0.55              |
| 6:N:402:PRO:HA   | 6:N:443:VAL:HG23  | 1.88                     | 0.55              |
| 6:N:1165:TYR:CE2 | 6:N:1214:PRO:HB3  | 2.42                     | 0.55              |
| 4:A:183:ASP:HB3  | 11:A:321:HOH:O    | 2.07                     | 0.55              |
| 4:B:30:ARG:HH22  | 5:C:854:PRO:HG2   | 1.72                     | 0.55              |
| 5:C:136:ILE:CG2  | 5:C:336:VAL:HG22  | 2.36                     | 0.55              |
| 5:C:401:LEU:HD21 | 5:C:565:GLN:HE21  | 1.71                     | 0.55              |
| 5:C:527:GLU:OE1  | 5:C:528:GLU:HG3   | 2.06                     | 0.55              |
| 5:C:780:GLU:HG2  | 11:C:1242:HOH:O   | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:887:ALA:HB3   | 11:D:8116:HOH:O   | 2.06                     | 0.55              |
| 6:D:1007:VAL:HG12 | 6:D:1011:PHE:CE2  | 2.40                     | 0.55              |
| 4:K:57:TYR:CE2    | 4:K:59:GLU:HA     | 2.41                     | 0.55              |
| 4:K:72:LYS:HE3    | 5:M:641:PRO:O     | 2.06                     | 0.55              |
| 5:M:115:LEU:O     | 5:M:115:LEU:HD12  | 2.06                     | 0.55              |
| 5:M:138:SER:HB3   | 5:M:333:ILE:HG23  | 1.88                     | 0.55              |
| 5:M:265:ARG:HB3   | 5:M:267:TYR:CD2   | 2.42                     | 0.55              |
| 5:M:671:ASN:N     | 5:M:671:ASN:ND2   | 2.50                     | 0.55              |
| 5:M:975:TYR:HA    | 5:M:982:PRO:HA    | 1.89                     | 0.55              |
| 6:N:710:ARG:C     | 6:N:712:GLY:H     | 2.14                     | 0.55              |
| 5:C:5:ARG:NE      | 5:C:8:ARG:HH12    | 2.00                     | 0.55              |
| 5:C:139:GLN:O     | 5:C:333:ILE:HA    | 2.07                     | 0.55              |
| 5:C:176:VAL:C     | 5:C:178:PRO:HD3   | 2.31                     | 0.55              |
| 6:D:117:ASP:H     | 6:D:150:ARG:HH12  | 1.55                     | 0.55              |
| 6:D:136:ASP:OD1   | 6:D:463:GLN:HB3   | 2.05                     | 0.55              |
| 5:M:285:LEU:HD23  | 5:M:285:LEU:O     | 2.06                     | 0.55              |
| 5:M:987:ILE:HG12  | 6:N:948:THR:HG21  | 1.88                     | 0.55              |
| 6:N:787:LEU:HD21  | 6:N:1023:MET:HE2  | 1.88                     | 0.55              |
| 6:N:1209:LEU:HG   | 6:N:1219:GLU:OE1  | 2.07                     | 0.55              |
| 6:N:1335:LEU:CD2  | 6:N:1344:VAL:HG22 | 2.27                     | 0.55              |
| 1:X:17:DC:H2''    | 1:X:18:DG:C5'     | 2.37                     | 0.55              |
| 4:A:153:ALA:HA    | 4:A:156:HIS:NE2   | 2.22                     | 0.55              |
| 4:B:41:ARG:HD2    | 4:B:177:VAL:CG2   | 2.37                     | 0.55              |
| 5:C:431:HIS:NE2   | 5:C:432:ARG:HB2   | 2.22                     | 0.55              |
| 5:C:1045:ALA:HB1  | 5:C:1048:THR:HB   | 1.89                     | 0.55              |
| 6:D:112:ILE:HB    | 6:D:512:MET:SD    | 2.46                     | 0.55              |
| 6:D:794:GLN:HB3   | 6:D:1017:PHE:HZ   | 1.72                     | 0.55              |
| 6:D:801:GLY:HA2   | 11:D:8362:HOH:O   | 2.06                     | 0.55              |
| 5:M:433:THR:CG2   | 5:M:488:ALA:HB1   | 2.35                     | 0.55              |
| 5:M:626:ARG:HH12  | 5:M:637:LEU:CB    | 2.17                     | 0.55              |
| 6:N:52:PRO:HD2    | 6:N:85:VAL:CG2    | 2.32                     | 0.55              |
| 6:N:116:LEU:HD21  | 6:N:464:LEU:HD22  | 1.88                     | 0.55              |
| 6:N:119:SER:N     | 6:N:123:LEU:HD22  | 2.17                     | 0.55              |
| 6:N:161:LEU:HD22  | 6:N:452:ILE:HG21  | 1.87                     | 0.55              |
| 6:N:827:ILE:HD12  | 6:N:827:ILE:H     | 1.72                     | 0.55              |
| 6:N:957:PRO:HG2   | 6:N:1007:VAL:HG22 | 1.87                     | 0.55              |
| 6:N:1027:GLY:HA2  | 11:N:9239:HOH:O   | 2.06                     | 0.55              |
| 6:N:1105:ILE:HD13 | 11:N:9367:HOH:O   | 2.05                     | 0.55              |
| 1:G:18:DG:H5'     | 1:G:18:DG:H8      | 1.72                     | 0.55              |
| 5:C:140:ILE:CG2   | 5:C:333:ILE:HG13  | 2.34                     | 0.55              |
| 5:C:141:HIS:HA    | 11:C:1222:HOH:O   | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:411:SER:OG    | 5:C:413:LEU:HD12  | 2.07                     | 0.55              |
| 5:C:949:LYS:HD3   | 6:D:796:ARG:NH2   | 2.19                     | 0.55              |
| 6:D:554:LEU:HD21  | 6:D:571:LYS:CE    | 2.36                     | 0.55              |
| 4:K:72:LYS:HG3    | 5:M:641:PRO:HB2   | 1.87                     | 0.55              |
| 4:K:177:VAL:O     | 5:M:864:GLY:CA    | 2.55                     | 0.55              |
| 4:K:181:VAL:HG21  | 5:M:939:ARG:NH1   | 2.20                     | 0.55              |
| 4:L:205:VAL:HG11  | 11:L:322:HOH:O    | 2.05                     | 0.55              |
| 5:M:141:HIS:CB    | 5:M:418:LEU:HD23  | 2.33                     | 0.55              |
| 5:M:660:ALA:HB1   | 5:M:667:ALA:O     | 2.06                     | 0.55              |
| 5:M:719:PRO:HB2   | 11:M:1137:HOH:O   | 2.07                     | 0.55              |
| 5:M:730:SER:O     | 5:M:734:LEU:HD13  | 2.07                     | 0.55              |
| 5:M:752:GLY:O     | 6:N:679:ARG:HG2   | 2.06                     | 0.55              |
| 5:M:1067:TYR:CE1  | 5:M:1071:ILE:HD11 | 2.41                     | 0.55              |
| 6:N:18:ILE:CG2    | 6:N:518:PRO:HG3   | 2.22                     | 0.55              |
| 6:N:43:GLY:N      | 11:N:9087:HOH:O   | 2.40                     | 0.55              |
| 6:N:137:PRO:HB2   | 6:N:138:LYS:HD3   | 1.89                     | 0.55              |
| 4:A:206:THR:HG23  | 4:A:208:LEU:H     | 1.72                     | 0.55              |
| 4:B:55:SER:OG     | 4:B:143:ARG:HD3   | 2.06                     | 0.55              |
| 5:C:290:LEU:HB3   | 5:C:302:VAL:HG12  | 1.88                     | 0.55              |
| 5:C:397:GLU:OE2   | 5:C:633:GLN:HG2   | 2.07                     | 0.55              |
| 5:C:433:THR:C     | 5:C:435:TYR:H     | 2.15                     | 0.55              |
| 5:C:437:ARG:NE    | 5:C:469:THR:HB    | 2.20                     | 0.55              |
| 5:C:753:ASP:O     | 5:C:792:VAL:HG23  | 2.07                     | 0.55              |
| 6:D:119:SER:N     | 6:D:123:LEU:HD22  | 2.18                     | 0.55              |
| 6:D:1147:ARG:HB3  | 6:D:1188:VAL:CG2  | 2.37                     | 0.55              |
| 6:D:1441:GLN:CD   | 6:D:1442:ASN:HB2  | 2.31                     | 0.55              |
| 6:D:1495:ILE:HG22 | 6:D:1499:ARG:HE   | 1.72                     | 0.55              |
| 4:K:5:LYS:O       | 4:K:8:ALA:HB2     | 2.07                     | 0.55              |
| 4:K:150:TYR:CE2   | 4:K:152:PRO:HG3   | 2.42                     | 0.55              |
| 4:K:161:ARG:HA    | 11:K:728:HOH:O    | 2.07                     | 0.55              |
| 5:M:1022:GLY:HA3  | 5:M:1026:GLN:O    | 2.07                     | 0.55              |
| 5:M:1098:ASP:HB2  | 6:N:21:TRP:CZ2    | 2.42                     | 0.55              |
| 6:N:123:LEU:O     | 6:N:126:VAL:HB    | 2.07                     | 0.55              |
| 6:N:183:GLU:HG2   | 6:N:184:GLU:N     | 2.21                     | 0.55              |
| 6:N:737:ASN:ND2   | 10:N:4999:APC:O3' | 2.37                     | 0.55              |
| 6:N:840:LYS:HE2   | 6:N:841:TYR:CE2   | 2.42                     | 0.55              |
| 6:N:1097:LYS:O    | 6:N:1101:VAL:HG23 | 2.07                     | 0.55              |
| 6:N:1425:THR:HG22 | 6:N:1429:LEU:CD1  | 2.36                     | 0.55              |
| 5:C:182:VAL:HG12  | 5:C:193:LEU:CD1   | 2.37                     | 0.55              |
| 5:C:194:VAL:HG12  | 5:C:204:GLN:HE22  | 1.72                     | 0.55              |
| 5:C:374:ASN:ND2   | 5:C:377:PRO:HD3   | 2.21                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:30:GLU:HB3    | 6:D:40:GLU:HB3    | 1.89                     | 0.55              |
| 6:D:57:GLU:HG2    | 6:D:58:CYS:N      | 2.21                     | 0.55              |
| 6:D:899:LEU:HD12  | 6:D:900:ILE:HG23  | 1.88                     | 0.55              |
| 6:D:1105:ILE:HD12 | 6:D:1373:ARG:NH2  | 2.19                     | 0.55              |
| 6:D:1266:ARG:HG2  | 6:D:1267:ARG:N    | 2.20                     | 0.55              |
| 6:D:1389:LEU:HG   | 6:D:1390:LEU:HG   | 1.89                     | 0.55              |
| 4:K:30:ARG:HH12   | 5:M:938:LYS:HD2   | 1.70                     | 0.55              |
| 5:M:12:VAL:HB     | 5:M:472:ARG:NH2   | 2.22                     | 0.55              |
| 5:M:139:GLN:HE21  | 5:M:418:LEU:HD22  | 1.72                     | 0.55              |
| 5:M:141:HIS:C     | 5:M:331:ARG:HG3   | 2.32                     | 0.55              |
| 5:M:239:PHE:CE1   | 5:M:254:VAL:HB    | 2.33                     | 0.55              |
| 5:M:609:ASN:N     | 5:M:609:ASN:ND2   | 2.54                     | 0.55              |
| 6:N:696:HIS:CD2   | 7:O:59:ASN:HB2    | 2.41                     | 0.55              |
| 6:N:1393:GLN:HB2  | 6:N:1398:TRP:CZ2  | 2.42                     | 0.55              |
| 6:N:1457:ASP:O    | 6:N:1459:LEU:HD12 | 2.07                     | 0.55              |
| 1:G:12:DG:H2''    | 1:G:13:DT:O5'     | 2.06                     | 0.55              |
| 2:H:3:G:H1'       | 11:C:1128:HOH:O   | 2.06                     | 0.55              |
| 4:B:7:LYS:HG2     | 11:B:368:HOH:O    | 2.07                     | 0.55              |
| 4:B:181:VAL:HB    | 11:B:355:HOH:O    | 2.06                     | 0.55              |
| 5:C:751:PRO:HA    | 5:C:792:VAL:HB    | 1.89                     | 0.55              |
| 6:D:119:SER:HB2   | 6:D:123:LEU:CB    | 2.37                     | 0.55              |
| 6:D:403:PHE:CD2   | 6:D:444:VAL:HG23  | 2.41                     | 0.55              |
| 6:D:474:GLU:O     | 6:D:478:LEU:HG    | 2.06                     | 0.55              |
| 6:D:618:LEU:HB3   | 6:D:619:LEU:HD23  | 1.89                     | 0.55              |
| 6:D:630:VAL:HA    | 6:D:744:GLN:CG    | 2.37                     | 0.55              |
| 4:K:73:GLU:OE1    | 4:K:130:ALA:HA    | 2.06                     | 0.55              |
| 5:M:173:ASP:O     | 5:M:184:MET:HA    | 2.06                     | 0.55              |
| 5:M:700:TYR:CB    | 5:M:833:LEU:HD22  | 2.37                     | 0.55              |
| 2:H:7:G:C8        | 2:H:7:G:C5'       | 2.91                     | 0.54              |
| 2:Y:7:G:H8        | 2:Y:7:G:O5'       | 1.90                     | 0.54              |
| 4:A:53:VAL:HG13   | 4:A:142:VAL:HG12  | 1.89                     | 0.54              |
| 4:B:24:VAL:HG22   | 4:B:196:THR:HB    | 1.90                     | 0.54              |
| 5:C:1:MET:CG      | 5:C:900:ARG:HH22  | 2.19                     | 0.54              |
| 5:C:20:GLU:O      | 5:C:24:GLU:HG2    | 2.07                     | 0.54              |
| 5:C:313:LEU:CB    | 5:C:321:GLU:HG3   | 2.37                     | 0.54              |
| 5:C:714:ASP:HB2   | 5:C:818:GLY:O     | 2.07                     | 0.54              |
| 5:C:1105:LYS:HZ2  | 5:C:1107:ASN:HD22 | 1.54                     | 0.54              |
| 6:D:447:VAL:HG23  | 6:D:448:GLU:N     | 2.21                     | 0.54              |
| 6:D:630:VAL:HA    | 6:D:744:GLN:HG2   | 1.89                     | 0.54              |
| 6:D:827:ILE:HG22  | 6:D:837:GLY:HA2   | 1.88                     | 0.54              |
| 6:D:890:VAL:HG11  | 6:D:922:LEU:CD1   | 2.37                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:1425:THR:HG21 | 11:D:8492:HOH:O   | 2.06                     | 0.54              |
| 4:L:219:ARG:HB2   | 11:L:344:HOH:O    | 2.06                     | 0.54              |
| 5:M:587:VAL:HG11  | 5:M:666:LEU:HD22  | 1.88                     | 0.54              |
| 5:M:716:LYS:NZ    | 6:N:36:THR:HA     | 2.21                     | 0.54              |
| 6:N:482:LYS:HB2   | 6:N:1388:ARG:NH2  | 2.21                     | 0.54              |
| 6:N:520:LEU:CD1   | 6:N:521:PRO:HD2   | 2.35                     | 0.54              |
| 6:N:1192:LEU:HD22 | 6:N:1345:GLU:HG2  | 1.89                     | 0.54              |
| 6:N:1263:PHE:O    | 6:N:1424:VAL:HG12 | 2.07                     | 0.54              |
| 6:N:1500:LYS:HB3  | 11:N:9412:HOH:O   | 2.07                     | 0.54              |
| 7:O:13:VAL:HG11   | 7:O:18:ARG:HB3    | 1.89                     | 0.54              |
| 5:C:814:GLU:HB3   | 11:C:1562:HOH:O   | 2.06                     | 0.54              |
| 5:C:842:ARG:HH21  | 5:C:993:PHE:HB3   | 1.73                     | 0.54              |
| 5:C:1032:PHE:O    | 5:C:1033:GLY:O    | 2.26                     | 0.54              |
| 6:D:115:LEU:HD13  | 6:D:502:PHE:CD1   | 2.42                     | 0.54              |
| 6:D:445:ARG:HG2   | 6:D:445:ARG:HH11  | 1.71                     | 0.54              |
| 6:D:967:ALA:HA    | 11:D:8411:HOH:O   | 2.06                     | 0.54              |
| 6:D:1087:ARG:HD2  | 6:D:1256:LEU:HD22 | 1.89                     | 0.54              |
| 5:M:15:LEU:HG     | 5:M:458:TYR:CE1   | 2.43                     | 0.54              |
| 5:M:244:PRO:CD    | 5:M:245:GLY:H     | 2.20                     | 0.54              |
| 5:M:607:ASP:HB2   | 5:M:610:ARG:O     | 2.06                     | 0.54              |
| 5:M:666:LEU:HD11  | 5:M:668:LEU:HD21  | 1.88                     | 0.54              |
| 6:N:141:ILE:HD13  | 6:N:450:TYR:O     | 2.07                     | 0.54              |
| 6:N:171:LEU:HD21  | 6:N:192:ALA:CB    | 2.37                     | 0.54              |
| 6:N:868:TYR:CE2   | 6:N:869:MET:HE3   | 2.42                     | 0.54              |
| 5:C:367:LEU:O     | 5:C:371:LYS:HB3   | 2.06                     | 0.54              |
| 5:C:413:LEU:HD11  | 5:C:452:ILE:HD11  | 1.89                     | 0.54              |
| 5:C:508:ILE:HG13  | 5:C:526:PRO:HB3   | 1.89                     | 0.54              |
| 5:C:526:PRO:HG2   | 11:C:1239:HOH:O   | 2.06                     | 0.54              |
| 5:C:702:SER:HB3   | 5:C:996:LYS:HZ2   | 1.71                     | 0.54              |
| 5:C:715:THR:HG22  | 5:C:717:LEU:HG    | 1.90                     | 0.54              |
| 5:C:1046:ALA:HB2  | 6:D:1476:THR:H    | 1.72                     | 0.54              |
| 6:D:119:SER:HB2   | 6:D:123:LEU:HD13  | 1.88                     | 0.54              |
| 6:D:133:ILE:HG12  | 6:D:153:LEU:O     | 2.07                     | 0.54              |
| 6:D:685:ASP:HA    | 6:D:688:TRP:CD1   | 2.41                     | 0.54              |
| 6:D:1128:VAL:O    | 6:D:1129:THR:C    | 2.50                     | 0.54              |
| 4:K:152:PRO:HB3   | 4:K:154:GLU:OE2   | 2.07                     | 0.54              |
| 4:L:59:GLU:CG     | 4:L:139:ASN:HD22  | 2.20                     | 0.54              |
| 5:M:22:GLN:C      | 5:M:121:MET:HE1   | 2.32                     | 0.54              |
| 5:M:250:ARG:HG2   | 5:M:253:ALA:HB3   | 1.90                     | 0.54              |
| 5:M:674:VAL:HG12  | 5:M:990:GLY:O     | 2.07                     | 0.54              |
| 5:M:851:LYS:HE2   | 5:M:852:ILE:O     | 2.08                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:1060:ILE:HG23 | 5:M:1061:GLU:H    | 1.73                     | 0.54              |
| 6:N:111:LYS:HG2   | 6:N:1452:ILE:HD11 | 1.89                     | 0.54              |
| 6:N:1120:VAL:O    | 6:N:1185:GLU:HA   | 2.08                     | 0.54              |
| 2:Y:5:C:H5'       | 5:M:764:GLU:OE2   | 2.06                     | 0.54              |
| 4:A:149:GLY:O     | 4:A:171:PHE:HB2   | 2.08                     | 0.54              |
| 5:C:1:MET:HE2     | 5:C:900:ARG:HH22  | 1.72                     | 0.54              |
| 5:C:12:VAL:HG12   | 5:C:534:VAL:HG13  | 1.89                     | 0.54              |
| 5:C:198:ARG:HH11  | 5:C:204:GLN:HG2   | 1.71                     | 0.54              |
| 5:C:289:THR:O     | 5:C:291:ALA:N     | 2.40                     | 0.54              |
| 5:C:292:ARG:HD2   | 5:C:299:LYS:HE2   | 1.90                     | 0.54              |
| 5:C:432:ARG:HH22  | 6:D:1053:PHE:HZ   | 1.55                     | 0.54              |
| 5:C:1060:ILE:HG23 | 5:C:1061:GLU:N    | 2.23                     | 0.54              |
| 6:D:137:PRO:HD2   | 6:D:453:ASP:OD2   | 2.07                     | 0.54              |
| 6:D:204:LEU:HD12  | 6:D:396:VAL:HB    | 1.88                     | 0.54              |
| 6:D:971:LEU:HG    | 6:D:972:LEU:HD22  | 1.89                     | 0.54              |
| 4:L:54:THR:HG22   | 4:L:158:ILE:HG13  | 1.89                     | 0.54              |
| 4:L:81:ASN:ND2    | 4:L:127:LEU:HD11  | 2.22                     | 0.54              |
| 5:M:598:GLU:HG3   | 5:M:623:TYR:OH    | 2.08                     | 0.54              |
| 5:M:983:ILE:HG21  | 5:M:987:ILE:CD1   | 2.37                     | 0.54              |
| 5:M:1008:ARG:NH2  | 5:M:1012:PRO:O    | 2.41                     | 0.54              |
| 5:M:1019:GLN:CD   | 6:N:616:GLN:HE22  | 2.15                     | 0.54              |
| 6:N:28:LYS:HB3    | 6:N:41:ARG:HD2    | 1.89                     | 0.54              |
| 7:O:28:GLN:CB     | 7:O:32:ARG:HH22   | 2.21                     | 0.54              |
| 7:O:51:LEU:CD2    | 7:O:52:GLU:H      | 2.19                     | 0.54              |
| 4:B:99:LEU:HD13   | 4:B:144:VAL:HG21  | 1.90                     | 0.54              |
| 5:C:897:LEU:O     | 5:C:899:GLN:HG2   | 2.08                     | 0.54              |
| 6:D:38:LYS:HG2    | 6:D:39:PRO:CD     | 2.37                     | 0.54              |
| 6:D:622:ARG:HD2   | 11:D:8134:HOH:O   | 2.07                     | 0.54              |
| 6:D:731:LEU:CD1   | 6:D:931:LEU:HB3   | 2.37                     | 0.54              |
| 6:D:1481:VAL:O    | 6:D:1481:VAL:HG12 | 2.07                     | 0.54              |
| 6:D:1485:GLN:NE2  | 7:E:79:LEU:N      | 2.55                     | 0.54              |
| 5:M:554:ASP:HB3   | 5:M:880:MET:HB2   | 1.87                     | 0.54              |
| 5:M:1008:ARG:NH1  | 5:M:1011:GLY:N    | 2.56                     | 0.54              |
| 5:M:1060:ILE:HD12 | 5:M:1064:ASN:HD21 | 1.72                     | 0.54              |
| 5:M:1067:TYR:CZ   | 5:M:1071:ILE:HD11 | 2.43                     | 0.54              |
| 5:M:1085:PHE:HE2  | 6:N:1468:LEU:HG   | 1.72                     | 0.54              |
| 6:N:132:TYR:O     | 6:N:456:MET:HB3   | 2.06                     | 0.54              |
| 6:N:462:GLN:CB    | 6:N:513:ILE:HD13  | 2.37                     | 0.54              |
| 6:N:1054:GLU:HB3  | 11:N:9098:HOH:O   | 2.07                     | 0.54              |
| 6:N:1192:LEU:HD21 | 6:N:1372:VAL:HG13 | 1.89                     | 0.54              |
| 6:N:1255:GLY:O    | 6:N:1259:VAL:HG23 | 2.08                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:N:9184:HOH:O  | 7:O:80:VAL:HG21   | 2.08                     | 0.54              |
| 4:B:33:GLY:O     | 4:B:195:LEU:HD13  | 2.08                     | 0.54              |
| 5:C:16:PRO:HD2   | 5:C:458:TYR:HA    | 1.89                     | 0.54              |
| 5:C:310:LEU:O    | 5:C:314:THR:HG23  | 2.07                     | 0.54              |
| 5:C:479:VAL:HG23 | 11:C:1232:HOH:O   | 2.08                     | 0.54              |
| 5:C:607:ASP:HB3  | 5:C:610:ARG:H     | 1.71                     | 0.54              |
| 5:C:806:LEU:CD1  | 5:C:813:VAL:HG21  | 2.37                     | 0.54              |
| 5:C:869:VAL:HA   | 11:C:1453:HOH:O   | 2.08                     | 0.54              |
| 6:D:135:LEU:HD13 | 6:D:148:GLU:HB2   | 1.89                     | 0.54              |
| 6:D:203:ALA:HB1  | 11:D:8118:HOH:O   | 2.06                     | 0.54              |
| 6:D:394:LEU:HD23 | 6:D:394:LEU:H     | 1.73                     | 0.54              |
| 6:D:737:ASN:CG   | 6:D:737:ASN:O     | 2.50                     | 0.54              |
| 6:D:989:TYR:O    | 6:D:993:LEU:HG    | 2.08                     | 0.54              |
| 6:D:1373:ARG:HE  | 6:D:1374:GLN:HE21 | 1.56                     | 0.54              |
| 4:L:92:PRO:HA    | 4:L:146:ARG:NH1   | 2.23                     | 0.54              |
| 5:M:89:THR:HG21  | 5:M:383:ARG:NH2   | 2.23                     | 0.54              |
| 5:M:121:MET:HE3  | 5:M:125:GLY:CA    | 2.32                     | 0.54              |
| 5:M:132:ALA:HB1  | 5:M:632:ASN:ND2   | 2.20                     | 0.54              |
| 5:M:164:PRO:HB2  | 11:M:1226:HOH:O   | 2.07                     | 0.54              |
| 5:M:332:ARG:HA   | 5:M:465:GLY:O     | 2.07                     | 0.54              |
| 5:M:943:VAL:HG11 | 5:M:973:VAL:HG21  | 1.90                     | 0.54              |
| 6:N:141:ILE:H    | 6:N:141:ILE:HD12  | 1.73                     | 0.54              |
| 6:N:754:PHE:HE2  | 6:N:1476:THR:HG21 | 1.72                     | 0.54              |
| 4:A:6:LEU:HD11   | 11:A:387:HOH:O    | 2.07                     | 0.54              |
| 4:A:115:LEU:HD22 | 11:A:317:HOH:O    | 2.07                     | 0.54              |
| 5:C:577:PRO:HA   | 5:C:671:ASN:HD21  | 1.71                     | 0.54              |
| 5:C:861:LEU:HD12 | 5:C:865:THR:HG23  | 1.88                     | 0.54              |
| 6:D:62:LYS:HD2   | 6:D:75:ARG:HD2    | 1.90                     | 0.54              |
| 6:D:133:ILE:CG2  | 6:D:454:ALA:HB1   | 2.37                     | 0.54              |
| 6:D:638:LYS:HD2  | 6:D:932:ASP:CG    | 2.33                     | 0.54              |
| 6:D:685:ASP:HA   | 6:D:688:TRP:NE1   | 2.22                     | 0.54              |
| 5:M:248:PRO:HA   | 11:M:1493:HOH:O   | 2.07                     | 0.54              |
| 5:M:304:LEU:CD2  | 5:M:305:PRO:HD3   | 2.29                     | 0.54              |
| 5:M:461:VAL:HA   | 11:M:1287:HOH:O   | 2.07                     | 0.54              |
| 5:M:837:ASP:O    | 5:M:848:VAL:HG13  | 2.06                     | 0.54              |
| 6:N:1246:VAL:HB  | 11:N:9392:HOH:O   | 2.07                     | 0.54              |
| 7:O:41:GLU:HG2   | 7:O:42:PRO:CD     | 2.37                     | 0.54              |
| 4:A:24:VAL:HG13  | 4:A:196:THR:HG22  | 1.89                     | 0.54              |
| 4:A:101:LEU:HB3  | 4:A:114:PHE:CD2   | 2.43                     | 0.54              |
| 11:B:382:HOH:O   | 6:D:685:ASP:HB3   | 2.08                     | 0.54              |
| 5:C:449:ILE:C    | 5:C:451:LEU:H     | 2.15                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:496:ILE:HD12  | 5:C:496:ILE:N     | 2.23                     | 0.54              |
| 5:C:668:LEU:O     | 5:C:995:MET:HB3   | 2.08                     | 0.54              |
| 5:C:833:LEU:HD11  | 5:C:839:LEU:HD21  | 1.89                     | 0.54              |
| 5:C:1017:THR:HB   | 6:D:613:ARG:NH2   | 2.22                     | 0.54              |
| 6:D:111:LYS:HG2   | 6:D:1452:ILE:HD11 | 1.90                     | 0.54              |
| 6:D:165:LYS:HA    | 6:D:199:LEU:CD1   | 2.38                     | 0.54              |
| 6:D:470:LEU:HD23  | 6:D:470:LEU:H     | 1.73                     | 0.54              |
| 6:D:708:LEU:HB3   | 6:D:1231:GLU:CB   | 2.35                     | 0.54              |
| 6:D:926:LYS:HA    | 6:D:929:ARG:HD2   | 1.88                     | 0.54              |
| 7:E:47:LYS:HA     | 7:E:54:LEU:HB3    | 1.88                     | 0.54              |
| 4:K:14:ARG:HH22   | 4:K:24:VAL:HG23   | 1.73                     | 0.54              |
| 4:L:159:LYS:HB2   | 11:L:316:HOH:O    | 2.08                     | 0.54              |
| 5:M:1097:LEU:HD22 | 5:M:1097:LEU:N    | 2.13                     | 0.54              |
| 6:N:583:ASP:OD1   | 6:N:586:ARG:HG3   | 2.07                     | 0.54              |
| 5:C:100:LEU:HD22  | 5:C:372:LEU:CD2   | 2.38                     | 0.54              |
| 5:C:397:GLU:OE1   | 5:C:631:SER:HB2   | 2.08                     | 0.54              |
| 5:C:1101:THR:OG1  | 5:C:1109:VAL:HB   | 2.08                     | 0.54              |
| 6:D:471:GLU:O     | 6:D:474:GLU:HB3   | 2.08                     | 0.54              |
| 6:D:799:LYS:O     | 6:D:829:VAL:HG22  | 2.08                     | 0.54              |
| 6:D:1209:LEU:HD21 | 7:E:16:LYS:HZ2    | 1.73                     | 0.54              |
| 5:M:620:LEU:HD12  | 5:M:620:LEU:H     | 1.72                     | 0.54              |
| 6:N:776:GLU:HB3   | 6:N:912:LYS:HE2   | 1.90                     | 0.54              |
| 4:A:42:ARG:HH12   | 4:B:34:VAL:HG11   | 1.72                     | 0.54              |
| 4:A:91:ASN:ND2    | 4:A:93:SER:H      | 2.06                     | 0.54              |
| 11:B:374:HOH:O    | 6:D:851:LEU:HD11  | 2.07                     | 0.54              |
| 5:C:684:PHE:N     | 5:C:687:ALA:HB3   | 2.19                     | 0.54              |
| 6:D:565:ILE:HB    | 6:D:566:ILE:HD12  | 1.90                     | 0.54              |
| 6:D:964:LEU:HD21  | 6:D:1058:ARG:NE   | 2.22                     | 0.54              |
| 6:D:1003:VAL:HG11 | 6:D:1041:LEU:HD23 | 1.90                     | 0.54              |
| 4:L:5:LYS:O       | 4:L:8:ALA:HB2     | 2.07                     | 0.54              |
| 5:M:225:SER:HB2   | 11:M:1245:HOH:O   | 2.08                     | 0.54              |
| 5:M:468:ARG:HE    | 5:M:487:THR:CA    | 2.21                     | 0.54              |
| 5:M:1095:LEU:HB2  | 5:M:1097:LEU:HD23 | 1.89                     | 0.54              |
| 6:N:131:LYS:HZ3   | 6:N:568:ARG:HB2   | 1.72                     | 0.54              |
| 6:N:177:ALA:HB3   | 6:N:205:TYR:OH    | 2.08                     | 0.54              |
| 6:N:436:GLU:HB2   | 6:N:445:ARG:HG3   | 1.89                     | 0.54              |
| 6:N:868:TYR:HB2   | 6:N:873:LEU:HD12  | 1.89                     | 0.54              |
| 6:N:996:TRP:HB2   | 11:N:9079:HOH:O   | 2.07                     | 0.54              |
| 4:A:22:GLU:OE2    | 4:A:198:ARG:HB3   | 2.08                     | 0.53              |
| 5:C:497:ALA:HA    | 5:C:515:ALA:HA    | 1.90                     | 0.53              |
| 5:C:758:ARG:HH22  | 5:C:788:THR:HB    | 1.73                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:911:GLU:HB3   | 5:C:912:PRO:HD3   | 1.90                     | 0.53              |
| 6:D:53:ILE:HA     | 6:D:86:ARG:NE     | 2.23                     | 0.53              |
| 6:D:127:LEU:HD22  | 6:D:460:ALA:HB3   | 1.90                     | 0.53              |
| 6:D:600:LEU:H     | 6:D:600:LEU:HD12  | 1.72                     | 0.53              |
| 6:D:754:PHE:CG    | 7:E:24:ALA:HB1    | 2.43                     | 0.53              |
| 5:M:57:GLU:O      | 5:M:62:GLY:HA3    | 2.07                     | 0.53              |
| 5:M:510:ALA:HB3   | 5:M:513:VAL:CG2   | 2.37                     | 0.53              |
| 6:N:478:LEU:O     | 6:N:1388:ARG:NH2  | 2.42                     | 0.53              |
| 6:N:1122:LEU:HB3  | 11:N:9164:HOH:O   | 2.09                     | 0.53              |
| 6:N:1462:LEU:O    | 6:N:1466:VAL:HG23 | 2.08                     | 0.53              |
| 2:H:13:C:C4'      | 5:C:409:ARG:HH22  | 2.13                     | 0.53              |
| 3:I:11:DC:H5      | 11:I:331:HOH:O    | 1.91                     | 0.53              |
| 3:Z:10:DA:H5''    | 6:N:121:THR:HG21  | 1.89                     | 0.53              |
| 4:A:102:LYS:HZ2   | 4:A:139:ASN:HD21  | 1.57                     | 0.53              |
| 5:C:157:ARG:NH1   | 5:C:217:LEU:HD22  | 2.23                     | 0.53              |
| 5:C:285:LEU:HD12  | 5:C:288:ARG:O     | 2.07                     | 0.53              |
| 6:D:22:SER:CB     | 6:D:92:HIS:HB3    | 2.37                     | 0.53              |
| 4:K:72:LYS:HD2    | 5:M:606:VAL:HG11  | 1.90                     | 0.53              |
| 4:L:73:GLU:HB3    | 4:L:77:GLU:CG     | 2.38                     | 0.53              |
| 4:L:176:ARG:HE    | 6:N:847:ASP:CG    | 2.17                     | 0.53              |
| 5:M:34:VAL:HB     | 5:M:38:LYS:CG     | 2.38                     | 0.53              |
| 5:M:259:GLY:HA3   | 11:M:1270:HOH:O   | 2.08                     | 0.53              |
| 6:N:168:THR:CG2   | 6:N:206:ARG:HH12  | 2.21                     | 0.53              |
| 6:N:462:GLN:HA    | 6:N:513:ILE:HD13  | 1.89                     | 0.53              |
| 6:N:714:GLN:CD    | 6:N:765:SER:HA    | 2.33                     | 0.53              |
| 6:N:875:THR:HB    | 6:N:880:ILE:HD11  | 1.90                     | 0.53              |
| 6:N:1191:PRO:HG2  | 6:N:1370:ILE:CD1  | 2.38                     | 0.53              |
| 6:N:1262:LEU:HD21 | 6:N:1351:GLU:HG3  | 1.91                     | 0.53              |
| 1:G:17:DC:H2''    | 1:G:18:DG:C5'     | 2.36                     | 0.53              |
| 5:C:134:ARG:HE    | 5:C:392:SER:HB3   | 1.72                     | 0.53              |
| 5:C:136:ILE:HG22  | 5:C:336:VAL:HG22  | 1.88                     | 0.53              |
| 5:C:438:ILE:HG23  | 5:C:453:THR:OG1   | 2.08                     | 0.53              |
| 5:C:462:ASP:OD1   | 5:C:462:ASP:N     | 2.41                     | 0.53              |
| 5:C:577:PRO:HG3   | 5:C:993:PHE:CE1   | 2.42                     | 0.53              |
| 5:C:1049:LEU:CD1  | 5:C:1053:LEU:HD11 | 2.39                     | 0.53              |
| 5:C:1054:THR:HG22 | 5:C:1082:PRO:HG3  | 1.89                     | 0.53              |
| 6:D:126:VAL:HG21  | 11:D:8125:HOH:O   | 2.07                     | 0.53              |
| 6:D:955:VAL:HG11  | 6:D:1015:TYR:CE2  | 2.42                     | 0.53              |
| 6:D:1063:GLU:HG3  | 6:D:1064:GLY:N    | 2.24                     | 0.53              |
| 6:D:1184:GLN:HB2  | 6:N:559:ALA:HA    | 1.90                     | 0.53              |
| 4:K:171:PHE:O     | 4:K:173:PRO:HD3   | 2.08                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:L:94:LEU:HD11  | 4:L:119:ASP:HB3   | 1.91                     | 0.53              |
| 4:L:201:THR:HG21 | 4:L:205:VAL:HG23  | 1.90                     | 0.53              |
| 5:M:512:ARG:HD3  | 5:M:523:ILE:HD11  | 1.90                     | 0.53              |
| 6:N:394:LEU:HG   | 6:N:396:VAL:CG2   | 2.38                     | 0.53              |
| 6:N:473:LEU:O    | 6:N:477:LEU:HG    | 2.08                     | 0.53              |
| 6:N:619:LEU:HD23 | 6:N:619:LEU:N     | 2.23                     | 0.53              |
| 6:N:817:GLU:O    | 6:N:821:VAL:HG23  | 2.08                     | 0.53              |
| 6:N:1114:THR:CG2 | 6:N:1195:GLN:HB3  | 2.38                     | 0.53              |
| 7:O:91:ARG:HG2   | 11:O:2238:HOH:O   | 2.08                     | 0.53              |
| 4:A:62:LEU:HD13  | 11:A:334:HOH:O    | 2.08                     | 0.53              |
| 4:B:5:LYS:O      | 4:B:8:ALA:HB2     | 2.08                     | 0.53              |
| 5:C:274:ARG:HB2  | 5:C:285:LEU:CD1   | 2.38                     | 0.53              |
| 6:D:781:PRO:O    | 6:D:786:ILE:HD11  | 2.07                     | 0.53              |
| 6:D:957:PRO:HG2  | 6:D:1007:VAL:HA   | 1.89                     | 0.53              |
| 6:D:1010:ASN:ND2 | 11:D:8083:HOH:O   | 2.41                     | 0.53              |
| 5:M:205:GLU:HB2  | 11:M:1398:HOH:O   | 2.07                     | 0.53              |
| 5:M:334:ARG:O    | 5:M:339:LEU:HD11  | 2.09                     | 0.53              |
| 5:M:344:PHE:HE2  | 5:M:378:LEU:HD21  | 1.74                     | 0.53              |
| 5:M:642:ARG:HD2  | 11:M:1230:HOH:O   | 2.08                     | 0.53              |
| 5:M:1045:ALA:HB1 | 5:M:1048:THR:HB   | 1.90                     | 0.53              |
| 6:N:878:GLY:HA2  | 6:N:881:LEU:HD23  | 1.90                     | 0.53              |
| 6:N:1078:ARG:HG3 | 6:N:1078:ARG:HH11 | 1.72                     | 0.53              |
| 1:X:17:DC:H4'    | 6:N:628:ARG:CD    | 2.38                     | 0.53              |
| 4:A:102:LYS:NZ   | 4:A:139:ASN:HD21  | 2.06                     | 0.53              |
| 4:A:159:LYS:HZ1  | 4:A:166:PRO:HD3   | 1.72                     | 0.53              |
| 4:A:175:ARG:CZ   | 4:A:176:ARG:HD3   | 2.37                     | 0.53              |
| 4:B:159:LYS:HD3  | 4:B:159:LYS:N     | 2.24                     | 0.53              |
| 5:C:167:LYS:HE3  | 11:C:1598:HOH:O   | 2.08                     | 0.53              |
| 5:C:309:TYR:HA   | 5:C:312:ALA:HB3   | 1.90                     | 0.53              |
| 5:C:872:ASN:ND2  | 5:C:874:LEU:H     | 2.06                     | 0.53              |
| 5:C:905:ILE:HG22 | 5:C:906:PHE:N     | 2.23                     | 0.53              |
| 6:D:152:LEU:HD11 | 11:D:8125:HOH:O   | 2.09                     | 0.53              |
| 6:D:191:LEU:HD11 | 6:D:395:VAL:CG2   | 2.38                     | 0.53              |
| 6:D:643:GLY:O    | 6:D:726:ILE:HG23  | 2.08                     | 0.53              |
| 6:D:758:GLU:O    | 6:D:762:GLN:HG2   | 2.08                     | 0.53              |
| 4:K:9:PRO:HB3    | 4:K:25:LEU:CG     | 2.38                     | 0.53              |
| 4:K:20:TYR:HD2   | 4:K:21:GLY:N      | 2.07                     | 0.53              |
| 4:K:57:TYR:CZ    | 4:K:59:GLU:HA     | 2.43                     | 0.53              |
| 4:K:176:ARG:HG3  | 4:K:200:TRP:CE3   | 2.44                     | 0.53              |
| 4:L:58:ILE:HB    | 4:L:61:VAL:CG1    | 2.39                     | 0.53              |
| 4:L:121:GLU:OE2  | 4:L:123:MET:HG2   | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:140:ILE:HD11  | 5:M:412:ALA:HB2   | 1.91                     | 0.53              |
| 5:M:224:GLU:HB2   | 5:M:227:PHE:CD1   | 2.44                     | 0.53              |
| 5:M:842:ARG:NH2   | 5:M:887:GLU:CD    | 2.66                     | 0.53              |
| 5:M:1019:GLN:HG2  | 5:M:1058:ASP:OD1  | 2.08                     | 0.53              |
| 6:N:769:LEU:HD11  | 6:N:919:PHE:CZ    | 2.43                     | 0.53              |
| 6:N:814:ALA:HB1   | 6:N:818:ARG:NH2   | 2.24                     | 0.53              |
| 6:N:886:VAL:HG13  | 6:N:930:LEU:HD11  | 1.89                     | 0.53              |
| 6:N:1026:SER:C    | 6:N:1028:ALA:H    | 2.16                     | 0.53              |
| 6:N:1148:VAL:HG13 | 6:N:1163:GLY:HA2  | 1.90                     | 0.53              |
| 6:N:1231:GLU:HB3  | 6:N:1232:PRO:CD   | 2.38                     | 0.53              |
| 1:X:22:DC:H4'     | 5:M:388:ARG:HG3   | 1.90                     | 0.53              |
| 5:C:880:MET:HE1   | 6:D:1037:GLN:OE1  | 2.09                     | 0.53              |
| 5:C:1006:HIS:HA   | 5:C:1027:PHE:CD1  | 2.43                     | 0.53              |
| 6:D:806:PHE:HE1   | 6:D:813:LEU:HD23  | 1.72                     | 0.53              |
| 6:D:864:VAL:HG12  | 6:D:865:THR:H     | 1.74                     | 0.53              |
| 4:K:20:TYR:HD2    | 4:K:21:GLY:H      | 1.55                     | 0.53              |
| 11:K:1782:HOH:O   | 5:M:640:ARG:HG2   | 2.08                     | 0.53              |
| 5:M:532:MET:HG2   | 5:M:533:ASP:O     | 2.08                     | 0.53              |
| 6:N:700:VAL:HG22  | 6:N:718:PRO:HG3   | 1.91                     | 0.53              |
| 6:N:996:TRP:CA    | 6:N:999:THR:HG22  | 2.29                     | 0.53              |
| 6:N:1112:CYS:SG   | 6:N:1195:GLN:HG2  | 2.49                     | 0.53              |
| 4:A:73:GLU:CD     | 4:A:73:GLU:H      | 2.17                     | 0.53              |
| 4:B:99:LEU:HD13   | 4:B:144:VAL:CG2   | 2.39                     | 0.53              |
| 5:C:218:VAL:HG23  | 5:C:311:PHE:HE1   | 1.72                     | 0.53              |
| 5:C:257:VAL:HG21  | 11:C:1481:HOH:O   | 2.08                     | 0.53              |
| 5:C:326:ASP:CB    | 5:C:431:HIS:HB2   | 2.37                     | 0.53              |
| 5:C:329:GLY:HA3   | 5:C:489:THR:HG23  | 1.89                     | 0.53              |
| 6:D:960:LYS:HE2   | 6:D:1041:LEU:HD22 | 1.91                     | 0.53              |
| 6:D:1041:LEU:HD12 | 6:D:1058:ARG:HA   | 1.90                     | 0.53              |
| 6:D:1221:VAL:HG12 | 6:D:1222:GLY:N    | 2.24                     | 0.53              |
| 7:E:25:LYS:HA     | 7:E:28:GLN:HE21   | 1.74                     | 0.53              |
| 4:L:33:GLY:O      | 4:L:195:LEU:HD22  | 2.09                     | 0.53              |
| 5:M:463:GLU:HB3   | 11:M:1525:HOH:O   | 2.09                     | 0.53              |
| 5:M:515:ALA:HB3   | 5:M:524:VAL:CG2   | 2.39                     | 0.53              |
| 2:Y:7:G:O6        | 5:M:1015:LEU:HB2  | 2.09                     | 0.53              |
| 4:B:50:GLY:HA3    | 4:B:171:PHE:O     | 2.08                     | 0.53              |
| 5:C:217:LEU:N     | 5:C:217:LEU:HD23  | 2.24                     | 0.53              |
| 6:D:43:GLY:N      | 11:D:8160:HOH:O   | 2.41                     | 0.53              |
| 6:D:592:THR:H     | 6:D:600:LEU:HD11  | 1.74                     | 0.53              |
| 6:D:995:LEU:HD11  | 11:D:8411:HOH:O   | 2.08                     | 0.53              |
| 7:E:18:ARG:HD3    | 11:E:116:HOH:O    | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:769:PRO:HG2   | 6:N:65:ARG:HD3    | 1.90                     | 0.53              |
| 6:N:1271:LYS:HZ1  | 6:N:1331:ASP:HB2  | 1.72                     | 0.53              |
| 5:C:305:PRO:HA    | 5:C:308:ARG:HB3   | 1.90                     | 0.53              |
| 5:C:545:ASN:OD1   | 5:C:583:LEU:HD13  | 2.08                     | 0.53              |
| 5:C:881:ASN:HD22  | 5:C:881:ASN:H     | 1.55                     | 0.53              |
| 6:D:161:LEU:HD22  | 6:D:452:ILE:HD13  | 1.91                     | 0.53              |
| 6:D:181:ASP:O     | 6:D:204:LEU:HA    | 2.08                     | 0.53              |
| 6:D:1258:ARG:HG2  | 11:D:8324:HOH:O   | 2.09                     | 0.53              |
| 6:D:1435:LEU:HD23 | 6:D:1467:ILE:HD12 | 1.91                     | 0.53              |
| 4:K:47:SER:HB3    | 4:K:217:ILE:HD13  | 1.90                     | 0.53              |
| 4:K:218:LEU:HG    | 11:K:1711:HOH:O   | 2.09                     | 0.53              |
| 5:M:142:ARG:HA    | 5:M:330:ASN:O     | 2.09                     | 0.53              |
| 5:M:549:PHE:CG    | 5:M:886:LEU:HD23  | 2.43                     | 0.53              |
| 5:M:644:VAL:HG22  | 5:M:647:GLN:OE1   | 2.08                     | 0.53              |
| 6:N:808:THR:OG1   | 6:N:809:PRO:HD3   | 2.09                     | 0.53              |
| 6:N:1200:VAL:HG22 | 6:N:1373:ARG:HH12 | 1.73                     | 0.53              |
| 7:O:73:LEU:N      | 7:O:73:LEU:HD12   | 2.24                     | 0.53              |
| 1:X:12:DG:H2''    | 1:X:13:DT:H5'     | 1.90                     | 0.53              |
| 4:B:206:THR:CG2   | 4:B:209:GLU:H     | 2.20                     | 0.53              |
| 5:C:195:LEU:HG    | 5:C:238:LEU:CD1   | 2.38                     | 0.53              |
| 5:C:442:GLU:HA    | 11:C:1416:HOH:O   | 2.08                     | 0.53              |
| 5:C:798:GLY:HA3   | 5:C:828:ALA:O     | 2.09                     | 0.53              |
| 5:C:957:LYS:HD3   | 5:C:961:GLU:OE1   | 2.09                     | 0.53              |
| 6:D:695:ILE:HG21  | 6:D:720:LEU:HD11  | 1.89                     | 0.53              |
| 6:D:827:ILE:O     | 6:D:837:GLY:HA3   | 2.09                     | 0.53              |
| 6:D:971:LEU:HG    | 6:D:972:LEU:N     | 2.22                     | 0.53              |
| 6:D:1037:GLN:OE1  | 6:D:1042:ARG:HD3  | 2.09                     | 0.53              |
| 6:D:1176:LYS:HA   | 6:D:1179:GLU:OE1  | 2.09                     | 0.53              |
| 6:D:1441:GLN:NE2  | 6:D:1442:ASN:HB2  | 2.25                     | 0.53              |
| 4:K:49:PRO:HG3    | 11:K:867:HOH:O    | 2.09                     | 0.53              |
| 4:K:100:LEU:HG    | 4:K:101:LEU:N     | 2.22                     | 0.53              |
| 4:L:10:VAL:HG23   | 4:L:26:GLU:O      | 2.09                     | 0.53              |
| 5:M:172:ILE:H     | 5:M:172:ILE:HD12  | 1.73                     | 0.53              |
| 5:M:264:PRO:HB3   | 5:M:289:THR:HB    | 1.90                     | 0.53              |
| 5:M:264:PRO:HB3   | 5:M:289:THR:CB    | 2.38                     | 0.53              |
| 5:M:394:PHE:HD1   | 5:M:633:GLN:HE22  | 1.56                     | 0.53              |
| 5:M:759:THR:HB    | 5:M:785:VAL:HG13  | 1.90                     | 0.53              |
| 5:M:1101:THR:HG21 | 5:M:1111:ILE:CG2  | 2.38                     | 0.53              |
| 5:M:1101:THR:OG1  | 5:M:1109:VAL:HB   | 2.08                     | 0.53              |
| 6:N:482:LYS:HB2   | 6:N:1388:ARG:HH21 | 1.73                     | 0.53              |
| 6:N:792:ILE:HG13  | 6:N:881:LEU:HD21  | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:1086:LEU:HB2  | 6:N:1087:ARG:NH1  | 2.23                     | 0.53              |
| 1:G:20:DG:H4'     | 5:C:394:PHE:CZ    | 2.44                     | 0.52              |
| 11:Z:1999:HOH:O   | 6:N:1426:LYS:HG3  | 2.08                     | 0.52              |
| 4:A:186:LEU:HB3   | 4:A:192:LEU:CD1   | 2.39                     | 0.52              |
| 4:B:28:LEU:HG     | 4:B:193:ASP:O     | 2.08                     | 0.52              |
| 5:C:1:MET:HG2     | 5:C:900:ARG:NH2   | 2.23                     | 0.52              |
| 5:C:443:THR:HA    | 5:C:452:ILE:O     | 2.09                     | 0.52              |
| 5:C:1031:ARG:HH21 | 6:D:621:LYS:HG3   | 1.73                     | 0.52              |
| 6:D:1026:SER:C    | 6:D:1028:ALA:H    | 2.17                     | 0.52              |
| 6:D:1269:LYS:NZ   | 6:D:1269:LYS:HB3  | 2.24                     | 0.52              |
| 6:D:1465:ASN:ND2  | 6:D:1470:ARG:HE   | 2.05                     | 0.52              |
| 4:L:37:GLY:HA3    | 4:L:179:PHE:CD1   | 2.45                     | 0.52              |
| 5:M:69:LEU:HB2    | 5:M:97:ARG:HB2    | 1.91                     | 0.52              |
| 5:M:367:LEU:HB3   | 5:M:371:LYS:HG2   | 1.90                     | 0.52              |
| 5:M:821:GLU:HB3   | 11:M:1453:HOH:O   | 2.08                     | 0.52              |
| 5:M:949:LYS:HD3   | 6:N:796:ARG:HH22  | 1.74                     | 0.52              |
| 5:M:953:VAL:HG22  | 5:M:966:LEU:HD11  | 1.90                     | 0.52              |
| 5:M:1008:ARG:HB2  | 5:M:1027:PHE:HB2  | 1.91                     | 0.52              |
| 6:N:166:GLN:HG2   | 6:N:396:VAL:HG13  | 1.91                     | 0.52              |
| 6:N:496:LEU:CD1   | 6:N:500:ARG:HG2   | 2.39                     | 0.52              |
| 6:N:705:ALA:CB    | 6:N:706:PRO:HD3   | 2.39                     | 0.52              |
| 6:N:882:PHE:O     | 6:N:886:VAL:HG23  | 2.08                     | 0.52              |
| 6:N:1058:ARG:HG2  | 11:N:9214:HOH:O   | 2.08                     | 0.52              |
| 6:N:1503:VAL:HG21 | 11:N:9060:HOH:O   | 2.07                     | 0.52              |
| 5:C:143:SER:HB2   | 5:C:276:LYS:NZ    | 2.24                     | 0.52              |
| 5:C:251:ASP:HB3   | 5:C:252:LYS:HD2   | 1.91                     | 0.52              |
| 5:C:260:LEU:HG    | 5:C:261:ILE:HG13  | 1.91                     | 0.52              |
| 5:C:1105:LYS:O    | 5:C:1107:ASN:N    | 2.42                     | 0.52              |
| 6:D:610:LYS:HA    | 6:D:615:ARG:CD    | 2.39                     | 0.52              |
| 7:E:32:ARG:HB2    | 7:E:32:ARG:HH11   | 1.74                     | 0.52              |
| 4:L:43:ILE:HG21   | 4:L:214:ALA:HA    | 1.91                     | 0.52              |
| 5:M:74:GLY:O      | 5:M:76:PRO:HD3    | 2.09                     | 0.52              |
| 5:M:89:THR:HA     | 5:M:129:ILE:O     | 2.08                     | 0.52              |
| 5:M:134:ARG:HH11  | 5:M:392:SER:HB3   | 1.74                     | 0.52              |
| 5:M:260:LEU:CB    | 5:M:291:ALA:HB1   | 2.36                     | 0.52              |
| 5:M:305:PRO:HA    | 5:M:308:ARG:HB3   | 1.91                     | 0.52              |
| 5:M:456:ALA:HB1   | 5:M:538:GLN:O     | 2.09                     | 0.52              |
| 6:N:204:LEU:HD13  | 6:N:445:ARG:HE    | 1.72                     | 0.52              |
| 6:N:520:LEU:HG    | 6:N:521:PRO:N     | 2.24                     | 0.52              |
| 6:N:1053:PHE:CE1  | 6:N:1072:ILE:HD12 | 2.44                     | 0.52              |
| 6:N:1236:LEU:HD11 | 6:N:1361:VAL:HG23 | 1.90                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:H:8:C:O5'       | 2:H:8:C:H6       | 1.92                     | 0.52              |
| 6:D:426:LYS:CE    | 6:D:427:VAL:HG23 | 2.40                     | 0.52              |
| 6:D:975:GLU:OE1   | 6:D:975:GLU:HA   | 2.08                     | 0.52              |
| 6:D:1081:GLY:HA2  | 6:D:1241:PHE:CD1 | 2.45                     | 0.52              |
| 4:K:163:ASN:HA    | 11:K:2179:HOH:O  | 2.10                     | 0.52              |
| 4:K:180:GLN:HA    | 5:M:937:ASP:OD1  | 2.08                     | 0.52              |
| 4:L:7:LYS:HE3     | 4:L:186:LEU:HD13 | 1.90                     | 0.52              |
| 5:M:218:VAL:HG22  | 5:M:221:LEU:CD2  | 2.39                     | 0.52              |
| 5:M:432:ARG:NH2   | 6:N:1047:LYS:HD3 | 2.22                     | 0.52              |
| 5:M:1092:LEU:HA   | 5:M:1095:LEU:CD1 | 2.39                     | 0.52              |
| 6:N:104:PHE:HD1   | 6:N:512:MET:HG2  | 1.74                     | 0.52              |
| 6:N:496:LEU:HD12  | 6:N:496:LEU:O    | 2.09                     | 0.52              |
| 6:N:789:LEU:O     | 6:N:793:THR:HG23 | 2.08                     | 0.52              |
| 6:N:800:LYS:HZ1   | 6:N:804:LEU:HD22 | 1.73                     | 0.52              |
| 6:N:899:LEU:HD12  | 6:N:900:ILE:HG23 | 1.91                     | 0.52              |
| 7:O:80:VAL:HG13   | 11:O:1385:HOH:O  | 2.09                     | 0.52              |
| 2:Y:7:G:H22       | 5:M:1014:SER:CA  | 2.23                     | 0.52              |
| 4:B:12:THR:OG1    | 4:B:24:VAL:HB    | 2.10                     | 0.52              |
| 4:B:43:ILE:HG23   | 4:B:47:SER:CB    | 2.40                     | 0.52              |
| 5:C:110:GLU:HG3   | 5:C:369:PRO:HB3  | 1.92                     | 0.52              |
| 5:C:230:ARG:HG2   | 5:C:230:ARG:HH11 | 1.73                     | 0.52              |
| 5:C:290:LEU:HB3   | 5:C:302:VAL:CG1  | 2.39                     | 0.52              |
| 5:C:487:THR:HB    | 5:C:490:GLU:HG3  | 1.90                     | 0.52              |
| 5:C:1105:LYS:HD2  | 5:C:1107:ASN:ND2 | 2.25                     | 0.52              |
| 6:D:42:ASP:CG     | 6:D:48:ARG:HH22  | 2.18                     | 0.52              |
| 6:D:64:LYS:HD2    | 11:D:8441:HOH:O  | 2.09                     | 0.52              |
| 6:D:202:VAL:HG11  | 6:D:400:VAL:HG12 | 1.91                     | 0.52              |
| 6:D:434:ARG:HB2   | 6:D:447:VAL:CG2  | 2.40                     | 0.52              |
| 6:D:557:LEU:HD11  | 11:D:8469:HOH:O  | 2.08                     | 0.52              |
| 6:D:628:ARG:HB2   | 11:D:8067:HOH:O  | 2.08                     | 0.52              |
| 6:D:1248:GLY:HA2  | 6:D:1251:ASP:OD2 | 2.09                     | 0.52              |
| 4:L:43:ILE:HG23   | 4:L:47:SER:CB    | 2.39                     | 0.52              |
| 5:M:674:VAL:HG23  | 5:M:869:VAL:HG13 | 1.92                     | 0.52              |
| 5:M:690:ILE:HD11  | 5:M:833:LEU:HD23 | 1.91                     | 0.52              |
| 5:M:807:ARG:HE    | 5:M:807:ARG:N    | 2.05                     | 0.52              |
| 5:M:850:ALA:HA    | 6:N:632:VAL:HG11 | 1.92                     | 0.52              |
| 5:M:860:HIS:CE1   | 5:M:975:TYR:HB2  | 2.45                     | 0.52              |
| 5:M:969:GLN:CD    | 5:M:971:LYS:HE3  | 2.34                     | 0.52              |
| 5:M:1001:VAL:HG22 | 11:M:1555:HOH:O  | 2.09                     | 0.52              |
| 5:M:1105:LYS:O    | 5:M:1107:ASN:N   | 2.42                     | 0.52              |
| 6:N:119:SER:CB    | 6:N:123:LEU:HB2  | 2.38                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:N:192:ALA:HB1   | 6:N:193:PRO:HD2  | 1.92                     | 0.52              |
| 6:N:584:ASN:HD22  | 6:N:585:GLY:N    | 2.08                     | 0.52              |
| 6:N:644:LEU:HD12  | 6:N:645:PRO:HD2  | 1.91                     | 0.52              |
| 6:N:1118:ILE:HD12 | 11:N:9016:HOH:O  | 2.09                     | 0.52              |
| 6:N:1121:PRO:CD   | 6:N:1346:ARG:HE  | 2.22                     | 0.52              |
| 1:X:13:DT:OP1     | 6:N:1093:TYR:HE2 | 1.93                     | 0.52              |
| 4:A:190:THR:HA    | 11:A:369:HOH:O   | 2.08                     | 0.52              |
| 5:C:173:ASP:O     | 5:C:184:MET:HA   | 2.09                     | 0.52              |
| 5:C:327:HIS:HA    | 5:C:431:HIS:CD2  | 2.44                     | 0.52              |
| 5:C:538:GLN:HG3   | 5:C:539:VAL:N    | 2.24                     | 0.52              |
| 5:C:559:LEU:HD23  | 5:C:563:ASN:OD1  | 2.10                     | 0.52              |
| 5:C:1062:GLY:HA2  | 11:C:1284:HOH:O  | 2.10                     | 0.52              |
| 6:D:52:PRO:CG     | 6:D:80:VAL:HG13  | 2.39                     | 0.52              |
| 6:D:95:LEU:HB3    | 6:D:515:GLU:O    | 2.09                     | 0.52              |
| 6:D:600:LEU:HD12  | 6:D:600:LEU:N    | 2.25                     | 0.52              |
| 6:D:820:GLU:HB2   | 6:D:836:VAL:HG11 | 1.92                     | 0.52              |
| 6:D:989:TYR:CE1   | 6:D:993:LEU:HD21 | 2.44                     | 0.52              |
| 6:D:1112:CYS:CB   | 6:D:1195:GLN:HG2 | 2.29                     | 0.52              |
| 6:D:1118:ILE:HD11 | 11:D:8142:HOH:O  | 2.09                     | 0.52              |
| 6:D:1184:GLN:HB2  | 6:N:559:ALA:CB   | 2.39                     | 0.52              |
| 6:D:1232:PRO:HA   | 6:D:1235:GLN:OE1 | 2.10                     | 0.52              |
| 4:L:27:PRO:HB3    | 4:L:192:LEU:HD22 | 1.91                     | 0.52              |
| 5:M:5:ARG:HE      | 5:M:8:ARG:NH2    | 2.02                     | 0.52              |
| 5:M:287:GLY:O     | 5:M:288:ARG:C    | 2.52                     | 0.52              |
| 5:M:328:LEU:HD13  | 5:M:433:THR:HB   | 1.90                     | 0.52              |
| 5:M:470:PRO:HB2   | 5:M:534:VAL:HG21 | 1.92                     | 0.52              |
| 5:M:684:PHE:N     | 5:M:687:ALA:HB3  | 2.21                     | 0.52              |
| 5:M:754:ILE:HG12  | 5:M:791:ARG:NH1  | 2.25                     | 0.52              |
| 5:M:839:LEU:HD23  | 5:M:996:LYS:HA   | 1.92                     | 0.52              |
| 5:M:1071:ILE:O    | 6:N:659:LYS:HD3  | 2.09                     | 0.52              |
| 6:N:44:LEU:H      | 6:N:44:LEU:HD12  | 1.75                     | 0.52              |
| 6:N:109:PRO:HB3   | 6:N:494:LYS:NZ   | 2.25                     | 0.52              |
| 6:N:568:ARG:O     | 6:N:572:ARG:HG3  | 2.08                     | 0.52              |
| 6:N:654:LYS:HB3   | 6:N:655:PRO:HD3  | 1.91                     | 0.52              |
| 6:N:787:LEU:CD1   | 6:N:1023:MET:HA  | 2.39                     | 0.52              |
| 6:N:832:ARG:HB3   | 6:N:833:GLU:OE1  | 2.09                     | 0.52              |
| 6:N:1165:TYR:OH   | 6:N:1202:GLN:HG2 | 2.09                     | 0.52              |
| 5:C:258:TYR:HB3   | 11:C:1335:HOH:O  | 2.08                     | 0.52              |
| 5:C:398:THR:HG21  | 5:C:567:GLN:C    | 2.34                     | 0.52              |
| 6:D:142:LEU:CD2   | 6:D:146:PRO:HA   | 2.40                     | 0.52              |
| 6:D:660:LYS:HD2   | 6:D:694:VAL:CG2  | 2.40                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:D:834:THR:HA    | 6:D:838:ARG:NH1  | 2.24                     | 0.52              |
| 7:E:45:ARG:HG2    | 11:E:129:HOH:O   | 2.09                     | 0.52              |
| 4:K:64:GLU:HA     | 4:K:165:ILE:HD13 | 1.91                     | 0.52              |
| 4:L:109:VAL:O     | 4:L:129:ILE:HG12 | 2.09                     | 0.52              |
| 5:M:5:ARG:CZ      | 5:M:8:ARG:HH12   | 2.22                     | 0.52              |
| 5:M:18:LEU:HD22   | 5:M:404:LEU:HD21 | 1.91                     | 0.52              |
| 5:M:218:VAL:O     | 5:M:221:LEU:HG   | 2.10                     | 0.52              |
| 5:M:516:ARG:NH2   | 6:N:1068:LEU:HB3 | 2.25                     | 0.52              |
| 5:M:971:LYS:HG2   | 5:M:988:VAL:CB   | 2.40                     | 0.52              |
| 5:M:1009:SER:OG   | 6:N:654:LYS:HD2  | 2.09                     | 0.52              |
| 6:N:1034:GLN:NE2  | 6:N:1243:THR:HB  | 2.25                     | 0.52              |
| 6:N:1204:CYS:C    | 11:N:9238:HOH:O  | 2.51                     | 0.52              |
| 6:N:1440:PHE:O    | 6:N:1441:GLN:O   | 2.28                     | 0.52              |
| 7:O:36:LYS:HE2    | 7:O:36:LYS:HA    | 1.90                     | 0.52              |
| 1:X:12:DG:H2''    | 1:X:13:DT:C5'    | 2.40                     | 0.52              |
| 4:A:14:ARG:HH22   | 4:A:24:VAL:CG2   | 2.23                     | 0.52              |
| 5:C:9:ILE:HD12    | 5:C:9:ILE:H      | 1.75                     | 0.52              |
| 5:C:13:ILE:HD11   | 5:C:483:VAL:HG21 | 1.92                     | 0.52              |
| 5:C:39:ARG:H      | 5:C:39:ARG:CD    | 2.03                     | 0.52              |
| 6:D:82:LYS:HD2    | 11:D:8499:HOH:O  | 2.08                     | 0.52              |
| 6:D:615:ARG:HH22  | 6:D:1096:ARG:CD  | 2.22                     | 0.52              |
| 6:D:1498:ALA:HB1  | 7:E:84:ARG:NH2   | 2.25                     | 0.52              |
| 7:E:48:MET:CB     | 7:E:54:LEU:HB2   | 2.39                     | 0.52              |
| 4:K:8:ALA:HB1     | 4:L:224:TYR:CE1  | 2.45                     | 0.52              |
| 4:L:206:THR:HG23  | 4:L:208:LEU:H    | 1.73                     | 0.52              |
| 5:M:589:ARG:HH11  | 5:M:589:ARG:HB2  | 1.73                     | 0.52              |
| 5:M:757:GLY:HA2   | 5:M:789:SER:OG   | 2.10                     | 0.52              |
| 5:M:1008:ARG:HH12 | 5:M:1011:GLY:H   | 1.58                     | 0.52              |
| 5:M:1019:GLN:HE22 | 6:N:616:GLN:HE22 | 1.58                     | 0.52              |
| 6:N:31:THR:HB     | 6:N:527:MET:HE2  | 1.91                     | 0.52              |
| 6:N:1492:LEU:HD12 | 6:N:1493:LYS:HZ1 | 1.73                     | 0.52              |
| 4:A:178:ALA:HB3   | 4:A:198:ARG:CG   | 2.37                     | 0.52              |
| 4:A:222:LEU:HD13  | 4:B:218:LEU:HD23 | 1.90                     | 0.52              |
| 5:C:65:VAL:CG2    | 5:C:101:ILE:HB   | 2.40                     | 0.52              |
| 5:C:260:LEU:C     | 5:C:260:LEU:HD12 | 2.34                     | 0.52              |
| 5:C:564:MET:SD    | 5:C:995:MET:HG3  | 2.50                     | 0.52              |
| 5:C:564:MET:HE2   | 5:C:565:GLN:HA   | 1.90                     | 0.52              |
| 5:C:748:GLU:CB    | 5:C:799:ILE:HD12 | 2.39                     | 0.52              |
| 5:C:859:PRO:O     | 5:C:867:VAL:HG22 | 2.09                     | 0.52              |
| 5:C:983:ILE:HB    | 11:C:1149:HOH:O  | 2.10                     | 0.52              |
| 6:D:684:LYS:HD3   | 6:D:686:GLU:OE1  | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:91:GLN:NE2    | 5:M:383:ARG:NH2   | 2.57                     | 0.52              |
| 5:M:157:ARG:HG2   | 11:M:1381:HOH:O   | 2.09                     | 0.52              |
| 5:M:352:ALA:HA    | 5:M:355:VAL:CG1   | 2.39                     | 0.52              |
| 5:M:436:GLY:HA2   | 5:M:538:GLN:C     | 2.35                     | 0.52              |
| 5:M:1032:PHE:HZ   | 5:M:1040:LEU:HD13 | 1.74                     | 0.52              |
| 6:N:141:ILE:HD12  | 6:N:141:ILE:N     | 2.25                     | 0.52              |
| 6:N:452:ILE:HG22  | 11:N:9064:HOH:O   | 2.10                     | 0.52              |
| 6:N:610:LYS:HG3   | 11:N:9272:HOH:O   | 2.09                     | 0.52              |
| 6:N:619:LEU:HD12  | 6:N:621:LYS:NZ    | 2.25                     | 0.52              |
| 6:N:756:GLN:NE2   | 6:N:760:ARG:HD2   | 2.24                     | 0.52              |
| 5:C:102:HIS:HB2   | 5:C:106:GLY:O     | 2.10                     | 0.52              |
| 5:C:287:GLY:O     | 5:C:288:ARG:C     | 2.53                     | 0.52              |
| 5:C:774:LEU:HD23  | 5:C:775:ARG:N     | 2.25                     | 0.52              |
| 5:C:996:LYS:HE3   | 11:C:1151:HOH:O   | 2.10                     | 0.52              |
| 6:D:543:LEU:O     | 6:D:546:ARG:HB2   | 2.10                     | 0.52              |
| 6:D:731:LEU:HD13  | 6:D:931:LEU:HB3   | 1.91                     | 0.52              |
| 4:K:156:HIS:CD2   | 4:K:157:GLY:N     | 2.77                     | 0.52              |
| 4:L:216:GLU:HG3   | 4:L:220:GLU:OE1   | 2.10                     | 0.52              |
| 5:M:212:GLY:HA3   | 5:M:218:VAL:HG21  | 1.91                     | 0.52              |
| 5:M:565:GLN:OE1   | 5:M:842:ARG:HG2   | 2.10                     | 0.52              |
| 6:N:204:LEU:HD12  | 6:N:396:VAL:CG2   | 2.40                     | 0.52              |
| 6:N:656:PHE:HB3   | 6:N:694:VAL:HG11  | 1.92                     | 0.52              |
| 6:N:1270:ALA:O    | 6:N:1329:ALA:HB3  | 2.09                     | 0.52              |
| 7:O:54:LEU:HA     | 7:O:58:PRO:CG     | 2.39                     | 0.52              |
| 4:B:124:ASN:N     | 4:B:125:PRO:HD3   | 2.23                     | 0.52              |
| 5:C:20:GLU:OE2    | 5:C:460:ARG:NH1   | 2.42                     | 0.52              |
| 5:C:1037:VAL:HG12 | 5:C:1041:GLU:OE2  | 2.10                     | 0.52              |
| 6:D:399:ARG:HD3   | 6:D:430:ASP:OD2   | 2.09                     | 0.52              |
| 6:D:525:ARG:HB2   | 6:D:538:SER:CB    | 2.40                     | 0.52              |
| 6:D:820:GLU:HA    | 6:D:825:ALA:O     | 2.10                     | 0.52              |
| 6:D:1267:ARG:HB2  | 6:D:1267:ARG:NH1  | 2.24                     | 0.52              |
| 4:K:1:MET:O       | 4:K:6:LEU:HD22    | 2.10                     | 0.52              |
| 5:M:353:ARG:HA    | 11:M:1274:HOH:O   | 2.09                     | 0.52              |
| 5:M:437:ARG:C     | 5:M:438:ILE:HD12  | 2.35                     | 0.52              |
| 5:M:1094:ALA:HA   | 6:N:90:MET:CE     | 2.39                     | 0.52              |
| 6:N:616:GLN:NE2   | 11:N:9292:HOH:O   | 2.43                     | 0.52              |
| 6:N:642:CYS:SG    | 6:N:716:PHE:HB2   | 2.50                     | 0.52              |
| 6:N:1403:LEU:O    | 6:N:1407:LEU:HD13 | 2.10                     | 0.52              |
| 6:N:1440:PHE:CG   | 6:N:1441:GLN:N    | 2.78                     | 0.52              |
| 7:O:67:GLU:HB3    | 7:O:73:LEU:HD11   | 1.91                     | 0.52              |
| 4:A:9:PRO:HD2     | 4:B:224:TYR:CE1   | 2.45                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:67:THR:CG2    | 5:C:609:ASN:HD21  | 2.23                     | 0.51              |
| 4:A:163:ASN:HD21  | 5:C:744:ARG:NH2   | 2.08                     | 0.51              |
| 5:C:286:SER:HB3   | 5:C:299:LYS:HE3   | 1.92                     | 0.51              |
| 6:D:206:ARG:CG    | 6:D:394:LEU:HD22  | 2.33                     | 0.51              |
| 6:D:396:VAL:CG1   | 6:D:447:VAL:HA    | 2.36                     | 0.51              |
| 5:M:557:ARG:NH1   | 5:M:879:ARG:HD3   | 2.25                     | 0.51              |
| 5:M:576:ALA:HB3   | 5:M:900:ARG:HH11  | 1.75                     | 0.51              |
| 5:M:1109:VAL:HA   | 6:N:3:LYS:HE3     | 1.92                     | 0.51              |
| 6:N:95:LEU:H      | 6:N:95:LEU:CD1    | 2.20                     | 0.51              |
| 6:N:396:VAL:CG1   | 6:N:447:VAL:HA    | 2.41                     | 0.51              |
| 6:N:461:ILE:O     | 6:N:465:LEU:HB2   | 2.09                     | 0.51              |
| 6:N:632:VAL:HG23  | 6:N:725:SER:HB2   | 1.92                     | 0.51              |
| 6:N:709:HIS:CD2   | 6:N:709:HIS:H     | 2.28                     | 0.51              |
| 6:N:960:LYS:HZ1   | 6:N:1041:LEU:HD13 | 1.75                     | 0.51              |
| 6:N:1020:LEU:HD21 | 6:N:1035:ILE:CG2  | 2.40                     | 0.51              |
| 4:A:73:GLU:CD     | 4:A:130:ALA:HA    | 2.35                     | 0.51              |
| 4:A:138:LEU:O     | 4:A:138:LEU:HD23  | 2.10                     | 0.51              |
| 4:A:188:GLN:HG3   | 4:A:189:ARG:H     | 1.74                     | 0.51              |
| 5:C:144:PRO:N     | 5:C:276:LYS:NZ    | 2.58                     | 0.51              |
| 5:C:157:ARG:HG3   | 5:C:314:THR:HG21  | 1.92                     | 0.51              |
| 5:C:198:ARG:CZ    | 5:C:203:ASP:HA    | 2.39                     | 0.51              |
| 5:C:843:HIS:CB    | 5:C:884:GLN:HG2   | 2.40                     | 0.51              |
| 6:D:710:ARG:C     | 6:D:712:GLY:H     | 2.18                     | 0.51              |
| 6:D:831:GLY:HA3   | 11:D:8198:HOH:O   | 2.09                     | 0.51              |
| 6:D:1098:LEU:CD2  | 6:D:1226:ALA:HA   | 2.38                     | 0.51              |
| 6:D:1118:ILE:HG13 | 6:D:1192:LEU:HD13 | 1.92                     | 0.51              |
| 4:K:41:ARG:O      | 4:K:45:LEU:HD12   | 2.10                     | 0.51              |
| 4:K:102:LYS:NZ    | 4:K:115:LEU:HD22  | 2.24                     | 0.51              |
| 4:L:182:GLU:OE1   | 4:L:194:LYS:O     | 2.29                     | 0.51              |
| 5:M:97:ARG:HA     | 5:M:111:ASP:O     | 2.10                     | 0.51              |
| 5:M:110:GLU:HG3   | 5:M:369:PRO:CB    | 2.29                     | 0.51              |
| 5:M:139:GLN:NE2   | 5:M:418:LEU:HD22  | 2.25                     | 0.51              |
| 5:M:557:ARG:HD3   | 5:M:560:MET:SD    | 2.50                     | 0.51              |
| 5:M:787:ASP:HB3   | 11:M:1300:HOH:O   | 2.09                     | 0.51              |
| 6:N:35:ARG:HG3    | 6:N:35:ARG:HH11   | 1.75                     | 0.51              |
| 6:N:50:PHE:CB     | 6:N:522:PRO:HG3   | 2.40                     | 0.51              |
| 6:N:52:PRO:CG     | 6:N:80:VAL:HG13   | 2.39                     | 0.51              |
| 6:N:754:PHE:O     | 6:N:758:GLU:HG2   | 2.10                     | 0.51              |
| 6:N:1121:PRO:HA   | 6:N:1185:GLU:HG2  | 1.90                     | 0.51              |
| 6:N:1248:GLY:O    | 6:N:1252:ILE:HG12 | 2.10                     | 0.51              |
| 6:N:1267:ARG:HA   | 6:N:1271:LYS:HZ1  | 1.75                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:N:1496:GLU:HA  | 6:N:1499:ARG:CZ   | 2.40                     | 0.51              |
| 1:G:19:DC:OP1    | 5:C:1001:VAL:HG11 | 2.10                     | 0.51              |
| 1:X:18:DG:H2''   | 1:X:19:DC:C5'     | 2.31                     | 0.51              |
| 4:A:26:GLU:HG3   | 4:A:184:THR:HG21  | 1.91                     | 0.51              |
| 4:B:206:THR:HG23 | 4:B:208:LEU:H     | 1.75                     | 0.51              |
| 5:C:69:LEU:C     | 5:C:70:GLU:HG2    | 2.35                     | 0.51              |
| 5:C:194:VAL:CG1  | 5:C:204:GLN:HE22  | 2.22                     | 0.51              |
| 5:C:841:ASN:HD21 | 5:C:845:ASN:N     | 2.08                     | 0.51              |
| 6:D:813:LEU:HD12 | 6:D:814:ALA:N     | 2.26                     | 0.51              |
| 7:E:39:VAL:HG22  | 7:E:67:GLU:HG2    | 1.92                     | 0.51              |
| 4:L:102:LYS:HZ2  | 4:L:137:ARG:HG2   | 1.72                     | 0.51              |
| 5:M:211:LEU:CD1  | 5:M:308:ARG:HA    | 2.40                     | 0.51              |
| 5:M:771:GLU:O    | 5:M:775:ARG:HG2   | 2.11                     | 0.51              |
| 5:M:841:ASN:HD21 | 5:M:845:ASN:H     | 1.58                     | 0.51              |
| 6:N:703:ASN:ND2  | 6:N:704:ARG:N     | 2.58                     | 0.51              |
| 6:N:879:ARG:HG3  | 6:N:879:ARG:NH1   | 2.25                     | 0.51              |
| 6:N:889:ALA:CB   | 6:N:930:LEU:HD12  | 2.39                     | 0.51              |
| 6:N:1442:ASN:CG  | 6:N:1444:THR:HB   | 2.36                     | 0.51              |
| 6:N:1476:THR:C   | 6:N:1478:SER:N    | 2.67                     | 0.51              |
| 4:B:216:GLU:HA   | 4:B:219:ARG:NH1   | 2.25                     | 0.51              |
| 5:C:163:ILE:O    | 5:C:163:ILE:HG13  | 2.08                     | 0.51              |
| 5:C:172:ILE:CG2  | 5:C:184:MET:HE3   | 2.40                     | 0.51              |
| 5:C:547:ILE:HD13 | 5:C:550:LEU:HD13  | 1.91                     | 0.51              |
| 5:C:552:HIS:CD2  | 6:D:1064:GLY:HA2  | 2.46                     | 0.51              |
| 5:C:580:MET:HB3  | 5:C:584:GLU:CD    | 2.35                     | 0.51              |
| 5:C:598:GLU:HG3  | 5:C:623:TYR:OH    | 2.10                     | 0.51              |
| 5:C:605:LYS:HD2  | 5:C:612:VAL:HB    | 1.92                     | 0.51              |
| 5:C:737:LEU:HD21 | 5:C:741:GLY:C     | 2.36                     | 0.51              |
| 5:C:946:ARG:HB3  | 5:C:946:ARG:NH1   | 2.25                     | 0.51              |
| 6:D:483:HIS:ND1  | 6:D:483:HIS:N     | 2.59                     | 0.51              |
| 6:D:690:ALA:O    | 6:D:694:VAL:HG23  | 2.10                     | 0.51              |
| 6:D:762:GLN:HE22 | 7:E:20:THR:HG21   | 1.75                     | 0.51              |
| 6:D:960:LYS:HZ1  | 6:D:1040:GLY:C    | 2.18                     | 0.51              |
| 6:D:1464:GLU:HA  | 6:D:1467:ILE:CD1  | 2.40                     | 0.51              |
| 4:K:9:PRO:HB3    | 4:K:25:LEU:HG     | 1.92                     | 0.51              |
| 4:L:36:LEU:O     | 4:L:39:PRO:HD2    | 2.10                     | 0.51              |
| 5:M:79:PRO:HD2   | 5:M:82:GLU:OE1    | 2.10                     | 0.51              |
| 5:M:173:ASP:OD1  | 5:M:185:LYS:HG3   | 2.11                     | 0.51              |
| 5:M:804:VAL:HB   | 5:M:824:ARG:HB2   | 1.93                     | 0.51              |
| 5:M:938:LYS:HB2  | 5:M:938:LYS:NZ    | 2.18                     | 0.51              |
| 5:M:976:ASP:HB2  | 11:M:1439:HOH:O   | 2.10                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:1087:VAL:HG23 | 6:N:524:LEU:HD21  | 1.92                     | 0.51              |
| 6:N:172:PRO:HG2   | 6:N:175:VAL:CG2   | 2.41                     | 0.51              |
| 6:N:793:THR:CB    | 6:N:879:ARG:HD3   | 2.31                     | 0.51              |
| 6:N:871:LYS:HB3   | 6:N:873:LEU:CD2   | 2.40                     | 0.51              |
| 6:N:977:ALA:HB1   | 6:N:983:LEU:HD21  | 1.91                     | 0.51              |
| 6:N:1377:LYS:HE3  | 6:N:1394:VAL:HG13 | 1.92                     | 0.51              |
| 2:H:8:C:H2'       | 2:H:9:G:C8        | 2.46                     | 0.51              |
| 4:A:98:THR:HG22   | 11:A:364:HOH:O    | 2.09                     | 0.51              |
| 4:B:102:LYS:NZ    | 4:B:137:ARG:NE    | 2.59                     | 0.51              |
| 5:C:195:LEU:HG    | 5:C:238:LEU:HD12  | 1.91                     | 0.51              |
| 5:C:328:LEU:HB3   | 5:C:488:ALA:HB2   | 1.93                     | 0.51              |
| 5:C:343:GLN:HB2   | 5:C:385:PHE:CD2   | 2.46                     | 0.51              |
| 5:C:640:ARG:O     | 5:C:642:ARG:HG2   | 2.10                     | 0.51              |
| 5:C:678:PRO:O     | 6:D:943:THR:HA    | 2.10                     | 0.51              |
| 6:D:145:VAL:CG2   | 6:D:146:PRO:HD2   | 2.33                     | 0.51              |
| 6:D:394:LEU:O     | 6:D:396:VAL:N     | 2.43                     | 0.51              |
| 6:D:582:LEU:HD23  | 6:D:603:LEU:CD1   | 2.41                     | 0.51              |
| 6:D:1100:ASP:CG   | 6:D:1463:LYS:HZ1  | 2.19                     | 0.51              |
| 6:D:1491:THR:O    | 6:D:1495:ILE:HD13 | 2.11                     | 0.51              |
| 4:K:158:ILE:O     | 4:K:159:LYS:HE2   | 2.11                     | 0.51              |
| 4:K:181:VAL:H     | 5:M:937:ASP:CG    | 2.19                     | 0.51              |
| 4:L:124:ASN:HD21  | 4:L:127:LEU:HD22  | 1.74                     | 0.51              |
| 4:L:202:ASP:HA    | 11:L:321:HOH:O    | 2.10                     | 0.51              |
| 5:M:351:LEU:HD22  | 5:M:377:PRO:HB2   | 1.92                     | 0.51              |
| 5:M:535:SER:HB3   | 5:M:537:LYS:HZ3   | 1.76                     | 0.51              |
| 5:M:855:VAL:HG11  | 11:M:1481:HOH:O   | 2.11                     | 0.51              |
| 6:N:701:LEU:HD12  | 6:N:701:LEU:H     | 1.74                     | 0.51              |
| 6:N:1090:ASP:HA   | 6:N:1093:TYR:HB2  | 1.91                     | 0.51              |
| 4:A:5:LYS:O       | 4:A:8:ALA:HB2     | 2.10                     | 0.51              |
| 4:A:88:ARG:HD2    | 4:A:121:GLU:OE1   | 2.10                     | 0.51              |
| 4:B:40:LEU:O      | 4:B:44:LEU:HG     | 2.11                     | 0.51              |
| 5:C:432:ARG:HH12  | 6:D:1072:ILE:HD11 | 1.75                     | 0.51              |
| 5:C:603:VAL:H     | 5:C:647:GLN:H     | 1.57                     | 0.51              |
| 5:C:612:VAL:HG12  | 11:C:1460:HOH:O   | 2.10                     | 0.51              |
| 5:C:835:VAL:HG13  | 5:C:836:GLY:N     | 2.25                     | 0.51              |
| 6:D:540:LEU:HA    | 6:D:543:LEU:CD1   | 2.40                     | 0.51              |
| 6:D:705:ALA:CB    | 6:D:706:PRO:HD3   | 2.40                     | 0.51              |
| 6:D:1101:VAL:HG21 | 6:D:1424:VAL:HA   | 1.93                     | 0.51              |
| 4:L:24:VAL:HG13   | 4:L:196:THR:CG2   | 2.39                     | 0.51              |
| 4:L:29:GLU:OE2    | 4:L:29:GLU:HA     | 2.10                     | 0.51              |
| 5:M:549:PHE:HA    | 11:M:1469:HOH:O   | 2.10                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:M:879:ARG:HH21  | 6:N:1029:ARG:NH2 | 2.08                     | 0.51              |
| 5:M:913:GLU:O     | 5:M:917:LEU:HG   | 2.11                     | 0.51              |
| 6:N:153:LEU:HD22  | 6:N:158:TYR:HB2  | 1.93                     | 0.51              |
| 6:N:396:VAL:C     | 6:N:398:ALA:N    | 2.69                     | 0.51              |
| 6:N:864:VAL:HB    | 11:N:9142:HOH:O  | 2.10                     | 0.51              |
| 6:N:1094:LEU:HB2  | 6:N:1260:ILE:CD1 | 2.38                     | 0.51              |
| 6:N:1100:ASP:HB3  | 6:N:1428:ALA:HB1 | 1.92                     | 0.51              |
| 6:N:1107:VAL:HA   | 6:N:1200:VAL:O   | 2.11                     | 0.51              |
| 6:N:1129:THR:O    | 6:N:1130:ARG:HD2 | 2.11                     | 0.51              |
| 6:N:1366:LYS:HA   | 6:N:1369:GLU:OE1 | 2.11                     | 0.51              |
| 4:A:221:HIS:HA    | 4:A:224:TYR:HD2  | 1.76                     | 0.51              |
| 4:B:40:LEU:HD21   | 4:B:215:VAL:HG12 | 1.93                     | 0.51              |
| 5:C:52:PHE:CG     | 5:C:68:PHE:HB2   | 2.46                     | 0.51              |
| 5:C:217:LEU:HD23  | 5:C:217:LEU:H    | 1.76                     | 0.51              |
| 5:C:1088:LEU:HD23 | 5:C:1089:VAL:N   | 2.26                     | 0.51              |
| 6:D:631:ILE:HG21  | 6:D:745:MET:SD   | 2.50                     | 0.51              |
| 6:D:903:ASP:O     | 6:D:904:VAL:HG13 | 2.11                     | 0.51              |
| 6:D:933:ALA:O     | 6:D:937:TYR:HD1  | 1.93                     | 0.51              |
| 4:L:102:LYS:HD3   | 4:L:139:ASN:CB   | 2.35                     | 0.51              |
| 5:M:64:LEU:HD13   | 5:M:359:MET:HG3  | 1.93                     | 0.51              |
| 5:M:163:ILE:HG13  | 5:M:163:ILE:O    | 2.09                     | 0.51              |
| 5:M:710:ILE:HD12  | 5:M:790:LEU:HB2  | 1.91                     | 0.51              |
| 5:M:892:LEU:HD11  | 5:M:967:PHE:CE1  | 2.45                     | 0.51              |
| 5:M:1090:LYS:HE3  | 5:M:1112:PHE:CE1 | 2.42                     | 0.51              |
| 6:N:415:VAL:O     | 6:N:432:TYR:HA   | 2.11                     | 0.51              |
| 6:N:634:GLY:O     | 6:N:637:LEU:HB3  | 2.11                     | 0.51              |
| 6:N:828:LYS:HD3   | 6:N:862:ASP:OD2  | 2.11                     | 0.51              |
| 6:N:1033:GLN:O    | 6:N:1037:GLN:HG3 | 2.10                     | 0.51              |
| 6:N:1117:TYR:CE2  | 6:N:1151:ARG:HD3 | 2.45                     | 0.51              |
| 6:N:1191:PRO:HB2  | 11:N:9021:HOH:O  | 2.10                     | 0.51              |
| 6:N:1452:ILE:HG22 | 6:N:1453:ALA:N   | 2.25                     | 0.51              |
| 6:N:1476:THR:HG23 | 7:O:21:VAL:HG22  | 1.92                     | 0.51              |
| 5:C:80:GLN:HE22   | 5:C:122:THR:HG23 | 1.76                     | 0.51              |
| 5:C:144:PRO:N     | 5:C:276:LYS:HZ1  | 2.08                     | 0.51              |
| 5:C:147:TYR:HB3   | 11:C:1186:HOH:O  | 2.10                     | 0.51              |
| 5:C:158:TYR:CE1   | 5:C:314:THR:HA   | 2.46                     | 0.51              |
| 5:C:352:ALA:HA    | 5:C:355:VAL:CG1  | 2.41                     | 0.51              |
| 5:C:573:ARG:CB    | 5:C:670:GLN:HE22 | 2.23                     | 0.51              |
| 5:C:878:SER:HA    | 6:D:1034:GLN:OE1 | 2.11                     | 0.51              |
| 5:C:1008:ARG:NH2  | 5:C:1011:GLY:H   | 2.09                     | 0.51              |
| 6:D:566:ILE:HD12  | 6:D:566:ILE:H    | 1.76                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:582:LEU:HD23  | 6:D:603:LEU:HD12  | 1.92                     | 0.51              |
| 6:D:1101:VAL:HG23 | 6:D:1424:VAL:HG23 | 1.93                     | 0.51              |
| 6:D:1347:TYR:CD2  | 6:D:1348:LEU:HD12 | 2.46                     | 0.51              |
| 4:K:26:GLU:HG2    | 4:K:27:PRO:CA     | 2.40                     | 0.51              |
| 4:L:160:ASP:HB3   | 4:L:161:ARG:HD2   | 1.92                     | 0.51              |
| 5:M:5:ARG:HB2     | 5:M:8:ARG:NH2     | 2.21                     | 0.51              |
| 5:M:169:GLY:HA2   | 5:M:263:ASP:OD1   | 2.11                     | 0.51              |
| 5:M:550:LEU:HD12  | 5:M:550:LEU:O     | 2.10                     | 0.51              |
| 6:N:62:LYS:HB2    | 6:N:73:CYS:SG     | 2.51                     | 0.51              |
| 6:N:542:ASP:O     | 6:N:546:ARG:HG3   | 2.10                     | 0.51              |
| 4:B:7:LYS:O       | 4:B:7:LYS:HD2     | 2.11                     | 0.51              |
| 5:C:604:ALA:HB3   | 5:C:612:VAL:O     | 2.10                     | 0.51              |
| 6:D:154:THR:HG22  | 6:D:157:GLU:OE2   | 2.10                     | 0.51              |
| 6:D:393:ILE:HG21  | 11:D:8118:HOH:O   | 2.11                     | 0.51              |
| 6:D:413:ASP:O     | 6:D:435:VAL:HG23  | 2.11                     | 0.51              |
| 6:D:671:LYS:HG3   | 11:D:8106:HOH:O   | 2.11                     | 0.51              |
| 6:D:1040:GLY:O    | 6:D:1060:SER:HB3  | 2.11                     | 0.51              |
| 6:D:1379:VAL:HG12 | 6:D:1419:PRO:HA   | 1.93                     | 0.51              |
| 7:E:41:GLU:CG     | 7:E:42:PRO:HD3    | 2.41                     | 0.51              |
| 5:M:160:ALA:HB3   | 5:M:174:LEU:HB2   | 1.93                     | 0.51              |
| 5:M:1047:HIS:H    | 5:M:1047:HIS:CD2  | 2.28                     | 0.51              |
| 6:N:481:MET:SD    | 6:N:493:ARG:HA    | 2.51                     | 0.51              |
| 6:N:1023:MET:HG2  | 6:N:1029:ARG:HB2  | 1.93                     | 0.51              |
| 7:O:10:PHE:CZ     | 7:O:16:LYS:HE3    | 2.46                     | 0.51              |
| 4:A:14:ARG:HG3    | 4:A:14:ARG:HH11   | 1.75                     | 0.51              |
| 4:B:48:ILE:HD12   | 4:B:48:ILE:H      | 1.76                     | 0.51              |
| 4:B:89:PHE:HB3    | 4:B:94:LEU:CD1    | 2.39                     | 0.51              |
| 5:C:3:ILE:HA      | 5:C:900:ARG:O     | 2.11                     | 0.51              |
| 5:C:288:ARG:NH1   | 5:C:288:ARG:HB2   | 2.26                     | 0.51              |
| 5:C:552:HIS:ND1   | 5:C:886:LEU:HD22  | 2.26                     | 0.51              |
| 5:C:730:SER:O     | 5:C:734:LEU:HD13  | 2.11                     | 0.51              |
| 5:C:1019:GLN:HE22 | 5:C:1058:ASP:CB   | 2.24                     | 0.51              |
| 6:D:181:ASP:HA    | 6:D:205:TYR:CD1   | 2.46                     | 0.51              |
| 6:D:785:ILE:HG13  | 6:D:939:PHE:HE2   | 1.74                     | 0.51              |
| 6:D:1151:ARG:HG2  | 6:D:1187:PRO:HB2  | 1.92                     | 0.51              |
| 7:E:27:ALA:HA     | 7:E:30:LEU:HD13   | 1.93                     | 0.51              |
| 7:E:33:HIS:CD2    | 7:E:89:MET:HG2    | 2.45                     | 0.51              |
| 7:E:48:MET:HG2    | 7:E:49:GLN:N      | 2.26                     | 0.51              |
| 5:M:571:LEU:HD21  | 5:M:700:TYR:HA    | 1.93                     | 0.51              |
| 5:M:628:PHE:HA    | 11:M:1256:HOH:O   | 2.10                     | 0.51              |
| 5:M:660:ALA:HA    | 11:M:1443:HOH:O   | 2.11                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:M:1007:ALA:HB2  | 6:N:648:MET:HG2  | 1.91                     | 0.51              |
| 5:M:1016:ILE:HG12 | 5:M:1017:THR:N   | 2.26                     | 0.51              |
| 6:N:90:MET:HE1    | 6:N:518:PRO:CB   | 2.40                     | 0.51              |
| 6:N:133:ILE:HD13  | 6:N:158:TYR:CD2  | 2.45                     | 0.51              |
| 6:N:155:ASP:N     | 11:N:9432:HOH:O  | 2.43                     | 0.51              |
| 6:N:409:VAL:CG1   | 6:N:435:VAL:HG11 | 2.41                     | 0.51              |
| 6:N:1087:ARG:HB3  | 6:N:1256:LEU:CD2 | 2.41                     | 0.51              |
| 6:N:1379:VAL:HA   | 6:N:1420:LEU:HB2 | 1.92                     | 0.51              |
| 4:A:18:ARG:CZ     | 4:A:123:MET:HE1  | 2.41                     | 0.50              |
| 4:B:27:PRO:C      | 4:B:28:LEU:HD23  | 2.35                     | 0.50              |
| 4:B:160:ASP:HA    | 11:B:363:HOH:O   | 2.09                     | 0.50              |
| 5:C:978:ARG:NH1   | 11:C:1599:HOH:O  | 2.44                     | 0.50              |
| 5:C:1034:GLU:HG2  | 6:D:619:LEU:HD13 | 1.93                     | 0.50              |
| 6:D:133:ILE:HG21  | 6:D:454:ALA:HB1  | 1.93                     | 0.50              |
| 6:D:550:ARG:HA    | 6:D:550:ARG:NE   | 2.20                     | 0.50              |
| 6:D:719:VAL:O     | 6:D:721:VAL:HG23 | 2.10                     | 0.50              |
| 6:D:978:TYR:HB2   | 6:D:983:LEU:HD12 | 1.93                     | 0.50              |
| 6:D:1023:MET:O    | 6:D:1028:ALA:HB3 | 2.11                     | 0.50              |
| 6:D:1031:ASN:HB3  | 6:D:1034:GLN:CD  | 2.36                     | 0.50              |
| 7:E:16:LYS:HA     | 11:E:128:HOH:O   | 2.10                     | 0.50              |
| 5:M:15:LEU:H      | 5:M:15:LEU:HD12  | 1.77                     | 0.50              |
| 5:M:692:GLU:O     | 5:M:696:LYS:HG3  | 2.10                     | 0.50              |
| 5:M:773:LEU:O     | 5:M:777:ILE:HG13 | 2.11                     | 0.50              |
| 5:M:1046:ALA:HB3  | 5:M:1047:HIS:HD2 | 1.76                     | 0.50              |
| 6:N:50:PHE:HB3    | 6:N:522:PRO:HG3  | 1.92                     | 0.50              |
| 6:N:1222:GLY:O    | 6:N:1225:ALA:HB3 | 2.11                     | 0.50              |
| 5:C:51:THR:HG23   | 5:C:348:LEU:HD23 | 1.93                     | 0.50              |
| 5:C:148:PHE:HB2   | 5:C:313:LEU:CD2  | 2.41                     | 0.50              |
| 5:C:338:GLU:HA    | 5:C:341:THR:HG22 | 1.93                     | 0.50              |
| 5:C:468:ARG:CZ    | 5:C:485:TYR:O    | 2.59                     | 0.50              |
| 5:C:564:MET:HE1   | 5:C:995:MET:HB2  | 1.92                     | 0.50              |
| 5:C:920:GLN:O     | 5:C:924:VAL:HG23 | 2.11                     | 0.50              |
| 6:D:133:ILE:HG13  | 6:D:153:LEU:HD12 | 1.93                     | 0.50              |
| 6:D:151:GLN:HA    | 11:D:8479:HOH:O  | 2.12                     | 0.50              |
| 6:D:611:GLN:HG3   | 6:D:611:GLN:O    | 2.11                     | 0.50              |
| 4:K:92:PRO:HG3    | 4:K:146:ARG:HH12 | 1.76                     | 0.50              |
| 5:M:144:PRO:HB2   | 11:M:1136:HOH:O  | 2.11                     | 0.50              |
| 5:M:289:THR:O     | 5:M:291:ALA:N    | 2.44                     | 0.50              |
| 5:M:439:CYS:HB2   | 5:M:541:SER:HB3  | 1.92                     | 0.50              |
| 5:M:888:THR:HG21  | 11:M:1248:HOH:O  | 2.10                     | 0.50              |
| 5:M:916:GLU:HG3   | 5:M:917:LEU:HD23 | 1.93                     | 0.50              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 5:M:943:VAL:HG11   | 5:M:973:VAL:CG2  | 2.41                     | 0.50              |
| 6:N:633:VAL:HB     | 6:N:740:PHE:CE1  | 2.46                     | 0.50              |
| 6:N:643:GLY:O      | 6:N:726:ILE:HG23 | 2.09                     | 0.50              |
| 6:N:937:TYR:CD1    | 6:N:937:TYR:N    | 2.79                     | 0.50              |
| 6:N:1101:VAL:HG22  | 6:N:1428:ALA:HB2 | 1.94                     | 0.50              |
| 6:N:1146:GLY:HA3   | 6:N:1207:TYR:CB  | 2.39                     | 0.50              |
| 10:N:4999:APC:H5'1 | 10:N:4999:APC:H8 | 1.93                     | 0.50              |
| 1:G:18:DG:O4'      | 5:C:1002:GLU:HB3 | 2.11                     | 0.50              |
| 4:A:111:ALA:HB3    | 4:A:124:ASN:O    | 2.11                     | 0.50              |
| 5:C:436:GLY:HA2    | 5:C:456:ALA:CB   | 2.41                     | 0.50              |
| 5:C:1021:LEU:HD23  | 11:C:1374:HOH:O  | 2.11                     | 0.50              |
| 5:C:1105:LYS:NZ    | 5:C:1107:ASN:HB2 | 2.26                     | 0.50              |
| 6:D:134:VAL:O      | 6:D:134:VAL:HG23 | 2.11                     | 0.50              |
| 6:D:657:LEU:HB2    | 6:D:691:LEU:HD22 | 1.93                     | 0.50              |
| 6:D:926:LYS:HA     | 6:D:929:ARG:CD   | 2.41                     | 0.50              |
| 6:D:1403:LEU:O     | 6:D:1407:LEU:HB2 | 2.11                     | 0.50              |
| 5:M:364:GLU:HB2    | 11:M:1318:HOH:O  | 2.10                     | 0.50              |
| 5:M:433:THR:C      | 5:M:435:TYR:H    | 2.18                     | 0.50              |
| 5:M:537:LYS:HG3    | 5:M:905:ILE:CD1  | 2.42                     | 0.50              |
| 5:M:589:ARG:HG3    | 5:M:596:TYR:CZ   | 2.46                     | 0.50              |
| 5:M:702:SER:OG     | 5:M:831:ARG:HB2  | 2.11                     | 0.50              |
| 5:M:726:ILE:HB     | 11:M:1385:HOH:O  | 2.10                     | 0.50              |
| 5:M:852:ILE:N      | 5:M:852:ILE:HD12 | 2.26                     | 0.50              |
| 5:M:1115:LEU:CG    | 6:N:85:VAL:HG12  | 2.40                     | 0.50              |
| 6:N:1424:VAL:CG1   | 6:N:1425:THR:H   | 2.22                     | 0.50              |
| 1:G:18:DG:H5''     | 6:D:628:ARG:NH2  | 2.26                     | 0.50              |
| 2:Y:2:A:C3'        | 2:Y:2:A:H8       | 2.12                     | 0.50              |
| 2:Y:7:G:OP1        | 6:N:530:VAL:HG13 | 2.11                     | 0.50              |
| 3:Z:10:DA:H5''     | 6:N:121:THR:CG2  | 2.41                     | 0.50              |
| 4:B:20:TYR:CE2     | 4:B:198:ARG:HB3  | 2.45                     | 0.50              |
| 5:C:610:ARG:HG3    | 5:C:622:GLU:HG3  | 1.94                     | 0.50              |
| 5:C:737:LEU:HD21   | 5:C:741:GLY:CA   | 2.42                     | 0.50              |
| 5:C:1019:GLN:HE21  | 5:C:1019:GLN:N   | 2.08                     | 0.50              |
| 6:D:87:ARG:HB2     | 6:D:523:ASP:HB3  | 1.93                     | 0.50              |
| 6:D:111:LYS:O      | 6:D:512:MET:HE1  | 2.11                     | 0.50              |
| 6:D:131:LYS:HG3    | 6:D:568:ARG:CG   | 2.41                     | 0.50              |
| 6:D:150:ARG:HG3    | 6:D:464:LEU:HD22 | 1.93                     | 0.50              |
| 6:D:434:ARG:H      | 6:D:447:VAL:CG2  | 2.20                     | 0.50              |
| 5:M:5:ARG:NE       | 5:M:8:ARG:NH1    | 2.57                     | 0.50              |
| 5:M:218:VAL:HA     | 5:M:221:LEU:HD23 | 1.93                     | 0.50              |
| 5:M:862:PRO:HA     | 5:M:975:TYR:CE2  | 2.47                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:1087:VAL:HG22 | 5:M:1091:GLU:OE1  | 2.10                     | 0.50              |
| 6:N:155:ASP:OD1   | 6:N:456:MET:HE1   | 2.11                     | 0.50              |
| 11:N:9174:HOH:O   | 7:O:81:PRO:HG2    | 2.11                     | 0.50              |
| 2:Y:6:U:OP1       | 6:N:528:VAL:HG13  | 2.12                     | 0.50              |
| 4:A:83:LYS:HZ1    | 4:A:168:ASP:HB2   | 1.76                     | 0.50              |
| 4:B:43:ILE:HG21   | 4:B:214:ALA:HA    | 1.94                     | 0.50              |
| 5:C:460:ARG:HB3   | 11:C:1158:HOH:O   | 2.11                     | 0.50              |
| 5:C:597:ALA:CA    | 5:C:655:LEU:HD11  | 2.41                     | 0.50              |
| 5:C:721:ARG:HA    | 5:C:820:ARG:NH2   | 2.26                     | 0.50              |
| 5:C:732:ALA:HA    | 5:C:735:ARG:NH1   | 2.26                     | 0.50              |
| 5:C:1006:HIS:HD1  | 5:C:1027:PHE:HD1  | 1.60                     | 0.50              |
| 11:C:1228:HOH:O   | 6:D:2:LYS:HA      | 2.11                     | 0.50              |
| 6:D:29:PRO:CB     | 6:D:549:ASN:HD21  | 2.23                     | 0.50              |
| 6:D:171:LEU:HD21  | 6:D:192:ALA:HB1   | 1.91                     | 0.50              |
| 6:D:542:ASP:N     | 6:D:542:ASP:OD2   | 2.42                     | 0.50              |
| 4:K:24:VAL:HG22   | 4:K:196:THR:CG2   | 2.41                     | 0.50              |
| 4:K:177:VAL:O     | 5:M:864:GLY:HA2   | 2.12                     | 0.50              |
| 4:L:62:LEU:HD12   | 4:L:62:LEU:N      | 2.22                     | 0.50              |
| 5:M:395:LYS:HE3   | 5:M:407:LYS:HE2   | 1.92                     | 0.50              |
| 5:M:757:GLY:HA2   | 5:M:789:SER:CB    | 2.42                     | 0.50              |
| 5:M:807:ARG:NE    | 5:M:807:ARG:N     | 2.59                     | 0.50              |
| 5:M:1055:LEU:HD11 | 5:M:1076:VAL:HB   | 1.94                     | 0.50              |
| 6:N:637:LEU:CD2   | 6:N:642:CYS:HA    | 2.41                     | 0.50              |
| 6:N:896:ALA:O     | 6:N:900:ILE:HG23  | 2.12                     | 0.50              |
| 6:N:1020:LEU:HD21 | 6:N:1035:ILE:HG23 | 1.93                     | 0.50              |
| 6:N:1195:GLN:HG3  | 6:N:1196:THR:N    | 2.27                     | 0.50              |
| 7:O:54:LEU:HG     | 7:O:58:PRO:CG     | 2.42                     | 0.50              |
| 2:H:14:G:P        | 5:C:409:ARG:HH12  | 2.35                     | 0.50              |
| 5:C:22:GLN:NE2    | 5:C:407:LYS:HG2   | 2.26                     | 0.50              |
| 5:C:275:TYR:HA    | 11:C:1297:HOH:O   | 2.11                     | 0.50              |
| 5:C:630:ARG:HA    | 5:C:705:ILE:CD1   | 2.41                     | 0.50              |
| 5:C:690:ILE:HD12  | 5:C:833:LEU:HD23  | 1.94                     | 0.50              |
| 5:C:713:ARG:NH2   | 6:D:532:GLY:H     | 2.09                     | 0.50              |
| 6:D:108:VAL:HG23  | 6:D:109:PRO:HD3   | 1.94                     | 0.50              |
| 6:D:155:ASP:O     | 6:D:159:ARG:N     | 2.41                     | 0.50              |
| 6:D:470:LEU:HD12  | 6:D:503:LEU:CD2   | 2.42                     | 0.50              |
| 5:M:158:TYR:HE1   | 5:M:314:THR:HA    | 1.76                     | 0.50              |
| 5:M:410:ILE:CD1   | 5:M:455:LEU:HB3   | 2.42                     | 0.50              |
| 5:M:754:ILE:HG12  | 5:M:791:ARG:HH12  | 1.77                     | 0.50              |
| 5:M:810:ASP:HB3   | 5:M:813:VAL:CG1   | 2.36                     | 0.50              |
| 5:M:836:GLY:HA3   | 6:N:724:GLN:HE21  | 1.76                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:613:ARG:HH11  | 6:N:616:GLN:HG2   | 1.76                     | 0.50              |
| 6:N:758:GLU:HA    | 7:O:20:THR:CG2    | 2.42                     | 0.50              |
| 6:N:890:VAL:O     | 6:N:890:VAL:HG23  | 2.11                     | 0.50              |
| 6:N:1240:THR:HB   | 6:N:1252:ILE:HD13 | 1.92                     | 0.50              |
| 6:N:1267:ARG:HA   | 6:N:1331:ASP:HB2  | 1.94                     | 0.50              |
| 7:O:28:GLN:HB3    | 7:O:32:ARG:NH2    | 2.25                     | 0.50              |
| 4:B:26:GLU:HB3    | 4:B:194:LYS:HG3   | 1.93                     | 0.50              |
| 4:B:174:VAL:HG13  | 4:B:200:TRP:O     | 2.12                     | 0.50              |
| 5:C:301:GLU:O     | 5:C:305:PRO:HG2   | 2.12                     | 0.50              |
| 5:C:580:MET:HB3   | 5:C:584:GLU:OE1   | 2.11                     | 0.50              |
| 5:C:627:ARG:CG    | 5:C:628:PHE:H     | 2.25                     | 0.50              |
| 5:C:702:SER:HB3   | 5:C:996:LYS:NZ    | 2.27                     | 0.50              |
| 5:C:820:ARG:HB2   | 11:C:1271:HOH:O   | 2.12                     | 0.50              |
| 6:D:902:LEU:HD23  | 6:D:902:LEU:H     | 1.75                     | 0.50              |
| 6:D:1103:HIS:NE2  | 6:D:1463:LYS:HB2  | 2.27                     | 0.50              |
| 6:D:1213:ARG:HH12 | 7:E:10:PHE:C      | 2.19                     | 0.50              |
| 6:D:1440:PHE:O    | 6:D:1441:GLN:O    | 2.30                     | 0.50              |
| 7:E:68:LEU:CD1    | 7:E:73:LEU:HD22   | 2.41                     | 0.50              |
| 5:M:120:LEU:HD13  | 5:M:121:MET:O     | 2.12                     | 0.50              |
| 5:M:192:PRO:HB2   | 5:M:195:LEU:HB2   | 1.93                     | 0.50              |
| 5:M:622:GLU:O     | 5:M:624:PRO:HD3   | 2.11                     | 0.50              |
| 5:M:837:ASP:HA    | 5:M:999:HIS:CE1   | 2.46                     | 0.50              |
| 5:M:876:VAL:O     | 5:M:879:ARG:O     | 2.30                     | 0.50              |
| 5:M:1105:LYS:C    | 5:M:1107:ASN:HD22 | 2.19                     | 0.50              |
| 6:N:150:ARG:CD    | 6:N:464:LEU:HD21  | 2.41                     | 0.50              |
| 6:N:619:LEU:HB2   | 6:N:621:LYS:HD3   | 1.92                     | 0.50              |
| 6:N:690:ALA:O     | 6:N:694:VAL:HG23  | 2.12                     | 0.50              |
| 6:N:845:ASN:N     | 6:N:848:GLU:HG3   | 2.26                     | 0.50              |
| 6:N:1037:GLN:HG2  | 6:N:1042:ARG:HB2  | 1.93                     | 0.50              |
| 6:N:1192:LEU:HD21 | 6:N:1372:VAL:CG1  | 2.42                     | 0.50              |
| 6:N:1394:VAL:HG11 | 6:N:1397:LYS:HE2  | 1.94                     | 0.50              |
| 1:X:8:DT:H2"      | 1:X:9:DG:C8       | 2.46                     | 0.50              |
| 5:C:57:GLU:O      | 5:C:62:GLY:HA3    | 2.12                     | 0.50              |
| 5:C:290:LEU:HD23  | 5:C:290:LEU:H     | 1.75                     | 0.50              |
| 5:C:999:HIS:HD2   | 5:C:1004:LYS:NZ   | 2.10                     | 0.50              |
| 6:D:54:LYS:CD     | 6:D:55:ASP:H      | 2.25                     | 0.50              |
| 6:D:397:LYS:O     | 6:D:448:GLU:HB2   | 2.12                     | 0.50              |
| 6:D:562:ALA:HB1   | 6:D:567:ILE:HD11  | 1.94                     | 0.50              |
| 6:D:634:GLY:CA    | 6:D:727:GLN:HE21  | 2.23                     | 0.50              |
| 5:M:5:ARG:NE      | 5:M:8:ARG:HH22    | 2.00                     | 0.50              |
| 5:M:1020:PRO:O    | 5:M:1021:LEU:HD12 | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:1034:GLU:HB3  | 6:N:619:LEU:CD2   | 2.40                     | 0.50              |
| 6:N:52:PRO:HG2    | 6:N:80:VAL:HG13   | 1.93                     | 0.50              |
| 6:N:79:GLU:HG3    | 11:N:9414:HOH:O   | 2.12                     | 0.50              |
| 6:N:475:LYS:HA    | 6:N:478:LEU:HG    | 1.94                     | 0.50              |
| 6:N:982:PHE:HB3   | 6:N:983:LEU:HD23  | 1.92                     | 0.50              |
| 6:N:1139:ASP:HB3  | 6:N:1357:ARG:NH2  | 2.27                     | 0.50              |
| 6:N:1237:THR:N    | 11:N:9434:HOH:O   | 2.45                     | 0.50              |
| 4:B:62:LEU:H      | 4:B:62:LEU:HD12   | 1.77                     | 0.50              |
| 5:C:265:ARG:HD2   | 5:C:267:TYR:CB    | 2.41                     | 0.50              |
| 5:C:906:PHE:CZ    | 6:D:1067:VAL:HA   | 2.46                     | 0.50              |
| 6:D:100:ALA:HA    | 6:D:514:LEU:H     | 1.76                     | 0.50              |
| 6:D:127:LEU:HD23  | 6:D:134:VAL:HG22  | 1.93                     | 0.50              |
| 6:D:133:ILE:HG13  | 6:D:153:LEU:CD1   | 2.41                     | 0.50              |
| 6:D:477:LEU:HD13  | 6:D:496:LEU:HA    | 1.94                     | 0.50              |
| 6:D:510:GLU:O     | 6:D:513:ILE:HD12  | 2.12                     | 0.50              |
| 6:D:683:ILE:HG23  | 6:D:687:VAL:HG21  | 1.94                     | 0.50              |
| 6:D:721:VAL:HG12  | 6:D:722:GLU:N     | 2.26                     | 0.50              |
| 6:D:739:ASP:O     | 6:D:741:ASP:N     | 2.45                     | 0.50              |
| 6:D:1021:TYR:HA   | 11:D:8152:HOH:O   | 2.11                     | 0.50              |
| 7:E:18:ARG:O      | 7:E:22:VAL:HG23   | 2.12                     | 0.50              |
| 5:M:17:PRO:HG3    | 11:M:1503:HOH:O   | 2.12                     | 0.50              |
| 5:M:22:GLN:OE1    | 5:M:407:LYS:HB3   | 2.12                     | 0.50              |
| 5:M:31:GLN:CD     | 5:M:34:VAL:HG23   | 2.36                     | 0.50              |
| 5:M:32:ALA:HB2    | 11:M:1235:HOH:O   | 2.12                     | 0.50              |
| 5:M:290:LEU:HB3   | 5:M:302:VAL:CG1   | 2.41                     | 0.50              |
| 5:M:432:ARG:HH21  | 6:N:1048:PRO:HD2  | 1.77                     | 0.50              |
| 5:M:662:GLU:HG2   | 5:M:663:ASN:CG    | 2.37                     | 0.50              |
| 6:N:637:LEU:HD12  | 6:N:641:GLN:OE1   | 2.12                     | 0.50              |
| 6:N:1087:ARG:HE   | 6:N:1253:THR:HG23 | 1.77                     | 0.50              |
| 6:N:1236:LEU:HD11 | 6:N:1361:VAL:CG2  | 2.42                     | 0.50              |
| 2:H:7:G:O5'       | 2:H:7:G:H8        | 1.95                     | 0.49              |
| 3:Z:9:DG:H2''     | 3:Z:10:DA:C8      | 2.47                     | 0.49              |
| 4:A:163:ASN:HD21  | 5:C:744:ARG:HH22  | 1.59                     | 0.49              |
| 5:C:73:LEU:N      | 5:C:73:LEU:HD23   | 2.27                     | 0.49              |
| 5:C:97:ARG:HA     | 5:C:111:ASP:O     | 2.12                     | 0.49              |
| 5:C:113:VAL:O     | 5:C:115:LEU:HG    | 2.11                     | 0.49              |
| 5:C:119:PRO:HG2   | 5:C:386:PHE:CD2   | 2.47                     | 0.49              |
| 5:C:408:ARG:CG    | 5:C:455:LEU:H     | 2.24                     | 0.49              |
| 6:D:82:LYS:CB     | 6:D:84:ILE:HG12   | 2.42                     | 0.49              |
| 6:D:926:LYS:HG3   | 11:D:8014:HOH:O   | 2.11                     | 0.49              |
| 6:D:977:ALA:CB    | 6:D:983:LEU:HD21  | 2.42                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:1144:LEU:HD11 | 6:D:1186:VAL:CG2  | 2.37                     | 0.49              |
| 6:D:1402:ALA:HB3  | 11:D:8309:HOH:O   | 2.11                     | 0.49              |
| 6:D:1443:THR:O    | 6:D:1447:LEU:HD13 | 2.11                     | 0.49              |
| 5:M:77:PRO:HG2    | 5:M:117:HIS:NE2   | 2.27                     | 0.49              |
| 5:M:134:ARG:CD    | 5:M:392:SER:HB3   | 2.42                     | 0.49              |
| 5:M:139:GLN:HE21  | 5:M:418:LEU:CD2   | 2.25                     | 0.49              |
| 6:N:143:ASN:OD1   | 6:N:145:VAL:HG12  | 2.11                     | 0.49              |
| 6:N:502:PHE:CZ    | 6:N:509:PRO:HB3   | 2.46                     | 0.49              |
| 6:N:838:ARG:NH1   | 6:N:838:ARG:HG2   | 2.26                     | 0.49              |
| 6:N:864:VAL:HB    | 11:N:9057:HOH:O   | 2.11                     | 0.49              |
| 6:N:1020:LEU:HD23 | 6:N:1021:TYR:N    | 2.27                     | 0.49              |
| 6:N:1042:ARG:NH2  | 11:N:9443:HOH:O   | 2.45                     | 0.49              |
| 6:N:1364:HIS:CE1  | 6:N:1366:LYS:HG3  | 2.47                     | 0.49              |
| 6:N:1459:LEU:HD21 | 6:N:1468:LEU:HD22 | 1.93                     | 0.49              |
| 6:N:1489:GLN:O    | 6:N:1493:LYS:HG2  | 2.12                     | 0.49              |
| 1:G:12:DG:H2''    | 1:G:13:DT:C5'     | 2.43                     | 0.49              |
| 4:B:86:VAL:HG12   | 4:B:124:ASN:HB2   | 1.94                     | 0.49              |
| 5:C:264:PRO:HD2   | 11:C:1410:HOH:O   | 2.12                     | 0.49              |
| 5:C:577:PRO:HB2   | 5:C:580:MET:HG2   | 1.93                     | 0.49              |
| 6:D:29:PRO:HB3    | 6:D:549:ASN:HD21  | 1.77                     | 0.49              |
| 6:D:185:VAL:HG21  | 6:D:203:ALA:HB2   | 1.93                     | 0.49              |
| 6:D:547:LEU:HB3   | 11:D:8068:HOH:O   | 2.11                     | 0.49              |
| 6:D:634:GLY:CA    | 6:D:727:GLN:HG2   | 2.43                     | 0.49              |
| 6:D:709:HIS:N     | 6:D:709:HIS:CD2   | 2.80                     | 0.49              |
| 7:E:83:ASP:O      | 7:E:86:GLN:HG3    | 2.13                     | 0.49              |
| 5:M:21:ILE:H      | 5:M:21:ILE:HD12   | 1.77                     | 0.49              |
| 5:M:198:ARG:HE    | 5:M:198:ARG:HA    | 1.77                     | 0.49              |
| 5:M:415:PRO:HD2   | 5:M:418:LEU:HD13  | 1.94                     | 0.49              |
| 5:M:583:LEU:N     | 5:M:584:GLU:OE2   | 2.45                     | 0.49              |
| 5:M:676:ILE:O     | 5:M:676:ILE:HG23  | 2.11                     | 0.49              |
| 5:M:959:PRO:O     | 5:M:963:LEU:HG    | 2.11                     | 0.49              |
| 6:N:522:PRO:HG2   | 6:N:523:ASP:N     | 2.26                     | 0.49              |
| 6:N:1010:ASN:HB3  | 11:N:9288:HOH:O   | 2.12                     | 0.49              |
| 5:C:54:ILE:HG22   | 5:C:66:LEU:HB3    | 1.95                     | 0.49              |
| 5:C:64:LEU:HD22   | 5:C:359:MET:HG3   | 1.93                     | 0.49              |
| 5:C:260:LEU:HA    | 5:C:291:ALA:CB    | 2.42                     | 0.49              |
| 5:C:881:ASN:N     | 5:C:881:ASN:ND2   | 2.60                     | 0.49              |
| 6:D:762:GLN:NE2   | 7:E:20:THR:OG1    | 2.45                     | 0.49              |
| 6:D:836:VAL:O     | 6:D:840:LYS:HG3   | 2.12                     | 0.49              |
| 6:D:1143:GLY:O    | 6:D:1147:ARG:NE   | 2.45                     | 0.49              |
| 6:D:1211:MET:HE1  | 6:D:1213:ARG:HD3  | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:1495:ILE:HG12 | 7:E:80:VAL:CG1    | 2.39                     | 0.49              |
| 4:L:47:SER:HB2    | 4:L:217:ILE:HD13  | 1.95                     | 0.49              |
| 4:L:103:ALA:HB1   | 4:L:107:LYS:CE    | 2.42                     | 0.49              |
| 5:M:276:LYS:O     | 5:M:280:LYS:HB3   | 2.12                     | 0.49              |
| 6:N:133:ILE:CG2   | 6:N:454:ALA:HB1   | 2.41                     | 0.49              |
| 6:N:437:VAL:HG13  | 6:N:444:VAL:HG22  | 1.94                     | 0.49              |
| 6:N:957:PRO:HG3   | 6:N:1007:VAL:HA   | 1.94                     | 0.49              |
| 6:N:996:TRP:CE2   | 6:N:1056:PRO:HG2  | 2.47                     | 0.49              |
| 6:N:1168:MET:CE   | 6:N:1171:VAL:HB   | 2.37                     | 0.49              |
| 6:N:1189:ARG:NH1  | 6:N:1203:LYS:HB2  | 2.28                     | 0.49              |
| 7:O:18:ARG:O      | 7:O:22:VAL:HG23   | 2.12                     | 0.49              |
| 7:O:68:LEU:HD12   | 7:O:73:LEU:HD22   | 1.93                     | 0.49              |
| 4:A:68:ILE:HD12   | 4:A:68:ILE:N      | 2.27                     | 0.49              |
| 4:A:83:LYS:HE2    | 4:A:170:VAL:HG13  | 1.93                     | 0.49              |
| 4:A:190:THR:HG23  | 11:A:369:HOH:O    | 2.12                     | 0.49              |
| 4:B:62:LEU:HD13   | 4:B:63:HIS:CE1    | 2.47                     | 0.49              |
| 5:C:8:ARG:N       | 5:C:907:ASP:OD2   | 2.45                     | 0.49              |
| 5:C:674:VAL:CG2   | 5:C:869:VAL:HG13  | 2.42                     | 0.49              |
| 5:C:689:VAL:HG11  | 5:C:870:ILE:HD11  | 1.94                     | 0.49              |
| 5:C:876:VAL:O     | 5:C:879:ARG:O     | 2.30                     | 0.49              |
| 5:C:1022:GLY:HA3  | 5:C:1026:GLN:O    | 2.12                     | 0.49              |
| 6:D:17:LYS:O      | 6:D:20:SER:HB3    | 2.12                     | 0.49              |
| 6:D:172:PRO:HG2   | 6:D:175:VAL:CG2   | 2.42                     | 0.49              |
| 6:D:519:VAL:HG12  | 6:D:544:TYR:CE2   | 2.48                     | 0.49              |
| 6:D:1124:GLN:HG2  | 6:D:1133:ARG:CG   | 2.42                     | 0.49              |
| 6:D:1258:ARG:HA   | 6:D:1261:GLU:OE2  | 2.12                     | 0.49              |
| 6:D:1384:PRO:HG3  | 6:D:1389:LEU:HA   | 1.92                     | 0.49              |
| 5:M:689:VAL:HG11  | 5:M:870:ILE:HD11  | 1.93                     | 0.49              |
| 5:M:817:PRO:C     | 5:M:819:VAL:H     | 2.20                     | 0.49              |
| 5:M:897:LEU:HD12  | 11:M:1461:HOH:O   | 2.12                     | 0.49              |
| 2:H:16:G:H21      | 6:D:705:ALA:HB1   | 1.78                     | 0.49              |
| 4:A:150:TYR:HH    | 5:C:696:LYS:HA    | 1.77                     | 0.49              |
| 4:A:199:ILE:HD12  | 4:A:199:ILE:N     | 2.26                     | 0.49              |
| 5:C:304:LEU:HA    | 11:C:1215:HOH:O   | 2.12                     | 0.49              |
| 5:C:432:ARG:HH12  | 6:D:1072:ILE:CD1  | 2.25                     | 0.49              |
| 5:C:490:GLU:HB3   | 5:C:493:ARG:CZ    | 2.42                     | 0.49              |
| 5:C:496:ILE:HA    | 5:C:531:PHE:O     | 2.11                     | 0.49              |
| 5:C:569:VAL:HG13  | 5:C:996:LYS:HZ3   | 1.77                     | 0.49              |
| 5:C:1001:VAL:O    | 5:C:1001:VAL:HG12 | 2.13                     | 0.49              |
| 6:D:118:LEU:HD21  | 6:D:464:LEU:HD13  | 1.94                     | 0.49              |
| 6:D:465:LEU:HD13  | 6:D:513:ILE:HD11  | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:1125:PRO:HB3  | 6:D:1130:ARG:NH1  | 2.27                     | 0.49              |
| 6:D:1374:GLN:OE1  | 6:D:1377:LYS:HD3  | 2.12                     | 0.49              |
| 4:K:30:ARG:NH2    | 5:M:938:LYS:HD2   | 2.25                     | 0.49              |
| 4:K:218:LEU:O     | 4:K:222:LEU:HD13  | 2.12                     | 0.49              |
| 5:M:340:MET:HG2   | 5:M:386:PHE:HE1   | 1.78                     | 0.49              |
| 5:M:574:ALA:HB2   | 11:M:1443:HOH:O   | 2.12                     | 0.49              |
| 5:M:736:ASP:HA    | 5:M:744:ARG:HH11  | 1.77                     | 0.49              |
| 5:M:1009:SER:HB3  | 6:N:651:GLU:O     | 2.13                     | 0.49              |
| 5:M:1016:ILE:HD13 | 5:M:1017:THR:H    | 1.78                     | 0.49              |
| 6:N:10:ILE:HG13   | 6:N:1434:TRP:CZ2  | 2.47                     | 0.49              |
| 6:N:516:ALA:O     | 6:N:518:PRO:HD3   | 2.13                     | 0.49              |
| 7:O:33:HIS:HB2    | 7:O:37:ASN:HD21   | 1.77                     | 0.49              |
| 5:C:127:PHE:O     | 5:C:133:ASP:HA    | 2.12                     | 0.49              |
| 5:C:150:PRO:HG3   | 5:C:158:TYR:HD2   | 1.78                     | 0.49              |
| 5:C:165:LEU:HD11  | 11:C:1123:HOH:O   | 2.13                     | 0.49              |
| 5:C:235:LEU:C     | 5:C:235:LEU:HD23  | 2.37                     | 0.49              |
| 5:C:409:ARG:HD2   | 5:C:452:ILE:CG2   | 2.42                     | 0.49              |
| 5:C:437:ARG:O     | 5:C:467:ILE:HD13  | 2.12                     | 0.49              |
| 5:C:537:LYS:H     | 5:C:537:LYS:HD2   | 1.78                     | 0.49              |
| 6:D:108:VAL:CB    | 6:D:109:PRO:HD3   | 2.42                     | 0.49              |
| 6:D:138:LYS:HD2   | 6:D:450:TYR:OH    | 2.13                     | 0.49              |
| 6:D:584:ASN:CG    | 6:D:590:PRO:HD2   | 2.37                     | 0.49              |
| 6:D:610:LYS:CA    | 6:D:615:ARG:HD3   | 2.42                     | 0.49              |
| 6:D:926:LYS:HA    | 6:D:929:ARG:HH11  | 1.78                     | 0.49              |
| 6:D:1087:ARG:HG3  | 6:D:1237:THR:CG2  | 2.40                     | 0.49              |
| 6:D:1263:PHE:O    | 6:D:1424:VAL:HG12 | 2.12                     | 0.49              |
| 6:D:1418:LYS:HD3  | 6:D:1419:PRO:CD   | 2.42                     | 0.49              |
| 5:M:127:PHE:O     | 5:M:133:ASP:HA    | 2.13                     | 0.49              |
| 5:M:265:ARG:HH22  | 5:M:332:ARG:HH22  | 1.60                     | 0.49              |
| 5:M:319:GLY:HA3   | 11:M:1388:HOH:O   | 2.11                     | 0.49              |
| 5:M:471:TYR:HB2   | 11:M:1201:HOH:O   | 2.11                     | 0.49              |
| 5:M:561:GLY:HA2   | 5:M:564:MET:HG3   | 1.93                     | 0.49              |
| 5:M:837:ASP:HA    | 5:M:999:HIS:HE1   | 1.78                     | 0.49              |
| 6:N:137:PRO:HD2   | 6:N:453:ASP:OD1   | 2.12                     | 0.49              |
| 6:N:641:GLN:HB3   | 6:N:717:GLN:O     | 2.12                     | 0.49              |
| 6:N:800:LYS:HE3   | 6:N:804:LEU:HB3   | 1.93                     | 0.49              |
| 6:N:897:TRP:HA    | 6:N:900:ILE:CG1   | 2.37                     | 0.49              |
| 6:N:947:ILE:HG23  | 11:N:9083:HOH:O   | 2.11                     | 0.49              |
| 6:N:1139:ASP:O    | 6:N:1142:ALA:HB3  | 2.13                     | 0.49              |
| 4:A:73:GLU:OE1    | 4:A:130:ALA:HA    | 2.12                     | 0.49              |
| 4:B:102:LYS:HZ1   | 4:B:137:ARG:NE    | 2.11                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:89:THR:HA     | 5:C:129:ILE:O     | 2.12                     | 0.49              |
| 5:C:101:ILE:HG22  | 5:C:102:HIS:N     | 2.27                     | 0.49              |
| 5:C:162:ILE:HD12  | 5:C:172:ILE:CB    | 2.43                     | 0.49              |
| 5:C:192:PRO:HB2   | 5:C:195:LEU:H     | 1.78                     | 0.49              |
| 5:C:264:PRO:HB3   | 5:C:289:THR:CB    | 2.43                     | 0.49              |
| 5:C:270:GLY:O     | 5:C:274:ARG:HD2   | 2.12                     | 0.49              |
| 5:C:596:TYR:HB2   | 11:C:1524:HOH:O   | 2.12                     | 0.49              |
| 5:C:1111:ILE:HD12 | 5:C:1112:PHE:H    | 1.78                     | 0.49              |
| 6:D:108:VAL:HB    | 6:D:109:PRO:HD3   | 1.94                     | 0.49              |
| 6:D:191:LEU:HG    | 6:D:197:SER:OG    | 2.13                     | 0.49              |
| 6:D:613:ARG:O     | 6:D:616:GLN:HB3   | 2.13                     | 0.49              |
| 6:D:899:LEU:HD13  | 6:D:914:LEU:CD2   | 2.37                     | 0.49              |
| 6:D:957:PRO:O     | 6:D:960:LYS:HB3   | 2.13                     | 0.49              |
| 6:D:1211:MET:SD   | 6:D:1213:ARG:HG2  | 2.52                     | 0.49              |
| 6:D:1376:MET:HE3  | 6:D:1421:LEU:HD22 | 1.95                     | 0.49              |
| 7:E:38:THR:HG23   | 7:E:41:GLU:OE2    | 2.13                     | 0.49              |
| 4:K:63:HIS:CD2    | 4:K:66:SER:HB2    | 2.48                     | 0.49              |
| 4:L:73:GLU:CD     | 4:L:130:ALA:HA    | 2.38                     | 0.49              |
| 5:M:25:SER:CB     | 5:M:335:THR:HB    | 2.42                     | 0.49              |
| 5:M:31:GLN:NE2    | 5:M:71:TYR:OH     | 2.45                     | 0.49              |
| 5:M:146:VAL:HG12  | 5:M:162:ILE:HA    | 1.93                     | 0.49              |
| 5:M:250:ARG:HG3   | 5:M:250:ARG:HH11  | 1.78                     | 0.49              |
| 5:M:403:SER:O     | 5:M:407:LYS:HG3   | 2.13                     | 0.49              |
| 5:M:902:ILE:O     | 5:M:904:PRO:HD3   | 2.12                     | 0.49              |
| 5:M:1065:ALA:HB1  | 5:M:1077:PRO:CG   | 2.36                     | 0.49              |
| 6:N:151:GLN:HG3   | 6:N:152:LEU:H     | 1.78                     | 0.49              |
| 6:N:1101:VAL:HG21 | 6:N:1424:VAL:HG23 | 1.95                     | 0.49              |
| 6:N:1338:ALA:HB2  | 11:N:9199:HOH:O   | 2.12                     | 0.49              |
| 6:N:1476:THR:C    | 6:N:1478:SER:H    | 2.19                     | 0.49              |
| 5:C:98:LEU:HD12   | 5:C:98:LEU:N      | 2.28                     | 0.49              |
| 5:C:141:HIS:CE1   | 5:C:334:ARG:HG3   | 2.47                     | 0.49              |
| 5:C:150:PRO:HG3   | 5:C:158:TYR:CD2   | 2.47                     | 0.49              |
| 5:C:162:ILE:O     | 5:C:164:PRO:HD3   | 2.12                     | 0.49              |
| 5:C:265:ARG:O     | 5:C:288:ARG:HD2   | 2.13                     | 0.49              |
| 5:C:537:LYS:HG3   | 5:C:545:ASN:HD21  | 1.78                     | 0.49              |
| 5:C:817:PRO:C     | 5:C:819:VAL:H     | 2.20                     | 0.49              |
| 5:C:918:LEU:HD23  | 5:C:968:LEU:HA    | 1.93                     | 0.49              |
| 6:D:204:LEU:O     | 6:D:394:LEU:HD23  | 2.13                     | 0.49              |
| 6:D:754:PHE:CE2   | 6:D:1476:THR:HG21 | 2.48                     | 0.49              |
| 6:D:1000:THR:HG23 | 6:D:1001:GLU:N    | 2.28                     | 0.49              |
| 6:D:1087:ARG:CG   | 6:D:1237:THR:HG21 | 2.41                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:1192:LEU:HD22 | 6:D:1345:GLU:CG   | 2.43                     | 0.49              |
| 4:L:111:ALA:HB3   | 4:L:124:ASN:O     | 2.13                     | 0.49              |
| 5:M:136:ILE:HD11  | 11:M:1417:HOH:O   | 2.12                     | 0.49              |
| 5:M:374:ASN:HD22  | 5:M:377:PRO:HD3   | 1.76                     | 0.49              |
| 6:N:116:LEU:HD22  | 6:N:118:LEU:HG    | 1.95                     | 0.49              |
| 6:N:827:ILE:O     | 6:N:837:GLY:HA3   | 2.12                     | 0.49              |
| 6:N:1156:LEU:HG   | 6:N:1177:ALA:HB2  | 1.94                     | 0.49              |
| 6:N:1213:ARG:NH2  | 7:O:15:SER:HA     | 2.27                     | 0.49              |
| 6:N:1487:VAL:HA   | 11:N:9036:HOH:O   | 2.11                     | 0.49              |
| 6:N:1488:ASP:OD1  | 6:N:1488:ASP:N    | 2.46                     | 0.49              |
| 4:A:173:PRO:HB2   | 4:A:205:VAL:HG22  | 1.94                     | 0.49              |
| 4:B:176:ARG:HG3   | 4:B:200:TRP:CE3   | 2.47                     | 0.49              |
| 5:C:106:GLY:C     | 5:C:107:LEU:HD23  | 2.38                     | 0.49              |
| 5:C:190:LYS:HB2   | 11:C:1219:HOH:O   | 2.13                     | 0.49              |
| 5:C:313:LEU:HA    | 5:C:321:GLU:HG3   | 1.94                     | 0.49              |
| 5:C:368:THR:N     | 5:C:369:PRO:HD2   | 2.28                     | 0.49              |
| 5:C:433:THR:CG2   | 5:C:488:ALA:HB1   | 2.28                     | 0.49              |
| 5:C:575:GLN:HG2   | 5:C:671:ASN:OD1   | 2.11                     | 0.49              |
| 5:C:689:VAL:O     | 5:C:869:VAL:HG23  | 2.13                     | 0.49              |
| 5:C:1040:LEU:HD21 | 5:C:1048:THR:HG22 | 1.95                     | 0.49              |
| 6:D:38:LYS:HZ1    | 6:D:59:ALA:HB1    | 1.77                     | 0.49              |
| 6:D:184:GLU:HG3   | 11:D:8384:HOH:O   | 2.13                     | 0.49              |
| 6:D:883:ALA:HB2   | 11:D:8066:HOH:O   | 2.12                     | 0.49              |
| 6:D:915:VAL:HG11  | 6:D:931:LEU:HD21  | 1.94                     | 0.49              |
| 4:L:121:GLU:CD    | 4:L:123:MET:HG2   | 2.37                     | 0.49              |
| 5:M:68:PHE:CZ     | 5:M:71:TYR:HD2    | 2.24                     | 0.49              |
| 5:M:301:GLU:O     | 5:M:305:PRO:HG2   | 2.13                     | 0.49              |
| 5:M:328:LEU:N     | 5:M:328:LEU:HD12  | 2.28                     | 0.49              |
| 5:M:328:LEU:HD11  | 5:M:434:HIS:CD2   | 2.47                     | 0.49              |
| 5:M:524:VAL:HG12  | 5:M:528:GLU:HB2   | 1.95                     | 0.49              |
| 5:M:971:LYS:HE2   | 11:M:1216:HOH:O   | 2.13                     | 0.49              |
| 6:N:92:HIS:HA     | 6:N:517:VAL:O     | 2.13                     | 0.49              |
| 6:N:538:SER:O     | 6:N:541:ASN:ND2   | 2.45                     | 0.49              |
| 6:N:565:ILE:HD12  | 6:N:565:ILE:N     | 2.26                     | 0.49              |
| 6:N:703:ASN:ND2   | 6:N:704:ARG:H     | 2.11                     | 0.49              |
| 6:N:1498:ALA:HB2  | 7:O:88:GLU:OE1    | 2.13                     | 0.49              |
| 4:B:57:TYR:CE2    | 4:B:161:ARG:HG2   | 2.48                     | 0.49              |
| 4:B:173:PRO:HA    | 4:B:202:ASP:OD2   | 2.13                     | 0.49              |
| 5:C:46:ALA:O      | 5:C:49:ARG:HG2    | 2.13                     | 0.49              |
| 5:C:722:ILE:O     | 5:C:722:ILE:HG23  | 2.13                     | 0.49              |
| 5:C:762:LYS:HD2   | 5:C:786:LYS:CB    | 2.42                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:860:HIS:CE1  | 5:C:975:TYR:HB2   | 2.48                     | 0.49              |
| 5:C:906:PHE:CD1  | 6:D:1067:VAL:HG13 | 2.48                     | 0.49              |
| 6:D:192:ALA:HB1  | 6:D:193:PRO:HD2   | 1.94                     | 0.49              |
| 6:D:396:VAL:CG1  | 6:D:447:VAL:HG12  | 2.42                     | 0.49              |
| 6:D:508:ARG:HD2  | 6:D:509:PRO:HD2   | 1.94                     | 0.49              |
| 6:D:729:HIS:CE1  | 6:D:731:LEU:HB2   | 2.48                     | 0.49              |
| 6:D:737:ASN:ND2  | 10:D:3999:APC:O3' | 2.38                     | 0.49              |
| 4:L:7:LYS:HD2    | 4:L:7:LYS:C       | 2.37                     | 0.49              |
| 5:M:433:THR:O    | 5:M:437:ARG:HD2   | 2.12                     | 0.49              |
| 5:M:498:GLN:NE2  | 6:N:1068:LEU:HG   | 2.28                     | 0.49              |
| 5:M:687:ALA:HB2  | 6:N:740:PHE:HB2   | 1.95                     | 0.49              |
| 5:M:728:HIS:C    | 5:M:729:LEU:HG    | 2.38                     | 0.49              |
| 5:M:759:THR:HB   | 5:M:785:VAL:HG22  | 1.95                     | 0.49              |
| 5:M:893:ALA:HB2  | 5:M:918:LEU:HD12  | 1.95                     | 0.49              |
| 5:M:981:GLU:HG3  | 5:M:982:PRO:HD2   | 1.94                     | 0.49              |
| 6:N:545:ARG:CZ   | 6:N:545:ARG:HB2   | 2.42                     | 0.49              |
| 6:N:829:VAL:O    | 6:N:835:SER:HB3   | 2.12                     | 0.49              |
| 6:N:1209:LEU:O   | 6:N:1210:SER:C    | 2.54                     | 0.49              |
| 2:Y:2:A:C8       | 2:Y:2:A:C4'       | 2.95                     | 0.48              |
| 5:C:18:LEU:HD22  | 5:C:404:LEU:CD2   | 2.43                     | 0.48              |
| 5:C:276:LYS:O    | 5:C:280:LYS:HB2   | 2.12                     | 0.48              |
| 5:C:439:CYS:SG   | 5:C:442:GLU:N     | 2.75                     | 0.48              |
| 5:C:439:CYS:SG   | 5:C:442:GLU:HB2   | 2.52                     | 0.48              |
| 5:C:579:VAL:CG1  | 5:C:887:GLU:HG3   | 2.33                     | 0.48              |
| 5:C:880:MET:HE3  | 6:D:1061:PHE:CE2  | 2.48                     | 0.48              |
| 11:C:1216:HOH:O  | 6:D:606:ILE:HD11  | 2.12                     | 0.48              |
| 6:D:675:ARG:HA   | 6:D:678:GLU:HG2   | 1.94                     | 0.48              |
| 6:D:699:VAL:H    | 6:D:756:GLN:HE22  | 1.55                     | 0.48              |
| 6:D:1033:GLN:N   | 11:D:8254:HOH:O   | 2.46                     | 0.48              |
| 6:D:1102:THR:CG2 | 6:D:1370:ILE:HG22 | 2.42                     | 0.48              |
| 6:D:1136:LYS:HB2 | 6:D:1139:ASP:OD1  | 2.13                     | 0.48              |
| 6:D:1231:GLU:CG  | 6:D:1232:PRO:HD3  | 2.43                     | 0.48              |
| 4:K:1:MET:O      | 4:K:6:LEU:HD13    | 2.12                     | 0.48              |
| 4:L:24:VAL:HG12  | 4:L:26:GLU:OE2    | 2.13                     | 0.48              |
| 4:L:89:PHE:CD1   | 4:L:120:VAL:HG13  | 2.48                     | 0.48              |
| 4:L:124:ASN:ND2  | 4:L:127:LEU:HB2   | 2.28                     | 0.48              |
| 5:M:95:TYR:CD2   | 5:M:114:PHE:HB2   | 2.47                     | 0.48              |
| 5:M:127:PHE:HZ   | 5:M:336:VAL:HG11  | 1.78                     | 0.48              |
| 5:M:174:LEU:HD13 | 5:M:307:LEU:HD13  | 1.94                     | 0.48              |
| 5:M:250:ARG:HG2  | 5:M:253:ALA:CB    | 2.43                     | 0.48              |
| 5:M:262:ALA:HB3  | 11:M:1334:HOH:O   | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:376:ARG:HG3   | 5:M:376:ARG:NH1   | 2.28                     | 0.48              |
| 5:M:490:GLU:HG2   | 5:M:493:ARG:CZ    | 2.42                     | 0.48              |
| 5:M:630:ARG:HA    | 11:M:1247:HOH:O   | 2.12                     | 0.48              |
| 5:M:642:ARG:HG3   | 5:M:657:ASP:OD2   | 2.13                     | 0.48              |
| 5:M:673:LEU:HB3   | 5:M:868:ASP:OD1   | 2.13                     | 0.48              |
| 6:N:470:LEU:CD2   | 6:N:470:LEU:H     | 2.24                     | 0.48              |
| 6:N:729:HIS:CE1   | 6:N:731:LEU:H     | 2.31                     | 0.48              |
| 6:N:739:ASP:O     | 6:N:741:ASP:N     | 2.45                     | 0.48              |
| 6:N:1114:THR:HG23 | 6:N:1114:THR:O    | 2.13                     | 0.48              |
| 4:A:108:GLU:OE2   | 4:A:131:THR:HG22  | 2.13                     | 0.48              |
| 4:A:180:GLN:HB3   | 4:A:182:GLU:OE2   | 2.11                     | 0.48              |
| 4:B:111:ALA:HB3   | 4:B:124:ASN:O     | 2.12                     | 0.48              |
| 5:C:571:LEU:HD12  | 5:C:996:LYS:HZ2   | 1.79                     | 0.48              |
| 5:C:723:THR:HG23  | 5:C:725:ASP:H     | 1.78                     | 0.48              |
| 5:C:1049:LEU:CD2  | 6:D:1472:ILE:HD12 | 2.37                     | 0.48              |
| 5:C:1102:LEU:N    | 6:D:7:LYS:O       | 2.46                     | 0.48              |
| 6:D:522:PRO:HG2   | 6:D:523:ASP:H     | 1.78                     | 0.48              |
| 6:D:689:ASP:O     | 6:D:693:GLU:HG3   | 2.12                     | 0.48              |
| 6:D:1217:ILE:HD12 | 6:D:1480:PHE:CE2  | 2.48                     | 0.48              |
| 6:D:1366:LYS:HA   | 6:D:1369:GLU:OE2  | 2.13                     | 0.48              |
| 6:D:1483:PHE:N    | 6:D:1483:PHE:CD1  | 2.81                     | 0.48              |
| 4:L:30:ARG:HH11   | 4:L:30:ARG:HB2    | 1.78                     | 0.48              |
| 5:M:19:THR:HG22   | 5:M:404:LEU:CD1   | 2.41                     | 0.48              |
| 5:M:39:ARG:H      | 5:M:39:ARG:CD     | 2.18                     | 0.48              |
| 5:M:165:LEU:HD12  | 5:M:166:PRO:C     | 2.38                     | 0.48              |
| 5:M:217:LEU:HD12  | 5:M:311:PHE:CD2   | 2.48                     | 0.48              |
| 5:M:302:VAL:O     | 5:M:306:THR:HG23  | 2.14                     | 0.48              |
| 5:M:642:ARG:NH1   | 11:M:1230:HOH:O   | 2.45                     | 0.48              |
| 5:M:854:PRO:HB2   | 5:M:856:GLU:CD    | 2.38                     | 0.48              |
| 5:M:1043:TYR:CE1  | 6:N:710:ARG:HG3   | 2.48                     | 0.48              |
| 6:N:646:LYS:NZ    | 6:N:722:GLU:HG2   | 2.28                     | 0.48              |
| 1:X:16:DG:N2      | 11:X:2005:HOH:O   | 2.46                     | 0.48              |
| 4:A:150:TYR:OH    | 5:C:696:LYS:HA    | 2.12                     | 0.48              |
| 4:B:115:LEU:HD12  | 4:B:115:LEU:O     | 2.13                     | 0.48              |
| 5:C:119:PRO:HB2   | 11:C:1174:HOH:O   | 2.12                     | 0.48              |
| 5:C:398:THR:HB    | 5:C:399:ASN:HD22  | 1.79                     | 0.48              |
| 5:C:548:PRO:HG3   | 5:C:842:ARG:NH1   | 2.28                     | 0.48              |
| 5:C:674:VAL:HG23  | 5:C:869:VAL:O     | 2.13                     | 0.48              |
| 5:C:874:LEU:C     | 5:C:877:PRO:HD2   | 2.38                     | 0.48              |
| 5:C:981:GLU:HG3   | 5:C:982:PRO:CD    | 2.43                     | 0.48              |
| 6:D:164:GLY:O     | 6:D:199:LEU:HD12  | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:764:LEU:HD12  | 6:D:766:ALA:H     | 1.79                     | 0.48              |
| 4:L:174:VAL:HG13  | 4:L:200:TRP:O     | 2.13                     | 0.48              |
| 5:M:98:LEU:HD21   | 5:M:373:VAL:HG21  | 1.95                     | 0.48              |
| 5:M:736:ASP:HA    | 5:M:744:ARG:HH12  | 1.75                     | 0.48              |
| 6:N:202:VAL:HB    | 6:N:398:ALA:O     | 2.13                     | 0.48              |
| 6:N:543:LEU:HA    | 6:N:546:ARG:HG3   | 1.96                     | 0.48              |
| 6:N:678:GLU:HB3   | 11:N:9222:HOH:O   | 2.13                     | 0.48              |
| 6:N:757:ALA:CB    | 7:O:24:ALA:HB2    | 2.42                     | 0.48              |
| 6:N:959:GLU:O     | 6:N:963:TYR:HD1   | 1.96                     | 0.48              |
| 6:N:1220:ALA:O    | 6:N:1224:VAL:HG23 | 2.14                     | 0.48              |
| 1:X:8:DT:H2''     | 1:X:9:DG:H8       | 1.77                     | 0.48              |
| 4:B:18:ARG:HH12   | 4:B:123:MET:CE    | 2.18                     | 0.48              |
| 5:C:98:LEU:HD13   | 5:C:110:GLU:O     | 2.13                     | 0.48              |
| 5:C:622:GLU:O     | 5:C:624:PRO:HD3   | 2.14                     | 0.48              |
| 5:C:1083:GLU:HA   | 5:C:1086:ARG:HE   | 1.79                     | 0.48              |
| 6:D:50:PHE:CB     | 6:D:522:PRO:HG3   | 2.43                     | 0.48              |
| 6:D:139:GLY:HA2   | 6:D:451:ASP:O     | 2.13                     | 0.48              |
| 6:D:827:ILE:H     | 6:D:827:ILE:HD12  | 1.77                     | 0.48              |
| 6:D:881:LEU:HA    | 11:D:8376:HOH:O   | 2.13                     | 0.48              |
| 6:D:1147:ARG:O    | 6:D:1166:LEU:HD23 | 2.12                     | 0.48              |
| 6:D:1213:ARG:HH12 | 7:E:11:GLY:HA2    | 1.78                     | 0.48              |
| 4:L:73:GLU:OE1    | 4:L:130:ALA:HA    | 2.13                     | 0.48              |
| 4:L:101:LEU:HD23  | 4:L:101:LEU:C     | 2.38                     | 0.48              |
| 5:M:52:PHE:HB3    | 5:M:53:PRO:HD3    | 1.95                     | 0.48              |
| 5:M:368:THR:N     | 5:M:369:PRO:HD2   | 2.29                     | 0.48              |
| 5:M:959:PRO:HB2   | 11:M:1487:HOH:O   | 2.13                     | 0.48              |
| 6:N:119:SER:N     | 6:N:123:LEU:HB2   | 2.28                     | 0.48              |
| 6:N:155:ASP:O     | 6:N:159:ARG:HB3   | 2.13                     | 0.48              |
| 6:N:181:ASP:O     | 6:N:204:LEU:HA    | 2.13                     | 0.48              |
| 6:N:606:ILE:HG23  | 11:N:9149:HOH:O   | 2.12                     | 0.48              |
| 6:N:619:LEU:HG    | 6:N:621:LYS:HE2   | 1.94                     | 0.48              |
| 6:N:759:ALA:O     | 6:N:763:MET:HB3   | 2.14                     | 0.48              |
| 6:N:1238:MET:HA   | 6:N:1241:PHE:HE2  | 1.76                     | 0.48              |
| 7:O:73:LEU:HD12   | 7:O:73:LEU:H      | 1.79                     | 0.48              |
| 1:X:12:DG:H2''    | 1:X:13:DT:O5'     | 2.14                     | 0.48              |
| 2:Y:7:G:C8        | 2:Y:7:G:H5''      | 2.49                     | 0.48              |
| 5:C:415:PRO:HD2   | 5:C:418:LEU:HD13  | 1.95                     | 0.48              |
| 5:C:601:GLY:HA3   | 5:C:615:TYR:HA    | 1.95                     | 0.48              |
| 5:C:675:ALA:CA    | 5:C:989:VAL:HG13  | 2.43                     | 0.48              |
| 5:C:688:ILE:CG2   | 5:C:871:LEU:HD23  | 2.43                     | 0.48              |
| 6:D:133:ILE:HG13  | 6:D:153:LEU:HG    | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:785:ILE:O     | 6:D:789:LEU:HG    | 2.14                     | 0.48              |
| 6:D:1495:ILE:HG22 | 6:D:1499:ARG:NH2  | 2.28                     | 0.48              |
| 5:M:342:ASP:HA    | 5:M:345:ARG:CD    | 2.43                     | 0.48              |
| 5:M:1103:ASP:OD1  | 6:N:3:LYS:HD2     | 2.13                     | 0.48              |
| 6:N:15:PRO:HB3    | 11:N:9303:HOH:O   | 2.12                     | 0.48              |
| 6:N:92:HIS:CA     | 6:N:519:VAL:HG23  | 2.43                     | 0.48              |
| 6:N:399:ARG:HH21  | 6:N:431:VAL:HG22  | 1.78                     | 0.48              |
| 6:N:584:ASN:HD21  | 6:N:590:PRO:HD2   | 1.77                     | 0.48              |
| 6:N:939:PHE:O     | 6:N:943:THR:HG23  | 2.13                     | 0.48              |
| 6:N:1378:TYR:O    | 6:N:1379:VAL:HG13 | 2.13                     | 0.48              |
| 2:H:11:C:C2'      | 2:H:12:G:H5''     | 2.44                     | 0.48              |
| 4:B:23:PHE:HZ     | 4:B:207:PRO:HB2   | 1.78                     | 0.48              |
| 5:C:159:ILE:HD11  | 11:C:1246:HOH:O   | 2.13                     | 0.48              |
| 5:C:168:ARG:HB2   | 11:C:1136:HOH:O   | 2.13                     | 0.48              |
| 5:C:326:ASP:HB2   | 5:C:431:HIS:CG    | 2.49                     | 0.48              |
| 5:C:409:ARG:NH1   | 5:C:444:PRO:HG2   | 2.28                     | 0.48              |
| 5:C:1034:GLU:HA   | 5:C:1037:VAL:CG2  | 2.43                     | 0.48              |
| 6:D:56:TYR:C      | 6:D:80:VAL:HG11   | 2.38                     | 0.48              |
| 6:D:110:SER:HB3   | 6:D:113:GLY:H     | 1.77                     | 0.48              |
| 7:E:41:GLU:H      | 7:E:41:GLU:CD     | 2.21                     | 0.48              |
| 5:M:16:PRO:HG2    | 5:M:485:TYR:OH    | 2.14                     | 0.48              |
| 5:M:21:ILE:HD11   | 11:M:1541:HOH:O   | 2.13                     | 0.48              |
| 5:M:44:ILE:HD12   | 5:M:344:PHE:CD1   | 2.48                     | 0.48              |
| 5:M:61:LYS:O      | 5:M:61:LYS:HD3    | 2.14                     | 0.48              |
| 5:M:95:TYR:HD2    | 5:M:114:PHE:HB2   | 1.79                     | 0.48              |
| 5:M:218:VAL:HG22  | 5:M:221:LEU:HD21  | 1.94                     | 0.48              |
| 5:M:260:LEU:HG    | 5:M:261:ILE:HG12  | 1.95                     | 0.48              |
| 5:M:607:ASP:HB3   | 5:M:609:ASN:H     | 1.79                     | 0.48              |
| 5:M:1012:PRO:HB2  | 5:M:1021:LEU:O    | 2.13                     | 0.48              |
| 6:N:42:ASP:O      | 6:N:43:GLY:O      | 2.32                     | 0.48              |
| 6:N:95:LEU:HA     | 6:N:551:ASN:ND2   | 2.28                     | 0.48              |
| 6:N:500:ARG:HG3   | 11:N:9399:HOH:O   | 2.14                     | 0.48              |
| 6:N:583:ASP:HB2   | 6:N:604:THR:OG1   | 2.14                     | 0.48              |
| 6:N:613:ARG:HD3   | 6:N:613:ARG:HA    | 1.62                     | 0.48              |
| 6:N:902:LEU:HB3   | 11:N:9040:HOH:O   | 2.13                     | 0.48              |
| 6:N:1066:THR:HG22 | 6:N:1069:GLU:OE1  | 2.12                     | 0.48              |
| 6:N:1441:GLN:OE1  | 6:N:1442:ASN:HB2  | 2.13                     | 0.48              |
| 7:O:41:GLU:N      | 7:O:42:PRO:CD     | 2.76                     | 0.48              |
| 2:Y:7:G:C5'       | 2:Y:7:G:H8        | 2.27                     | 0.48              |
| 5:C:176:VAL:HG13  | 11:C:1142:HOH:O   | 2.14                     | 0.48              |
| 5:C:205:GLU:O     | 5:C:209:ARG:HD2   | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:691:SER:HB2   | 5:C:858:MET:SD    | 2.53                     | 0.48              |
| 5:C:758:ARG:NH2   | 5:C:788:THR:HB    | 2.29                     | 0.48              |
| 5:C:1103:ASP:OD1  | 5:C:1109:VAL:HG22 | 2.14                     | 0.48              |
| 6:D:42:ASP:O      | 6:D:43:GLY:O      | 2.31                     | 0.48              |
| 6:D:462:GLN:HA    | 6:D:513:ILE:HD13  | 1.94                     | 0.48              |
| 6:D:762:GLN:CB    | 7:E:16:LYS:HE2    | 2.44                     | 0.48              |
| 6:D:963:TYR:HE2   | 6:D:1002:LYS:HB3  | 1.78                     | 0.48              |
| 6:D:1381:VAL:HG13 | 11:D:8400:HOH:O   | 2.14                     | 0.48              |
| 7:E:23:VAL:HG22   | 7:E:68:LEU:HD23   | 1.96                     | 0.48              |
| 4:K:224:TYR:HD1   | 11:K:1342:HOH:O   | 1.96                     | 0.48              |
| 4:L:52:ALA:HB2    | 4:L:170:VAL:C     | 2.38                     | 0.48              |
| 4:L:124:ASN:N     | 4:L:125:PRO:HD3   | 2.29                     | 0.48              |
| 4:L:173:PRO:HG3   | 11:L:367:HOH:O    | 2.14                     | 0.48              |
| 5:M:260:LEU:HA    | 5:M:291:ALA:CB    | 2.43                     | 0.48              |
| 5:M:567:GLN:C     | 5:M:997:LEU:HD12  | 2.38                     | 0.48              |
| 5:M:626:ARG:HB3   | 5:M:626:ARG:HH11  | 1.79                     | 0.48              |
| 5:M:767:PRO:HD3   | 11:M:1522:HOH:O   | 2.14                     | 0.48              |
| 5:M:845:ASN:ND2   | 11:M:1407:HOH:O   | 2.46                     | 0.48              |
| 6:N:490:ALA:HA    | 6:N:1390:LEU:CD1  | 2.44                     | 0.48              |
| 6:N:1102:THR:HG22 | 6:N:1222:GLY:HA3  | 1.95                     | 0.48              |
| 6:N:1152:GLU:OE2  | 6:N:1154:GLU:HG3  | 2.13                     | 0.48              |
| 6:N:1378:TYR:HA   | 6:N:1395:LEU:H    | 1.78                     | 0.48              |
| 4:A:215:VAL:HG21  | 4:B:225:PHE:CD1   | 2.49                     | 0.48              |
| 4:B:102:LYS:HZ2   | 4:B:139:ASN:HB2   | 1.78                     | 0.48              |
| 5:C:265:ARG:H     | 5:C:289:THR:HG21  | 1.78                     | 0.48              |
| 5:C:317:VAL:HG23  | 11:C:1254:HOH:O   | 2.14                     | 0.48              |
| 5:C:405:ARG:NE    | 5:C:566:THR:HG21  | 2.28                     | 0.48              |
| 5:C:562:SER:HB3   | 11:C:1416:HOH:O   | 2.12                     | 0.48              |
| 5:C:587:VAL:HG23  | 11:C:1190:HOH:O   | 2.12                     | 0.48              |
| 5:C:610:ARG:HD3   | 5:C:622:GLU:CD    | 2.38                     | 0.48              |
| 6:D:81:THR:HB     | 6:D:85:VAL:HG22   | 1.95                     | 0.48              |
| 6:D:119:SER:N     | 6:D:123:LEU:HB2   | 2.29                     | 0.48              |
| 6:D:562:ALA:HB1   | 6:D:567:ILE:CD1   | 2.44                     | 0.48              |
| 6:D:644:LEU:HD23  | 6:D:718:PRO:CB    | 2.43                     | 0.48              |
| 6:D:671:LYS:O     | 6:D:675:ARG:HG3   | 2.14                     | 0.48              |
| 6:D:792:ILE:O     | 6:D:792:ILE:HG12  | 2.13                     | 0.48              |
| 6:D:1112:CYS:HB2  | 6:D:1195:GLN:CG   | 2.32                     | 0.48              |
| 6:D:1209:LEU:O    | 6:D:1210:SER:C    | 2.53                     | 0.48              |
| 6:D:1381:VAL:HB   | 6:D:1389:LEU:O    | 2.14                     | 0.48              |
| 4:K:38:ASN:CB     | 5:M:980:GLY:HA3   | 2.40                     | 0.48              |
| 4:L:23:PHE:O      | 4:L:196:THR:HA    | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:L:226:SER:O     | 4:L:228:PRO:HD3   | 2.14                     | 0.48              |
| 5:M:172:ILE:HG23  | 5:M:184:MET:SD    | 2.54                     | 0.48              |
| 5:M:399:ASN:O     | 5:M:400:PRO:C     | 2.57                     | 0.48              |
| 5:M:853:LEU:HB3   | 5:M:858:MET:HE2   | 1.94                     | 0.48              |
| 5:M:1095:LEU:HD21 | 6:N:603:LEU:HB3   | 1.95                     | 0.48              |
| 5:M:1101:THR:C    | 5:M:1102:LEU:HD12 | 2.38                     | 0.48              |
| 6:N:93:ILE:HB     | 6:N:517:VAL:HB    | 1.96                     | 0.48              |
| 6:N:394:LEU:HD21  | 6:N:445:ARG:CZ    | 2.43                     | 0.48              |
| 6:N:804:LEU:HD23  | 6:N:804:LEU:H     | 1.79                     | 0.48              |
| 6:N:1098:LEU:HD23 | 6:N:1371:VAL:HG21 | 1.96                     | 0.48              |
| 6:N:1336:LEU:CD1  | 6:N:1341:PRO:HG3  | 2.44                     | 0.48              |
| 6:N:1383:ASP:HB2  | 6:N:1416:ALA:HB3  | 1.96                     | 0.48              |
| 6:N:1484:THR:H    | 7:O:25:LYS:NZ     | 2.11                     | 0.48              |
| 6:N:1499:ARG:HB2  | 6:N:1499:ARG:HH11 | 1.78                     | 0.48              |
| 7:O:57:ASP:H      | 7:O:58:PRO:HD3    | 1.79                     | 0.48              |
| 1:G:23:DG:N2      | 11:G:185:HOH:O    | 2.46                     | 0.48              |
| 2:Y:7:G:H2'       | 2:Y:8:C:OP1       | 2.14                     | 0.48              |
| 2:Y:9:G:C8        | 2:Y:9:G:C5'       | 2.97                     | 0.48              |
| 4:A:156:HIS:CD2   | 4:A:157:GLY:N     | 2.82                     | 0.48              |
| 5:C:260:LEU:CD1   | 5:C:261:ILE:HG13  | 2.43                     | 0.48              |
| 5:C:774:LEU:HD11  | 11:D:8351:HOH:O   | 2.14                     | 0.48              |
| 5:C:833:LEU:HD13  | 5:C:996:LYS:HD2   | 1.96                     | 0.48              |
| 6:D:33:ASN:HB2    | 6:D:40:GLU:CD     | 2.38                     | 0.48              |
| 6:D:153:LEU:HB3   | 11:D:8252:HOH:O   | 2.14                     | 0.48              |
| 6:D:581:LEU:HD23  | 6:D:581:LEU:H     | 1.77                     | 0.48              |
| 6:D:651:GLU:HA    | 6:D:654:LYS:HZ2   | 1.78                     | 0.48              |
| 6:D:727:GLN:NE2   | 11:D:8105:HOH:O   | 2.46                     | 0.48              |
| 6:D:1094:LEU:O    | 6:D:1098:LEU:HD13 | 2.14                     | 0.48              |
| 6:D:1120:VAL:HB   | 6:D:1144:LEU:HD21 | 1.96                     | 0.48              |
| 6:D:1221:VAL:O    | 6:D:1224:VAL:HB   | 2.14                     | 0.48              |
| 7:E:5:GLY:HA3     | 7:E:8:LYS:HD2     | 1.96                     | 0.48              |
| 4:K:36:LEU:O      | 4:K:39:PRO:HD2    | 2.14                     | 0.48              |
| 5:M:21:ILE:HD12   | 5:M:21:ILE:N      | 2.29                     | 0.48              |
| 5:M:129:ILE:HG22  | 5:M:130:ASN:N     | 2.29                     | 0.48              |
| 5:M:256:TYR:HB2   | 11:M:1408:HOH:O   | 2.13                     | 0.48              |
| 5:M:352:ALA:C     | 5:M:355:VAL:HG12  | 2.39                     | 0.48              |
| 5:M:616:GLU:OE1   | 5:M:616:GLU:HA    | 2.11                     | 0.48              |
| 6:N:546:ARG:HB3   | 6:N:546:ARG:HH11  | 1.78                     | 0.48              |
| 6:N:786:ILE:HD13  | 6:N:1027:GLY:CA   | 2.44                     | 0.48              |
| 6:N:974:ILE:HD11  | 6:N:995:LEU:HD22  | 1.95                     | 0.48              |
| 6:N:1109:GLU:CG   | 6:N:1201:CYS:HA   | 2.34                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:1223:ILE:H    | 6:N:1223:ILE:CD1  | 2.19                     | 0.48              |
| 7:O:22:VAL:CG1    | 7:O:68:LEU:HD21   | 2.44                     | 0.48              |
| 3:I:4:DC:H2''     | 3:I:5:DG:O5'      | 2.14                     | 0.48              |
| 4:A:36:LEU:HD11   | 4:B:221:HIS:CD2   | 2.49                     | 0.48              |
| 4:B:153:ALA:HA    | 4:B:156:HIS:CE1   | 2.49                     | 0.48              |
| 5:C:322:VAL:HG23  | 5:C:322:VAL:O     | 2.14                     | 0.48              |
| 5:C:681:GLY:O     | 6:D:633:VAL:HG11  | 2.14                     | 0.48              |
| 5:C:964:LYS:HZ2   | 5:C:968:LEU:HD21  | 1.79                     | 0.48              |
| 6:D:93:ILE:HG13   | 6:D:519:VAL:CG2   | 2.43                     | 0.48              |
| 6:D:650:LEU:HD23  | 6:D:691:LEU:CD2   | 2.43                     | 0.48              |
| 6:D:675:ARG:HB3   | 6:D:675:ARG:CZ    | 2.43                     | 0.48              |
| 6:D:769:LEU:HB2   | 6:D:919:PHE:CE1   | 2.49                     | 0.48              |
| 6:D:1097:LYS:O    | 6:D:1101:VAL:HG23 | 2.13                     | 0.48              |
| 6:D:1105:ILE:HG23 | 6:D:1373:ARG:NH2  | 2.28                     | 0.48              |
| 6:D:1462:LEU:HD21 | 6:D:1474:ALA:CB   | 2.42                     | 0.48              |
| 4:L:7:LYS:HD2     | 4:L:7:LYS:O       | 2.14                     | 0.48              |
| 5:M:91:GLN:NE2    | 5:M:383:ARG:HH22  | 2.12                     | 0.48              |
| 5:M:101:ILE:HG22  | 5:M:102:HIS:N     | 2.29                     | 0.48              |
| 5:M:684:PHE:HD2   | 11:N:9180:HOH:O   | 1.97                     | 0.48              |
| 5:M:1013:TYR:HB3  | 5:M:1018:GLN:OE1  | 2.13                     | 0.48              |
| 5:M:1030:GLN:HE22 | 6:N:628:ARG:HD3   | 1.78                     | 0.48              |
| 5:M:1040:LEU:N    | 5:M:1040:LEU:HD12 | 2.29                     | 0.48              |
| 6:N:9:ARG:HA      | 6:N:1455:LYS:O    | 2.13                     | 0.48              |
| 6:N:573:MET:HE1   | 11:N:9034:HOH:O   | 2.13                     | 0.48              |
| 1:G:18:DG:H5''    | 6:D:628:ARG:HH22  | 1.79                     | 0.47              |
| 4:A:150:TYR:CE1   | 5:C:696:LYS:HA    | 2.49                     | 0.47              |
| 5:C:144:PRO:HA    | 5:C:163:ILE:CD1   | 2.44                     | 0.47              |
| 5:C:193:LEU:HD12  | 5:C:193:LEU:N     | 2.29                     | 0.47              |
| 5:C:433:THR:O     | 5:C:437:ARG:HD2   | 2.14                     | 0.47              |
| 5:C:715:THR:CG2   | 5:C:717:LEU:HG    | 2.43                     | 0.47              |
| 6:D:117:ASP:N     | 6:D:150:ARG:HH11  | 2.12                     | 0.47              |
| 6:D:796:ARG:O     | 6:D:797:LYS:HD2   | 2.14                     | 0.47              |
| 6:D:932:ASP:O     | 6:D:935:LYS:HB3   | 2.14                     | 0.47              |
| 4:K:213:GLN:O     | 4:K:217:ILE:HG13  | 2.13                     | 0.47              |
| 5:M:129:ILE:HG13  | 5:M:386:PHE:HB3   | 1.96                     | 0.47              |
| 5:M:152:PRO:HB2   | 11:M:1160:HOH:O   | 2.14                     | 0.47              |
| 5:M:257:VAL:HG22  | 11:M:1151:HOH:O   | 2.13                     | 0.47              |
| 5:M:503:LEU:HD23  | 5:M:507:ARG:O     | 2.14                     | 0.47              |
| 5:M:571:LEU:HD21  | 5:M:700:TYR:CD2   | 2.49                     | 0.47              |
| 5:M:604:ALA:HB3   | 5:M:612:VAL:O     | 2.14                     | 0.47              |
| 5:M:687:ALA:C     | 5:M:688:ILE:HG13  | 2.39                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:M:780:GLU:HG3  | 5:M:781:LYS:HD3   | 1.96                     | 0.47              |
| 5:M:833:LEU:HD21 | 5:M:839:LEU:HD11  | 1.96                     | 0.47              |
| 6:N:84:ILE:O     | 6:N:87:ARG:HG3    | 2.13                     | 0.47              |
| 6:N:94:GLU:O     | 6:N:551:ASN:ND2   | 2.45                     | 0.47              |
| 6:N:137:PRO:HD2  | 6:N:453:ASP:CG    | 2.39                     | 0.47              |
| 6:N:525:ARG:HB2  | 6:N:538:SER:CB    | 2.43                     | 0.47              |
| 6:N:783:ARG:HH12 | 6:N:1029:ARG:NH2  | 2.12                     | 0.47              |
| 6:N:1378:TYR:OH  | 6:N:1431:THR:HA   | 2.14                     | 0.47              |
| 3:I:9:DG:H2''    | 3:I:10:DA:C8      | 2.50                     | 0.47              |
| 4:A:18:ARG:NH1   | 4:A:123:MET:HE1   | 2.29                     | 0.47              |
| 5:C:158:TYR:CD1  | 5:C:314:THR:HG22  | 2.44                     | 0.47              |
| 5:C:185:LYS:HB3  | 5:C:188:LYS:O     | 2.13                     | 0.47              |
| 6:D:440:VAL:CB   | 6:D:441:ARG:HH21  | 2.26                     | 0.47              |
| 6:D:756:GLN:CG   | 6:D:760:ARG:HH11  | 2.25                     | 0.47              |
| 6:D:810:GLU:C    | 6:D:813:LEU:HG    | 2.39                     | 0.47              |
| 6:D:902:LEU:HD13 | 11:D:8066:HOH:O   | 2.12                     | 0.47              |
| 6:D:1087:ARG:NH2 | 6:D:1253:THR:HG22 | 2.27                     | 0.47              |
| 6:D:1124:GLN:HA  | 6:D:1125:PRO:HD3  | 1.65                     | 0.47              |
| 6:D:1147:ARG:HB2 | 6:D:1166:LEU:HD21 | 1.96                     | 0.47              |
| 6:D:1147:ARG:HD2 | 6:D:1188:VAL:HG21 | 1.96                     | 0.47              |
| 6:D:1228:SER:HA  | 11:D:8193:HOH:O   | 2.14                     | 0.47              |
| 6:D:1429:LEU:HG  | 6:D:1441:GLN:HG3  | 1.96                     | 0.47              |
| 4:K:2:LEU:HA     | 4:K:6:LEU:HD22    | 1.96                     | 0.47              |
| 4:K:111:ALA:HB3  | 4:K:124:ASN:O     | 2.13                     | 0.47              |
| 5:M:111:ASP:CG   | 5:M:112:GLU:HG2   | 2.39                     | 0.47              |
| 5:M:252:LYS:HZ2  | 5:M:296:GLY:HA3   | 1.77                     | 0.47              |
| 5:M:487:THR:OG1  | 5:M:490:GLU:HG3   | 2.13                     | 0.47              |
| 6:N:47:GLU:O     | 6:N:51:GLY:N      | 2.47                     | 0.47              |
| 6:N:58:CYS:HA    | 6:N:78:VAL:HG11   | 1.96                     | 0.47              |
| 6:N:838:ARG:HH11 | 6:N:838:ARG:HG2   | 1.79                     | 0.47              |
| 6:N:861:GLN:NE2  | 6:N:861:GLN:H     | 2.12                     | 0.47              |
| 7:O:57:ASP:N     | 7:O:58:PRO:HD3    | 2.30                     | 0.47              |
| 2:Y:7:G:O6       | 5:M:1015:LEU:N    | 2.45                     | 0.47              |
| 3:Z:4:DC:H4'     | 11:Z:1418:HOH:O   | 2.15                     | 0.47              |
| 4:A:26:GLU:HG2   | 4:A:27:PRO:HG3    | 1.96                     | 0.47              |
| 4:A:171:PHE:O    | 4:A:173:PRO:HD3   | 2.15                     | 0.47              |
| 5:C:31:GLN:O     | 5:C:31:GLN:HG2    | 2.14                     | 0.47              |
| 5:C:77:PRO:HB2   | 5:C:78:PHE:CD1    | 2.49                     | 0.47              |
| 5:C:1102:LEU:HB2 | 6:D:7:LYS:HB2     | 1.96                     | 0.47              |
| 6:D:520:LEU:HD12 | 6:D:521:PRO:HD2   | 1.97                     | 0.47              |
| 6:D:583:ASP:OD2  | 6:D:604:THR:HG21  | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:619:LEU:HD23  | 6:D:619:LEU:N     | 2.29                     | 0.47              |
| 6:D:1101:VAL:HG21 | 6:D:1424:VAL:CA   | 2.44                     | 0.47              |
| 6:D:1441:GLN:OE1  | 6:D:1442:ASN:HB2  | 2.13                     | 0.47              |
| 5:M:620:LEU:HD12  | 5:M:620:LEU:N     | 2.29                     | 0.47              |
| 5:M:734:LEU:HD11  | 11:M:1385:HOH:O   | 2.14                     | 0.47              |
| 6:N:628:ARG:HG3   | 6:N:628:ARG:NH1   | 2.30                     | 0.47              |
| 6:N:1130:ARG:HD3  | 11:N:9173:HOH:O   | 2.13                     | 0.47              |
| 4:A:67:THR:HG23   | 5:C:609:ASN:HD21  | 1.79                     | 0.47              |
| 4:A:101:LEU:HD22  | 4:A:114:PHE:CZ    | 2.49                     | 0.47              |
| 4:B:64:GLU:O      | 4:B:64:GLU:HG2    | 2.14                     | 0.47              |
| 5:C:18:LEU:HD22   | 5:C:404:LEU:HD21  | 1.95                     | 0.47              |
| 5:C:148:PHE:HZ    | 5:C:281:LEU:HB3   | 1.78                     | 0.47              |
| 5:C:158:TYR:HE1   | 5:C:314:THR:HA    | 1.79                     | 0.47              |
| 5:C:244:PRO:CD    | 5:C:245:GLY:H     | 2.26                     | 0.47              |
| 5:C:361:MET:HG3   | 5:C:371:LYS:HD2   | 1.96                     | 0.47              |
| 5:C:437:ARG:HH21  | 5:C:469:THR:HG22  | 1.80                     | 0.47              |
| 5:C:625:LEU:O     | 5:C:627:ARG:N     | 2.47                     | 0.47              |
| 6:D:147:VAL:HG12  | 11:D:8415:HOH:O   | 2.14                     | 0.47              |
| 6:D:159:ARG:HB3   | 6:D:163:TYR:OH    | 2.14                     | 0.47              |
| 6:D:1033:GLN:O    | 6:D:1037:GLN:HG3  | 2.14                     | 0.47              |
| 6:D:1200:VAL:N    | 11:D:8286:HOH:O   | 2.47                     | 0.47              |
| 6:D:1262:LEU:HD23 | 6:D:1352:ILE:CG1  | 2.44                     | 0.47              |
| 7:E:16:LYS:HD3    | 7:E:17:TYR:CE1    | 2.49                     | 0.47              |
| 4:K:9:PRO:HB3     | 4:K:25:LEU:HD21   | 1.95                     | 0.47              |
| 4:K:64:GLU:O      | 4:K:64:GLU:HG3    | 2.13                     | 0.47              |
| 5:M:65:VAL:HG12   | 5:M:67:ASP:OD2    | 2.14                     | 0.47              |
| 5:M:474:VAL:HG12  | 5:M:531:PHE:HA    | 1.96                     | 0.47              |
| 5:M:610:ARG:NH1   | 5:M:612:VAL:HG23  | 2.30                     | 0.47              |
| 5:M:675:ALA:CA    | 5:M:989:VAL:HG12  | 2.38                     | 0.47              |
| 5:M:734:LEU:HD21  | 11:M:1385:HOH:O   | 2.14                     | 0.47              |
| 5:M:764:GLU:HG3   | 6:N:54:LYS:HD3    | 1.96                     | 0.47              |
| 5:M:798:GLY:H     | 5:M:827:VAL:CG1   | 2.28                     | 0.47              |
| 5:M:1049:LEU:HD23 | 6:N:1472:ILE:HD12 | 1.95                     | 0.47              |
| 5:M:1067:TYR:HB3  | 11:M:1303:HOH:O   | 2.13                     | 0.47              |
| 6:N:95:LEU:HD12   | 6:N:95:LEU:N      | 2.24                     | 0.47              |
| 6:N:394:LEU:O     | 6:N:396:VAL:N     | 2.47                     | 0.47              |
| 6:N:457:GLY:C     | 6:N:459:GLU:N     | 2.72                     | 0.47              |
| 6:N:610:LYS:HB2   | 11:N:9190:HOH:O   | 2.15                     | 0.47              |
| 6:N:756:GLN:HE22  | 6:N:760:ARG:HB3   | 1.80                     | 0.47              |
| 6:N:820:GLU:HA    | 6:N:825:ALA:O     | 2.15                     | 0.47              |
| 6:N:1231:GLU:HB3  | 6:N:1232:PRO:HD3  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:O:26:ARG:NH1    | 7:O:29:GLN:HE21   | 2.13                     | 0.47              |
| 4:B:40:LEU:HD22   | 4:B:211:LEU:CD1   | 2.43                     | 0.47              |
| 5:C:759:THR:HG21  | 5:C:783:ARG:NH2   | 2.30                     | 0.47              |
| 6:D:683:ILE:N     | 6:D:683:ILE:HD12  | 2.29                     | 0.47              |
| 6:D:783:ARG:HA    | 6:D:1028:ALA:CA   | 2.29                     | 0.47              |
| 6:D:876:SER:O     | 6:D:880:ILE:HG12  | 2.15                     | 0.47              |
| 6:D:884:ARG:HG2   | 11:D:8116:HOH:O   | 2.14                     | 0.47              |
| 6:D:1220:ALA:HB1  | 6:D:1223:ILE:CD1  | 2.40                     | 0.47              |
| 5:M:310:LEU:O     | 5:M:314:THR:HG23  | 2.14                     | 0.47              |
| 5:M:537:LYS:H     | 5:M:537:LYS:CD    | 2.20                     | 0.47              |
| 5:M:684:PHE:O     | 5:M:685:GLU:C     | 2.58                     | 0.47              |
| 6:N:493:ARG:CZ    | 6:N:1391:GLU:HA   | 2.45                     | 0.47              |
| 6:N:1023:MET:HG2  | 6:N:1029:ARG:H    | 1.80                     | 0.47              |
| 6:N:1268:PRO:HD3  | 6:N:1331:ASP:HB2  | 1.96                     | 0.47              |
| 7:O:8:LYS:O       | 7:O:12:MET:HG3    | 2.14                     | 0.47              |
| 7:O:13:VAL:HG12   | 7:O:14:ASP:N      | 2.29                     | 0.47              |
| 4:A:79:ILE:HG21   | 4:A:165:ILE:HD11  | 1.94                     | 0.47              |
| 4:B:45:LEU:HD21   | 6:D:855:HIS:NE2   | 2.30                     | 0.47              |
| 5:C:626:ARG:N     | 5:C:639:GLN:HE21  | 2.13                     | 0.47              |
| 5:C:722:ILE:CD1   | 5:C:823:VAL:HG21  | 2.39                     | 0.47              |
| 5:C:874:LEU:HD11  | 6:D:787:LEU:HD23  | 1.97                     | 0.47              |
| 6:D:23:TYR:O      | 6:D:91:GLY:HA2    | 2.14                     | 0.47              |
| 6:D:138:LYS:HE2   | 11:D:8030:HOH:O   | 2.14                     | 0.47              |
| 6:D:401:TYR:HB2   | 11:D:8164:HOH:O   | 2.14                     | 0.47              |
| 6:D:610:LYS:C     | 6:D:615:ARG:HD3   | 2.39                     | 0.47              |
| 6:D:634:GLY:HA3   | 6:D:727:GLN:HG2   | 1.97                     | 0.47              |
| 6:D:1107:VAL:HA   | 6:D:1200:VAL:O    | 2.14                     | 0.47              |
| 6:D:1160:LEU:CD1  | 6:D:1174:LEU:HD21 | 2.42                     | 0.47              |
| 6:D:1223:ILE:HG22 | 6:D:1227:GLN:NE2  | 2.16                     | 0.47              |
| 5:M:7:GLY:O       | 5:M:8:ARG:NE      | 2.48                     | 0.47              |
| 5:M:68:PHE:HZ     | 5:M:71:TYR:CD2    | 2.23                     | 0.47              |
| 5:M:86:LYS:HD2    | 11:M:1208:HOH:O   | 2.14                     | 0.47              |
| 5:M:462:ASP:CG    | 5:M:463:GLU:N     | 2.67                     | 0.47              |
| 5:M:764:GLU:CB    | 6:N:54:LYS:HD3    | 2.44                     | 0.47              |
| 5:M:1090:LYS:CD   | 6:N:90:MET:HG3    | 2.40                     | 0.47              |
| 6:N:119:SER:H     | 6:N:123:LEU:HB2   | 1.79                     | 0.47              |
| 6:N:493:ARG:NH2   | 6:N:1391:GLU:HA   | 2.29                     | 0.47              |
| 6:N:520:LEU:HD11  | 6:N:524:LEU:HD23  | 1.96                     | 0.47              |
| 6:N:1220:ALA:CB   | 6:N:1223:ILE:HD13 | 2.27                     | 0.47              |
| 6:N:1432:LYS:HA   | 11:N:9333:HOH:O   | 2.13                     | 0.47              |
| 2:Y:8:C:H2'       | 2:Y:9:G:N7        | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Y:16:G:H5'     | 6:N:742:GLY:C    | 2.39                     | 0.47              |
| 4:A:69:PRO:HA    | 5:C:607:ASP:OD1  | 2.14                     | 0.47              |
| 4:A:101:LEU:HD23 | 4:A:140:MET:HG2  | 1.95                     | 0.47              |
| 4:B:101:LEU:HD23 | 4:B:101:LEU:C    | 2.40                     | 0.47              |
| 4:B:117:VAL:HG11 | 11:B:324:HOH:O   | 2.14                     | 0.47              |
| 4:B:124:ASN:HD21 | 4:B:127:LEU:HD22 | 1.78                     | 0.47              |
| 5:C:322:VAL:HB   | 11:C:1379:HOH:O  | 2.15                     | 0.47              |
| 5:C:352:ALA:C    | 5:C:355:VAL:HG12 | 2.39                     | 0.47              |
| 5:C:361:MET:HE2  | 5:C:371:LYS:CD   | 2.44                     | 0.47              |
| 5:C:564:MET:HG3  | 5:C:565:GLN:N    | 2.29                     | 0.47              |
| 5:C:663:ASN:C    | 5:C:665:PHE:H    | 2.23                     | 0.47              |
| 5:C:747:ALA:C    | 5:C:799:ILE:HG23 | 2.39                     | 0.47              |
| 5:C:807:ARG:C    | 11:C:1277:HOH:O  | 2.58                     | 0.47              |
| 5:C:874:LEU:HD11 | 6:D:787:LEU:CD2  | 2.44                     | 0.47              |
| 5:C:1008:ARG:NH2 | 5:C:1011:GLY:N   | 2.62                     | 0.47              |
| 5:C:1030:GLN:NE2 | 5:C:1030:GLN:HA  | 2.29                     | 0.47              |
| 5:C:1115:LEU:HG  | 6:D:85:VAL:HG12  | 1.97                     | 0.47              |
| 6:D:137:PRO:HD3  | 6:D:455:ARG:HH21 | 1.80                     | 0.47              |
| 6:D:206:ARG:HB2  | 6:D:392:SER:O    | 2.14                     | 0.47              |
| 6:D:398:ALA:HA   | 6:D:446:VAL:O    | 2.15                     | 0.47              |
| 6:D:455:ARG:CB   | 6:D:460:ALA:CA   | 2.86                     | 0.47              |
| 6:D:638:LYS:HD2  | 6:D:932:ASP:OD1  | 2.14                     | 0.47              |
| 6:D:800:LYS:HE3  | 6:D:804:LEU:HD13 | 1.96                     | 0.47              |
| 6:D:1496:GLU:HA  | 6:D:1499:ARG:CZ  | 2.44                     | 0.47              |
| 4:K:177:VAL:O    | 5:M:864:GLY:HA3  | 2.15                     | 0.47              |
| 4:L:43:ILE:HG23  | 4:L:47:SER:HB3   | 1.97                     | 0.47              |
| 4:L:81:ASN:O     | 4:L:127:LEU:HD21 | 2.15                     | 0.47              |
| 4:L:161:ARG:HD2  | 4:L:161:ARG:N    | 2.30                     | 0.47              |
| 5:M:27:ARG:HD3   | 5:M:28:ARG:N     | 2.29                     | 0.47              |
| 5:M:45:GLN:HE21  | 5:M:68:PHE:HE2   | 1.62                     | 0.47              |
| 5:M:119:PRO:HG2  | 5:M:386:PHE:CD2  | 2.49                     | 0.47              |
| 5:M:162:ILE:HB   | 5:M:172:ILE:HB   | 1.96                     | 0.47              |
| 5:M:172:ILE:HG23 | 5:M:184:MET:CE   | 2.45                     | 0.47              |
| 5:M:331:ARG:CB   | 5:M:331:ARG:HH11 | 2.27                     | 0.47              |
| 5:M:430:VAL:HG13 | 6:N:1075:HIS:ND1 | 2.30                     | 0.47              |
| 5:M:589:ARG:HG3  | 5:M:596:TYR:CE1  | 2.50                     | 0.47              |
| 5:M:689:VAL:HG11 | 5:M:870:ILE:CD1  | 2.44                     | 0.47              |
| 5:M:769:PRO:HG2  | 6:N:65:ARG:CD    | 2.45                     | 0.47              |
| 5:M:926:PHE:HD2  | 5:M:930:LYS:HE3  | 1.80                     | 0.47              |
| 5:M:1056:LYS:HD3 | 6:N:625:TYR:CD1  | 2.50                     | 0.47              |
| 5:M:1090:LYS:HG2 | 5:M:1112:PHE:CZ  | 2.48                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:N:127:LEU:HD13  | 6:N:128:TYR:CD2  | 2.49                     | 0.47              |
| 6:N:204:LEU:O     | 6:N:394:LEU:HD23 | 2.14                     | 0.47              |
| 6:N:481:MET:CE    | 6:N:1388:ARG:HG3 | 2.44                     | 0.47              |
| 6:N:634:GLY:HA2   | 6:N:727:GLN:HE21 | 1.79                     | 0.47              |
| 6:N:666:ILE:H     | 6:N:666:ILE:HG13 | 1.41                     | 0.47              |
| 6:N:1197:ARG:HH11 | 6:N:1197:ARG:HB2 | 1.80                     | 0.47              |
| 6:N:1353:GLN:HG2  | 6:N:1368:ILE:CD1 | 2.45                     | 0.47              |
| 2:H:10:G:C2'      | 2:H:11:C:H5'     | 2.45                     | 0.47              |
| 4:B:58:ILE:HD13   | 4:B:140:MET:HB3  | 1.96                     | 0.47              |
| 5:C:26:TYR:CD2    | 5:C:121:MET:HB2  | 2.49                     | 0.47              |
| 5:C:204:GLN:OE1   | 5:C:222:MET:HA   | 2.15                     | 0.47              |
| 5:C:573:ARG:HG2   | 5:C:670:GLN:OE1  | 2.15                     | 0.47              |
| 5:C:688:ILE:N     | 11:C:1474:HOH:O  | 2.47                     | 0.47              |
| 5:C:964:LYS:NZ    | 5:C:968:LEU:HD21 | 2.29                     | 0.47              |
| 6:D:53:ILE:HA     | 6:D:86:ARG:CZ    | 2.44                     | 0.47              |
| 6:D:135:LEU:HB2   | 6:D:148:GLU:O    | 2.15                     | 0.47              |
| 6:D:173:PRO:HB2   | 11:D:8270:HOH:O  | 2.13                     | 0.47              |
| 6:D:720:LEU:H     | 6:D:720:LEU:HD12 | 1.80                     | 0.47              |
| 6:D:1384:PRO:HG3  | 6:D:1389:LEU:CA  | 2.45                     | 0.47              |
| 6:D:1462:LEU:HD23 | 6:D:1473:PRO:HD2 | 1.96                     | 0.47              |
| 7:E:64:ALA:O      | 7:E:68:LEU:HD13  | 2.14                     | 0.47              |
| 4:L:152:PRO:HG2   | 6:N:857:ILE:HD12 | 1.96                     | 0.47              |
| 5:M:78:PHE:HB3    | 5:M:82:GLU:OE1   | 2.14                     | 0.47              |
| 5:M:376:ARG:HG3   | 5:M:376:ARG:HH11 | 1.80                     | 0.47              |
| 5:M:603:VAL:H     | 5:M:647:GLN:H    | 1.63                     | 0.47              |
| 5:M:996:LYS:HE3   | 11:M:1161:HOH:O  | 2.14                     | 0.47              |
| 5:M:1031:ARG:NH1  | 6:N:621:LYS:HZ2  | 2.13                     | 0.47              |
| 5:M:1070:ILE:HG23 | 6:N:656:PHE:CD1  | 2.50                     | 0.47              |
| 6:N:519:VAL:HA    | 6:N:544:TYR:OH   | 2.15                     | 0.47              |
| 1:G:19:DC:P       | 5:C:1001:VAL:HB  | 2.55                     | 0.47              |
| 2:H:7:G:C8        | 2:H:7:G:H5''     | 2.50                     | 0.47              |
| 1:X:21:DC:H3'     | 11:X:589:HOH:O   | 2.14                     | 0.47              |
| 4:A:89:PHE:HZ     | 4:A:146:ARG:HB2  | 1.80                     | 0.47              |
| 4:B:162:ILE:HD12  | 4:B:163:ASN:N    | 2.29                     | 0.47              |
| 5:C:470:PRO:HD3   | 5:C:485:TYR:HE2  | 1.79                     | 0.47              |
| 5:C:553:ASP:OD1   | 5:C:843:HIS:HB3  | 2.14                     | 0.47              |
| 5:C:769:PRO:HB3   | 11:D:8366:HOH:O  | 2.15                     | 0.47              |
| 5:C:937:ASP:HB2   | 5:C:940:GLU:CG   | 2.43                     | 0.47              |
| 5:C:1016:ILE:HG12 | 5:C:1017:THR:N   | 2.29                     | 0.47              |
| 5:C:1036:GLU:O    | 5:C:1039:ALA:HB3 | 2.14                     | 0.47              |
| 6:D:116:LEU:HD22  | 6:D:118:LEU:CD2  | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:704:ARG:HH12  | 6:D:743:ASP:CB    | 2.28                     | 0.47              |
| 6:D:1472:ILE:HD13 | 6:D:1472:ILE:N    | 2.29                     | 0.47              |
| 4:K:112:ARG:HG2   | 4:K:125:PRO:CA    | 2.45                     | 0.47              |
| 4:L:140:MET:HG2   | 4:L:141:GLU:N     | 2.28                     | 0.47              |
| 4:L:222:LEU:HA    | 4:L:225:PHE:CE1   | 2.50                     | 0.47              |
| 5:M:69:LEU:HD21   | 5:M:99:GLN:HG3    | 1.97                     | 0.47              |
| 5:M:625:LEU:O     | 5:M:627:ARG:N     | 2.48                     | 0.47              |
| 5:M:677:MET:HE1   | 5:M:679:PHE:CD1   | 2.44                     | 0.47              |
| 5:M:688:ILE:CD1   | 5:M:847:GLY:HA3   | 2.45                     | 0.47              |
| 5:M:842:ARG:HH22  | 5:M:887:GLU:CD    | 2.23                     | 0.47              |
| 6:N:26:VAL:HG21   | 6:N:519:VAL:HG11  | 1.97                     | 0.47              |
| 6:N:439:LEU:HG    | 11:N:9125:HOH:O   | 2.15                     | 0.47              |
| 6:N:506:GLY:O     | 6:N:507:ASN:C     | 2.58                     | 0.47              |
| 6:N:711:LEU:HD21  | 6:N:768:ASN:HB2   | 1.95                     | 0.47              |
| 6:N:756:GLN:NE2   | 6:N:756:GLN:O     | 2.48                     | 0.47              |
| 6:N:845:ASN:ND2   | 6:N:846:PRO:HD2   | 2.30                     | 0.47              |
| 6:N:884:ARG:HG2   | 11:N:9101:HOH:O   | 2.14                     | 0.47              |
| 6:N:1156:LEU:HD21 | 6:N:1177:ALA:HA   | 1.97                     | 0.47              |
| 6:N:1221:VAL:HG12 | 6:N:1222:GLY:N    | 2.30                     | 0.47              |
| 7:O:38:THR:HG21   | 7:O:63:TRP:CZ3    | 2.50                     | 0.47              |
| 2:H:8:C:H2'       | 2:H:9:G:N7        | 2.30                     | 0.47              |
| 4:A:48:ILE:CD1    | 4:A:210:ALA:HB1   | 2.44                     | 0.47              |
| 4:B:51:THR:HG23   | 11:B:316:HOH:O    | 2.15                     | 0.47              |
| 4:B:110:LYS:HD3   | 4:B:112:ARG:HG2   | 1.97                     | 0.47              |
| 5:C:146:VAL:CG2   | 5:C:162:ILE:HG23  | 2.43                     | 0.47              |
| 5:C:437:ARG:HG2   | 5:C:467:ILE:O     | 2.15                     | 0.47              |
| 5:C:674:VAL:HG11  | 5:C:992:MET:HB3   | 1.97                     | 0.47              |
| 5:C:1095:LEU:HD22 | 6:D:101:HIS:CE1   | 2.49                     | 0.47              |
| 6:D:130:SER:HB3   | 6:D:132:TYR:CE1   | 2.50                     | 0.47              |
| 6:D:796:ARG:HH21  | 6:D:828:LYS:CE    | 2.27                     | 0.47              |
| 6:D:896:ALA:O     | 6:D:899:LEU:HD12  | 2.15                     | 0.47              |
| 6:D:1191:PRO:HB3  | 6:D:1370:ILE:HD13 | 1.95                     | 0.47              |
| 4:L:34:VAL:HA     | 4:L:179:PHE:HE1   | 1.79                     | 0.47              |
| 5:M:151:ASP:OD1   | 5:M:154:ARG:HB3   | 2.15                     | 0.47              |
| 5:M:806:LEU:HD11  | 5:M:824:ARG:HH22  | 1.79                     | 0.47              |
| 5:M:822:VAL:CB    | 5:M:824:ARG:HH21  | 2.28                     | 0.47              |
| 5:M:876:VAL:HG13  | 5:M:881:ASN:HD21  | 1.79                     | 0.47              |
| 6:N:1118:ILE:HG12 | 6:N:1193:THR:HG23 | 1.97                     | 0.47              |
| 6:N:1462:LEU:HD21 | 6:N:1474:ALA:HB3  | 1.97                     | 0.47              |
| 2:H:4:U:O2'       | 2:H:5:C:H5'       | 2.15                     | 0.46              |
| 2:Y:15:C:H2'      | 2:Y:16:G:C8       | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:88:ARG:NH1    | 4:A:89:PHE:O      | 2.47                     | 0.46              |
| 4:A:133:GLU:OE1   | 5:C:605:LYS:HB3   | 2.16                     | 0.46              |
| 4:A:175:ARG:NH2   | 4:A:176:ARG:HD3   | 2.30                     | 0.46              |
| 5:C:23:VAL:HA     | 5:C:121:MET:HE2   | 1.98                     | 0.46              |
| 5:C:265:ARG:HD2   | 5:C:267:TYR:CG    | 2.50                     | 0.46              |
| 5:C:292:ARG:HB2   | 5:C:299:LYS:HG2   | 1.97                     | 0.46              |
| 5:C:394:PHE:CE1   | 5:C:632:ASN:HB3   | 2.49                     | 0.46              |
| 5:C:872:ASN:ND2   | 5:C:874:LEU:N     | 2.63                     | 0.46              |
| 5:C:900:ARG:NH1   | 11:C:1210:HOH:O   | 2.48                     | 0.46              |
| 5:C:999:HIS:HB2   | 11:C:1358:HOH:O   | 2.15                     | 0.46              |
| 5:C:1098:ASP:O    | 6:D:10:ILE:HA     | 2.15                     | 0.46              |
| 5:C:1103:ASP:N    | 5:C:1107:ASN:O    | 2.44                     | 0.46              |
| 6:D:118:LEU:HD13  | 6:D:461:ILE:HD12  | 1.97                     | 0.46              |
| 6:D:161:LEU:HD21  | 6:D:452:ILE:CG2   | 2.27                     | 0.46              |
| 6:D:502:PHE:HA    | 11:D:8084:HOH:O   | 2.14                     | 0.46              |
| 6:D:502:PHE:CZ    | 6:D:509:PRO:HB3   | 2.50                     | 0.46              |
| 6:D:843:PHE:CE1   | 6:D:864:VAL:HG11  | 2.50                     | 0.46              |
| 6:D:1198:TYR:HE2  | 6:D:1377:LYS:HD2  | 1.80                     | 0.46              |
| 6:D:1451:ALA:O    | 6:D:1452:ILE:C    | 2.57                     | 0.46              |
| 7:E:54:LEU:HA     | 7:E:58:PRO:CG     | 2.44                     | 0.46              |
| 4:K:111:ALA:HB2   | 4:K:127:LEU:CD2   | 2.45                     | 0.46              |
| 4:K:177:VAL:HG13  | 4:K:199:ILE:CD1   | 2.45                     | 0.46              |
| 4:L:94:LEU:HD11   | 4:L:119:ASP:HB2   | 1.97                     | 0.46              |
| 5:M:2:GLU:O       | 5:M:3:ILE:HD13    | 2.15                     | 0.46              |
| 5:M:23:VAL:HA     | 5:M:121:MET:HE2   | 1.96                     | 0.46              |
| 5:M:498:GLN:HE22  | 6:N:1067:VAL:CG1  | 2.28                     | 0.46              |
| 5:M:678:PRO:HD2   | 11:N:9146:HOH:O   | 2.14                     | 0.46              |
| 6:N:10:ILE:HD11   | 6:N:1434:TRP:NE1  | 2.30                     | 0.46              |
| 6:N:134:VAL:CG1   | 6:N:152:LEU:HD22  | 2.45                     | 0.46              |
| 6:N:462:GLN:O     | 6:N:466:LYS:HG3   | 2.15                     | 0.46              |
| 6:N:493:ARG:HD2   | 6:N:494:LYS:N     | 2.30                     | 0.46              |
| 6:N:1121:PRO:HB2  | 6:N:1135:ARG:HH12 | 1.79                     | 0.46              |
| 6:N:1122:LEU:HD11 | 6:N:1186:VAL:HG23 | 1.97                     | 0.46              |
| 6:N:1149:LEU:HD23 | 6:N:1187:PRO:O    | 2.15                     | 0.46              |
| 6:N:1221:VAL:O    | 6:N:1222:GLY:C    | 2.58                     | 0.46              |
| 6:N:1389:LEU:HG   | 6:N:1390:LEU:H    | 1.79                     | 0.46              |
| 7:O:91:ARG:HH11   | 7:O:92:LEU:HD21   | 1.80                     | 0.46              |
| 2:H:9:G:C8        | 2:H:9:G:C5'       | 2.98                     | 0.46              |
| 4:A:7:LYS:HE3     | 4:A:186:LEU:HD22  | 1.97                     | 0.46              |
| 4:A:42:ARG:HH12   | 4:B:34:VAL:CG1    | 2.28                     | 0.46              |
| 5:C:172:ILE:H     | 5:C:172:ILE:HD12  | 1.80                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:193:LEU:CD1  | 5:C:193:LEU:N     | 2.78                     | 0.46              |
| 5:C:207:LEU:HD22 | 5:C:221:LEU:HD13  | 1.97                     | 0.46              |
| 5:C:292:ARG:HD2  | 5:C:299:LYS:CE    | 2.46                     | 0.46              |
| 5:C:713:ARG:HH22 | 6:D:532:GLY:H     | 1.62                     | 0.46              |
| 5:C:718:GLY:HA3  | 5:C:761:PHE:CE1   | 2.50                     | 0.46              |
| 5:C:859:PRO:HB3  | 5:C:974:LEU:CD2   | 2.44                     | 0.46              |
| 5:C:1100:GLN:HB3 | 6:D:9:ARG:HH21    | 1.80                     | 0.46              |
| 6:D:66:GLN:O     | 6:D:69:GLU:HB3    | 2.16                     | 0.46              |
| 6:D:69:GLU:HG2   | 6:D:70:GLY:N      | 2.30                     | 0.46              |
| 6:D:136:ASP:OD2  | 6:D:464:LEU:HD23  | 2.15                     | 0.46              |
| 6:D:540:LEU:HA   | 6:D:543:LEU:HD11  | 1.97                     | 0.46              |
| 6:D:647:ARG:HA   | 6:D:650:LEU:HD12  | 1.96                     | 0.46              |
| 6:D:871:LYS:NZ   | 6:N:442:ASN:HD22  | 2.13                     | 0.46              |
| 6:D:1100:ASP:HB3 | 6:D:1428:ALA:HB1  | 1.97                     | 0.46              |
| 6:D:1468:LEU:O   | 6:D:1468:LEU:HD23 | 2.15                     | 0.46              |
| 7:E:48:MET:HB2   | 7:E:54:LEU:HB2    | 1.96                     | 0.46              |
| 4:L:124:ASN:HD21 | 4:L:127:LEU:HB2   | 1.80                     | 0.46              |
| 5:M:79:PRO:HA    | 5:M:90:TYR:HE2    | 1.80                     | 0.46              |
| 5:M:512:ARG:HB3  | 5:M:523:ILE:HD11  | 1.97                     | 0.46              |
| 5:M:668:LEU:HD13 | 5:M:995:MET:CE    | 2.44                     | 0.46              |
| 5:M:689:VAL:CG1  | 5:M:690:ILE:H     | 2.25                     | 0.46              |
| 5:M:716:LYS:HZ1  | 6:N:36:THR:HG23   | 1.80                     | 0.46              |
| 5:M:751:PRO:HB2  | 6:N:680:GLN:NE2   | 2.30                     | 0.46              |
| 5:M:862:PRO:HD3  | 5:M:973:VAL:O     | 2.14                     | 0.46              |
| 5:M:897:LEU:HD11 | 5:M:920:GLN:HB3   | 1.97                     | 0.46              |
| 5:M:911:GLU:HB2  | 5:M:912:PRO:HD3   | 1.97                     | 0.46              |
| 5:M:940:GLU:HG3  | 11:M:1220:HOH:O   | 2.15                     | 0.46              |
| 5:M:1050:GLN:NE2 | 6:N:1471:LEU:N    | 2.58                     | 0.46              |
| 6:N:33:ASN:O     | 6:N:36:THR:O      | 2.33                     | 0.46              |
| 6:N:92:HIS:HA    | 6:N:519:VAL:HG23  | 1.96                     | 0.46              |
| 6:N:133:ILE:HB   | 6:N:153:LEU:CD1   | 2.45                     | 0.46              |
| 6:N:434:ARG:NH2  | 6:N:447:VAL:HG11  | 2.29                     | 0.46              |
| 6:N:452:ILE:HB   | 11:N:9092:HOH:O   | 2.14                     | 0.46              |
| 6:N:1381:VAL:HB  | 6:N:1389:LEU:O    | 2.14                     | 0.46              |
| 4:B:170:VAL:O    | 4:B:170:VAL:HG23  | 2.16                     | 0.46              |
| 4:B:206:THR:HG23 | 4:B:208:LEU:N     | 2.29                     | 0.46              |
| 5:C:212:GLY:HA3  | 5:C:218:VAL:HG21  | 1.96                     | 0.46              |
| 5:C:361:MET:HE2  | 5:C:371:LYS:HD3   | 1.96                     | 0.46              |
| 5:C:399:ASN:O    | 5:C:400:PRO:C     | 2.57                     | 0.46              |
| 5:C:456:ALA:HA   | 5:C:541:SER:HA    | 1.97                     | 0.46              |
| 5:C:494:TYR:HD2  | 5:C:530:GLU:HB3   | 1.81                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:600:ASP:OD1  | 5:C:651:LYS:HB2   | 2.15                     | 0.46              |
| 6:D:82:LYS:C     | 6:D:84:ILE:N      | 2.74                     | 0.46              |
| 6:D:119:SER:HB2  | 6:D:123:LEU:N     | 2.29                     | 0.46              |
| 6:D:164:GLY:HA3  | 11:D:8094:HOH:O   | 2.15                     | 0.46              |
| 4:K:26:GLU:HG3   | 4:K:184:THR:HG21  | 1.95                     | 0.46              |
| 4:K:200:TRP:HZ2  | 11:M:1430:HOH:O   | 1.97                     | 0.46              |
| 5:M:677:MET:HB3  | 5:M:987:ILE:HD13  | 1.96                     | 0.46              |
| 5:M:798:GLY:HA3  | 5:M:828:ALA:O     | 2.15                     | 0.46              |
| 5:M:831:ARG:NH1  | 5:M:999:HIS:HB3   | 2.31                     | 0.46              |
| 5:M:1094:ALA:HA  | 6:N:90:MET:HE3    | 1.97                     | 0.46              |
| 6:N:133:ILE:HG22 | 6:N:455:ARG:N     | 2.30                     | 0.46              |
| 6:N:564:GLU:O    | 6:N:567:ILE:HG13  | 2.16                     | 0.46              |
| 6:N:793:THR:OG1  | 6:N:905:PRO:HA    | 2.14                     | 0.46              |
| 6:N:799:LYS:HB3  | 6:N:826:PRO:HG2   | 1.97                     | 0.46              |
| 6:N:890:VAL:HG12 | 6:N:926:LYS:CD    | 2.35                     | 0.46              |
| 6:N:1252:ILE:HA  | 11:N:9048:HOH:O   | 2.14                     | 0.46              |
| 6:N:1369:GLU:HA  | 6:N:1372:VAL:HG12 | 1.97                     | 0.46              |
| 2:H:5:C:H6       | 2:H:5:C:O5'       | 1.98                     | 0.46              |
| 1:X:14:DT:H3'    | 6:N:610:LYS:HZ1   | 1.81                     | 0.46              |
| 1:X:15:DC:H2''   | 1:X:16:DG:H8      | 1.80                     | 0.46              |
| 4:A:18:ARG:O     | 4:A:207:PRO:HD3   | 2.15                     | 0.46              |
| 4:A:156:HIS:CD2  | 4:A:157:GLY:H     | 2.32                     | 0.46              |
| 5:C:75:GLU:HA    | 5:C:76:PRO:HD3    | 1.79                     | 0.46              |
| 5:C:159:ILE:CG2  | 5:C:175:GLU:HB2   | 2.45                     | 0.46              |
| 5:C:197:LEU:HB3  | 5:C:202:TYR:HB2   | 1.97                     | 0.46              |
| 5:C:889:HIS:CE1  | 6:D:951:ILE:HG22  | 2.50                     | 0.46              |
| 6:D:116:LEU:HG   | 6:D:468:LEU:CD1   | 2.46                     | 0.46              |
| 6:D:117:ASP:O    | 6:D:150:ARG:HD2   | 2.16                     | 0.46              |
| 6:D:407:VAL:HG13 | 6:D:422:ALA:HB2   | 1.97                     | 0.46              |
| 6:D:844:ALA:O    | 6:D:867:ARG:HB3   | 2.15                     | 0.46              |
| 6:D:1394:VAL:HB  | 6:D:1397:LYS:HB2  | 1.97                     | 0.46              |
| 4:L:39:PRO:HD3   | 11:L:348:HOH:O    | 2.16                     | 0.46              |
| 4:L:43:ILE:HD12  | 4:L:217:ILE:CG2   | 2.45                     | 0.46              |
| 4:L:102:LYS:HD2  | 4:L:138:LEU:O     | 2.15                     | 0.46              |
| 4:L:106:PRO:HG3  | 4:L:134:GLU:CD    | 2.41                     | 0.46              |
| 4:L:184:THR:CG2  | 4:L:194:LYS:HB2   | 2.45                     | 0.46              |
| 5:M:286:SER:OG   | 5:M:299:LYS:HE3   | 2.15                     | 0.46              |
| 5:M:381:ALA:HB2  | 11:M:1457:HOH:O   | 2.15                     | 0.46              |
| 5:M:401:LEU:HG   | 5:M:402:SER:N     | 2.29                     | 0.46              |
| 5:M:611:ILE:HD11 | 5:M:641:PRO:HG3   | 1.97                     | 0.46              |
| 5:M:739:GLU:OE2  | 5:M:744:ARG:HA    | 2.14                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:948:GLU:OE1   | 5:M:955:PRO:HA    | 2.16                     | 0.46              |
| 5:M:984:GLU:HG3   | 6:N:944:THR:O     | 2.15                     | 0.46              |
| 6:N:18:ILE:HG23   | 6:N:518:PRO:CG    | 2.23                     | 0.46              |
| 6:N:107:ASP:O     | 6:N:108:VAL:C     | 2.57                     | 0.46              |
| 6:N:204:LEU:HB3   | 6:N:445:ARG:HH21  | 1.81                     | 0.46              |
| 6:N:792:ILE:HD13  | 6:N:793:THR:CG2   | 2.44                     | 0.46              |
| 6:N:820:GLU:CB    | 6:N:836:VAL:HG21  | 2.45                     | 0.46              |
| 6:N:911:LEU:O     | 6:N:915:VAL:HG23  | 2.14                     | 0.46              |
| 6:N:1335:LEU:HD13 | 6:N:1347:TYR:CE2  | 2.50                     | 0.46              |
| 1:X:14:DT:H3'     | 6:N:610:LYS:HZ3   | 1.80                     | 0.46              |
| 4:A:101:LEU:HD22  | 4:A:114:PHE:CE2   | 2.49                     | 0.46              |
| 4:A:173:PRO:O     | 4:A:201:THR:HG22  | 2.16                     | 0.46              |
| 5:C:198:ARG:HD3   | 5:C:228:ALA:HA    | 1.98                     | 0.46              |
| 5:C:605:LYS:CD    | 5:C:612:VAL:HB    | 2.45                     | 0.46              |
| 5:C:669:GLY:C     | 5:C:670:GLN:HG2   | 2.41                     | 0.46              |
| 5:C:1046:ALA:HB3  | 6:D:1476:THR:HB   | 1.98                     | 0.46              |
| 6:D:123:LEU:HD11  | 6:D:152:LEU:CD2   | 2.39                     | 0.46              |
| 6:D:399:ARG:HH11  | 6:D:430:ASP:CB    | 2.25                     | 0.46              |
| 6:D:420:VAL:C     | 6:D:421:LEU:HD23  | 2.40                     | 0.46              |
| 6:D:434:ARG:HB2   | 6:D:447:VAL:HG22  | 1.98                     | 0.46              |
| 6:D:1184:GLN:N    | 6:N:559:ALA:O     | 2.47                     | 0.46              |
| 4:K:30:ARG:NH1    | 5:M:938:LYS:HD2   | 2.31                     | 0.46              |
| 4:K:52:ALA:HB2    | 4:K:170:VAL:O     | 2.15                     | 0.46              |
| 5:M:61:LYS:NZ     | 11:M:1290:HOH:O   | 2.48                     | 0.46              |
| 5:M:109:LYS:HE2   | 5:M:111:ASP:HA    | 1.97                     | 0.46              |
| 5:M:217:LEU:HD12  | 5:M:311:PHE:HA    | 1.96                     | 0.46              |
| 5:M:326:ASP:OD1   | 5:M:427:VAL:HG22  | 2.14                     | 0.46              |
| 5:M:468:ARG:HB3   | 5:M:486:MET:O     | 2.14                     | 0.46              |
| 6:N:637:LEU:CD1   | 6:N:641:GLN:HB2   | 2.45                     | 0.46              |
| 6:N:1146:GLY:O    | 6:N:1207:TYR:N    | 2.48                     | 0.46              |
| 6:N:1221:VAL:O    | 6:N:1224:VAL:HB   | 2.15                     | 0.46              |
| 5:C:98:LEU:C      | 5:C:109:LYS:HD2   | 2.40                     | 0.46              |
| 5:C:181:VAL:HG12  | 5:C:182:VAL:N     | 2.30                     | 0.46              |
| 5:C:226:VAL:HG13  | 5:C:227:PHE:CD1   | 2.51                     | 0.46              |
| 5:C:732:ALA:HA    | 5:C:735:ARG:CZ    | 2.45                     | 0.46              |
| 5:C:737:LEU:HD21  | 5:C:741:GLY:N     | 2.30                     | 0.46              |
| 5:C:1083:GLU:CG   | 5:C:1086:ARG:HH21 | 2.25                     | 0.46              |
| 6:D:785:ILE:HG22  | 6:D:789:LEU:CD1   | 2.36                     | 0.46              |
| 6:D:1002:LYS:HA   | 11:D:8149:HOH:O   | 2.16                     | 0.46              |
| 6:D:1110:ALA:O    | 6:D:1111:ASP:C    | 2.58                     | 0.46              |
| 6:D:1335:LEU:CD2  | 6:D:1344:VAL:HG22 | 2.46                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:K:23:PHE:O      | 4:K:196:THR:HA   | 2.16                     | 0.46              |
| 4:K:224:TYR:HB3   | 4:L:9:PRO:CB     | 2.45                     | 0.46              |
| 5:M:689:VAL:O     | 5:M:869:VAL:HG23 | 2.15                     | 0.46              |
| 5:M:937:ASP:O     | 5:M:941:VAL:HG23 | 2.16                     | 0.46              |
| 5:M:939:ARG:CB    | 5:M:982:PRO:HG3  | 2.33                     | 0.46              |
| 5:M:1047:HIS:CD2  | 5:M:1047:HIS:N   | 2.83                     | 0.46              |
| 5:M:1093:GLN:HB3  | 6:N:90:MET:SD    | 2.55                     | 0.46              |
| 6:N:400:VAL:HG13  | 6:N:400:VAL:O    | 2.16                     | 0.46              |
| 6:N:633:VAL:C     | 6:N:635:PRO:HD3  | 2.40                     | 0.46              |
| 6:N:654:LYS:HB2   | 6:N:654:LYS:NZ   | 2.31                     | 0.46              |
| 6:N:880:ILE:O     | 6:N:883:ALA:HB3  | 2.15                     | 0.46              |
| 6:N:1440:PHE:C    | 6:N:1440:PHE:CD2 | 2.93                     | 0.46              |
| 4:A:86:VAL:HG12   | 4:A:124:ASN:HB2  | 1.97                     | 0.46              |
| 4:B:154:GLU:HB3   | 4:B:155:LYS:HZ2  | 1.79                     | 0.46              |
| 5:C:445:GLU:HA    | 5:C:449:ILE:HD12 | 1.97                     | 0.46              |
| 5:C:902:ILE:O     | 5:C:904:PRO:HD3  | 2.15                     | 0.46              |
| 5:C:971:LYS:HB2   | 5:C:986:PRO:HB2  | 1.97                     | 0.46              |
| 5:C:1082:PRO:HD2  | 6:D:1468:LEU:O   | 2.15                     | 0.46              |
| 6:D:436:GLU:HB2   | 6:D:445:ARG:CG   | 2.45                     | 0.46              |
| 6:D:618:LEU:HD12  | 6:D:1439:SER:HB3 | 1.96                     | 0.46              |
| 6:D:987:GLU:O     | 6:D:991:GLN:HB2  | 2.15                     | 0.46              |
| 6:D:1042:ARG:NH2  | 6:D:1061:PHE:HZ  | 2.12                     | 0.46              |
| 6:D:1372:VAL:HA   | 6:D:1375:MET:HE3 | 1.96                     | 0.46              |
| 6:D:1393:GLN:HE22 | 6:D:1394:VAL:HB  | 1.80                     | 0.46              |
| 4:L:68:ILE:HG21   | 11:L:362:HOH:O   | 2.15                     | 0.46              |
| 5:M:146:VAL:CG2   | 5:M:281:LEU:HD11 | 2.46                     | 0.46              |
| 5:M:260:LEU:HA    | 5:M:291:ALA:HB2  | 1.98                     | 0.46              |
| 5:M:467:ILE:HG23  | 11:M:1287:HOH:O  | 2.15                     | 0.46              |
| 5:M:748:GLU:HA    | 5:M:799:ILE:HD13 | 1.97                     | 0.46              |
| 6:N:30:GLU:HB3    | 6:N:40:GLU:HB3   | 1.96                     | 0.46              |
| 6:N:611:GLN:HG3   | 6:N:611:GLN:O    | 2.14                     | 0.46              |
| 1:X:15:DC:H2"     | 1:X:16:DG:C8     | 2.51                     | 0.46              |
| 5:C:141:HIS:C     | 5:C:141:HIS:CD2  | 2.93                     | 0.46              |
| 5:C:218:VAL:O     | 5:C:221:LEU:HG   | 2.16                     | 0.46              |
| 5:C:232:GLU:O     | 5:C:236:ILE:HD12 | 2.16                     | 0.46              |
| 5:C:522:VAL:HG21  | 11:C:1425:HOH:O  | 2.15                     | 0.46              |
| 5:C:524:VAL:HG13  | 5:C:528:GLU:HB2  | 1.98                     | 0.46              |
| 5:C:545:ASN:OD1   | 5:C:583:LEU:HD22 | 2.16                     | 0.46              |
| 5:C:834:GLN:HB2   | 5:C:834:GLN:HE21 | 1.58                     | 0.46              |
| 5:C:1081:VAL:HG23 | 11:C:1198:HOH:O  | 2.16                     | 0.46              |
| 5:C:1101:THR:HG23 | 5:C:1109:VAL:O   | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:31:THR:HB     | 6:D:527:MET:CE    | 2.46                     | 0.46              |
| 6:D:438:ASP:HB2   | 6:D:445:ARG:NH1   | 2.31                     | 0.46              |
| 6:D:785:ILE:H     | 6:D:785:ILE:CD1   | 2.13                     | 0.46              |
| 6:D:786:ILE:CG2   | 6:D:1026:SER:HB3  | 2.37                     | 0.46              |
| 6:D:939:PHE:O     | 6:D:943:THR:HG23  | 2.16                     | 0.46              |
| 6:D:1101:VAL:HG12 | 6:D:1374:GLN:HB3  | 1.97                     | 0.46              |
| 5:M:567:GLN:HG2   | 11:M:1537:HOH:O   | 2.15                     | 0.46              |
| 5:M:694:LEU:HD21  | 5:M:868:ASP:OD2   | 2.15                     | 0.46              |
| 5:M:906:PHE:CZ    | 6:N:1067:VAL:HA   | 2.51                     | 0.46              |
| 5:M:1036:GLU:O    | 5:M:1039:ALA:HB3  | 2.16                     | 0.46              |
| 6:N:62:LYS:HG3    | 6:N:75:ARG:HD2    | 1.98                     | 0.46              |
| 6:N:397:LYS:HB3   | 6:N:448:GLU:CB    | 2.46                     | 0.46              |
| 6:N:403:PHE:CE2   | 6:N:444:VAL:HG23  | 2.51                     | 0.46              |
| 6:N:960:LYS:HD3   | 11:N:9374:HOH:O   | 2.15                     | 0.46              |
| 6:N:984:THR:CG2   | 6:N:987:GLU:H     | 2.29                     | 0.46              |
| 6:N:1145:TYR:HD2  | 6:N:1168:MET:SD   | 2.39                     | 0.46              |
| 6:N:1209:LEU:CD2  | 6:N:1210:SER:H    | 2.28                     | 0.46              |
| 6:N:1402:ALA:HB2  | 6:N:1415:VAL:CG2  | 2.46                     | 0.46              |
| 5:C:231:PRO:HD2   | 11:C:1261:HOH:O   | 2.16                     | 0.46              |
| 5:C:401:LEU:CD2   | 5:C:565:GLN:HE21  | 2.29                     | 0.46              |
| 5:C:404:LEU:HD22  | 5:C:591:SER:HB3   | 1.98                     | 0.46              |
| 5:C:418:LEU:N     | 5:C:418:LEU:HD12  | 2.31                     | 0.46              |
| 5:C:437:ARG:HG2   | 5:C:467:ILE:HB    | 1.98                     | 0.46              |
| 5:C:516:ARG:HH21  | 6:D:1068:LEU:HB3  | 1.81                     | 0.46              |
| 6:D:33:ASN:HB2    | 6:D:40:GLU:OE1    | 2.16                     | 0.46              |
| 6:D:749:VAL:HA    | 6:D:750:PRO:HD3   | 1.82                     | 0.46              |
| 6:D:783:ARG:HH22  | 6:D:1239:ARG:HH22 | 1.64                     | 0.46              |
| 6:D:800:LYS:CE    | 6:D:804:LEU:HD22  | 2.43                     | 0.46              |
| 6:D:951:ILE:O     | 6:D:951:ILE:HD13  | 2.16                     | 0.46              |
| 6:D:1228:SER:O    | 6:D:1232:PRO:CD   | 2.58                     | 0.46              |
| 4:K:185:ARG:O     | 4:K:185:ARG:HD2   | 2.15                     | 0.46              |
| 5:M:91:GLN:NE2    | 5:M:117:HIS:O     | 2.49                     | 0.46              |
| 5:M:674:VAL:HG21  | 5:M:871:LEU:HG    | 1.98                     | 0.46              |
| 5:M:745:ILE:H     | 5:M:745:ILE:CD1   | 2.22                     | 0.46              |
| 5:M:864:GLY:O     | 5:M:866:PRO:HD3   | 2.15                     | 0.46              |
| 5:M:1008:ARG:HH12 | 5:M:1011:GLY:N    | 2.14                     | 0.46              |
| 6:N:543:LEU:CD1   | 6:N:581:LEU:HA    | 2.38                     | 0.46              |
| 6:N:707:THR:HG22  | 6:N:712:GLY:HA3   | 1.96                     | 0.46              |
| 6:N:760:ARG:NH1   | 7:O:61:VAL:HG23   | 2.27                     | 0.46              |
| 6:N:968:ASP:O     | 6:N:971:LEU:HB3   | 2.16                     | 0.46              |
| 6:N:974:ILE:CD1   | 6:N:995:LEU:HD22  | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:1112:CYS:CB   | 6:N:1195:GLN:HG2  | 2.44                     | 0.46              |
| 6:N:1349:VAL:HA   | 6:N:1368:ILE:HG21 | 1.98                     | 0.46              |
| 5:C:124:ASP:OD1   | 5:C:124:ASP:N     | 2.48                     | 0.46              |
| 5:C:169:GLY:CA    | 5:C:263:ASP:HB3   | 2.44                     | 0.46              |
| 5:C:217:LEU:HD11  | 5:C:314:THR:OG1   | 2.16                     | 0.46              |
| 5:C:322:VAL:HG13  | 11:C:1193:HOH:O   | 2.14                     | 0.46              |
| 5:C:333:ILE:N     | 5:C:333:ILE:HD12  | 2.31                     | 0.46              |
| 5:C:359:MET:HE2   | 5:C:359:MET:O     | 2.15                     | 0.46              |
| 5:C:737:LEU:HD21  | 5:C:741:GLY:H     | 1.81                     | 0.46              |
| 5:C:758:ARG:HG2   | 5:C:758:ARG:HH11  | 1.81                     | 0.46              |
| 6:D:19:ARG:H      | 6:D:19:ARG:HG2    | 1.51                     | 0.46              |
| 6:D:71:LYS:HB2    | 6:D:71:LYS:HZ3    | 1.79                     | 0.46              |
| 6:D:407:VAL:HA    | 6:D:422:ALA:CB    | 2.46                     | 0.46              |
| 6:D:443:VAL:CG1   | 6:D:445:ARG:HH22  | 2.29                     | 0.46              |
| 6:D:617:ASN:HA    | 11:D:8092:HOH:O   | 2.15                     | 0.46              |
| 6:D:638:LYS:NZ    | 11:D:8121:HOH:O   | 2.48                     | 0.46              |
| 6:D:899:LEU:HB3   | 6:D:921:ARG:NH1   | 2.31                     | 0.46              |
| 6:D:926:LYS:HG2   | 6:D:929:ARG:NH1   | 2.30                     | 0.46              |
| 6:D:1166:LEU:HD12 | 6:D:1171:VAL:HG22 | 1.98                     | 0.46              |
| 4:L:124:ASN:CG    | 4:L:127:LEU:HB2   | 2.41                     | 0.46              |
| 4:L:175:ARG:HD3   | 4:L:202:ASP:HB3   | 1.98                     | 0.46              |
| 5:M:342:ASP:O     | 5:M:346:VAL:HG23  | 2.16                     | 0.46              |
| 5:M:568:ALA:HB3   | 11:M:1233:HOH:O   | 2.15                     | 0.46              |
| 5:M:1019:GLN:NE2  | 11:N:9292:HOH:O   | 2.48                     | 0.46              |
| 5:M:1031:ARG:HE   | 6:N:621:LYS:HB3   | 1.80                     | 0.46              |
| 5:M:1060:ILE:CD1  | 5:M:1064:ASN:HD21 | 2.29                     | 0.46              |
| 6:N:30:GLU:HB3    | 6:N:40:GLU:CB     | 2.45                     | 0.46              |
| 6:N:65:ARG:HD2    | 6:N:65:ARG:HA     | 1.70                     | 0.46              |
| 6:N:115:LEU:HB2   | 6:N:498:VAL:HG11  | 1.98                     | 0.46              |
| 6:N:491:LYS:HD2   | 6:N:491:LYS:O     | 2.16                     | 0.46              |
| 6:N:644:LEU:HD12  | 6:N:645:PRO:CD    | 2.46                     | 0.46              |
| 6:N:902:LEU:HD13  | 11:N:9040:HOH:O   | 2.14                     | 0.46              |
| 6:N:959:GLU:O     | 6:N:963:TYR:CD1   | 2.70                     | 0.46              |
| 6:N:1002:LYS:HA   | 11:N:9185:HOH:O   | 2.15                     | 0.46              |
| 6:N:1353:GLN:HG2  | 6:N:1368:ILE:HD11 | 1.98                     | 0.46              |
| 6:N:1366:LYS:O    | 6:N:1370:ILE:HG12 | 2.15                     | 0.46              |
| 6:N:1394:VAL:HB   | 6:N:1397:LYS:CB   | 2.43                     | 0.46              |
| 6:N:1437:ALA:C    | 6:N:1446:VAL:HG21 | 2.40                     | 0.46              |
| 7:O:36:LYS:HZ2    | 7:O:45:ARG:HH22   | 1.63                     | 0.46              |
| 5:C:5:ARG:HE      | 5:C:5:ARG:HB2     | 1.65                     | 0.45              |
| 5:C:430:VAL:HG12  | 6:D:1078:ARG:HG3  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:950:LEU:HB3   | 5:C:952:LEU:CD2   | 2.44                     | 0.45              |
| 6:D:14:SER:O      | 6:D:17:LYS:N      | 2.49                     | 0.45              |
| 6:D:496:LEU:HD21  | 6:D:1388:ARG:CG   | 2.44                     | 0.45              |
| 6:D:639:LEU:HD12  | 6:D:640:HIS:H     | 1.81                     | 0.45              |
| 6:D:1123:PHE:CZ   | 6:D:1178:ALA:HB1  | 2.51                     | 0.45              |
| 6:D:1218:GLY:HA2  | 11:D:8043:HOH:O   | 2.15                     | 0.45              |
| 4:K:198:ARG:NH2   | 5:M:932:GLU:HB3   | 2.30                     | 0.45              |
| 5:M:100:LEU:HD12  | 5:M:101:ILE:O     | 2.16                     | 0.45              |
| 5:M:195:LEU:O     | 5:M:199:VAL:HG23  | 2.16                     | 0.45              |
| 5:M:352:ALA:CA    | 5:M:355:VAL:HG12  | 2.44                     | 0.45              |
| 5:M:1043:TYR:HA   | 6:N:710:ARG:NH1   | 2.30                     | 0.45              |
| 6:N:631:ILE:HG21  | 6:N:745:MET:HG3   | 1.97                     | 0.45              |
| 6:N:770:LEU:HD11  | 6:N:919:PHE:HE2   | 1.80                     | 0.45              |
| 6:N:783:ARG:NH1   | 6:N:1029:ARG:CZ   | 2.79                     | 0.45              |
| 6:N:1051:GLU:HB3  | 11:N:9122:HOH:O   | 2.15                     | 0.45              |
| 6:N:1192:LEU:HD22 | 6:N:1345:GLU:CG   | 2.46                     | 0.45              |
| 6:N:1262:LEU:HD21 | 6:N:1351:GLU:CG   | 2.46                     | 0.45              |
| 3:I:8:DA:H1'      | 3:I:9:DG:C5'      | 2.46                     | 0.45              |
| 4:A:154:GLU:H     | 4:A:154:GLU:CD    | 2.24                     | 0.45              |
| 5:C:146:VAL:HG13  | 5:C:162:ILE:HA    | 1.97                     | 0.45              |
| 5:C:189:ARG:HD3   | 5:C:190:LYS:H     | 1.81                     | 0.45              |
| 5:C:203:ASP:O     | 5:C:207:LEU:HB2   | 2.16                     | 0.45              |
| 5:C:573:ARG:HH11  | 5:C:573:ARG:CB    | 2.19                     | 0.45              |
| 5:C:669:GLY:HA3   | 5:C:995:MET:HA    | 1.98                     | 0.45              |
| 6:D:114:THR:HB    | 6:D:498:VAL:HG21  | 1.98                     | 0.45              |
| 6:D:1098:LEU:CD2  | 6:D:1229:ILE:HD12 | 2.44                     | 0.45              |
| 4:K:39:PRO:O      | 4:K:43:ILE:HG12   | 2.17                     | 0.45              |
| 4:K:198:ARG:HH22  | 5:M:932:GLU:CB    | 2.26                     | 0.45              |
| 4:L:121:GLU:OE1   | 4:L:123:MET:HG2   | 2.16                     | 0.45              |
| 5:M:30:LEU:O      | 5:M:30:LEU:HD12   | 2.17                     | 0.45              |
| 5:M:44:ILE:HG23   | 5:M:344:PHE:CE1   | 2.47                     | 0.45              |
| 5:M:146:VAL:HG21  | 5:M:281:LEU:HD11  | 1.98                     | 0.45              |
| 5:M:192:PRO:HD2   | 5:M:195:LEU:HD22  | 1.98                     | 0.45              |
| 5:M:211:LEU:HD22  | 11:M:1152:HOH:O   | 2.17                     | 0.45              |
| 5:M:688:ILE:HD12  | 5:M:847:GLY:HA3   | 1.99                     | 0.45              |
| 6:N:119:SER:OG    | 6:N:123:LEU:HD13  | 2.16                     | 0.45              |
| 6:N:206:ARG:HH11  | 6:N:206:ARG:HG3   | 1.81                     | 0.45              |
| 6:N:409:VAL:HG11  | 6:N:435:VAL:HG21  | 1.98                     | 0.45              |
| 6:N:470:LEU:H     | 6:N:470:LEU:HD23  | 1.81                     | 0.45              |
| 6:N:772:PRO:HB2   | 11:N:9024:HOH:O   | 2.15                     | 0.45              |
| 6:N:1136:LYS:O    | 6:N:1140:ILE:HG13 | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:1380:GLU:OE2 | 6:N:1390:LEU:HA  | 2.15                     | 0.45              |
| 5:C:10:ARG:HH11  | 5:C:11:GLU:H     | 1.63                     | 0.45              |
| 5:C:398:THR:HG21 | 5:C:567:GLN:CA   | 2.46                     | 0.45              |
| 5:C:640:ARG:HA   | 11:C:1183:HOH:O  | 2.16                     | 0.45              |
| 5:C:832:LYS:HE3  | 11:C:1519:HOH:O  | 2.15                     | 0.45              |
| 6:D:508:ARG:NH1  | 11:D:8038:HOH:O  | 2.50                     | 0.45              |
| 6:D:530:VAL:HB   | 6:D:534:ARG:HB2  | 1.99                     | 0.45              |
| 6:D:884:ARG:HA   | 11:D:8116:HOH:O  | 2.16                     | 0.45              |
| 6:D:896:ALA:O    | 6:D:900:ILE:HG23 | 2.17                     | 0.45              |
| 6:D:1135:ARG:HD2 | 6:D:1139:ASP:OD2 | 2.17                     | 0.45              |
| 6:D:1207:TYR:HA  | 6:D:1214:PRO:HA  | 1.97                     | 0.45              |
| 6:D:1402:ALA:HB2 | 6:D:1415:VAL:CG2 | 2.46                     | 0.45              |
| 4:K:16:GLN:NE2   | 11:K:788:HOH:O   | 2.47                     | 0.45              |
| 4:L:50:GLY:HA3   | 4:L:171:PHE:O    | 2.16                     | 0.45              |
| 4:L:59:GLU:HG2   | 4:L:139:ASN:HD22 | 1.80                     | 0.45              |
| 4:L:112:ARG:H    | 4:L:112:ARG:HG2  | 1.48                     | 0.45              |
| 5:M:350:ARG:HB3  | 5:M:377:PRO:HB3  | 1.97                     | 0.45              |
| 5:M:479:VAL:HG22 | 5:M:506:ASN:HA   | 1.98                     | 0.45              |
| 5:M:577:PRO:HB3  | 5:M:842:ARG:NH1  | 2.31                     | 0.45              |
| 5:M:801:VAL:HG23 | 5:M:802:ARG:N    | 2.31                     | 0.45              |
| 5:M:1103:ASP:CG  | 6:N:3:LYS:HD2    | 2.42                     | 0.45              |
| 5:M:1115:LEU:O   | 6:N:89:ARG:CZ    | 2.64                     | 0.45              |
| 6:N:31:THR:OG1   | 6:N:32:ILE:N     | 2.49                     | 0.45              |
| 6:N:95:LEU:HA    | 6:N:551:ASN:HD21 | 1.81                     | 0.45              |
| 6:N:169:TYR:HB3  | 6:N:195:VAL:HG11 | 1.99                     | 0.45              |
| 6:N:465:LEU:HD22 | 6:N:510:GLU:HA   | 1.97                     | 0.45              |
| 6:N:710:ARG:C    | 6:N:712:GLY:N    | 2.74                     | 0.45              |
| 6:N:756:GLN:HE21 | 6:N:760:ARG:HD2  | 1.82                     | 0.45              |
| 6:N:796:ARG:NE   | 6:N:828:LYS:NZ   | 2.61                     | 0.45              |
| 6:N:907:GLU:O    | 6:N:911:LEU:HG   | 2.15                     | 0.45              |
| 6:N:954:ALA:C    | 6:N:1039:CYS:SG  | 2.99                     | 0.45              |
| 6:N:963:TYR:HD1  | 6:N:963:TYR:H    | 1.63                     | 0.45              |
| 4:A:186:LEU:HB2  | 11:A:361:HOH:O   | 2.17                     | 0.45              |
| 4:A:206:THR:HG23 | 4:A:208:LEU:N    | 2.31                     | 0.45              |
| 5:C:263:ASP:C    | 5:C:264:PRO:O    | 2.59                     | 0.45              |
| 5:C:265:ARG:HB3  | 5:C:267:TYR:CE2  | 2.51                     | 0.45              |
| 5:C:385:PHE:O    | 5:C:389:SER:HB2  | 2.16                     | 0.45              |
| 5:C:401:LEU:HD22 | 5:C:546:LEU:HD13 | 1.99                     | 0.45              |
| 5:C:403:SER:O    | 5:C:407:LYS:HD3  | 2.16                     | 0.45              |
| 5:C:431:HIS:CD2  | 5:C:432:ARG:N    | 2.85                     | 0.45              |
| 5:C:523:ILE:HG23 | 5:C:523:ILE:O    | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:569:VAL:HA    | 5:C:570:PRO:HD3   | 1.85                     | 0.45              |
| 5:C:625:LEU:HA    | 5:C:639:GLN:NE2   | 2.24                     | 0.45              |
| 5:C:810:ASP:HA    | 5:C:811:PRO:HD3   | 1.68                     | 0.45              |
| 5:C:1008:ARG:HB2  | 5:C:1027:PHE:HB2  | 1.99                     | 0.45              |
| 5:C:1055:LEU:HD22 | 5:C:1066:ALA:CB   | 2.37                     | 0.45              |
| 5:C:1063:ARG:O    | 5:C:1066:ALA:HB3  | 2.16                     | 0.45              |
| 6:D:44:LEU:O      | 6:D:525:ARG:NH2   | 2.49                     | 0.45              |
| 6:D:136:ASP:HB3   | 6:D:137:PRO:CD    | 2.33                     | 0.45              |
| 6:D:165:LYS:HA    | 6:D:199:LEU:HD13  | 1.97                     | 0.45              |
| 6:D:396:VAL:CG1   | 6:D:398:ALA:HB2   | 2.46                     | 0.45              |
| 6:D:606:ILE:O     | 6:D:613:ARG:HB2   | 2.16                     | 0.45              |
| 6:D:819:GLY:HA2   | 11:D:8465:HOH:O   | 2.17                     | 0.45              |
| 6:D:1145:TYR:HB2  | 6:D:1168:MET:HE1  | 1.97                     | 0.45              |
| 6:D:1376:MET:CE   | 6:D:1421:LEU:HD22 | 2.46                     | 0.45              |
| 4:K:38:ASN:CG     | 5:M:980:GLY:CA    | 2.89                     | 0.45              |
| 4:K:41:ARG:HA     | 4:K:44:LEU:HD12   | 1.97                     | 0.45              |
| 4:K:101:LEU:C     | 4:K:101:LEU:HD23  | 2.41                     | 0.45              |
| 4:K:158:ILE:HA    | 11:K:1352:HOH:O   | 2.15                     | 0.45              |
| 5:M:77:PRO:HG2    | 5:M:117:HIS:CE1   | 2.51                     | 0.45              |
| 5:M:310:LEU:HD11  | 11:M:1381:HOH:O   | 2.15                     | 0.45              |
| 5:M:468:ARG:NE    | 5:M:487:THR:HG23  | 2.32                     | 0.45              |
| 5:M:479:VAL:HG21  | 5:M:503:LEU:CD1   | 2.46                     | 0.45              |
| 5:M:601:GLY:HA3   | 5:M:615:TYR:HA    | 1.97                     | 0.45              |
| 5:M:817:PRO:O     | 6:N:532:GLY:HA2   | 2.15                     | 0.45              |
| 5:M:1007:ALA:HB1  | 6:N:652:LEU:CD1   | 2.46                     | 0.45              |
| 6:N:106:LYS:CE    | 6:N:125:GLN:HE22  | 2.30                     | 0.45              |
| 6:N:781:PRO:O     | 6:N:786:ILE:HD11  | 2.17                     | 0.45              |
| 6:N:800:LYS:HE3   | 6:N:804:LEU:HD22  | 1.98                     | 0.45              |
| 1:G:15:DC:H2''    | 1:G:16:DG:H8      | 1.82                     | 0.45              |
| 3:Z:4:DC:H2''     | 3:Z:5:DG:O5'      | 2.16                     | 0.45              |
| 4:A:9:PRO:HB3     | 4:A:25:LEU:CG     | 2.46                     | 0.45              |
| 4:B:48:ILE:HG22   | 4:B:173:PRO:HD2   | 1.99                     | 0.45              |
| 5:C:146:VAL:HG11  | 5:C:306:THR:CB    | 2.41                     | 0.45              |
| 5:C:168:ARG:HH11  | 5:C:168:ARG:HG3   | 1.82                     | 0.45              |
| 5:C:260:LEU:HA    | 5:C:291:ALA:HB2   | 1.97                     | 0.45              |
| 5:C:267:TYR:O     | 5:C:268:ASP:C     | 2.59                     | 0.45              |
| 6:D:68:PHE:HZ     | 11:D:8399:HOH:O   | 1.98                     | 0.45              |
| 6:D:158:TYR:CZ    | 6:D:456:MET:HE1   | 2.51                     | 0.45              |
| 6:D:618:LEU:CD1   | 6:D:1439:SER:HB3  | 2.47                     | 0.45              |
| 6:D:794:GLN:OE1   | 6:D:905:PRO:HG3   | 2.15                     | 0.45              |
| 6:D:1344:VAL:HG12 | 6:D:1348:LEU:CD1  | 2.46                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:1476:THR:O    | 6:D:1482:ARG:HA   | 2.17                     | 0.45              |
| 7:E:45:ARG:HE     | 7:E:45:ARG:HB2    | 1.62                     | 0.45              |
| 4:K:13:VAL:HG22   | 4:K:23:PHE:HD1    | 1.82                     | 0.45              |
| 4:K:94:LEU:HD11   | 4:K:119:ASP:HB3   | 1.98                     | 0.45              |
| 4:L:2:LEU:O       | 4:L:6:LEU:HD23    | 2.16                     | 0.45              |
| 5:M:43:GLY:HA2    | 5:M:341:THR:HG21  | 1.96                     | 0.45              |
| 5:M:122:THR:HB    | 5:M:124:ASP:OD1   | 2.17                     | 0.45              |
| 5:M:165:LEU:HA    | 5:M:166:PRO:O     | 2.16                     | 0.45              |
| 5:M:250:ARG:HG3   | 5:M:250:ARG:NH1   | 2.31                     | 0.45              |
| 5:M:375:SER:HA    | 11:M:1564:HOH:O   | 2.14                     | 0.45              |
| 5:M:474:VAL:HG13  | 5:M:530:GLU:C     | 2.42                     | 0.45              |
| 5:M:769:PRO:HD2   | 6:N:65:ARG:NE     | 2.32                     | 0.45              |
| 6:N:41:ARG:CD     | 6:N:42:ASP:H      | 2.28                     | 0.45              |
| 6:N:152:LEU:HD23  | 6:N:152:LEU:N     | 2.31                     | 0.45              |
| 6:N:204:LEU:HD12  | 6:N:396:VAL:HG21  | 1.97                     | 0.45              |
| 6:N:497:GLU:O     | 6:N:500:ARG:HB2   | 2.16                     | 0.45              |
| 6:N:1045:MET:HE2  | 6:N:1073:SER:CB   | 2.39                     | 0.45              |
| 3:I:3:DA:H4'      | 5:C:423:ALA:HB1   | 1.97                     | 0.45              |
| 1:X:13:DT:OP1     | 6:N:1093:TYR:CE2  | 2.70                     | 0.45              |
| 5:C:51:THR:CG2    | 5:C:348:LEU:HD23  | 2.46                     | 0.45              |
| 5:C:329:GLY:CA    | 5:C:489:THR:HG23  | 2.46                     | 0.45              |
| 5:C:567:GLN:HB2   | 5:C:997:LEU:HD12  | 1.98                     | 0.45              |
| 5:C:833:LEU:CD1   | 5:C:996:LYS:HD2   | 2.47                     | 0.45              |
| 5:C:1016:ILE:HD13 | 5:C:1016:ILE:N    | 2.24                     | 0.45              |
| 6:D:32:ILE:HD12   | 6:D:527:MET:HG2   | 1.97                     | 0.45              |
| 6:D:36:THR:O      | 6:D:38:LYS:N      | 2.49                     | 0.45              |
| 6:D:107:ASP:O     | 6:D:108:VAL:C     | 2.60                     | 0.45              |
| 6:D:1057:VAL:HG13 | 6:D:1069:GLU:HB3  | 1.98                     | 0.45              |
| 6:D:1135:ARG:HB3  | 6:D:1140:ILE:CG1  | 2.47                     | 0.45              |
| 6:D:1153:VAL:CG1  | 6:N:561:GLY:HA3   | 2.41                     | 0.45              |
| 6:D:1198:TYR:N    | 11:D:8501:HOH:O   | 2.48                     | 0.45              |
| 6:D:1213:ARG:NH2  | 7:E:10:PHE:O      | 2.44                     | 0.45              |
| 6:D:1221:VAL:O    | 6:D:1222:GLY:C    | 2.59                     | 0.45              |
| 6:D:1389:LEU:HD13 | 11:D:8087:HOH:O   | 2.17                     | 0.45              |
| 6:D:1477:GLY:O    | 6:D:1478:SER:C    | 2.59                     | 0.45              |
| 4:L:73:GLU:HB3    | 4:L:77:GLU:HG3    | 1.97                     | 0.45              |
| 5:M:121:MET:CE    | 5:M:125:GLY:HA2   | 2.34                     | 0.45              |
| 5:M:139:GLN:HA    | 5:M:411:SER:O     | 2.17                     | 0.45              |
| 5:M:516:ARG:CZ    | 6:N:1068:LEU:HD13 | 2.44                     | 0.45              |
| 5:M:690:ILE:CG2   | 5:M:852:ILE:HG13  | 2.47                     | 0.45              |
| 5:M:695:LEU:HD23  | 5:M:695:LEU:O     | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:168:THR:OG1   | 6:N:206:ARG:NH2   | 2.49                     | 0.45              |
| 6:N:179:VAL:HG21  | 6:N:191:LEU:HD23  | 1.99                     | 0.45              |
| 6:N:618:LEU:HD22  | 6:N:619:LEU:HD22  | 1.98                     | 0.45              |
| 6:N:682:ASP:OD1   | 6:N:682:ASP:N     | 2.49                     | 0.45              |
| 6:N:701:LEU:HD12  | 6:N:701:LEU:N     | 2.32                     | 0.45              |
| 6:N:787:LEU:CD2   | 6:N:1023:MET:HE2  | 2.46                     | 0.45              |
| 6:N:845:ASN:H     | 6:N:848:GLU:HG3   | 1.81                     | 0.45              |
| 6:N:945:SER:OG    | 6:N:947:ILE:HG13  | 2.16                     | 0.45              |
| 6:N:1031:ASN:HB3  | 6:N:1034:GLN:OE1  | 2.15                     | 0.45              |
| 6:N:1412:LYS:NZ   | 6:N:1414:PRO:HG3  | 2.32                     | 0.45              |
| 6:N:1475:GLY:O    | 6:N:1478:SER:HB3  | 2.16                     | 0.45              |
| 7:O:28:GLN:HB3    | 7:O:32:ARG:HH12   | 1.82                     | 0.45              |
| 2:H:9:G:C5'       | 2:H:9:G:H8        | 2.30                     | 0.45              |
| 4:A:41:ARG:HH11   | 4:A:177:VAL:HB    | 1.82                     | 0.45              |
| 4:A:193:ASP:CG    | 5:C:938:LYS:HZ1   | 2.24                     | 0.45              |
| 5:C:56:GLU:CB     | 5:C:64:LEU:HD23   | 2.46                     | 0.45              |
| 5:C:160:ALA:HB3   | 5:C:174:LEU:HB2   | 1.97                     | 0.45              |
| 5:C:551:GLU:HB3   | 5:C:906:PHE:CD2   | 2.52                     | 0.45              |
| 5:C:570:PRO:O     | 5:C:702:SER:HB2   | 2.16                     | 0.45              |
| 5:C:603:VAL:O     | 5:C:646:GLY:HA2   | 2.16                     | 0.45              |
| 5:C:837:ASP:OD1   | 5:C:999:HIS:NE2   | 2.50                     | 0.45              |
| 5:C:910:LYS:HG3   | 5:C:912:PRO:HD2   | 1.99                     | 0.45              |
| 6:D:10:ILE:HD11   | 6:D:1434:TRP:CE2  | 2.51                     | 0.45              |
| 6:D:576:GLU:HA    | 6:D:579:ASP:OD2   | 2.17                     | 0.45              |
| 6:D:992:ILE:HG21  | 11:D:8500:HOH:O   | 2.16                     | 0.45              |
| 6:D:1102:THR:HG23 | 6:D:1370:ILE:HG22 | 1.99                     | 0.45              |
| 6:D:1406:ARG:HB2  | 6:D:1412:LYS:HZ3  | 1.82                     | 0.45              |
| 6:D:1484:THR:O    | 7:E:25:LYS:HD3    | 2.17                     | 0.45              |
| 4:K:58:ILE:HG21   | 4:K:68:ILE:CD1    | 2.46                     | 0.45              |
| 5:M:615:TYR:HB3   | 5:M:617:ASP:OD1   | 2.16                     | 0.45              |
| 5:M:829:GLN:NE2   | 5:M:831:ARG:HH21  | 2.15                     | 0.45              |
| 5:M:899:GLN:HG3   | 5:M:901:TYR:CZ    | 2.51                     | 0.45              |
| 5:M:987:ILE:HG12  | 6:N:948:THR:CG2   | 2.46                     | 0.45              |
| 5:M:1034:GLU:CB   | 6:N:619:LEU:HD13  | 2.45                     | 0.45              |
| 6:N:515:GLU:HG3   | 11:N:9303:HOH:O   | 2.16                     | 0.45              |
| 6:N:587:ARG:HG2   | 6:N:587:ARG:HH11  | 1.81                     | 0.45              |
| 6:N:784:ASP:HB3   | 6:N:939:PHE:CE2   | 2.51                     | 0.45              |
| 6:N:1232:PRO:O    | 6:N:1236:LEU:HG   | 2.16                     | 0.45              |
| 4:A:13:VAL:HG22   | 4:A:23:PHE:CD1    | 2.51                     | 0.45              |
| 4:B:97:VAL:HG13   | 11:B:325:HOH:O    | 2.17                     | 0.45              |
| 5:C:906:PHE:CE1   | 6:D:1067:VAL:HG13 | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:1060:ILE:O    | 5:C:1063:ARG:HG2  | 2.15                     | 0.45              |
| 6:D:36:THR:C      | 6:D:38:LYS:N      | 2.75                     | 0.45              |
| 6:D:407:VAL:HA    | 6:D:422:ALA:HB2   | 1.99                     | 0.45              |
| 6:D:506:GLY:O     | 6:D:507:ASN:C     | 2.59                     | 0.45              |
| 6:D:633:VAL:HG22  | 6:D:635:PRO:HD3   | 1.98                     | 0.45              |
| 6:D:974:ILE:O     | 6:D:983:LEU:HD11  | 2.16                     | 0.45              |
| 6:D:998:GLU:O     | 6:D:1002:LYS:HG3  | 2.17                     | 0.45              |
| 6:D:1225:ALA:HB2  | 6:D:1367:HIS:ND1  | 2.32                     | 0.45              |
| 6:D:1261:GLU:O    | 6:D:1264:GLU:O    | 2.35                     | 0.45              |
| 6:D:1492:LEU:O    | 6:D:1492:LEU:HD22 | 2.16                     | 0.45              |
| 7:E:80:VAL:HG11   | 7:E:85:LEU:HD23   | 1.98                     | 0.45              |
| 5:M:806:LEU:O     | 5:M:821:GLU:HB2   | 2.17                     | 0.45              |
| 5:M:844:GLY:O     | 5:M:846:LYS:HG3   | 2.16                     | 0.45              |
| 5:M:860:HIS:CE1   | 5:M:977:GLY:HA2   | 2.52                     | 0.45              |
| 6:N:36:THR:O      | 6:N:38:LYS:N      | 2.49                     | 0.45              |
| 6:N:777:PRO:HG2   | 6:N:916:TYR:HB2   | 1.98                     | 0.45              |
| 6:N:954:ALA:HB1   | 6:N:1039:CYS:SG   | 2.57                     | 0.45              |
| 6:N:969:ARG:O     | 6:N:973:GLN:HG3   | 2.17                     | 0.45              |
| 6:N:987:GLU:O     | 6:N:991:GLN:HG3   | 2.16                     | 0.45              |
| 6:N:993:LEU:HA    | 11:N:9079:HOH:O   | 2.17                     | 0.45              |
| 6:N:1262:LEU:HD23 | 6:N:1352:ILE:HA   | 1.99                     | 0.45              |
| 1:G:15:DC:H2"     | 1:G:16:DG:C8      | 2.52                     | 0.45              |
| 11:A:316:HOH:O    | 4:B:148:VAL:HG23  | 2.17                     | 0.45              |
| 4:B:213:GLN:HG2   | 11:B:331:HOH:O    | 2.17                     | 0.45              |
| 5:C:14:PRO:HB2    | 11:C:1307:HOH:O   | 2.17                     | 0.45              |
| 5:C:22:GLN:OE1    | 5:C:407:LYS:HB3   | 2.16                     | 0.45              |
| 5:C:76:PRO:HA     | 5:C:77:PRO:HD3    | 1.89                     | 0.45              |
| 5:C:855:VAL:HG13  | 5:C:856:GLU:OE2   | 2.17                     | 0.45              |
| 5:C:1046:ALA:O    | 6:D:1472:ILE:HD11 | 2.16                     | 0.45              |
| 11:C:1135:HOH:O   | 6:D:750:PRO:HB3   | 2.16                     | 0.45              |
| 6:D:33:ASN:O      | 6:D:36:THR:O      | 2.34                     | 0.45              |
| 6:D:481:MET:CE    | 6:D:493:ARG:HB2   | 2.47                     | 0.45              |
| 6:D:525:ARG:HB2   | 6:D:538:SER:OG    | 2.17                     | 0.45              |
| 6:D:1141:GLU:OE2  | 6:D:1168:MET:HE2  | 2.16                     | 0.45              |
| 6:D:1345:GLU:O    | 6:D:1349:VAL:HG23 | 2.16                     | 0.45              |
| 4:K:189:ARG:HG3   | 4:K:191:ASP:OD1   | 2.17                     | 0.45              |
| 4:L:1:MET:HB2     | 11:L:357:HOH:O    | 2.17                     | 0.45              |
| 4:L:19:GLU:OE2    | 4:L:19:GLU:N      | 2.49                     | 0.45              |
| 4:L:45:LEU:HD22   | 6:N:851:LEU:CD2   | 2.47                     | 0.45              |
| 5:M:243:ARG:HB3   | 11:M:1168:HOH:O   | 2.16                     | 0.45              |
| 5:M:265:ARG:H     | 5:M:289:THR:HG21  | 1.80                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:358:ARG:HB3   | 5:M:371:LYS:O     | 2.17                     | 0.45              |
| 5:M:564:MET:SD    | 5:M:565:GLN:N     | 2.90                     | 0.45              |
| 5:M:689:VAL:CG1   | 5:M:690:ILE:N     | 2.79                     | 0.45              |
| 5:M:882:LEU:N     | 5:M:882:LEU:HD23  | 2.32                     | 0.45              |
| 6:N:28:LYS:CG     | 6:N:29:PRO:HD2    | 2.47                     | 0.45              |
| 6:N:542:ASP:HA    | 6:N:545:ARG:NE    | 2.30                     | 0.45              |
| 6:N:634:GLY:N     | 6:N:635:PRO:HD3   | 2.32                     | 0.45              |
| 6:N:646:LYS:HZ2   | 6:N:721:VAL:C     | 2.25                     | 0.45              |
| 6:N:837:GLY:O     | 6:N:841:TYR:CD1   | 2.70                     | 0.45              |
| 6:N:1147:ARG:CB   | 6:N:1188:VAL:HG21 | 2.44                     | 0.45              |
| 6:N:1336:LEU:HD11 | 6:N:1341:PRO:HG3  | 1.99                     | 0.45              |
| 7:O:28:GLN:C      | 7:O:32:ARG:HH12   | 2.25                     | 0.45              |
| 7:O:41:GLU:HG2    | 7:O:42:PRO:N      | 2.31                     | 0.45              |
| 7:O:84:ARG:HB3    | 11:O:1385:HOH:O   | 2.15                     | 0.45              |
| 1:X:6:DT:H2'      | 1:X:7:DC:C5       | 2.52                     | 0.45              |
| 2:Y:8:C:H2'       | 2:Y:9:G:C8        | 2.52                     | 0.45              |
| 5:C:54:ILE:CG2    | 5:C:66:LEU:HB3    | 2.47                     | 0.45              |
| 5:C:248:PRO:HG3   | 11:C:1252:HOH:O   | 2.17                     | 0.45              |
| 5:C:703:ILE:H     | 5:C:703:ILE:CD1   | 2.17                     | 0.45              |
| 5:C:813:VAL:HG22  | 5:C:814:GLU:N     | 2.32                     | 0.45              |
| 5:C:899:GLN:NE2   | 5:C:901:TYR:OH    | 2.50                     | 0.45              |
| 5:C:1095:LEU:CD2  | 6:D:582:LEU:HD22  | 2.43                     | 0.45              |
| 6:D:484:PRO:HB3   | 6:D:488:ARG:NE    | 2.17                     | 0.45              |
| 6:D:1010:ASN:HB3  | 11:D:8019:HOH:O   | 2.17                     | 0.45              |
| 6:D:1102:THR:HG22 | 6:D:1222:GLY:HA3  | 1.99                     | 0.45              |
| 6:D:1369:GLU:HA   | 6:D:1372:VAL:HG12 | 1.98                     | 0.45              |
| 6:D:1426:LYS:HA   | 6:D:1429:LEU:HD13 | 1.99                     | 0.45              |
| 6:D:1465:ASN:ND2  | 6:D:1471:LEU:O    | 2.50                     | 0.45              |
| 5:M:36:PRO:HB2    | 5:M:70:GLU:HG2    | 1.98                     | 0.45              |
| 5:M:263:ASP:C     | 5:M:264:PRO:O     | 2.59                     | 0.45              |
| 5:M:678:PRO:HG2   | 6:N:943:THR:HA    | 1.99                     | 0.45              |
| 5:M:798:GLY:H     | 5:M:827:VAL:HG11  | 1.82                     | 0.45              |
| 6:N:45:PHE:O      | 6:N:46:ASP:C      | 2.60                     | 0.45              |
| 6:N:127:LEU:H     | 6:N:127:LEU:HD12  | 1.82                     | 0.45              |
| 6:N:675:ARG:O     | 6:N:678:GLU:HG2   | 2.17                     | 0.45              |
| 6:N:777:PRO:CG    | 6:N:916:TYR:HB2   | 2.47                     | 0.45              |
| 6:N:876:SER:HB3   | 11:N:9301:HOH:O   | 2.17                     | 0.45              |
| 4:A:20:TYR:HE2    | 4:A:198:ARG:HB2   | 1.82                     | 0.44              |
| 4:A:83:LYS:HG3    | 4:A:170:VAL:HG21  | 1.98                     | 0.44              |
| 4:A:179:PHE:HB2   | 4:A:195:LEU:CD1   | 2.45                     | 0.44              |
| 5:C:689:VAL:HG21  | 5:C:870:ILE:HD12  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:1008:ARG:HH12 | 5:C:1010:THR:HA   | 1.81                     | 0.44              |
| 5:C:1084:SER:HA   | 5:C:1087:VAL:HG12 | 1.99                     | 0.44              |
| 6:D:6:ARG:HG2     | 6:D:6:ARG:HH11    | 1.82                     | 0.44              |
| 6:D:112:ILE:HD11  | 6:D:461:ILE:CG2   | 2.47                     | 0.44              |
| 6:D:950:GLY:O     | 6:D:953:ASP:HB2   | 2.16                     | 0.44              |
| 6:D:1119:SER:O    | 6:D:1121:PRO:HD3  | 2.16                     | 0.44              |
| 6:D:1147:ARG:O    | 6:D:1165:TYR:HA   | 2.18                     | 0.44              |
| 6:D:1487:VAL:HG12 | 6:D:1488:ASP:N    | 2.31                     | 0.44              |
| 4:L:102:LYS:HE3   | 4:L:104:GLU:CG    | 2.43                     | 0.44              |
| 5:M:80:GLN:HE21   | 5:M:84:ARG:NH2    | 2.15                     | 0.44              |
| 5:M:199:VAL:HG13  | 5:M:235:LEU:HG    | 1.99                     | 0.44              |
| 5:M:265:ARG:HB3   | 5:M:267:TYR:CZ    | 2.52                     | 0.44              |
| 5:M:334:ARG:HG3   | 11:M:1156:HOH:O   | 2.17                     | 0.44              |
| 5:M:400:PRO:HG2   | 5:M:593:ALA:CB    | 2.47                     | 0.44              |
| 5:M:461:VAL:HG13  | 5:M:465:GLY:HA2   | 1.98                     | 0.44              |
| 5:M:490:GLU:HG2   | 5:M:493:ARG:NH2   | 2.32                     | 0.44              |
| 5:M:992:MET:C     | 11:M:1511:HOH:O   | 2.60                     | 0.44              |
| 5:M:1003:ASP:OD1  | 5:M:1004:LYS:HG2  | 2.16                     | 0.44              |
| 6:N:700:VAL:HG13  | 6:N:718:PRO:HG2   | 2.00                     | 0.44              |
| 6:N:754:PHE:CZ    | 6:N:1476:THR:HG21 | 2.52                     | 0.44              |
| 6:N:793:THR:O     | 6:N:879:ARG:HD3   | 2.17                     | 0.44              |
| 6:N:999:THR:HA    | 6:N:1002:LYS:HD2  | 1.98                     | 0.44              |
| 6:N:1151:ARG:HG2  | 6:N:1187:PRO:CB   | 2.45                     | 0.44              |
| 6:N:1231:GLU:HA   | 6:N:1234:THR:OG1  | 2.17                     | 0.44              |
| 6:N:1425:THR:O    | 6:N:1429:LEU:HD12 | 2.16                     | 0.44              |
| 2:Y:4:U:O2'       | 2:Y:5:C:H5'       | 2.16                     | 0.44              |
| 4:A:229:GLN:C     | 4:B:12:THR:HA     | 2.42                     | 0.44              |
| 4:B:84:GLU:OE1    | 4:B:127:LEU:HD11  | 2.17                     | 0.44              |
| 5:C:422:ARG:HB2   | 11:C:1579:HOH:O   | 2.17                     | 0.44              |
| 5:C:674:VAL:HG12  | 5:C:990:GLY:O     | 2.18                     | 0.44              |
| 5:C:676:ILE:O     | 6:D:948:THR:HB    | 2.17                     | 0.44              |
| 5:C:783:ARG:HG2   | 5:C:785:VAL:HB    | 1.98                     | 0.44              |
| 5:C:1038:TRP:HA   | 5:C:1041:GLU:OE1  | 2.17                     | 0.44              |
| 6:D:15:PRO:O      | 6:D:19:ARG:HG2    | 2.18                     | 0.44              |
| 6:D:111:LYS:C     | 6:D:512:MET:HE1   | 2.42                     | 0.44              |
| 6:D:116:LEU:HD11  | 6:D:464:LEU:CB    | 2.46                     | 0.44              |
| 6:D:783:ARG:HH12  | 6:D:1239:ARG:NH2  | 2.15                     | 0.44              |
| 6:D:1014:ASN:O    | 6:D:1016:PRO:HD3  | 2.17                     | 0.44              |
| 6:D:1183:ILE:HG13 | 6:D:1183:ILE:O    | 2.16                     | 0.44              |
| 6:D:1184:GLN:HB2  | 6:N:559:ALA:CA    | 2.47                     | 0.44              |
| 6:D:1232:PRO:HB3  | 6:D:1361:VAL:HG21 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:D:1271:LYS:HD3 | 6:D:1331:ASP:N    | 2.32                     | 0.44              |
| 6:D:1377:LYS:O   | 6:D:1395:LEU:HB3  | 2.18                     | 0.44              |
| 6:D:1486:VAL:CG1 | 7:E:22:VAL:HG13   | 2.46                     | 0.44              |
| 4:K:26:GLU:HG2   | 4:K:27:PRO:N      | 2.32                     | 0.44              |
| 4:L:94:LEU:HD21  | 4:L:119:ASP:HB2   | 1.99                     | 0.44              |
| 5:M:9:ILE:HD12   | 5:M:9:ILE:O       | 2.18                     | 0.44              |
| 5:M:13:ILE:HD12  | 5:M:13:ILE:O      | 2.17                     | 0.44              |
| 5:M:582:GLY:C    | 5:M:583:LEU:HD12  | 2.42                     | 0.44              |
| 5:M:670:GLN:NE2  | 5:M:699:PHE:O     | 2.51                     | 0.44              |
| 5:M:676:ILE:HG21 | 5:M:988:VAL:HG13  | 1.99                     | 0.44              |
| 5:M:716:LYS:NZ   | 6:N:36:THR:HG23   | 2.31                     | 0.44              |
| 6:N:54:LYS:HE3   | 6:N:55:ASP:HB2    | 1.99                     | 0.44              |
| 6:N:400:VAL:HG22 | 6:N:443:VAL:CG2   | 2.41                     | 0.44              |
| 6:N:434:ARG:H    | 6:N:447:VAL:HG22  | 1.82                     | 0.44              |
| 6:N:470:LEU:HD12 | 6:N:503:LEU:HD21  | 1.99                     | 0.44              |
| 6:N:705:ALA:HB3  | 6:N:706:PRO:HD3   | 1.99                     | 0.44              |
| 6:N:1026:SER:C   | 6:N:1028:ALA:N    | 2.74                     | 0.44              |
| 6:N:1472:ILE:O   | 6:N:1477:GLY:HA3  | 2.17                     | 0.44              |
| 1:X:18:DG:P      | 6:N:628:ARG:HH21  | 2.40                     | 0.44              |
| 2:Y:11:C:C2'     | 2:Y:12:G:H5''     | 2.47                     | 0.44              |
| 3:Z:6:DC:P       | 6:N:1266:ARG:HH12 | 2.41                     | 0.44              |
| 4:B:30:ARG:CZ    | 4:B:30:ARG:HB3    | 2.47                     | 0.44              |
| 5:C:44:ILE:HG22  | 5:C:45:GLN:N      | 2.31                     | 0.44              |
| 5:C:97:ARG:HB3   | 5:C:109:LYS:HE3   | 1.99                     | 0.44              |
| 5:C:352:ALA:CA   | 5:C:355:VAL:HG12  | 2.47                     | 0.44              |
| 5:C:595:LEU:HD22 | 5:C:625:LEU:HD23  | 2.00                     | 0.44              |
| 5:C:748:GLU:HA   | 5:C:799:ILE:HD12  | 1.99                     | 0.44              |
| 6:D:10:ILE:O     | 6:D:1451:ALA:HA   | 2.18                     | 0.44              |
| 6:D:156:GLU:O    | 6:D:159:ARG:HB2   | 2.18                     | 0.44              |
| 6:D:396:VAL:HB   | 6:D:398:ALA:HB3   | 1.98                     | 0.44              |
| 6:D:420:VAL:O    | 6:D:421:LEU:HD23  | 2.17                     | 0.44              |
| 6:D:471:GLU:H    | 6:D:471:GLU:HG2   | 1.52                     | 0.44              |
| 6:D:525:ARG:O    | 6:D:525:ARG:HG2   | 2.17                     | 0.44              |
| 6:D:593:ASN:HB2  | 11:D:8122:HOH:O   | 2.18                     | 0.44              |
| 6:D:1432:LYS:NZ  | 6:D:1432:LYS:HB3  | 2.32                     | 0.44              |
| 4:L:19:GLU:O     | 4:L:200:TRP:HA    | 2.18                     | 0.44              |
| 4:L:201:THR:HG21 | 4:L:205:VAL:O     | 2.17                     | 0.44              |
| 5:M:208:ALA:O    | 5:M:218:VAL:HG21  | 2.17                     | 0.44              |
| 5:M:405:ARG:NH2  | 5:M:566:THR:CG2   | 2.79                     | 0.44              |
| 5:M:663:ASN:C    | 5:M:665:PHE:H     | 2.25                     | 0.44              |
| 5:M:780:GLU:HG3  | 5:M:781:LYS:H     | 1.83                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:859:PRO:HB3   | 5:M:974:LEU:HD23  | 1.99                     | 0.44              |
| 5:M:1013:TYR:CZ   | 5:M:1063:ARG:HD2  | 2.52                     | 0.44              |
| 5:M:1043:TYR:CE2  | 6:N:763:MET:HA    | 2.53                     | 0.44              |
| 6:N:35:ARG:HG3    | 6:N:35:ARG:NH1    | 2.33                     | 0.44              |
| 6:N:85:VAL:HG23   | 6:N:86:ARG:N      | 2.33                     | 0.44              |
| 6:N:784:ASP:HB3   | 6:N:939:PHE:HE2   | 1.82                     | 0.44              |
| 2:H:7:G:C5'       | 2:H:7:G:H8        | 2.29                     | 0.44              |
| 2:Y:16:G:H3'      | 11:Y:968:HOH:O    | 2.17                     | 0.44              |
| 4:A:47:SER:HB3    | 4:A:217:ILE:HD13  | 2.00                     | 0.44              |
| 4:A:150:TYR:CZ    | 5:C:696:LYS:HA    | 2.53                     | 0.44              |
| 4:A:219:ARG:HD3   | 4:B:219:ARG:HG3   | 1.99                     | 0.44              |
| 4:B:95:GLN:HA     | 4:B:146:ARG:HD2   | 1.99                     | 0.44              |
| 5:C:52:PHE:O      | 5:C:54:ILE:N      | 2.50                     | 0.44              |
| 5:C:172:ILE:HG12  | 11:C:1177:HOH:O   | 2.17                     | 0.44              |
| 5:C:189:ARG:NH1   | 5:C:190:LYS:HD2   | 2.33                     | 0.44              |
| 5:C:479:VAL:HG22  | 5:C:506:ASN:HA    | 1.99                     | 0.44              |
| 5:C:503:LEU:HD23  | 5:C:507:ARG:O     | 2.17                     | 0.44              |
| 5:C:553:ASP:OD1   | 5:C:881:ASN:HB2   | 2.17                     | 0.44              |
| 5:C:721:ARG:CG    | 5:C:820:ARG:HH12  | 2.29                     | 0.44              |
| 5:C:952:LEU:HB3   | 5:C:966:LEU:HD11  | 2.00                     | 0.44              |
| 5:C:957:LYS:HB2   | 5:C:957:LYS:NZ    | 2.33                     | 0.44              |
| 6:D:34:TYR:O      | 6:D:35:ARG:C      | 2.60                     | 0.44              |
| 6:D:651:GLU:HG2   | 11:D:8181:HOH:O   | 2.17                     | 0.44              |
| 6:D:654:LYS:O     | 6:D:658:LEU:HG    | 2.17                     | 0.44              |
| 6:D:796:ARG:C     | 6:D:797:LYS:HD2   | 2.42                     | 0.44              |
| 6:D:1000:THR:HG23 | 6:D:1001:GLU:H    | 1.82                     | 0.44              |
| 6:D:1010:ASN:CG   | 6:D:1014:ASN:HD22 | 2.26                     | 0.44              |
| 4:L:124:ASN:ND2   | 4:L:127:LEU:HD22  | 2.32                     | 0.44              |
| 5:M:94:LEU:HD12   | 5:M:95:TYR:N      | 2.32                     | 0.44              |
| 5:M:252:LYS:HD2   | 5:M:252:LYS:N     | 2.32                     | 0.44              |
| 5:M:949:LYS:CD    | 6:N:796:ARG:HH22  | 2.29                     | 0.44              |
| 5:M:1084:SER:HA   | 5:M:1087:VAL:HG12 | 1.98                     | 0.44              |
| 6:N:436:GLU:OE2   | 6:N:445:ARG:HD3   | 2.18                     | 0.44              |
| 6:N:530:VAL:HB    | 6:N:534:ARG:HB2   | 1.99                     | 0.44              |
| 6:N:1213:ARG:HH22 | 7:O:15:SER:HA     | 1.83                     | 0.44              |
| 6:N:1262:LEU:HD12 | 6:N:1262:LEU:HA   | 1.77                     | 0.44              |
| 7:O:24:ALA:O      | 7:O:28:GLN:HG3    | 2.17                     | 0.44              |
| 1:G:12:DG:H1'     | 1:G:13:DT:H5'     | 1.99                     | 0.44              |
| 4:A:165:ILE:O     | 4:A:165:ILE:HG13  | 2.18                     | 0.44              |
| 4:B:47:SER:OG     | 4:B:48:ILE:N      | 2.49                     | 0.44              |
| 5:C:170:PRO:HB2   | 11:C:1335:HOH:O   | 2.17                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:C:189:ARG:HD3   | 5:C:190:LYS:N    | 2.33                     | 0.44              |
| 5:C:393:GLN:HE21  | 5:C:393:GLN:HB2  | 1.62                     | 0.44              |
| 5:C:566:THR:O     | 5:C:566:THR:HG22 | 2.18                     | 0.44              |
| 5:C:673:LEU:HD21  | 5:C:867:VAL:HG12 | 2.00                     | 0.44              |
| 5:C:689:VAL:CG1   | 5:C:853:LEU:HD13 | 2.47                     | 0.44              |
| 6:D:15:PRO:HD3    | 6:D:511:TRP:CE3  | 2.52                     | 0.44              |
| 6:D:95:LEU:HD23   | 6:D:96:ALA:H     | 1.82                     | 0.44              |
| 6:D:531:ASP:C     | 6:D:533:GLY:H    | 2.26                     | 0.44              |
| 6:D:550:ARG:NH1   | 6:D:573:MET:SD   | 2.88                     | 0.44              |
| 6:D:554:LEU:HD12  | 6:D:570:GLU:HB3  | 2.00                     | 0.44              |
| 6:D:800:LYS:O     | 6:D:800:LYS:HD3  | 2.18                     | 0.44              |
| 6:D:875:THR:HG22  | 6:D:879:ARG:HB2  | 2.00                     | 0.44              |
| 6:D:1344:VAL:HG11 | 6:D:1421:LEU:CD2 | 2.48                     | 0.44              |
| 6:D:1380:GLU:HA   | 6:D:1391:GLU:O   | 2.18                     | 0.44              |
| 7:E:13:VAL:HG11   | 7:E:18:ARG:HB3   | 2.00                     | 0.44              |
| 4:K:73:GLU:CD     | 4:K:73:GLU:H     | 2.25                     | 0.44              |
| 4:L:38:ASN:HB3    | 4:L:39:PRO:HD3   | 2.00                     | 0.44              |
| 5:M:15:LEU:HD12   | 5:M:15:LEU:N     | 2.31                     | 0.44              |
| 5:M:18:LEU:HD23   | 5:M:542:VAL:HG21 | 2.00                     | 0.44              |
| 5:M:69:LEU:HD12   | 5:M:97:ARG:HB3   | 1.98                     | 0.44              |
| 5:M:140:ILE:HG22  | 5:M:333:ILE:CD1  | 2.48                     | 0.44              |
| 5:M:548:PRO:HB2   | 5:M:843:HIS:HE1  | 1.83                     | 0.44              |
| 5:M:1034:GLU:CB   | 6:N:619:LEU:HD22 | 2.44                     | 0.44              |
| 6:N:50:PHE:HB3    | 6:N:522:PRO:CD   | 2.47                     | 0.44              |
| 6:N:899:LEU:CB    | 6:N:917:GLN:HG2  | 2.48                     | 0.44              |
| 6:N:1139:ASP:HB3  | 6:N:1357:ARG:CZ  | 2.48                     | 0.44              |
| 6:N:1149:LEU:HD22 | 6:N:1187:PRO:HG2 | 2.00                     | 0.44              |
| 6:N:1336:LEU:CD2  | 6:N:1421:LEU:HB2 | 2.48                     | 0.44              |
| 7:O:62:THR:HB     | 11:O:844:HOH:O   | 2.18                     | 0.44              |
| 4:A:132:LEU:N     | 4:A:132:LEU:HD12 | 2.32                     | 0.44              |
| 4:A:151:VAL:HB    | 4:A:169:ALA:HB3  | 2.00                     | 0.44              |
| 4:B:48:ILE:HD12   | 4:B:48:ILE:N     | 2.32                     | 0.44              |
| 5:C:41:ASN:O      | 5:C:46:ALA:HB2   | 2.17                     | 0.44              |
| 5:C:69:LEU:CD1    | 5:C:109:LYS:HE3  | 2.45                     | 0.44              |
| 5:C:148:PHE:HB2   | 5:C:313:LEU:HD22 | 1.99                     | 0.44              |
| 5:C:473:ARG:HA    | 5:C:531:PHE:CD1  | 2.53                     | 0.44              |
| 5:C:524:VAL:CG1   | 5:C:528:GLU:HB2  | 2.48                     | 0.44              |
| 5:C:549:PHE:CD2   | 5:C:886:LEU:HB3  | 2.52                     | 0.44              |
| 5:C:579:VAL:HB    | 5:C:890:LEU:HD21 | 1.98                     | 0.44              |
| 5:C:650:ARG:CG    | 5:C:653:ASP:HB2  | 2.44                     | 0.44              |
| 5:C:690:ILE:HG23  | 5:C:852:ILE:HA   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:33:ASN:HB2    | 6:D:40:GLU:OE2    | 2.18                     | 0.44              |
| 6:D:119:SER:H     | 6:D:123:LEU:HB2   | 1.83                     | 0.44              |
| 6:D:1080:GLY:O    | 6:D:1083:ASP:N    | 2.50                     | 0.44              |
| 6:D:1201:CYS:SG   | 6:D:1204:CYS:HB2  | 2.57                     | 0.44              |
| 6:D:1367:HIS:O    | 6:D:1371:VAL:HG23 | 2.17                     | 0.44              |
| 5:M:23:VAL:HA     | 5:M:121:MET:CE    | 2.48                     | 0.44              |
| 5:M:198:ARG:HG2   | 5:M:204:GLN:HE22  | 1.82                     | 0.44              |
| 5:M:260:LEU:C     | 5:M:260:LEU:HD12  | 2.42                     | 0.44              |
| 5:M:496:ILE:HA    | 5:M:531:PHE:O     | 2.18                     | 0.44              |
| 5:M:1034:GLU:HB3  | 6:N:619:LEU:CD1   | 2.46                     | 0.44              |
| 6:N:644:LEU:HD12  | 6:N:645:PRO:N     | 2.33                     | 0.44              |
| 6:N:1147:ARG:O    | 6:N:1166:LEU:HD23 | 2.17                     | 0.44              |
| 7:O:5:GLY:HA3     | 7:O:8:LYS:HD2     | 1.99                     | 0.44              |
| 1:X:13:DT:OP2     | 6:N:1096:ARG:NH2  | 2.45                     | 0.44              |
| 4:B:19:GLU:O      | 4:B:200:TRP:HA    | 2.18                     | 0.44              |
| 4:B:58:ILE:HG21   | 4:B:61:VAL:HG23   | 2.00                     | 0.44              |
| 5:C:329:GLY:CA    | 5:C:488:ALA:HB3   | 2.48                     | 0.44              |
| 5:C:546:LEU:HD13  | 5:C:565:GLN:HE22  | 1.82                     | 0.44              |
| 5:C:862:PRO:HD3   | 5:C:973:VAL:O     | 2.18                     | 0.44              |
| 6:D:115:LEU:HD12  | 6:D:499:VAL:HG22  | 2.00                     | 0.44              |
| 6:D:123:LEU:CD1   | 6:D:152:LEU:HD22  | 2.41                     | 0.44              |
| 6:D:710:ARG:C     | 6:D:712:GLY:N     | 2.76                     | 0.44              |
| 6:D:1432:LYS:HG2  | 6:D:1433:SER:N    | 2.33                     | 0.44              |
| 6:D:1463:LYS:O    | 6:D:1467:ILE:HG13 | 2.18                     | 0.44              |
| 4:L:73:GLU:OE1    | 4:L:131:THR:N     | 2.51                     | 0.44              |
| 4:L:143:ARG:NE    | 4:L:145:ASP:OD1   | 2.51                     | 0.44              |
| 5:M:284:ARG:O     | 5:M:301:GLU:HB2   | 2.18                     | 0.44              |
| 5:M:728:HIS:O     | 5:M:729:LEU:HG    | 2.17                     | 0.44              |
| 6:N:95:LEU:HA     | 6:N:551:ASN:OD1   | 2.17                     | 0.44              |
| 6:N:121:THR:HB    | 11:N:9300:HOH:O   | 2.17                     | 0.44              |
| 6:N:124:GLU:O     | 6:N:127:LEU:HD12  | 2.18                     | 0.44              |
| 6:N:131:LYS:NZ    | 6:N:568:ARG:HB2   | 2.32                     | 0.44              |
| 6:N:637:LEU:HD11  | 6:N:642:CYS:N     | 2.33                     | 0.44              |
| 6:N:711:LEU:HD22  | 6:N:714:GLN:NE2   | 2.33                     | 0.44              |
| 6:N:884:ARG:CZ    | 6:N:884:ARG:HB3   | 2.45                     | 0.44              |
| 6:N:955:VAL:HG11  | 6:N:1015:TYR:CE2  | 2.52                     | 0.44              |
| 6:N:1192:LEU:HD23 | 11:N:9021:HOH:O   | 2.17                     | 0.44              |
| 2:Y:10:G:C2'      | 2:Y:11:C:H5'      | 2.47                     | 0.44              |
| 5:C:31:GLN:HB3    | 5:C:71:TYR:HH     | 1.82                     | 0.44              |
| 5:C:137:VAL:HG22  | 5:C:391:LEU:HG    | 2.00                     | 0.44              |
| 5:C:288:ARG:CB    | 5:C:288:ARG:HH11  | 2.31                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:C:964:LYS:O     | 5:C:968:LEU:HG   | 2.17                     | 0.44              |
| 6:D:8:VAL:HG23    | 6:D:1457:ASP:CB  | 2.37                     | 0.44              |
| 6:D:95:LEU:HD23   | 6:D:96:ALA:N     | 2.32                     | 0.44              |
| 6:D:128:TYR:O     | 6:D:457:GLY:HA2  | 2.17                     | 0.44              |
| 6:D:418:GLY:O     | 6:D:428:LYS:HB3  | 2.18                     | 0.44              |
| 6:D:489:ARG:NH1   | 11:D:8508:HOH:O  | 2.49                     | 0.44              |
| 6:D:554:LEU:CD1   | 6:D:571:LYS:HD3  | 2.45                     | 0.44              |
| 6:D:615:ARG:NH2   | 6:D:1096:ARG:CZ  | 2.81                     | 0.44              |
| 6:D:1098:LEU:HD21 | 6:D:1229:ILE:CD1 | 2.44                     | 0.44              |
| 6:D:1481:VAL:HG22 | 7:E:18:ARG:HH21  | 1.83                     | 0.44              |
| 7:E:41:GLU:HB2    | 7:E:45:ARG:CZ    | 2.48                     | 0.44              |
| 4:K:26:GLU:HG2    | 4:K:27:PRO:HA    | 1.99                     | 0.44              |
| 4:K:34:VAL:HG23   | 4:K:179:PHE:HZ   | 1.82                     | 0.44              |
| 4:K:44:LEU:HD13   | 4:K:177:VAL:HG11 | 2.00                     | 0.44              |
| 4:K:185:ARG:HB2   | 11:K:1437:HOH:O  | 2.17                     | 0.44              |
| 5:M:12:VAL:HG13   | 5:M:13:ILE:HG13  | 2.00                     | 0.44              |
| 5:M:41:ASN:O      | 5:M:46:ALA:HB2   | 2.18                     | 0.44              |
| 5:M:84:ARG:HG2    | 5:M:131:GLY:O    | 2.18                     | 0.44              |
| 5:M:479:VAL:HG21  | 5:M:503:LEU:HD11 | 1.98                     | 0.44              |
| 5:M:721:ARG:HH21  | 5:M:783:ARG:NH1  | 2.15                     | 0.44              |
| 5:M:808:ARG:NH2   | 5:M:820:ARG:NH2  | 2.65                     | 0.44              |
| 5:M:971:LYS:HG2   | 5:M:988:VAL:HB   | 2.00                     | 0.44              |
| 5:M:1060:ILE:HG21 | 5:M:1083:GLU:OE1 | 2.17                     | 0.44              |
| 6:N:493:ARG:HG2   | 6:N:1390:LEU:CB  | 2.43                     | 0.44              |
| 6:N:578:VAL:O     | 6:N:581:LEU:HD23 | 2.17                     | 0.44              |
| 6:N:984:THR:HG22  | 6:N:987:GLU:HG3  | 1.99                     | 0.44              |
| 3:I:4:DC:H3'      | 11:I:2461:HOH:O  | 2.18                     | 0.44              |
| 4:A:5:LYS:HE2     | 4:B:224:TYR:OH   | 2.18                     | 0.44              |
| 4:A:26:GLU:HG2    | 4:A:27:PRO:N     | 2.33                     | 0.44              |
| 5:C:127:PHE:CE1   | 5:C:136:ILE:HG12 | 2.53                     | 0.44              |
| 5:C:355:VAL:CG2   | 5:C:372:LEU:HG   | 2.48                     | 0.44              |
| 5:C:573:ARG:HD2   | 5:C:699:PHE:HA   | 2.00                     | 0.44              |
| 5:C:1055:LEU:CD2  | 5:C:1066:ALA:HB2 | 2.37                     | 0.44              |
| 6:D:18:ILE:HD12   | 6:D:518:PRO:HG3  | 1.99                     | 0.44              |
| 6:D:19:ARG:NE     | 6:D:94:GLU:OE1   | 2.51                     | 0.44              |
| 6:D:81:THR:HB     | 6:D:85:VAL:CG2   | 2.48                     | 0.44              |
| 6:D:569:ASN:HA    | 6:D:572:ARG:NE   | 2.33                     | 0.44              |
| 6:D:675:ARG:HA    | 6:D:678:GLU:CG   | 2.48                     | 0.44              |
| 6:D:867:ARG:HD2   | 6:D:867:ARG:C    | 2.42                     | 0.44              |
| 6:D:1045:MET:O    | 6:D:1053:PHE:HD1 | 2.01                     | 0.44              |
| 4:K:102:LYS:HZ1   | 4:K:115:LEU:HD22 | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:L:43:ILE:HD12   | 4:L:217:ILE:HG21  | 2.00                     | 0.44              |
| 5:M:140:ILE:O     | 5:M:140:ILE:HD12  | 2.18                     | 0.44              |
| 5:M:198:ARG:HG2   | 5:M:204:GLN:NE2   | 2.33                     | 0.44              |
| 5:M:486:MET:HG3   | 5:M:490:GLU:HB2   | 2.00                     | 0.44              |
| 6:N:163:TYR:HE1   | 6:N:198:ARG:HH12  | 1.66                     | 0.44              |
| 6:N:486:ARG:CA    | 6:N:489:ARG:HG2   | 2.45                     | 0.44              |
| 6:N:639:LEU:HD23  | 6:N:639:LEU:H     | 1.83                     | 0.44              |
| 6:N:646:LYS:HG2   | 6:N:720:LEU:HB3   | 1.99                     | 0.44              |
| 6:N:962:GLN:O     | 6:N:966:GLU:HG3   | 2.18                     | 0.44              |
| 6:N:1037:GLN:OE1  | 6:N:1042:ARG:HD2  | 2.17                     | 0.44              |
| 6:N:1100:ASP:HB3  | 6:N:1428:ALA:CB   | 2.47                     | 0.44              |
| 6:N:1102:THR:HG22 | 6:N:1102:THR:O    | 2.18                     | 0.44              |
| 6:N:1209:LEU:C    | 6:N:1211:MET:N    | 2.74                     | 0.44              |
| 6:N:1221:VAL:O    | 6:N:1224:VAL:N    | 2.50                     | 0.44              |
| 6:N:1478:SER:O    | 6:N:1482:ARG:N    | 2.51                     | 0.44              |
| 6:N:1481:VAL:O    | 6:N:1481:VAL:HG12 | 2.18                     | 0.44              |
| 1:G:11:DC:H5''    | 6:D:1442:ASN:ND2  | 2.33                     | 0.43              |
| 1:X:15:DC:P       | 6:N:610:LYS:HE2   | 2.58                     | 0.43              |
| 2:Y:5:C:O5'       | 2:Y:5:C:H6        | 2.00                     | 0.43              |
| 4:A:222:LEU:HD22  | 4:B:218:LEU:HD23  | 2.00                     | 0.43              |
| 4:B:40:LEU:HD22   | 4:B:211:LEU:HD12  | 1.99                     | 0.43              |
| 5:C:279:GLU:HG3   | 5:C:280:LYS:N     | 2.33                     | 0.43              |
| 5:C:285:LEU:HD23  | 5:C:285:LEU:O     | 2.18                     | 0.43              |
| 5:C:409:ARG:HB3   | 5:C:454:SER:OG    | 2.17                     | 0.43              |
| 5:C:436:GLY:C     | 5:C:456:ALA:HB3   | 2.43                     | 0.43              |
| 5:C:563:ASN:O     | 5:C:567:GLN:HG2   | 2.18                     | 0.43              |
| 5:C:703:ILE:HD11  | 11:C:1597:HOH:O   | 2.17                     | 0.43              |
| 5:C:745:ILE:HD11  | 5:C:803:THR:OG1   | 2.18                     | 0.43              |
| 6:D:26:VAL:HG11   | 6:D:44:LEU:HD23   | 2.00                     | 0.43              |
| 6:D:60:CYS:SG     | 6:D:62:LYS:HG3    | 2.58                     | 0.43              |
| 6:D:393:ILE:HD12  | 11:D:8204:HOH:O   | 2.18                     | 0.43              |
| 6:D:632:VAL:O     | 6:D:727:GLN:HA    | 2.18                     | 0.43              |
| 6:D:675:ARG:O     | 6:D:678:GLU:HG2   | 2.17                     | 0.43              |
| 6:D:834:THR:CG2   | 6:D:838:ARG:HH11  | 2.27                     | 0.43              |
| 7:E:28:GLN:HE21   | 7:E:28:GLN:HB2    | 1.56                     | 0.43              |
| 5:M:52:PHE:O      | 5:M:54:ILE:N      | 2.51                     | 0.43              |
| 5:M:177:GLU:N     | 5:M:178:PRO:HD3   | 2.32                     | 0.43              |
| 5:M:578:VAL:HG21  | 5:M:991:GLN:O     | 2.18                     | 0.43              |
| 5:M:669:GLY:HA3   | 5:M:995:MET:HA    | 1.99                     | 0.43              |
| 5:M:940:GLU:N     | 11:M:1220:HOH:O   | 2.51                     | 0.43              |
| 5:M:971:LYS:HG2   | 5:M:988:VAL:N     | 2.33                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:165:LYS:HG2   | 6:N:397:LYS:HD3   | 2.00                     | 0.43              |
| 6:N:1045:MET:CB   | 6:N:1073:SER:HA   | 2.48                     | 0.43              |
| 6:N:1164:ARG:NH1  | 6:N:1170:ASP:OD2  | 2.51                     | 0.43              |
| 5:C:101:ILE:HD12  | 5:C:107:LEU:HD13  | 2.00                     | 0.43              |
| 5:C:532:MET:HG2   | 5:C:533:ASP:N     | 2.32                     | 0.43              |
| 5:C:568:ALA:HB1   | 5:C:668:LEU:HB2   | 2.00                     | 0.43              |
| 5:C:841:ASN:HD21  | 5:C:845:ASN:H     | 1.65                     | 0.43              |
| 5:C:872:ASN:C     | 5:C:872:ASN:ND2   | 2.70                     | 0.43              |
| 5:C:1058:ASP:O    | 5:C:1060:ILE:N    | 2.51                     | 0.43              |
| 6:D:576:GLU:C     | 6:D:576:GLU:CD    | 2.85                     | 0.43              |
| 6:D:827:ILE:HG23  | 6:D:840:LYS:NZ    | 2.33                     | 0.43              |
| 6:D:1066:THR:OG1  | 6:D:1067:VAL:N    | 2.51                     | 0.43              |
| 6:D:1262:LEU:HD21 | 6:D:1351:GLU:CG   | 2.43                     | 0.43              |
| 6:D:1438:ALA:CA   | 6:D:1446:VAL:HG11 | 2.48                     | 0.43              |
| 4:K:114:PHE:O     | 4:K:116:PRO:HD3   | 2.18                     | 0.43              |
| 4:L:83:LYS:HE2    | 4:L:168:ASP:HB2   | 2.00                     | 0.43              |
| 4:L:86:VAL:HG12   | 4:L:124:ASN:HB2   | 1.99                     | 0.43              |
| 5:M:22:GLN:CD     | 5:M:407:LYS:HB3   | 2.42                     | 0.43              |
| 5:M:147:TYR:CE2   | 5:M:280:LYS:HE2   | 2.52                     | 0.43              |
| 5:M:307:LEU:CD1   | 5:M:310:LEU:HD23  | 2.48                     | 0.43              |
| 5:M:573:ARG:HB3   | 5:M:670:GLN:OE1   | 2.18                     | 0.43              |
| 5:M:672:VAL:HG12  | 5:M:699:PHE:HE1   | 1.82                     | 0.43              |
| 5:M:842:ARG:NH2   | 5:M:887:GLU:OE1   | 2.51                     | 0.43              |
| 5:M:1008:ARG:NH2  | 5:M:1020:PRO:HB3  | 2.33                     | 0.43              |
| 11:M:1170:HOH:O   | 6:N:754:PHE:HB2   | 2.18                     | 0.43              |
| 11:M:1450:HOH:O   | 6:N:1456:LYS:HB3  | 2.17                     | 0.43              |
| 6:N:155:ASP:O     | 6:N:159:ARG:N     | 2.49                     | 0.43              |
| 6:N:204:LEU:HB3   | 6:N:445:ARG:NH2   | 2.32                     | 0.43              |
| 6:N:732:VAL:O     | 6:N:732:VAL:HG12  | 2.18                     | 0.43              |
| 6:N:1087:ARG:HB3  | 6:N:1237:THR:HG21 | 2.00                     | 0.43              |
| 6:N:1165:TYR:HB2  | 11:N:9241:HOH:O   | 2.18                     | 0.43              |
| 6:N:1261:GLU:O    | 6:N:1264:GLU:O    | 2.35                     | 0.43              |
| 6:N:1383:ASP:HA   | 6:N:1384:PRO:HD3  | 1.71                     | 0.43              |
| 6:N:1423:GLY:O    | 6:N:1424:VAL:C    | 2.62                     | 0.43              |
| 2:H:5:C:H2'       | 2:H:6:U:C5        | 2.52                     | 0.43              |
| 2:Y:9:G:C5'       | 2:Y:9:G:H8        | 2.30                     | 0.43              |
| 4:B:65:PHE:CE1    | 6:D:813:LEU:HD13  | 2.54                     | 0.43              |
| 5:C:71:TYR:HA     | 5:C:96:ALA:HB2    | 2.00                     | 0.43              |
| 5:C:124:ASP:OD2   | 5:C:592:LEU:HD12  | 2.19                     | 0.43              |
| 5:C:360:LEU:HD22  | 11:C:1160:HOH:O   | 2.17                     | 0.43              |
| 5:C:391:LEU:C     | 5:C:391:LEU:HD23  | 2.43                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:C:431:HIS:CG    | 5:C:432:ARG:H    | 2.35                     | 0.43              |
| 5:C:1031:ARG:CZ   | 6:D:621:LYS:NZ   | 2.81                     | 0.43              |
| 6:D:409:VAL:CG1   | 6:D:435:VAL:HG11 | 2.48                     | 0.43              |
| 6:D:411:THR:HG23  | 6:D:436:GLU:HA   | 2.01                     | 0.43              |
| 6:D:477:LEU:HD21  | 6:D:495:ARG:NH1  | 2.33                     | 0.43              |
| 6:D:827:ILE:HG22  | 6:D:837:GLY:CA   | 2.47                     | 0.43              |
| 6:D:957:PRO:HG3   | 6:D:1007:VAL:HA  | 2.00                     | 0.43              |
| 4:K:30:ARG:HH22   | 5:M:938:LYS:CD   | 2.28                     | 0.43              |
| 4:K:133:GLU:OE2   | 4:K:134:GLU:HB2  | 2.17                     | 0.43              |
| 4:L:91:ASN:OD1    | 4:L:91:ASN:N     | 2.51                     | 0.43              |
| 5:M:198:ARG:HE    | 5:M:198:ARG:CA   | 2.32                     | 0.43              |
| 5:M:342:ASP:HA    | 5:M:345:ARG:HD3  | 1.99                     | 0.43              |
| 5:M:351:LEU:HD11  | 11:M:1564:HOH:O  | 2.17                     | 0.43              |
| 5:M:569:VAL:HA    | 5:M:570:PRO:HD3  | 1.88                     | 0.43              |
| 5:M:601:GLY:O     | 5:M:648:ARG:HA   | 2.18                     | 0.43              |
| 5:M:816:LYS:HB2   | 5:M:819:VAL:CG2  | 2.47                     | 0.43              |
| 5:M:873:PRO:O     | 5:M:877:PRO:HD3  | 2.18                     | 0.43              |
| 5:M:876:VAL:H     | 5:M:877:PRO:CD   | 2.31                     | 0.43              |
| 5:M:1045:ALA:HA   | 6:N:758:GLU:CD   | 2.44                     | 0.43              |
| 6:N:53:ILE:HA     | 6:N:86:ARG:HD2   | 1.99                     | 0.43              |
| 6:N:57:GLU:OE2    | 6:N:61:GLY:HA2   | 2.18                     | 0.43              |
| 6:N:154:THR:HG23  | 6:N:157:GLU:H    | 1.82                     | 0.43              |
| 6:N:436:GLU:OE1   | 6:N:445:ARG:O    | 2.36                     | 0.43              |
| 6:N:481:MET:CE    | 6:N:496:LEU:HD23 | 2.48                     | 0.43              |
| 6:N:645:PRO:HG3   | 6:N:725:SER:O    | 2.18                     | 0.43              |
| 6:N:813:LEU:HB2   | 6:N:839:LEU:HD21 | 1.99                     | 0.43              |
| 1:X:17:DC:O3'     | 6:N:628:ARG:NE   | 2.51                     | 0.43              |
| 4:A:48:ILE:HD11   | 4:A:210:ALA:HB1  | 2.00                     | 0.43              |
| 5:C:36:PRO:CG     | 5:C:70:GLU:HB3   | 2.36                     | 0.43              |
| 5:C:142:ARG:NH2   | 5:C:325:ILE:HG12 | 2.34                     | 0.43              |
| 5:C:256:TYR:CE1   | 5:C:293:PHE:HB2  | 2.53                     | 0.43              |
| 5:C:466:PHE:O     | 5:C:468:ARG:N    | 2.52                     | 0.43              |
| 6:D:957:PRO:HG3   | 11:D:8019:HOH:O  | 2.17                     | 0.43              |
| 6:D:1046:GLN:HG2  | 6:D:1052:THR:CG2 | 2.44                     | 0.43              |
| 6:D:1105:ILE:HG22 | 11:D:8286:HOH:O  | 2.17                     | 0.43              |
| 6:D:1117:TYR:CE1  | 6:D:1187:PRO:HA  | 2.53                     | 0.43              |
| 6:D:1471:LEU:HD21 | 6:D:1477:GLY:HA2 | 1.99                     | 0.43              |
| 6:D:1486:VAL:HG12 | 7:E:22:VAL:HG13  | 2.00                     | 0.43              |
| 5:M:166:PRO:HA    | 11:M:1128:HOH:O  | 2.17                     | 0.43              |
| 5:M:328:LEU:HD11  | 5:M:434:HIS:HD2  | 1.82                     | 0.43              |
| 5:M:462:ASP:HB3   | 5:M:468:ARG:CD   | 2.43                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:490:GLU:HG2   | 5:M:493:ARG:NH1   | 2.33                     | 0.43              |
| 5:M:587:VAL:CG1   | 5:M:588:VAL:N     | 2.79                     | 0.43              |
| 5:M:876:VAL:O     | 5:M:876:VAL:HG12  | 2.17                     | 0.43              |
| 5:M:879:ARG:HH21  | 6:N:1029:ARG:HH22 | 1.65                     | 0.43              |
| 5:M:1003:ASP:OD2  | 6:N:724:GLN:NE2   | 2.52                     | 0.43              |
| 6:N:471:GLU:OE1   | 6:N:503:LEU:HD21  | 2.18                     | 0.43              |
| 6:N:606:ILE:CG2   | 6:N:607:LEU:HG    | 2.48                     | 0.43              |
| 6:N:615:ARG:NH2   | 6:N:1096:ARG:HD2  | 2.34                     | 0.43              |
| 6:N:794:GLN:HG2   | 6:N:1017:PHE:CE1  | 2.53                     | 0.43              |
| 6:N:832:ARG:NE    | 6:N:832:ARG:HA    | 2.33                     | 0.43              |
| 6:N:970:LYS:HE2   | 11:N:9402:HOH:O   | 2.18                     | 0.43              |
| 6:N:1145:TYR:CD1  | 6:N:1145:TYR:C    | 2.95                     | 0.43              |
| 6:N:1209:LEU:HD21 | 7:O:17:TYR:OH     | 2.19                     | 0.43              |
| 6:N:1453:ALA:O    | 6:N:1455:LYS:HG2  | 2.18                     | 0.43              |
| 7:O:21:VAL:HG12   | 7:O:25:LYS:HD2    | 1.99                     | 0.43              |
| 7:O:65:MET:O      | 7:O:69:LEU:HD12   | 2.17                     | 0.43              |
| 4:B:216:GLU:HA    | 4:B:219:ARG:HH12  | 1.83                     | 0.43              |
| 4:B:223:THR:C     | 4:B:225:PHE:H     | 2.27                     | 0.43              |
| 5:C:250:ARG:HG2   | 5:C:253:ALA:HB3   | 2.00                     | 0.43              |
| 5:C:433:THR:C     | 5:C:435:TYR:N     | 2.75                     | 0.43              |
| 5:C:474:VAL:HG23  | 5:C:478:VAL:C     | 2.44                     | 0.43              |
| 5:C:814:GLU:O     | 5:C:816:LYS:NZ    | 2.52                     | 0.43              |
| 5:C:976:ASP:HB3   | 5:C:979:THR:HG22  | 2.00                     | 0.43              |
| 5:C:1058:ASP:CG   | 5:C:1084:SER:H    | 2.22                     | 0.43              |
| 6:D:95:LEU:CD2    | 6:D:574:LEU:HD21  | 2.45                     | 0.43              |
| 6:D:108:VAL:CG2   | 6:D:109:PRO:HD3   | 2.47                     | 0.43              |
| 6:D:415:VAL:O     | 6:D:432:TYR:HA    | 2.18                     | 0.43              |
| 6:D:711:LEU:HD21  | 6:D:768:ASN:CB    | 2.49                     | 0.43              |
| 6:D:899:LEU:HB3   | 6:D:921:ARG:HH12  | 1.83                     | 0.43              |
| 6:D:1099:VAL:HG23 | 6:D:1226:ALA:HB1  | 2.00                     | 0.43              |
| 6:D:1108:ARG:HH21 | 6:D:1198:TYR:C    | 2.27                     | 0.43              |
| 6:D:1122:LEU:O    | 6:D:1135:ARG:HB2  | 2.18                     | 0.43              |
| 6:D:1271:LYS:CE   | 6:D:1331:ASP:H    | 2.32                     | 0.43              |
| 6:D:1406:ARG:CB   | 6:D:1412:LYS:HZ3  | 2.31                     | 0.43              |
| 6:D:1436:SER:N    | 11:D:8024:HOH:O   | 2.49                     | 0.43              |
| 7:E:37:ASN:HD22   | 7:E:89:MET:CE     | 2.29                     | 0.43              |
| 4:K:55:SER:HB2    | 4:K:158:ILE:HB    | 2.00                     | 0.43              |
| 4:K:116:PRO:HG3   | 11:K:2001:HOH:O   | 2.17                     | 0.43              |
| 4:K:127:LEU:HA    | 11:K:827:HOH:O    | 2.17                     | 0.43              |
| 5:M:37:GLU:HA     | 11:M:1579:HOH:O   | 2.18                     | 0.43              |
| 5:M:39:ARG:HG3    | 5:M:39:ARG:NH1    | 2.29                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:144:PRO:N     | 5:M:276:LYS:HZ3   | 2.16                     | 0.43              |
| 5:M:162:ILE:HB    | 5:M:172:ILE:HD13  | 2.00                     | 0.43              |
| 5:M:1095:LEU:HB2  | 5:M:1097:LEU:CD2  | 2.47                     | 0.43              |
| 5:M:1095:LEU:O    | 5:M:1096:ALA:C    | 2.62                     | 0.43              |
| 6:N:40:GLU:HB3    | 6:N:41:ARG:H      | 1.68                     | 0.43              |
| 6:N:111:LYS:HG2   | 6:N:1452:ILE:CD1  | 2.48                     | 0.43              |
| 6:N:615:ARG:HH22  | 6:N:1096:ARG:CD   | 2.31                     | 0.43              |
| 6:N:1467:ILE:H    | 6:N:1467:ILE:HG13 | 1.55                     | 0.43              |
| 4:A:19:GLU:O      | 4:A:200:TRP:HA    | 2.18                     | 0.43              |
| 5:C:18:LEU:HD13   | 5:C:590:ASP:CB    | 2.48                     | 0.43              |
| 5:C:230:ARG:HA    | 5:C:231:PRO:HD3   | 1.84                     | 0.43              |
| 5:C:496:ILE:HG13  | 5:C:531:PHE:HB2   | 2.01                     | 0.43              |
| 5:C:602:GLU:OE1   | 5:C:648:ARG:HG2   | 2.18                     | 0.43              |
| 5:C:975:TYR:N     | 5:C:975:TYR:CD1   | 2.86                     | 0.43              |
| 6:D:52:PRO:HG2    | 6:D:80:VAL:HA     | 2.00                     | 0.43              |
| 6:D:127:LEU:CD2   | 6:D:134:VAL:HG22  | 2.49                     | 0.43              |
| 6:D:475:LYS:NZ    | 11:D:8306:HOH:O   | 2.51                     | 0.43              |
| 6:D:522:PRO:HG2   | 6:D:523:ASP:N     | 2.33                     | 0.43              |
| 6:D:554:LEU:HD11  | 6:D:571:LYS:CD    | 2.48                     | 0.43              |
| 6:D:683:ILE:HG23  | 6:D:687:VAL:CG2   | 2.48                     | 0.43              |
| 6:D:695:ILE:HD13  | 6:D:720:LEU:HD11  | 2.00                     | 0.43              |
| 6:D:716:PHE:CZ    | 6:D:765:SER:HB3   | 2.54                     | 0.43              |
| 6:D:741:ASP:O     | 6:D:741:ASP:CG    | 2.60                     | 0.43              |
| 6:D:959:GLU:CD    | 6:D:959:GLU:N     | 2.73                     | 0.43              |
| 4:L:86:VAL:HG13   | 4:L:86:VAL:O      | 2.18                     | 0.43              |
| 4:L:99:LEU:HD13   | 4:L:144:VAL:CG2   | 2.49                     | 0.43              |
| 5:M:179:ASN:ND2   | 11:M:1597:HOH:O   | 2.50                     | 0.43              |
| 5:M:666:LEU:HD11  | 5:M:668:LEU:CD2   | 2.48                     | 0.43              |
| 5:M:771:GLU:HB2   | 11:M:1204:HOH:O   | 2.18                     | 0.43              |
| 6:N:41:ARG:HB2    | 11:N:9006:HOH:O   | 2.18                     | 0.43              |
| 6:N:62:LYS:HG3    | 6:N:75:ARG:HH11   | 1.84                     | 0.43              |
| 6:N:525:ARG:HB2   | 6:N:538:SER:HB3   | 2.00                     | 0.43              |
| 6:N:781:PRO:HB3   | 6:N:785:ILE:CG2   | 2.49                     | 0.43              |
| 6:N:893:GLU:O     | 6:N:896:ALA:HB3   | 2.18                     | 0.43              |
| 6:N:961:LYS:HG2   | 11:N:9172:HOH:O   | 2.17                     | 0.43              |
| 6:N:1101:VAL:HG13 | 6:N:1427:SER:OG   | 2.18                     | 0.43              |
| 6:N:1148:VAL:HG11 | 6:N:1203:LYS:HB3  | 2.00                     | 0.43              |
| 6:N:1372:VAL:HA   | 6:N:1375:MET:HE2  | 2.00                     | 0.43              |
| 6:N:1431:THR:OG1  | 6:N:1432:LYS:N    | 2.51                     | 0.43              |
| 6:N:1451:ALA:O    | 6:N:1452:ILE:C    | 2.61                     | 0.43              |
| 7:O:26:ARG:HE     | 7:O:30:LEU:HD12   | 1.84                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:O:67:GLU:HB3    | 7:O:73:LEU:CD1    | 2.48                     | 0.43              |
| 2:Y:5:C:H2'       | 2:Y:6:U:C5        | 2.50                     | 0.43              |
| 4:B:23:PHE:O      | 4:B:196:THR:HA    | 2.19                     | 0.43              |
| 4:B:100:LEU:O     | 4:B:115:LEU:HG    | 2.19                     | 0.43              |
| 4:B:103:ALA:N     | 11:B:348:HOH:O    | 2.51                     | 0.43              |
| 5:C:140:ILE:HG13  | 5:C:411:SER:O     | 2.18                     | 0.43              |
| 5:C:602:GLU:CD    | 5:C:648:ARG:HG2   | 2.43                     | 0.43              |
| 5:C:631:SER:CB    | 5:C:637:LEU:HD11  | 2.45                     | 0.43              |
| 5:C:815:LEU:HD23  | 11:C:1323:HOH:O   | 2.19                     | 0.43              |
| 5:C:1118:LYS:O    | 5:C:1119:ARG:HB2  | 2.18                     | 0.43              |
| 6:D:80:VAL:HG12   | 6:D:81:THR:O      | 2.18                     | 0.43              |
| 6:D:171:LEU:HD11  | 11:D:8204:HOH:O   | 2.19                     | 0.43              |
| 6:D:556:LYS:O     | 6:D:560:GLN:HG3   | 2.19                     | 0.43              |
| 6:D:586:ARG:HH22  | 6:D:1444:THR:HG21 | 1.83                     | 0.43              |
| 6:D:849:ALA:O     | 6:D:853:VAL:HG23  | 2.18                     | 0.43              |
| 6:D:1098:LEU:HD11 | 6:D:1263:PHE:CE2  | 2.53                     | 0.43              |
| 6:D:1422:MET:CE   | 6:D:1427:SER:HA   | 2.48                     | 0.43              |
| 4:L:54:THR:CG2    | 4:L:158:ILE:HG13  | 2.48                     | 0.43              |
| 4:L:223:THR:HG23  | 11:L:379:HOH:O    | 2.18                     | 0.43              |
| 4:L:227:ASN:ND2   | 4:L:227:ASN:H     | 2.16                     | 0.43              |
| 5:M:31:GLN:NE2    | 5:M:31:GLN:O      | 2.52                     | 0.43              |
| 5:M:222:MET:HE1   | 11:M:1174:HOH:O   | 2.18                     | 0.43              |
| 5:M:285:LEU:HD12  | 5:M:288:ARG:O     | 2.19                     | 0.43              |
| 5:M:771:GLU:O     | 5:M:771:GLU:HG2   | 2.19                     | 0.43              |
| 5:M:834:GLN:HB3   | 11:M:1436:HOH:O   | 2.19                     | 0.43              |
| 5:M:882:LEU:HD11  | 6:N:1038:LEU:HB3  | 2.00                     | 0.43              |
| 6:N:12:LEU:HD21   | 6:N:104:PHE:CE1   | 2.52                     | 0.43              |
| 6:N:69:GLU:H      | 6:N:69:GLU:CD     | 2.26                     | 0.43              |
| 6:N:396:VAL:CG1   | 6:N:447:VAL:HG12  | 2.47                     | 0.43              |
| 6:N:826:PRO:O     | 6:N:836:VAL:HG13  | 2.18                     | 0.43              |
| 6:N:994:GLN:O     | 6:N:998:GLU:HG3   | 2.17                     | 0.43              |
| 7:O:70:THR:HG22   | 7:O:71:GLY:N      | 2.33                     | 0.43              |
| 5:C:17:PRO:O      | 5:C:20:GLU:HB3    | 2.19                     | 0.43              |
| 5:C:140:ILE:HA    | 5:C:332:ARG:O     | 2.18                     | 0.43              |
| 5:C:250:ARG:HD2   | 11:C:1278:HOH:O   | 2.18                     | 0.43              |
| 5:C:269:LEU:C     | 5:C:269:LEU:HD23  | 2.43                     | 0.43              |
| 5:C:493:ARG:HE    | 5:C:493:ARG:HB2   | 1.53                     | 0.43              |
| 5:C:949:LYS:CD    | 6:D:796:ARG:HH22  | 2.24                     | 0.43              |
| 5:C:1003:ASP:OD1  | 5:C:1004:LYS:HD3  | 2.19                     | 0.43              |
| 6:D:400:VAL:CG2   | 6:D:443:VAL:HG21  | 2.48                     | 0.43              |
| 6:D:470:LEU:H     | 6:D:470:LEU:CD2   | 2.31                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:D:496:LEU:HD11 | 6:D:1388:ARG:HG3  | 2.01                     | 0.43              |
| 6:D:662:GLU:OE2  | 6:D:669:ASN:HA    | 2.18                     | 0.43              |
| 6:D:699:VAL:H    | 6:D:756:GLN:HE21  | 1.62                     | 0.43              |
| 6:D:782:SER:O    | 6:D:786:ILE:HG13  | 2.18                     | 0.43              |
| 6:D:867:ARG:HD2  | 6:D:867:ARG:O     | 2.19                     | 0.43              |
| 6:D:935:LYS:HE3  | 11:D:8312:HOH:O   | 2.18                     | 0.43              |
| 6:D:1026:SER:C   | 6:D:1028:ALA:N    | 2.77                     | 0.43              |
| 6:D:1209:LEU:C   | 6:D:1211:MET:N    | 2.75                     | 0.43              |
| 6:D:1336:LEU:CD1 | 6:D:1341:PRO:HG3  | 2.49                     | 0.43              |
| 6:D:1438:ALA:O   | 6:D:1443:THR:HG22 | 2.18                     | 0.43              |
| 4:K:7:LYS:HD2    | 4:K:186:LEU:HD21  | 2.00                     | 0.43              |
| 5:M:99:GLN:NE2   | 5:M:109:LYS:HB2   | 2.33                     | 0.43              |
| 5:M:151:ASP:OD2  | 5:M:152:PRO:HD2   | 2.19                     | 0.43              |
| 5:M:194:VAL:CG1  | 5:M:221:LEU:HB2   | 2.48                     | 0.43              |
| 5:M:672:VAL:HG12 | 5:M:699:PHE:CE1   | 2.54                     | 0.43              |
| 5:M:805:ARG:NH1  | 5:M:807:ARG:HD3   | 2.34                     | 0.43              |
| 6:N:106:LYS:HE2  | 6:N:125:GLN:HE22  | 1.84                     | 0.43              |
| 6:N:179:VAL:CG1  | 6:N:183:GLU:HB3   | 2.45                     | 0.43              |
| 6:N:207:PHE:HB3  | 11:N:9229:HOH:O   | 2.18                     | 0.43              |
| 6:N:399:ARG:NE   | 6:N:430:ASP:HB2   | 2.33                     | 0.43              |
| 6:N:816:HIS:ND1  | 6:N:816:HIS:N     | 2.65                     | 0.43              |
| 6:N:949:ILE:N    | 11:N:9020:HOH:O   | 2.51                     | 0.43              |
| 6:N:1148:VAL:CG1 | 6:N:1163:GLY:HA2  | 2.48                     | 0.43              |
| 6:N:1207:TYR:HA  | 6:N:1214:PRO:HA   | 2.00                     | 0.43              |
| 4:A:43:ILE:HD11  | 4:B:35:THR:HG21   | 2.00                     | 0.43              |
| 4:A:108:GLU:HB3  | 4:A:110:LYS:CE    | 2.49                     | 0.43              |
| 5:C:7:GLY:H      | 5:C:904:PRO:HD2   | 1.84                     | 0.43              |
| 5:C:145:GLY:H    | 5:C:163:ILE:HG13  | 1.83                     | 0.43              |
| 5:C:258:TYR:N    | 5:C:258:TYR:CD2   | 2.84                     | 0.43              |
| 5:C:441:VAL:O    | 5:C:559:LEU:HG    | 2.18                     | 0.43              |
| 5:C:626:ARG:HH11 | 5:C:626:ARG:HG3   | 1.84                     | 0.43              |
| 5:C:714:ASP:N    | 5:C:818:GLY:O     | 2.52                     | 0.43              |
| 5:C:751:PRO:HA   | 5:C:792:VAL:CG1   | 2.49                     | 0.43              |
| 5:C:759:THR:HG23 | 11:C:1516:HOH:O   | 2.19                     | 0.43              |
| 5:C:875:GLY:O    | 5:C:879:ARG:HD2   | 2.19                     | 0.43              |
| 5:C:909:ALA:HB1  | 5:C:914:ILE:CD1   | 2.47                     | 0.43              |
| 5:C:981:GLU:HG3  | 5:C:982:PRO:HD3   | 2.01                     | 0.43              |
| 5:C:1103:ASP:OD2 | 5:C:1108:PRO:O    | 2.37                     | 0.43              |
| 6:D:189:GLN:HG3  | 11:D:8023:HOH:O   | 2.19                     | 0.43              |
| 6:D:440:VAL:CG2  | 6:D:441:ARG:HH21  | 2.32                     | 0.43              |
| 6:D:787:LEU:HD13 | 6:D:1023:MET:HA   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:1262:LEU:HD23 | 6:D:1352:ILE:HG12 | 2.00                     | 0.43              |
| 6:D:1268:PRO:HD2  | 6:D:1271:LYS:HD3  | 2.01                     | 0.43              |
| 6:D:1365:ASP:O    | 6:D:1366:LYS:C    | 2.62                     | 0.43              |
| 5:M:193:LEU:HD22  | 5:M:307:LEU:HD21  | 2.00                     | 0.43              |
| 5:M:553:ASP:OD2   | 5:M:883:GLY:HA3   | 2.18                     | 0.43              |
| 5:M:1019:GLN:HA   | 5:M:1020:PRO:HD3  | 1.86                     | 0.43              |
| 6:N:69:GLU:CD     | 6:N:69:GLU:N      | 2.77                     | 0.43              |
| 6:N:191:LEU:HD22  | 6:N:393:ILE:HD13  | 2.00                     | 0.43              |
| 6:N:455:ARG:HD3   | 6:N:463:GLN:CD    | 2.44                     | 0.43              |
| 6:N:456:MET:HG2   | 11:N:9491:HOH:O   | 2.18                     | 0.43              |
| 6:N:525:ARG:H     | 6:N:525:ARG:CD    | 2.31                     | 0.43              |
| 6:N:607:LEU:HD23  | 11:N:9149:HOH:O   | 2.19                     | 0.43              |
| 6:N:619:LEU:O     | 6:N:620:GLY:C     | 2.62                     | 0.43              |
| 6:N:1144:LEU:HA   | 6:N:1147:ARG:HG3  | 2.00                     | 0.43              |
| 6:N:1424:VAL:CG1  | 6:N:1425:THR:N    | 2.82                     | 0.43              |
| 6:N:1498:ALA:CB   | 7:O:84:ARG:HE     | 2.31                     | 0.43              |
| 7:O:28:GLN:CA     | 7:O:32:ARG:HH22   | 2.32                     | 0.43              |
| 1:G:23:DG:OP1     | 5:C:388:ARG:NH1   | 2.52                     | 0.43              |
| 3:I:8:DA:OP1      | 6:D:1426:LYS:HE3  | 2.19                     | 0.43              |
| 2:Y:7:G:N2        | 5:M:1014:SER:HA   | 2.32                     | 0.43              |
| 3:Z:5:DG:H3'      | 11:Z:945:HOH:O    | 2.18                     | 0.43              |
| 4:A:215:VAL:HG11  | 4:B:225:PHE:HD1   | 1.84                     | 0.43              |
| 5:C:121:MET:HE3   | 5:C:125:GLY:CA    | 2.41                     | 0.43              |
| 5:C:262:ALA:O     | 5:C:264:PRO:O     | 2.37                     | 0.43              |
| 5:C:894:GLY:HA2   | 5:C:901:TYR:OH    | 2.19                     | 0.43              |
| 5:C:946:ARG:HD3   | 5:C:984:GLU:HB3   | 2.01                     | 0.43              |
| 5:C:983:ILE:HG21  | 5:C:987:ILE:CD1   | 2.49                     | 0.43              |
| 6:D:30:GLU:N      | 11:D:8061:HOH:O   | 2.52                     | 0.43              |
| 6:D:45:PHE:O      | 6:D:46:ASP:C      | 2.62                     | 0.43              |
| 6:D:497:GLU:O     | 6:D:500:ARG:HB2   | 2.19                     | 0.43              |
| 6:D:764:LEU:HD12  | 6:D:765:SER:N     | 2.34                     | 0.43              |
| 6:D:767:HIS:CE1   | 7:E:6:ILE:HG21    | 2.54                     | 0.43              |
| 6:D:799:LYS:N     | 11:D:8279:HOH:O   | 2.52                     | 0.43              |
| 6:D:820:GLU:HG3   | 6:D:836:VAL:HG11  | 1.99                     | 0.43              |
| 6:D:1441:GLN:NE2  | 6:D:1442:ASN:H    | 2.17                     | 0.43              |
| 4:K:36:LEU:C      | 4:K:39:PRO:HD2    | 2.44                     | 0.43              |
| 4:L:9:PRO:HB3     | 4:L:25:LEU:CD2    | 2.49                     | 0.43              |
| 4:L:26:GLU:HB2    | 4:L:27:PRO:HA     | 2.01                     | 0.43              |
| 4:L:70:GLY:N      | 11:L:402:HOH:O    | 2.50                     | 0.43              |
| 4:L:76:VAL:HA     | 4:L:79:ILE:HG12   | 2.00                     | 0.43              |
| 5:M:175:GLU:HB3   | 5:M:183:SER:OG    | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:290:LEU:HD23  | 5:M:290:LEU:N     | 2.32                     | 0.43              |
| 5:M:299:LYS:HG3   | 11:M:1441:HOH:O   | 2.19                     | 0.43              |
| 5:M:564:MET:CB    | 11:M:1517:HOH:O   | 2.67                     | 0.43              |
| 5:M:701:THR:CG2   | 5:M:830:LYS:HE2   | 2.46                     | 0.43              |
| 5:M:822:VAL:HB    | 5:M:824:ARG:HH21  | 1.84                     | 0.43              |
| 5:M:851:LYS:HD2   | 5:M:852:ILE:H     | 1.84                     | 0.43              |
| 5:M:1103:ASP:OD2  | 6:N:3:LYS:HD2     | 2.18                     | 0.43              |
| 6:N:407:VAL:HA    | 6:N:422:ALA:CB    | 2.49                     | 0.43              |
| 6:N:508:ARG:HD3   | 11:N:9337:HOH:O   | 2.18                     | 0.43              |
| 6:N:695:ILE:CD1   | 6:N:718:PRO:HB2   | 2.48                     | 0.43              |
| 6:N:826:PRO:HD2   | 6:N:829:VAL:HG22  | 2.00                     | 0.43              |
| 6:N:953:ASP:OD2   | 6:N:953:ASP:N     | 2.52                     | 0.43              |
| 6:N:1112:CYS:O    | 6:N:1189:ARG:NH2  | 2.52                     | 0.43              |
| 6:N:1150:ALA:CB   | 6:N:1151:ARG:HD2  | 2.48                     | 0.43              |
| 6:N:1264:GLU:HG3  | 6:N:1425:THR:OG1  | 2.19                     | 0.43              |
| 5:C:139:GLN:HE21  | 5:C:334:ARG:CD    | 2.25                     | 0.42              |
| 5:C:183:SER:OG    | 5:C:190:LYS:HG2   | 2.18                     | 0.42              |
| 5:C:251:ASP:HB3   | 5:C:252:LYS:CD    | 2.48                     | 0.42              |
| 5:C:265:ARG:NH1   | 11:C:1308:HOH:O   | 2.51                     | 0.42              |
| 5:C:313:LEU:HD13  | 5:C:321:GLU:CG    | 2.49                     | 0.42              |
| 5:C:399:ASN:ND2   | 5:C:402:SER:OG    | 2.52                     | 0.42              |
| 5:C:500:ASN:HA    | 11:C:1162:HOH:O   | 2.19                     | 0.42              |
| 5:C:583:LEU:O     | 5:C:587:VAL:HG23  | 2.20                     | 0.42              |
| 5:C:599:GLU:HA    | 5:C:651:LYS:HG3   | 2.00                     | 0.42              |
| 5:C:614:ARG:HG3   | 5:C:620:LEU:CD2   | 2.43                     | 0.42              |
| 6:D:101:HIS:HD2   | 6:D:514:LEU:HD11  | 1.83                     | 0.42              |
| 6:D:133:ILE:HG13  | 6:D:153:LEU:CG    | 2.48                     | 0.42              |
| 6:D:175:VAL:HG21  | 11:D:8081:HOH:O   | 2.19                     | 0.42              |
| 6:D:397:LYS:HB3   | 6:D:448:GLU:CB    | 2.49                     | 0.42              |
| 6:D:397:LYS:HD3   | 6:D:448:GLU:OE1   | 2.19                     | 0.42              |
| 6:D:701:LEU:O     | 6:D:747:VAL:HA    | 2.20                     | 0.42              |
| 6:D:739:ASP:OD1   | 6:D:741:ASP:OD1   | 2.37                     | 0.42              |
| 6:D:786:ILE:CD1   | 6:D:908:LYS:HD3   | 2.49                     | 0.42              |
| 6:D:1123:PHE:CE2  | 6:D:1184:GLN:HA   | 2.54                     | 0.42              |
| 6:D:1344:VAL:HG12 | 6:D:1348:LEU:HD13 | 2.00                     | 0.42              |
| 6:D:1490:LYS:HB2  | 7:E:93:TYR:OH     | 2.19                     | 0.42              |
| 7:E:41:GLU:N      | 7:E:42:PRO:CD     | 2.81                     | 0.42              |
| 4:K:133:GLU:HG3   | 5:M:605:LYS:HA    | 2.01                     | 0.42              |
| 4:L:59:GLU:HB2    | 4:L:137:ARG:CZ    | 2.49                     | 0.42              |
| 5:M:141:HIS:NE2   | 5:M:332:ARG:HD2   | 2.34                     | 0.42              |
| 5:M:208:ALA:HB3   | 5:M:209:ARG:NH2   | 2.33                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:M:433:THR:C    | 5:M:435:TYR:N     | 2.77                     | 0.42              |
| 5:M:458:TYR:N    | 5:M:458:TYR:CD1   | 2.86                     | 0.42              |
| 5:M:515:ALA:HB3  | 5:M:524:VAL:HG21  | 2.01                     | 0.42              |
| 5:M:519:GLY:HA3  | 11:M:1314:HOH:O   | 2.19                     | 0.42              |
| 5:M:874:LEU:HD23 | 6:N:783:ARG:HB3   | 2.01                     | 0.42              |
| 6:N:586:ARG:HH22 | 6:N:1444:THR:HG21 | 1.84                     | 0.42              |
| 6:N:692:GLU:C    | 6:N:692:GLU:CD    | 2.86                     | 0.42              |
| 6:N:860:LEU:HD22 | 6:N:881:LEU:HD23  | 2.01                     | 0.42              |
| 6:N:963:TYR:HA   | 6:N:966:GLU:OE2   | 2.19                     | 0.42              |
| 6:N:984:THR:HG23 | 6:N:987:GLU:H     | 1.84                     | 0.42              |
| 6:N:1153:VAL:O   | 6:N:1160:LEU:HG   | 2.19                     | 0.42              |
| 7:O:26:ARG:HD3   | 7:O:73:LEU:CD2    | 2.49                     | 0.42              |
| 7:O:51:LEU:HD12  | 11:O:1058:HOH:O   | 2.19                     | 0.42              |
| 1:G:23:DG:H5"    | 5:C:388:ARG:NH2   | 2.35                     | 0.42              |
| 4:A:152:PRO:HB3  | 4:A:154:GLU:OE1   | 2.19                     | 0.42              |
| 5:C:313:LEU:CA   | 5:C:321:GLU:HG3   | 2.48                     | 0.42              |
| 5:C:352:ALA:O    | 5:C:355:VAL:HG12  | 2.19                     | 0.42              |
| 5:C:580:MET:CE   | 5:C:584:GLU:HG3   | 2.49                     | 0.42              |
| 5:C:816:LYS:HB2  | 5:C:819:VAL:HG21  | 2.00                     | 0.42              |
| 6:D:26:VAL:HG11  | 6:D:44:LEU:CD2    | 2.48                     | 0.42              |
| 6:D:171:LEU:HD21 | 6:D:192:ALA:HB3   | 2.00                     | 0.42              |
| 6:D:564:GLU:HA   | 6:D:567:ILE:HD12  | 2.01                     | 0.42              |
| 6:D:699:VAL:HG21 | 6:D:760:ARG:HB3   | 2.01                     | 0.42              |
| 6:D:794:GLN:HB3  | 6:D:1017:PHE:CZ   | 2.51                     | 0.42              |
| 6:D:796:ARG:HE   | 6:D:828:LYS:HZ3   | 1.67                     | 0.42              |
| 6:D:893:GLU:O    | 6:D:896:ALA:HB3   | 2.20                     | 0.42              |
| 6:D:969:ARG:HA   | 11:D:8045:HOH:O   | 2.19                     | 0.42              |
| 6:D:1046:GLN:HG2 | 6:D:1052:THR:CA   | 2.49                     | 0.42              |
| 6:D:1231:GLU:OE2 | 6:D:1232:PRO:HD3  | 2.18                     | 0.42              |
| 4:L:106:PRO:HG3  | 4:L:133:GLU:O     | 2.19                     | 0.42              |
| 5:M:12:VAL:HB    | 5:M:472:ARG:NH1   | 2.34                     | 0.42              |
| 5:M:136:ILE:HD13 | 5:M:136:ILE:HA    | 1.93                     | 0.42              |
| 5:M:191:PHE:HB2  | 5:M:192:PRO:HD3   | 2.01                     | 0.42              |
| 5:M:235:LEU:HD21 | 11:M:1276:HOH:O   | 2.18                     | 0.42              |
| 5:M:460:ARG:C    | 11:M:1287:HOH:O   | 2.62                     | 0.42              |
| 5:M:960:GLU:HG3  | 5:M:961:GLU:N     | 2.32                     | 0.42              |
| 5:M:1058:ASP:O   | 5:M:1060:ILE:N    | 2.51                     | 0.42              |
| 5:M:1103:ASP:N   | 5:M:1107:ASN:O    | 2.49                     | 0.42              |
| 6:N:161:LEU:HB2  | 11:N:9073:HOH:O   | 2.19                     | 0.42              |
| 6:N:407:VAL:HA   | 6:N:422:ALA:HB2   | 2.01                     | 0.42              |
| 6:N:501:ALA:CB   | 6:N:1453:ALA:HB2  | 2.38                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:522:PRO:HA   | 6:N:525:ARG:NE   | 2.34                     | 0.42              |
| 6:N:714:GLN:HE22 | 6:N:768:ASN:HD22 | 1.67                     | 0.42              |
| 6:N:756:GLN:NE2  | 6:N:760:ARG:HB3  | 2.34                     | 0.42              |
| 6:N:783:ARG:H    | 6:N:783:ARG:HG3  | 1.53                     | 0.42              |
| 4:A:55:SER:HB2   | 4:A:158:ILE:HB   | 2.01                     | 0.42              |
| 4:B:102:LYS:HZ3  | 4:B:139:ASN:HB2  | 1.84                     | 0.42              |
| 4:B:169:ALA:HB1  | 4:B:171:PHE:CE2  | 2.54                     | 0.42              |
| 5:C:259:GLY:O    | 5:C:290:LEU:O    | 2.37                     | 0.42              |
| 5:C:267:TYR:CD2  | 5:C:267:TYR:N    | 2.87                     | 0.42              |
| 5:C:297:GLU:HG3  | 11:C:1205:HOH:O  | 2.18                     | 0.42              |
| 5:C:437:ARG:CB   | 5:C:467:ILE:HB   | 2.49                     | 0.42              |
| 5:C:492:ASP:OD2  | 5:C:518:LYS:HB3  | 2.18                     | 0.42              |
| 5:C:573:ARG:CD   | 5:C:670:GLN:HE22 | 2.32                     | 0.42              |
| 5:C:971:LYS:HB3  | 5:C:987:ILE:C    | 2.43                     | 0.42              |
| 6:D:32:ILE:HD13  | 6:D:37:LEU:O     | 2.19                     | 0.42              |
| 6:D:98:PRO:HG3   | 6:D:462:GLN:HE22 | 1.85                     | 0.42              |
| 6:D:137:PRO:HG3  | 6:D:467:GLU:OE1  | 2.20                     | 0.42              |
| 6:D:185:VAL:HG21 | 6:D:191:LEU:CD2  | 2.49                     | 0.42              |
| 6:D:191:LEU:HB2  | 6:D:195:VAL:HG12 | 2.00                     | 0.42              |
| 6:D:423:ASP:OD1  | 6:D:423:ASP:N    | 2.52                     | 0.42              |
| 6:D:440:VAL:HB   | 6:D:441:ARG:NH2  | 2.30                     | 0.42              |
| 6:D:625:TYR:CD1  | 6:D:625:TYR:N    | 2.88                     | 0.42              |
| 6:D:701:LEU:CD1  | 6:D:715:ALA:HB2  | 2.49                     | 0.42              |
| 6:D:711:LEU:HD22 | 6:D:714:GLN:NE2  | 2.34                     | 0.42              |
| 6:D:829:VAL:O    | 6:D:835:SER:HB2  | 2.19                     | 0.42              |
| 6:D:1047:LYS:HG2 | 6:D:1053:PHE:CE2 | 2.54                     | 0.42              |
| 4:K:206:THR:HG23 | 4:K:207:PRO:CD   | 2.49                     | 0.42              |
| 4:L:56:VAL:HG12  | 4:L:57:TYR:N     | 2.34                     | 0.42              |
| 5:M:203:ASP:O    | 5:M:207:LEU:HB2  | 2.18                     | 0.42              |
| 5:M:617:ASP:HB2  | 5:M:619:ARG:NE   | 2.33                     | 0.42              |
| 5:M:869:VAL:HG22 | 5:M:871:LEU:HD23 | 2.01                     | 0.42              |
| 6:N:45:PHE:HB3   | 6:N:86:ARG:HH22  | 1.83                     | 0.42              |
| 6:N:63:TYR:HB3   | 6:N:68:PHE:CE1   | 2.54                     | 0.42              |
| 6:N:206:ARG:HG3  | 6:N:206:ARG:NH1  | 2.34                     | 0.42              |
| 6:N:631:ILE:HG21 | 6:N:745:MET:CG   | 2.49                     | 0.42              |
| 6:N:840:LYS:HE2  | 6:N:841:TYR:HE2  | 1.84                     | 0.42              |
| 2:H:2:A:H2'      | 2:H:3:G:O5'      | 2.20                     | 0.42              |
| 3:Z:8:DA:H1'     | 3:Z:9:DG:C5'     | 2.46                     | 0.42              |
| 4:A:221:HIS:HA   | 4:A:224:TYR:CD2  | 2.54                     | 0.42              |
| 5:C:86:LYS:HB2   | 5:C:88:LEU:HD23  | 2.01                     | 0.42              |
| 5:C:214:TYR:OH   | 5:C:312:ALA:HB2  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:362:GLY:HA2  | 5:C:371:LYS:NZ    | 2.34                     | 0.42              |
| 5:C:588:VAL:HA   | 5:C:591:SER:OG    | 2.19                     | 0.42              |
| 5:C:626:ARG:O    | 5:C:638:ASP:HA    | 2.19                     | 0.42              |
| 5:C:690:ILE:HD11 | 5:C:833:LEU:HD23  | 2.00                     | 0.42              |
| 5:C:695:LEU:HD11 | 5:C:832:LYS:HB3   | 2.02                     | 0.42              |
| 5:C:1085:PHE:O   | 5:C:1088:LEU:HB3  | 2.18                     | 0.42              |
| 6:D:193:PRO:HG2  | 11:D:8081:HOH:O   | 2.18                     | 0.42              |
| 6:D:455:ARG:NH1  | 6:D:463:GLN:HG3   | 2.35                     | 0.42              |
| 6:D:1109:GLU:CG  | 6:D:1201:CYS:HA   | 2.31                     | 0.42              |
| 4:K:9:PRO:HB3    | 4:K:25:LEU:CD2    | 2.50                     | 0.42              |
| 5:M:146:VAL:CG1  | 5:M:162:ILE:HG12  | 2.48                     | 0.42              |
| 5:M:244:PRO:HD2  | 5:M:245:GLY:N     | 2.28                     | 0.42              |
| 5:M:334:ARG:HA   | 5:M:338:GLU:OE2   | 2.19                     | 0.42              |
| 5:M:364:GLU:O    | 5:M:367:LEU:HG    | 2.18                     | 0.42              |
| 5:M:526:PRO:HA   | 5:M:529:VAL:CG2   | 2.50                     | 0.42              |
| 5:M:526:PRO:HA   | 5:M:529:VAL:HG23  | 2.01                     | 0.42              |
| 5:M:654:LEU:HD13 | 5:M:664:GLY:N     | 2.34                     | 0.42              |
| 5:M:695:LEU:CD2  | 5:M:832:LYS:HD3   | 2.29                     | 0.42              |
| 5:M:894:GLY:HA2  | 5:M:901:TYR:OH    | 2.19                     | 0.42              |
| 6:N:409:VAL:HG12 | 6:N:435:VAL:HG11  | 2.01                     | 0.42              |
| 6:N:441:ARG:HH22 | 6:N:445:ARG:NH2   | 2.16                     | 0.42              |
| 6:N:462:GLN:CA   | 6:N:513:ILE:HD13  | 2.49                     | 0.42              |
| 6:N:653:PHE:N    | 6:N:653:PHE:CD1   | 2.87                     | 0.42              |
| 6:N:688:TRP:HA   | 6:N:688:TRP:CE3   | 2.54                     | 0.42              |
| 6:N:785:ILE:CG1  | 6:N:935:LYS:HA    | 2.43                     | 0.42              |
| 6:N:903:ASP:O    | 6:N:904:VAL:HG13  | 2.19                     | 0.42              |
| 6:N:921:ARG:HH11 | 6:N:921:ARG:CB    | 2.15                     | 0.42              |
| 6:N:1329:ALA:C   | 6:N:1330:ILE:HD12 | 2.44                     | 0.42              |
| 1:G:12:DG:H2''   | 1:G:13:DT:H5'     | 2.01                     | 0.42              |
| 5:C:191:PHE:CE2  | 5:C:196:LEU:HD12  | 2.55                     | 0.42              |
| 5:C:227:PHE:HB3  | 11:C:1552:HOH:O   | 2.20                     | 0.42              |
| 5:C:609:ASN:N    | 5:C:609:ASN:ND2   | 2.63                     | 0.42              |
| 5:C:689:VAL:CG1  | 5:C:690:ILE:N     | 2.82                     | 0.42              |
| 5:C:839:LEU:CD2  | 5:C:996:LYS:HA    | 2.47                     | 0.42              |
| 5:C:924:VAL:HG12 | 11:C:1285:HOH:O   | 2.18                     | 0.42              |
| 6:D:29:PRO:HD3   | 11:D:8201:HOH:O   | 2.18                     | 0.42              |
| 6:D:79:GLU:HG2   | 6:D:80:VAL:N      | 2.33                     | 0.42              |
| 6:D:114:THR:CG2  | 6:D:495:ARG:HA    | 2.49                     | 0.42              |
| 6:D:118:LEU:O    | 6:D:120:ALA:N     | 2.53                     | 0.42              |
| 6:D:118:LEU:CD1  | 6:D:461:ILE:HD12  | 2.50                     | 0.42              |
| 6:D:440:VAL:HB   | 6:D:441:ARG:NE    | 2.32                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:D:486:ARG:CA   | 6:D:489:ARG:HG2   | 2.47                     | 0.42              |
| 6:D:817:GLU:HA   | 6:D:836:VAL:HG21  | 2.02                     | 0.42              |
| 6:D:838:ARG:NH1  | 6:D:838:ARG:HG2   | 2.34                     | 0.42              |
| 6:D:1389:LEU:HG  | 6:D:1390:LEU:N    | 2.24                     | 0.42              |
| 6:D:1487:VAL:HB  | 7:E:74:VAL:HG23   | 2.00                     | 0.42              |
| 7:E:47:LYS:C     | 7:E:54:LEU:HD13   | 2.44                     | 0.42              |
| 4:K:179:PHE:CD1  | 4:K:179:PHE:C     | 2.97                     | 0.42              |
| 4:L:56:VAL:HG22  | 4:L:142:VAL:HG12  | 2.01                     | 0.42              |
| 4:L:106:PRO:HA   | 4:L:133:GLU:O     | 2.20                     | 0.42              |
| 4:L:142:VAL:HG23 | 4:L:142:VAL:O     | 2.18                     | 0.42              |
| 4:L:182:GLU:OE1  | 4:L:194:LYS:HD2   | 2.20                     | 0.42              |
| 5:M:208:ALA:CB   | 5:M:209:ARG:HH21  | 2.32                     | 0.42              |
| 5:M:566:THR:O    | 5:M:566:THR:HG22  | 2.18                     | 0.42              |
| 5:M:602:GLU:OE1  | 5:M:648:ARG:HB3   | 2.18                     | 0.42              |
| 5:M:937:ASP:OD2  | 5:M:939:ARG:HG2   | 2.20                     | 0.42              |
| 5:M:1032:PHE:HB3 | 6:N:620:GLY:O     | 2.20                     | 0.42              |
| 6:N:739:ASP:OD1  | 6:N:741:ASP:OD1   | 2.36                     | 0.42              |
| 6:N:955:VAL:HG11 | 6:N:1015:TYR:CZ   | 2.54                     | 0.42              |
| 6:N:989:TYR:CE1  | 6:N:993:LEU:HD21  | 2.54                     | 0.42              |
| 6:N:1365:ASP:O   | 6:N:1369:GLU:HG3  | 2.19                     | 0.42              |
| 6:N:1401:GLU:OE2 | 6:N:1415:VAL:HG21 | 2.20                     | 0.42              |
| 2:H:9:G:N2       | 11:H:26:HOH:O     | 2.53                     | 0.42              |
| 1:X:19:DC:H3'    | 11:X:2000:HOH:O   | 2.19                     | 0.42              |
| 5:C:77:PRO:HD3   | 5:C:91:GLN:O      | 2.20                     | 0.42              |
| 5:C:333:ILE:HG12 | 5:C:467:ILE:HD11  | 2.01                     | 0.42              |
| 5:C:408:ARG:O    | 5:C:454:SER:HA    | 2.19                     | 0.42              |
| 5:C:431:HIS:HD2  | 5:C:433:THR:OG1   | 2.03                     | 0.42              |
| 5:C:606:VAL:HG23 | 5:C:645:VAL:HG12  | 2.02                     | 0.42              |
| 5:C:620:LEU:HD11 | 11:C:1436:HOH:O   | 2.19                     | 0.42              |
| 5:C:644:VAL:HB   | 11:C:1372:HOH:O   | 2.20                     | 0.42              |
| 5:C:693:GLU:HA   | 5:C:696:LYS:HE3   | 2.00                     | 0.42              |
| 5:C:710:ILE:CD1  | 5:C:790:LEU:HD13  | 2.49                     | 0.42              |
| 5:C:874:LEU:HA   | 6:D:1023:MET:SD   | 2.60                     | 0.42              |
| 5:C:895:TYR:HA   | 11:C:1275:HOH:O   | 2.20                     | 0.42              |
| 5:C:1096:ALA:HB2 | 6:D:101:HIS:NE2   | 2.34                     | 0.42              |
| 5:C:1111:ILE:H   | 5:C:1111:ILE:HG13 | 1.48                     | 0.42              |
| 6:D:54:LYS:CG    | 6:D:55:ASP:H      | 2.32                     | 0.42              |
| 6:D:116:LEU:HD23 | 6:D:150:ARG:HH11  | 1.85                     | 0.42              |
| 6:D:709:HIS:CD2  | 6:D:709:HIS:H     | 2.37                     | 0.42              |
| 6:D:841:TYR:HB3  | 6:D:843:PHE:CZ    | 2.54                     | 0.42              |
| 6:D:1121:PRO:HG3 | 6:D:1185:GLU:OE2  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:1393:GLN:CD   | 6:D:1394:VAL:N    | 2.67                     | 0.42              |
| 4:K:13:VAL:HG22   | 4:K:23:PHE:CD1    | 2.55                     | 0.42              |
| 5:M:473:ARG:HG3   | 5:M:474:VAL:N     | 2.35                     | 0.42              |
| 5:M:536:PRO:HB3   | 5:M:906:PHE:HD1   | 1.84                     | 0.42              |
| 5:M:575:GLN:NE2   | 5:M:670:GLN:OE1   | 2.52                     | 0.42              |
| 5:M:810:ASP:HA    | 5:M:811:PRO:HD3   | 1.67                     | 0.42              |
| 5:M:833:LEU:HD11  | 5:M:839:LEU:HD21  | 2.01                     | 0.42              |
| 5:M:889:HIS:HE1   | 6:N:951:ILE:H     | 1.67                     | 0.42              |
| 5:M:1060:ILE:O    | 5:M:1064:ASN:ND2  | 2.53                     | 0.42              |
| 5:M:1111:ILE:HG13 | 5:M:1112:PHE:N    | 2.31                     | 0.42              |
| 6:N:131:LYS:HZ3   | 6:N:568:ARG:CB    | 2.32                     | 0.42              |
| 6:N:166:GLN:OE1   | 6:N:396:VAL:HG22  | 2.20                     | 0.42              |
| 6:N:656:PHE:HB3   | 6:N:694:VAL:CG1   | 2.50                     | 0.42              |
| 6:N:692:GLU:CD    | 6:N:692:GLU:O     | 2.63                     | 0.42              |
| 6:N:1036:ARG:HB3  | 6:N:1036:ARG:HH11 | 1.82                     | 0.42              |
| 6:N:1158:VAL:HG12 | 6:N:1159:ARG:N    | 2.35                     | 0.42              |
| 4:A:161:ARG:HA    | 4:A:161:ARG:NE    | 2.34                     | 0.42              |
| 4:B:142:VAL:HG23  | 4:B:142:VAL:O     | 2.18                     | 0.42              |
| 5:C:95:TYR:HD1    | 5:C:112:GLU:CD    | 2.27                     | 0.42              |
| 5:C:137:VAL:N     | 5:C:391:LEU:HD21  | 2.33                     | 0.42              |
| 5:C:140:ILE:HD11  | 5:C:412:ALA:HB2   | 2.01                     | 0.42              |
| 5:C:966:LEU:HD12  | 5:C:966:LEU:HA    | 1.94                     | 0.42              |
| 6:D:711:LEU:HD21  | 6:D:768:ASN:HB2   | 2.01                     | 0.42              |
| 6:D:806:PHE:HE1   | 6:D:813:LEU:HB3   | 1.79                     | 0.42              |
| 6:D:820:GLU:OE1   | 6:D:840:LYS:HE3   | 2.20                     | 0.42              |
| 6:D:1103:HIS:HD2  | 6:D:1463:LYS:H    | 1.59                     | 0.42              |
| 4:K:213:GLN:NE2   | 11:K:1765:HOH:O   | 2.51                     | 0.42              |
| 4:L:75:VAL:O      | 4:L:79:ILE:HG23   | 2.19                     | 0.42              |
| 4:L:189:ARG:HG3   | 4:L:189:ARG:O     | 2.19                     | 0.42              |
| 5:M:69:LEU:HD12   | 5:M:97:ARG:CB     | 2.49                     | 0.42              |
| 5:M:98:LEU:N      | 5:M:98:LEU:HD12   | 2.35                     | 0.42              |
| 5:M:458:TYR:N     | 5:M:458:TYR:HD1   | 2.18                     | 0.42              |
| 5:M:580:MET:O     | 5:M:902:ILE:HA    | 2.19                     | 0.42              |
| 5:M:783:ARG:HE    | 5:M:785:VAL:CG1   | 2.32                     | 0.42              |
| 5:M:1009:SER:OG   | 5:M:1010:THR:N    | 2.53                     | 0.42              |
| 6:N:19:ARG:HE     | 6:N:516:ALA:CB    | 2.32                     | 0.42              |
| 6:N:959:GLU:CD    | 6:N:959:GLU:H     | 2.27                     | 0.42              |
| 6:N:998:GLU:O     | 6:N:1002:LYS:HG3  | 2.20                     | 0.42              |
| 6:N:1023:MET:HB2  | 6:N:1023:MET:HE3  | 1.85                     | 0.42              |
| 6:N:1047:LYS:HG2  | 6:N:1053:PHE:CE1  | 2.54                     | 0.42              |
| 6:N:1055:VAL:HA   | 6:N:1056:PRO:HD3  | 1.90                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:1146:GLY:C    | 6:N:1207:TYR:HB2  | 2.45                     | 0.42              |
| 3:I:3:DA:O4'      | 5:C:423:ALA:HB2   | 2.20                     | 0.42              |
| 4:A:184:THR:N     | 11:A:321:HOH:O    | 2.53                     | 0.42              |
| 5:C:401:LEU:HD21  | 5:C:565:GLN:NE2   | 2.34                     | 0.42              |
| 5:C:541:SER:OG    | 5:C:542:VAL:N     | 2.52                     | 0.42              |
| 5:C:780:GLU:H     | 5:C:780:GLU:HG3   | 1.53                     | 0.42              |
| 5:C:1105:LYS:HD2  | 5:C:1107:ASN:HD22 | 1.83                     | 0.42              |
| 6:D:54:LYS:HB3    | 6:D:57:GLU:OE2    | 2.20                     | 0.42              |
| 6:D:87:ARG:NH2    | 11:D:8227:HOH:O   | 2.53                     | 0.42              |
| 6:D:462:GLN:HG2   | 6:D:466:LYS:HZ2   | 1.85                     | 0.42              |
| 6:D:470:LEU:HD21  | 11:D:8038:HOH:O   | 2.19                     | 0.42              |
| 6:D:695:ILE:HD13  | 6:D:720:LEU:CD1   | 2.50                     | 0.42              |
| 6:D:698:LYS:HE3   | 6:D:698:LYS:HB3   | 1.92                     | 0.42              |
| 6:D:780:LYS:HD2   | 6:D:912:LYS:HB2   | 2.02                     | 0.42              |
| 6:D:1072:ILE:HG12 | 11:D:8010:HOH:O   | 2.20                     | 0.42              |
| 6:D:1341:PRO:O    | 6:D:1343:ALA:N    | 2.52                     | 0.42              |
| 7:E:66:LYS:HD2    | 7:E:69:LEU:HD23   | 2.02                     | 0.42              |
| 5:M:628:PHE:CZ    | 5:M:703:ILE:HD13  | 2.55                     | 0.42              |
| 5:M:1111:ILE:H    | 5:M:1111:ILE:HG12 | 1.43                     | 0.42              |
| 6:N:584:ASN:HD22  | 6:N:584:ASN:C     | 2.28                     | 0.42              |
| 6:N:879:ARG:CG    | 6:N:879:ARG:HH11  | 2.32                     | 0.42              |
| 3:I:13:DG:H2''    | 3:I:14:DG:C8      | 2.55                     | 0.42              |
| 4:A:8:ALA:HB1     | 4:B:224:TYR:CE1   | 2.51                     | 0.42              |
| 4:A:182:GLU:HG2   | 4:A:194:LYS:HG2   | 2.02                     | 0.42              |
| 4:B:81:ASN:O      | 4:B:127:LEU:HD21  | 2.20                     | 0.42              |
| 5:C:139:GLN:HA    | 5:C:411:SER:O     | 2.19                     | 0.42              |
| 5:C:431:HIS:CD2   | 5:C:432:ARG:HB2   | 2.55                     | 0.42              |
| 5:C:442:GLU:HG2   | 5:C:454:SER:H     | 1.84                     | 0.42              |
| 5:C:719:PRO:HD2   | 11:C:1241:HOH:O   | 2.20                     | 0.42              |
| 6:D:48:ARG:HE     | 6:D:48:ARG:HB3    | 1.53                     | 0.42              |
| 6:D:116:LEU:HD23  | 6:D:150:ARG:NH1   | 2.35                     | 0.42              |
| 6:D:127:LEU:CD1   | 6:D:128:TYR:N     | 2.80                     | 0.42              |
| 6:D:1444:THR:OG1  | 6:D:1445:HIS:N    | 2.53                     | 0.42              |
| 7:E:33:HIS:CE1    | 7:E:89:MET:HB3    | 2.55                     | 0.42              |
| 4:K:107:LYS:HD3   | 4:K:108:GLU:O     | 2.20                     | 0.42              |
| 4:L:58:ILE:HG21   | 4:L:61:VAL:HB     | 2.00                     | 0.42              |
| 4:L:73:GLU:CB     | 4:L:77:GLU:HG3    | 2.50                     | 0.42              |
| 5:M:20:GLU:OE2    | 5:M:460:ARG:HD3   | 2.20                     | 0.42              |
| 5:M:874:LEU:C     | 5:M:877:PRO:HD2   | 2.44                     | 0.42              |
| 5:M:909:ALA:CB    | 5:M:914:ILE:HD11  | 2.47                     | 0.42              |
| 5:M:1035:MET:H    | 5:M:1035:MET:HG3  | 1.65                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:M:1043:TYR:C    | 5:M:1045:ALA:H   | 2.28                     | 0.42              |
| 6:N:19:ARG:HH11   | 6:N:19:ARG:HG3   | 1.85                     | 0.42              |
| 6:N:31:THR:CB     | 6:N:527:MET:HE2  | 2.49                     | 0.42              |
| 6:N:403:PHE:CD2   | 6:N:444:VAL:HG23 | 2.55                     | 0.42              |
| 6:N:574:LEU:O     | 6:N:578:VAL:HG23 | 2.19                     | 0.42              |
| 6:N:596:SER:HB3   | 6:N:598:ARG:NE   | 2.35                     | 0.42              |
| 6:N:600:LEU:HD12  | 6:N:600:LEU:H    | 1.83                     | 0.42              |
| 6:N:673:ALA:O     | 6:N:677:LEU:HD12 | 2.19                     | 0.42              |
| 6:N:683:ILE:HG23  | 6:N:687:VAL:HG21 | 2.01                     | 0.42              |
| 6:N:774:SER:C     | 6:N:776:GLU:H    | 2.27                     | 0.42              |
| 6:N:1078:ARG:HG3  | 6:N:1078:ARG:NH1 | 2.34                     | 0.42              |
| 6:N:1365:ASP:O    | 6:N:1366:LYS:C   | 2.62                     | 0.42              |
| 6:N:1415:VAL:HG22 | 11:N:9043:HOH:O  | 2.19                     | 0.42              |
| 2:Y:7:G:H22       | 5:M:1014:SER:HA  | 1.84                     | 0.42              |
| 4:A:70:GLY:O      | 4:A:132:LEU:HA   | 2.19                     | 0.42              |
| 4:B:22:GLU:HG2    | 4:B:198:ARG:HG2  | 2.00                     | 0.42              |
| 4:B:152:PRO:HG2   | 6:D:857:ILE:HD12 | 2.01                     | 0.42              |
| 5:C:6:PHE:HB2     | 5:C:908:GLY:C    | 2.44                     | 0.42              |
| 5:C:71:TYR:HA     | 5:C:96:ALA:CB    | 2.50                     | 0.42              |
| 5:C:143:SER:CB    | 5:C:276:LYS:NZ   | 2.83                     | 0.42              |
| 5:C:182:VAL:HG12  | 5:C:193:LEU:HD13 | 2.01                     | 0.42              |
| 5:C:208:ALA:HB1   | 5:C:218:VAL:CG1  | 2.50                     | 0.42              |
| 5:C:208:ALA:O     | 5:C:218:VAL:HG21 | 2.19                     | 0.42              |
| 5:C:537:LYS:CG    | 5:C:545:ASN:HD21 | 2.33                     | 0.42              |
| 5:C:577:PRO:HA    | 5:C:993:PHE:CD2  | 2.54                     | 0.42              |
| 5:C:598:GLU:O     | 5:C:651:LYS:HG3  | 2.20                     | 0.42              |
| 6:D:50:PHE:HB3    | 6:D:522:PRO:CG   | 2.46                     | 0.42              |
| 6:D:82:LYS:HB2    | 11:D:8499:HOH:O  | 2.20                     | 0.42              |
| 6:D:461:ILE:O     | 6:D:465:LEU:HB2  | 2.18                     | 0.42              |
| 6:D:1001:GLU:O    | 6:D:1004:THR:HB  | 2.20                     | 0.42              |
| 6:D:1341:PRO:O    | 6:D:1344:VAL:N   | 2.53                     | 0.42              |
| 6:D:1492:LEU:HD13 | 6:D:1492:LEU:C   | 2.45                     | 0.42              |
| 7:E:59:ASN:N      | 7:E:59:ASN:ND2   | 2.68                     | 0.42              |
| 4:K:91:ASN:HB3    | 11:K:1721:HOH:O  | 2.20                     | 0.42              |
| 4:L:25:LEU:CD2    | 4:L:28:LEU:HD21  | 2.40                     | 0.42              |
| 5:M:63:GLY:HA3    | 5:M:103:LYS:HG3  | 2.02                     | 0.42              |
| 5:M:456:ALA:HA    | 5:M:541:SER:HA   | 2.01                     | 0.42              |
| 5:M:549:PHE:HE2   | 5:M:887:GLU:HA   | 1.85                     | 0.42              |
| 5:M:605:LYS:O     | 5:M:611:ILE:HA   | 2.20                     | 0.42              |
| 5:M:728:HIS:NE2   | 5:M:775:ARG:NH1  | 2.67                     | 0.42              |
| 5:M:757:GLY:HA2   | 5:M:789:SER:HB3  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:872:ASN:HD21  | 5:M:874:LEU:HD13  | 1.85                     | 0.42              |
| 5:M:917:LEU:HB3   | 11:M:1461:HOH:O   | 2.20                     | 0.42              |
| 5:M:1049:LEU:HD23 | 6:N:1472:ILE:CD1  | 2.49                     | 0.42              |
| 6:N:397:LYS:HB3   | 6:N:448:GLU:HB3   | 2.01                     | 0.42              |
| 6:N:446:VAL:O     | 6:N:447:VAL:O     | 2.38                     | 0.42              |
| 6:N:628:ARG:HG3   | 6:N:628:ARG:HH11  | 1.84                     | 0.42              |
| 6:N:632:VAL:O     | 6:N:727:GLN:HA    | 2.20                     | 0.42              |
| 6:N:804:LEU:HD12  | 6:N:830:ALA:O     | 2.20                     | 0.42              |
| 6:N:859:ASP:HB3   | 6:N:861:GLN:NE2   | 2.35                     | 0.42              |
| 6:N:1137:ARG:HG3  | 11:N:9103:HOH:O   | 2.19                     | 0.42              |
| 6:N:1463:LYS:O    | 6:N:1467:ILE:HG13 | 2.19                     | 0.42              |
| 7:O:47:LYS:CA     | 7:O:54:LEU:HB3    | 2.49                     | 0.42              |
| 2:H:13:C:C3'      | 5:C:409:ARG:HH22  | 2.32                     | 0.41              |
| 4:A:89:PHE:CE2    | 4:A:146:ARG:HB2   | 2.55                     | 0.41              |
| 5:C:129:ILE:CG1   | 5:C:134:ARG:HD3   | 2.50                     | 0.41              |
| 5:C:186:VAL:HG23  | 5:C:187:ASN:N     | 2.26                     | 0.41              |
| 5:C:243:ARG:N     | 5:C:244:PRO:HD3   | 2.32                     | 0.41              |
| 5:C:848:VAL:HG12  | 5:C:849:VAL:N     | 2.35                     | 0.41              |
| 5:C:1031:ARG:NH1  | 6:D:621:LYS:NZ    | 2.68                     | 0.41              |
| 5:C:1084:SER:O    | 5:C:1087:VAL:HG12 | 2.20                     | 0.41              |
| 6:D:105:VAL:HG12  | 11:D:8237:HOH:O   | 2.20                     | 0.41              |
| 6:D:566:ILE:HD12  | 6:D:566:ILE:N     | 2.35                     | 0.41              |
| 6:D:581:LEU:HG    | 6:D:582:LEU:N     | 2.35                     | 0.41              |
| 6:D:789:LEU:HD13  | 6:D:911:LEU:HD21  | 2.02                     | 0.41              |
| 6:D:890:VAL:HG23  | 6:D:890:VAL:O     | 2.19                     | 0.41              |
| 6:D:926:LYS:HE2   | 6:D:926:LYS:HB3   | 1.93                     | 0.41              |
| 6:D:1042:ARG:HD2  | 6:D:1045:MET:CE   | 2.50                     | 0.41              |
| 6:D:1495:ILE:HG22 | 6:D:1499:ARG:NE   | 2.35                     | 0.41              |
| 4:K:14:ARG:HH11   | 4:K:14:ARG:HG3    | 1.85                     | 0.41              |
| 4:K:30:ARG:HA     | 4:K:30:ARG:HD2    | 1.87                     | 0.41              |
| 4:L:43:ILE:HG23   | 4:L:217:ILE:HG21  | 2.02                     | 0.41              |
| 4:L:143:ARG:NH1   | 4:L:158:ILE:HG21  | 2.35                     | 0.41              |
| 5:M:263:ASP:HB2   | 5:M:264:PRO:HD3   | 2.02                     | 0.41              |
| 5:M:292:ARG:HD2   | 5:M:299:LYS:CE    | 2.49                     | 0.41              |
| 5:M:745:ILE:HG21  | 11:M:1187:HOH:O   | 2.19                     | 0.41              |
| 5:M:756:VAL:O     | 5:M:789:SER:CB    | 2.66                     | 0.41              |
| 5:M:842:ARG:HG3   | 5:M:995:MET:HE3   | 2.02                     | 0.41              |
| 5:M:940:GLU:O     | 5:M:943:VAL:HG12  | 2.19                     | 0.41              |
| 5:M:1013:TYR:CE1  | 5:M:1020:PRO:HG3  | 2.55                     | 0.41              |
| 6:N:12:LEU:HD23   | 6:N:12:LEU:HA     | 1.84                     | 0.41              |
| 6:N:95:LEU:HA     | 6:N:551:ASN:CG    | 2.45                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:206:ARG:CG    | 6:N:394:LEU:HD22  | 2.36                     | 0.41              |
| 6:N:485:SER:HA    | 11:N:9344:HOH:O   | 2.19                     | 0.41              |
| 6:N:1000:THR:HG23 | 6:N:1001:GLU:N    | 2.34                     | 0.41              |
| 6:N:1206:GLY:O    | 6:N:1215:VAL:HG23 | 2.20                     | 0.41              |
| 6:N:1267:ARG:HD2  | 6:N:1271:LYS:HE2  | 2.01                     | 0.41              |
| 6:N:1381:VAL:HG22 | 6:N:1398:TRP:CZ2  | 2.54                     | 0.41              |
| 6:N:1399:ASP:O    | 6:N:1403:LEU:HB2  | 2.19                     | 0.41              |
| 2:Y:7:G:H22       | 5:M:1014:SER:N    | 2.17                     | 0.41              |
| 5:C:22:GLN:CB     | 5:C:121:MET:HE1   | 2.49                     | 0.41              |
| 5:C:68:PHE:HZ     | 5:C:71:TYR:HD2    | 1.68                     | 0.41              |
| 5:C:89:THR:O      | 5:C:91:GLN:HG3    | 2.20                     | 0.41              |
| 5:C:636:ALA:HB3   | 5:C:703:ILE:CD1   | 2.33                     | 0.41              |
| 5:C:704:HIS:O     | 5:C:829:GLN:OE1   | 2.38                     | 0.41              |
| 5:C:873:PRO:O     | 5:C:877:PRO:HD3   | 2.20                     | 0.41              |
| 5:C:1031:ARG:CZ   | 6:D:621:LYS:HZ2   | 2.34                     | 0.41              |
| 6:D:12:LEU:HD21   | 6:D:104:PHE:CZ    | 2.55                     | 0.41              |
| 6:D:134:VAL:HA    | 6:D:151:GLN:O     | 2.19                     | 0.41              |
| 6:D:457:GLY:C     | 6:D:459:GLU:N     | 2.77                     | 0.41              |
| 6:D:522:PRO:HA    | 6:D:525:ARG:NE    | 2.34                     | 0.41              |
| 6:D:984:THR:HG23  | 6:D:986:ARG:H     | 1.84                     | 0.41              |
| 6:D:1248:GLY:O    | 6:D:1252:ILE:HG12 | 2.20                     | 0.41              |
| 6:D:1472:ILE:O    | 6:D:1477:GLY:HA3  | 2.19                     | 0.41              |
| 7:E:44:GLU:HA     | 11:E:110:HOH:O    | 2.20                     | 0.41              |
| 4:L:9:PRO:HB3     | 4:L:25:LEU:HG     | 2.03                     | 0.41              |
| 4:L:175:ARG:H     | 4:L:175:ARG:HG2   | 1.61                     | 0.41              |
| 5:M:39:ARG:NH2    | 11:M:1341:HOH:O   | 2.52                     | 0.41              |
| 5:M:217:LEU:HD13  | 11:M:1269:HOH:O   | 2.20                     | 0.41              |
| 5:M:274:ARG:HG3   | 5:M:285:LEU:HD22  | 2.02                     | 0.41              |
| 5:M:354:GLY:O     | 5:M:358:ARG:HD3   | 2.19                     | 0.41              |
| 5:M:957:LYS:HB2   | 5:M:957:LYS:NZ    | 2.35                     | 0.41              |
| 5:M:1016:ILE:CG1  | 5:M:1017:THR:N    | 2.82                     | 0.41              |
| 6:N:52:PRO:CB     | 6:N:80:VAL:HG13   | 2.50                     | 0.41              |
| 6:N:66:GLN:O      | 6:N:69:GLU:HB3    | 2.20                     | 0.41              |
| 6:N:394:LEU:HD11  | 6:N:445:ARG:HH12  | 1.81                     | 0.41              |
| 6:N:709:HIS:CD2   | 6:N:709:HIS:N     | 2.89                     | 0.41              |
| 6:N:1209:LEU:HD13 | 11:N:9248:HOH:O   | 2.20                     | 0.41              |
| 6:N:1363:LEU:HD12 | 6:N:1363:LEU:O    | 2.20                     | 0.41              |
| 6:N:1498:ALA:HB1  | 7:O:84:ARG:HE     | 1.86                     | 0.41              |
| 4:A:42:ARG:HH22   | 4:B:34:VAL:HB     | 1.85                     | 0.41              |
| 4:A:111:ALA:CB    | 4:A:127:LEU:HD23  | 2.42                     | 0.41              |
| 4:A:128:HIS:HE1   | 4:A:131:THR:HG23  | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:132:LEU:HD23  | 4:B:136:GLY:O     | 2.20                     | 0.41              |
| 5:C:6:PHE:CD1     | 5:C:6:PHE:N       | 2.88                     | 0.41              |
| 5:C:115:LEU:HG    | 5:C:115:LEU:H     | 1.70                     | 0.41              |
| 5:C:182:VAL:CG2   | 5:C:220:GLY:O     | 2.67                     | 0.41              |
| 5:C:468:ARG:NH2   | 11:C:1462:HOH:O   | 2.53                     | 0.41              |
| 5:C:552:HIS:HD2   | 6:D:1064:GLY:HA2  | 1.86                     | 0.41              |
| 5:C:1006:HIS:HA   | 5:C:1027:PHE:HD1  | 1.83                     | 0.41              |
| 5:C:1102:LEU:HD23 | 5:C:1106:ASP:C    | 2.45                     | 0.41              |
| 6:D:412:GLY:HA2   | 6:D:434:ARG:NH1   | 2.34                     | 0.41              |
| 6:D:1464:GLU:HA   | 6:D:1467:ILE:HD11 | 2.02                     | 0.41              |
| 7:E:8:LYS:O       | 7:E:12:MET:HG3    | 2.20                     | 0.41              |
| 7:E:28:GLN:HG2    | 7:E:32:ARG:HH22   | 1.86                     | 0.41              |
| 4:K:41:ARG:HG3    | 4:K:177:VAL:CG1   | 2.50                     | 0.41              |
| 4:K:91:ASN:O      | 4:K:94:LEU:HD12   | 2.20                     | 0.41              |
| 4:L:48:ILE:HG22   | 4:L:173:PRO:HD2   | 2.03                     | 0.41              |
| 4:L:88:ARG:HD2    | 4:L:123:MET:SD    | 2.61                     | 0.41              |
| 5:M:29:ALA:HB2    | 5:M:337:GLY:HA3   | 2.01                     | 0.41              |
| 5:M:211:LEU:HD11  | 5:M:308:ARG:HA    | 2.02                     | 0.41              |
| 5:M:666:LEU:HD12  | 5:M:667:ALA:N     | 2.35                     | 0.41              |
| 5:M:670:GLN:NE2   | 5:M:699:PHE:CG    | 2.88                     | 0.41              |
| 5:M:913:GLU:O     | 5:M:916:GLU:HB3   | 2.20                     | 0.41              |
| 5:M:1070:ILE:HG23 | 6:N:656:PHE:HD1   | 1.84                     | 0.41              |
| 6:N:531:ASP:C     | 6:N:533:GLY:H     | 2.28                     | 0.41              |
| 6:N:704:ARG:CZ    | 6:N:737:ASN:O     | 2.69                     | 0.41              |
| 3:Z:13:DG:H2"     | 3:Z:14:DG:C8      | 2.55                     | 0.41              |
| 5:C:1016:ILE:HG12 | 5:C:1017:THR:H    | 1.84                     | 0.41              |
| 6:D:10:ILE:C      | 6:D:1451:ALA:HA   | 2.46                     | 0.41              |
| 6:D:98:PRO:HA     | 6:D:515:GLU:HA    | 2.01                     | 0.41              |
| 6:D:124:GLU:O     | 6:D:128:TYR:HB2   | 2.19                     | 0.41              |
| 6:D:496:LEU:HD12  | 6:D:500:ARG:HG2   | 2.03                     | 0.41              |
| 6:D:672:ALA:C     | 11:D:8039:HOH:O   | 2.63                     | 0.41              |
| 6:D:754:PHE:O     | 6:D:758:GLU:HG2   | 2.20                     | 0.41              |
| 6:D:783:ARG:HD2   | 6:D:1029:ARG:HG2  | 2.02                     | 0.41              |
| 6:D:972:LEU:HD23  | 11:D:8045:HOH:O   | 2.19                     | 0.41              |
| 6:D:1100:ASP:HB3  | 6:D:1428:ALA:CB   | 2.49                     | 0.41              |
| 6:D:1236:LEU:HD12 | 6:D:1359:GLN:HB3  | 2.03                     | 0.41              |
| 4:K:36:LEU:HD11   | 11:L:365:HOH:O    | 2.20                     | 0.41              |
| 4:K:42:ARG:HH11   | 5:M:978:ARG:CA    | 2.28                     | 0.41              |
| 4:K:181:VAL:O     | 5:M:938:LYS:N     | 2.54                     | 0.41              |
| 5:M:13:ILE:HG23   | 5:M:483:VAL:HG21  | 2.02                     | 0.41              |
| 5:M:23:VAL:HG13   | 11:M:1414:HOH:O   | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:632:ASN:HB3   | 5:M:633:GLN:NE2   | 2.35                     | 0.41              |
| 5:M:1067:TYR:O    | 5:M:1071:ILE:HG12 | 2.20                     | 0.41              |
| 5:M:1085:PHE:CE2  | 6:N:1468:LEU:HG   | 2.52                     | 0.41              |
| 6:N:36:THR:C      | 6:N:38:LYS:N      | 2.74                     | 0.41              |
| 6:N:159:ARG:NH2   | 11:N:9468:HOH:O   | 2.53                     | 0.41              |
| 6:N:470:LEU:HD12  | 6:N:503:LEU:CD2   | 2.50                     | 0.41              |
| 6:N:493:ARG:CG    | 6:N:1390:LEU:HB2  | 2.45                     | 0.41              |
| 6:N:782:SER:O     | 6:N:786:ILE:HG13  | 2.20                     | 0.41              |
| 6:N:899:LEU:HB3   | 6:N:917:GLN:HG2   | 2.01                     | 0.41              |
| 6:N:1124:GLN:HA   | 6:N:1125:PRO:HD3  | 1.60                     | 0.41              |
| 6:N:1155:VAL:HG12 | 11:N:9051:HOH:O   | 2.20                     | 0.41              |
| 2:H:2:A:C2'       | 2:H:3:G:O5'       | 2.68                     | 0.41              |
| 1:X:11:DC:H2''    | 1:X:12:DG:H8      | 1.85                     | 0.41              |
| 1:X:12:DG:H2'     | 1:X:13:DT:H72     | 2.02                     | 0.41              |
| 5:C:118:ILE:HG22  | 5:C:382:ILE:HD13  | 2.01                     | 0.41              |
| 5:C:137:VAL:CG2   | 5:C:391:LEU:HG    | 2.50                     | 0.41              |
| 5:C:603:VAL:HG11  | 5:C:606:VAL:HG22  | 2.03                     | 0.41              |
| 5:C:692:GLU:O     | 5:C:696:LYS:HG3   | 2.20                     | 0.41              |
| 5:C:715:THR:HA    | 11:C:1542:HOH:O   | 2.20                     | 0.41              |
| 5:C:791:ARG:O     | 5:C:793:PRO:HD3   | 2.20                     | 0.41              |
| 6:D:28:LYS:HD2    | 11:D:8201:HOH:O   | 2.20                     | 0.41              |
| 6:D:510:GLU:HG2   | 11:D:8320:HOH:O   | 2.20                     | 0.41              |
| 6:D:702:LEU:HD12  | 6:D:702:LEU:N     | 2.35                     | 0.41              |
| 6:D:906:GLN:HB3   | 6:D:911:LEU:CD1   | 2.49                     | 0.41              |
| 6:D:1046:GLN:HG2  | 6:D:1052:THR:CB   | 2.51                     | 0.41              |
| 6:D:1154:GLU:HB3  | 6:N:563:PRO:HB3   | 2.01                     | 0.41              |
| 6:D:1481:VAL:HG11 | 7:E:18:ARG:CA     | 2.42                     | 0.41              |
| 6:D:1481:VAL:HG22 | 7:E:18:ARG:NE     | 2.28                     | 0.41              |
| 7:E:41:GLU:CD     | 7:E:42:PRO:HD3    | 2.44                     | 0.41              |
| 7:E:43:GLU:H      | 7:E:43:GLU:HG3    | 1.69                     | 0.41              |
| 4:K:94:LEU:HD11   | 4:K:119:ASP:CB    | 2.51                     | 0.41              |
| 4:K:174:VAL:HG13  | 4:K:200:TRP:O     | 2.20                     | 0.41              |
| 5:M:25:SER:OG     | 5:M:335:THR:HB    | 2.20                     | 0.41              |
| 5:M:217:LEU:CD1   | 5:M:311:PHE:HA    | 2.50                     | 0.41              |
| 5:M:259:GLY:O     | 5:M:290:LEU:O     | 2.38                     | 0.41              |
| 5:M:292:ARG:HB2   | 5:M:299:LYS:HG2   | 2.02                     | 0.41              |
| 5:M:309:TYR:HA    | 5:M:312:ALA:HB3   | 2.02                     | 0.41              |
| 5:M:780:GLU:HG3   | 5:M:781:LYS:N     | 2.35                     | 0.41              |
| 5:M:928:LYS:O     | 5:M:932:GLU:HG3   | 2.21                     | 0.41              |
| 5:M:1003:ASP:CG   | 5:M:1004:LYS:N    | 2.78                     | 0.41              |
| 6:N:8:VAL:HG12    | 6:N:9:ARG:N       | 2.34                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:800:LYS:CE    | 6:N:804:LEU:HD13  | 2.50                     | 0.41              |
| 6:N:1330:ILE:HB   | 6:N:1347:TYR:OH   | 2.20                     | 0.41              |
| 2:H:7:G:H2'       | 2:H:8:C:OP1       | 2.20                     | 0.41              |
| 2:Y:16:G:O3'      | 6:N:741:ASP:OD1   | 2.39                     | 0.41              |
| 4:A:191:ASP:C     | 4:A:192:LEU:HG    | 2.45                     | 0.41              |
| 5:C:1:MET:HE2     | 5:C:900:ARG:NH2   | 2.34                     | 0.41              |
| 5:C:265:ARG:HB2   | 11:C:1165:HOH:O   | 2.21                     | 0.41              |
| 5:C:318:PRO:HB2   | 11:C:1545:HOH:O   | 2.20                     | 0.41              |
| 5:C:348:LEU:HD12  | 5:C:348:LEU:HA    | 1.90                     | 0.41              |
| 5:C:668:LEU:H     | 5:C:668:LEU:HD12  | 1.86                     | 0.41              |
| 5:C:673:LEU:CD2   | 5:C:867:VAL:HG12  | 2.50                     | 0.41              |
| 5:C:684:PHE:O     | 5:C:685:GLU:C     | 2.64                     | 0.41              |
| 5:C:754:ILE:HD12  | 5:C:789:SER:HB3   | 2.02                     | 0.41              |
| 5:C:764:GLU:HG3   | 6:D:54:LYS:HZ3    | 1.85                     | 0.41              |
| 5:C:1012:PRO:HB2  | 5:C:1021:LEU:O    | 2.20                     | 0.41              |
| 6:D:641:GLN:HB3   | 6:D:717:GLN:O     | 2.20                     | 0.41              |
| 6:D:838:ARG:HH11  | 6:D:838:ARG:HG2   | 1.86                     | 0.41              |
| 6:D:1153:VAL:HG12 | 6:D:1155:VAL:HG22 | 2.02                     | 0.41              |
| 6:D:1457:ASP:O    | 6:D:1459:LEU:HD12 | 2.21                     | 0.41              |
| 6:D:1485:GLN:H    | 6:D:1485:GLN:HG2  | 1.75                     | 0.41              |
| 6:D:1494:ALA:HB1  | 7:E:88:GLU:OE2    | 2.21                     | 0.41              |
| 5:M:23:VAL:HA     | 11:M:1414:HOH:O   | 2.21                     | 0.41              |
| 5:M:80:GLN:HE21   | 5:M:84:ARG:HH21   | 1.68                     | 0.41              |
| 5:M:395:LYS:HE2   | 5:M:403:SER:CB    | 2.36                     | 0.41              |
| 5:M:713:ARG:HB3   | 5:M:720:GLU:OE2   | 2.20                     | 0.41              |
| 5:M:983:ILE:O     | 5:M:983:ILE:HG22  | 2.20                     | 0.41              |
| 5:M:993:PHE:HE1   | 5:M:995:MET:HE2   | 1.85                     | 0.41              |
| 5:M:1008:ARG:HA   | 5:M:1027:PHE:CD2  | 2.54                     | 0.41              |
| 6:N:63:TYR:HB3    | 6:N:68:PHE:CD1    | 2.55                     | 0.41              |
| 6:N:90:MET:HE2    | 6:N:519:VAL:O     | 2.19                     | 0.41              |
| 6:N:716:PHE:O     | 6:N:718:PRO:HD3   | 2.21                     | 0.41              |
| 6:N:729:HIS:HE1   | 6:N:731:LEU:HG    | 1.85                     | 0.41              |
| 6:N:937:TYR:H     | 6:N:937:TYR:HD1   | 1.66                     | 0.41              |
| 6:N:956:ILE:HA    | 6:N:957:PRO:HD3   | 1.93                     | 0.41              |
| 6:N:1406:ARG:HE   | 6:N:1407:LEU:HD12 | 1.84                     | 0.41              |
| 7:O:9:LEU:HB3     | 7:O:19:LEU:CD2    | 2.50                     | 0.41              |
| 1:G:14:DT:H5''    | 11:D:8242:HOH:O   | 2.21                     | 0.41              |
| 4:B:52:ALA:HB2    | 4:B:170:VAL:C     | 2.45                     | 0.41              |
| 4:B:229:GLN:HE21  | 4:B:229:GLN:HB2   | 1.62                     | 0.41              |
| 5:C:358:ARG:CA    | 5:C:361:MET:HG2   | 2.51                     | 0.41              |
| 5:C:443:THR:HG21  | 6:D:1078:ARG:NH2  | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:491:GLU:CB    | 11:C:1287:HOH:O   | 2.68                     | 0.41              |
| 5:C:595:LEU:HD12  | 11:C:1444:HOH:O   | 2.21                     | 0.41              |
| 5:C:694:LEU:HD21  | 5:C:868:ASP:CB    | 2.47                     | 0.41              |
| 6:D:717:GLN:HG2   | 11:D:8027:HOH:O   | 2.21                     | 0.41              |
| 6:D:764:LEU:HD23  | 6:D:767:HIS:CD2   | 2.54                     | 0.41              |
| 6:D:1107:VAL:HG12 | 6:D:1217:ILE:HA   | 2.02                     | 0.41              |
| 6:D:1136:LYS:HB2  | 6:D:1139:ASP:CG   | 2.45                     | 0.41              |
| 6:D:1223:ILE:HD11 | 6:D:1462:LEU:HD12 | 2.03                     | 0.41              |
| 6:D:1393:GLN:NE2  | 6:D:1394:VAL:HB   | 2.36                     | 0.41              |
| 4:L:11:PHE:CE1    | 4:L:23:PHE:HB3    | 2.55                     | 0.41              |
| 5:M:73:LEU:O      | 5:M:73:LEU:HD12   | 2.21                     | 0.41              |
| 5:M:158:TYR:CZ    | 5:M:313:LEU:HG    | 2.55                     | 0.41              |
| 5:M:469:THR:OG1   | 5:M:470:PRO:HD2   | 2.21                     | 0.41              |
| 5:M:668:LEU:H     | 5:M:668:LEU:HD12  | 1.86                     | 0.41              |
| 5:M:738:ASP:HB2   | 5:M:744:ARG:HB3   | 2.02                     | 0.41              |
| 5:M:1092:LEU:HD23 | 5:M:1095:LEU:HD13 | 2.03                     | 0.41              |
| 6:N:701:LEU:O     | 6:N:747:VAL:HA    | 2.21                     | 0.41              |
| 6:N:709:HIS:HA    | 6:N:1227:GLN:HB3  | 2.01                     | 0.41              |
| 6:N:759:ALA:HA    | 6:N:763:MET:HE2   | 2.03                     | 0.41              |
| 6:N:916:TYR:O     | 6:N:919:PHE:HB3   | 2.19                     | 0.41              |
| 6:N:1110:ALA:O    | 6:N:1111:ASP:C    | 2.61                     | 0.41              |
| 6:N:1134:LEU:HB3  | 11:N:9479:HOH:O   | 2.20                     | 0.41              |
| 7:O:93:TYR:HA     | 7:O:94:PRO:HD2    | 1.87                     | 0.41              |
| 1:G:6:DT:H2''     | 1:G:7:DC:C5       | 2.55                     | 0.41              |
| 2:H:14:G:C2'      | 2:H:15:C:H5'      | 2.48                     | 0.41              |
| 1:X:15:DC:OP2     | 6:N:610:LYS:HE2   | 2.21                     | 0.41              |
| 4:A:178:ALA:HA    | 11:C:1156:HOH:O   | 2.20                     | 0.41              |
| 4:A:186:LEU:O     | 4:A:187:GLY:C     | 2.64                     | 0.41              |
| 5:C:242:LEU:HD11  | 11:C:1327:HOH:O   | 2.21                     | 0.41              |
| 5:C:599:GLU:OE2   | 5:C:619:ARG:NH2   | 2.54                     | 0.41              |
| 5:C:619:ARG:C     | 5:C:620:LEU:HD23  | 2.46                     | 0.41              |
| 5:C:639:GLN:HG2   | 11:C:1396:HOH:O   | 2.19                     | 0.41              |
| 5:C:1079:PRO:HB2  | 11:D:8463:HOH:O   | 2.19                     | 0.41              |
| 6:D:185:VAL:HG11  | 6:D:197:SER:OG    | 2.20                     | 0.41              |
| 6:D:446:VAL:O     | 6:D:447:VAL:O     | 2.39                     | 0.41              |
| 6:D:525:ARG:HA    | 6:D:526:PRO:HD3   | 1.73                     | 0.41              |
| 6:D:568:ARG:O     | 6:D:569:ASN:C     | 2.64                     | 0.41              |
| 6:D:833:GLU:CD    | 6:N:426:LYS:HE2   | 2.46                     | 0.41              |
| 6:D:1086:LEU:HA   | 11:D:8250:HOH:O   | 2.21                     | 0.41              |
| 6:D:1197:ARG:CB   | 6:D:1396:GLU:HG3  | 2.45                     | 0.41              |
| 7:E:76:GLY:N      | 7:E:79:LEU:HD22   | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:K:224:TYR:HB3   | 4:L:9:PRO:CG      | 2.51                     | 0.41              |
| 4:L:81:ASN:HD21   | 4:L:127:LEU:HD11  | 1.85                     | 0.41              |
| 5:M:393:GLN:NE2   | 5:M:406:HIS:HE1   | 2.18                     | 0.41              |
| 5:M:674:VAL:HG11  | 5:M:992:MET:HB3   | 2.02                     | 0.41              |
| 5:M:1021:LEU:HA   | 11:M:1512:HOH:O   | 2.21                     | 0.41              |
| 5:M:1096:ALA:O    | 6:N:13:ALA:CB     | 2.68                     | 0.41              |
| 6:N:28:LYS:CB     | 6:N:41:ARG:HD2    | 2.50                     | 0.41              |
| 6:N:407:VAL:HG12  | 6:N:409:VAL:H     | 1.85                     | 0.41              |
| 6:N:769:LEU:HD11  | 6:N:919:PHE:CE2   | 2.56                     | 0.41              |
| 6:N:832:ARG:HA    | 6:N:832:ARG:CZ    | 2.51                     | 0.41              |
| 6:N:879:ARG:HG3   | 6:N:879:ARG:HH11  | 1.84                     | 0.41              |
| 6:N:965:GLU:OE1   | 6:N:965:GLU:HA    | 2.20                     | 0.41              |
| 6:N:1007:VAL:HA   | 11:N:9288:HOH:O   | 2.21                     | 0.41              |
| 6:N:1117:TYR:CD2  | 6:N:1117:TYR:N    | 2.88                     | 0.41              |
| 6:N:1341:PRO:C    | 6:N:1343:ALA:N    | 2.77                     | 0.41              |
| 6:N:1401:GLU:CD   | 6:N:1415:VAL:HG11 | 2.46                     | 0.41              |
| 6:N:1406:ARG:HE   | 6:N:1407:LEU:CD1  | 2.33                     | 0.41              |
| 6:N:1425:THR:HG22 | 6:N:1429:LEU:HD12 | 2.01                     | 0.41              |
| 7:O:19:LEU:O      | 7:O:23:VAL:HG23   | 2.20                     | 0.41              |
| 3:Z:5:DG:H1'      | 3:Z:6:DC:H5'      | 2.01                     | 0.41              |
| 4:B:64:GLU:CA     | 4:B:165:ILE:HD13  | 2.48                     | 0.41              |
| 4:B:65:PHE:CD1    | 4:B:65:PHE:N      | 2.88                     | 0.41              |
| 5:C:61:LYS:O      | 5:C:359:MET:HE1   | 2.21                     | 0.41              |
| 5:C:140:ILE:HD13  | 5:C:331:ARG:CZ    | 2.51                     | 0.41              |
| 5:C:150:PRO:HA    | 5:C:158:TYR:HD2   | 1.86                     | 0.41              |
| 5:C:385:PHE:HA    | 5:C:389:SER:OG    | 2.21                     | 0.41              |
| 5:C:588:VAL:HA    | 5:C:591:SER:HG    | 1.86                     | 0.41              |
| 5:C:663:ASN:C     | 5:C:665:PHE:N     | 2.79                     | 0.41              |
| 5:C:676:ILE:HD13  | 5:C:676:ILE:O     | 2.21                     | 0.41              |
| 5:C:690:ILE:HG13  | 5:C:694:LEU:HD12  | 2.01                     | 0.41              |
| 5:C:838:LYS:C     | 5:C:839:LEU:HD23  | 2.45                     | 0.41              |
| 5:C:957:LYS:HG2   | 5:C:961:GLU:CB    | 2.51                     | 0.41              |
| 5:C:1046:ALA:HA   | 6:D:1472:ILE:CG1  | 2.44                     | 0.41              |
| 5:C:1067:TYR:HB3  | 11:C:1435:HOH:O   | 2.21                     | 0.41              |
| 5:C:1112:PHE:O    | 5:C:1113:GLU:C    | 2.64                     | 0.41              |
| 6:D:434:ARG:HB2   | 6:D:447:VAL:HG21  | 2.03                     | 0.41              |
| 6:D:470:LEU:HD23  | 6:D:470:LEU:N     | 2.36                     | 0.41              |
| 6:D:651:GLU:HA    | 6:D:654:LYS:HZ3   | 1.84                     | 0.41              |
| 6:D:703:ASN:ND2   | 6:D:704:ARG:N     | 2.67                     | 0.41              |
| 6:D:938:GLY:O     | 6:D:942:SER:HB3   | 2.21                     | 0.41              |
| 6:D:996:TRP:CE3   | 6:D:996:TRP:HA    | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:1063:GLU:HG3  | 6:D:1064:GLY:H    | 1.84                     | 0.41              |
| 6:D:1492:LEU:HD11 | 11:D:8102:HOH:O   | 2.21                     | 0.41              |
| 7:E:4:PRO:HG3     | 11:E:115:HOH:O    | 2.21                     | 0.41              |
| 7:E:89:MET:HE3    | 7:E:93:TYR:CD1    | 2.56                     | 0.41              |
| 4:K:3:ASP:CG      | 4:K:4:SER:N       | 2.79                     | 0.41              |
| 4:K:10:VAL:HG12   | 4:K:12:THR:HG22   | 2.02                     | 0.41              |
| 4:K:14:ARG:CZ     | 4:K:14:ARG:HB2    | 2.50                     | 0.41              |
| 4:K:159:LYS:NZ    | 4:K:164:ALA:O     | 2.50                     | 0.41              |
| 4:K:173:PRO:HB2   | 4:K:205:VAL:HG22  | 2.03                     | 0.41              |
| 4:L:209:GLU:HG2   | 11:L:361:HOH:O    | 2.21                     | 0.41              |
| 5:M:86:LYS:HZ3    | 5:M:812:GLY:H     | 1.69                     | 0.41              |
| 5:M:140:ILE:HG13  | 5:M:411:SER:O     | 2.20                     | 0.41              |
| 5:M:193:LEU:HD21  | 11:M:1471:HOH:O   | 2.21                     | 0.41              |
| 5:M:280:LYS:NZ    | 5:M:280:LYS:HB2   | 2.35                     | 0.41              |
| 5:M:471:TYR:CD2   | 5:M:533:ASP:HA    | 2.56                     | 0.41              |
| 5:M:495:THR:HG21  | 5:M:524:VAL:HG11  | 2.03                     | 0.41              |
| 5:M:704:HIS:HA    | 11:M:1346:HOH:O   | 2.21                     | 0.41              |
| 5:M:848:VAL:HG12  | 5:M:849:VAL:N     | 2.36                     | 0.41              |
| 5:M:878:SER:OG    | 6:N:1029:ARG:HD2  | 2.20                     | 0.41              |
| 6:N:89:ARG:O      | 6:N:521:PRO:HB3   | 2.20                     | 0.41              |
| 6:N:119:SER:HB2   | 6:N:123:LEU:N     | 2.31                     | 0.41              |
| 6:N:165:LYS:O     | 6:N:167:GLU:HG3   | 2.20                     | 0.41              |
| 6:N:708:LEU:HD22  | 6:N:1234:THR:OG1  | 2.21                     | 0.41              |
| 6:N:728:LEU:HD12  | 6:N:729:HIS:N     | 2.36                     | 0.41              |
| 6:N:749:VAL:HA    | 6:N:750:PRO:HD3   | 1.87                     | 0.41              |
| 6:N:791:TYR:CD2   | 6:N:945:SER:HB2   | 2.56                     | 0.41              |
| 6:N:796:ARG:O     | 6:N:828:LYS:HD2   | 2.21                     | 0.41              |
| 6:N:811:GLU:CD    | 6:N:811:GLU:C     | 2.89                     | 0.41              |
| 6:N:875:THR:HG22  | 6:N:879:ARG:HB2   | 2.03                     | 0.41              |
| 6:N:1114:THR:CG2  | 6:N:1114:THR:O    | 2.68                     | 0.41              |
| 6:N:1336:LEU:HD22 | 6:N:1421:LEU:HB2  | 2.03                     | 0.41              |
| 6:N:1336:LEU:CA   | 6:N:1344:VAL:HG21 | 2.50                     | 0.41              |
| 6:N:1472:ILE:HB   | 6:N:1474:ALA:O    | 2.21                     | 0.41              |
| 1:G:8:DT:H2''     | 1:G:9:DG:C8       | 2.55                     | 0.41              |
| 1:G:12:DG:H2'     | 1:G:13:DT:H72     | 2.02                     | 0.41              |
| 3:I:7:DC:OP2      | 6:D:1266:ARG:NE   | 2.54                     | 0.41              |
| 4:B:80:LEU:HA     | 4:B:83:LYS:HD2    | 2.03                     | 0.41              |
| 4:B:137:ARG:CZ    | 4:B:139:ASN:HB3   | 2.51                     | 0.41              |
| 5:C:160:ALA:HB2   | 5:C:310:LEU:HB2   | 2.02                     | 0.41              |
| 5:C:438:ILE:HA    | 5:C:455:LEU:HA    | 2.03                     | 0.41              |
| 5:C:468:ARG:NE    | 5:C:485:TYR:O     | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:606:VAL:HG11  | 5:C:643:VAL:O     | 2.21                     | 0.41              |
| 5:C:715:THR:C     | 5:C:717:LEU:H     | 2.28                     | 0.41              |
| 5:C:808:ARG:NH2   | 5:C:820:ARG:CZ    | 2.84                     | 0.41              |
| 5:C:876:VAL:H     | 5:C:877:PRO:CD    | 2.33                     | 0.41              |
| 5:C:911:GLU:OE1   | 6:D:951:ILE:HD12  | 2.21                     | 0.41              |
| 5:C:945:ARG:NE    | 11:C:1564:HOH:O   | 2.54                     | 0.41              |
| 5:C:1030:GLN:O    | 6:D:622:ARG:HA    | 2.21                     | 0.41              |
| 5:C:1095:LEU:O    | 5:C:1096:ALA:C    | 2.64                     | 0.41              |
| 6:D:456:MET:N     | 6:D:459:GLU:OE1   | 2.49                     | 0.41              |
| 6:D:1003:VAL:O    | 6:D:1006:ALA:HB3  | 2.21                     | 0.41              |
| 6:D:1117:TYR:HB2  | 6:D:1188:VAL:O    | 2.21                     | 0.41              |
| 6:D:1191:PRO:CB   | 6:D:1370:ILE:HD13 | 2.51                     | 0.41              |
| 6:D:1425:THR:HG22 | 6:D:1429:LEU:CD1  | 2.50                     | 0.41              |
| 6:D:1429:LEU:HD12 | 6:D:1440:PHE:HE1  | 1.85                     | 0.41              |
| 6:D:1435:LEU:HB2  | 6:D:1457:ASP:OD2  | 2.21                     | 0.41              |
| 4:L:26:GLU:HB3    | 4:L:194:LYS:HG3   | 2.03                     | 0.41              |
| 4:L:49:PRO:HG3    | 11:L:364:HOH:O    | 2.20                     | 0.41              |
| 5:M:102:HIS:CE1   | 5:M:365:ASP:HA    | 2.55                     | 0.41              |
| 5:M:674:VAL:CG2   | 5:M:871:LEU:HG    | 2.51                     | 0.41              |
| 5:M:874:LEU:H     | 5:M:874:LEU:CD1   | 2.34                     | 0.41              |
| 6:N:47:GLU:HG3    | 6:N:51:GLY:O      | 2.21                     | 0.41              |
| 6:N:180:LYS:CG    | 6:N:183:GLU:HB2   | 2.31                     | 0.41              |
| 6:N:668:PRO:HB3   | 11:N:9371:HOH:O   | 2.20                     | 0.41              |
| 6:N:773:ALA:HB2   | 11:N:9308:HOH:O   | 2.21                     | 0.41              |
| 6:N:1041:LEU:HD23 | 6:N:1041:LEU:O    | 2.21                     | 0.41              |
| 6:N:1147:ARG:HB3  | 6:N:1188:VAL:CG2  | 2.50                     | 0.41              |
| 6:N:1406:ARG:NE   | 6:N:1407:LEU:HD12 | 2.36                     | 0.41              |
| 6:N:1438:ALA:CA   | 6:N:1446:VAL:HG11 | 2.51                     | 0.41              |
| 1:G:11:DC:H2"     | 1:G:12:DG:H8      | 1.85                     | 0.40              |
| 4:A:223:THR:C     | 4:A:225:PHE:H     | 2.29                     | 0.40              |
| 4:B:48:ILE:HA     | 4:B:49:PRO:HD3    | 1.88                     | 0.40              |
| 4:B:66:SER:O      | 4:B:75:VAL:HG23   | 2.21                     | 0.40              |
| 4:B:80:LEU:HG     | 6:D:844:ALA:HA    | 2.02                     | 0.40              |
| 5:C:52:PHE:CE1    | 5:C:66:LEU:HG     | 2.56                     | 0.40              |
| 5:C:174:LEU:O     | 5:C:310:LEU:HD22  | 2.22                     | 0.40              |
| 5:C:250:ARG:HG2   | 5:C:253:ALA:CB    | 2.51                     | 0.40              |
| 5:C:436:GLY:O     | 5:C:459:ALA:CB    | 2.65                     | 0.40              |
| 5:C:1065:ALA:HB3  | 11:C:1284:HOH:O   | 2.20                     | 0.40              |
| 6:D:495:ARG:O     | 6:D:499:VAL:HG23  | 2.21                     | 0.40              |
| 6:D:645:PRO:CD    | 6:D:726:ILE:HG12  | 2.51                     | 0.40              |
| 6:D:972:LEU:HD13  | 6:D:972:LEU:HA    | 1.94                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:1403:LEU:HD22 | 11:D:8028:HOH:O   | 2.21                     | 0.40              |
| 4:K:44:LEU:HD13   | 4:K:177:VAL:CG1   | 2.51                     | 0.40              |
| 4:L:172:SER:HA    | 4:L:173:PRO:HD3   | 1.88                     | 0.40              |
| 5:M:43:GLY:O      | 5:M:44:ILE:C      | 2.63                     | 0.40              |
| 5:M:256:TYR:HE1   | 11:M:1452:HOH:O   | 2.04                     | 0.40              |
| 5:M:494:TYR:HB3   | 5:M:530:GLU:OE2   | 2.21                     | 0.40              |
| 5:M:572:ILE:HD11  | 5:M:701:THR:CB    | 2.51                     | 0.40              |
| 5:M:685:GLU:HG3   | 5:M:686:ASP:N     | 2.36                     | 0.40              |
| 5:M:776:SER:HA    | 5:M:780:GLU:HB3   | 2.02                     | 0.40              |
| 5:M:1112:PHE:O    | 5:M:1113:GLU:C    | 2.64                     | 0.40              |
| 6:N:50:PHE:HB3    | 6:N:522:PRO:CG    | 2.51                     | 0.40              |
| 6:N:127:LEU:HA    | 6:N:132:TYR:HD1   | 1.86                     | 0.40              |
| 6:N:137:PRO:HD2   | 6:N:453:ASP:CB    | 2.50                     | 0.40              |
| 6:N:434:ARG:HH22  | 6:N:447:VAL:HG11  | 1.86                     | 0.40              |
| 6:N:792:ILE:HG22  | 6:N:792:ILE:H     | 1.63                     | 0.40              |
| 6:N:957:PRO:HG3   | 11:N:9288:HOH:O   | 2.20                     | 0.40              |
| 6:N:1213:ARG:HD2  | 6:N:1214:PRO:N    | 2.35                     | 0.40              |
| 1:G:20:DG:H3'     | 11:G:38:HOH:O     | 2.20                     | 0.40              |
| 3:Z:3:DA:H1'      | 11:Z:824:HOH:O    | 2.20                     | 0.40              |
| 4:A:107:LYS:HE2   | 4:A:113:ASP:OD2   | 2.21                     | 0.40              |
| 4:A:182:GLU:OE2   | 4:A:182:GLU:N     | 2.54                     | 0.40              |
| 5:C:5:ARG:HB3     | 5:C:902:ILE:HD12  | 2.02                     | 0.40              |
| 5:C:80:GLN:HG2    | 5:C:90:TYR:CE2    | 2.56                     | 0.40              |
| 5:C:80:GLN:HE21   | 5:C:80:GLN:HB3    | 1.63                     | 0.40              |
| 5:C:150:PRO:HA    | 5:C:158:TYR:CD2   | 2.56                     | 0.40              |
| 5:C:164:PRO:HD2   | 5:C:170:PRO:O     | 2.20                     | 0.40              |
| 5:C:260:LEU:CB    | 5:C:291:ALA:HB1   | 2.37                     | 0.40              |
| 5:C:327:HIS:CD2   | 5:C:431:HIS:NE2   | 2.88                     | 0.40              |
| 5:C:410:ILE:HD12  | 5:C:438:ILE:HG12  | 2.00                     | 0.40              |
| 5:C:474:VAL:HG23  | 5:C:478:VAL:O     | 2.21                     | 0.40              |
| 5:C:605:LYS:O     | 5:C:611:ILE:HA    | 2.21                     | 0.40              |
| 5:C:874:LEU:HD12  | 5:C:874:LEU:N     | 2.30                     | 0.40              |
| 5:C:958:THR:CG2   | 5:C:961:GLU:HB2   | 2.46                     | 0.40              |
| 5:C:1008:ARG:NH1  | 5:C:1010:THR:HA   | 2.37                     | 0.40              |
| 5:C:1053:LEU:CD1  | 6:D:1466:VAL:HG22 | 2.51                     | 0.40              |
| 5:C:1078:GLU:HA   | 5:C:1079:PRO:HD3  | 1.93                     | 0.40              |
| 5:C:1090:LYS:HE2  | 5:C:1112:PHE:CE1  | 2.56                     | 0.40              |
| 5:C:1095:LEU:HD23 | 5:C:1095:LEU:HA   | 1.93                     | 0.40              |
| 6:D:141:ILE:CD1   | 6:D:450:TYR:HB3   | 2.48                     | 0.40              |
| 6:D:398:ALA:HB2   | 6:D:446:VAL:C     | 2.45                     | 0.40              |
| 6:D:629:SER:C     | 6:D:744:GLN:HG2   | 2.46                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:D:767:HIS:O    | 6:D:924:MET:HE2  | 2.21                     | 0.40              |
| 6:D:965:GLU:HA   | 6:D:968:ASP:HB3  | 2.02                     | 0.40              |
| 6:D:999:THR:O    | 6:D:1002:LYS:HB2 | 2.21                     | 0.40              |
| 6:D:1093:TYR:CE1 | 6:D:1097:LYS:HE2 | 2.57                     | 0.40              |
| 6:D:1184:GLN:HB2 | 6:N:559:ALA:HB1  | 2.02                     | 0.40              |
| 4:K:101:LEU:HD12 | 4:K:114:PHE:N    | 2.36                     | 0.40              |
| 4:K:159:LYS:HD3  | 4:K:159:LYS:HA   | 1.90                     | 0.40              |
| 4:K:219:ARG:HG2  | 4:L:222:LEU:HD12 | 2.03                     | 0.40              |
| 11:K:1711:HOH:O  | 4:L:222:LEU:HD11 | 2.21                     | 0.40              |
| 4:L:70:GLY:O     | 4:L:132:LEU:HA   | 2.21                     | 0.40              |
| 4:L:90:LEU:HD12  | 4:L:90:LEU:O     | 2.21                     | 0.40              |
| 4:L:137:ARG:CZ   | 4:L:139:ASN:HB3  | 2.52                     | 0.40              |
| 4:L:185:ARG:NH1  | 11:L:381:HOH:O   | 2.55                     | 0.40              |
| 5:M:80:GLN:HG2   | 5:M:90:TYR:CZ    | 2.56                     | 0.40              |
| 5:M:395:LYS:O    | 5:M:633:GLN:NE2  | 2.54                     | 0.40              |
| 6:N:493:ARG:NE   | 6:N:1390:LEU:O   | 2.54                     | 0.40              |
| 6:N:628:ARG:C    | 6:N:648:MET:HE1  | 2.46                     | 0.40              |
| 6:N:646:LYS:HG3  | 6:N:721:VAL:O    | 2.20                     | 0.40              |
| 6:N:701:LEU:HD13 | 6:N:748:HIS:HB2  | 2.03                     | 0.40              |
| 6:N:738:ALA:CB   | 6:N:745:MET:HE3  | 2.52                     | 0.40              |
| 6:N:955:VAL:HG11 | 6:N:1015:TYR:OH  | 2.21                     | 0.40              |
| 6:N:996:TRP:CZ2  | 6:N:1056:PRO:HG2 | 2.57                     | 0.40              |
| 6:N:1105:ILE:HA  | 11:N:9367:HOH:O  | 2.21                     | 0.40              |
| 6:N:1271:LYS:HZ3 | 6:N:1271:LYS:HB2 | 1.86                     | 0.40              |
| 6:N:1365:ASP:OD2 | 6:N:1365:ASP:N   | 2.53                     | 0.40              |
| 1:X:12:DG:C8     | 1:X:13:DT:H72    | 2.56                     | 0.40              |
| 2:Y:12:G:C8      | 2:Y:12:G:C5'     | 2.96                     | 0.40              |
| 4:A:156:HIS:HD2  | 4:A:157:GLY:N    | 2.20                     | 0.40              |
| 4:A:175:ARG:HH21 | 4:A:176:ARG:HE   | 1.68                     | 0.40              |
| 5:C:97:ARG:HB3   | 5:C:109:LYS:CE   | 2.51                     | 0.40              |
| 5:C:408:ARG:NE   | 5:C:542:VAL:HG23 | 2.37                     | 0.40              |
| 5:C:676:ILE:HG22 | 5:C:988:VAL:O    | 2.21                     | 0.40              |
| 5:C:697:ARG:O    | 5:C:697:ARG:HG3  | 2.21                     | 0.40              |
| 5:C:710:ILE:HB   | 5:C:790:LEU:CD2  | 2.43                     | 0.40              |
| 5:C:909:ALA:CB   | 5:C:914:ILE:HD11 | 2.45                     | 0.40              |
| 6:D:82:LYS:C     | 6:D:84:ILE:H     | 2.28                     | 0.40              |
| 6:D:131:LYS:C    | 6:D:456:MET:HB3  | 2.47                     | 0.40              |
| 6:D:400:VAL:O    | 6:D:402:PRO:HD3  | 2.20                     | 0.40              |
| 6:D:421:LEU:HD21 | 6:D:429:SER:OG   | 2.21                     | 0.40              |
| 6:D:456:MET:HG3  | 11:D:8208:HOH:O  | 2.21                     | 0.40              |
| 6:D:681:ARG:HE   | 6:D:681:ARG:HB2  | 1.66                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:D:1046:GLN:HG2 | 6:D:1052:THR:HA   | 2.03                     | 0.40              |
| 6:D:1071:PHE:HB3 | 11:D:8010:HOH:O   | 2.22                     | 0.40              |
| 6:D:1117:TYR:CD1 | 6:D:1187:PRO:HA   | 2.57                     | 0.40              |
| 4:K:42:ARG:NH2   | 4:L:31:GLY:O      | 2.40                     | 0.40              |
| 4:K:223:THR:C    | 4:K:225:PHE:H     | 2.29                     | 0.40              |
| 5:M:80:GLN:HG2   | 5:M:90:TYR:CE1    | 2.57                     | 0.40              |
| 5:M:141:HIS:CA   | 5:M:331:ARG:HG3   | 2.52                     | 0.40              |
| 5:M:217:LEU:HD11 | 5:M:314:THR:OG1   | 2.21                     | 0.40              |
| 5:M:437:ARG:HB3  | 5:M:467:ILE:HB    | 2.03                     | 0.40              |
| 5:M:610:ARG:HD2  | 5:M:622:GLU:HG3   | 2.04                     | 0.40              |
| 5:M:626:ARG:NH1  | 5:M:629:TYR:HB2   | 2.37                     | 0.40              |
| 5:M:720:GLU:OE1  | 5:M:758:ARG:HD2   | 2.21                     | 0.40              |
| 5:M:909:ALA:HB1  | 5:M:914:ILE:CD1   | 2.48                     | 0.40              |
| 6:N:12:LEU:HD21  | 6:N:104:PHE:CZ    | 2.57                     | 0.40              |
| 6:N:168:THR:HG21 | 6:N:206:ARG:HH12  | 1.86                     | 0.40              |
| 6:N:415:VAL:HG12 | 6:N:416:ALA:N     | 2.37                     | 0.40              |
| 6:N:481:MET:HE2  | 6:N:492:ALA:C     | 2.46                     | 0.40              |
| 6:N:525:ARG:HB2  | 6:N:538:SER:HB2   | 2.03                     | 0.40              |
| 6:N:563:PRO:O    | 6:N:564:GLU:C     | 2.64                     | 0.40              |
| 6:N:1087:ARG:CB  | 6:N:1256:LEU:HD22 | 2.49                     | 0.40              |
| 1:G:14:DT:C2'    | 1:G:15:DC:H5'     | 2.49                     | 0.40              |
| 2:H:16:G:H5'     | 6:D:742:GLY:HA3   | 2.04                     | 0.40              |
| 4:B:43:ILE:HG23  | 4:B:47:SER:HB3    | 2.02                     | 0.40              |
| 4:B:43:ILE:HG23  | 4:B:47:SER:OG     | 2.20                     | 0.40              |
| 4:B:67:THR:HB    | 4:B:74:ASP:OD1    | 2.21                     | 0.40              |
| 5:C:431:HIS:CD2  | 5:C:433:THR:OG1   | 2.74                     | 0.40              |
| 5:C:739:GLU:H    | 5:C:739:GLU:HG2   | 1.62                     | 0.40              |
| 5:C:773:LEU:O    | 5:C:777:ILE:HG13  | 2.20                     | 0.40              |
| 5:C:782:ALA:O    | 5:C:784:ASP:N     | 2.54                     | 0.40              |
| 6:D:700:VAL:HG13 | 6:D:718:PRO:HG2   | 2.03                     | 0.40              |
| 6:D:789:LEU:O    | 6:D:793:THR:HG23  | 2.21                     | 0.40              |
| 6:D:817:GLU:O    | 6:D:821:VAL:HG23  | 2.21                     | 0.40              |
| 6:D:1221:VAL:O   | 6:D:1224:VAL:N    | 2.54                     | 0.40              |
| 6:D:1453:ALA:O   | 6:D:1454:GLY:C    | 2.64                     | 0.40              |
| 6:D:1481:VAL:CG2 | 7:E:18:ARG:HE     | 2.30                     | 0.40              |
| 4:K:35:THR:HG23  | 4:L:39:PRO:HA     | 2.03                     | 0.40              |
| 4:K:67:THR:HG22  | 5:M:627:ARG:HH21  | 1.87                     | 0.40              |
| 4:K:88:ARG:NH1   | 4:K:88:ARG:HG2    | 2.37                     | 0.40              |
| 4:L:58:ILE:HG22  | 4:L:61:VAL:HB     | 2.03                     | 0.40              |
| 5:M:139:GLN:OE1  | 5:M:415:PRO:HD3   | 2.22                     | 0.40              |
| 5:M:267:TYR:O    | 5:M:268:ASP:C     | 2.63                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:684:PHE:CG    | 5:M:685:GLU:N     | 2.90                     | 0.40              |
| 5:M:926:PHE:CD2   | 5:M:930:LYS:HE3   | 2.55                     | 0.40              |
| 5:M:1034:GLU:H    | 6:N:619:LEU:HB3   | 1.79                     | 0.40              |
| 5:M:1091:GLU:HA   | 6:N:520:LEU:HD13  | 2.03                     | 0.40              |
| 6:N:44:LEU:H      | 6:N:44:LEU:CD1    | 2.34                     | 0.40              |
| 6:N:135:LEU:HD22  | 6:N:147:VAL:HG23  | 2.02                     | 0.40              |
| 6:N:501:ALA:HB1   | 6:N:1453:ALA:CB   | 2.40                     | 0.40              |
| 6:N:691:LEU:HG    | 6:N:720:LEU:HD21  | 2.02                     | 0.40              |
| 6:N:1108:ARG:NH1  | 11:N:9097:HOH:O   | 2.54                     | 0.40              |
| 3:I:8:DA:H2"      | 3:I:9:DG:OP2      | 2.22                     | 0.40              |
| 4:A:82:LEU:CD2    | 4:A:142:VAL:HG11  | 2.43                     | 0.40              |
| 4:A:206:THR:CG2   | 4:A:209:GLU:H     | 2.32                     | 0.40              |
| 4:B:165:ILE:HA    | 4:B:166:PRO:HD3   | 1.95                     | 0.40              |
| 5:C:7:GLY:O       | 5:C:8:ARG:HD2     | 2.21                     | 0.40              |
| 5:C:144:PRO:CG    | 5:C:265:ARG:NH2   | 2.80                     | 0.40              |
| 5:C:160:ALA:HB1   | 5:C:306:THR:OG1   | 2.21                     | 0.40              |
| 5:C:182:VAL:HG12  | 5:C:193:LEU:HD11  | 2.02                     | 0.40              |
| 5:C:300:ASP:OD2   | 5:C:303:PHE:HB3   | 2.22                     | 0.40              |
| 5:C:520:GLU:HA    | 5:C:521:PRO:HD3   | 1.96                     | 0.40              |
| 5:C:626:ARG:HG2   | 11:C:1192:HOH:O   | 2.21                     | 0.40              |
| 5:C:636:ALA:CB    | 5:C:703:ILE:HD13  | 2.34                     | 0.40              |
| 5:C:743:VAL:HG13  | 5:C:800:VAL:HG11  | 2.02                     | 0.40              |
| 5:C:1006:HIS:O    | 6:D:627:GLY:HA2   | 2.21                     | 0.40              |
| 5:C:1019:GLN:HE22 | 5:C:1058:ASP:HB2  | 1.86                     | 0.40              |
| 6:D:51:GLY:HA3    | 6:D:86:ARG:HA     | 2.04                     | 0.40              |
| 6:D:630:VAL:HA    | 6:D:744:GLN:HG3   | 2.03                     | 0.40              |
| 6:D:1037:GLN:CG   | 6:D:1042:ARG:HB3  | 2.47                     | 0.40              |
| 6:D:1083:ASP:OD2  | 6:D:1241:PHE:HB3  | 2.21                     | 0.40              |
| 6:D:1269:LYS:HB3  | 6:D:1269:LYS:HZ2  | 1.85                     | 0.40              |
| 6:D:1441:GLN:CD   | 6:D:1442:ASN:N    | 2.80                     | 0.40              |
| 4:K:18:ARG:O      | 4:K:207:PRO:HD3   | 2.22                     | 0.40              |
| 4:K:170:VAL:HG13  | 11:M:1536:HOH:O   | 2.20                     | 0.40              |
| 4:L:133:GLU:HB3   | 4:L:134:GLU:H     | 1.62                     | 0.40              |
| 5:M:194:VAL:HG11  | 5:M:221:LEU:C     | 2.46                     | 0.40              |
| 5:M:324:ASP:HA    | 11:M:1465:HOH:O   | 2.22                     | 0.40              |
| 5:M:663:ASN:C     | 5:M:665:PHE:N     | 2.79                     | 0.40              |
| 5:M:1094:ALA:HA   | 6:N:90:MET:HE1    | 2.03                     | 0.40              |
| 6:N:34:TYR:O      | 6:N:35:ARG:C      | 2.65                     | 0.40              |
| 6:N:112:ILE:O     | 6:N:112:ILE:HD12  | 2.22                     | 0.40              |
| 6:N:637:LEU:HD21  | 6:N:641:GLN:O     | 2.22                     | 0.40              |
| 6:N:1044:LEU:HD13 | 6:N:1052:THR:HG21 | 2.04                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 6:N:1047:LYS:HB3 | 6:N:1048:PRO:CD | 2.51                     | 0.40              |
| 6:N:1147:ARG:O   | 6:N:1165:TYR:HA | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|------------------|------------|-----------|----------|-------------|----|
| 4   | A     | 227/315 (72%)    | 206 (91%)  | 14 (6%)   | 7 (3%)   | 3           | 19 |
| 4   | B     | 227/315 (72%)    | 206 (91%)  | 15 (7%)   | 6 (3%)   | 4           | 23 |
| 4   | K     | 227/315 (72%)    | 208 (92%)  | 13 (6%)   | 6 (3%)   | 4           | 23 |
| 4   | L     | 227/315 (72%)    | 206 (91%)  | 15 (7%)   | 6 (3%)   | 4           | 23 |
| 5   | C     | 1117/1119 (100%) | 919 (82%)  | 136 (12%) | 62 (6%)  | 1           | 8  |
| 5   | M     | 1117/1119 (100%) | 923 (83%)  | 133 (12%) | 61 (6%)  | 1           | 8  |
| 6   | D     | 1258/1524 (82%)  | 1051 (84%) | 149 (12%) | 58 (5%)  | 2           | 11 |
| 6   | N     | 1258/1524 (82%)  | 1058 (84%) | 140 (11%) | 60 (5%)  | 2           | 11 |
| 7   | E     | 93/99 (94%)      | 76 (82%)   | 11 (12%)  | 6 (6%)   | 1           | 5  |
| 7   | O     | 93/99 (94%)      | 74 (80%)   | 12 (13%)  | 7 (8%)   | 1           | 4  |
| All | All   | 5844/6744 (87%)  | 4927 (84%) | 638 (11%) | 279 (5%) | 2           | 11 |

All (279) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | A     | 29  | GLU  |
| 4   | A     | 187 | GLY  |
| 4   | B     | 29  | GLU  |
| 4   | B     | 187 | GLY  |
| 5   | C     | 178 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | C     | 231  | PRO  |
| 5   | C     | 244  | PRO  |
| 5   | C     | 288  | ARG  |
| 5   | C     | 290  | LEU  |
| 5   | C     | 369  | PRO  |
| 5   | C     | 462  | ASP  |
| 5   | C     | 465  | GLY  |
| 5   | C     | 548  | PRO  |
| 5   | C     | 627  | ARG  |
| 5   | C     | 680  | ASP  |
| 5   | C     | 727  | PRO  |
| 5   | C     | 908  | GLY  |
| 5   | C     | 1033 | GLY  |
| 5   | C     | 1106 | ASP  |
| 6   | D     | 40   | GLU  |
| 6   | D     | 43   | GLY  |
| 6   | D     | 55   | ASP  |
| 6   | D     | 137  | PRO  |
| 6   | D     | 447  | VAL  |
| 6   | D     | 705  | ALA  |
| 6   | D     | 742  | GLY  |
| 6   | D     | 832  | ARG  |
| 6   | D     | 844  | ALA  |
| 6   | D     | 1028 | ALA  |
| 6   | D     | 1129 | THR  |
| 6   | D     | 1389 | LEU  |
| 6   | D     | 1441 | GLN  |
| 7   | E     | 42   | PRO  |
| 4   | K     | 29   | GLU  |
| 4   | K     | 187  | GLY  |
| 4   | L     | 29   | GLU  |
| 4   | L     | 187  | GLY  |
| 5   | M     | 170  | PRO  |
| 5   | M     | 178  | PRO  |
| 5   | M     | 191  | PHE  |
| 5   | M     | 231  | PRO  |
| 5   | M     | 244  | PRO  |
| 5   | M     | 288  | ARG  |
| 5   | M     | 290  | LEU  |
| 5   | M     | 369  | PRO  |
| 5   | M     | 462  | ASP  |
| 5   | M     | 465  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | M     | 548  | PRO  |
| 5   | M     | 680  | ASP  |
| 5   | M     | 727  | PRO  |
| 5   | M     | 908  | GLY  |
| 5   | M     | 1033 | GLY  |
| 5   | M     | 1106 | ASP  |
| 6   | N     | 40   | GLU  |
| 6   | N     | 43   | GLY  |
| 6   | N     | 55   | ASP  |
| 6   | N     | 137  | PRO  |
| 6   | N     | 447  | VAL  |
| 6   | N     | 705  | ALA  |
| 6   | N     | 742  | GLY  |
| 6   | N     | 832  | ARG  |
| 6   | N     | 844  | ALA  |
| 6   | N     | 1028 | ALA  |
| 6   | N     | 1129 | THR  |
| 6   | N     | 1389 | LEU  |
| 6   | N     | 1441 | GLN  |
| 7   | O     | 42   | PRO  |
| 5   | C     | 40   | GLU  |
| 5   | C     | 44   | ILE  |
| 5   | C     | 59   | LYS  |
| 5   | C     | 152  | PRO  |
| 5   | C     | 156  | GLY  |
| 5   | C     | 170  | PRO  |
| 5   | C     | 191  | PHE  |
| 5   | C     | 251  | ASP  |
| 5   | C     | 363  | SER  |
| 5   | C     | 418  | LEU  |
| 5   | C     | 457  | ALA  |
| 5   | C     | 529  | VAL  |
| 5   | C     | 626  | ARG  |
| 5   | C     | 698  | ASP  |
| 5   | C     | 783  | ARG  |
| 5   | C     | 784  | ASP  |
| 5   | C     | 864  | GLY  |
| 5   | C     | 1059 | ASP  |
| 6   | D     | 34   | TYR  |
| 6   | D     | 120  | ALA  |
| 6   | D     | 164  | GLY  |
| 6   | D     | 620  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | D     | 740  | PHE  |
| 6   | D     | 803  | GLY  |
| 6   | D     | 1208 | ASP  |
| 6   | D     | 1342 | GLU  |
| 6   | D     | 1385 | GLY  |
| 6   | D     | 1452 | ILE  |
| 6   | D     | 1454 | GLY  |
| 7   | E     | 53   | GLY  |
| 7   | E     | 58   | PRO  |
| 5   | M     | 40   | GLU  |
| 5   | M     | 44   | ILE  |
| 5   | M     | 59   | LYS  |
| 5   | M     | 152  | PRO  |
| 5   | M     | 156  | GLY  |
| 5   | M     | 223  | ASP  |
| 5   | M     | 251  | ASP  |
| 5   | M     | 363  | SER  |
| 5   | M     | 418  | LEU  |
| 5   | M     | 529  | VAL  |
| 5   | M     | 626  | ARG  |
| 5   | M     | 627  | ARG  |
| 5   | M     | 698  | ASP  |
| 5   | M     | 905  | ILE  |
| 5   | M     | 1005 | MET  |
| 5   | M     | 1059 | ASP  |
| 6   | N     | 120  | ALA  |
| 6   | N     | 164  | GLY  |
| 6   | N     | 594  | PRO  |
| 6   | N     | 620  | GLY  |
| 6   | N     | 740  | PHE  |
| 6   | N     | 803  | GLY  |
| 6   | N     | 1125 | PRO  |
| 6   | N     | 1208 | ASP  |
| 6   | N     | 1221 | VAL  |
| 6   | N     | 1385 | GLY  |
| 6   | N     | 1424 | VAL  |
| 6   | N     | 1452 | ILE  |
| 6   | N     | 1454 | GLY  |
| 7   | O     | 53   | GLY  |
| 7   | O     | 58   | PRO  |
| 4   | A     | 3    | ASP  |
| 5   | C     | 74   | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | C     | 164  | PRO  |
| 5   | C     | 188  | LYS  |
| 5   | C     | 223  | ASP  |
| 5   | C     | 262  | ALA  |
| 5   | C     | 268  | ASP  |
| 5   | C     | 325  | ILE  |
| 5   | C     | 424  | GLY  |
| 5   | C     | 517  | ARG  |
| 5   | C     | 740  | GLU  |
| 5   | C     | 808  | ARG  |
| 6   | D     | 37   | LEU  |
| 6   | D     | 96   | ALA  |
| 6   | D     | 110  | SER  |
| 6   | D     | 395  | VAL  |
| 6   | D     | 507  | ASN  |
| 6   | D     | 594  | PRO  |
| 6   | D     | 696  | HIS  |
| 6   | D     | 822  | ALA  |
| 6   | D     | 924  | MET  |
| 6   | D     | 1125 | PRO  |
| 6   | D     | 1196 | THR  |
| 6   | D     | 1341 | PRO  |
| 7   | E     | 43   | GLU  |
| 4   | L     | 191  | ASP  |
| 5   | M     | 74   | GLY  |
| 5   | M     | 164  | PRO  |
| 5   | M     | 188  | LYS  |
| 5   | M     | 268  | ASP  |
| 5   | M     | 424  | GLY  |
| 5   | M     | 457  | ALA  |
| 5   | M     | 517  | ARG  |
| 5   | M     | 808  | ARG  |
| 5   | M     | 864  | GLY  |
| 5   | M     | 984  | GLU  |
| 6   | N     | 37   | LEU  |
| 6   | N     | 96   | ALA  |
| 6   | N     | 395  | VAL  |
| 6   | N     | 397  | LYS  |
| 6   | N     | 507  | ASN  |
| 6   | N     | 539  | ASP  |
| 6   | N     | 807  | ALA  |
| 6   | N     | 830  | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | N     | 924  | MET  |
| 6   | N     | 1196 | THR  |
| 6   | N     | 1269 | LYS  |
| 7   | O     | 43   | GLU  |
| 5   | C     | 80   | GLN  |
| 5   | C     | 180  | GLY  |
| 5   | C     | 282  | GLY  |
| 5   | C     | 984  | GLU  |
| 5   | C     | 1004 | LYS  |
| 5   | C     | 1024 | LYS  |
| 5   | C     | 1045 | ALA  |
| 6   | D     | 808  | THR  |
| 6   | D     | 830  | ALA  |
| 6   | D     | 1221 | VAL  |
| 6   | D     | 1244 | GLY  |
| 6   | D     | 1269 | LYS  |
| 6   | D     | 1390 | LEU  |
| 4   | K     | 3    | ASP  |
| 5   | M     | 180  | GLY  |
| 5   | M     | 262  | ALA  |
| 5   | M     | 767  | PRO  |
| 5   | M     | 1024 | LYS  |
| 6   | N     | 34   | TYR  |
| 6   | N     | 110  | SER  |
| 6   | N     | 735  | ALA  |
| 6   | N     | 808  | THR  |
| 6   | N     | 822  | ALA  |
| 6   | N     | 1244 | GLY  |
| 7   | O     | 32   | ARG  |
| 7   | O     | 82   | GLU  |
| 5   | C     | 767  | PRO  |
| 5   | C     | 877  | PRO  |
| 6   | D     | 31   | THR  |
| 6   | D     | 807  | ALA  |
| 7   | E     | 82   | GLU  |
| 5   | M     | 80   | GLN  |
| 5   | M     | 264  | PRO  |
| 5   | M     | 877  | PRO  |
| 5   | M     | 1004 | LYS  |
| 5   | M     | 1045 | ALA  |
| 6   | N     | 181  | ASP  |
| 6   | N     | 601  | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | N     | 1390 | LEU  |
| 4   | A     | 118  | ALA  |
| 4   | B     | 48   | ILE  |
| 4   | B     | 191  | ASP  |
| 5   | C     | 11   | GLU  |
| 5   | C     | 264  | PRO  |
| 5   | C     | 905  | ILE  |
| 5   | C     | 1114 | GLY  |
| 6   | D     | 406  | ASP  |
| 6   | D     | 483  | HIS  |
| 6   | D     | 525  | ARG  |
| 6   | D     | 530  | VAL  |
| 6   | D     | 601  | ARG  |
| 4   | L     | 48   | ILE  |
| 5   | M     | 740  | GLU  |
| 5   | M     | 781  | LYS  |
| 6   | N     | 24   | GLY  |
| 6   | N     | 483  | HIS  |
| 6   | N     | 696  | HIS  |
| 6   | N     | 1222 | GLY  |
| 6   | N     | 1341 | PRO  |
| 5   | C     | 646  | GLY  |
| 5   | C     | 779  | GLY  |
| 7   | E     | 5    | GLY  |
| 4   | L     | 157  | GLY  |
| 5   | M     | 144  | PRO  |
| 5   | M     | 646  | GLY  |
| 5   | M     | 779  | GLY  |
| 5   | M     | 1114 | GLY  |
| 6   | N     | 136  | ASP  |
| 6   | N     | 526  | PRO  |
| 6   | N     | 1214 | PRO  |
| 4   | A     | 157  | GLY  |
| 4   | B     | 157  | GLY  |
| 5   | C     | 1079 | PRO  |
| 6   | D     | 565  | ILE  |
| 6   | D     | 1214 | PRO  |
| 4   | K     | 9    | PRO  |
| 5   | M     | 53   | PRO  |
| 4   | A     | 9    | PRO  |
| 5   | C     | 53   | PRO  |
| 6   | D     | 134  | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | D     | 136  | ASP  |
| 6   | D     | 1050 | GLY  |
| 4   | K     | 125  | PRO  |
| 4   | K     | 157  | GLY  |
| 4   | L     | 125  | PRO  |
| 5   | M     | 282  | GLY  |
| 5   | M     | 876  | VAL  |
| 6   | N     | 146  | PRO  |
| 6   | N     | 530  | VAL  |
| 4   | A     | 125  | PRO  |
| 4   | B     | 125  | PRO  |
| 6   | D     | 484  | PRO  |
| 6   | D     | 595  | GLY  |
| 5   | M     | 336  | VAL  |
| 6   | N     | 484  | PRO  |
| 6   | N     | 595  | GLY  |
| 6   | N     | 1050 | GLY  |
| 5   | C     | 876  | VAL  |
| 6   | D     | 98   | PRO  |
| 6   | D     | 1222 | GLY  |
| 6   | N     | 565  | ILE  |
| 7   | O     | 5    | GLY  |

### 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 |   |
|-----|-------|-----------------|-----------|-----------|-------------|---|
| 4   | A     | 202/273 (74%)   | 159 (79%) | 43 (21%)  | 1           | 6 |
| 4   | B     | 202/273 (74%)   | 158 (78%) | 44 (22%)  | 1           | 6 |
| 4   | K     | 202/273 (74%)   | 155 (77%) | 47 (23%)  | 1           | 4 |
| 4   | L     | 202/273 (74%)   | 152 (75%) | 50 (25%)  | 1           | 3 |
| 5   | C     | 941/941 (100%)  | 690 (73%) | 251 (27%) | 0           | 3 |
| 5   | M     | 941/941 (100%)  | 690 (73%) | 251 (27%) | 0           | 3 |
| 6   | D     | 1063/1279 (83%) | 813 (76%) | 250 (24%) | 1           | 4 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|-----------------|------------|------------|-------------|----|
| 6   | N     | 1063/1279 (83%) | 820 (77%)  | 243 (23%)  | 1           | 5  |
| 7   | E     | 84/88 (96%)     | 57 (68%)   | 27 (32%)   | 0           | 1  |
| 7   | O     | 84/88 (96%)     | 69 (82%)   | 15 (18%)   | 2           | 10 |
| All | All   | 4984/5708 (87%) | 3763 (76%) | 1221 (24%) | 1           | 4  |

All (1221) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | A     | 5   | LYS  |
| 4   | A     | 9   | PRO  |
| 4   | A     | 15  | THR  |
| 4   | A     | 16  | GLN  |
| 4   | A     | 26  | GLU  |
| 4   | A     | 29  | GLU  |
| 4   | A     | 47  | SER  |
| 4   | A     | 60  | ASP  |
| 4   | A     | 68  | ILE  |
| 4   | A     | 73  | GLU  |
| 4   | A     | 74  | ASP  |
| 4   | A     | 79  | ILE  |
| 4   | A     | 80  | LEU  |
| 4   | A     | 84  | GLU  |
| 4   | A     | 89  | PHE  |
| 4   | A     | 92  | PRO  |
| 4   | A     | 99  | LEU  |
| 4   | A     | 100 | LEU  |
| 4   | A     | 101 | LEU  |
| 4   | A     | 102 | LYS  |
| 4   | A     | 104 | GLU  |
| 4   | A     | 115 | LEU  |
| 4   | A     | 127 | LEU  |
| 4   | A     | 138 | LEU  |
| 4   | A     | 140 | MET  |
| 4   | A     | 141 | GLU  |
| 4   | A     | 142 | VAL  |
| 4   | A     | 143 | ARG  |
| 4   | A     | 148 | VAL  |
| 4   | A     | 168 | ASP  |
| 4   | A     | 174 | VAL  |
| 4   | A     | 176 | ARG  |
| 4   | A     | 180 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | A     | 182 | GLU  |
| 4   | A     | 183 | ASP  |
| 4   | A     | 185 | ARG  |
| 4   | A     | 189 | ARG  |
| 4   | A     | 191 | ASP  |
| 4   | A     | 201 | THR  |
| 4   | A     | 206 | THR  |
| 4   | A     | 216 | GLU  |
| 4   | A     | 218 | LEU  |
| 4   | A     | 219 | ARG  |
| 4   | B     | 1   | MET  |
| 4   | B     | 2   | LEU  |
| 4   | B     | 3   | ASP  |
| 4   | B     | 4   | SER  |
| 4   | B     | 19  | GLU  |
| 4   | B     | 25  | LEU  |
| 4   | B     | 26  | GLU  |
| 4   | B     | 28  | LEU  |
| 4   | B     | 32  | PHE  |
| 4   | B     | 41  | ARG  |
| 4   | B     | 42  | ARG  |
| 4   | B     | 47  | SER  |
| 4   | B     | 60  | ASP  |
| 4   | B     | 62  | LEU  |
| 4   | B     | 63  | HIS  |
| 4   | B     | 66  | SER  |
| 4   | B     | 67  | THR  |
| 4   | B     | 73  | GLU  |
| 4   | B     | 77  | GLU  |
| 4   | B     | 81  | ASN  |
| 4   | B     | 85  | LEU  |
| 4   | B     | 90  | LEU  |
| 4   | B     | 93  | SER  |
| 4   | B     | 95  | GLN  |
| 4   | B     | 101 | LEU  |
| 4   | B     | 110 | LYS  |
| 4   | B     | 112 | ARG  |
| 4   | B     | 122 | ILE  |
| 4   | B     | 140 | MET  |
| 4   | B     | 155 | LYS  |
| 4   | B     | 156 | HIS  |
| 4   | B     | 159 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 163 | ASN  |
| 4   | B     | 167 | VAL  |
| 4   | B     | 189 | ARG  |
| 4   | B     | 195 | LEU  |
| 4   | B     | 196 | THR  |
| 4   | B     | 197 | LEU  |
| 4   | B     | 201 | THR  |
| 4   | B     | 206 | THR  |
| 4   | B     | 213 | GLN  |
| 4   | B     | 216 | GLU  |
| 4   | B     | 221 | HIS  |
| 4   | B     | 229 | GLN  |
| 5   | C     | 2   | GLU  |
| 5   | C     | 8   | ARG  |
| 5   | C     | 9   | ILE  |
| 5   | C     | 10  | ARG  |
| 5   | C     | 13  | ILE  |
| 5   | C     | 26  | TYR  |
| 5   | C     | 30  | LEU  |
| 5   | C     | 34  | VAL  |
| 5   | C     | 38  | LYS  |
| 5   | C     | 39  | ARG  |
| 5   | C     | 40  | GLU  |
| 5   | C     | 41  | ASN  |
| 5   | C     | 48  | PHE  |
| 5   | C     | 49  | ARG  |
| 5   | C     | 50  | GLU  |
| 5   | C     | 51  | THR  |
| 5   | C     | 64  | LEU  |
| 5   | C     | 65  | VAL  |
| 5   | C     | 66  | LEU  |
| 5   | C     | 70  | GLU  |
| 5   | C     | 73  | LEU  |
| 5   | C     | 80  | GLN  |
| 5   | C     | 82  | GLU  |
| 5   | C     | 88  | LEU  |
| 5   | C     | 91  | GLN  |
| 5   | C     | 94  | LEU  |
| 5   | C     | 95  | TYR  |
| 5   | C     | 98  | LEU  |
| 5   | C     | 105 | THR  |
| 5   | C     | 107 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | C     | 114 | PHE  |
| 5   | C     | 115 | LEU  |
| 5   | C     | 121 | MET  |
| 5   | C     | 123 | GLU  |
| 5   | C     | 124 | ASP  |
| 5   | C     | 133 | ASP  |
| 5   | C     | 139 | GLN  |
| 5   | C     | 142 | ARG  |
| 5   | C     | 147 | TYR  |
| 5   | C     | 148 | PHE  |
| 5   | C     | 151 | ASP  |
| 5   | C     | 152 | PRO  |
| 5   | C     | 158 | TYR  |
| 5   | C     | 161 | SER  |
| 5   | C     | 163 | ILE  |
| 5   | C     | 170 | PRO  |
| 5   | C     | 171 | TRP  |
| 5   | C     | 177 | GLU  |
| 5   | C     | 178 | PRO  |
| 5   | C     | 182 | VAL  |
| 5   | C     | 183 | SER  |
| 5   | C     | 184 | MET  |
| 5   | C     | 187 | ASN  |
| 5   | C     | 188 | LYS  |
| 5   | C     | 193 | LEU  |
| 5   | C     | 194 | VAL  |
| 5   | C     | 196 | LEU  |
| 5   | C     | 198 | ARG  |
| 5   | C     | 205 | GLU  |
| 5   | C     | 209 | ARG  |
| 5   | C     | 217 | LEU  |
| 5   | C     | 218 | VAL  |
| 5   | C     | 221 | LEU  |
| 5   | C     | 225 | SER  |
| 5   | C     | 226 | VAL  |
| 5   | C     | 229 | MET  |
| 5   | C     | 233 | GLU  |
| 5   | C     | 235 | LEU  |
| 5   | C     | 237 | ARG  |
| 5   | C     | 238 | LEU  |
| 5   | C     | 241 | LEU  |
| 5   | C     | 252 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | C     | 254 | VAL  |
| 5   | C     | 260 | LEU  |
| 5   | C     | 266 | ARG  |
| 5   | C     | 267 | TYR  |
| 5   | C     | 268 | ASP  |
| 5   | C     | 275 | TYR  |
| 5   | C     | 278 | GLU  |
| 5   | C     | 279 | GLU  |
| 5   | C     | 284 | ARG  |
| 5   | C     | 285 | LEU  |
| 5   | C     | 286 | SER  |
| 5   | C     | 290 | LEU  |
| 5   | C     | 293 | PHE  |
| 5   | C     | 294 | GLU  |
| 5   | C     | 301 | GLU  |
| 5   | C     | 309 | TYR  |
| 5   | C     | 321 | GLU  |
| 5   | C     | 327 | HIS  |
| 5   | C     | 328 | LEU  |
| 5   | C     | 330 | ASN  |
| 5   | C     | 345 | ARG  |
| 5   | C     | 351 | LEU  |
| 5   | C     | 359 | MET  |
| 5   | C     | 360 | LEU  |
| 5   | C     | 363 | SER  |
| 5   | C     | 365 | ASP  |
| 5   | C     | 367 | LEU  |
| 5   | C     | 368 | THR  |
| 5   | C     | 379 | GLU  |
| 5   | C     | 385 | PHE  |
| 5   | C     | 387 | SER  |
| 5   | C     | 390 | GLN  |
| 5   | C     | 393 | GLN  |
| 5   | C     | 394 | PHE  |
| 5   | C     | 397 | GLU  |
| 5   | C     | 398 | THR  |
| 5   | C     | 399 | ASN  |
| 5   | C     | 401 | LEU  |
| 5   | C     | 405 | ARG  |
| 5   | C     | 407 | LYS  |
| 5   | C     | 408 | ARG  |
| 5   | C     | 413 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | C     | 419 | THR  |
| 5   | C     | 422 | ARG  |
| 5   | C     | 426 | ASP  |
| 5   | C     | 433 | THR  |
| 5   | C     | 441 | VAL  |
| 5   | C     | 442 | GLU  |
| 5   | C     | 445 | GLU  |
| 5   | C     | 453 | THR  |
| 5   | C     | 455 | LEU  |
| 5   | C     | 460 | ARG  |
| 5   | C     | 469 | THR  |
| 5   | C     | 484 | VAL  |
| 5   | C     | 491 | GLU  |
| 5   | C     | 492 | ASP  |
| 5   | C     | 498 | GLN  |
| 5   | C     | 503 | LEU  |
| 5   | C     | 507 | ARG  |
| 5   | C     | 508 | ILE  |
| 5   | C     | 518 | LYS  |
| 5   | C     | 525 | SER  |
| 5   | C     | 527 | GLU  |
| 5   | C     | 530 | GLU  |
| 5   | C     | 538 | GLN  |
| 5   | C     | 560 | MET  |
| 5   | C     | 562 | SER  |
| 5   | C     | 564 | MET  |
| 5   | C     | 567 | GLN  |
| 5   | C     | 569 | VAL  |
| 5   | C     | 572 | ILE  |
| 5   | C     | 573 | ARG  |
| 5   | C     | 578 | VAL  |
| 5   | C     | 579 | VAL  |
| 5   | C     | 584 | GLU  |
| 5   | C     | 586 | ARG  |
| 5   | C     | 590 | ASP  |
| 5   | C     | 602 | GLU  |
| 5   | C     | 605 | LYS  |
| 5   | C     | 609 | ASN  |
| 5   | C     | 610 | ARG  |
| 5   | C     | 611 | ILE  |
| 5   | C     | 620 | LEU  |
| 5   | C     | 621 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | C     | 638 | ASP  |
| 5   | C     | 639 | GLN  |
| 5   | C     | 644 | VAL  |
| 5   | C     | 647 | GLN  |
| 5   | C     | 649 | VAL  |
| 5   | C     | 668 | LEU  |
| 5   | C     | 670 | GLN  |
| 5   | C     | 676 | ILE  |
| 5   | C     | 677 | MET  |
| 5   | C     | 701 | THR  |
| 5   | C     | 703 | ILE  |
| 5   | C     | 705 | ILE  |
| 5   | C     | 715 | THR  |
| 5   | C     | 721 | ARG  |
| 5   | C     | 727 | PRO  |
| 5   | C     | 729 | LEU  |
| 5   | C     | 739 | GLU  |
| 5   | C     | 740 | GLU  |
| 5   | C     | 748 | GLU  |
| 5   | C     | 750 | LYS  |
| 5   | C     | 766 | GLU  |
| 5   | C     | 770 | GLU  |
| 5   | C     | 774 | LEU  |
| 5   | C     | 780 | GLU  |
| 5   | C     | 784 | ASP  |
| 5   | C     | 785 | VAL  |
| 5   | C     | 794 | PRO  |
| 5   | C     | 805 | ARG  |
| 5   | C     | 807 | ARG  |
| 5   | C     | 814 | GLU  |
| 5   | C     | 816 | LYS  |
| 5   | C     | 821 | GLU  |
| 5   | C     | 822 | VAL  |
| 5   | C     | 825 | VAL  |
| 5   | C     | 834 | GLN  |
| 5   | C     | 841 | ASN  |
| 5   | C     | 846 | LYS  |
| 5   | C     | 856 | GLU  |
| 5   | C     | 858 | MET  |
| 5   | C     | 862 | PRO  |
| 5   | C     | 865 | THR  |
| 5   | C     | 870 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | C     | 872  | ASN  |
| 5   | C     | 881  | ASN  |
| 5   | C     | 882  | LEU  |
| 5   | C     | 884  | GLN  |
| 5   | C     | 890  | LEU  |
| 5   | C     | 900  | ARG  |
| 5   | C     | 904  | PRO  |
| 5   | C     | 918  | LEU  |
| 5   | C     | 920  | GLN  |
| 5   | C     | 923  | GLU  |
| 5   | C     | 924  | VAL  |
| 5   | C     | 937  | ASP  |
| 5   | C     | 938  | LYS  |
| 5   | C     | 939  | ARG  |
| 5   | C     | 946  | ARG  |
| 5   | C     | 950  | LEU  |
| 5   | C     | 953  | VAL  |
| 5   | C     | 957  | LYS  |
| 5   | C     | 958  | THR  |
| 5   | C     | 960  | GLU  |
| 5   | C     | 961  | GLU  |
| 5   | C     | 963  | LEU  |
| 5   | C     | 966  | LEU  |
| 5   | C     | 971  | LYS  |
| 5   | C     | 981  | GLU  |
| 5   | C     | 988  | VAL  |
| 5   | C     | 989  | VAL  |
| 5   | C     | 995  | MET  |
| 5   | C     | 999  | HIS  |
| 5   | C     | 1002 | GLU  |
| 5   | C     | 1005 | MET  |
| 5   | C     | 1016 | ILE  |
| 5   | C     | 1019 | GLN  |
| 5   | C     | 1021 | LEU  |
| 5   | C     | 1030 | GLN  |
| 5   | C     | 1031 | ARG  |
| 5   | C     | 1035 | MET  |
| 5   | C     | 1040 | LEU  |
| 5   | C     | 1051 | GLU  |
| 5   | C     | 1052 | MET  |
| 5   | C     | 1061 | GLU  |
| 5   | C     | 1072 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | C     | 1080 | SER  |
| 5   | C     | 1085 | PHE  |
| 5   | C     | 1097 | LEU  |
| 5   | C     | 1098 | ASP  |
| 5   | C     | 1101 | THR  |
| 5   | C     | 1104 | GLU  |
| 5   | C     | 1105 | LYS  |
| 5   | C     | 1108 | PRO  |
| 5   | C     | 1110 | ASP  |
| 5   | C     | 1111 | ILE  |
| 5   | C     | 1118 | LYS  |
| 6   | D     | 6    | ARG  |
| 6   | D     | 8    | VAL  |
| 6   | D     | 10   | ILE  |
| 6   | D     | 17   | LYS  |
| 6   | D     | 29   | PRO  |
| 6   | D     | 34   | TYR  |
| 6   | D     | 41   | ARG  |
| 6   | D     | 42   | ASP  |
| 6   | D     | 45   | PHE  |
| 6   | D     | 53   | ILE  |
| 6   | D     | 56   | TYR  |
| 6   | D     | 57   | GLU  |
| 6   | D     | 58   | CYS  |
| 6   | D     | 67   | ARG  |
| 6   | D     | 68   | PHE  |
| 6   | D     | 69   | GLU  |
| 6   | D     | 71   | LYS  |
| 6   | D     | 76   | CYS  |
| 6   | D     | 82   | LYS  |
| 6   | D     | 85   | VAL  |
| 6   | D     | 87   | ARG  |
| 6   | D     | 95   | LEU  |
| 6   | D     | 97   | THR  |
| 6   | D     | 101  | HIS  |
| 6   | D     | 103  | TRP  |
| 6   | D     | 106  | LYS  |
| 6   | D     | 108  | VAL  |
| 6   | D     | 111  | LYS  |
| 6   | D     | 112  | ILE  |
| 6   | D     | 116  | LEU  |
| 6   | D     | 124  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | D     | 127 | LEU  |
| 6   | D     | 128 | TYR  |
| 6   | D     | 133 | ILE  |
| 6   | D     | 145 | VAL  |
| 6   | D     | 149 | LYS  |
| 6   | D     | 151 | GLN  |
| 6   | D     | 152 | LEU  |
| 6   | D     | 153 | LEU  |
| 6   | D     | 155 | ASP  |
| 6   | D     | 161 | LEU  |
| 6   | D     | 163 | TYR  |
| 6   | D     | 169 | TYR  |
| 6   | D     | 180 | LYS  |
| 6   | D     | 189 | GLN  |
| 6   | D     | 196 | VAL  |
| 6   | D     | 198 | ARG  |
| 6   | D     | 199 | LEU  |
| 6   | D     | 206 | ARG  |
| 6   | D     | 207 | PHE  |
| 6   | D     | 394 | LEU  |
| 6   | D     | 407 | VAL  |
| 6   | D     | 410 | SER  |
| 6   | D     | 423 | ASP  |
| 6   | D     | 430 | ASP  |
| 6   | D     | 439 | LEU  |
| 6   | D     | 443 | VAL  |
| 6   | D     | 447 | VAL  |
| 6   | D     | 452 | ILE  |
| 6   | D     | 456 | MET  |
| 6   | D     | 465 | LEU  |
| 6   | D     | 466 | LYS  |
| 6   | D     | 470 | LEU  |
| 6   | D     | 471 | GLU  |
| 6   | D     | 474 | GLU  |
| 6   | D     | 481 | MET  |
| 6   | D     | 483 | HIS  |
| 6   | D     | 485 | SER  |
| 6   | D     | 493 | ARG  |
| 6   | D     | 496 | LEU  |
| 6   | D     | 505 | SER  |
| 6   | D     | 513 | ILE  |
| 6   | D     | 519 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | D     | 522 | PRO  |
| 6   | D     | 523 | ASP  |
| 6   | D     | 525 | ARG  |
| 6   | D     | 538 | SER  |
| 6   | D     | 542 | ASP  |
| 6   | D     | 543 | LEU  |
| 6   | D     | 550 | ARG  |
| 6   | D     | 554 | LEU  |
| 6   | D     | 564 | GLU  |
| 6   | D     | 570 | GLU  |
| 6   | D     | 590 | PRO  |
| 6   | D     | 594 | PRO  |
| 6   | D     | 607 | LEU  |
| 6   | D     | 611 | GLN  |
| 6   | D     | 615 | ARG  |
| 6   | D     | 619 | LEU  |
| 6   | D     | 621 | LYS  |
| 6   | D     | 639 | LEU  |
| 6   | D     | 642 | CYS  |
| 6   | D     | 644 | LEU  |
| 6   | D     | 651 | GLU  |
| 6   | D     | 652 | LEU  |
| 6   | D     | 654 | LYS  |
| 6   | D     | 659 | LYS  |
| 6   | D     | 662 | GLU  |
| 6   | D     | 669 | ASN  |
| 6   | D     | 670 | VAL  |
| 6   | D     | 676 | MET  |
| 6   | D     | 678 | GLU  |
| 6   | D     | 679 | ARG  |
| 6   | D     | 682 | ASP  |
| 6   | D     | 691 | LEU  |
| 6   | D     | 692 | GLU  |
| 6   | D     | 698 | LYS  |
| 6   | D     | 702 | LEU  |
| 6   | D     | 709 | HIS  |
| 6   | D     | 710 | ARG  |
| 6   | D     | 724 | GLN  |
| 6   | D     | 733 | CYS  |
| 6   | D     | 734 | GLU  |
| 6   | D     | 736 | PHE  |
| 6   | D     | 737 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | D     | 741 | ASP  |
| 6   | D     | 743 | ASP  |
| 6   | D     | 744 | GLN  |
| 6   | D     | 754 | PHE  |
| 6   | D     | 758 | GLU  |
| 6   | D     | 762 | GLN  |
| 6   | D     | 763 | MET  |
| 6   | D     | 764 | LEU  |
| 6   | D     | 770 | LEU  |
| 6   | D     | 778 | LEU  |
| 6   | D     | 782 | SER  |
| 6   | D     | 783 | ARG  |
| 6   | D     | 785 | ILE  |
| 6   | D     | 792 | ILE  |
| 6   | D     | 796 | ARG  |
| 6   | D     | 808 | THR  |
| 6   | D     | 810 | GLU  |
| 6   | D     | 811 | GLU  |
| 6   | D     | 816 | HIS  |
| 6   | D     | 826 | PRO  |
| 6   | D     | 827 | ILE  |
| 6   | D     | 833 | GLU  |
| 6   | D     | 834 | THR  |
| 6   | D     | 839 | LEU  |
| 6   | D     | 842 | VAL  |
| 6   | D     | 859 | ASP  |
| 6   | D     | 863 | VAL  |
| 6   | D     | 864 | VAL  |
| 6   | D     | 869 | MET  |
| 6   | D     | 876 | SER  |
| 6   | D     | 897 | TRP  |
| 6   | D     | 899 | LEU  |
| 6   | D     | 901 | GLN  |
| 6   | D     | 904 | VAL  |
| 6   | D     | 907 | GLU  |
| 6   | D     | 913 | ASP  |
| 6   | D     | 914 | LEU  |
| 6   | D     | 922 | LEU  |
| 6   | D     | 932 | ASP  |
| 6   | D     | 947 | ILE  |
| 6   | D     | 951 | ILE  |
| 6   | D     | 959 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | D     | 971  | LEU  |
| 6   | D     | 972  | LEU  |
| 6   | D     | 975  | GLU  |
| 6   | D     | 980  | MET  |
| 6   | D     | 982  | PHE  |
| 6   | D     | 983  | LEU  |
| 6   | D     | 988  | ARG  |
| 6   | D     | 991  | GLN  |
| 6   | D     | 1005 | GLN  |
| 6   | D     | 1013 | GLU  |
| 6   | D     | 1014 | ASN  |
| 6   | D     | 1019 | PRO  |
| 6   | D     | 1033 | GLN  |
| 6   | D     | 1038 | LEU  |
| 6   | D     | 1044 | LEU  |
| 6   | D     | 1052 | THR  |
| 6   | D     | 1060 | SER  |
| 6   | D     | 1062 | ARG  |
| 6   | D     | 1063 | GLU  |
| 6   | D     | 1066 | THR  |
| 6   | D     | 1067 | VAL  |
| 6   | D     | 1070 | TYR  |
| 6   | D     | 1074 | SER  |
| 6   | D     | 1083 | ASP  |
| 6   | D     | 1084 | THR  |
| 6   | D     | 1093 | TYR  |
| 6   | D     | 1096 | ARG  |
| 6   | D     | 1100 | ASP  |
| 6   | D     | 1112 | CYS  |
| 6   | D     | 1114 | THR  |
| 6   | D     | 1118 | ILE  |
| 6   | D     | 1119 | SER  |
| 6   | D     | 1134 | LEU  |
| 6   | D     | 1135 | ARG  |
| 6   | D     | 1139 | ASP  |
| 6   | D     | 1151 | ARG  |
| 6   | D     | 1152 | GLU  |
| 6   | D     | 1155 | VAL  |
| 6   | D     | 1164 | ARG  |
| 6   | D     | 1166 | LEU  |
| 6   | D     | 1167 | SER  |
| 6   | D     | 1196 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | D     | 1197 | ARG  |
| 6   | D     | 1207 | TYR  |
| 6   | D     | 1211 | MET  |
| 6   | D     | 1214 | PRO  |
| 6   | D     | 1231 | GLU  |
| 6   | D     | 1232 | PRO  |
| 6   | D     | 1234 | THR  |
| 6   | D     | 1237 | THR  |
| 6   | D     | 1242 | HIS  |
| 6   | D     | 1256 | LEU  |
| 6   | D     | 1257 | PRO  |
| 6   | D     | 1259 | VAL  |
| 6   | D     | 1260 | ILE  |
| 6   | D     | 1264 | GLU  |
| 6   | D     | 1267 | ARG  |
| 6   | D     | 1271 | LYS  |
| 6   | D     | 1330 | ILE  |
| 6   | D     | 1331 | ASP  |
| 6   | D     | 1332 | PRO  |
| 6   | D     | 1337 | GLU  |
| 6   | D     | 1344 | VAL  |
| 6   | D     | 1346 | ARG  |
| 6   | D     | 1347 | TYR  |
| 6   | D     | 1354 | LYS  |
| 6   | D     | 1363 | LEU  |
| 6   | D     | 1376 | MET  |
| 6   | D     | 1377 | LYS  |
| 6   | D     | 1383 | ASP  |
| 6   | D     | 1393 | GLN  |
| 6   | D     | 1395 | LEU  |
| 6   | D     | 1397 | LYS  |
| 6   | D     | 1403 | LEU  |
| 6   | D     | 1404 | ASN  |
| 6   | D     | 1410 | GLU  |
| 6   | D     | 1415 | VAL  |
| 6   | D     | 1422 | MET  |
| 6   | D     | 1424 | VAL  |
| 6   | D     | 1426 | LYS  |
| 6   | D     | 1429 | LEU  |
| 6   | D     | 1432 | LYS  |
| 6   | D     | 1435 | LEU  |
| 6   | D     | 1436 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | D     | 1440 | PHE  |
| 6   | D     | 1464 | GLU  |
| 6   | D     | 1465 | ASN  |
| 6   | D     | 1466 | VAL  |
| 6   | D     | 1470 | ARG  |
| 6   | D     | 1471 | LEU  |
| 6   | D     | 1472 | ILE  |
| 6   | D     | 1483 | PHE  |
| 6   | D     | 1488 | ASP  |
| 7   | E     | 13   | VAL  |
| 7   | E     | 28   | GLN  |
| 7   | E     | 30   | LEU  |
| 7   | E     | 31   | LEU  |
| 7   | E     | 32   | ARG  |
| 7   | E     | 40   | LEU  |
| 7   | E     | 41   | GLU  |
| 7   | E     | 42   | PRO  |
| 7   | E     | 47   | LYS  |
| 7   | E     | 49   | GLN  |
| 7   | E     | 51   | LEU  |
| 7   | E     | 57   | ASP  |
| 7   | E     | 67   | GLU  |
| 7   | E     | 68   | LEU  |
| 7   | E     | 69   | LEU  |
| 7   | E     | 70   | THR  |
| 7   | E     | 72   | ARG  |
| 7   | E     | 74   | VAL  |
| 7   | E     | 77   | GLU  |
| 7   | E     | 79   | LEU  |
| 7   | E     | 81   | PRO  |
| 7   | E     | 82   | GLU  |
| 7   | E     | 83   | ASP  |
| 7   | E     | 85   | LEU  |
| 7   | E     | 86   | GLN  |
| 7   | E     | 94   | PRO  |
| 7   | E     | 96   | GLU  |
| 4   | K     | 1    | MET  |
| 4   | K     | 5    | LYS  |
| 4   | K     | 9    | PRO  |
| 4   | K     | 26   | GLU  |
| 4   | K     | 43   | ILE  |
| 4   | K     | 45   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | K     | 49  | PRO  |
| 4   | K     | 54  | THR  |
| 4   | K     | 58  | ILE  |
| 4   | K     | 64  | GLU  |
| 4   | K     | 73  | GLU  |
| 4   | K     | 76  | VAL  |
| 4   | K     | 80  | LEU  |
| 4   | K     | 86  | VAL  |
| 4   | K     | 89  | PHE  |
| 4   | K     | 92  | PRO  |
| 4   | K     | 93  | SER  |
| 4   | K     | 96  | THR  |
| 4   | K     | 98  | THR  |
| 4   | K     | 99  | LEU  |
| 4   | K     | 109 | VAL  |
| 4   | K     | 115 | LEU  |
| 4   | K     | 116 | PRO  |
| 4   | K     | 126 | ASP  |
| 4   | K     | 127 | LEU  |
| 4   | K     | 131 | THR  |
| 4   | K     | 133 | GLU  |
| 4   | K     | 134 | GLU  |
| 4   | K     | 137 | ARG  |
| 4   | K     | 141 | GLU  |
| 4   | K     | 143 | ARG  |
| 4   | K     | 145 | ASP  |
| 4   | K     | 154 | GLU  |
| 4   | K     | 167 | VAL  |
| 4   | K     | 179 | PHE  |
| 4   | K     | 180 | GLN  |
| 4   | K     | 182 | GLU  |
| 4   | K     | 183 | ASP  |
| 4   | K     | 189 | ARG  |
| 4   | K     | 197 | LEU  |
| 4   | K     | 201 | THR  |
| 4   | K     | 204 | SER  |
| 4   | K     | 206 | THR  |
| 4   | K     | 208 | LEU  |
| 4   | K     | 216 | GLU  |
| 4   | K     | 219 | ARG  |
| 4   | K     | 229 | GLN  |
| 4   | L     | 3   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | L     | 4   | SER  |
| 4   | L     | 7   | LYS  |
| 4   | L     | 10  | VAL  |
| 4   | L     | 15  | THR  |
| 4   | L     | 24  | VAL  |
| 4   | L     | 26  | GLU  |
| 4   | L     | 30  | ARG  |
| 4   | L     | 41  | ARG  |
| 4   | L     | 47  | SER  |
| 4   | L     | 51  | THR  |
| 4   | L     | 58  | ILE  |
| 4   | L     | 60  | ASP  |
| 4   | L     | 61  | VAL  |
| 4   | L     | 62  | LEU  |
| 4   | L     | 63  | HIS  |
| 4   | L     | 64  | GLU  |
| 4   | L     | 66  | SER  |
| 4   | L     | 67  | THR  |
| 4   | L     | 73  | GLU  |
| 4   | L     | 77  | GLU  |
| 4   | L     | 80  | LEU  |
| 4   | L     | 81  | ASN  |
| 4   | L     | 95  | GLN  |
| 4   | L     | 100 | LEU  |
| 4   | L     | 115 | LEU  |
| 4   | L     | 117 | VAL  |
| 4   | L     | 122 | ILE  |
| 4   | L     | 129 | ILE  |
| 4   | L     | 132 | LEU  |
| 4   | L     | 140 | MET  |
| 4   | L     | 151 | VAL  |
| 4   | L     | 152 | PRO  |
| 4   | L     | 160 | ASP  |
| 4   | L     | 163 | ASN  |
| 4   | L     | 172 | SER  |
| 4   | L     | 177 | VAL  |
| 4   | L     | 179 | PHE  |
| 4   | L     | 180 | GLN  |
| 4   | L     | 182 | GLU  |
| 4   | L     | 184 | THR  |
| 4   | L     | 190 | THR  |
| 4   | L     | 191 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | L     | 196 | THR  |
| 4   | L     | 200 | TRP  |
| 4   | L     | 206 | THR  |
| 4   | L     | 215 | VAL  |
| 4   | L     | 223 | THR  |
| 4   | L     | 224 | TYR  |
| 4   | L     | 227 | ASN  |
| 5   | M     | 1   | MET  |
| 5   | M     | 9   | ILE  |
| 5   | M     | 10  | ARG  |
| 5   | M     | 27  | ARG  |
| 5   | M     | 30  | LEU  |
| 5   | M     | 31  | GLN  |
| 5   | M     | 33  | ASP  |
| 5   | M     | 39  | ARG  |
| 5   | M     | 42  | VAL  |
| 5   | M     | 45  | GLN  |
| 5   | M     | 51  | THR  |
| 5   | M     | 54  | ILE  |
| 5   | M     | 61  | LYS  |
| 5   | M     | 77  | PRO  |
| 5   | M     | 80  | GLN  |
| 5   | M     | 82  | GLU  |
| 5   | M     | 95  | TYR  |
| 5   | M     | 98  | LEU  |
| 5   | M     | 99  | GLN  |
| 5   | M     | 100 | LEU  |
| 5   | M     | 107 | LEU  |
| 5   | M     | 115 | LEU  |
| 5   | M     | 117 | HIS  |
| 5   | M     | 118 | ILE  |
| 5   | M     | 120 | LEU  |
| 5   | M     | 126 | SER  |
| 5   | M     | 128 | ILE  |
| 5   | M     | 133 | ASP  |
| 5   | M     | 142 | ARG  |
| 5   | M     | 158 | TYR  |
| 5   | M     | 163 | ILE  |
| 5   | M     | 170 | PRO  |
| 5   | M     | 173 | ASP  |
| 5   | M     | 178 | PRO  |
| 5   | M     | 179 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | M     | 181 | VAL  |
| 5   | M     | 182 | VAL  |
| 5   | M     | 184 | MET  |
| 5   | M     | 185 | LYS  |
| 5   | M     | 186 | VAL  |
| 5   | M     | 188 | LYS  |
| 5   | M     | 190 | LYS  |
| 5   | M     | 193 | LEU  |
| 5   | M     | 194 | VAL  |
| 5   | M     | 198 | ARG  |
| 5   | M     | 205 | GLU  |
| 5   | M     | 209 | ARG  |
| 5   | M     | 210 | GLU  |
| 5   | M     | 216 | GLU  |
| 5   | M     | 218 | VAL  |
| 5   | M     | 221 | LEU  |
| 5   | M     | 222 | MET  |
| 5   | M     | 224 | GLU  |
| 5   | M     | 225 | SER  |
| 5   | M     | 226 | VAL  |
| 5   | M     | 230 | ARG  |
| 5   | M     | 233 | GLU  |
| 5   | M     | 241 | LEU  |
| 5   | M     | 243 | ARG  |
| 5   | M     | 252 | LYS  |
| 5   | M     | 260 | LEU  |
| 5   | M     | 261 | ILE  |
| 5   | M     | 264 | PRO  |
| 5   | M     | 266 | ARG  |
| 5   | M     | 267 | TYR  |
| 5   | M     | 271 | GLU  |
| 5   | M     | 280 | LYS  |
| 5   | M     | 283 | ILE  |
| 5   | M     | 285 | LEU  |
| 5   | M     | 289 | THR  |
| 5   | M     | 290 | LEU  |
| 5   | M     | 293 | PHE  |
| 5   | M     | 294 | GLU  |
| 5   | M     | 301 | GLU  |
| 5   | M     | 304 | LEU  |
| 5   | M     | 309 | TYR  |
| 5   | M     | 317 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | M     | 320 | HIS  |
| 5   | M     | 323 | ASP  |
| 5   | M     | 331 | ARG  |
| 5   | M     | 332 | ARG  |
| 5   | M     | 342 | ASP  |
| 5   | M     | 350 | ARG  |
| 5   | M     | 351 | LEU  |
| 5   | M     | 359 | MET  |
| 5   | M     | 361 | MET  |
| 5   | M     | 365 | ASP  |
| 5   | M     | 367 | LEU  |
| 5   | M     | 376 | ARG  |
| 5   | M     | 382 | ILE  |
| 5   | M     | 383 | ARG  |
| 5   | M     | 387 | SER  |
| 5   | M     | 393 | GLN  |
| 5   | M     | 394 | PHE  |
| 5   | M     | 398 | THR  |
| 5   | M     | 401 | LEU  |
| 5   | M     | 413 | LEU  |
| 5   | M     | 419 | THR  |
| 5   | M     | 422 | ARG  |
| 5   | M     | 426 | ASP  |
| 5   | M     | 430 | VAL  |
| 5   | M     | 433 | THR  |
| 5   | M     | 440 | PRO  |
| 5   | M     | 443 | THR  |
| 5   | M     | 451 | LEU  |
| 5   | M     | 452 | ILE  |
| 5   | M     | 458 | TYR  |
| 5   | M     | 471 | TYR  |
| 5   | M     | 473 | ARG  |
| 5   | M     | 474 | VAL  |
| 5   | M     | 480 | THR  |
| 5   | M     | 487 | THR  |
| 5   | M     | 489 | THR  |
| 5   | M     | 503 | LEU  |
| 5   | M     | 508 | ILE  |
| 5   | M     | 511 | GLU  |
| 5   | M     | 513 | VAL  |
| 5   | M     | 517 | ARG  |
| 5   | M     | 520 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | M     | 530 | GLU  |
| 5   | M     | 532 | MET  |
| 5   | M     | 543 | ASN  |
| 5   | M     | 553 | ASP  |
| 5   | M     | 554 | ASP  |
| 5   | M     | 572 | ILE  |
| 5   | M     | 579 | VAL  |
| 5   | M     | 581 | THR  |
| 5   | M     | 584 | GLU  |
| 5   | M     | 585 | GLU  |
| 5   | M     | 586 | ARG  |
| 5   | M     | 587 | VAL  |
| 5   | M     | 589 | ARG  |
| 5   | M     | 599 | GLU  |
| 5   | M     | 602 | GLU  |
| 5   | M     | 607 | ASP  |
| 5   | M     | 609 | ASN  |
| 5   | M     | 613 | VAL  |
| 5   | M     | 616 | GLU  |
| 5   | M     | 617 | ASP  |
| 5   | M     | 620 | LEU  |
| 5   | M     | 625 | LEU  |
| 5   | M     | 627 | ARG  |
| 5   | M     | 628 | PHE  |
| 5   | M     | 645 | VAL  |
| 5   | M     | 647 | GLN  |
| 5   | M     | 654 | LEU  |
| 5   | M     | 662 | GLU  |
| 5   | M     | 668 | LEU  |
| 5   | M     | 671 | ASN  |
| 5   | M     | 677 | MET  |
| 5   | M     | 678 | PRO  |
| 5   | M     | 686 | ASP  |
| 5   | M     | 699 | PHE  |
| 5   | M     | 701 | THR  |
| 5   | M     | 711 | GLU  |
| 5   | M     | 715 | THR  |
| 5   | M     | 717 | LEU  |
| 5   | M     | 722 | ILE  |
| 5   | M     | 727 | PRO  |
| 5   | M     | 728 | HIS  |
| 5   | M     | 731 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | M     | 735 | ARG  |
| 5   | M     | 736 | ASP  |
| 5   | M     | 737 | LEU  |
| 5   | M     | 738 | ASP  |
| 5   | M     | 739 | GLU  |
| 5   | M     | 745 | ILE  |
| 5   | M     | 751 | PRO  |
| 5   | M     | 765 | SER  |
| 5   | M     | 766 | GLU  |
| 5   | M     | 769 | PRO  |
| 5   | M     | 781 | LYS  |
| 5   | M     | 783 | ARG  |
| 5   | M     | 784 | ASP  |
| 5   | M     | 785 | VAL  |
| 5   | M     | 787 | ASP  |
| 5   | M     | 792 | VAL  |
| 5   | M     | 794 | PRO  |
| 5   | M     | 803 | THR  |
| 5   | M     | 805 | ARG  |
| 5   | M     | 806 | LEU  |
| 5   | M     | 807 | ARG  |
| 5   | M     | 808 | ARG  |
| 5   | M     | 814 | GLU  |
| 5   | M     | 815 | LEU  |
| 5   | M     | 822 | VAL  |
| 5   | M     | 824 | ARG  |
| 5   | M     | 833 | LEU  |
| 5   | M     | 834 | GLN  |
| 5   | M     | 841 | ASN  |
| 5   | M     | 856 | GLU  |
| 5   | M     | 857 | ASP  |
| 5   | M     | 862 | PRO  |
| 5   | M     | 870 | ILE  |
| 5   | M     | 878 | SER  |
| 5   | M     | 881 | ASN  |
| 5   | M     | 882 | LEU  |
| 5   | M     | 884 | GLN  |
| 5   | M     | 892 | LEU  |
| 5   | M     | 904 | PRO  |
| 5   | M     | 905 | ILE  |
| 5   | M     | 907 | ASP  |
| 5   | M     | 913 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | M     | 916  | GLU  |
| 5   | M     | 918  | LEU  |
| 5   | M     | 920  | GLN  |
| 5   | M     | 928  | LYS  |
| 5   | M     | 937  | ASP  |
| 5   | M     | 938  | LYS  |
| 5   | M     | 939  | ARG  |
| 5   | M     | 944  | LEU  |
| 5   | M     | 946  | ARG  |
| 5   | M     | 953  | VAL  |
| 5   | M     | 957  | LYS  |
| 5   | M     | 958  | THR  |
| 5   | M     | 960  | GLU  |
| 5   | M     | 966  | LEU  |
| 5   | M     | 974  | LEU  |
| 5   | M     | 981  | GLU  |
| 5   | M     | 983  | ILE  |
| 5   | M     | 984  | GLU  |
| 5   | M     | 988  | VAL  |
| 5   | M     | 995  | MET  |
| 5   | M     | 997  | LEU  |
| 5   | M     | 999  | HIS  |
| 5   | M     | 1003 | ASP  |
| 5   | M     | 1005 | MET  |
| 5   | M     | 1006 | HIS  |
| 5   | M     | 1016 | ILE  |
| 5   | M     | 1017 | THR  |
| 5   | M     | 1018 | GLN  |
| 5   | M     | 1021 | LEU  |
| 5   | M     | 1027 | PHE  |
| 5   | M     | 1035 | MET  |
| 5   | M     | 1053 | LEU  |
| 5   | M     | 1054 | THR  |
| 5   | M     | 1055 | LEU  |
| 5   | M     | 1058 | ASP  |
| 5   | M     | 1060 | ILE  |
| 5   | M     | 1072 | LYS  |
| 5   | M     | 1074 | GLU  |
| 5   | M     | 1078 | GLU  |
| 5   | M     | 1079 | PRO  |
| 5   | M     | 1081 | VAL  |
| 5   | M     | 1092 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | M     | 1095 | LEU  |
| 5   | M     | 1097 | LEU  |
| 5   | M     | 1098 | ASP  |
| 5   | M     | 1101 | THR  |
| 5   | M     | 1103 | ASP  |
| 5   | M     | 1115 | LEU  |
| 6   | N     | 4    | GLU  |
| 6   | N     | 5    | VAL  |
| 6   | N     | 20   | SER  |
| 6   | N     | 25   | GLU  |
| 6   | N     | 26   | VAL  |
| 6   | N     | 36   | THR  |
| 6   | N     | 40   | GLU  |
| 6   | N     | 41   | ARG  |
| 6   | N     | 42   | ASP  |
| 6   | N     | 44   | LEU  |
| 6   | N     | 56   | TYR  |
| 6   | N     | 57   | GLU  |
| 6   | N     | 64   | LYS  |
| 6   | N     | 65   | ARG  |
| 6   | N     | 67   | ARG  |
| 6   | N     | 68   | PHE  |
| 6   | N     | 69   | GLU  |
| 6   | N     | 75   | ARG  |
| 6   | N     | 79   | GLU  |
| 6   | N     | 80   | VAL  |
| 6   | N     | 82   | LYS  |
| 6   | N     | 87   | ARG  |
| 6   | N     | 95   | LEU  |
| 6   | N     | 97   | THR  |
| 6   | N     | 98   | PRO  |
| 6   | N     | 101  | HIS  |
| 6   | N     | 108  | VAL  |
| 6   | N     | 112  | ILE  |
| 6   | N     | 116  | LEU  |
| 6   | N     | 122  | GLU  |
| 6   | N     | 123  | LEU  |
| 6   | N     | 124  | GLU  |
| 6   | N     | 127  | LEU  |
| 6   | N     | 131  | LYS  |
| 6   | N     | 133  | ILE  |
| 6   | N     | 145  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | N     | 147 | VAL  |
| 6   | N     | 148 | GLU  |
| 6   | N     | 149 | LYS  |
| 6   | N     | 152 | LEU  |
| 6   | N     | 153 | LEU  |
| 6   | N     | 155 | ASP  |
| 6   | N     | 157 | GLU  |
| 6   | N     | 160 | GLU  |
| 6   | N     | 166 | GLN  |
| 6   | N     | 167 | GLU  |
| 6   | N     | 176 | ASP  |
| 6   | N     | 178 | LEU  |
| 6   | N     | 180 | LYS  |
| 6   | N     | 199 | LEU  |
| 6   | N     | 405 | ASP  |
| 6   | N     | 406 | ASP  |
| 6   | N     | 414 | ARG  |
| 6   | N     | 434 | ARG  |
| 6   | N     | 437 | VAL  |
| 6   | N     | 446 | VAL  |
| 6   | N     | 451 | ASP  |
| 6   | N     | 455 | ARG  |
| 6   | N     | 456 | MET  |
| 6   | N     | 462 | GLN  |
| 6   | N     | 464 | LEU  |
| 6   | N     | 465 | LEU  |
| 6   | N     | 467 | GLU  |
| 6   | N     | 469 | ASP  |
| 6   | N     | 470 | LEU  |
| 6   | N     | 471 | GLU  |
| 6   | N     | 477 | LEU  |
| 6   | N     | 493 | ARG  |
| 6   | N     | 496 | LEU  |
| 6   | N     | 499 | VAL  |
| 6   | N     | 507 | ASN  |
| 6   | N     | 511 | TRP  |
| 6   | N     | 512 | MET  |
| 6   | N     | 513 | ILE  |
| 6   | N     | 522 | PRO  |
| 6   | N     | 523 | ASP  |
| 6   | N     | 525 | ARG  |
| 6   | N     | 537 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | N     | 538 | SER  |
| 6   | N     | 539 | ASP  |
| 6   | N     | 544 | TYR  |
| 6   | N     | 548 | ILE  |
| 6   | N     | 550 | ARG  |
| 6   | N     | 565 | ILE  |
| 6   | N     | 567 | ILE  |
| 6   | N     | 576 | GLU  |
| 6   | N     | 581 | LEU  |
| 6   | N     | 584 | ASN  |
| 6   | N     | 594 | PRO  |
| 6   | N     | 613 | ARG  |
| 6   | N     | 617 | ASN  |
| 6   | N     | 619 | LEU  |
| 6   | N     | 629 | SER  |
| 6   | N     | 635 | PRO  |
| 6   | N     | 639 | LEU  |
| 6   | N     | 641 | GLN  |
| 6   | N     | 644 | LEU  |
| 6   | N     | 647 | ARG  |
| 6   | N     | 654 | LYS  |
| 6   | N     | 660 | LYS  |
| 6   | N     | 661 | MET  |
| 6   | N     | 666 | ILE  |
| 6   | N     | 669 | ASN  |
| 6   | N     | 680 | GLN  |
| 6   | N     | 682 | ASP  |
| 6   | N     | 684 | LYS  |
| 6   | N     | 688 | TRP  |
| 6   | N     | 692 | GLU  |
| 6   | N     | 699 | VAL  |
| 6   | N     | 701 | LEU  |
| 6   | N     | 707 | THR  |
| 6   | N     | 709 | HIS  |
| 6   | N     | 728 | LEU  |
| 6   | N     | 733 | CYS  |
| 6   | N     | 734 | GLU  |
| 6   | N     | 737 | ASN  |
| 6   | N     | 740 | PHE  |
| 6   | N     | 741 | ASP  |
| 6   | N     | 743 | ASP  |
| 6   | N     | 764 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | N     | 769 | LEU  |
| 6   | N     | 792 | ILE  |
| 6   | N     | 794 | GLN  |
| 6   | N     | 795 | VAL  |
| 6   | N     | 797 | LYS  |
| 6   | N     | 816 | HIS  |
| 6   | N     | 817 | GLU  |
| 6   | N     | 818 | ARG  |
| 6   | N     | 823 | LEU  |
| 6   | N     | 824 | ASN  |
| 6   | N     | 826 | PRO  |
| 6   | N     | 832 | ARG  |
| 6   | N     | 834 | THR  |
| 6   | N     | 836 | VAL  |
| 6   | N     | 838 | ARG  |
| 6   | N     | 840 | LYS  |
| 6   | N     | 841 | TYR  |
| 6   | N     | 847 | ASP  |
| 6   | N     | 848 | GLU  |
| 6   | N     | 861 | GLN  |
| 6   | N     | 864 | VAL  |
| 6   | N     | 874 | GLU  |
| 6   | N     | 879 | ARG  |
| 6   | N     | 881 | LEU  |
| 6   | N     | 888 | GLU  |
| 6   | N     | 897 | TRP  |
| 6   | N     | 902 | LEU  |
| 6   | N     | 907 | GLU  |
| 6   | N     | 914 | LEU  |
| 6   | N     | 921 | ARG  |
| 6   | N     | 926 | LYS  |
| 6   | N     | 930 | LEU  |
| 6   | N     | 935 | LYS  |
| 6   | N     | 939 | PHE  |
| 6   | N     | 947 | ILE  |
| 6   | N     | 951 | ILE  |
| 6   | N     | 952 | ASP  |
| 6   | N     | 959 | GLU  |
| 6   | N     | 968 | ASP  |
| 6   | N     | 976 | GLN  |
| 6   | N     | 983 | LEU  |
| 6   | N     | 985 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | N     | 988  | ARG  |
| 6   | N     | 1001 | GLU  |
| 6   | N     | 1020 | LEU  |
| 6   | N     | 1032 | PRO  |
| 6   | N     | 1034 | GLN  |
| 6   | N     | 1039 | CYS  |
| 6   | N     | 1041 | LEU  |
| 6   | N     | 1042 | ARG  |
| 6   | N     | 1046 | GLN  |
| 6   | N     | 1053 | PHE  |
| 6   | N     | 1060 | SER  |
| 6   | N     | 1062 | ARG  |
| 6   | N     | 1063 | GLU  |
| 6   | N     | 1070 | TYR  |
| 6   | N     | 1083 | ASP  |
| 6   | N     | 1088 | THR  |
| 6   | N     | 1097 | LYS  |
| 6   | N     | 1098 | LEU  |
| 6   | N     | 1100 | ASP  |
| 6   | N     | 1104 | GLU  |
| 6   | N     | 1109 | GLU  |
| 6   | N     | 1112 | CYS  |
| 6   | N     | 1115 | THR  |
| 6   | N     | 1116 | ASN  |
| 6   | N     | 1129 | THR  |
| 6   | N     | 1130 | ARG  |
| 6   | N     | 1144 | LEU  |
| 6   | N     | 1151 | ARG  |
| 6   | N     | 1152 | GLU  |
| 6   | N     | 1155 | VAL  |
| 6   | N     | 1160 | LEU  |
| 6   | N     | 1166 | LEU  |
| 6   | N     | 1170 | ASP  |
| 6   | N     | 1197 | ARG  |
| 6   | N     | 1204 | CYS  |
| 6   | N     | 1207 | TYR  |
| 6   | N     | 1208 | ASP  |
| 6   | N     | 1211 | MET  |
| 6   | N     | 1219 | GLU  |
| 6   | N     | 1228 | SER  |
| 6   | N     | 1232 | PRO  |
| 6   | N     | 1237 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | N     | 1238 | MET  |
| 6   | N     | 1242 | HIS  |
| 6   | N     | 1251 | ASP  |
| 6   | N     | 1257 | PRO  |
| 6   | N     | 1260 | ILE  |
| 6   | N     | 1262 | LEU  |
| 6   | N     | 1264 | GLU  |
| 6   | N     | 1333 | HIS  |
| 6   | N     | 1334 | GLN  |
| 6   | N     | 1337 | GLU  |
| 6   | N     | 1345 | GLU  |
| 6   | N     | 1348 | LEU  |
| 6   | N     | 1350 | GLU  |
| 6   | N     | 1365 | ASP  |
| 6   | N     | 1380 | GLU  |
| 6   | N     | 1381 | VAL  |
| 6   | N     | 1389 | LEU  |
| 6   | N     | 1391 | GLU  |
| 6   | N     | 1397 | LYS  |
| 6   | N     | 1412 | LYS  |
| 6   | N     | 1415 | VAL  |
| 6   | N     | 1418 | LYS  |
| 6   | N     | 1422 | MET  |
| 6   | N     | 1429 | LEU  |
| 6   | N     | 1431 | THR  |
| 6   | N     | 1432 | LYS  |
| 6   | N     | 1433 | SER  |
| 6   | N     | 1435 | LEU  |
| 6   | N     | 1440 | PHE  |
| 6   | N     | 1441 | GLN  |
| 6   | N     | 1449 | GLU  |
| 6   | N     | 1452 | ILE  |
| 6   | N     | 1455 | LYS  |
| 6   | N     | 1464 | GLU  |
| 6   | N     | 1471 | LEU  |
| 6   | N     | 1472 | ILE  |
| 6   | N     | 1481 | VAL  |
| 6   | N     | 1489 | GLN  |
| 6   | N     | 1492 | LEU  |
| 7   | O     | 20   | THR  |
| 7   | O     | 30   | LEU  |
| 7   | O     | 41   | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | O     | 43  | GLU  |
| 7   | O     | 46  | PRO  |
| 7   | O     | 48  | MET  |
| 7   | O     | 59  | ASN  |
| 7   | O     | 69  | LEU  |
| 7   | O     | 72  | ARG  |
| 7   | O     | 81  | PRO  |
| 7   | O     | 82  | GLU  |
| 7   | O     | 86  | GLN  |
| 7   | O     | 89  | MET  |
| 7   | O     | 94  | PRO  |
| 7   | O     | 96  | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | A     | 38  | ASN  |
| 4   | A     | 91  | ASN  |
| 4   | A     | 124 | ASN  |
| 4   | A     | 163 | ASN  |
| 4   | A     | 180 | GLN  |
| 4   | A     | 212 | ASN  |
| 4   | A     | 221 | HIS  |
| 4   | B     | 95  | GLN  |
| 4   | B     | 124 | ASN  |
| 4   | B     | 128 | HIS  |
| 4   | B     | 139 | ASN  |
| 4   | B     | 180 | GLN  |
| 4   | B     | 212 | ASN  |
| 4   | B     | 221 | HIS  |
| 4   | B     | 229 | GLN  |
| 5   | C     | 22  | GLN  |
| 5   | C     | 80  | GLN  |
| 5   | C     | 130 | ASN  |
| 5   | C     | 139 | GLN  |
| 5   | C     | 187 | ASN  |
| 5   | C     | 320 | HIS  |
| 5   | C     | 327 | HIS  |
| 5   | C     | 343 | GLN  |
| 5   | C     | 390 | GLN  |
| 5   | C     | 393 | GLN  |
| 5   | C     | 399 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | C     | 406  | HIS  |
| 5   | C     | 431  | HIS  |
| 5   | C     | 434  | HIS  |
| 5   | C     | 500  | ASN  |
| 5   | C     | 565  | GLN  |
| 5   | C     | 567  | GLN  |
| 5   | C     | 575  | GLN  |
| 5   | C     | 609  | ASN  |
| 5   | C     | 639  | GLN  |
| 5   | C     | 663  | ASN  |
| 5   | C     | 834  | GLN  |
| 5   | C     | 841  | ASN  |
| 5   | C     | 872  | ASN  |
| 5   | C     | 881  | ASN  |
| 5   | C     | 889  | HIS  |
| 5   | C     | 899  | GLN  |
| 5   | C     | 969  | GLN  |
| 5   | C     | 1019 | GLN  |
| 5   | C     | 1026 | GLN  |
| 5   | C     | 1030 | GLN  |
| 5   | C     | 1050 | GLN  |
| 5   | C     | 1100 | GLN  |
| 5   | C     | 1107 | ASN  |
| 6   | D     | 33   | ASN  |
| 6   | D     | 143  | ASN  |
| 6   | D     | 166  | GLN  |
| 6   | D     | 189  | GLN  |
| 6   | D     | 463  | GLN  |
| 6   | D     | 549  | ASN  |
| 6   | D     | 616  | GLN  |
| 6   | D     | 636  | GLN  |
| 6   | D     | 703  | ASN  |
| 6   | D     | 709  | HIS  |
| 6   | D     | 714  | GLN  |
| 6   | D     | 727  | GLN  |
| 6   | D     | 756  | GLN  |
| 6   | D     | 762  | GLN  |
| 6   | D     | 824  | ASN  |
| 6   | D     | 917  | GLN  |
| 6   | D     | 962  | GLN  |
| 6   | D     | 973  | GLN  |
| 6   | D     | 976  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | D     | 1005 | GLN  |
| 6   | D     | 1010 | ASN  |
| 6   | D     | 1014 | ASN  |
| 6   | D     | 1033 | GLN  |
| 6   | D     | 1103 | HIS  |
| 6   | D     | 1195 | GLN  |
| 6   | D     | 1227 | GLN  |
| 6   | D     | 1334 | GLN  |
| 6   | D     | 1359 | GLN  |
| 6   | D     | 1441 | GLN  |
| 6   | D     | 1442 | ASN  |
| 6   | D     | 1445 | HIS  |
| 6   | D     | 1465 | ASN  |
| 6   | D     | 1485 | GLN  |
| 7   | E     | 28   | GLN  |
| 7   | E     | 29   | GLN  |
| 7   | E     | 33   | HIS  |
| 7   | E     | 37   | ASN  |
| 7   | E     | 59   | ASN  |
| 7   | E     | 86   | GLN  |
| 4   | K     | 16   | GLN  |
| 4   | K     | 38   | ASN  |
| 4   | K     | 95   | GLN  |
| 4   | K     | 124  | ASN  |
| 4   | K     | 139  | ASN  |
| 4   | K     | 156  | HIS  |
| 4   | K     | 212  | ASN  |
| 4   | K     | 213  | GLN  |
| 4   | K     | 229  | GLN  |
| 4   | L     | 38   | ASN  |
| 4   | L     | 81   | ASN  |
| 4   | L     | 95   | GLN  |
| 4   | L     | 124  | ASN  |
| 4   | L     | 128  | HIS  |
| 4   | L     | 212  | ASN  |
| 4   | L     | 227  | ASN  |
| 5   | M     | 31   | GLN  |
| 5   | M     | 45   | GLN  |
| 5   | M     | 80   | GLN  |
| 5   | M     | 91   | GLN  |
| 5   | M     | 139  | GLN  |
| 5   | M     | 187  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | M     | 204  | GLN  |
| 5   | M     | 343  | GLN  |
| 5   | M     | 374  | ASN  |
| 5   | M     | 406  | HIS  |
| 5   | M     | 552  | HIS  |
| 5   | M     | 565  | GLN  |
| 5   | M     | 575  | GLN  |
| 5   | M     | 609  | ASN  |
| 5   | M     | 633  | GLN  |
| 5   | M     | 639  | GLN  |
| 5   | M     | 704  | HIS  |
| 5   | M     | 829  | GLN  |
| 5   | M     | 834  | GLN  |
| 5   | M     | 841  | ASN  |
| 5   | M     | 845  | ASN  |
| 5   | M     | 872  | ASN  |
| 5   | M     | 881  | ASN  |
| 5   | M     | 889  | HIS  |
| 5   | M     | 899  | GLN  |
| 5   | M     | 991  | GLN  |
| 5   | M     | 1047 | HIS  |
| 5   | M     | 1050 | GLN  |
| 5   | M     | 1064 | ASN  |
| 5   | M     | 1107 | ASN  |
| 6   | N     | 125  | GLN  |
| 6   | N     | 151  | GLN  |
| 6   | N     | 442  | ASN  |
| 6   | N     | 507  | ASN  |
| 6   | N     | 529  | GLN  |
| 6   | N     | 541  | ASN  |
| 6   | N     | 549  | ASN  |
| 6   | N     | 552  | ASN  |
| 6   | N     | 575  | GLN  |
| 6   | N     | 584  | ASN  |
| 6   | N     | 616  | GLN  |
| 6   | N     | 680  | GLN  |
| 6   | N     | 696  | HIS  |
| 6   | N     | 703  | ASN  |
| 6   | N     | 714  | GLN  |
| 6   | N     | 727  | GLN  |
| 6   | N     | 737  | ASN  |
| 6   | N     | 744  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | N     | 756  | GLN  |
| 6   | N     | 845  | ASN  |
| 6   | N     | 861  | GLN  |
| 6   | N     | 906  | GLN  |
| 6   | N     | 976  | GLN  |
| 6   | N     | 1010 | ASN  |
| 6   | N     | 1014 | ASN  |
| 6   | N     | 1025 | GLN  |
| 6   | N     | 1033 | GLN  |
| 6   | N     | 1124 | GLN  |
| 6   | N     | 1195 | GLN  |
| 6   | N     | 1334 | GLN  |
| 6   | N     | 1445 | HIS  |
| 6   | N     | 1465 | ASN  |
| 7   | O     | 29   | GLN  |
| 7   | O     | 78   | ASN  |
| 7   | O     | 86   | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed     | Backbone Outliers | Pucker Outliers |
|-----|-------|--------------|-------------------|-----------------|
| 2   | H     | 16/16 (100%) | 12 (75%)          | 8 (50%)         |
| 2   | Y     | 16/16 (100%) | 11 (68%)          | 8 (50%)         |
| All | All   | 32/32 (100%) | 23 (71%)          | 16 (50%)        |

All (23) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 2   | A    |
| 2   | H     | 3   | G    |
| 2   | H     | 6   | U    |
| 2   | H     | 7   | G    |
| 2   | H     | 8   | C    |
| 2   | H     | 9   | G    |
| 2   | H     | 10  | G    |
| 2   | H     | 12  | G    |
| 2   | H     | 13  | C    |
| 2   | H     | 14  | G    |
| 2   | H     | 15  | C    |
| 2   | H     | 16  | G    |
| 2   | Y     | 2   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Y     | 3   | G    |
| 2   | Y     | 6   | U    |
| 2   | Y     | 7   | G    |
| 2   | Y     | 8   | C    |
| 2   | Y     | 9   | G    |
| 2   | Y     | 10  | G    |
| 2   | Y     | 12  | G    |
| 2   | Y     | 13  | C    |
| 2   | Y     | 14  | G    |
| 2   | Y     | 15  | C    |

All (16) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 1   | G    |
| 2   | H     | 6   | U    |
| 2   | H     | 7   | G    |
| 2   | H     | 8   | C    |
| 2   | H     | 9   | G    |
| 2   | H     | 12  | G    |
| 2   | H     | 13  | C    |
| 2   | H     | 15  | C    |
| 2   | Y     | 1   | G    |
| 2   | Y     | 6   | U    |
| 2   | Y     | 7   | G    |
| 2   | Y     | 8   | C    |
| 2   | Y     | 9   | G    |
| 2   | Y     | 12  | G    |
| 2   | Y     | 13  | C    |
| 2   | Y     | 15  | 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

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 10  | APC  | D     | 3999 | 9    | 29,33,33     | 1.30 | 4 (13%)  | 44,52,52    | 1.67 | 8 (18%)  |
| 10  | APC  | N     | 4999 | 9    | 29,33,33     | 1.11 | 3 (10%)  | 44,52,52    | 1.69 | 8 (18%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|------|------|---------|-------------|---------|
| 10  | APC  | D     | 3999 | 9    | -       | 10/19/38/38 | 0/3/3/3 |
| 10  | APC  | N     | 4999 | 9    | -       | 8/19/38/38  | 0/3/3/3 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 10  | D     | 3999 | APC  | PB-O3B | 3.51  | 1.62        | 1.58     |
| 10  | D     | 3999 | APC  | PB-O2B | -3.41 | 1.48        | 1.56     |
| 10  | N     | 4999 | APC  | PB-O3B | 3.11  | 1.61        | 1.58     |
| 10  | D     | 3999 | APC  | PA-O2A | -3.02 | 1.49        | 1.56     |
| 10  | N     | 4999 | APC  | PB-O2B | -2.91 | 1.49        | 1.56     |
| 10  | N     | 4999 | APC  | PA-O2A | -2.69 | 1.49        | 1.56     |
| 10  | D     | 3999 | APC  | C2-N3  | -2.33 | 1.29        | 1.33     |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 10  | N     | 4999 | APC  | C1'-N9-C8 | 5.00  | 138.20      | 127.09   |
| 10  | D     | 3999 | APC  | C1'-N9-C8 | 4.91  | 138.00      | 127.09   |
| 10  | N     | 4999 | APC  | C4-N9-C1' | -4.51 | 116.08      | 126.63   |
| 10  | D     | 3999 | APC  | C4-N9-C1' | -4.24 | 116.72      | 126.63   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10  | N     | 4999 | APC  | PB-O3B-PG   | -3.62 | 119.47      | 132.45   |
| 10  | D     | 3999 | APC  | PB-O3B-PG   | -3.57 | 119.65      | 132.45   |
| 10  | N     | 4999 | APC  | O4'-C1'-N9  | 3.20  | 114.23      | 108.09   |
| 10  | D     | 3999 | APC  | O2A-PA-O1A  | 3.12  | 120.11      | 109.95   |
| 10  | N     | 4999 | APC  | O2A-PA-O1A  | 3.08  | 119.98      | 109.95   |
| 10  | N     | 4999 | APC  | O2B-PB-O1B  | 3.07  | 119.93      | 109.95   |
| 10  | D     | 3999 | APC  | O2B-PB-O1B  | 3.01  | 119.75      | 109.95   |
| 10  | D     | 3999 | APC  | O2'-C2'-C3' | -2.90 | 102.51      | 111.82   |
| 10  | D     | 3999 | APC  | O4'-C1'-N9  | 2.84  | 113.55      | 108.09   |
| 10  | N     | 4999 | APC  | C2'-C3'-C4' | 2.44  | 107.31      | 102.61   |
| 10  | D     | 3999 | APC  | C2'-C3'-C4' | 2.37  | 107.20      | 102.61   |
| 10  | N     | 4999 | APC  | C2'-C1'-N9  | -2.34 | 107.48      | 113.30   |

There are no chirality outliers.

All (18) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 10  | D     | 3999 | APC  | PA-C3A-PB-O1B   |
| 10  | D     | 3999 | APC  | PA-C3A-PB-O3B   |
| 10  | D     | 3999 | APC  | PB-C3A-PA-O1A   |
| 10  | D     | 3999 | APC  | PB-C3A-PA-O5'   |
| 10  | N     | 4999 | APC  | PA-C3A-PB-O1B   |
| 10  | N     | 4999 | APC  | PA-C3A-PB-O3B   |
| 10  | N     | 4999 | APC  | PB-C3A-PA-O1A   |
| 10  | N     | 4999 | APC  | PB-C3A-PA-O5'   |
| 10  | N     | 4999 | APC  | C5'-O5'-PA-O2A  |
| 10  | D     | 3999 | APC  | O4'-C4'-C5'-O5' |
| 10  | N     | 4999 | APC  | O4'-C4'-C5'-O5' |
| 10  | N     | 4999 | APC  | C4'-C5'-O5'-PA  |
| 10  | D     | 3999 | APC  | C3'-C4'-C5'-O5' |
| 10  | D     | 3999 | APC  | PA-C3A-PB-O2B   |
| 10  | N     | 4999 | APC  | PA-C3A-PB-O2B   |
| 10  | D     | 3999 | APC  | C4'-C5'-O5'-PA  |
| 10  | D     | 3999 | APC  | C5'-O5'-PA-O2A  |
| 10  | D     | 3999 | APC  | C5'-O5'-PA-O1A  |

There are no ring outliers.

2 monomers are involved in 4 short contacts:

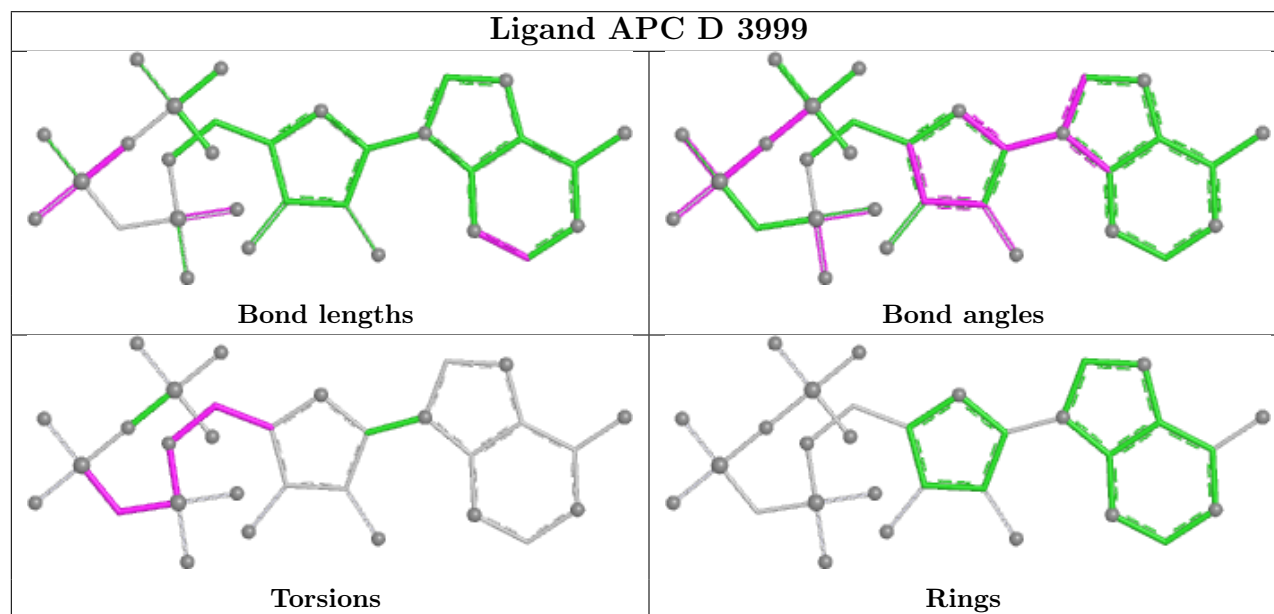
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 10  | D     | 3999 | APC  | 2       | 0            |

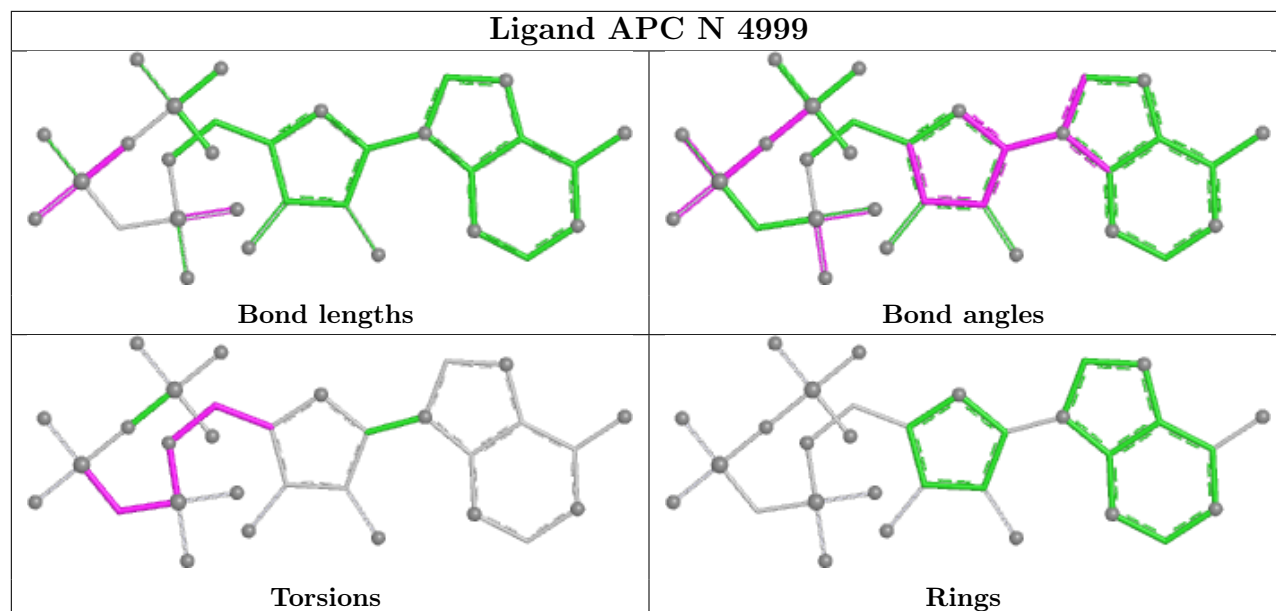
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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 10  | N     | 4999 | APC  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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   | G     | 23/23 (100%)     | -1.77  | 0 100 100 | 22, 46, 76, 79        | 0     |
| 1   | X     | 23/23 (100%)     | -1.81  | 0 100 100 | 21, 38, 71, 90        | 0     |
| 2   | H     | 16/16 (100%)     | -1.92  | 0 100 100 | 36, 56, 100, 102      | 0     |
| 2   | Y     | 16/16 (100%)     | -1.96  | 0 100 100 | 21, 73, 101, 103      | 0     |
| 3   | I     | 13/14 (92%)      | -1.69  | 0 100 100 | 49, 65, 74, 85        | 0     |
| 3   | Z     | 13/14 (92%)      | -1.75  | 0 100 100 | 54, 67, 80, 81        | 0     |
| 4   | A     | 229/315 (72%)    | -1.53  | 0 100 100 | 41, 66, 86, 94        | 0     |
| 4   | B     | 229/315 (72%)    | -1.48  | 0 100 100 | 43, 70, 85, 101       | 0     |
| 4   | K     | 229/315 (72%)    | -1.53  | 0 100 100 | 41, 65, 81, 93        | 0     |
| 4   | L     | 229/315 (72%)    | -1.50  | 0 100 100 | 38, 68, 80, 90        | 0     |
| 5   | C     | 1119/1119 (100%) | -1.50  | 0 100 100 | 26, 64, 86, 101       | 0     |
| 5   | M     | 1119/1119 (100%) | -1.49  | 0 100 100 | 25, 65, 89, 109       | 0     |
| 6   | D     | 1264/1524 (82%)  | -1.52  | 0 100 100 | 23, 61, 83, 100       | 0     |
| 6   | N     | 1264/1524 (82%)  | -1.53  | 0 100 100 | 26, 60, 84, 100       | 0     |
| 7   | E     | 95/99 (95%)      | -1.54  | 0 100 100 | 35, 59, 74, 82        | 0     |
| 7   | O     | 95/99 (95%)      | -1.56  | 0 100 100 | 45, 66, 80, 84        | 0     |
| All | All   | 5976/6850 (87%)  | -1.52  | 0 100 100 | 21, 64, 86, 109       | 0     |

There are no RSRZ outliers to report.

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

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](#)

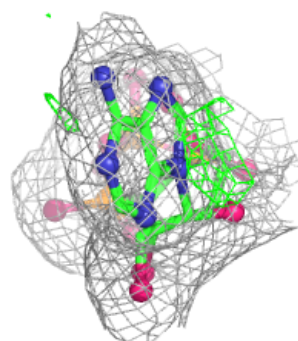
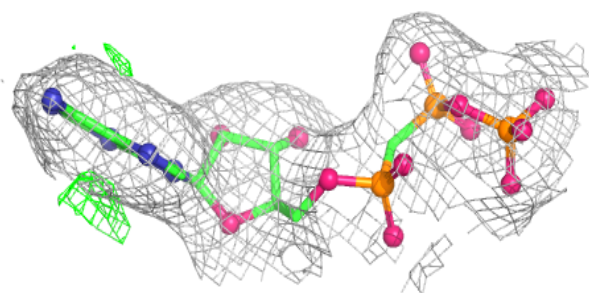
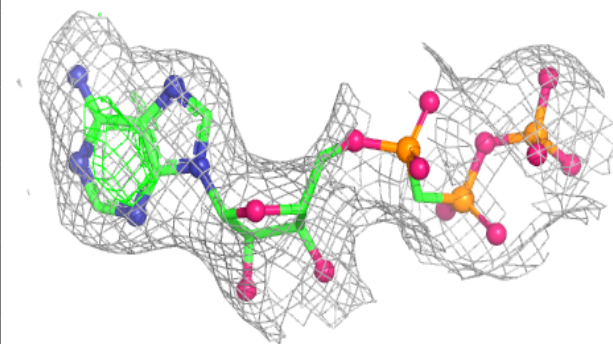
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 8   | ZN   | D     | 4058 | 1/1   | 1.00 | 0.02 | 66,66,66,66                 | 0     |
| 8   | ZN   | D     | 6112 | 1/1   | 1.00 | 0.01 | 59,59,59,59                 | 0     |
| 8   | ZN   | N     | 5058 | 1/1   | 1.00 | 0.02 | 66,66,66,66                 | 0     |
| 8   | ZN   | N     | 7112 | 1/1   | 1.00 | 0.01 | 65,65,65,65                 | 0     |
| 9   | MG   | D     | 8001 | 1/1   | 1.00 | 0.01 | 23,23,23,23                 | 0     |
| 9   | MG   | D     | 8002 | 1/1   | 1.00 | 0.01 | 25,25,25,25                 | 0     |
| 9   | MG   | N     | 9001 | 1/1   | 1.00 | 0.01 | 21,21,21,21                 | 0     |
| 9   | MG   | N     | 9002 | 1/1   | 1.00 | 0.01 | 23,23,23,23                 | 0     |
| 10  | APC  | D     | 3999 | 31/31 | 1.00 | 0.03 | 41,49,52,54                 | 0     |
| 10  | APC  | N     | 4999 | 31/31 | 1.00 | 0.03 | 45,49,51,54                 | 0     |

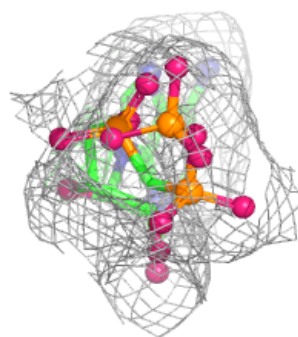
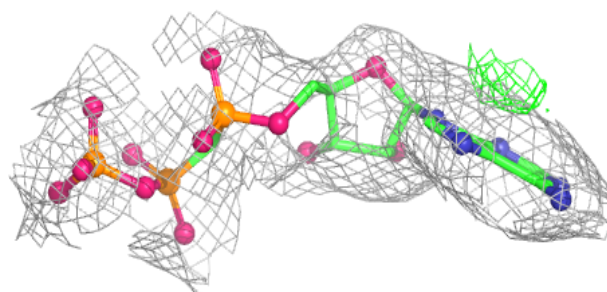
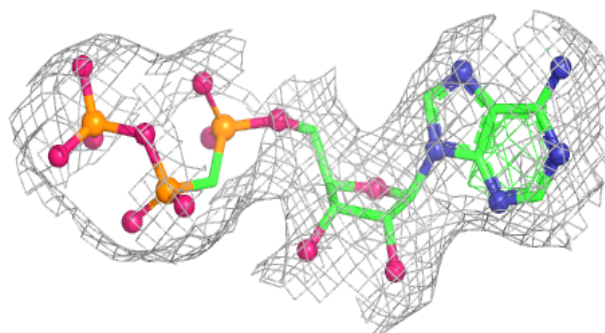
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around APC D 3999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around APC N 4999:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.