



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:59 AM EDT

PDB ID : 1SFO / pdb\_00001sfo  
Title : RNA POLYMERASE II STRAND SEPARATED ELONGATION COMPLEX  
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.  
Deposited on : 2004-02-20  
Resolution : 3.61 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

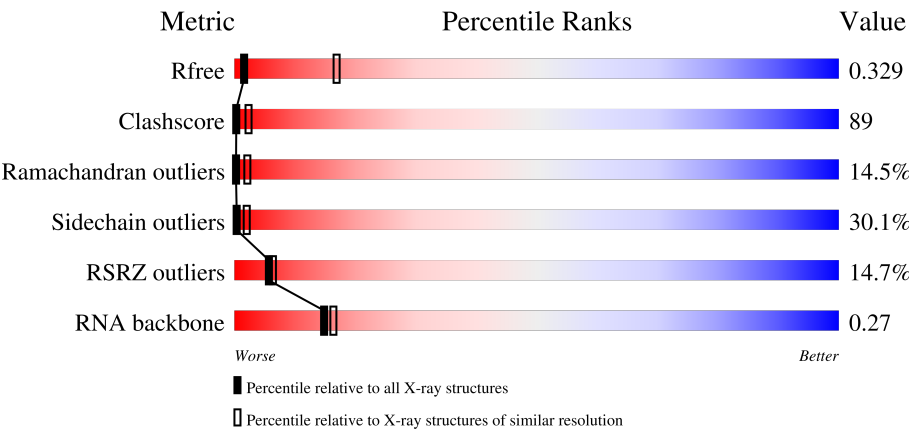
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.61 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 <sub>free</sub>     | 180053                      | 1062 (3.72-3.52)                                      |
| Clashscore            | 190562                      | 1092 (3.72-3.52)                                      |
| Ramachandran outliers | 187476                      | 1057 (3.72-3.52)                                      |
| Sidechain outliers    | 187428                      | 1055 (3.72-3.52)                                      |
| RSRZ outliers         | 180081                      | 1060 (3.72-3.52)                                      |
| RNA backbone          | 3983                        | 1018 (4.18-3.06)                                      |

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   | R     | 10     | <div><div>100%</div><div><div></div><div></div><div></div><div></div></div><div>40%40%20%</div></div>      |
| 2   | T     | 14     | <div><div>93%</div><div><div></div><div></div><div></div><div></div></div><div>21%64%14%</div></div>       |
| 3   | A     | 1733   | <div><div>12%</div><div><div></div><div></div><div></div><div></div></div><div>9%34%27%11%20%</div></div>  |
| 4   | B     | 1224   | <div><div>12%</div><div><div></div><div></div><div></div><div></div></div><div>12%39%29%10%10%</div></div> |

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| Mol | Chain | Length | Quality of chain                                                                                         |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------|
| 5   | C     | 318    | <div><div></div><div>4%</div><div>15%</div><div>34%</div><div>28%</div><div>6%</div><div>16%</div></div> |
| 6   | E     | 215    | <div><div></div><div>30%</div><div>11%</div><div>40%</div><div>38%</div><div>11%</div></div>             |
| 7   | F     | 155    | <div><div></div><div>6%</div><div>8%</div><div>27%</div><div>18%</div><div>46%</div></div>               |
| 8   | H     | 146    | <div><div></div><div>17%</div><div>9%</div><div>30%</div><div>34%</div><div>18%</div><div>9%</div></div> |
| 9   | I     | 122    | <div><div></div><div>14%</div><div>16%</div><div>30%</div><div>39%</div><div>12%</div></div>             |
| 10  | J     | 70     | <div><div></div><div>6%</div><div>13%</div><div>41%</div><div>24%</div><div>14%</div><div>7%</div></div> |
| 11  | K     | 120    | <div><div></div><div>2%</div><div>10%</div><div>53%</div><div>25%</div><div>7%</div><div>5%</div></div>  |
| 12  | L     | 70     | <div><div></div><div>10%</div><div>26%</div><div>20%</div><div>17%</div><div>34%</div></div>             |

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 28647 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 RNA chain called RNA STRAND.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 1   | R     | 10       | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 217   | 98 | 45 | 65 | 9 |         |         |       |

- Molecule 2 is a DNA chain called DNA STRAND.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 2   | T     | 14       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 279   | 135 | 48 | 83 | 13 |         |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase II largest subunit.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | A     | 1395     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10969 | 6917 | 1923 | 2068 | 61 |         |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 4   | B     | 1106     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8793  | 5568 | 1538 | 1632 | 55 |         |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 5   | C     | 266      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2095  | 1317 | 348 | 417 | 13 |         |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 6   | E     | 214      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1752  | 1111 | 309 | 321 | 11 |         |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | F     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 679   | 434 | 115 | 127 | 3 |         |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 133      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1068  | 673 | 180 | 211 | 4 |         |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 9   | I     | 119      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 971   | 596 | 179 | 186 | 10 |         |         |       |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | J     | 65       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 532   | 339 | 93 | 94 | 6 |         |         |       |

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | K     | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 919   | 590 | 156 | 171 | 2 |         |         |       |

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | L     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 364   | 224 | 72 | 64 | 4 |         |         |       |

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 13  | A     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 13  | B     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 13  | C     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 13  | I     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 13  | J     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 13  | L     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

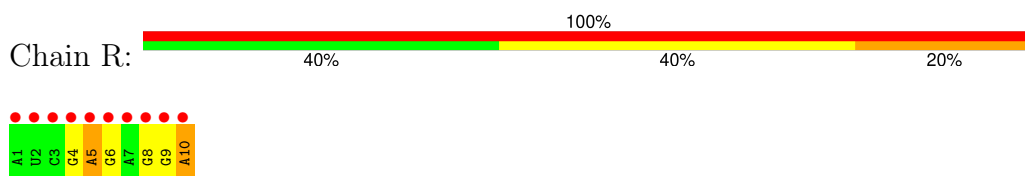
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 14  | A     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

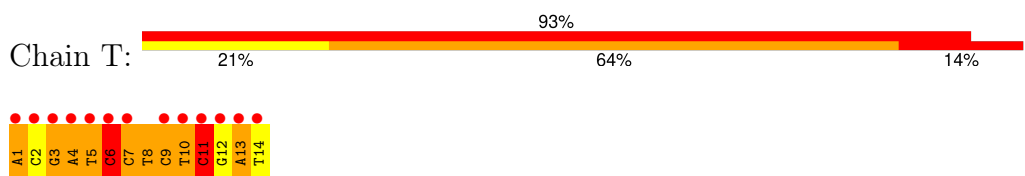
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

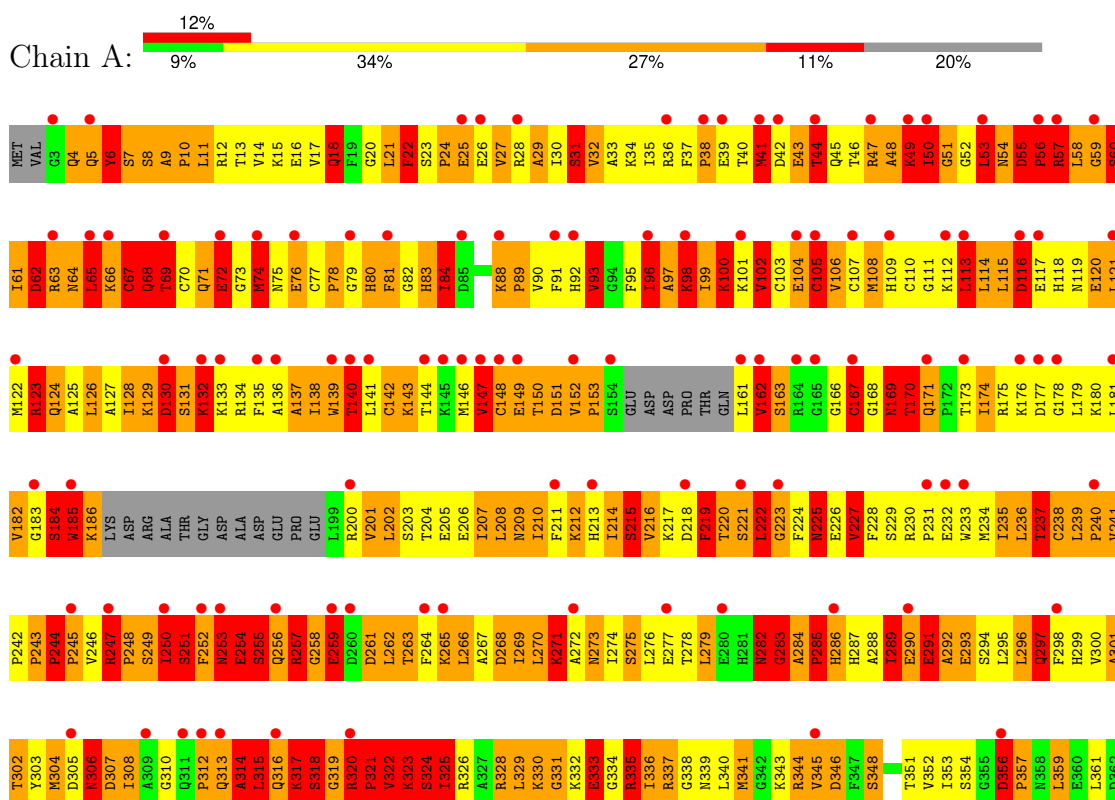
#### • Molecule 1: RNA STRAND



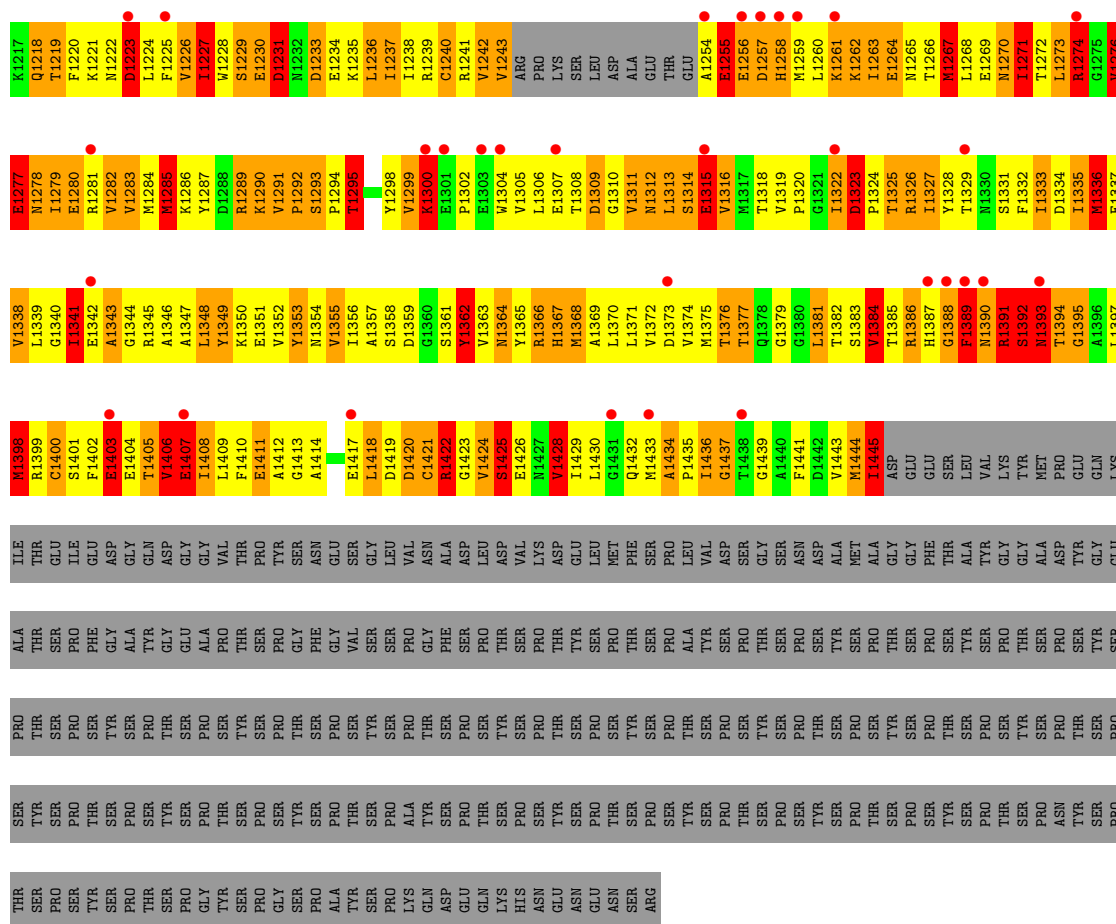
#### • Molecule 2: DNA STRAND



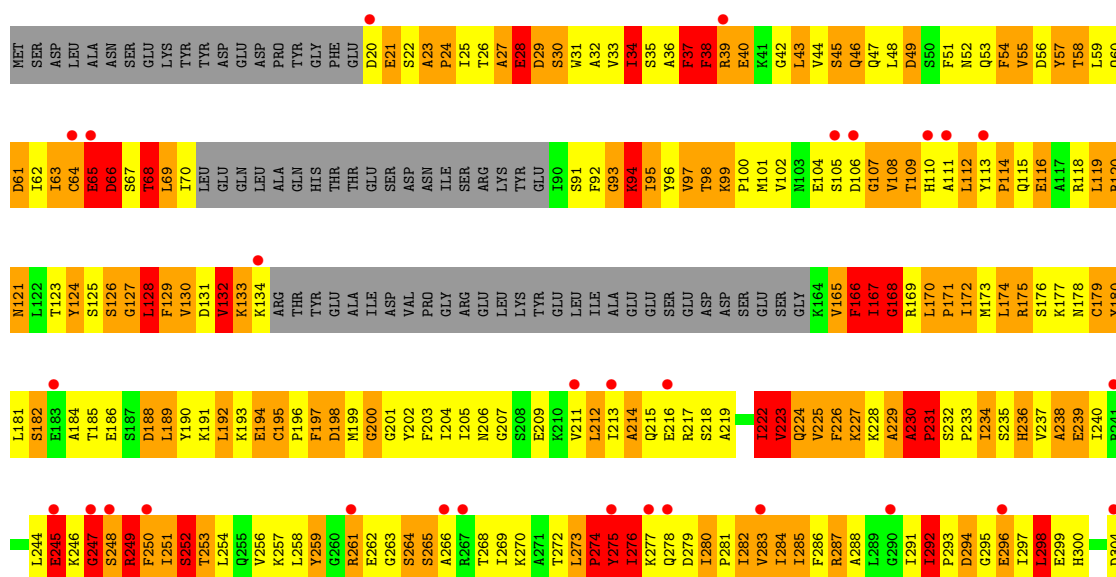
#### • Molecule 3: DNA-directed RNA polymerase II largest subunit



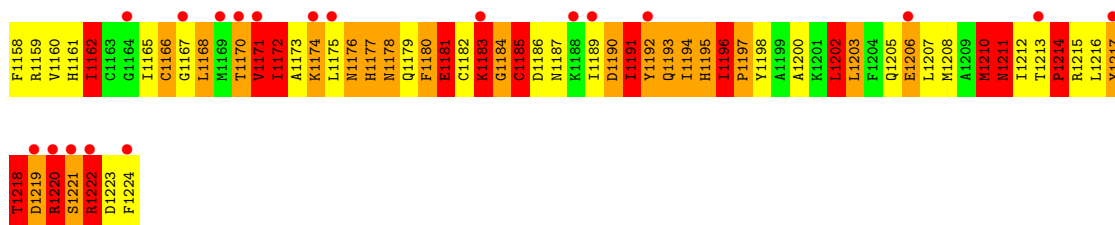
|       |       |       |       |      |      |       |      |      |      |      |      |      |      |      |
|-------|-------|-------|-------|------|------|-------|------|------|------|------|------|------|------|------|
| D1157 | P1156 | G1097 | L1037 | K977 | S917 | R857  | E795 | A733 | G673 | Q611 | Y551 | M487 | Q425 | Q363 |
| P1158 | P1159 | V1095 | T1038 | P978 | E918 | N858  | S796 | E734 | P674 | I612 | W552 | M487 | L426 | V364 |
| S1160 | R1100 | R1099 | K1039 | S979 | I919 | S859  | K797 | N735 | T675 | I613 | P553 | H490 | Q427 | G365 |
| T1161 | L1101 | R1100 | Q1040 | D980 | L920 | L860  |      | N736 | M676 | F614 | P554 | H491 | Y428 | P366 |
| V1162 | F1042 | K1102 | A1041 | L981 | G921 | G861  | E801 | K738 | R677 | G615 | W555 | Q493 | G429 | P367 |
| I1163 | D1043 | E1103 | D1043 | T982 | D922 | N862  | N802 | N738 | E678 | V616 | W556 | Q493 | M430 | K368 |
| P1164 | W1044 | L1104 | K984  | L983 | L923 | V863  | N802 | K738 | T679 | V617 | D557 | S494 | K431 | S369 |
| E1165 | V1045 | D985  | L925  | K924 | L925 | I864  | S803 | L740 | T680 | E618 | G558 | E496 | V432 | I370 |
| D1166 | L1046 | R986  | V926  | F926 | Q926 | F866  | Y804 | N742 | E681 | K619 | V559 | E496 | E433 | T373 |
| E1167 | S1047 | V987  | Q927  | F987 | Q927 | F866  | L805 | N742 | T682 | I620 | I560 | T497 | R435 | L374 |
| I1168 | N1048 | L988  | L928  | L928 | L928 | Y868  | R806 | V743 | T683 | T621 | R434 | R498 | R435 | L374 |
| E1169 | T1049 | G989  | L929  | L929 | L929 | G869  | G807 | K744 | A684 | G623 | T562 | A499 | L436 | T375 |
| I1170 | E1050 | E870  | T809  | T809 | T809 | E870  | T809 | N746 | A686 | S624 | A564 | E500 | M437 | Y376 |
| Q1171 | A1051 | D871  | P810  | P810 | P810 | D871  | P810 | N747 | K687 | S625 | I565 | E500 | P377 | P377 |
| L1172 | Q1052 | G872  | Q811  | Q811 | Q811 | G872  | Q811 | N748 | K688 | N626 | I566 | E500 | P378 | E378 |
| H1173 | F1053 | M873  | E812  | E812 | E812 | M873  | E812 | N748 | K689 | S627 | I566 | A506 | P441 | V379 |
| L1174 | L1054 | D874  | F813  | F813 | F813 | D874  | F813 | N749 | K690 | G628 | K567 | A506 | V442 | T381 |
| S1175 | R1055 | A875  | F814  | F814 | F814 | A875  | F814 | N751 | V690 | L629 | K569 | V507 | L443 | P382 |
| L1176 | S1056 | H876  | F815  | F815 | F815 | H876  | F815 | N752 | V692 | I630 | P570 | V507 | F444 | Y383 |
| LEU   | V1057 | H877  | H816  | H816 | H816 | H877  | H816 | N753 | D692 |      | L571 | T511 | M445 | N384 |
| ASP   | W1058 | I878  | A817  | A817 | A817 | I878  | A817 | N754 | T694 | V633 | W572 | S513 | R446 | T385 |
| GLU   | V1059 | E879  | M818  | M818 | M818 | E879  | M818 | N755 | T694 | T634 | S573 | S513 | Q447 | D386 |
| ALA   | P1060 | K880  | G819  | G819 | G819 | K880  | G819 | N756 | E696 | R635 | K574 | P514 | P448 | R387 |
| GLU   | G1061 | Q881  | G820  | G820 | G820 | Q881  | G820 | N757 | A697 |      | K575 | Q515 | S449 | L388 |
| GLN   | E1062 | S882  | E822  | E822 | E822 | S882  | E822 | N758 | Q698 | G638 | Q576 | S516 | L450 | T389 |
| SER   | V1064 | L843  | E823  | E823 | E823 | L843  | E823 | N759 | A699 | P639 | I577 | N517 | H451 | Q390 |
| PHE   | G1065 | D884  | G824  | G824 | G824 | D884  | G824 | N760 | A700 | Q640 | L578 | K518 | R452 | Q391 |
| ASP   | V1066 | E845  | L824  | L824 | L824 | E845  | L824 | N761 | V641 | G642 | S579 | P519 | Q447 | V392 |
| Q1187 | L1067 | I886  | I825  | I825 | I825 | I886  | I825 | N762 | W702 | C642 | V580 | C520 | S454 | R393 |
| Q1188 | A1068 | G887  | D826  | D826 | D826 | G887  | D826 | N763 | T703 | A643 | A581 | N521 | M455 | N394 |
| S1189 | R1069 | Q888  | T827  | T827 | T827 | Q888  | T827 | N764 | A704 | K644 | I582 | G522 | M456 | G395 |
| P1190 | A1070 | S889  | T828  | T828 | T828 | S889  | T828 | N765 | A705 | L645 | P583 | G522 | M457 | P396 |
| W1191 | Q1071 | D890  | V829  | V829 | V829 | D890  | V829 | N766 | Q767 | F646 | N584 | G525 | H458 | N397 |
| L1192 | L1072 | A891  | K830  | K830 | K830 | A891  | K830 | N767 | Q768 | G647 | V524 | G525 |      | E398 |
| L1193 | G1073 | E892  | T831  | T831 | T831 | E892  | T831 | N768 | W708 | N648 | I586 | D526 | V462 | H399 |
| I1194 | E1074 | F893  | A832  | A832 | A832 | F893  | A832 | N769 | T709 | I649 | H587 | T527 | T463 | P400 |
| L1195 | P1075 | E894  | E833  | E833 | E833 | E894  | E833 | N770 | L710 | Q650 | L588 | L528 | P464 | G401 |
| S1196 | L1015 | K895  | T834  | T834 | T834 | K895  | T834 | N771 | R711 | K651 | Q589 | C529 | Y465 | C402 |
| L1197 | L1016 | R896  | G835  | G835 | G835 | R896  | G835 | N772 | E712 | V652 | R590 | G530 | S466 | X403 |
| T1197 | L1017 | Y897  | Y836  | Y836 | Y836 | Y897  | Y836 | N773 | S713 | V653 | F591 | I531 | T467 | Y404 |
| L1198 | F1018 | R898  | I837  | I837 | I837 | R898  | I837 | N774 | F714 | N654 | D592 | R532 | F468 | V405 |
| R1199 | G1019 | V899  | Q838  | Q838 | Q838 | V899  | Q838 | N775 | E715 | F655 | E593 | K533 | R469 | I406 |
| H1200 | C1020 | D900  | R839  | R839 | R839 | D900  | R839 | N776 | D716 | V656 | G594 | L534 | L470 | R407 |
| A1201 | L1021 | L901  | R840  | R840 | R840 | L901  | R840 | N777 | N717 | L657 | T595 | T635 | M471 | D408 |
| M1202 | L1022 | L902  | L841  | L841 | L841 | L902  | L841 | N778 | W718 | L658 | T596 | L536 | L472 | S409 |
| N1203 | R1023 | N903  | V842  | V842 | V842 | N903  | V842 | N779 | V719 | L659 | T597 | L537 | L472 |      |
| PHE   | S1024 | T904  | K843  | K843 | K843 | T904  | K843 | N780 | W720 | H659 | L597 | R537 | S473 | R412 |
| HIS   | R1025 | D905  | A844  | A844 | A844 | D905  | A844 | N781 | R721 | N660 | L598 | D538 | V474 | I413 |
| PHE   | L1026 | H906  | L845  | L845 | L845 | H906  | L845 | N782 | F721 | G661 | D599 | T539 | T475 | I413 |
| ALA   | A1027 | T807  | E846  | E846 | E846 | T807  | E846 | N783 | L722 | F662 | P600 | F540 | S476 | D414 |
| GLY   | T1028 | L908  | D847  | D847 | D847 | L908  | D847 | N784 | N723 | S663 | K601 | I541 | P477 | L415 |
| VAL   | R1029 | Q969  | P848  | P848 | P848 | Q969  | P848 | N785 | E724 | T664 | D602 | E542 | Y478 | R416 |
| ALA   | R1030 | P910  | M849  | M849 | M849 | P910  | M849 | N786 | W725 | G665 | N603 | L543 | P477 | R416 |
| SER   | V1031 | S911  | H852  | H852 | H852 | V1031 | H852 | N787 | R726 | I666 | N603 | L543 | Y417 | S418 |
| K1032 | L1032 | L912  | G852  | G852 | G852 | L1032 | G852 | N788 | D727 | G667 | G804 | D544 | A480 | S418 |
| Q1033 | Q1033 | L913  | D853  | D853 | D853 | Q1033 | D853 | N789 | K728 | D668 | M605 | Q545 | F482 | K419 |
| E1034 | E1034 | E914  | N854  | N854 | N854 | E1034 | N854 | N790 | A729 | T669 | L606 | V546 | D482 | R420 |
| T1095 | T1095 | S915  | T855  | T855 | T855 | T1095 | T855 | N791 | W730 | I670 | I607 | L547 | D483 | A421 |
| S1096 | S1096 | T976  | T856  | T856 | T856 | S1096 | T856 | N792 | G730 | I671 | I608 | N548 | G484 | G422 |
|       |       |       |       |      |      |       |      | N794 | L732 | D672 | G610 | L550 | E496 | I424 |



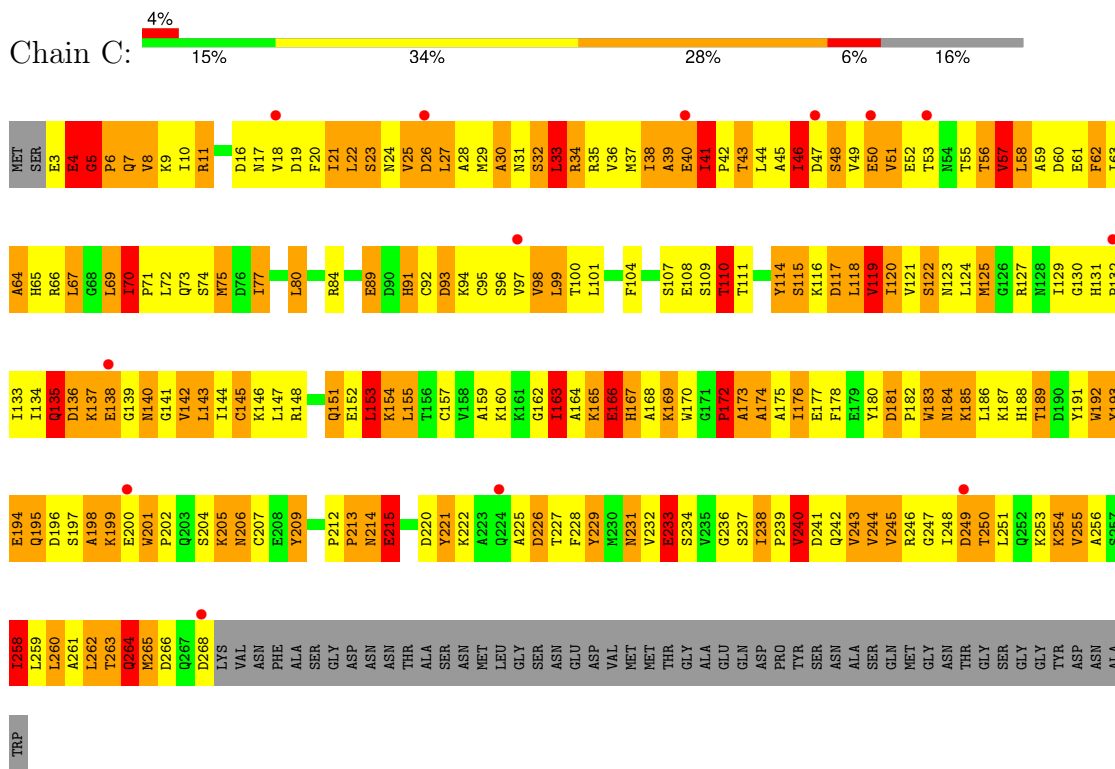
• Molecule 4: DNA-directed RNA polymerase II 140 kDa polypeptide



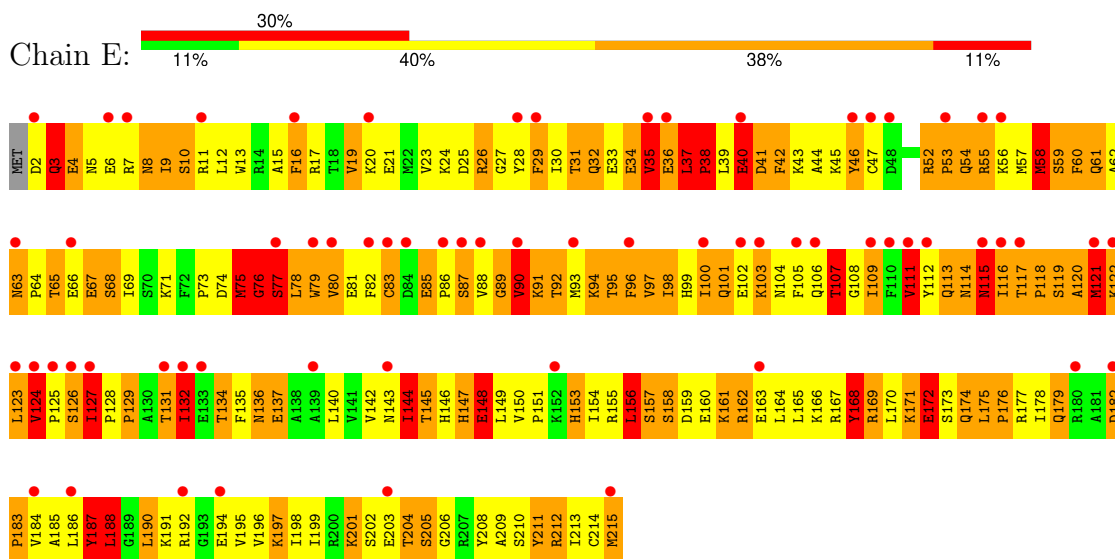
|       |       |       |      |      |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|
| H1097 | A1035 | Q975  | K914 | S853 | M792 | S732 | GLY  | E612 | Q548 | Y488 | D427 | T365 | V305 |
| M1098 | A1036 | I976  | T915 | L854 | A793 | H733 | PHE  | V613 | T549 | S489 | I428 | Q366 | M306 |
| V1099 | L1037 | G977  | T916 | F855 | M794 | H734 | GLU  | S614 | D550 | S490 | F429 | L367 | D307 |
| D1100 | S1038 | D978  | F917 | F856 | I795 | A735 | ASP  | M615 | P551 | T491 | R430 | E368 | W308 |
| D1101 | G1039 | K979  | I918 | R857 | L796 | T736 | VAL  | I616 | M552 | L492 | M431 | Q369 | Q309 |
| K1102 | S919  | F980  | S919 | S858 | L797 | T737 | GLU  | R617 | P553 | S493 | M432 | F370 | M310 |
| A1103 | G1042 | A981  | PRD  | M859 | L798 | F738 | VAL  | D618 | I554 | H494 | M433 | E371 | L311 |
| H1104 | D1043 | S982  | ASP  | M860 | P799 | F739 | P679 | R619 | I555 | L495 | R434 | S372 | E312 |
| A1105 | G1044 | R983  | GLU  | D861 | Q800 | H740 | T680 | R620 | T556 | L496 | T435 | S373 | M313 |
| R1106 | S1045 | H984  | GLU  | K862 | K801 | C741 | M681 | E621 | T556 | L497 | V436 | K374 | L314 |
| A1107 | P1046 | G985  | GLU  | E863 | P802 | E742 | S682 | K622 | F557 | T498 | R497 | A375 | K315 |
| A1108 | G1047 | Q986  | LEU  | K864 | L803 | I743 | S683 | E623 | E560 | M499 | E437 | F376 | P316 |
| G1109 | T1048 | K987  | GLY  | K865 | G804 | H744 | L684 | L624 | E561 | T500 | GLU  | F377 | C317 |
| D1110 | D1049 | G988  | GLN  | Y866 | T805 | P745 | L685 | K625 | Q562 | ALA  | HIS  | L378 | V318 |
| M1111 | I1050 | T989  | ARG  | G867 | R806 | S746 | M686 | I626 | M563 | ASP  | PHE  | G379 | E319 |
| T1112 | T1051 | I990  | THR  | M688 | R807 | M747 | E687 | F627 | GLY  | ASP  | ASP  | D320 | D320 |
| V1113 | V1052 | G991  | ALA  | S869 | A808 | I748 | G688 | T628 | P565 | ASN  | MET  | M381 | G321 |
| L1114 | G1053 | I992  | TYR  | R870 | M809 | L749 | L689 | D629 | L566 | ASP  | GLY  | T382 | F322 |
| T1115 | G1054 | T993  | HIS  | T871 | E810 | G750 | V690 | A630 | E567 | LYS  | L446 | M383 | V323 |
| R1116 | I1055 | Y994  | S933 | E872 | Y811 | V751 | E691 | G631 | D688 | LYS  | L447 | K384 | Y324 |
| Q1117 | S1056 | R995  | K934 | T873 | L812 | A752 | V692 | R632 | V569 | LEU  | A447 | K385 | Q325 |
| P1118 | K1057 | R996  | R935 | K876 | K813 | A753 | L693 | V633 | V570 | A509 | I448 | L386 | D326 |
| V1119 | L1058 | E997  | D936 | R878 | F814 | S754 | D694 | Y634 | K510 | K510 | N449 | L387 | R327 |
| E1120 | L1059 | D998  | A937 | P877 | R815 | I755 | A695 | R635 | P511 | P511 | K450 | C388 | E328 |
| G1121 | R1060 | M999  | S938 | Q878 | E816 | I756 | S696 | P636 | H572 | R512 | K451 | C389 | T329 |
| R1122 | E1061 | P1000 | T939 | R879 | L817 | P757 | E697 | L637 | S574 | Q513 | T452 | L390 | A330 |
| S1123 | H1062 | F1001 | P940 | T880 | P818 | F758 | E699 | F638 | P575 | H515 | T453 | D391 | L331 |
| R1124 | G1063 | T1002 | L941 | T881 | A819 | P759 | E699 | T639 | D576 | L514 | T454 | R392 | D332 |
| G1125 | Y1064 | A1003 | R942 | T882 | G820 | D760 | S700 | V640 | A577 | N516 | S455 | K393 | F333 |
| G1126 | Q1065 | E1004 | K883 | L883 | Q821 | H761 | I701 | E641 | T578 | T517 | G456 | D394 | I334 |
| G1127 | S1066 | G1005 | T944 | R884 | N822 | N822 | L702 | D642 | R579 | H518 | L457 | Q395 | G335 |
| L1128 | L1067 | I1006 | E945 | R885 | A823 | Q763 | L703 | D643 | V580 | H519 | K458 | ARG  | ARG  |
| R1129 | G1068 | V1007 | R946 | K886 | I824 | S764 | A704 | E644 | F581 | G520 | L461 | GLY  | GLY  |
| F1130 | F1069 | D1008 | G947 | R887 | V825 | P765 | M705 | S645 | V582 | L521 | A462 | THR  | THR  |
| G1131 | D1069 | L1009 | R948 | G888 | A826 | R766 | Q706 | L646 | N583 | C523 | T463 | ALA  | ALA  |
| E1132 | V949  | L1010 | T889 | T889 | I827 | N767 | P707 | O647 | G584 | P524 | G464 | LEU  | LEU  |
| M1133 | M1072 | I1011 | R950 | Y890 | A828 | T768 | E708 | K648 | V585 | A525 | N465 | GLY  | GLY  |
| E1134 | Q851  | I1012 | D891 | D891 | C829 | Y769 | D709 | E650 | H587 | E526 | G467 | ILE  | ILE  |
| R1135 | V952  | M1013 | K892 | K892 | Y830 | Q770 | L710 | L651 | G588 | P528 | E468 | LYS  | LYS  |
| D1136 | L953  | H1014 | D894 | D894 | S831 | S771 | E711 | K652 | V589 | E529 | Q469 | E346 | E346 |
| C1137 | V954  | H1015 | D895 | D895 | M773 | A772 | P712 | V653 | H590 | G530 | K470 | K347 | K347 |
| M1138 | T955  | L1016 | T895 | D896 | K835 | G774 | E714 | R654 | R591 | Q531 | K471 | K348 | K348 |
| I1139 | N956  | I1017 | R957 | G897 | E836 | K775 | A715 | K655 | N592 | A532 | A472 | I349 | I349 |
| A1140 | N957  | P1018 | L898 | L898 | D837 | Q776 | ASN  | G656 | P593 | A533 | A473 | Q350 | Q350 |
| H1141 | Q958  | S1019 | D959 | T899 | S838 | A777 | GLU  | H657 | A594 | C533 | M473 | Y351 | Y351 |
| A1144 | A1082 | R1020 | G960 | A900 | M839 | M778 | GLU  | T658 | R595 | G534 | S474 | A414 | A414 |
| S1145 | Q1084 | T1022 | L961 | P901 | I840 | G779 | ASN  | A659 | L596 | L535 | R475 | K352 | K352 |
| F1146 | I1085 | V1023 | G902 | G902 | M841 | V780 | ASP  | K660 | M597 | V536 | R476 | D354 | D354 |
| L1147 | F1086 | A1024 | K962 | K962 | N842 | F781 | LEU  | L661 | T599 | K537 | A477 | I355 | I355 |
| K1148 | F1087 | H1025 | V964 | R904 | Q843 | L782 | D722 | M682 | T599 | M538 | G478 | L356 | L356 |
| E1149 | G1088 | L1026 | V965 | V905 | S844 | T783 | V723 | A663 | L600 | L539 | V479 | K418 | K418 |
| R1150 | P1089 | I1027 | S966 | S906 | N784 | T784 | D724 | T664 | E540 | S540 | S480 | T419 | T419 |
| L1151 | T1090 | E1028 | G967 | G907 | I846 | V785 | P725 | E665 | R604 | L541 | Q481 | K358 | K358 |
| M1152 | Y1091 | C1029 | V968 | E908 | D847 | N786 | A726 | V666 | R605 | M542 | V482 | F421 | F421 |
| E1153 | Y1092 | L1030 | R969 | D909 | R848 | V787 | K727 | O667 | K606 | S543 | L483 | K422 | K422 |
| A1154 | Q1093 | L1031 | T970 | V910 | C849 | R788 | R728 | D688 | I609 | C544 | M484 | K423 | K423 |
| S1155 | S1032 | S1032 | T971 | I911 | L950 | M789 | I729 | D688 | N610 | I545 | R485 | L424 | L424 |
| D1156 | K1033 | K1033 | R951 | R951 | D790 | R790 | R730 | ILE  | N610 | S546 | R486 | T425 | T425 |
| A1157 | R1096 | V1034 | G913 | G913 | R852 | T791 | V731 | GLY  | P611 | V547 | T487 | K426 | K426 |



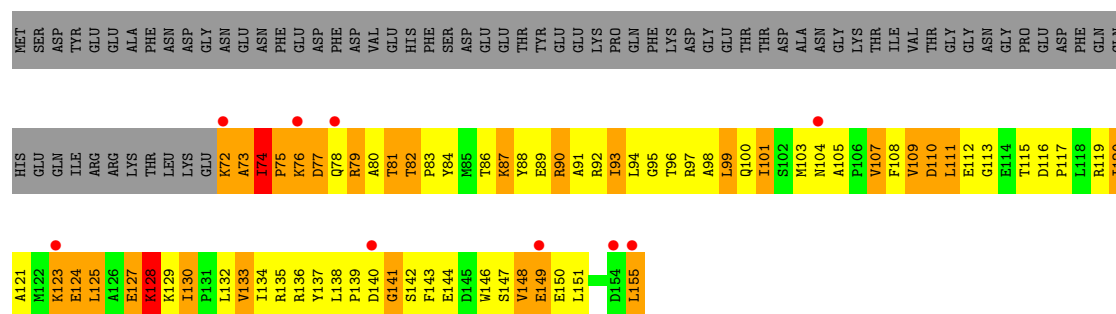
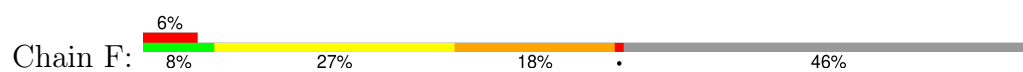
• Molecule 5: DNA-directed RNA polymerase II 45 kDa polypeptide



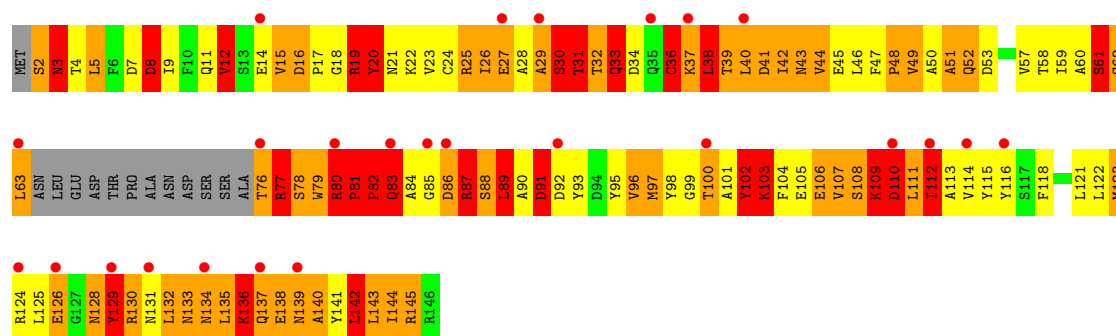
• Molecule 6: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



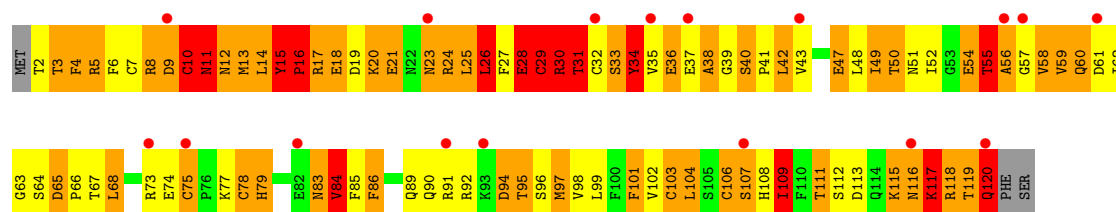
• Molecule 7: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



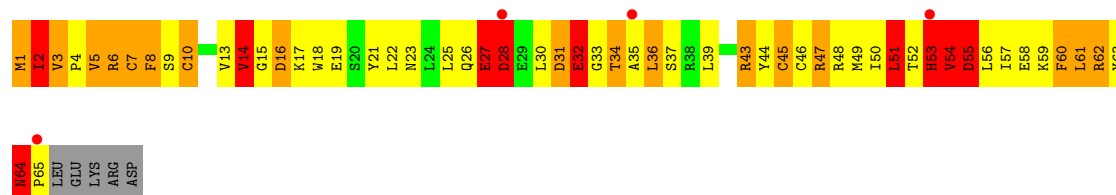
- Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



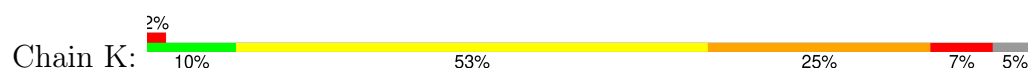
- Molecule 9: DNA-directed RNA polymerase II 14.2 kDa polypeptide



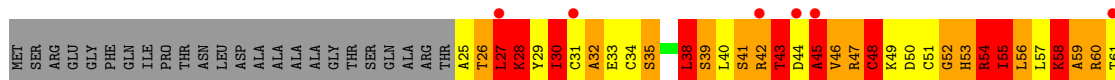
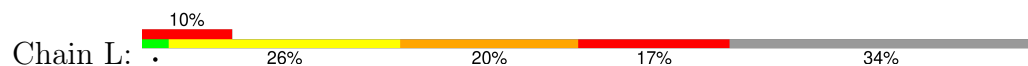
- Molecule 10: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide



- Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 167.08Å 221.26Å 193.69Å<br>90.00° 100.10° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 39.86 – 3.61<br>39.86 – 3.61                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 92.7 (39.86-3.61)<br>92.6 (39.86-3.61)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.13 (at 3.57Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.315 , 0.343<br>0.309 , 0.329                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 8031 reflections (10.04%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 47.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.357                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 18.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.76                                                        | EDS              |
| Total number of atoms                                                   | 28647                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 53.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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   | R     | 0.56         | 0/244           | 0.91        | 0/380             |
| 2   | T     | 0.49         | 0/311           | 1.62        | 9/477 (1.9%)      |
| 3   | A     | 1.14         | 45/11163 (0.4%) | 2.10        | 539/15091 (3.6%)  |
| 4   | B     | 1.09         | 31/8964 (0.3%)  | 1.96        | 353/12086 (2.9%)  |
| 5   | C     | 0.96         | 0/2133          | 1.85        | 77/2891 (2.7%)    |
| 6   | E     | 1.10         | 4/1788 (0.2%)   | 2.08        | 74/2406 (3.1%)    |
| 7   | F     | 1.06         | 0/691           | 2.06        | 18/933 (1.9%)     |
| 8   | H     | 1.12         | 3/1086 (0.3%)   | 2.15        | 60/1470 (4.1%)    |
| 9   | I     | 1.28         | 6/989 (0.6%)    | 2.24        | 59/1331 (4.4%)    |
| 10  | J     | 0.94         | 0/541           | 2.02        | 18/727 (2.5%)     |
| 11  | K     | 0.89         | 0/937           | 1.71        | 29/1265 (2.3%)    |
| 12  | L     | 1.16         | 0/366           | 2.38        | 23/485 (4.7%)     |
| All | All   | 1.09         | 89/29213 (0.3%) | 2.02        | 1259/39542 (3.2%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | T     | 0                   | 5                   |
| 3   | A     | 1                   | 6                   |
| 4   | B     | 0                   | 7                   |
| 5   | C     | 0                   | 2                   |
| 6   | E     | 0                   | 1                   |
| 9   | I     | 0                   | 1                   |
| All | All   | 1                   | 22                  |

All (89) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | A     | 319  | GLY  | C-O   | 12.81 | 1.41        | 1.23     |
| 3   | A     | 320  | ARG  | CA-CB | 12.00 | 1.72        | 1.53     |
| 3   | A     | 323  | LYS  | N-CA  | 9.82  | 1.58        | 1.46     |
| 4   | B     | 981  | ALA  | CA-C  | -9.07 | 1.40        | 1.52     |
| 3   | A     | 531  | ILE  | CA-CB | 8.73  | 1.66        | 1.54     |
| 3   | A     | 325  | ILE  | CA-CB | 8.43  | 1.66        | 1.54     |
| 3   | A     | 256  | GLN  | CA-C  | 8.25  | 1.63        | 1.52     |
| 3   | A     | 325  | ILE  | N-CA  | 8.03  | 1.56        | 1.46     |
| 3   | A     | 322  | VAL  | CA-C  | 8.01  | 1.62        | 1.52     |
| 3   | A     | 320  | ARG  | CA-C  | -7.86 | 1.43        | 1.52     |
| 3   | A     | 1398 | MET  | SD-CE | -7.63 | 1.60        | 1.79     |
| 3   | A     | 50   | ILE  | CA-CB | 7.58  | 1.64        | 1.54     |
| 4   | B     | 315  | LYS  | CA-CB | 7.53  | 1.60        | 1.54     |
| 4   | B     | 868  | MET  | SD-CE | 7.45  | 1.98        | 1.79     |
| 3   | A     | 1368 | MET  | SD-CE | -7.36 | 1.61        | 1.79     |
| 3   | A     | 255  | SER  | CA-CB | 7.32  | 1.65        | 1.53     |
| 6   | E     | 132  | ILE  | N-CA  | -7.18 | 1.37        | 1.46     |
| 4   | B     | 1223 | ASP  | CA-C  | 7.00  | 1.62        | 1.52     |
| 3   | A     | 323  | LYS  | CA-CB | 6.76  | 1.64        | 1.53     |
| 3   | A     | 320  | ARG  | C-N   | 6.75  | 1.47        | 1.34     |
| 4   | B     | 595  | ARG  | CA-C  | 6.73  | 1.61        | 1.52     |
| 3   | A     | 49   | LYS  | CA-C  | 6.73  | 1.55        | 1.52     |
| 9   | I     | 29   | CYS  | CA-CB | 6.71  | 1.62        | 1.53     |
| 3   | A     | 320  | ARG  | C-O   | -6.62 | 1.15        | 1.24     |
| 9   | I     | 28   | GLU  | CA-C  | 6.53  | 1.61        | 1.52     |
| 3   | A     | 257  | ARG  | CA-CB | 6.49  | 1.64        | 1.53     |
| 3   | A     | 67   | CYS  | CA-CB | 6.45  | 1.64        | 1.53     |
| 3   | A     | 320  | ARG  | CG-CD | 6.36  | 1.71        | 1.52     |
| 9   | I     | 10   | CYS  | CA-C  | 6.34  | 1.61        | 1.52     |
| 9   | I     | 117  | LYS  | CA-C  | 6.34  | 1.62        | 1.53     |
| 9   | I     | 118  | ARG  | N-CA  | 6.32  | 1.53        | 1.46     |
| 4   | B     | 595  | ARG  | CB-CG | 6.29  | 1.71        | 1.52     |
| 3   | A     | 1175 | SER  | CA-C  | 6.28  | 1.61        | 1.52     |
| 4   | B     | 510  | LYS  | CA-C  | 6.25  | 1.59        | 1.52     |
| 3   | A     | 128  | ILE  | CA-CB | 6.22  | 1.61        | 1.53     |
| 8   | H     | 126  | GLU  | CA-C  | 6.19  | 1.59        | 1.52     |
| 4   | B     | 880  | THR  | CA-CB | -6.13 | 1.45        | 1.53     |
| 4   | B     | 132  | VAL  | CA-C  | 6.13  | 1.60        | 1.52     |
| 4   | B     | 595  | ARG  | CG-CD | 6.07  | 1.70        | 1.52     |
| 3   | A     | 254  | GLU  | CA-C  | 6.01  | 1.60        | 1.52     |
| 4   | B     | 133  | LYS  | CA-C  | 5.98  | 1.61        | 1.53     |
| 4   | B     | 132  | VAL  | CA-CB | 5.87  | 1.62        | 1.54     |
| 3   | A     | 1336 | MET  | SD-CE | -5.87 | 1.64        | 1.79     |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | A     | 977  | LYS  | CA-C  | 5.85  | 1.60        | 1.52     |
| 3   | A     | 973  | ILE  | CA-C  | 5.82  | 1.59        | 1.52     |
| 9   | I     | 9    | ASP  | CA-C  | 5.76  | 1.60        | 1.52     |
| 4   | B     | 863  | GLU  | CA-C  | 5.75  | 1.59        | 1.52     |
| 4   | B     | 841  | MET  | SD-CE | -5.74 | 1.65        | 1.79     |
| 3   | A     | 249  | SER  | C-O   | 5.72  | 1.31        | 1.24     |
| 4   | B     | 648  | HIS  | N-CA  | 5.70  | 1.53        | 1.46     |
| 4   | B     | 250  | PHE  | CA-C  | 5.69  | 1.60        | 1.53     |
| 3   | A     | 249  | SER  | CA-C  | 5.67  | 1.60        | 1.52     |
| 3   | A     | 423  | ASP  | CA-C  | -5.64 | 1.50        | 1.53     |
| 4   | B     | 1072 | MET  | SD-CE | -5.64 | 1.65        | 1.79     |
| 3   | A     | 905  | ASP  | CA-C  | 5.59  | 1.60        | 1.52     |
| 3   | A     | 256  | GLN  | CA-CB | 5.55  | 1.60        | 1.52     |
| 4   | B     | 447  | ALA  | CA-CB | -5.51 | 1.44        | 1.53     |
| 8   | H     | 108  | SER  | CA-C  | -5.51 | 1.45        | 1.52     |
| 8   | H     | 79   | TRP  | N-CA  | -5.50 | 1.39        | 1.46     |
| 4   | B     | 429  | PHE  | CA-C  | 5.47  | 1.60        | 1.52     |
| 3   | A     | 324  | SER  | CA-C  | 5.47  | 1.59        | 1.52     |
| 3   | A     | 152  | VAL  | CA-C  | 5.47  | 1.58        | 1.52     |
| 6   | E     | 124  | VAL  | CA-CB | 5.47  | 1.61        | 1.54     |
| 3   | A     | 55   | ASP  | CA-C  | 5.43  | 1.59        | 1.52     |
| 3   | A     | 11   | LEU  | N-CA  | -5.43 | 1.40        | 1.46     |
| 4   | B     | 473  | MET  | N-CA  | -5.41 | 1.39        | 1.46     |
| 4   | B     | 981  | ALA  | N-CA  | -5.38 | 1.39        | 1.46     |
| 3   | A     | 57   | ARG  | CA-C  | 5.38  | 1.59        | 1.52     |
| 3   | A     | 1255 | GLU  | CA-C  | 5.36  | 1.59        | 1.52     |
| 3   | A     | 322  | VAL  | C-O   | -5.36 | 1.17        | 1.24     |
| 3   | A     | 1393 | ASN  | N-CA  | 5.32  | 1.53        | 1.46     |
| 4   | B     | 595  | ARG  | CA-CB | 5.21  | 1.62        | 1.53     |
| 4   | B     | 637  | LEU  | C-O   | 5.20  | 1.30        | 1.24     |
| 4   | B     | 275  | TYR  | CA-C  | 5.20  | 1.59        | 1.52     |
| 4   | B     | 864  | LYS  | N-CA  | 5.17  | 1.52        | 1.46     |
| 3   | A     | 1289 | ARG  | CA-C  | 5.16  | 1.58        | 1.52     |
| 4   | B     | 1224 | PHE  | N-CA  | 5.15  | 1.56        | 1.46     |
| 4   | B     | 737  | THR  | N-CA  | -5.15 | 1.39        | 1.46     |
| 6   | E     | 116  | ILE  | CA-CB | 5.15  | 1.61        | 1.54     |
| 4   | B     | 132  | VAL  | N-CA  | 5.15  | 1.52        | 1.46     |
| 4   | B     | 596  | LEU  | N-CA  | 5.14  | 1.52        | 1.46     |
| 4   | B     | 1166 | CYS  | CA-CB | 5.14  | 1.62        | 1.53     |
| 3   | A     | 1267 | MET  | SD-CE | -5.12 | 1.66        | 1.79     |
| 3   | A     | 202  | LEU  | CA-C  | -5.12 | 1.46        | 1.53     |
| 3   | A     | 277  | GLU  | CA-C  | 5.12  | 1.59        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | A     | 321 | PRO  | CA-CB | -5.12 | 1.44        | 1.53     |
| 4   | B     | 865 | LYS  | N-CA  | 5.09  | 1.52        | 1.46     |
| 3   | A     | 317 | LYS  | CA-C  | 5.09  | 1.59        | 1.52     |
| 6   | E     | 115 | ASN  | CA-C  | 5.07  | 1.59        | 1.52     |

All (1259) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 3   | A     | 821  | ARG  | N-CA-C | -26.04 | 79.39       | 112.72   |
| 4   | B     | 479  | VAL  | N-CA-C | -22.98 | 84.24       | 110.21   |
| 7   | F     | 74   | ILE  | CA-C-N | 20.19  | 140.48      | 119.89   |
| 7   | F     | 74   | ILE  | C-N-CA | 20.19  | 140.48      | 119.89   |
| 3   | A     | 322  | VAL  | N-CA-C | 19.68  | 150.26      | 109.34   |
| 3   | A     | 321  | PRO  | N-CA-C | -18.56 | 63.84       | 112.10   |
| 3   | A     | 121  | LEU  | N-CA-C | -18.26 | 87.91       | 114.39   |
| 3   | A     | 170  | THR  | N-CA-C | 17.99  | 134.73      | 109.18   |
| 3   | A     | 890  | ASP  | N-CA-C | -17.69 | 91.33       | 113.97   |
| 10  | J     | 3    | VAL  | CA-C-N | -17.48 | 97.99       | 119.84   |
| 10  | J     | 3    | VAL  | C-N-CA | -17.48 | 97.99       | 119.84   |
| 4   | B     | 296  | GLU  | N-CA-C | -17.30 | 91.44       | 112.89   |
| 4   | B     | 69   | LEU  | N-CA-C | 17.20  | 137.03      | 109.85   |
| 9   | I     | 75   | CYS  | N-CA-C | -16.94 | 88.20       | 110.40   |
| 5   | C     | 41   | ILE  | CA-C-N | 16.24  | 136.45      | 119.89   |
| 5   | C     | 41   | ILE  | C-N-CA | 16.24  | 136.45      | 119.89   |
| 4   | B     | 706  | GLN  | N-CA-C | -16.19 | 91.52       | 110.13   |
| 3   | A     | 152  | VAL  | N-CA-C | 16.08  | 127.18      | 109.01   |
| 4   | B     | 430  | ARG  | N-CA-C | 15.92  | 132.96      | 113.38   |
| 8   | H     | 137  | GLN  | N-CA-C | 15.56  | 133.52      | 110.48   |
| 4   | B     | 474  | SER  | N-CA-C | -15.22 | 92.36       | 113.37   |
| 3   | A     | 1405 | THR  | N-CA-C | 15.17  | 127.90      | 111.36   |
| 7   | F     | 130  | ILE  | CA-C-N | 14.88  | 138.44      | 119.84   |
| 7   | F     | 130  | ILE  | C-N-CA | 14.88  | 138.44      | 119.84   |
| 4   | B     | 1154 | ALA  | N-CA-C | -14.82 | 91.41       | 110.53   |
| 6   | E     | 5    | ASN  | N-CA-C | -14.77 | 93.38       | 111.40   |
| 3   | A     | 1111 | MET  | N-CA-C | 14.74  | 132.07      | 109.96   |
| 6   | E     | 52   | ARG  | CA-C-N | 14.48  | 137.95      | 119.84   |
| 6   | E     | 52   | ARG  | C-N-CA | 14.48  | 137.95      | 119.84   |
| 3   | A     | 259  | GLU  | N-CA-C | 14.45  | 141.58      | 110.80   |
| 4   | B     | 550  | ASP  | CA-C-N | 14.43  | 133.98      | 118.97   |
| 4   | B     | 550  | ASP  | C-N-CA | 14.43  | 133.98      | 118.97   |
| 3   | A     | 1311 | VAL  | N-CA-C | 14.43  | 129.28      | 107.78   |
| 4   | B     | 431  | TYR  | N-CA-C | -14.35 | 80.23       | 110.80   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 4   | B     | 230  | ALA  | CA-C-N | 14.26  | 137.66      | 119.84   |
| 4   | B     | 230  | ALA  | C-N-CA | 14.26  | 137.66      | 119.84   |
| 3   | A     | 513  | SER  | CA-C-N | 14.24  | 133.94      | 119.56   |
| 3   | A     | 513  | SER  | C-N-CA | 14.24  | 133.94      | 119.56   |
| 4   | B     | 429  | PHE  | N-CA-C | -14.10 | 94.01       | 112.34   |
| 4   | B     | 637  | LEU  | N-CA-C | 14.01  | 140.64      | 110.80   |
| 4   | B     | 711  | GLU  | CA-C-N | 13.97  | 137.31      | 119.84   |
| 4   | B     | 711  | GLU  | C-N-CA | 13.97  | 137.31      | 119.84   |
| 3   | A     | 973  | ILE  | N-CA-C | 13.84  | 128.05      | 109.37   |
| 4   | B     | 1221 | SER  | N-CA-C | 13.81  | 130.53      | 109.96   |
| 8   | H     | 133  | ASN  | N-CA-C | 13.75  | 132.05      | 114.31   |
| 3   | A     | 236  | LEU  | N-CA-C | 13.75  | 128.95      | 109.15   |
| 4   | B     | 99   | LYS  | N-CA-C | -13.68 | 92.46       | 109.83   |
| 6   | E     | 157  | SER  | N-CA-C | 13.67  | 130.51      | 110.28   |
| 3   | A     | 152  | VAL  | CA-C-N | 13.59  | 136.83      | 119.84   |
| 3   | A     | 152  | VAL  | C-N-CA | 13.59  | 136.83      | 119.84   |
| 4   | B     | 427  | ASP  | N-CA-C | -13.59 | 96.38       | 113.23   |
| 8   | H     | 110  | ASP  | N-CA-C | -13.57 | 96.74       | 113.02   |
| 3   | A     | 81   | PHE  | N-CA-C | 13.52  | 129.84      | 110.23   |
| 3   | A     | 330  | LYS  | N-CA-C | 13.48  | 130.18      | 109.96   |
| 3   | A     | 1172 | LEU  | N-CA-C | 13.46  | 133.28      | 107.98   |
| 3   | A     | 1323 | ASP  | CA-C-N | 13.46  | 135.06      | 120.12   |
| 3   | A     | 1323 | ASP  | C-N-CA | 13.46  | 135.06      | 120.12   |
| 4   | B     | 635  | ARG  | N-CA-C | 13.41  | 139.44      | 109.81   |
| 4   | B     | 744  | HIS  | CA-C-N | 13.39  | 136.58      | 119.84   |
| 4   | B     | 744  | HIS  | C-N-CA | 13.39  | 136.58      | 119.84   |
| 3   | A     | 163  | SER  | N-CA-C | 13.25  | 131.59      | 109.06   |
| 3   | A     | 532  | ARG  | N-CA-C | 13.16  | 130.43      | 112.93   |
| 4   | B     | 523  | CYS  | CA-C-N | 13.13  | 133.10      | 119.19   |
| 4   | B     | 523  | CYS  | C-N-CA | 13.13  | 133.10      | 119.19   |
| 8   | H     | 31   | THR  | N-CA-C | -13.09 | 94.31       | 110.41   |
| 6   | E     | 63   | ASN  | CA-C-N | 13.05  | 133.89      | 119.93   |
| 6   | E     | 63   | ASN  | C-N-CA | 13.05  | 133.89      | 119.93   |
| 5   | C     | 89   | GLU  | N-CA-C | -12.94 | 89.75       | 110.32   |
| 3   | A     | 1109 | LYS  | N-CA-C | -12.92 | 97.19       | 111.14   |
| 9   | I     | 55   | THR  | N-CA-C | -12.91 | 93.49       | 110.53   |
| 4   | B     | 66   | ASP  | N-CA-C | -12.71 | 98.70       | 112.93   |
| 3   | A     | 291  | GLU  | N-CA-C | -12.64 | 97.58       | 111.36   |
| 3   | A     | 1094 | VAL  | N-CA-C | 12.61  | 126.81      | 108.53   |
| 4   | B     | 276  | ILE  | N-CA-C | 12.60  | 126.63      | 108.48   |
| 4   | B     | 838  | SER  | N-CA-C | -12.57 | 91.84       | 109.95   |
| 3   | A     | 78   | PRO  | N-CA-C | -12.53 | 90.83       | 110.50   |

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| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 4   | B     | 478  | GLY  | N-CA-C   | -12.44 | 83.71       | 113.18   |
| 4   | B     | 764  | SER  | CA-C-N   | -12.42 | 107.09      | 119.64   |
| 4   | B     | 764  | SER  | C-N-CA   | -12.42 | 107.09      | 119.64   |
| 12  | L     | 60   | ARG  | N-CA-C   | -12.33 | 92.19       | 108.34   |
| 3   | A     | 322  | VAL  | CB-CA-C  | -12.31 | 91.10       | 111.29   |
| 9   | I     | 118  | ARG  | N-CA-C   | 12.30  | 127.04      | 108.46   |
| 5   | C     | 7    | GLN  | N-CA-C   | 12.29  | 129.26      | 108.13   |
| 3   | A     | 893  | PHE  | N-CA-C   | -12.27 | 97.99       | 111.36   |
| 7   | F     | 105  | ALA  | N-CA-C   | -12.19 | 94.54       | 110.39   |
| 12  | L     | 44   | ASP  | N-CA-C   | -12.15 | 94.75       | 111.87   |
| 3   | A     | 252  | PHE  | N-CA-C   | -12.13 | 99.15       | 114.56   |
| 3   | A     | 183  | GLY  | N-CA-C   | 12.11  | 132.26      | 110.71   |
| 3   | A     | 366  | VAL  | CA-C-N   | -12.05 | 107.71      | 119.76   |
| 3   | A     | 366  | VAL  | C-N-CA   | -12.05 | 107.71      | 119.76   |
| 12  | L     | 41   | SER  | N-CA-C   | 12.04  | 129.47      | 110.32   |
| 4   | B     | 484  | ASN  | N-CA-C   | -12.04 | 88.93       | 108.07   |
| 3   | A     | 320  | ARG  | CA-CB-CG | -11.92 | 90.26       | 114.10   |
| 3   | A     | 974  | ASP  | N-CA-C   | 11.90  | 128.13      | 108.73   |
| 3   | A     | 1207 | LEU  | N-CA-C   | 11.71  | 128.97      | 109.06   |
| 8   | H     | 100  | THR  | N-CA-C   | -11.71 | 91.32       | 110.17   |
| 6   | E     | 119  | SER  | N-CA-C   | -11.66 | 98.30       | 111.82   |
| 3   | A     | 43   | GLU  | N-CA-C   | -11.61 | 89.59       | 108.52   |
| 3   | A     | 88   | LYS  | CA-C-N   | 11.59  | 134.32      | 119.84   |
| 3   | A     | 88   | LYS  | C-N-CA   | 11.59  | 134.32      | 119.84   |
| 4   | B     | 868  | MET  | N-CA-C   | -11.54 | 85.79       | 107.71   |
| 3   | A     | 328  | ARG  | N-CA-C   | -11.51 | 98.42       | 110.97   |
| 3   | A     | 55   | ASP  | N-CA-C   | 11.47  | 135.15      | 109.81   |
| 3   | A     | 896  | ARG  | N-CA-C   | 11.46  | 128.43      | 113.18   |
| 3   | A     | 1005 | GLU  | N-CA-C   | 11.46  | 126.36      | 112.38   |
| 3   | A     | 257  | ARG  | N-CA-C   | 11.45  | 135.18      | 110.80   |
| 4   | B     | 68   | THR  | N-CA-C   | 11.42  | 127.19      | 110.28   |
| 3   | A     | 491  | VAL  | CA-C-N   | 11.42  | 131.55      | 119.90   |
| 3   | A     | 491  | VAL  | C-N-CA   | 11.42  | 131.55      | 119.90   |
| 3   | A     | 120  | GLU  | N-CA-C   | 11.41  | 128.25      | 111.81   |
| 4   | B     | 1168 | LEU  | N-CA-C   | 11.40  | 127.52      | 109.50   |
| 3   | A     | 1112 | LYS  | N-CA-C   | 11.36  | 125.00      | 111.82   |
| 3   | A     | 452  | LYS  | N-CA-C   | -11.34 | 97.74       | 111.69   |
| 9   | I     | 79   | HIS  | N-CA-C   | 11.34  | 134.96      | 110.80   |
| 4   | B     | 330  | ALA  | N-CA-C   | -11.33 | 94.23       | 111.56   |
| 4   | B     | 647  | GLY  | N-CA-C   | 11.32  | 140.01      | 113.18   |
| 3   | A     | 993  | LEU  | N-CA-C   | -11.30 | 95.77       | 112.04   |
| 3   | A     | 1229 | SER  | N-CA-C   | -11.27 | 92.96       | 110.42   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 8   | H     | 121  | LEU  | N-CA-C | -11.25 | 91.87       | 109.76   |
| 6   | E     | 205  | SER  | N-CA-C | -11.23 | 88.26       | 108.48   |
| 8   | H     | 16   | ASP  | N-CA-C | 11.23  | 132.92      | 108.66   |
| 3   | A     | 258  | GLY  | N-CA-C | 11.12  | 139.54      | 113.18   |
| 3   | A     | 972  | HIS  | CA-C-N | 11.11  | 135.41      | 120.63   |
| 3   | A     | 972  | HIS  | C-N-CA | 11.11  | 135.41      | 120.63   |
| 4   | B     | 252  | SER  | N-CA-C | 11.11  | 127.73      | 107.73   |
| 3   | A     | 474  | VAL  | N-CA-C | -11.11 | 100.11      | 111.88   |
| 3   | A     | 249  | SER  | N-CA-C | 11.07  | 134.38      | 110.80   |
| 3   | A     | 293  | GLU  | N-CA-C | -11.06 | 100.52      | 114.56   |
| 3   | A     | 1121 | GLU  | N-CA-C | -11.03 | 94.86       | 110.08   |
| 9   | I     | 18   | GLU  | N-CA-C | 11.01  | 127.27      | 109.76   |
| 4   | B     | 39   | ARG  | N-CA-C | -10.99 | 99.27       | 111.14   |
| 3   | A     | 977  | LYS  | CA-C-N | 10.94  | 133.52      | 119.84   |
| 3   | A     | 977  | LYS  | C-N-CA | 10.94  | 133.52      | 119.84   |
| 12  | L     | 58   | LYS  | N-CA-C | 10.94  | 125.79      | 113.21   |
| 5   | C     | 199  | LYS  | N-CA-C | -10.92 | 99.35       | 112.89   |
| 4   | B     | 253  | THR  | N-CA-C | 10.88  | 125.53      | 108.67   |
| 3   | A     | 1163 | ILE  | N-CA-C | 10.80  | 119.16      | 107.60   |
| 4   | B     | 468  | GLU  | N-CA-C | 10.79  | 133.79      | 110.80   |
| 3   | A     | 173  | THR  | N-CA-C | -10.71 | 91.17       | 108.41   |
| 3   | A     | 137  | ALA  | N-CA-C | -10.69 | 97.49       | 112.13   |
| 3   | A     | 918  | GLU  | N-CA-C | -10.60 | 96.93       | 111.56   |
| 5   | C     | 30   | ALA  | N-CA-C | -10.59 | 99.61       | 112.54   |
| 11  | K     | 2    | ASN  | N-CA-C | -10.56 | 99.15       | 113.30   |
| 6   | E     | 107  | THR  | N-CA-C | 10.55  | 127.36      | 108.69   |
| 3   | A     | 317  | LYS  | CA-C-N | 10.54  | 141.68      | 121.54   |
| 3   | A     | 317  | LYS  | C-N-CA | 10.54  | 141.68      | 121.54   |
| 3   | A     | 833  | GLU  | N-CA-C | -10.53 | 98.18       | 111.02   |
| 3   | A     | 946  | VAL  | N-CA-C | 10.45  | 120.43      | 110.30   |
| 3   | A     | 1226 | VAL  | N-CA-C | 10.44  | 123.90      | 108.45   |
| 9   | I     | 26   | LEU  | N-CA-C | 10.43  | 128.48      | 107.41   |
| 5   | C     | 255  | VAL  | N-CA-C | -10.42 | 100.41      | 110.42   |
| 5   | C     | 167  | HIS  | N-CA-C | -10.40 | 92.41       | 108.42   |
| 3   | A     | 1283 | VAL  | N-CA-C | 10.37  | 125.61      | 108.81   |
| 4   | B     | 95   | ILE  | N-CA-C | -10.33 | 93.26       | 109.17   |
| 3   | A     | 254  | GLU  | CA-C-N | 10.33  | 141.26      | 121.54   |
| 3   | A     | 254  | GLU  | C-N-CA | 10.33  | 141.26      | 121.54   |
| 3   | A     | 1289 | ARG  | N-CA-C | 10.30  | 125.23      | 108.34   |
| 3   | A     | 216  | VAL  | N-CA-C | -10.24 | 100.80      | 110.42   |
| 5   | C     | 238  | ILE  | CA-C-N | -10.23 | 109.30      | 120.14   |
| 5   | C     | 238  | ILE  | C-N-CA | -10.23 | 109.30      | 120.14   |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 10  | J     | 45   | CYS  | N-CA-C  | -10.22 | 100.10      | 111.14   |
| 3   | A     | 251  | SER  | N-CA-C  | 10.22  | 132.57      | 110.80   |
| 9   | I     | 120  | GLN  | N-CA-C  | 10.20  | 139.56      | 111.00   |
| 3   | A     | 1072 | ILE  | N-CA-C  | -10.19 | 103.56      | 112.12   |
| 4   | B     | 349  | ILE  | N-CA-C  | -10.17 | 100.86      | 110.42   |
| 3   | A     | 21   | LEU  | N-CA-C  | 10.15  | 124.31      | 109.69   |
| 4   | B     | 772  | ALA  | N-CA-C  | -10.14 | 100.99      | 113.97   |
| 5   | C     | 181  | ASP  | CA-C-N  | 10.12  | 129.77      | 119.24   |
| 5   | C     | 181  | ASP  | C-N-CA  | 10.12  | 129.77      | 119.24   |
| 9   | I     | 8    | ARG  | N-CA-C  | -10.12 | 89.24       | 110.80   |
| 3   | A     | 602  | ASP  | N-CA-C  | -10.10 | 97.30       | 111.24   |
| 9   | I     | 65   | ASP  | CA-C-N  | 10.08  | 133.09      | 120.89   |
| 9   | I     | 65   | ASP  | C-N-CA  | 10.08  | 133.09      | 120.89   |
| 4   | B     | 712  | PRO  | N-CA-C  | -10.08 | 91.70       | 112.47   |
| 4   | B     | 981  | ALA  | N-CA-C  | 10.08  | 132.26      | 110.80   |
| 3   | A     | 878  | ILE  | N-CA-C  | 10.05  | 124.56      | 108.97   |
| 6   | E     | 53   | PRO  | CA-C-N  | -10.00 | 106.26      | 122.26   |
| 6   | E     | 53   | PRO  | C-N-CA  | -10.00 | 106.26      | 122.26   |
| 11  | K     | 16   | GLU  | N-CA-C  | -9.97  | 94.09       | 109.85   |
| 4   | B     | 475  | SER  | N-CA-C  | -9.96  | 89.59       | 110.80   |
| 6   | E     | 33   | GLU  | N-CA-C  | -9.95  | 100.39      | 111.14   |
| 6   | E     | 42   | PHE  | CA-C-N  | 9.95   | 133.78      | 120.65   |
| 6   | E     | 42   | PHE  | C-N-CA  | 9.95   | 133.78      | 120.65   |
| 8   | H     | 129  | TYR  | N-CA-C  | -9.94  | 100.79      | 113.72   |
| 3   | A     | 277  | GLU  | N-CA-C  | -9.93  | 100.43      | 112.54   |
| 4   | B     | 107  | GLY  | N-CA-C  | 9.90   | 124.98      | 110.63   |
| 3   | A     | 22   | PHE  | N-CA-C  | 9.84   | 126.06      | 107.75   |
| 5   | C     | 51   | VAL  | N-CA-C  | 9.82   | 122.09      | 107.75   |
| 10  | J     | 64   | ASN  | N-CA-C  | 9.82   | 131.52      | 109.81   |
| 4   | B     | 1180 | PHE  | N-CA-C  | 9.81   | 125.28      | 112.72   |
| 4   | B     | 511  | PRO  | N-CA-C  | 9.81   | 127.51      | 114.27   |
| 4   | B     | 1174 | LYS  | N-CA-C  | -9.81  | 97.69       | 111.81   |
| 9   | I     | 78   | CYS  | N-CA-CB | -9.73  | 94.05       | 110.49   |
| 4   | B     | 1131 | GLY  | N-CA-C  | 9.71   | 123.09      | 111.93   |
| 3   | A     | 148  | CYS  | N-CA-C  | -9.70  | 99.06       | 112.25   |
| 4   | B     | 413  | LEU  | N-CA-C  | -9.69  | 99.48       | 111.11   |
| 3   | A     | 317  | LYS  | N-CA-C  | 9.69   | 131.43      | 110.80   |
| 3   | A     | 535  | THR  | N-CA-C  | 9.67   | 123.04      | 111.82   |
| 3   | A     | 225  | ASN  | N-CA-C  | 9.66   | 122.03      | 110.44   |
| 3   | A     | 7    | SER  | N-CA-C  | -9.64  | 94.57       | 109.52   |
| 3   | A     | 879  | GLU  | N-CA-C  | 9.64   | 124.16      | 108.55   |
| 4   | B     | 706  | GLN  | CA-C-N  | -9.60  | 107.84      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4   | B     | 706  | GLN  | C-N-CA   | -9.60 | 107.84      | 119.84   |
| 3   | A     | 65   | LEU  | N-CA-C   | 9.58  | 124.06      | 112.38   |
| 3   | A     | 318  | SER  | N-CA-C   | -9.56 | 90.43       | 110.80   |
| 3   | A     | 182  | VAL  | N-CA-C   | 9.52  | 121.66      | 107.75   |
| 3   | A     | 102  | VAL  | CB-CA-C  | -9.52 | 96.84       | 112.26   |
| 3   | A     | 113  | LEU  | N-CA-C   | -9.51 | 96.41       | 110.48   |
| 7   | F     | 124  | GLU  | N-CA-C   | -9.47 | 101.49      | 113.23   |
| 4   | B     | 244  | LEU  | N-CA-C   | 9.46  | 124.20      | 110.10   |
| 4   | B     | 1223 | ASP  | N-CA-C   | 9.45  | 130.92      | 110.80   |
| 4   | B     | 1019 | SER  | N-CA-C   | 9.44  | 124.33      | 113.01   |
| 4   | B     | 591  | ARG  | N-CA-C   | -9.43 | 96.56       | 110.52   |
| 3   | A     | 283  | GLY  | N-CA-C   | 9.41  | 135.49      | 113.18   |
| 3   | A     | 1143 | LEU  | N-CA-C   | -9.40 | 100.59      | 111.03   |
| 4   | B     | 640  | VAL  | N-CA-C   | 9.40  | 122.64      | 113.71   |
| 4   | B     | 456  | GLY  | N-CA-C   | -9.40 | 101.11      | 112.49   |
| 7   | F     | 93   | ILE  | N-CA-C   | -9.40 | 101.18      | 110.30   |
| 3   | A     | 316  | GLN  | CA-C-N   | 9.39  | 139.47      | 121.54   |
| 3   | A     | 316  | GLN  | C-N-CA   | 9.39  | 139.47      | 121.54   |
| 4   | B     | 392  | ARG  | N-CA-C   | -9.38 | 101.26      | 112.89   |
| 6   | E     | 55   | ARG  | N-CA-C   | 9.37  | 122.45      | 111.02   |
| 3   | A     | 906  | HIS  | N-CA-C   | 9.37  | 122.90      | 112.97   |
| 3   | A     | 93   | VAL  | N-CA-C   | 9.37  | 128.82      | 109.34   |
| 8   | H     | 45   | GLU  | N-CA-C   | -9.37 | 101.63      | 113.43   |
| 5   | C     | 139  | GLY  | N-CA-C   | 9.35  | 127.73      | 114.64   |
| 3   | A     | 253  | ASN  | N-CA-C   | 9.35  | 130.71      | 110.80   |
| 4   | B     | 1192 | TYR  | N-CA-C   | 9.34  | 125.22      | 108.69   |
| 6   | E     | 67   | GLU  | N-CA-C   | -9.34 | 100.51      | 112.93   |
| 3   | A     | 666  | ILE  | N-CA-C   | -9.34 | 99.52       | 112.50   |
| 4   | B     | 1218 | THR  | N-CA-C   | 9.34  | 123.99      | 112.23   |
| 6   | E     | 106  | GLN  | N-CA-C   | -9.33 | 102.47      | 114.04   |
| 3   | A     | 398  | GLU  | N-CA-C   | -9.32 | 94.47       | 109.76   |
| 3   | A     | 1392 | SER  | N-CA-C   | 9.32  | 130.66      | 110.80   |
| 4   | B     | 54   | PHE  | N-CA-C   | -9.32 | 90.95       | 110.80   |
| 3   | A     | 886  | ILE  | N-CA-C   | 9.32  | 119.92      | 110.23   |
| 9   | I     | 40   | SER  | N-CA-C   | -9.30 | 99.80       | 108.07   |
| 3   | A     | 98   | LYS  | N-CA-C   | -9.29 | 91.02       | 110.80   |
| 9   | I     | 25   | LEU  | N-CA-C   | 9.27  | 124.35      | 109.24   |
| 4   | B     | 1048 | THR  | N-CA-C   | 9.27  | 122.77      | 108.96   |
| 3   | A     | 4    | GLN  | N-CA-C   | -9.26 | 95.35       | 109.14   |
| 3   | A     | 221  | SER  | N-CA-C   | -9.23 | 99.76       | 111.02   |
| 10  | J     | 5    | VAL  | N-CA-C   | -9.23 | 96.66       | 109.21   |
| 10  | J     | 10   | CYS  | CA-CB-SG | 9.22  | 135.61      | 114.40   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 7   | F     | 149  | GLU  | N-CA-C  | -9.22 | 98.77       | 112.04   |
| 4   | B     | 280  | ILE  | CA-C-N  | -9.21 | 109.72      | 120.13   |
| 4   | B     | 280  | ILE  | C-N-CA  | -9.21 | 109.72      | 120.13   |
| 8   | H     | 36   | CYS  | N-CA-C  | 9.20  | 124.69      | 109.06   |
| 6   | E     | 182  | ASP  | CA-C-N  | 9.18  | 131.32      | 119.84   |
| 6   | E     | 182  | ASP  | C-N-CA  | 9.18  | 131.32      | 119.84   |
| 9   | I     | 74   | GLU  | N-CA-C  | -9.17 | 94.59       | 108.99   |
| 3   | A     | 723  | ASN  | N-CA-C  | -9.16 | 100.86      | 111.03   |
| 4   | B     | 882  | THR  | N-CA-C  | 9.13  | 121.32      | 111.36   |
| 4   | B     | 166  | PHE  | N-CA-C  | 9.12  | 124.27      | 109.59   |
| 4   | B     | 756  | ILE  | N-CA-C  | 9.09  | 117.86      | 108.95   |
| 8   | H     | 80   | ARG  | N-CA-C  | -9.09 | 89.73       | 109.81   |
| 3   | A     | 324  | SER  | N-CA-C  | 9.07  | 131.81      | 113.31   |
| 6   | E     | 153  | HIS  | N-CA-C  | -9.06 | 98.85       | 110.53   |
| 3   | A     | 524  | VAL  | N-CA-C  | 9.05  | 123.11      | 108.99   |
| 4   | B     | 766  | ARG  | N-CA-C  | -9.02 | 101.14      | 110.97   |
| 3   | A     | 1444 | MET  | N-CA-C  | 9.01  | 120.50      | 108.07   |
| 9   | I     | 77   | LYS  | CA-C-N  | 8.99  | 138.72      | 121.54   |
| 9   | I     | 77   | LYS  | C-N-CA  | 8.99  | 138.72      | 121.54   |
| 3   | A     | 126  | LEU  | N-CA-C  | 8.99  | 123.84      | 113.15   |
| 3   | A     | 1279 | ILE  | N-CA-C  | 8.98  | 115.82      | 106.21   |
| 3   | A     | 463  | ILE  | CA-C-N  | 8.98  | 129.41      | 120.52   |
| 3   | A     | 463  | ILE  | C-N-CA  | 8.98  | 129.41      | 120.52   |
| 3   | A     | 1313 | LEU  | N-CA-C  | -8.98 | 97.12       | 111.04   |
| 3   | A     | 793  | SER  | CA-C-N  | 8.96  | 131.04      | 119.84   |
| 3   | A     | 793  | SER  | C-N-CA  | 8.96  | 131.04      | 119.84   |
| 9   | I     | 10   | CYS  | N-CA-C  | 8.95  | 129.87      | 110.80   |
| 3   | A     | 384  | ASN  | N-CA-C  | 8.94  | 124.88      | 112.45   |
| 4   | B     | 276  | ILE  | CB-CA-C | -8.94 | 97.29       | 110.62   |
| 4   | B     | 723  | VAL  | N-CA-C  | 8.91  | 127.87      | 109.34   |
| 3   | A     | 316  | GLN  | CB-CA-C | 8.91  | 128.14      | 110.42   |
| 11  | K     | 20   | LYS  | N-CA-C  | -8.90 | 94.37       | 109.24   |
| 3   | A     | 1408 | ILE  | N-CA-C  | -8.88 | 99.99       | 111.09   |
| 3   | A     | 954  | TRP  | N-CA-C  | 8.85  | 124.01      | 109.58   |
| 4   | B     | 167  | ILE  | CB-CA-C | -8.81 | 97.47       | 110.33   |
| 6   | E     | 120  | ALA  | N-CA-C  | 8.81  | 123.86      | 113.20   |
| 3   | A     | 125  | ALA  | N-CA-C  | 8.80  | 123.79      | 112.34   |
| 4   | B     | 21   | GLU  | N-CA-C  | 8.79  | 129.53      | 110.80   |
| 6   | E     | 147  | HIS  | N-CA-C  | 8.79  | 123.73      | 109.76   |
| 4   | B     | 606  | LYS  | N-CA-C  | -8.77 | 100.26      | 112.45   |
| 8   | H     | 83   | GLN  | N-CA-C  | -8.76 | 92.14       | 110.80   |
| 3   | A     | 861  | GLY  | N-CA-C  | -8.73 | 103.57      | 114.92   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4   | B     | 486  | TYR  | N-CA-C   | -8.73 | 100.96      | 111.69   |
| 4   | B     | 758  | PHE  | CA-C-N   | -8.73 | 110.44      | 120.12   |
| 4   | B     | 758  | PHE  | C-N-CA   | -8.73 | 110.44      | 120.12   |
| 4   | B     | 764  | SER  | N-CA-C   | 8.72  | 125.58      | 113.45   |
| 4   | B     | 127  | GLY  | N-CA-C   | 8.72  | 123.24      | 111.03   |
| 3   | A     | 1269 | GLU  | N-CA-C   | 8.70  | 129.33      | 110.80   |
| 3   | A     | 675  | THR  | N-CA-C   | -8.69 | 102.80      | 113.41   |
| 6   | E     | 126  | SER  | N-CA-C   | 8.68  | 121.53      | 111.11   |
| 4   | B     | 1172 | ILE  | N-CA-CB  | -8.68 | 102.02      | 112.35   |
| 3   | A     | 766  | GLY  | N-CA-C   | 8.67  | 122.88      | 111.52   |
| 4   | B     | 197  | PHE  | N-CA-C   | -8.67 | 102.84      | 113.50   |
| 3   | A     | 284  | ALA  | N-CA-C   | 8.66  | 128.96      | 109.81   |
| 3   | A     | 1381 | LEU  | N-CA-C   | -8.65 | 95.14       | 109.07   |
| 4   | B     | 370  | PHE  | N-CA-C   | -8.64 | 89.48       | 107.37   |
| 5   | C     | 183  | TRP  | N-CA-C   | -8.63 | 95.45       | 109.96   |
| 8   | H     | 92   | ASP  | N-CA-C   | -8.58 | 102.81      | 113.28   |
| 9   | I     | 78   | CYS  | CA-CB-SG | 8.56  | 134.10      | 114.40   |
| 3   | A     | 599  | SER  | CA-C-N   | -8.55 | 109.15      | 119.84   |
| 3   | A     | 599  | SER  | C-N-CA   | -8.55 | 109.15      | 119.84   |
| 4   | B     | 227  | LYS  | N-CA-C   | -8.53 | 97.66       | 110.28   |
| 3   | A     | 585  | GLY  | N-CA-C   | -8.51 | 102.94      | 115.63   |
| 3   | A     | 1276 | VAL  | N-CA-C   | 8.51  | 120.86      | 108.53   |
| 3   | A     | 50   | ILE  | CB-CA-C  | -8.50 | 97.34       | 111.29   |
| 4   | B     | 588  | GLY  | N-CA-C   | 8.49  | 121.25      | 110.38   |
| 4   | B     | 265  | SER  | N-CA-C   | 8.48  | 128.86      | 110.80   |
| 6   | E     | 46   | TYR  | N-CA-C   | 8.47  | 123.18      | 113.01   |
| 5   | C     | 115  | SER  | N-CA-C   | -8.46 | 102.01      | 111.82   |
| 4   | B     | 901  | PRO  | N-CA-C   | 8.45  | 125.55      | 113.47   |
| 9   | I     | 48   | LEU  | N-CA-C   | -8.45 | 101.80      | 114.64   |
| 3   | A     | 735  | VAL  | N-CA-C   | 8.44  | 124.25      | 112.35   |
| 6   | E     | 197  | LYS  | N-CA-C   | -8.43 | 96.01       | 109.59   |
| 6   | E     | 192  | ARG  | N-CA-C   | -8.43 | 97.32       | 109.96   |
| 3   | A     | 8    | SER  | N-CA-C   | -8.36 | 100.83      | 112.45   |
| 3   | A     | 227  | VAL  | N-CA-C   | 8.35  | 126.71      | 109.34   |
| 3   | A     | 1237 | ILE  | N-CA-C   | 8.35  | 121.38      | 108.44   |
| 7   | F     | 138  | LEU  | CA-C-N   | -8.35 | 110.85      | 120.12   |
| 7   | F     | 138  | LEU  | C-N-CA   | -8.35 | 110.85      | 120.12   |
| 3   | A     | 447  | GLN  | C-N-CD   | 8.33  | 138.93      | 120.60   |
| 3   | A     | 1120 | LEU  | N-CA-C   | 8.33  | 120.66      | 110.41   |
| 4   | B     | 578  | THR  | N-CA-C   | -8.33 | 97.35       | 109.59   |
| 3   | A     | 483  | ASP  | N-CA-C   | -8.31 | 100.09      | 111.56   |
| 3   | A     | 906  | HIS  | CB-CA-C  | -8.30 | 98.46       | 111.17   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 4   | B     | 168  | GLY  | N-CA-C     | 8.29  | 132.82      | 113.18   |
| 3   | A     | 750  | GLY  | N-CA-C     | -8.28 | 101.51      | 115.08   |
| 3   | A     | 1377 | THR  | N-CA-C     | 8.27  | 124.47      | 113.72   |
| 8   | H     | 111  | LEU  | N-CA-C     | 8.26  | 122.72      | 108.76   |
| 8   | H     | 141  | TYR  | N-CA-C     | -8.26 | 97.06       | 109.86   |
| 3   | A     | 356  | ASP  | CA-C-N     | 8.25  | 127.91      | 119.82   |
| 3   | A     | 356  | ASP  | C-N-CA     | 8.25  | 127.91      | 119.82   |
| 4   | B     | 916  | THR  | CA-C-N     | 8.23  | 130.13      | 119.84   |
| 4   | B     | 916  | THR  | C-N-CA     | 8.23  | 130.13      | 119.84   |
| 3   | A     | 286  | HIS  | N-CA-C     | 8.23  | 128.32      | 110.80   |
| 3   | A     | 1137 | ALA  | N-CA-C     | -8.23 | 103.76      | 113.88   |
| 4   | B     | 748  | ILE  | N-CA-C     | -8.22 | 101.89      | 113.07   |
| 4   | B     | 961  | LEU  | N-CA-C     | 8.22  | 122.15      | 110.23   |
| 3   | A     | 9    | ALA  | CA-C-N     | -8.22 | 109.57      | 119.84   |
| 3   | A     | 9    | ALA  | C-N-CA     | -8.22 | 109.57      | 119.84   |
| 3   | A     | 273  | ASN  | CA-C-N     | -8.20 | 109.97      | 121.77   |
| 3   | A     | 273  | ASN  | C-N-CA     | -8.20 | 109.97      | 121.77   |
| 3   | A     | 531  | ILE  | N-CA-C     | -8.18 | 92.33       | 109.34   |
| 3   | A     | 619  | LYS  | N-CA-C     | 8.17  | 119.81      | 111.07   |
| 9   | I     | 58   | VAL  | N-CA-C     | -8.17 | 96.06       | 107.99   |
| 3   | A     | 967  | ALA  | N-CA-C     | -8.17 | 101.17      | 112.12   |
| 2   | T     | 3    | DG   | N9-C1'-C2' | -8.16 | 101.26      | 113.50   |
| 3   | A     | 6    | TYR  | N-CA-C     | -8.14 | 98.43       | 110.48   |
| 12  | L     | 65   | VAL  | N-CA-C     | 8.14  | 120.30      | 108.58   |
| 3   | A     | 1256 | GLU  | N-CA-C     | 8.12  | 128.09      | 110.80   |
| 3   | A     | 223  | GLY  | N-CA-C     | 8.10  | 132.38      | 113.18   |
| 3   | A     | 1262 | LYS  | N-CA-C     | -8.10 | 103.15      | 112.87   |
| 4   | B     | 97   | VAL  | N-CA-C     | 8.09  | 119.77      | 108.12   |
| 3   | A     | 417  | TYR  | N-CA-C     | -8.08 | 97.19       | 109.96   |
| 8   | H     | 85   | GLY  | N-CA-C     | -8.08 | 94.02       | 113.18   |
| 3   | A     | 885  | THR  | N-CA-C     | -8.08 | 101.22      | 112.45   |
| 3   | A     | 582  | ILE  | CA-C-N     | 8.07  | 129.92      | 119.84   |
| 3   | A     | 582  | ILE  | C-N-CA     | 8.07  | 129.92      | 119.84   |
| 2   | T     | 6    | DC   | N1-C1'-C2' | -8.05 | 101.42      | 113.50   |
| 3   | A     | 316  | GLN  | CA-CB-CG   | -8.02 | 98.06       | 114.10   |
| 3   | A     | 624  | SER  | N-CA-C     | -8.02 | 101.67      | 112.26   |
| 8   | H     | 145  | ARG  | N-CA-C     | 8.02  | 122.63      | 109.24   |
| 4   | B     | 222  | ILE  | CA-C-N     | 8.01  | 136.40      | 121.97   |
| 4   | B     | 222  | ILE  | C-N-CA     | 8.01  | 136.40      | 121.97   |
| 3   | A     | 270  | LEU  | N-CA-C     | -7.99 | 103.42      | 113.01   |
| 6   | E     | 79   | TRP  | N-CA-C     | 7.98  | 123.73      | 107.69   |
| 4   | B     | 132  | VAL  | N-CA-C     | 7.98  | 125.93      | 109.34   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 5   | C     | 39   | ALA  | N-CA-C     | 7.95  | 123.14      | 112.88   |
| 4   | B     | 432  | MET  | N-CA-C     | 7.95  | 127.74      | 110.80   |
| 4   | B     | 305  | VAL  | N-CA-C     | 7.93  | 125.84      | 109.34   |
| 3   | A     | 978  | PRO  | N-CA-C     | 7.93  | 128.81      | 112.47   |
| 3   | A     | 887  | GLY  | N-CA-C     | 7.93  | 124.30      | 112.41   |
| 4   | B     | 37   | PHE  | N-CA-C     | -7.90 | 93.98       | 110.80   |
| 12  | L     | 38   | LEU  | N-CA-C     | -7.88 | 100.36      | 110.53   |
| 3   | A     | 249  | SER  | CA-C-N     | 7.88  | 136.16      | 121.97   |
| 3   | A     | 249  | SER  | C-N-CA     | 7.88  | 136.16      | 121.97   |
| 3   | A     | 310  | GLY  | N-CA-C     | 7.87  | 120.79      | 111.35   |
| 10  | J     | 54   | VAL  | N-CA-C     | 7.84  | 117.98      | 106.85   |
| 10  | J     | 27   | GLU  | N-CA-C     | 7.83  | 123.34      | 112.93   |
| 4   | B     | 165  | VAL  | N-CA-C     | 7.82  | 120.12      | 108.46   |
| 3   | A     | 50   | ILE  | N-CA-C     | 7.82  | 125.61      | 109.34   |
| 4   | B     | 846  | ILE  | N-CA-C     | -7.81 | 103.19      | 110.53   |
| 3   | A     | 714  | PHE  | N-CA-C     | -7.80 | 101.88      | 111.40   |
| 3   | A     | 442  | VAL  | N-CA-C     | 7.79  | 119.56      | 108.42   |
| 3   | A     | 31   | SER  | N-CA-C     | 7.78  | 121.09      | 110.35   |
| 3   | A     | 100  | LYS  | N-CA-C     | -7.78 | 101.90      | 111.40   |
| 6   | E     | 89   | GLY  | N-CA-C     | 7.77  | 122.44      | 111.10   |
| 4   | B     | 570  | VAL  | CA-C-N     | 7.76  | 128.17      | 119.32   |
| 4   | B     | 570  | VAL  | C-N-CA     | 7.76  | 128.17      | 119.32   |
| 9   | I     | 111  | THR  | N-CA-C     | 7.76  | 121.55      | 109.52   |
| 2   | T     | 7    | DC   | N1-C1'-C2' | -7.76 | 101.87      | 113.50   |
| 8   | H     | 62   | SER  | N-CA-C     | 7.75  | 127.32      | 110.80   |
| 3   | A     | 950  | GLY  | N-CA-C     | -7.74 | 103.87      | 115.32   |
| 4   | B     | 172  | ILE  | N-CA-C     | 7.74  | 119.00      | 108.17   |
| 4   | B     | 167  | ILE  | N-CA-C     | -7.74 | 96.98       | 108.12   |
| 3   | A     | 778  | GLY  | N-CA-C     | -7.74 | 103.13      | 112.49   |
| 5   | C     | 40   | GLU  | CA-C-N     | -7.74 | 114.97      | 123.02   |
| 5   | C     | 40   | GLU  | C-N-CA     | -7.74 | 114.97      | 123.02   |
| 3   | A     | 924  | LYS  | N-CA-C     | -7.73 | 102.91      | 112.88   |
| 3   | A     | 1006 | ILE  | CB-CA-C    | -7.73 | 101.92      | 112.04   |
| 3   | A     | 1291 | VAL  | CA-C-N     | 7.72  | 129.49      | 119.84   |
| 3   | A     | 1291 | VAL  | C-N-CA     | 7.72  | 129.49      | 119.84   |
| 5   | C     | 205  | LYS  | N-CA-C     | -7.72 | 101.99      | 111.33   |
| 3   | A     | 595  | THR  | N-CA-C     | 7.71  | 122.41      | 109.76   |
| 6   | E     | 75   | MET  | N-CA-C     | 7.71  | 120.96      | 110.55   |
| 8   | H     | 102  | TYR  | N-CA-C     | 7.71  | 124.35      | 114.56   |
| 4   | B     | 1170 | THR  | N-CA-C     | -7.71 | 102.94      | 112.88   |
| 3   | A     | 1001 | ARG  | N-CA-C     | 7.70  | 123.12      | 112.04   |
| 6   | E     | 74   | ASP  | N-CA-C     | 7.70  | 122.34      | 112.34   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 5   | C     | 38   | ILE  | CB-CA-C  | -7.69 | 102.12      | 111.97   |
| 3   | A     | 915  | SER  | N-CA-C   | -7.69 | 102.74      | 113.20   |
| 11  | K     | 34   | THR  | N-CA-C   | -7.68 | 99.45       | 110.59   |
| 3   | A     | 881  | GLN  | N-CA-C   | -7.68 | 97.64       | 109.24   |
| 5   | C     | 109  | SER  | N-CA-C   | 7.67  | 127.14      | 110.80   |
| 10  | J     | 61   | LEU  | N-CA-C   | -7.67 | 102.92      | 111.82   |
| 4   | B     | 1193 | GLN  | N-CA-C   | -7.67 | 96.73       | 109.46   |
| 5   | C     | 155  | LEU  | N-CA-C   | 7.67  | 121.54      | 109.81   |
| 3   | A     | 1211 | GLN  | N-CA-C   | -7.65 | 101.93      | 111.11   |
| 4   | B     | 43   | LEU  | N-CA-C   | 7.64  | 122.64      | 113.16   |
| 10  | J     | 2    | ILE  | N-CA-C   | 7.64  | 125.23      | 109.34   |
| 4   | B     | 238  | ALA  | N-CA-C   | -7.64 | 97.29       | 109.59   |
| 3   | A     | 36   | ARG  | N-CA-C   | 7.62  | 121.83      | 112.54   |
| 3   | A     | 1171 | GLN  | N-CA-C   | -7.60 | 101.99      | 111.11   |
| 6   | E     | 34   | GLU  | N-CA-C   | 7.60  | 121.47      | 111.75   |
| 4   | B     | 1096 | ARG  | N-CA-C   | -7.58 | 94.65       | 110.80   |
| 4   | B     | 247  | GLY  | N-CA-C   | 7.58  | 131.14      | 113.18   |
| 5   | C     | 125  | MET  | N-CA-C   | -7.57 | 103.34      | 112.58   |
| 8   | H     | 112  | ILE  | N-CA-C   | 7.56  | 121.06      | 108.81   |
| 3   | A     | 1155 | ASP  | CA-C-N   | 7.55  | 129.28      | 119.84   |
| 3   | A     | 1155 | ASP  | C-N-CA   | 7.55  | 129.28      | 119.84   |
| 3   | A     | 1428 | VAL  | N-CA-C   | -7.55 | 102.77      | 111.00   |
| 4   | B     | 1066 | SER  | N-CA-C   | 7.55  | 126.87      | 110.80   |
| 3   | A     | 243  | PRO  | CA-C-N   | 7.54  | 128.15      | 120.38   |
| 3   | A     | 243  | PRO  | C-N-CA   | 7.54  | 128.15      | 120.38   |
| 3   | A     | 1293 | SER  | N-CA-C   | -7.53 | 99.07       | 110.07   |
| 4   | B     | 638  | PHE  | N-CA-CB  | 7.52  | 121.19      | 110.44   |
| 5   | C     | 173  | ALA  | N-CA-C   | 7.51  | 126.80      | 110.80   |
| 3   | A     | 830  | LYS  | N-CA-C   | -7.49 | 103.05      | 111.07   |
| 4   | B     | 379  | GLY  | N-CA-C   | -7.49 | 103.43      | 112.49   |
| 3   | A     | 67   | CYS  | N-CA-C   | -7.49 | 94.69       | 108.24   |
| 3   | A     | 315  | LEU  | CA-CB-CG | 7.49  | 142.50      | 116.30   |
| 3   | A     | 481  | ASP  | N-CA-C   | -7.48 | 98.56       | 109.18   |
| 11  | K     | 75   | ILE  | N-CA-C   | 7.48  | 118.89      | 108.12   |
| 4   | B     | 648  | HIS  | N-CA-C   | 7.47  | 126.72      | 110.80   |
| 3   | A     | 250  | ILE  | N-CA-C   | 7.47  | 124.88      | 109.34   |
| 9   | I     | 38   | ALA  | N-CA-C   | 7.47  | 121.22      | 110.24   |
| 6   | E     | 33   | GLU  | CA-C-N   | 7.46  | 131.27      | 120.38   |
| 6   | E     | 33   | GLU  | C-N-CA   | 7.46  | 131.27      | 120.38   |
| 8   | H     | 110  | ASP  | N-CA-CB  | -7.45 | 99.67       | 110.47   |
| 3   | A     | 1293 | SER  | CA-C-N   | 7.45  | 129.15      | 119.84   |
| 3   | A     | 1293 | SER  | C-N-CA   | 7.45  | 129.15      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 9   | I     | 90   | GLN  | N-CA-C   | -7.44 | 98.44       | 110.20   |
| 4   | B     | 195  | CYS  | CA-C-N   | 7.43  | 128.70      | 120.45   |
| 4   | B     | 195  | CYS  | C-N-CA   | 7.43  | 128.70      | 120.45   |
| 4   | B     | 564  | GLU  | N-CA-C   | -7.43 | 100.43      | 109.57   |
| 12  | L     | 32   | ALA  | N-CA-C   | 7.43  | 119.17      | 111.14   |
| 3   | A     | 1053 | PHE  | N-CA-C   | -7.43 | 94.97       | 110.80   |
| 5   | C     | 153  | LEU  | N-CA-C   | -7.43 | 96.30       | 108.41   |
| 8   | H     | 81   | PRO  | N-CA-C   | -7.43 | 101.64      | 110.70   |
| 12  | L     | 33   | GLU  | N-CA-C   | 7.42  | 119.00      | 111.07   |
| 3   | A     | 1279 | ILE  | CB-CA-C  | -7.40 | 104.94      | 113.22   |
| 3   | A     | 818  | MET  | N-CA-C   | -7.40 | 103.24      | 111.82   |
| 4   | B     | 552  | MET  | N-CA-C   | 7.40  | 122.86      | 113.25   |
| 3   | A     | 899  | VAL  | CB-CA-C  | 7.39  | 118.84      | 110.41   |
| 3   | A     | 513  | SER  | N-CA-C   | 7.38  | 118.95      | 109.72   |
| 4   | B     | 1128 | LEU  | N-CA-C   | -7.38 | 97.91       | 109.72   |
| 3   | A     | 451  | HIS  | CB-CA-C  | -7.37 | 97.19       | 111.78   |
| 3   | A     | 1422 | ARG  | N-CA-C   | -7.36 | 102.05      | 113.02   |
| 3   | A     | 1434 | ALA  | CA-C-N   | -7.36 | 110.64      | 119.84   |
| 3   | A     | 1434 | ALA  | C-N-CA   | -7.36 | 110.64      | 119.84   |
| 6   | E     | 65   | THR  | N-CA-C   | -7.35 | 99.40       | 110.28   |
| 3   | A     | 1343 | ALA  | N-CA-C   | -7.35 | 102.43      | 111.40   |
| 4   | B     | 275  | TYR  | CA-CB-CG | 7.34  | 127.11      | 113.90   |
| 3   | A     | 205  | GLU  | N-CA-C   | 7.34  | 120.21      | 111.33   |
| 3   | A     | 506  | ALA  | N-CA-C   | 7.34  | 121.80      | 110.20   |
| 4   | B     | 861  | ASP  | N-CA-C   | 7.34  | 120.51      | 108.99   |
| 4   | B     | 251  | ILE  | N-CA-C   | 7.33  | 119.16      | 107.73   |
| 7   | F     | 75   | PRO  | N-CA-C   | 7.33  | 122.76      | 111.11   |
| 3   | A     | 532  | ARG  | CA-C-N   | -7.32 | 109.74      | 120.28   |
| 3   | A     | 532  | ARG  | C-N-CA   | -7.32 | 109.74      | 120.28   |
| 3   | A     | 58   | LEU  | N-CA-C   | 7.32  | 121.17      | 109.24   |
| 9   | I     | 90   | GLN  | CA-C-N   | -7.32 | 113.10      | 123.20   |
| 9   | I     | 90   | GLN  | C-N-CA   | -7.32 | 113.10      | 123.20   |
| 3   | A     | 252  | PHE  | O-C-N    | 7.31  | 129.85      | 122.10   |
| 4   | B     | 133  | LYS  | N-CA-C   | 7.31  | 120.17      | 110.53   |
| 3   | A     | 42   | ASP  | N-CA-C   | 7.30  | 119.67      | 109.15   |
| 4   | B     | 323  | VAL  | N-CA-C   | -7.30 | 94.16       | 109.34   |
| 4   | B     | 273  | LEU  | CA-C-N   | 7.29  | 128.95      | 119.84   |
| 4   | B     | 273  | LEU  | C-N-CA   | 7.29  | 128.95      | 119.84   |
| 11  | K     | 27   | ALA  | CA-C-N   | 7.29  | 128.95      | 119.84   |
| 11  | K     | 27   | ALA  | C-N-CA   | 7.29  | 128.95      | 119.84   |
| 4   | B     | 880  | THR  | N-CA-C   | 7.29  | 119.44      | 110.91   |
| 4   | B     | 1052 | VAL  | N-CA-C   | -7.28 | 103.19      | 110.62   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | B     | 644  | GLU  | N-CA-C  | 7.26  | 121.55      | 108.48   |
| 5   | C     | 108  | GLU  | N-CA-C  | -7.25 | 104.96      | 113.88   |
| 4   | B     | 1093 | GLN  | N-CA-C  | 7.24  | 120.73      | 109.07   |
| 3   | A     | 780  | VAL  | N-CA-C  | 7.24  | 118.40      | 108.84   |
| 3   | A     | 1295 | THR  | N-CA-C  | 7.22  | 121.73      | 112.34   |
| 3   | A     | 1038 | THR  | N-CA-C  | -7.22 | 98.10       | 109.07   |
| 4   | B     | 723  | VAL  | CB-CA-C | -7.22 | 99.45       | 111.29   |
| 4   | B     | 976  | ILE  | N-CA-C  | 7.22  | 117.20      | 110.42   |
| 6   | E     | 114  | ASN  | N-CA-C  | 7.20  | 123.70      | 114.56   |
| 9   | I     | 118  | ARG  | CB-CA-C | -7.20 | 98.14       | 109.72   |
| 4   | B     | 729  | ILE  | N-CA-C  | 7.19  | 116.67      | 106.53   |
| 3   | A     | 289  | ILE  | N-CA-C  | -7.18 | 94.40       | 109.34   |
| 3   | A     | 567  | LYS  | CA-C-N  | 7.18  | 128.81      | 119.84   |
| 3   | A     | 567  | LYS  | C-N-CA  | 7.18  | 128.81      | 119.84   |
| 11  | K     | 14   | GLU  | N-CA-C  | 7.18  | 120.47      | 108.20   |
| 3   | A     | 1033 | GLN  | N-CA-C  | 7.17  | 120.51      | 111.69   |
| 3   | A     | 562  | THR  | CA-C-N  | 7.16  | 128.23      | 120.13   |
| 3   | A     | 562  | THR  | C-N-CA  | 7.16  | 128.23      | 120.13   |
| 9   | I     | 103  | CYS  | N-CA-C  | -7.16 | 101.61      | 110.41   |
| 6   | E     | 95   | THR  | N-CA-C  | -7.15 | 104.55      | 113.28   |
| 5   | C     | 221  | TYR  | N-CA-C  | 7.12  | 122.14      | 113.38   |
| 5   | C     | 226  | ASP  | N-CA-C  | -7.12 | 98.19       | 109.23   |
| 3   | A     | 177  | ASP  | N-CA-C  | -7.12 | 95.22       | 107.61   |
| 4   | B     | 1191 | ILE  | N-CA-C  | 7.12  | 120.71      | 108.90   |
| 3   | A     | 256  | GLN  | N-CA-C  | 7.10  | 121.33      | 107.98   |
| 3   | A     | 60   | SER  | N-CA-C  | 7.10  | 125.92      | 110.80   |
| 3   | A     | 440  | ASP  | CA-C-N  | 7.10  | 128.71      | 119.84   |
| 3   | A     | 440  | ASP  | C-N-CA  | 7.10  | 128.71      | 119.84   |
| 4   | B     | 250  | PHE  | N-CA-C  | -7.08 | 94.58       | 107.75   |
| 3   | A     | 256  | GLN  | CA-C-N  | 7.08  | 135.06      | 121.54   |
| 3   | A     | 256  | GLN  | C-N-CA  | 7.08  | 135.06      | 121.54   |
| 3   | A     | 710  | LEU  | N-CA-C  | -7.08 | 104.38      | 112.87   |
| 4   | B     | 825  | VAL  | N-CA-C  | 7.07  | 118.67      | 108.48   |
| 6   | E     | 10   | SER  | N-CA-C  | -7.07 | 102.62      | 111.11   |
| 5   | C     | 251  | LEU  | N-CA-C  | -7.07 | 103.27      | 110.97   |
| 4   | B     | 662  | MET  | N-CA-C  | -7.05 | 103.35      | 112.23   |
| 3   | A     | 505  | CYS  | N-CA-C  | 7.04  | 121.89      | 113.16   |
| 4   | B     | 326  | ASP  | N-CA-C  | 7.04  | 125.80      | 110.80   |
| 3   | A     | 568  | PRO  | N-CA-C  | 7.04  | 126.97      | 112.47   |
| 3   | A     | 909  | ASP  | CA-C-N  | -7.04 | 111.04      | 119.84   |
| 3   | A     | 909  | ASP  | C-N-CA  | -7.04 | 111.04      | 119.84   |
| 7   | F     | 127  | GLU  | N-CA-C  | -7.04 | 95.94       | 109.24   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 6   | E     | 54   | GLN  | CA-CB-CG | -7.03 | 100.03      | 114.10   |
| 3   | A     | 285  | PRO  | N-CA-C   | 7.03  | 126.95      | 112.47   |
| 4   | B     | 223  | VAL  | N-CA-CB  | -7.03 | 99.63       | 111.23   |
| 4   | B     | 801  | LYS  | N-CA-C   | -7.02 | 99.99       | 110.24   |
| 5   | C     | 177  | GLU  | N-CA-C   | -7.02 | 101.08      | 110.55   |
| 10  | J     | 30   | LEU  | N-CA-C   | 7.01  | 120.58      | 109.50   |
| 3   | A     | 683  | ILE  | N-CA-C   | -7.01 | 103.94      | 110.53   |
| 8   | H     | 128  | ASN  | N-CA-C   | 6.99  | 125.69      | 110.80   |
| 3   | A     | 130  | ASP  | N-CA-C   | 6.98  | 125.67      | 110.80   |
| 4   | B     | 170  | LEU  | CA-C-N   | 6.97  | 128.56      | 119.84   |
| 4   | B     | 170  | LEU  | C-N-CA   | 6.97  | 128.56      | 119.84   |
| 6   | E     | 176  | PRO  | N-CA-C   | -6.97 | 100.13      | 111.21   |
| 4   | B     | 1157 | ALA  | N-CA-C   | -6.95 | 95.99       | 110.80   |
| 4   | B     | 1177 | HIS  | N-CA-C   | -6.95 | 101.81      | 111.81   |
| 12  | L     | 65   | VAL  | CA-C-N   | 6.94  | 131.78      | 121.72   |
| 12  | L     | 65   | VAL  | C-N-CA   | 6.94  | 131.78      | 121.72   |
| 3   | A     | 253  | ASN  | CA-C-N   | 6.94  | 134.79      | 121.54   |
| 3   | A     | 253  | ASN  | C-N-CA   | 6.94  | 134.79      | 121.54   |
| 3   | A     | 147  | VAL  | CB-CA-C  | -6.93 | 101.67      | 111.38   |
| 3   | A     | 541  | ILE  | CA-C-N   | -6.93 | 110.65      | 123.05   |
| 3   | A     | 541  | ILE  | C-N-CA   | -6.93 | 110.65      | 123.05   |
| 4   | B     | 510  | LYS  | N-CA-C   | 6.93  | 124.81      | 108.40   |
| 4   | B     | 884  | ARG  | N-CA-C   | -6.93 | 94.07       | 107.44   |
| 3   | A     | 247  | ARG  | CA-C-N   | -6.92 | 111.19      | 119.84   |
| 3   | A     | 247  | ARG  | C-N-CA   | -6.92 | 111.19      | 119.84   |
| 11  | K     | 82   | ASP  | CA-C-N   | 6.91  | 128.48      | 119.84   |
| 11  | K     | 82   | ASP  | C-N-CA   | 6.91  | 128.48      | 119.84   |
| 4   | B     | 112  | LEU  | N-CA-C   | 6.91  | 120.93      | 109.46   |
| 3   | A     | 345  | VAL  | N-CA-C   | 6.90  | 119.13      | 108.44   |
| 9   | I     | 78   | CYS  | N-CA-C   | 6.89  | 125.48      | 110.80   |
| 6   | E     | 90   | VAL  | N-CA-C   | 6.89  | 123.67      | 109.34   |
| 5   | C     | 80   | LEU  | N-CA-C   | -6.89 | 98.84       | 109.52   |
| 4   | B     | 860  | MET  | N-CA-C   | 6.89  | 119.90      | 109.23   |
| 3   | A     | 836  | TYR  | N-CA-C   | -6.88 | 103.71      | 111.14   |
| 4   | B     | 900  | ALA  | N-CA-C   | -6.88 | 101.14      | 110.36   |
| 4   | B     | 424  | LEU  | N-CA-C   | -6.88 | 102.86      | 111.11   |
| 10  | J     | 53   | HIS  | CA-C-N   | -6.87 | 113.48      | 123.10   |
| 10  | J     | 53   | HIS  | C-N-CA   | -6.87 | 113.48      | 123.10   |
| 3   | A     | 454  | SER  | N-CA-C   | -6.86 | 104.79      | 113.02   |
| 4   | B     | 316  | PRO  | N-CA-C   | 6.85  | 122.46      | 114.03   |
| 4   | B     | 126  | SER  | N-CA-C   | 6.83  | 120.18      | 110.14   |
| 5   | C     | 225  | ALA  | N-CA-C   | 6.83  | 120.06      | 109.07   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | A     | 1123 | GLY  | N-CA-C   | -6.83 | 103.62      | 113.86   |
| 3   | A     | 779  | PHE  | N-CA-C   | -6.80 | 102.04      | 110.41   |
| 5   | C     | 169  | LYS  | N-CA-C   | -6.80 | 104.24      | 112.54   |
| 3   | A     | 244  | PRO  | N-CA-C   | 6.80  | 119.00      | 110.70   |
| 10  | J     | 28   | ASP  | N-CA-C   | -6.78 | 105.78      | 112.97   |
| 5   | C     | 220  | ASP  | N-CA-C   | -6.78 | 98.18       | 108.96   |
| 9   | I     | 68   | LEU  | CA-C-N   | 6.78  | 126.74      | 120.03   |
| 9   | I     | 68   | LEU  | C-N-CA   | 6.78  | 126.74      | 120.03   |
| 3   | A     | 1170 | ILE  | N-CA-C   | -6.77 | 106.41      | 111.90   |
| 3   | A     | 24   | PRO  | N-CA-C   | -6.77 | 104.00      | 113.81   |
| 3   | A     | 376  | TYR  | CA-C-N   | 6.77  | 128.30      | 119.84   |
| 3   | A     | 376  | TYR  | C-N-CA   | 6.77  | 128.30      | 119.84   |
| 3   | A     | 11   | LEU  | N-CA-C   | 6.76  | 120.05      | 108.02   |
| 6   | E     | 121  | MET  | N-CA-C   | -6.76 | 105.19      | 113.50   |
| 7   | F     | 142  | SER  | N-CA-C   | 6.76  | 120.37      | 110.17   |
| 3   | A     | 74   | MET  | N-CA-C   | 6.75  | 125.17      | 110.80   |
| 3   | A     | 914  | GLU  | N-CA-C   | -6.75 | 105.18      | 113.41   |
| 4   | B     | 639  | ILE  | N-CA-C   | 6.74  | 119.56      | 109.17   |
| 4   | B     | 1057 | LYS  | N-CA-C   | -6.74 | 103.86      | 111.07   |
| 5   | C     | 201  | TRP  | CA-C-N   | -6.74 | 111.41      | 119.84   |
| 5   | C     | 201  | TRP  | C-N-CA   | -6.74 | 111.41      | 119.84   |
| 8   | H     | 134  | ASN  | N-CA-C   | -6.72 | 92.08       | 107.48   |
| 4   | B     | 883  | LEU  | N-CA-C   | 6.72  | 125.11      | 110.80   |
| 3   | A     | 468  | PHE  | N-CA-C   | -6.71 | 99.89       | 109.96   |
| 3   | A     | 1348 | LEU  | N-CA-C   | -6.70 | 103.22      | 111.33   |
| 3   | A     | 425  | GLN  | N-CA-C   | -6.70 | 97.81       | 108.73   |
| 4   | B     | 707  | PRO  | N-CA-C   | -6.69 | 98.69       | 112.47   |
| 5   | C     | 5    | GLY  | N-CA-C   | 6.69  | 125.99      | 112.34   |
| 5   | C     | 7    | GLN  | CB-CA-C  | -6.68 | 100.48      | 110.24   |
| 8   | H     | 96   | VAL  | N-CA-C   | 6.68  | 117.43      | 108.27   |
| 11  | K     | 79   | GLU  | N-CA-C   | -6.68 | 100.00      | 109.96   |
| 3   | A     | 1161 | THR  | N-CA-C   | 6.68  | 119.15      | 110.53   |
| 3   | A     | 533  | LYS  | CA-CB-CG | 6.68  | 127.46      | 114.10   |
| 4   | B     | 222  | ILE  | N-CA-C   | 6.68  | 118.41      | 108.46   |
| 3   | A     | 621  | THR  | N-CA-C   | 6.67  | 121.73      | 112.45   |
| 3   | A     | 1300 | LYS  | N-CA-C   | 6.67  | 120.17      | 108.56   |
| 3   | A     | 1270 | ASN  | N-CA-C   | -6.67 | 96.59       | 110.80   |
| 3   | A     | 1278 | ASN  | N-CA-C   | 6.66  | 124.99      | 110.80   |
| 3   | A     | 1271 | ILE  | N-CA-C   | 6.65  | 118.10      | 107.73   |
| 4   | B     | 837  | ASP  | N-CA-C   | 6.64  | 120.82      | 111.52   |
| 3   | A     | 50   | ILE  | N-CA-CB  | 6.64  | 122.18      | 111.23   |
| 3   | A     | 1122 | PRO  | N-CA-C   | 6.64  | 126.14      | 112.47   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | A     | 1294 | PRO  | N-CA-C   | -6.63 | 98.81       | 112.47   |
| 5   | C     | 262  | LEU  | N-CA-C   | -6.63 | 104.13      | 111.36   |
| 4   | B     | 636  | PRO  | CA-N-CD  | -6.62 | 102.72      | 112.00   |
| 4   | B     | 1214 | PRO  | N-CA-C   | -6.62 | 98.83       | 112.47   |
| 6   | E     | 179  | GLN  | N-CA-C   | 6.62  | 120.45      | 109.46   |
| 3   | A     | 941  | LYS  | N-CA-C   | -6.61 | 102.71      | 111.24   |
| 12  | L     | 39   | SER  | N-CA-C   | -6.61 | 96.72       | 110.80   |
| 3   | A     | 1196 | GLU  | N-CA-C   | -6.60 | 100.19      | 110.42   |
| 4   | B     | 637  | LEU  | O-C-N    | 6.60  | 131.37      | 122.59   |
| 4   | B     | 431  | TYR  | CA-CB-CG | 6.60  | 125.78      | 113.90   |
| 6   | E     | 199  | ILE  | N-CA-C   | 6.59  | 117.21      | 106.72   |
| 4   | B     | 1092 | TYR  | N-CA-C   | 6.59  | 120.43      | 109.95   |
| 4   | B     | 610  | ASN  | N-CA-C   | 6.58  | 117.67      | 109.57   |
| 3   | A     | 380  | VAL  | CB-CA-C  | -6.58 | 101.32      | 111.71   |
| 4   | B     | 971  | THR  | N-CA-C   | -6.56 | 98.50       | 109.07   |
| 3   | A     | 1208 | THR  | N-CA-C   | 6.56  | 119.10      | 108.34   |
| 6   | E     | 184  | VAL  | N-CA-C   | -6.56 | 106.17      | 111.81   |
| 11  | K     | 105  | PHE  | N-CA-C   | -6.55 | 104.06      | 111.14   |
| 3   | A     | 569  | LYS  | N-CA-C   | -6.55 | 95.33       | 109.81   |
| 3   | A     | 56   | PRO  | N-CA-C   | 6.55  | 125.97      | 112.47   |
| 3   | A     | 1341 | ILE  | N-CA-C   | 6.55  | 117.24      | 110.36   |
| 3   | A     | 1315 | GLU  | CA-C-N   | -6.55 | 114.44      | 121.84   |
| 3   | A     | 1315 | GLU  | C-N-CA   | -6.55 | 114.44      | 121.84   |
| 3   | A     | 1403 | GLU  | N-CA-C   | 6.54  | 124.74      | 110.80   |
| 6   | E     | 111  | VAL  | N-CA-C   | 6.54  | 122.95      | 109.34   |
| 3   | A     | 174  | ILE  | N-CA-C   | 6.54  | 117.18      | 110.05   |
| 4   | B     | 1113 | VAL  | CB-CA-C  | -6.54 | 103.70      | 111.94   |
| 9   | I     | 50   | THR  | N-CA-C   | 6.54  | 120.06      | 109.40   |
| 3   | A     | 254  | GLU  | CB-CA-C  | 6.54  | 123.43      | 110.42   |
| 4   | B     | 1109 | GLY  | CA-C-N   | 6.53  | 126.48      | 120.21   |
| 4   | B     | 1109 | GLY  | C-N-CA   | 6.53  | 126.48      | 120.21   |
| 3   | A     | 1418 | LEU  | N-CA-C   | -6.52 | 97.78       | 108.41   |
| 3   | A     | 1009 | ASN  | N-CA-C   | -6.51 | 105.34      | 113.28   |
| 3   | A     | 255  | SER  | CA-C-N   | -6.49 | 111.96      | 122.34   |
| 3   | A     | 255  | SER  | C-N-CA   | -6.49 | 111.96      | 122.34   |
| 4   | B     | 292  | ILE  | N-CA-C   | 6.49  | 122.90      | 108.88   |
| 3   | A     | 490  | HIS  | CA-C-N   | -6.48 | 117.21      | 122.85   |
| 3   | A     | 490  | HIS  | C-N-CA   | -6.48 | 117.21      | 122.85   |
| 3   | A     | 704  | ALA  | N-CA-C   | 6.47  | 119.15      | 109.25   |
| 3   | A     | 11   | LEU  | CA-C-N   | -6.47 | 111.94      | 122.81   |
| 3   | A     | 11   | LEU  | C-N-CA   | -6.47 | 111.94      | 122.81   |
| 3   | A     | 252  | PHE  | CA-C-N   | 6.47  | 133.90      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | A     | 252  | PHE  | C-N-CA  | 6.47  | 133.90      | 121.54   |
| 3   | A     | 1163 | ILE  | CA-C-N  | 6.47  | 127.92      | 119.84   |
| 3   | A     | 1163 | ILE  | C-N-CA  | 6.47  | 127.92      | 119.84   |
| 4   | B     | 250  | PHE  | CA-C-N  | -6.46 | 114.28      | 122.43   |
| 4   | B     | 250  | PHE  | C-N-CA  | -6.46 | 114.28      | 122.43   |
| 3   | A     | 797  | LYS  | N-CA-C  | 6.46  | 120.08      | 112.72   |
| 3   | A     | 1361 | SER  | N-CA-C  | 6.45  | 119.38      | 110.35   |
| 6   | E     | 54   | GLN  | CA-C-N  | 6.45  | 129.75      | 120.79   |
| 6   | E     | 54   | GLN  | C-N-CA  | 6.45  | 129.75      | 120.79   |
| 5   | C     | 9    | LYS  | N-CA-C  | -6.44 | 97.09       | 110.80   |
| 4   | B     | 809  | MET  | N-CA-C  | -6.44 | 104.12      | 112.23   |
| 5   | C     | 98   | VAL  | N-CA-C  | 6.42  | 118.28      | 108.71   |
| 3   | A     | 596  | THR  | N-CA-C  | 6.42  | 124.46      | 110.80   |
| 5   | C     | 46   | ILE  | N-CA-C  | 6.41  | 122.67      | 109.34   |
| 3   | A     | 638  | GLY  | CA-C-N  | -6.40 | 111.84      | 119.84   |
| 3   | A     | 638  | GLY  | C-N-CA  | -6.40 | 111.84      | 119.84   |
| 3   | A     | 1406 | VAL  | N-CA-C  | 6.40  | 117.18      | 110.72   |
| 4   | B     | 889  | THR  | N-CA-C  | 6.40  | 120.25      | 109.76   |
| 6   | E     | 127  | ILE  | CA-C-N  | 6.40  | 126.97      | 120.38   |
| 6   | E     | 127  | ILE  | C-N-CA  | 6.40  | 126.97      | 120.38   |
| 3   | A     | 755  | PHE  | N-CA-C  | -6.39 | 104.00      | 110.97   |
| 3   | A     | 169  | ASN  | CA-C-N  | -6.39 | 111.64      | 123.01   |
| 3   | A     | 169  | ASN  | C-N-CA  | -6.39 | 111.64      | 123.01   |
| 12  | L     | 68   | GLU  | N-CA-C  | -6.39 | 98.80       | 108.96   |
| 4   | B     | 681  | TRP  | N-CA-C  | -6.38 | 103.23      | 111.02   |
| 3   | A     | 1127 | ASP  | N-CA-C  | -6.38 | 97.20       | 110.80   |
| 4   | B     | 184  | ALA  | N-CA-C  | 6.38  | 119.62      | 110.24   |
| 3   | A     | 1066 | VAL  | CB-CA-C | -6.38 | 103.80      | 111.97   |
| 4   | B     | 433  | GLN  | N-CA-C  | -6.38 | 103.84      | 111.69   |
| 3   | A     | 997  | LEU  | N-CA-C  | -6.38 | 103.59      | 111.75   |
| 6   | E     | 58   | MET  | N-CA-C  | -6.38 | 101.84      | 111.34   |
| 4   | B     | 170  | LEU  | N-CA-C  | 6.37  | 122.89      | 108.74   |
| 4   | B     | 959  | ASP  | N-CA-C  | 6.37  | 124.37      | 110.80   |
| 3   | A     | 1121 | GLU  | CA-C-N  | 6.37  | 127.80      | 119.84   |
| 3   | A     | 1121 | GLU  | C-N-CA  | 6.37  | 127.80      | 119.84   |
| 6   | E     | 53   | PRO  | N-CA-C  | 6.36  | 125.58      | 112.47   |
| 5   | C     | 175  | ALA  | N-CA-C  | 6.36  | 118.82      | 108.26   |
| 8   | H     | 122  | LEU  | N-CA-C  | 6.36  | 120.28      | 110.42   |
| 4   | B     | 453  | ILE  | N-CA-C  | 6.36  | 116.40      | 110.42   |
| 4   | B     | 1196 | ILE  | CA-C-N  | 6.35  | 126.69      | 119.83   |
| 4   | B     | 1196 | ILE  | C-N-CA  | 6.35  | 126.69      | 119.83   |
| 3   | A     | 1118 | VAL  | N-CA-C  | 6.35  | 118.17      | 108.71   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | B     | 1076 | HIS  | CB-CA-C     | -6.34 | 100.89      | 110.90   |
| 9   | I     | 49   | ILE  | N-CA-C      | -6.33 | 96.61       | 107.24   |
| 11  | K     | 56   | VAL  | CB-CA-C     | -6.33 | 101.72      | 110.96   |
| 8   | H     | 91   | ASP  | N-CA-C      | 6.32  | 124.27      | 110.80   |
| 3   | A     | 1227 | ILE  | N-CA-C      | 6.32  | 117.81      | 108.65   |
| 3   | A     | 116  | ASP  | N-CA-C      | 6.32  | 119.05      | 109.95   |
| 3   | A     | 282  | ASN  | N-CA-C      | -6.31 | 100.07      | 108.34   |
| 5   | C     | 194  | GLU  | N-CA-C      | -6.31 | 107.43      | 114.62   |
| 3   | A     | 434  | ARG  | N-CA-C      | 6.31  | 118.76      | 109.24   |
| 6   | E     | 41   | ASP  | N-CA-C      | 6.31  | 120.83      | 113.20   |
| 3   | A     | 841  | LEU  | N-CA-C      | -6.30 | 103.55      | 111.11   |
| 3   | A     | 895  | LYS  | CG-CD-CE    | 6.29  | 125.78      | 111.30   |
| 4   | B     | 1184 | GLY  | N-CA-C      | -6.28 | 98.30       | 113.18   |
| 3   | A     | 496  | GLU  | N-CA-C      | -6.28 | 104.13      | 110.97   |
| 6   | E     | 29   | PHE  | N-CA-C      | 6.27  | 118.94      | 108.96   |
| 2   | T     | 1    | DA   | C2'-C3'-O3' | 6.27  | 120.91      | 111.50   |
| 7   | F     | 101  | ILE  | N-CA-C      | -6.27 | 103.78      | 110.36   |
| 11  | K     | 31   | VAL  | N-CA-C      | 6.27  | 119.30      | 108.95   |
| 5   | C     | 8    | VAL  | N-CA-C      | 6.27  | 116.88      | 110.05   |
| 4   | B     | 1138 | MET  | N-CA-C      | -6.27 | 104.36      | 111.07   |
| 3   | A     | 320  | ARG  | C-N-CD      | -6.26 | 106.82      | 120.60   |
| 5   | C     | 118  | LEU  | N-CA-C      | -6.26 | 101.83      | 110.35   |
| 3   | A     | 67   | CYS  | CA-C-O      | -6.26 | 115.05      | 122.13   |
| 3   | A     | 1138 | ILE  | N-CA-C      | 6.24  | 116.92      | 111.56   |
| 7   | F     | 77   | ASP  | CB-CA-C     | -6.24 | 99.16       | 112.63   |
| 4   | B     | 262  | GLU  | N-CA-C      | 6.23  | 118.12      | 109.15   |
| 3   | A     | 373  | THR  | N-CA-C      | 6.22  | 120.74      | 111.96   |
| 4   | B     | 618  | ASP  | N-CA-C      | -6.22 | 98.58       | 108.73   |
| 6   | E     | 171  | LYS  | N-CA-C      | -6.22 | 98.85       | 109.24   |
| 4   | B     | 1084 | GLN  | N-CA-C      | -6.21 | 101.29      | 110.48   |
| 3   | A     | 97   | ALA  | N-CA-C      | 6.21  | 119.95      | 112.38   |
| 4   | B     | 520  | GLY  | N-CA-C      | 6.21  | 122.47      | 115.08   |
| 8   | H     | 41   | ASP  | N-CA-C      | -6.20 | 99.17       | 109.46   |
| 3   | A     | 215  | SER  | N-CA-C      | 6.19  | 119.57      | 110.59   |
| 4   | B     | 865  | LYS  | CA-C-N      | -6.19 | 113.31      | 122.41   |
| 4   | B     | 865  | LYS  | C-N-CA      | -6.19 | 113.31      | 122.41   |
| 4   | B     | 909  | ASP  | N-CA-C      | 6.19  | 119.33      | 110.24   |
| 4   | B     | 620  | ARG  | N-CA-C      | 6.18  | 120.55      | 113.19   |
| 4   | B     | 604  | ARG  | N-CA-C      | -6.18 | 103.86      | 112.45   |
| 4   | B     | 473  | MET  | CB-CA-C     | 6.18  | 122.71      | 110.42   |
| 3   | A     | 775  | ILE  | N-CA-C      | 6.17  | 122.18      | 109.34   |
| 3   | A     | 447  | GLN  | CA-C-N      | -6.17 | 112.19      | 127.00   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | A     | 447  | GLN  | C-N-CA     | -6.17 | 112.19      | 127.00   |
| 3   | A     | 136  | ALA  | N-CA-C     | -6.17 | 105.07      | 112.59   |
| 4   | B     | 885  | MET  | N-CA-C     | -6.17 | 100.04      | 109.41   |
| 12  | L     | 48   | CYS  | N-CA-C     | 6.17  | 123.93      | 110.80   |
| 3   | A     | 711  | ARG  | N-CA-C     | -6.16 | 104.11      | 111.69   |
| 3   | A     | 301  | ALA  | N-CA-C     | -6.16 | 105.42      | 113.12   |
| 3   | A     | 84   | ILE  | N-CA-C     | 6.14  | 122.12      | 109.34   |
| 3   | A     | 867  | ILE  | CB-CA-C    | -6.13 | 101.23      | 111.29   |
| 4   | B     | 689  | LEU  | N-CA-C     | -6.13 | 104.21      | 113.89   |
| 3   | A     | 241  | VAL  | CA-C-N     | 6.13  | 126.69      | 120.38   |
| 3   | A     | 241  | VAL  | C-N-CA     | 6.13  | 126.69      | 120.38   |
| 4   | B     | 40   | GLU  | N-CA-C     | 6.12  | 118.92      | 111.82   |
| 8   | H     | 57   | VAL  | N-CA-C     | 6.12  | 117.18      | 108.42   |
| 6   | E     | 93   | MET  | N-CA-C     | -6.12 | 104.52      | 112.23   |
| 3   | A     | 652  | VAL  | CB-CA-C    | -6.12 | 104.03      | 112.04   |
| 4   | B     | 249  | ARG  | CA-C-N     | 6.12  | 131.35      | 122.85   |
| 4   | B     | 249  | ARG  | C-N-CA     | 6.12  | 131.35      | 122.85   |
| 5   | C     | 222  | LYS  | N-CA-C     | -6.11 | 104.99      | 112.88   |
| 4   | B     | 222  | ILE  | O-C-N      | 6.11  | 129.64      | 123.10   |
| 3   | A     | 895  | LYS  | CA-CB-CG   | 6.10  | 126.30      | 114.10   |
| 12  | L     | 30   | ILE  | N-CA-C     | -6.10 | 96.66       | 109.34   |
| 5   | C     | 57   | VAL  | N-CA-C     | -6.09 | 104.36      | 111.00   |
| 3   | A     | 357  | PRO  | N-CA-C     | 6.09  | 121.84      | 113.98   |
| 3   | A     | 1193 | LEU  | N-CA-C     | -6.08 | 99.33       | 109.24   |
| 4   | B     | 595  | ARG  | CB-CG-CD   | 6.08  | 125.29      | 111.30   |
| 4   | B     | 655  | LYS  | N-CA-C     | -6.08 | 103.97      | 111.75   |
| 3   | A     | 44   | THR  | N-CA-C     | 6.08  | 123.75      | 110.80   |
| 4   | B     | 422  | LYS  | N-CA-C     | -6.08 | 105.35      | 112.89   |
| 2   | T     | 11   | DC   | N1-C1'-C2' | -6.08 | 104.39      | 113.50   |
| 3   | A     | 1010 | ALA  | N-CA-C     | -6.07 | 103.99      | 111.40   |
| 4   | B     | 64   | CYS  | N-CA-C     | -6.07 | 99.34       | 109.24   |
| 4   | B     | 421  | PHE  | N-CA-C     | -6.07 | 104.97      | 112.38   |
| 3   | A     | 1414 | ALA  | N-CA-C     | 6.07  | 118.39      | 111.11   |
| 4   | B     | 886  | LYS  | N-CA-C     | 6.07  | 119.46      | 110.48   |
| 4   | B     | 1210 | MET  | N-CA-C     | -6.06 | 103.19      | 111.56   |
| 9   | I     | 109  | ILE  | N-CA-C     | 6.06  | 116.33      | 107.37   |
| 4   | B     | 876  | LYS  | CA-C-N     | 6.05  | 127.41      | 119.84   |
| 4   | B     | 876  | LYS  | C-N-CA     | 6.05  | 127.41      | 119.84   |
| 4   | B     | 1122 | ARG  | N-CA-C     | -6.05 | 104.80      | 111.82   |
| 3   | A     | 284  | ALA  | CA-C-N     | 6.05  | 127.40      | 119.84   |
| 3   | A     | 284  | ALA  | C-N-CA     | 6.05  | 127.40      | 119.84   |
| 4   | B     | 819  | ALA  | N-CA-C     | -6.05 | 98.40       | 108.32   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | E     | 80   | VAL  | N-CA-C      | -6.04 | 101.21      | 109.55   |
| 4   | B     | 358  | LYS  | N-CA-C      | 6.04  | 119.84      | 112.23   |
| 3   | A     | 5    | GLN  | N-CA-C      | 6.04  | 123.66      | 110.80   |
| 3   | A     | 679  | ILE  | CB-CA-C     | -6.03 | 104.25      | 111.97   |
| 3   | A     | 437  | MET  | N-CA-C      | 6.03  | 119.01      | 110.14   |
| 8   | H     | 30   | SER  | N-CA-C      | 6.03  | 117.83      | 109.15   |
| 3   | A     | 1006 | ILE  | CA-C-N      | 6.03  | 128.23      | 120.70   |
| 3   | A     | 1006 | ILE  | C-N-CA      | 6.03  | 128.23      | 120.70   |
| 4   | B     | 426  | LYS  | N-CA-C      | 6.03  | 120.65      | 112.88   |
| 4   | B     | 473  | MET  | CB-CG-SD    | 6.01  | 130.73      | 112.70   |
| 3   | A     | 784  | LEU  | N-CA-C      | -6.01 | 101.23      | 108.14   |
| 4   | B     | 236  | HIS  | N-CA-C      | -6.01 | 99.17       | 108.42   |
| 3   | A     | 1155 | ASP  | N-CA-C      | -6.01 | 95.40       | 108.74   |
| 10  | J     | 34   | THR  | N-CA-C      | -6.01 | 103.39      | 112.04   |
| 4   | B     | 863  | GLU  | N-CA-C      | 6.00  | 118.19      | 108.34   |
| 3   | A     | 842  | VAL  | CB-CA-C     | -6.00 | 103.94      | 112.22   |
| 4   | B     | 791  | THR  | N-CA-C      | -6.00 | 100.07      | 109.25   |
| 8   | H     | 29   | ALA  | CA-C-N      | 6.00  | 131.01      | 121.66   |
| 8   | H     | 29   | ALA  | C-N-CA      | 6.00  | 131.01      | 121.66   |
| 3   | A     | 320  | ARG  | CB-CA-C     | 6.00  | 121.98      | 110.17   |
| 3   | A     | 123  | ARG  | N-CA-C      | -5.99 | 98.04       | 110.80   |
| 5   | C     | 84   | ARG  | N-CA-C      | -5.99 | 105.23      | 112.54   |
| 8   | H     | 38   | LEU  | N-CA-C      | 5.99  | 118.51      | 109.23   |
| 10  | J     | 16   | ASP  | N-CA-C      | -5.99 | 105.63      | 113.17   |
| 3   | A     | 412  | ARG  | N-CA-C      | 5.98  | 119.18      | 107.57   |
| 4   | B     | 1074 | ASN  | N-CA-C      | -5.98 | 100.54      | 109.15   |
| 4   | B     | 1211 | ASN  | N-CA-C      | 5.98  | 119.89      | 112.24   |
| 3   | A     | 1384 | VAL  | N-CA-C      | -5.97 | 106.59      | 111.91   |
| 4   | B     | 34   | ILE  | CB-CA-C     | -5.97 | 104.06      | 111.70   |
| 8   | H     | 31   | THR  | N-CA-CB     | 5.96  | 118.55      | 110.38   |
| 12  | L     | 28   | LYS  | N-CA-C      | 5.96  | 123.50      | 110.80   |
| 3   | A     | 1020 | CYS  | N-CA-C      | -5.96 | 103.96      | 111.11   |
| 4   | B     | 1222 | ARG  | N-CA-C      | -5.96 | 99.57       | 109.46   |
| 3   | A     | 855  | THR  | N-CA-C      | -5.95 | 102.14      | 110.35   |
| 12  | L     | 45   | ALA  | N-CA-C      | 5.95  | 123.47      | 110.80   |
| 3   | A     | 1227 | ILE  | CB-CA-C     | -5.95 | 101.19      | 110.52   |
| 2   | T     | 3    | DG   | C2'-C3'-O3' | -5.94 | 102.59      | 111.50   |
| 4   | B     | 1195 | HIS  | N-CA-C      | 5.94  | 118.08      | 107.80   |
| 3   | A     | 254  | GLU  | CA-CB-CG    | -5.94 | 102.23      | 114.10   |
| 3   | A     | 569  | LYS  | CA-C-N      | -5.93 | 112.42      | 119.84   |
| 3   | A     | 569  | LYS  | C-N-CA      | -5.93 | 112.42      | 119.84   |
| 3   | A     | 1445 | ILE  | N-CA-C      | 5.93  | 127.61      | 111.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | B     | 939  | THR  | CA-C-N      | 5.93  | 127.25      | 119.84   |
| 4   | B     | 939  | THR  | C-N-CA      | 5.93  | 127.25      | 119.84   |
| 5   | C     | 7    | GLN  | CA-C-N      | 5.93  | 129.43      | 120.95   |
| 5   | C     | 7    | GLN  | C-N-CA      | 5.93  | 129.43      | 120.95   |
| 5   | C     | 258  | ILE  | CA-C-N      | 5.93  | 128.69      | 120.63   |
| 5   | C     | 258  | ILE  | C-N-CA      | 5.93  | 128.69      | 120.63   |
| 9   | I     | 5    | ARG  | N-CA-C      | 5.93  | 118.71      | 109.52   |
| 4   | B     | 871  | THR  | N-CA-C      | 5.93  | 120.08      | 107.70   |
| 8   | H     | 27   | GLU  | N-CA-C      | -5.92 | 98.75       | 108.41   |
| 3   | A     | 269  | ILE  | N-CA-C      | 5.92  | 116.13      | 110.74   |
| 2   | T     | 9    | DC   | C5'-C4'-C3' | -5.92 | 106.02      | 114.90   |
| 3   | A     | 378  | GLU  | CA-C-N      | -5.91 | 114.46      | 122.91   |
| 3   | A     | 378  | GLU  | C-N-CA      | -5.91 | 114.46      | 122.91   |
| 4   | B     | 684  | LEU  | N-CA-C      | -5.91 | 104.75      | 111.07   |
| 4   | B     | 226  | PHE  | N-CA-C      | 5.91  | 118.03      | 108.34   |
| 3   | A     | 403  | LYS  | N-CA-C      | -5.90 | 100.44      | 109.41   |
| 4   | B     | 198  | ASP  | N-CA-C      | -5.90 | 101.30      | 110.10   |
| 3   | A     | 321  | PRO  | CA-C-N      | -5.89 | 111.37      | 121.97   |
| 3   | A     | 321  | PRO  | C-N-CA      | -5.89 | 111.37      | 121.97   |
| 12  | L     | 27   | LEU  | N-CA-C      | 5.88  | 118.81      | 109.81   |
| 3   | A     | 292  | ALA  | N-CA-C      | 5.88  | 119.60      | 111.55   |
| 3   | A     | 746  | MET  | N-CA-C      | -5.88 | 105.20      | 112.90   |
| 3   | A     | 934  | LYS  | CA-C-N      | 5.88  | 128.96      | 120.79   |
| 3   | A     | 934  | LYS  | C-N-CA      | 5.88  | 128.96      | 120.79   |
| 3   | A     | 433  | GLU  | CA-C-N      | -5.87 | 112.70      | 122.21   |
| 3   | A     | 433  | GLU  | C-N-CA      | -5.87 | 112.70      | 122.21   |
| 4   | B     | 837  | ASP  | CB-CA-C     | -5.87 | 103.99      | 111.86   |
| 9   | I     | 95   | THR  | N-CA-C      | 5.87  | 119.52      | 110.42   |
| 12  | L     | 52   | GLY  | N-CA-C      | 5.87  | 127.10      | 113.18   |
| 11  | K     | 47   | ARG  | N-CA-C      | 5.87  | 117.68      | 111.28   |
| 6   | E     | 32   | GLN  | N-CA-C      | -5.86 | 105.90      | 113.16   |
| 7   | F     | 76   | LYS  | N-CA-C      | -5.85 | 104.73      | 112.34   |
| 3   | A     | 435  | HIS  | N-CA-C      | -5.85 | 101.99      | 110.24   |
| 4   | B     | 1085 | ILE  | N-CA-C      | 5.85  | 117.86      | 108.85   |
| 4   | B     | 510  | LYS  | CA-C-N      | 5.85  | 126.36      | 120.04   |
| 4   | B     | 510  | LYS  | C-N-CA      | 5.85  | 126.36      | 120.04   |
| 4   | B     | 596  | LEU  | N-CA-C      | 5.85  | 118.53      | 111.40   |
| 3   | A     | 344  | ARG  | N-CA-C      | -5.84 | 101.03      | 110.32   |
| 4   | B     | 805  | THR  | N-CA-C      | 5.84  | 118.36      | 109.95   |
| 8   | H     | 19   | ARG  | N-CA-C      | -5.84 | 98.35       | 110.80   |
| 3   | A     | 1219 | THR  | N-CA-C      | -5.84 | 106.69      | 113.88   |
| 3   | A     | 259  | GLU  | CA-CB-CG    | -5.83 | 102.43      | 114.10   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | A     | 1214 | GLU  | N-CA-C      | -5.83 | 105.26      | 112.38   |
| 5   | C     | 38   | ILE  | N-CA-C      | 5.83  | 116.02      | 110.42   |
| 3   | A     | 399  | HIS  | N-CA-C      | 5.82  | 122.67      | 109.81   |
| 3   | A     | 904  | THR  | CB-CA-C     | 5.82  | 122.00      | 110.42   |
| 11  | K     | 80   | GLY  | CA-C-N      | 5.82  | 128.97      | 120.71   |
| 11  | K     | 80   | GLY  | C-N-CA      | 5.82  | 128.97      | 120.71   |
| 4   | B     | 896  | ASP  | N-CA-C      | -5.82 | 105.02      | 111.71   |
| 8   | H     | 133  | ASN  | CB-CA-C     | -5.82 | 99.25       | 109.02   |
| 3   | A     | 316  | GLN  | CB-CG-CD    | 5.82  | 122.48      | 112.60   |
| 3   | A     | 1393 | ASN  | N-CA-C      | 5.82  | 123.19      | 110.80   |
| 2   | T     | 5    | DT   | N1-C1'-C2'  | -5.81 | 104.78      | 113.50   |
| 5   | C     | 176  | ILE  | N-CA-C      | 5.81  | 116.47      | 107.99   |
| 2   | T     | 4    | DA   | C5'-C4'-C3' | -5.80 | 106.21      | 114.90   |
| 3   | A     | 1126 | ALA  | N-CA-C      | 5.79  | 119.90      | 112.26   |
| 4   | B     | 245  | GLU  | N-CA-C      | 5.79  | 117.67      | 111.36   |
| 4   | B     | 882  | THR  | CB-CA-C     | -5.78 | 101.02      | 110.85   |
| 6   | E     | 144  | ILE  | N-CA-C      | -5.78 | 105.09      | 110.53   |
| 3   | A     | 601  | LYS  | N-CA-C      | -5.78 | 105.56      | 113.30   |
| 8   | H     | 3    | ASN  | N-CA-C      | 5.78  | 123.10      | 110.80   |
| 3   | A     | 274  | ILE  | CB-CA-C     | 5.77  | 121.39      | 110.94   |
| 3   | A     | 687  | LYS  | N-CA-C      | -5.77 | 104.59      | 111.69   |
| 3   | A     | 948  | VAL  | N-CA-C      | -5.77 | 103.21      | 111.17   |
| 4   | B     | 471  | LYS  | N-CA-C      | -5.77 | 98.51       | 110.80   |
| 3   | A     | 449  | SER  | N-CA-C      | 5.77  | 118.56      | 109.39   |
| 3   | A     | 1277 | GLU  | N-CA-C      | -5.76 | 102.75      | 110.24   |
| 12  | L     | 30   | ILE  | CB-CA-C     | -5.76 | 101.85      | 111.29   |
| 4   | B     | 1171 | VAL  | N-CA-C      | 5.75  | 121.31      | 109.34   |
| 9   | I     | 31   | THR  | N-CA-C      | -5.75 | 105.28      | 112.93   |
| 4   | B     | 420  | LEU  | N-CA-C      | -5.75 | 106.31      | 113.55   |
| 5   | C     | 233  | GLU  | N-CA-C      | -5.75 | 99.92       | 109.46   |
| 11  | K     | 18   | LYS  | CA-C-N      | -5.75 | 114.60      | 122.93   |
| 11  | K     | 18   | LYS  | C-N-CA      | -5.75 | 114.60      | 122.93   |
| 4   | B     | 687  | GLU  | N-CA-C      | -5.75 | 106.60      | 113.21   |
| 4   | B     | 1133 | MET  | N-CA-C      | 5.74  | 117.54      | 111.28   |
| 4   | B     | 306  | ASN  | N-CA-C      | -5.74 | 105.86      | 112.92   |
| 4   | B     | 514  | LEU  | N-CA-C      | -5.74 | 101.55      | 110.10   |
| 5   | C     | 163  | ILE  | N-CA-C      | 5.74  | 118.11      | 108.81   |
| 5   | C     | 266  | ASP  | N-CA-C      | -5.73 | 105.78      | 112.89   |
| 12  | L     | 49   | LYS  | CA-C-N      | 5.73  | 136.59      | 126.45   |
| 12  | L     | 49   | LYS  | C-N-CA      | 5.73  | 136.59      | 126.45   |
| 9   | I     | 11   | ASN  | N-CA-CB     | 5.73  | 120.17      | 110.49   |
| 4   | B     | 361  | LEU  | CA-C-N      | 5.72  | 127.00      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4   | B     | 361  | LEU  | C-N-CA   | 5.72  | 127.00      | 119.84   |
| 3   | A     | 653  | VAL  | CB-CA-C  | -5.72 | 104.41      | 112.14   |
| 5   | C     | 21   | ILE  | N-CA-C   | -5.72 | 100.10      | 108.11   |
| 3   | A     | 404  | TYR  | N-CA-C   | 5.72  | 122.99      | 110.80   |
| 3   | A     | 317  | LYS  | CA-CB-CG | -5.72 | 102.66      | 114.10   |
| 3   | A     | 938  | LYS  | N-CA-C   | -5.72 | 104.25      | 111.11   |
| 6   | E     | 76   | GLY  | N-CA-C   | 5.71  | 126.72      | 113.18   |
| 6   | E     | 91   | LYS  | N-CA-C   | -5.71 | 104.43      | 111.40   |
| 8   | H     | 37   | LYS  | N-CA-C   | 5.71  | 117.86      | 109.24   |
| 11  | K     | 22   | ASP  | CA-C-N   | 5.70  | 126.97      | 119.84   |
| 11  | K     | 22   | ASP  | C-N-CA   | 5.70  | 126.97      | 119.84   |
| 9   | I     | 5    | ARG  | N-CA-CB  | -5.70 | 101.64      | 111.55   |
| 3   | A     | 1007 | ILE  | CB-CA-C  | -5.69 | 104.69      | 111.81   |
| 3   | A     | 68   | GLN  | N-CA-C   | 5.69  | 122.92      | 110.80   |
| 3   | A     | 1000 | LEU  | CA-CB-CG | -5.69 | 96.38       | 116.30   |
| 4   | B     | 581  | PHE  | CA-C-N   | -5.69 | 115.09      | 122.99   |
| 4   | B     | 581  | PHE  | C-N-CA   | -5.69 | 115.09      | 122.99   |
| 3   | A     | 902  | LEU  | N-CA-C   | -5.68 | 98.69       | 110.80   |
| 4   | B     | 699  | GLU  | N-CA-C   | 5.68  | 119.03      | 111.75   |
| 5   | C     | 40   | GLU  | N-CA-C   | 5.68  | 122.87      | 113.89   |
| 9   | I     | 94   | ASP  | N-CA-C   | 5.68  | 120.44      | 112.72   |
| 3   | A     | 29   | ALA  | N-CA-C   | -5.68 | 104.71      | 111.69   |
| 4   | B     | 128  | LEU  | N-CA-C   | 5.67  | 118.31      | 107.75   |
| 4   | B     | 616  | ILE  | N-CA-C   | 5.67  | 116.03      | 107.80   |
| 8   | H     | 42   | ILE  | N-CA-C   | 5.67  | 121.14      | 109.34   |
| 3   | A     | 609  | ASP  | N-CA-C   | -5.67 | 98.72       | 110.80   |
| 5   | C     | 198  | ALA  | N-CA-C   | 5.67  | 120.85      | 113.88   |
| 6   | E     | 156  | LEU  | CA-C-N   | 5.66  | 128.91      | 120.87   |
| 6   | E     | 156  | LEU  | C-N-CA   | 5.66  | 128.91      | 120.87   |
| 3   | A     | 907  | THR  | CB-CA-C  | -5.66 | 100.42      | 112.63   |
| 4   | B     | 1076 | HIS  | N-CA-C   | -5.65 | 105.03      | 111.14   |
| 4   | B     | 431  | TYR  | CB-CA-C  | 5.65  | 121.67      | 110.42   |
| 6   | E     | 209  | ALA  | N-CA-C   | 5.65  | 117.86      | 108.20   |
| 4   | B     | 651  | LEU  | N-CA-C   | -5.65 | 100.47      | 109.96   |
| 4   | B     | 986  | GLN  | N-CA-C   | 5.65  | 117.67      | 109.71   |
| 3   | A     | 316  | GLN  | O-C-N    | 5.64  | 130.10      | 122.59   |
| 4   | B     | 473  | MET  | CA-C-O   | 5.64  | 128.58      | 120.51   |
| 3   | A     | 945  | GLU  | N-CA-C   | -5.64 | 98.79       | 110.80   |
| 4   | B     | 335  | GLY  | N-CA-C   | -5.64 | 96.95       | 113.30   |
| 11  | K     | 81   | TYR  | CA-CB-CG | 5.63  | 124.04      | 113.90   |
| 3   | A     | 315  | LEU  | CB-CA-C  | -5.63 | 99.21       | 110.42   |
| 4   | B     | 466  | TRP  | N-CA-C   | 5.63  | 122.80      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 5   | C     | 215  | GLU  | N-CA-C   | 5.62  | 122.77      | 110.80   |
| 4   | B     | 250  | PHE  | CA-CB-CG | 5.62  | 119.42      | 113.80   |
| 4   | B     | 1162 | ILE  | N-CA-C   | 5.62  | 116.45      | 108.42   |
| 4   | B     | 481  | GLN  | N-CA-C   | -5.62 | 101.20      | 109.18   |
| 4   | B     | 638  | PHE  | CB-CA-C  | -5.61 | 98.78       | 110.40   |
| 8   | H     | 103  | LYS  | N-CA-C   | 5.61  | 118.57      | 108.48   |
| 4   | B     | 933  | SER  | CA-C-N   | -5.60 | 113.60      | 122.23   |
| 4   | B     | 933  | SER  | C-N-CA   | -5.60 | 113.60      | 122.23   |
| 8   | H     | 132  | LEU  | N-CA-C   | -5.59 | 105.65      | 113.37   |
| 4   | B     | 899  | ILE  | CB-CA-C  | -5.59 | 102.12      | 111.29   |
| 9   | I     | 36   | GLU  | CA-CB-CG | 5.59  | 125.28      | 114.10   |
| 8   | H     | 123  | MET  | N-CA-C   | 5.59  | 118.20      | 108.76   |
| 3   | A     | 318  | SER  | N-CA-CB  | 5.58  | 119.93      | 110.49   |
| 3   | A     | 888  | GLY  | N-CA-C   | 5.58  | 126.40      | 113.18   |
| 3   | A     | 237  | THR  | CB-CA-C  | -5.58 | 99.33       | 110.42   |
| 3   | A     | 729  | ALA  | N-CA-C   | -5.57 | 104.42      | 111.11   |
| 11  | K     | 17   | SER  | CA-C-N   | -5.57 | 113.02      | 120.54   |
| 11  | K     | 17   | SER  | C-N-CA   | -5.57 | 113.02      | 120.54   |
| 3   | A     | 257  | ARG  | CG-CD-NE | 5.57  | 124.26      | 112.00   |
| 4   | B     | 981  | ALA  | O-C-N    | 5.57  | 130.00      | 122.59   |
| 8   | H     | 142  | LEU  | N-CA-C   | -5.57 | 99.19       | 108.32   |
| 3   | A     | 18   | GLN  | N-CA-C   | 5.55  | 118.62      | 107.41   |
| 3   | A     | 764  | CYS  | N-CA-C   | -5.55 | 99.62       | 109.06   |
| 3   | A     | 1139 | GLU  | N-CA-C   | 5.55  | 122.62      | 110.80   |
| 9   | I     | 84   | VAL  | N-CA-C   | -5.55 | 97.80       | 109.34   |
| 5   | C     | 119  | VAL  | N-CA-CB  | -5.55 | 104.28      | 111.82   |
| 3   | A     | 1010 | ALA  | CA-C-N   | 5.54  | 128.02      | 120.54   |
| 3   | A     | 1010 | ALA  | C-N-CA   | 5.54  | 128.02      | 120.54   |
| 7   | F     | 109  | VAL  | CB-CA-C  | -5.54 | 102.20      | 111.29   |
| 6   | E     | 156  | LEU  | N-CA-C   | 5.54  | 117.61      | 109.24   |
| 4   | B     | 346  | GLU  | N-CA-C   | 5.54  | 122.60      | 110.80   |
| 6   | E     | 35   | VAL  | CB-CA-C  | 5.54  | 120.37      | 111.29   |
| 3   | A     | 946  | VAL  | CB-CA-C  | -5.53 | 104.89      | 111.81   |
| 11  | K     | 66   | PRO  | N-CA-C   | 5.53  | 120.82      | 113.57   |
| 4   | B     | 980  | PHE  | CB-CA-C  | -5.53 | 102.46      | 113.80   |
| 3   | A     | 307  | ASP  | N-CA-C   | -5.53 | 103.93      | 111.56   |
| 9   | I     | 59   | VAL  | N-CA-CB  | -5.53 | 103.81      | 111.99   |
| 5   | C     | 91   | HIS  | N-CA-C   | 5.53  | 118.61      | 109.94   |
| 3   | A     | 1160 | SER  | N-CA-C   | 5.52  | 117.49      | 108.76   |
| 4   | B     | 977  | GLY  | N-CA-C   | 5.52  | 122.16      | 115.31   |
| 4   | B     | 1172 | ILE  | N-CA-C   | 5.52  | 116.43      | 106.61   |
| 3   | A     | 481  | ASP  | N-CA-CB  | 5.51  | 119.93      | 111.22   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 8   | H     | 20   | TYR  | CB-CA-C  | -5.51 | 99.45       | 110.42   |
| 8   | H     | 107  | VAL  | N-CA-C   | -5.51 | 97.88       | 109.34   |
| 3   | A     | 329  | LEU  | N-CA-C   | 5.50  | 118.04      | 111.71   |
| 5   | C     | 120  | ILE  | CA-C-N   | -5.50 | 117.32      | 122.66   |
| 5   | C     | 120  | ILE  | C-N-CA   | -5.50 | 117.32      | 122.66   |
| 6   | E     | 201  | LYS  | N-CA-C   | -5.50 | 103.64      | 110.41   |
| 3   | A     | 904  | THR  | N-CA-CB  | -5.50 | 101.19      | 110.49   |
| 4   | B     | 259  | TYR  | N-CA-C   | -5.50 | 103.09      | 110.24   |
| 3   | A     | 532  | ARG  | CB-CA-C  | -5.50 | 101.44      | 110.08   |
| 8   | H     | 81   | PRO  | CA-C-N   | 5.49  | 126.71      | 119.84   |
| 8   | H     | 81   | PRO  | C-N-CA   | 5.49  | 126.71      | 119.84   |
| 8   | H     | 126  | GLU  | N-CA-C   | 5.49  | 118.41      | 108.69   |
| 4   | B     | 758  | PHE  | N-CA-C   | 5.49  | 121.94      | 109.81   |
| 4   | B     | 634  | TYR  | CA-C-N   | -5.49 | 108.41      | 121.80   |
| 4   | B     | 634  | TYR  | C-N-CA   | -5.49 | 108.41      | 121.80   |
| 3   | A     | 1395 | GLY  | N-CA-C   | -5.48 | 104.12      | 112.51   |
| 4   | B     | 212  | LEU  | CA-CB-CG | -5.48 | 97.12       | 116.30   |
| 8   | H     | 5    | LEU  | N-CA-C   | 5.48  | 122.33      | 114.39   |
| 4   | B     | 680  | THR  | CB-CA-C  | -5.48 | 100.98      | 110.45   |
| 4   | B     | 880  | THR  | CA-C-N   | 5.47  | 132.00      | 121.54   |
| 4   | B     | 880  | THR  | C-N-CA   | 5.47  | 132.00      | 121.54   |
| 4   | B     | 214  | ALA  | N-CA-C   | -5.47 | 103.12      | 110.24   |
| 3   | A     | 171  | GLN  | N-CA-C   | -5.47 | 101.69      | 109.62   |
| 3   | A     | 439  | ASN  | N-CA-C   | 5.47  | 119.53      | 112.86   |
| 3   | A     | 980  | ASP  | CB-CA-C  | 5.46  | 121.30      | 110.42   |
| 4   | B     | 93   | GLY  | N-CA-C   | -5.46 | 103.27      | 111.19   |
| 4   | B     | 363  | HIS  | N-CA-C   | -5.46 | 99.17       | 110.80   |
| 10  | J     | 10   | CYS  | N-CA-CB  | -5.46 | 101.27      | 110.49   |
| 12  | L     | 68   | GLU  | CB-CG-CD | 5.46  | 121.88      | 112.60   |
| 3   | A     | 275  | SER  | N-CA-C   | -5.45 | 105.73      | 112.38   |
| 4   | B     | 131  | ASP  | CA-C-N   | 5.45  | 131.78      | 121.97   |
| 4   | B     | 131  | ASP  | C-N-CA   | 5.45  | 131.78      | 121.97   |
| 9   | I     | 18   | GLU  | CA-C-N   | -5.45 | 113.62      | 122.34   |
| 9   | I     | 18   | GLU  | C-N-CA   | -5.45 | 113.62      | 122.34   |
| 8   | H     | 33   | GLN  | CA-CB-CG | -5.45 | 103.21      | 114.10   |
| 3   | A     | 41   | MET  | N-CA-C   | 5.44  | 122.39      | 110.80   |
| 3   | A     | 261  | ASP  | N-CA-C   | 5.44  | 119.78      | 113.20   |
| 4   | B     | 230  | ALA  | C-N-CD   | -5.44 | 102.68      | 125.00   |
| 4   | B     | 1023 | VAL  | N-CA-C   | 5.44  | 116.82      | 110.62   |
| 11  | K     | 72   | LYS  | N-CA-C   | 5.44  | 117.28      | 108.41   |
| 3   | A     | 202  | LEU  | CA-CB-CG | -5.44 | 97.27       | 116.30   |
| 9   | I     | 17   | ARG  | CA-C-N   | 5.44  | 129.28      | 121.50   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 9   | I     | 17   | ARG  | C-N-CA   | 5.44  | 129.28      | 121.50   |
| 3   | A     | 321  | PRO  | N-CA-CB  | -5.44 | 96.62       | 102.60   |
| 3   | A     | 182  | VAL  | N-CA-CB  | -5.43 | 104.58      | 111.64   |
| 4   | B     | 650  | GLU  | N-CA-C   | 5.43  | 116.90      | 109.18   |
| 12  | L     | 43   | THR  | N-CA-C   | 5.43  | 122.38      | 110.80   |
| 8   | H     | 109  | LYS  | CA-C-O   | 5.43  | 128.28      | 120.51   |
| 3   | A     | 627  | GLY  | N-CA-C   | -5.43 | 106.81      | 115.66   |
| 6   | E     | 188  | LEU  | N-CA-C   | -5.43 | 107.20      | 113.88   |
| 6   | E     | 85   | GLU  | N-CA-C   | 5.42  | 121.80      | 109.81   |
| 9   | I     | 75   | CYS  | CA-C-N   | 5.42  | 126.62      | 119.84   |
| 9   | I     | 75   | CYS  | C-N-CA   | 5.42  | 126.62      | 119.84   |
| 4   | B     | 32   | ALA  | N-CA-C   | -5.42 | 105.28      | 111.14   |
| 5   | C     | 33   | LEU  | N-CA-C   | -5.42 | 102.64      | 111.04   |
| 3   | A     | 1392 | SER  | CA-C-N   | 5.41  | 131.88      | 121.54   |
| 3   | A     | 1392 | SER  | C-N-CA   | 5.41  | 131.88      | 121.54   |
| 7   | F     | 87   | LYS  | N-CA-C   | -5.40 | 105.29      | 111.07   |
| 4   | B     | 616  | ILE  | CB-CA-C  | -5.40 | 103.08      | 110.96   |
| 11  | K     | 85   | ASP  | N-CA-C   | -5.40 | 105.31      | 111.14   |
| 3   | A     | 75   | ASN  | N-CA-C   | -5.39 | 99.04       | 109.24   |
| 3   | A     | 1407 | GLU  | N-CA-CB  | -5.39 | 102.16      | 110.20   |
| 8   | H     | 61   | SER  | N-CA-C   | -5.39 | 99.31       | 110.80   |
| 5   | C     | 70   | ILE  | N-CA-CB  | -5.39 | 105.07      | 110.08   |
| 4   | B     | 903  | VAL  | N-CA-C   | 5.38  | 116.02      | 109.30   |
| 3   | A     | 110  | CYS  | N-CA-C   | -5.38 | 107.27      | 113.88   |
| 4   | B     | 638  | PHE  | CA-C-N   | 5.37  | 129.81      | 122.34   |
| 4   | B     | 638  | PHE  | C-N-CA   | 5.37  | 129.81      | 122.34   |
| 3   | A     | 43   | GLU  | CB-CA-C  | 5.37  | 119.00      | 110.19   |
| 3   | A     | 1145 | SER  | N-CA-C   | 5.37  | 119.31      | 112.87   |
| 10  | J     | 54   | VAL  | CB-CA-C  | 5.37  | 118.50      | 111.53   |
| 4   | B     | 317  | CYS  | N-CA-C   | -5.36 | 102.73      | 111.04   |
| 3   | A     | 970  | THR  | N-CA-C   | -5.36 | 106.52      | 113.16   |
| 3   | A     | 642  | CYS  | N-CA-C   | -5.35 | 105.34      | 111.07   |
| 3   | A     | 907  | THR  | N-CA-C   | 5.35  | 118.34      | 109.94   |
| 3   | A     | 1194 | ARG  | N-CA-C   | 5.35  | 118.88      | 107.70   |
| 11  | K     | 33   | ILE  | CB-CA-C  | -5.34 | 104.83      | 111.08   |
| 9   | I     | 10   | CYS  | CA-CB-SG | 5.34  | 126.68      | 114.40   |
| 3   | A     | 1218 | GLN  | N-CA-C   | 5.34  | 119.35      | 113.21   |
| 3   | A     | 1002 | GLY  | N-CA-C   | 5.34  | 125.83      | 113.18   |
| 8   | H     | 136  | LYS  | N-CA-CB  | -5.34 | 102.59      | 110.49   |
| 3   | A     | 1391 | ARG  | CG-CD-NE | 5.33  | 123.73      | 112.00   |
| 5   | C     | 50   | GLU  | N-CA-C   | -5.33 | 100.55      | 109.24   |
| 8   | H     | 144  | ILE  | N-CA-CB  | -5.33 | 104.05      | 111.41   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | A     | 1189 | SER  | CA-C-N   | 5.33  | 125.41      | 119.87   |
| 3   | A     | 1189 | SER  | C-N-CA   | 5.33  | 125.41      | 119.87   |
| 4   | B     | 239  | GLU  | CA-CB-CG | 5.33  | 124.76      | 114.10   |
| 3   | A     | 105  | CYS  | N-CA-C   | 5.32  | 120.64      | 114.04   |
| 3   | A     | 895  | LYS  | CD-CE-NZ | 5.32  | 128.93      | 111.90   |
| 4   | B     | 1130 | PHE  | N-CA-C   | -5.32 | 98.61       | 108.24   |
| 4   | B     | 1087 | PHE  | N-CA-C   | 5.32  | 117.06      | 108.34   |
| 3   | A     | 346  | ASP  | N-CA-C   | 5.31  | 116.94      | 110.41   |
| 4   | B     | 636  | PRO  | N-CA-C   | 5.31  | 123.41      | 112.47   |
| 4   | B     | 888  | GLY  | N-CA-C   | 5.31  | 125.76      | 113.18   |
| 3   | A     | 453  | MET  | N-CA-C   | 5.31  | 118.85      | 112.38   |
| 3   | A     | 320  | ARG  | N-CA-C   | 5.30  | 121.53      | 109.81   |
| 4   | B     | 788  | ARG  | N-CA-C   | -5.30 | 101.64      | 110.17   |
| 3   | A     | 69   | THR  | N-CA-CB  | 5.30  | 119.44      | 110.49   |
| 3   | A     | 314  | ALA  | N-CA-C   | 5.30  | 122.08      | 110.80   |
| 4   | B     | 1197 | PRO  | N-CA-C   | -5.30 | 102.87      | 111.03   |
| 4   | B     | 1045 | SER  | N-CA-C   | -5.29 | 102.77      | 110.08   |
| 3   | A     | 255  | SER  | N-CA-C   | -5.29 | 99.53       | 110.80   |
| 4   | B     | 1115 | THR  | N-CA-C   | 5.29  | 117.12      | 111.36   |
| 3   | A     | 919  | ILE  | CB-CA-C  | -5.29 | 102.62      | 111.29   |
| 4   | B     | 1217 | TYR  | CA-C-N   | 5.29  | 129.67      | 120.68   |
| 4   | B     | 1217 | TYR  | C-N-CA   | 5.29  | 129.67      | 120.68   |
| 4   | B     | 851  | PHE  | N-CA-C   | 5.28  | 118.68      | 111.39   |
| 3   | A     | 322  | VAL  | O-C-N    | -5.28 | 115.97      | 122.57   |
| 4   | B     | 978  | ASP  | N-CA-C   | 5.28  | 118.09      | 110.28   |
| 3   | A     | 143  | LYS  | N-CA-C   | -5.28 | 105.11      | 112.45   |
| 4   | B     | 1078 | GLY  | N-CA-C   | -5.28 | 108.80      | 115.08   |
| 9   | I     | 37   | GLU  | N-CA-C   | -5.28 | 103.06      | 110.50   |
| 4   | B     | 638  | PHE  | CA-CB-CG | 5.28  | 119.08      | 113.80   |
| 4   | B     | 980  | PHE  | CA-C-O   | 5.27  | 125.67      | 120.56   |
| 3   | A     | 1336 | MET  | N-CA-C   | 5.27  | 117.44      | 111.11   |
| 4   | B     | 182  | SER  | N-CA-C   | 5.27  | 119.34      | 113.01   |
| 3   | A     | 262  | LEU  | N-CA-C   | -5.27 | 106.00      | 112.90   |
| 5   | C     | 62   | PHE  | N-CA-C   | -5.27 | 105.43      | 111.07   |
| 5   | C     | 93   | ASP  | N-CA-C   | -5.27 | 106.80      | 113.18   |
| 4   | B     | 589  | VAL  | N-CA-C   | 5.27  | 116.49      | 108.80   |
| 3   | A     | 1199 | ARG  | N-CA-C   | -5.26 | 104.79      | 111.11   |
| 4   | B     | 116  | GLU  | N-CA-C   | 5.26  | 117.70      | 111.33   |
| 6   | E     | 83   | CYS  | N-CA-C   | 5.26  | 117.82      | 109.24   |
| 3   | A     | 1389 | PHE  | N-CA-C   | 5.26  | 122.00      | 110.80   |
| 8   | H     | 137  | GLN  | CA-C-N   | 5.26  | 129.55      | 121.19   |
| 8   | H     | 137  | GLN  | C-N-CA   | 5.26  | 129.55      | 121.19   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | A     | 815  | PHE  | CB-CA-C  | -5.25 | 102.81      | 110.95   |
| 3   | A     | 1316 | VAL  | CB-CA-C  | -5.25 | 106.44      | 111.06   |
| 5   | C     | 135  | GLN  | N-CA-C   | -5.25 | 105.19      | 113.02   |
| 9   | I     | 40   | SER  | CA-C-N   | 5.25  | 125.71      | 120.04   |
| 9   | I     | 40   | SER  | C-N-CA   | 5.25  | 125.71      | 120.04   |
| 3   | A     | 127  | ALA  | N-CA-C   | -5.25 | 99.61       | 110.80   |
| 6   | E     | 96   | PHE  | N-CA-C   | -5.25 | 99.62       | 110.80   |
| 3   | A     | 66   | LYS  | N-CA-C   | 5.24  | 121.97      | 110.80   |
| 3   | A     | 1161 | THR  | CA-C-N   | 5.24  | 129.00      | 121.55   |
| 3   | A     | 1161 | THR  | C-N-CA   | 5.24  | 129.00      | 121.55   |
| 3   | A     | 1403 | GLU  | CA-CB-CG | -5.24 | 103.61      | 114.10   |
| 4   | B     | 273  | LEU  | N-CA-C   | 5.24  | 116.73      | 108.55   |
| 4   | B     | 793  | ALA  | N-CA-C   | -5.24 | 99.63       | 110.80   |
| 3   | A     | 735  | VAL  | CA-C-N   | -5.24 | 113.51      | 120.63   |
| 3   | A     | 735  | VAL  | C-N-CA   | -5.24 | 113.51      | 120.63   |
| 3   | A     | 786  | HIS  | N-CA-C   | -5.23 | 106.13      | 112.88   |
| 4   | B     | 609  | ILE  | CB-CA-C  | -5.22 | 102.84      | 110.62   |
| 4   | B     | 1220 | ARG  | CA-C-N   | 5.22  | 128.75      | 121.02   |
| 4   | B     | 1220 | ARG  | C-N-CA   | 5.22  | 128.75      | 121.02   |
| 4   | B     | 960  | GLY  | CA-C-N   | 5.22  | 128.12      | 120.71   |
| 4   | B     | 960  | GLY  | C-N-CA   | 5.22  | 128.12      | 120.71   |
| 5   | C     | 172  | PRO  | N-CA-C   | -5.22 | 101.72      | 112.47   |
| 3   | A     | 560  | ILE  | CA-C-N   | -5.22 | 114.61      | 120.14   |
| 3   | A     | 560  | ILE  | C-N-CA   | -5.22 | 114.61      | 120.14   |
| 3   | A     | 414  | ASP  | N-CA-C   | 5.21  | 117.68      | 107.57   |
| 3   | A     | 498  | ARG  | N-CA-C   | -5.21 | 105.49      | 111.07   |
| 3   | A     | 886  | ILE  | CA-C-N   | -5.21 | 117.11      | 122.27   |
| 3   | A     | 886  | ILE  | C-N-CA   | -5.21 | 117.11      | 122.27   |
| 3   | A     | 1323 | ASP  | N-CA-C   | -5.21 | 99.15       | 108.47   |
| 3   | A     | 49   | LYS  | CA-C-O   | -5.21 | 116.38      | 119.55   |
| 3   | A     | 201  | VAL  | CA-C-N   | -5.20 | 115.62      | 122.85   |
| 3   | A     | 201  | VAL  | C-N-CA   | -5.20 | 115.62      | 122.85   |
| 3   | A     | 1113 | THR  | CA-C-N   | -5.20 | 113.34      | 119.84   |
| 3   | A     | 1113 | THR  | C-N-CA   | -5.20 | 113.34      | 119.84   |
| 3   | A     | 1236 | LEU  | N-CA-C   | 5.20  | 117.20      | 109.25   |
| 5   | C     | 166  | GLU  | N-CA-C   | 5.20  | 119.67      | 112.45   |
| 3   | A     | 623  | GLY  | N-CA-C   | -5.19 | 102.72      | 112.64   |
| 6   | E     | 26   | ARG  | N-CA-C   | -5.19 | 105.11      | 111.75   |
| 3   | A     | 53   | LEU  | CA-CB-CG | 5.18  | 134.45      | 116.30   |
| 3   | A     | 222  | LEU  | N-CA-C   | -5.18 | 102.08      | 110.32   |
| 4   | B     | 400  | HIS  | N-CA-C   | -5.18 | 100.79      | 109.24   |
| 4   | B     | 1181 | GLU  | N-CA-C   | 5.18  | 121.84      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | A     | 842  | VAL  | N-CA-C   | 5.18  | 115.95      | 110.72   |
| 4   | B     | 492  | LEU  | CA-CB-CG | -5.18 | 98.16       | 116.30   |
| 4   | B     | 621  | GLU  | N-CA-C   | -5.18 | 105.70      | 113.89   |
| 3   | A     | 743  | VAL  | CB-CA-C  | -5.18 | 105.33      | 111.81   |
| 4   | B     | 807  | ARG  | N-CA-C   | -5.18 | 105.70      | 112.23   |
| 4   | B     | 38   | PHE  | N-CA-C   | 5.18  | 121.83      | 110.80   |
| 3   | A     | 1094 | VAL  | CB-CA-C  | -5.17 | 102.94      | 110.81   |
| 4   | B     | 384  | ARG  | N-CA-C   | -5.17 | 105.72      | 111.36   |
| 3   | A     | 252  | PHE  | CA-C-O   | 5.17  | 124.45      | 118.55   |
| 3   | A     | 1107 | VAL  | N-CA-C   | -5.17 | 98.58       | 109.34   |
| 4   | B     | 1009 | ASP  | N-CA-C   | -5.17 | 105.26      | 112.45   |
| 3   | A     | 97   | ALA  | CA-C-N   | -5.17 | 111.67      | 121.54   |
| 3   | A     | 97   | ALA  | C-N-CA   | -5.17 | 111.67      | 121.54   |
| 9   | I     | 106  | CYS  | N-CA-C   | -5.17 | 105.03      | 113.19   |
| 3   | A     | 1166 | ASP  | CB-CA-C  | -5.16 | 101.88      | 110.81   |
| 9   | I     | 30   | ARG  | CB-CA-C  | 5.16  | 117.57      | 111.22   |
| 4   | B     | 222  | ILE  | CA-C-O   | 5.15  | 126.44      | 120.67   |
| 4   | B     | 287  | ARG  | N-CA-C   | -5.15 | 105.56      | 111.07   |
| 4   | B     | 937  | ALA  | N-CA-C   | -5.15 | 99.83       | 110.80   |
| 3   | A     | 88   | LYS  | N-CA-C   | -5.14 | 98.51       | 108.59   |
| 3   | A     | 128  | ILE  | N-CA-C   | -5.14 | 101.23      | 108.12   |
| 4   | B     | 876  | LYS  | N-CA-C   | -5.14 | 98.38       | 109.01   |
| 8   | H     | 87   | ARG  | N-CA-C   | 5.13  | 115.31      | 108.38   |
| 3   | A     | 673  | GLY  | CA-C-N   | -5.13 | 115.60      | 120.83   |
| 3   | A     | 673  | GLY  | C-N-CA   | -5.13 | 115.60      | 120.83   |
| 8   | H     | 12   | VAL  | N-CA-C   | 5.13  | 115.97      | 108.58   |
| 3   | A     | 665  | GLY  | CA-C-O   | -5.13 | 116.03      | 121.88   |
| 3   | A     | 1285 | MET  | CA-CB-CG | 5.12  | 124.34      | 114.10   |
| 4   | B     | 394  | ASP  | N-CA-C   | 5.12  | 121.71      | 110.80   |
| 3   | A     | 1406 | VAL  | CA-C-N   | 5.12  | 129.33      | 120.58   |
| 3   | A     | 1406 | VAL  | C-N-CA   | 5.12  | 129.33      | 120.58   |
| 4   | B     | 577  | ALA  | N-CA-C   | 5.12  | 117.00      | 107.99   |
| 4   | B     | 321  | GLY  | N-CA-C   | 5.11  | 125.30      | 113.18   |
| 3   | A     | 1072 | ILE  | CB-CA-C  | -5.11 | 105.90      | 110.91   |
| 4   | B     | 473  | MET  | O-C-N    | 5.11  | 129.39      | 122.59   |
| 5   | C     | 41   | ILE  | CA-C-O   | 5.11  | 122.93      | 119.20   |
| 3   | A     | 846  | GLU  | N-CA-C   | 5.11  | 121.68      | 110.80   |
| 3   | A     | 253  | ASN  | O-C-N    | 5.10  | 129.38      | 122.59   |
| 5   | C     | 263  | THR  | N-CA-C   | -5.10 | 99.93       | 110.80   |
| 3   | A     | 533  | LYS  | N-CA-CB  | 5.10  | 118.08      | 110.22   |
| 3   | A     | 736  | ASN  | N-CA-C   | -5.10 | 105.37      | 111.03   |
| 3   | A     | 1443 | VAL  | N-CA-C   | 5.10  | 115.25      | 108.11   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4   | B     | 224  | GLN  | N-CA-C   | 5.10  | 117.72      | 108.69   |
| 9   | I     | 56   | ALA  | N-CA-C   | -5.10 | 99.94       | 110.80   |
| 3   | A     | 857  | ARG  | N-CA-C   | 5.09  | 117.16      | 109.41   |
| 9   | I     | 39   | GLY  | N-CA-C   | -5.09 | 101.11      | 113.18   |
| 3   | A     | 1407 | GLU  | CA-CB-CG | -5.09 | 103.92      | 114.10   |
| 4   | B     | 1196 | ILE  | N-CA-C   | 5.08  | 119.86      | 108.88   |
| 4   | B     | 552  | MET  | CA-C-N   | -5.08 | 113.49      | 119.84   |
| 4   | B     | 552  | MET  | C-N-CA   | -5.08 | 113.49      | 119.84   |
| 8   | H     | 40   | LEU  | N-CA-C   | 5.08  | 117.17      | 108.90   |
| 4   | B     | 893  | LEU  | CA-CB-CG | 5.07  | 134.05      | 116.30   |
| 3   | A     | 542  | GLU  | N-CA-C   | 5.07  | 117.59      | 110.14   |
| 4   | B     | 612  | GLU  | CB-CA-C  | -5.07 | 103.09      | 110.95   |
| 6   | E     | 42   | PHE  | N-CA-C   | -5.07 | 105.41      | 112.45   |
| 3   | A     | 49   | LYS  | N-CA-C   | 5.06  | 116.17      | 108.12   |
| 3   | A     | 800  | VAL  | N-CA-C   | -5.06 | 102.21      | 108.89   |
| 6   | E     | 113  | GLN  | CA-CB-CG | 5.06  | 124.23      | 114.10   |
| 6   | E     | 115  | ASN  | N-CA-C   | 5.06  | 121.58      | 110.80   |
| 3   | A     | 670  | ILE  | CB-CA-C  | -5.06 | 103.34      | 111.59   |
| 9   | I     | 28   | GLU  | N-CA-C   | 5.06  | 121.58      | 110.80   |
| 3   | A     | 652  | VAL  | N-CA-C   | 5.06  | 115.73      | 110.82   |
| 3   | A     | 1312 | ASN  | CA-C-N   | 5.06  | 128.48      | 120.89   |
| 3   | A     | 1312 | ASN  | C-N-CA   | 5.06  | 128.48      | 120.89   |
| 3   | A     | 259  | GLU  | CA-C-N   | 5.05  | 130.56      | 121.06   |
| 3   | A     | 259  | GLU  | C-N-CA   | 5.05  | 130.56      | 121.06   |
| 4   | B     | 419  | THR  | N-CA-C   | 5.05  | 121.56      | 110.80   |
| 11  | K     | 111  | LEU  | N-CA-C   | 5.04  | 119.19      | 113.19   |
| 4   | B     | 324  | ILE  | CB-CA-C  | -5.04 | 103.02      | 111.29   |
| 3   | A     | 385  | ILE  | N-CA-C   | 5.04  | 119.83      | 109.34   |
| 4   | B     | 841  | MET  | N-CA-C   | 5.04  | 117.11      | 108.90   |
| 4   | B     | 129  | PHE  | N-CA-C   | 5.03  | 117.11      | 108.90   |
| 3   | A     | 297  | GLN  | N-CA-C   | -5.03 | 105.26      | 111.40   |
| 3   | A     | 323  | LYS  | CB-CG-CD | 5.03  | 122.87      | 111.30   |
| 3   | A     | 727  | ASP  | N-CA-C   | 5.03  | 117.15      | 111.11   |
| 3   | A     | 968  | GLN  | CA-C-N   | -5.03 | 114.44      | 122.29   |
| 3   | A     | 968  | GLN  | C-N-CA   | -5.03 | 114.44      | 122.29   |
| 3   | A     | 1362 | TYR  | N-CA-C   | -5.03 | 102.35      | 110.14   |
| 3   | A     | 415  | LEU  | N-CA-C   | 5.03  | 121.50      | 110.80   |
| 4   | B     | 315  | LYS  | N-CA-C   | -5.03 | 107.14      | 113.77   |
| 4   | B     | 473  | MET  | CA-CB-CG | -5.03 | 104.05      | 114.10   |
| 4   | B     | 43   | LEU  | CA-CB-CG | -5.02 | 98.73       | 116.30   |
| 3   | A     | 923  | LEU  | N-CA-C   | 5.02  | 121.48      | 110.80   |
| 4   | B     | 93   | GLY  | CA-C-O   | -5.02 | 116.64      | 121.41   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | A     | 539  | THR  | N-CA-C   | 5.01  | 116.77      | 108.20   |
| 4   | B     | 250  | PHE  | CB-CA-C  | -5.01 | 102.89      | 111.31   |
| 9   | I     | 17   | ARG  | CG-CD-NE | -5.01 | 100.97      | 112.00   |
| 3   | A     | 1071 | SER  | N-CA-C   | 5.01  | 118.88      | 112.87   |
| 9   | I     | 30   | ARG  | N-CA-C   | -5.01 | 105.91      | 112.72   |
| 3   | A     | 735  | VAL  | CA-C-O   | -5.00 | 114.67      | 119.92   |
| 4   | B     | 905  | VAL  | N-CA-C   | -5.00 | 101.86      | 108.96   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3   | A     | 322 | VAL  | CA   |

All (22) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 3   | A     | 1035 | TYR  | Sidechain |
| 3   | A     | 320  | ARG  | Mainchain |
| 3   | A     | 322  | VAL  | Mainchain |
| 3   | A     | 376  | TYR  | Sidechain |
| 3   | A     | 6    | TYR  | Sidechain |
| 3   | A     | 814  | PHE  | Sidechain |
| 4   | B     | 250  | PHE  | Sidechain |
| 4   | B     | 275  | TYR  | Sidechain |
| 4   | B     | 431  | TYR  | Sidechain |
| 4   | B     | 636  | PRO  | Mainchain |
| 4   | B     | 638  | PHE  | Sidechain |
| 4   | B     | 797  | TYR  | Sidechain |
| 4   | B     | 798  | TYR  | Sidechain |
| 5   | C     | 114  | TYR  | Sidechain |
| 5   | C     | 209  | TYR  | Sidechain |
| 6   | E     | 187  | TYR  | Sidechain |
| 9   | I     | 4    | PHE  | Sidechain |
| 2   | T     | 10   | DT   | Sidechain |
| 2   | T     | 11   | DC   | Sidechain |
| 2   | T     | 13   | DA   | Sidechain |
| 2   | T     | 6    | DC   | Sidechain |
| 2   | T     | 8    | DT   | 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   | R     | 217   | 0        | 110      | 19      | 0            |
| 2   | T     | 279   | 0        | 160      | 43      | 0            |
| 3   | A     | 10969 | 0        | 11070    | 2196    | 0            |
| 4   | B     | 8793  | 0        | 8823     | 1668    | 0            |
| 5   | C     | 2095  | 0        | 2051     | 355     | 0            |
| 6   | E     | 1752  | 0        | 1776     | 310     | 0            |
| 7   | F     | 679   | 0        | 701      | 133     | 0            |
| 8   | H     | 1068  | 0        | 1040     | 204     | 0            |
| 9   | I     | 971   | 0        | 929      | 173     | 0            |
| 10  | J     | 532   | 0        | 542      | 127     | 0            |
| 11  | K     | 919   | 0        | 929      | 181     | 0            |
| 12  | L     | 364   | 0        | 387      | 66      | 0            |
| 13  | A     | 2     | 0        | 0        | 0       | 0            |
| 13  | B     | 1     | 0        | 0        | 0       | 0            |
| 13  | C     | 1     | 0        | 0        | 0       | 0            |
| 13  | I     | 2     | 0        | 0        | 0       | 0            |
| 13  | J     | 1     | 0        | 0        | 0       | 0            |
| 13  | L     | 1     | 0        | 0        | 0       | 0            |
| 14  | A     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 28647 | 0        | 28518    | 5075    | 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 89.

All (5075) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:853:ASP:OD1  | 3:A:855:THR:HB    | 1.32                     | 1.25              |
| 3:A:90:VAL:HG12  | 3:A:297:GLN:NE2   | 1.49                     | 1.24              |
| 4:B:635:ARG:HB2  | 4:B:636:PRO:CD    | 1.65                     | 1.21              |
| 3:A:321:PRO:O    | 3:A:322:VAL:HG22  | 1.41                     | 1.18              |
| 3:A:351:THR:HG23 | 4:B:1103:ILE:HD12 | 1.23                     | 1.18              |
| 3:A:61:ILE:O     | 3:A:63:ARG:N      | 1.78                     | 1.17              |
| 3:A:312:PRO:O    | 3:A:313:GLN:HG3   | 1.44                     | 1.16              |
| 4:B:477:ALA:HB3  | 4:B:479:VAL:HG22  | 1.21                     | 1.16              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:67:CYS:O      | 3:A:70:CYS:HB3    | 1.39                     | 1.16              |
| 3:A:855:THR:HG21  | 3:A:857:ARG:HE    | 1.11                     | 1.16              |
| 4:B:1175:LEU:O    | 4:B:1176:ASN:HB2  | 1.40                     | 1.16              |
| 2:T:2:DC:H2'      | 2:T:3:DG:C8       | 1.82                     | 1.15              |
| 4:B:174:LEU:HD22  | 4:B:204:ILE:HD11  | 1.20                     | 1.15              |
| 3:A:1015:VAL:HG12 | 3:A:1019:CYS:SG   | 1.87                     | 1.14              |
| 3:A:1242:VAL:HG12 | 3:A:1243:VAL:H    | 1.13                     | 1.14              |
| 3:A:90:VAL:HG11   | 3:A:297:GLN:HA    | 1.19                     | 1.14              |
| 4:B:120:ARG:HD2   | 4:B:955:THR:HG21  | 1.22                     | 1.14              |
| 3:A:899:VAL:HG12  | 3:A:929:LEU:HD12  | 1.27                     | 1.14              |
| 4:B:471:LYS:HG3   | 4:B:472:ALA:H     | 0.97                     | 1.14              |
| 4:B:635:ARG:CB    | 4:B:636:PRO:HD3   | 1.77                     | 1.14              |
| 3:A:913:LEU:CD1   | 3:A:914:GLU:H     | 1.59                     | 1.13              |
| 6:E:52:ARG:HB3    | 6:E:53:PRO:HD2    | 1.23                     | 1.13              |
| 5:C:3:GLU:HG3     | 5:C:4:GLU:H       | 1.01                     | 1.13              |
| 4:B:977:GLY:HA3   | 4:B:1099:VAL:HG21 | 1.26                     | 1.13              |
| 4:B:955:THR:HG22  | 4:B:956:THR:H     | 1.07                     | 1.13              |
| 3:A:1364:ASN:ND2  | 3:A:1366:ARG:HG2  | 1.63                     | 1.13              |
| 7:F:155:LEU:HD23  | 7:F:155:LEU:H     | 1.04                     | 1.12              |
| 3:A:278:THR:O     | 3:A:278:THR:HG22  | 1.50                     | 1.12              |
| 3:A:353:ILE:HD13  | 3:A:487:MET:HE3   | 1.18                     | 1.12              |
| 3:A:913:LEU:HD12  | 3:A:914:GLU:N     | 1.64                     | 1.11              |
| 5:C:22:LEU:CD2    | 5:C:25:VAL:HG21   | 1.80                     | 1.11              |
| 3:A:892:ALA:HA    | 3:A:895:LYS:HB2   | 1.20                     | 1.11              |
| 4:B:167:ILE:HG23  | 4:B:424:LEU:HD13  | 1.14                     | 1.10              |
| 3:A:320:ARG:H     | 3:A:320:ARG:HD2   | 0.99                     | 1.10              |
| 3:A:1161:THR:HG22 | 3:A:1163:ILE:H    | 0.96                     | 1.10              |
| 4:B:882:THR:HG21  | 4:B:935:ARG:HA    | 1.30                     | 1.10              |
| 4:B:474:SER:HA    | 4:B:476:ARG:HG3   | 1.29                     | 1.10              |
| 4:B:1051:THR:HG22 | 4:B:1053:GLU:H    | 1.10                     | 1.09              |
| 10:J:43:ARG:HG3   | 10:J:46:CYS:HB2   | 1.32                     | 1.09              |
| 4:B:549:THR:HG22  | 4:B:550:ASP:H     | 0.99                     | 1.09              |
| 4:B:1171:VAL:HG12 | 4:B:1172:ILE:H    | 1.14                     | 1.09              |
| 4:B:658:ILE:HA    | 4:B:661:LEU:HD12  | 1.35                     | 1.09              |
| 3:A:630:ILE:H     | 3:A:630:ILE:HD12  | 1.15                     | 1.09              |
| 3:A:901:LEU:HG    | 3:A:926:GLN:HE21  | 1.13                     | 1.08              |
| 4:B:711:GLU:H     | 4:B:712:PRO:HD3   | 1.05                     | 1.08              |
| 3:A:59:GLY:HA2    | 3:A:67:CYS:SG     | 1.91                     | 1.08              |
| 4:B:65:GLU:HG2    | 4:B:66:ASP:N      | 1.51                     | 1.08              |
| 3:A:49:LYS:O      | 3:A:50:ILE:HG12   | 1.54                     | 1.08              |
| 3:A:169:ASN:ND2   | 3:A:169:ASN:H     | 1.37                     | 1.08              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:169:ASN:HD22  | 3:A:169:ASN:N     | 1.47                     | 1.08              |
| 3:A:672:ASP:HB2   | 3:A:736:ASN:OD1   | 1.53                     | 1.08              |
| 3:A:868:TYR:CE1   | 3:A:1064:VAL:HG11 | 1.87                     | 1.08              |
| 3:A:89:PRO:O      | 3:A:204:THR:HG21  | 1.52                     | 1.08              |
| 4:B:169:ARG:HB2   | 4:B:454:THR:HG23  | 1.35                     | 1.08              |
| 3:A:261:ASP:HB3   | 3:A:323:LYS:CD    | 1.83                     | 1.07              |
| 3:A:649:ILE:O     | 3:A:653:VAL:HG23  | 1.53                     | 1.07              |
| 4:B:1099:VAL:HG12 | 4:B:1103:ILE:HD11 | 1.33                     | 1.07              |
| 10:J:10:CYS:SG    | 10:J:43:ARG:HD2   | 1.93                     | 1.07              |
| 3:A:380:VAL:HG21  | 3:A:430:TRP:H     | 1.20                     | 1.07              |
| 8:H:81:PRO:HB2    | 8:H:82:PRO:HD2    | 1.14                     | 1.07              |
| 3:A:322:VAL:CG1   | 3:A:323:LYS:HD3   | 1.83                     | 1.07              |
| 3:A:1169:ILE:H    | 3:A:1169:ILE:HD12 | 1.16                     | 1.07              |
| 4:B:1103:ILE:HD13 | 4:B:1103:ILE:N    | 1.70                     | 1.07              |
| 3:A:7:SER:HB3     | 4:B:1193:GLN:NE2  | 1.67                     | 1.07              |
| 4:B:287:ARG:HG2   | 4:B:292:ILE:HD13  | 1.37                     | 1.07              |
| 3:A:868:TYR:HE1   | 3:A:1064:VAL:HG11 | 1.00                     | 1.06              |
| 4:B:65:GLU:CG     | 4:B:66:ASP:H      | 1.67                     | 1.06              |
| 6:E:46:TYR:HE2    | 6:E:58:MET:HA     | 1.14                     | 1.06              |
| 8:H:32:THR:HG22   | 8:H:33:GLN:HG2    | 1.32                     | 1.06              |
| 3:A:567:LYS:HB2   | 3:A:568:PRO:HD2   | 1.09                     | 1.06              |
| 3:A:1299:VAL:HG12 | 3:A:1300:LYS:H    | 1.19                     | 1.06              |
| 11:K:53:ASP:O     | 11:K:56:VAL:HG23  | 1.55                     | 1.06              |
| 3:A:265:LYS:HE2   | 3:A:323:LYS:HE2   | 1.35                     | 1.06              |
| 3:A:1004:ASN:ND2  | 6:E:167:ARG:HD2   | 1.69                     | 1.06              |
| 3:A:114:LEU:O     | 3:A:115:LEU:HD23  | 1.53                     | 1.05              |
| 3:A:380:VAL:CG2   | 3:A:430:TRP:H     | 1.67                     | 1.05              |
| 3:A:406:ILE:CD1   | 3:A:431:LYS:HB2   | 1.84                     | 1.05              |
| 4:B:473:MET:C     | 4:B:475:SER:H     | 1.46                     | 1.05              |
| 3:A:71:GLN:O      | 3:A:73:GLY:N      | 1.89                     | 1.05              |
| 4:B:464:GLY:HA3   | 4:B:478:GLY:HA2   | 1.38                     | 1.05              |
| 9:I:10:CYS:HB3    | 9:I:31:THR:HG21   | 1.13                     | 1.05              |
| 4:B:917:PRO:HA    | 4:B:933:SER:O     | 1.54                     | 1.05              |
| 3:A:1025:ARG:HG2  | 3:A:1025:ARG:HH11 | 1.20                     | 1.05              |
| 4:B:635:ARG:HD2   | 4:B:636:PRO:HD3   | 1.32                     | 1.05              |
| 3:A:913:LEU:HD12  | 3:A:914:GLU:H     | 0.93                     | 1.05              |
| 3:A:981:LEU:HD21  | 3:A:1039:LYS:HA   | 1.32                     | 1.05              |
| 4:B:235:SER:O     | 4:B:236:HIS:ND1   | 1.87                     | 1.05              |
| 5:C:60:ASP:HB3    | 12:L:67:PHE:CE1   | 1.91                     | 1.05              |
| 3:A:315:LEU:HD12  | 3:A:319:GLY:HA2   | 1.39                     | 1.04              |
| 4:B:471:LYS:HG3   | 4:B:472:ALA:N     | 1.63                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:E:135:PHE:HB3   | 6:E:140:LEU:HD11  | 1.37                     | 1.04              |
| 4:B:254:LEU:HD22  | 4:B:361:LEU:HD11  | 1.39                     | 1.04              |
| 3:A:530:GLY:C     | 3:A:532:ARG:N     | 2.03                     | 1.04              |
| 3:A:320:ARG:HD2   | 3:A:320:ARG:N     | 1.70                     | 1.04              |
| 3:A:565:ILE:HG23  | 3:A:567:LYS:HE3   | 1.33                     | 1.04              |
| 3:A:406:ILE:HD13  | 3:A:431:LYS:HB2   | 1.04                     | 1.03              |
| 3:A:1214:GLU:O    | 3:A:1218:GLN:HG2  | 1.57                     | 1.03              |
| 3:A:146:MET:O     | 3:A:170:THR:HG22  | 1.54                     | 1.03              |
| 6:E:28:TYR:HE1    | 6:E:78:LEU:HD13   | 1.18                     | 1.03              |
| 10:J:64:ASN:HB3   | 10:J:65:PRO:HD3   | 1.40                     | 1.03              |
| 3:A:278:THR:O     | 3:A:279:LEU:HD23  | 1.58                     | 1.03              |
| 3:A:1422:ARG:HH21 | 4:B:1220:ARG:HD3  | 1.24                     | 1.03              |
| 7:F:73:ALA:O      | 7:F:74:ILE:HG12   | 1.56                     | 1.03              |
| 3:A:265:LYS:NZ    | 3:A:322:VAL:HG21  | 1.72                     | 1.03              |
| 3:A:452:LYS:HB2   | 4:B:1141:HIS:CE1  | 1.93                     | 1.03              |
| 3:A:901:LEU:HD23  | 3:A:907:THR:CG2   | 1.89                     | 1.03              |
| 4:B:280:ILE:HG21  | 4:B:285:ILE:HG12  | 1.39                     | 1.03              |
| 5:C:18:VAL:HG23   | 5:C:240:VAL:HG11  | 1.36                     | 1.03              |
| 3:A:783:THR:HG22  | 3:A:784:LEU:HG    | 1.37                     | 1.03              |
| 5:C:60:ASP:HB3    | 12:L:67:PHE:HE1   | 1.18                     | 1.03              |
| 3:A:320:ARG:CB    | 3:A:321:PRO:HB3   | 1.87                     | 1.02              |
| 3:A:1004:ASN:HD22 | 6:E:167:ARG:CD    | 1.72                     | 1.02              |
| 3:A:320:ARG:HB2   | 3:A:321:PRO:HB3   | 1.03                     | 1.02              |
| 4:B:329:THR:HA    | 4:B:332:ASP:HB2   | 1.36                     | 1.02              |
| 5:C:57:VAL:HG11   | 10:J:60:PHE:HB2   | 1.40                     | 1.02              |
| 3:A:567:LYS:HB3   | 8:H:96:VAL:N      | 1.75                     | 1.02              |
| 9:I:17:ARG:HG2    | 9:I:18:GLU:H      | 1.21                     | 1.01              |
| 12:L:51:CYS:SG    | 12:L:51:CYS:O     | 2.18                     | 1.01              |
| 3:A:531:ILE:HG12  | 3:A:622:VAL:HG11  | 1.36                     | 1.01              |
| 4:B:634:TYR:HE1   | 4:B:692:TYR:CD1   | 1.78                     | 1.01              |
| 9:I:17:ARG:HG2    | 9:I:18:GLU:N      | 1.72                     | 1.01              |
| 2:T:6:DC:H2''     | 2:T:7:DC:H5'      | 1.41                     | 1.01              |
| 3:A:215:SER:HB3   | 3:A:218:ASP:OD2   | 1.59                     | 1.01              |
| 4:B:284:ILE:HD12  | 4:B:324:ILE:HD12  | 1.42                     | 1.01              |
| 4:B:635:ARG:HB2   | 4:B:636:PRO:HD3   | 1.03                     | 1.01              |
| 11:K:49:GLU:HG3   | 11:K:94:ILE:HD11  | 1.41                     | 1.01              |
| 3:A:91:PHE:HD2    | 3:A:297:GLN:OE1   | 1.43                     | 1.01              |
| 3:A:1312:ASN:O    | 3:A:1316:VAL:HG23 | 1.61                     | 1.01              |
| 3:A:65:LEU:HD23   | 3:A:65:LEU:H      | 1.25                     | 1.01              |
| 3:A:1445:ILE:H    | 3:A:1445:ILE:HD12 | 1.23                     | 1.01              |
| 4:B:701:ILE:HB    | 4:B:740:HIS:HE1   | 1.22                     | 1.00              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:E:65:THR:OG1    | 6:E:67:GLU:HB3    | 1.61                     | 1.00              |
| 4:B:108:VAL:HG12  | 4:B:109:THR:H     | 1.27                     | 1.00              |
| 5:C:133:ILE:O     | 5:C:134:ILE:HD13  | 1.59                     | 1.00              |
| 2:T:1:DA:H2''     | 2:T:2:DC:O5'      | 1.57                     | 1.00              |
| 3:A:351:THR:HG22  | 3:A:352:VAL:H     | 1.26                     | 1.00              |
| 3:A:1067:LEU:HD21 | 3:A:1367:HIS:HE1  | 1.23                     | 1.00              |
| 3:A:1079:MET:O    | 3:A:1080:THR:OG1  | 1.78                     | 1.00              |
| 6:E:64:PRO:CG     | 6:E:76:GLY:HA2    | 1.92                     | 1.00              |
| 4:B:167:ILE:CG2   | 4:B:424:LEU:HD13  | 1.90                     | 1.00              |
| 4:B:1165:ILE:HG22 | 4:B:1166:CYS:N    | 1.75                     | 1.00              |
| 5:C:46:ILE:HD13   | 5:C:159:ALA:HB2   | 1.42                     | 1.00              |
| 3:A:320:ARG:HH21  | 4:B:471:LYS:HB3   | 1.25                     | 1.00              |
| 3:A:1134:ILE:O    | 3:A:1138:ILE:HG12 | 1.61                     | 1.00              |
| 3:A:567:LYS:HB3   | 8:H:96:VAL:H      | 1.22                     | 0.99              |
| 5:C:44:LEU:HB2    | 5:C:77:ILE:HD11   | 1.03                     | 0.99              |
| 7:F:81:THR:HG22   | 7:F:136:ARG:NH1   | 1.76                     | 0.99              |
| 4:B:1084:GLN:NE2  | 5:C:191:TYR:HA    | 1.77                     | 0.99              |
| 9:I:10:CYS:CB     | 9:I:31:THR:HG21   | 1.92                     | 0.99              |
| 6:E:46:TYR:CE2    | 6:E:58:MET:HA     | 1.96                     | 0.99              |
| 3:A:367:PRO:HG2   | 3:A:370:ILE:HD12  | 1.44                     | 0.99              |
| 4:B:1002:THR:HG21 | 4:B:1006:ILE:HB   | 1.41                     | 0.99              |
| 3:A:567:LYS:CB    | 3:A:568:PRO:HD2   | 1.89                     | 0.98              |
| 3:A:40:THR:HG22   | 3:A:41:MET:HE3    | 1.46                     | 0.98              |
| 4:B:256:VAL:HG11  | 4:B:382:ILE:CD1   | 1.93                     | 0.98              |
| 3:A:99:ILE:HA     | 3:A:102:VAL:CG2   | 1.93                     | 0.98              |
| 4:B:955:THR:HG22  | 4:B:956:THR:N     | 1.72                     | 0.98              |
| 6:E:113:GLN:HA    | 6:E:137:GLU:HG3   | 1.45                     | 0.98              |
| 3:A:901:LEU:HA    | 3:A:907:THR:HG23  | 1.44                     | 0.98              |
| 4:B:168:GLY:HA2   | 4:B:454:THR:OG1   | 1.64                     | 0.98              |
| 4:B:1103:ILE:HD13 | 4:B:1103:ILE:H    | 1.27                     | 0.98              |
| 5:C:229:TYR:N     | 5:C:229:TYR:HD1   | 1.62                     | 0.98              |
| 7:F:81:THR:HG21   | 7:F:136:ARG:HD3   | 1.42                     | 0.98              |
| 8:H:116:TYR:HB2   | 8:H:123:MET:HB3   | 1.46                     | 0.98              |
| 11:K:51:LEU:CD1   | 11:K:59:ALA:HB3   | 1.93                     | 0.98              |
| 3:A:406:ILE:HD13  | 3:A:431:LYS:CB    | 1.93                     | 0.97              |
| 3:A:302:THR:HG23  | 3:A:313:GLN:HE22  | 1.26                     | 0.97              |
| 3:A:1004:ASN:HD22 | 6:E:167:ARG:HD2   | 0.84                     | 0.97              |
| 4:B:563:MET:HG3   | 4:B:563:MET:O     | 1.61                     | 0.97              |
| 4:B:711:GLU:N     | 4:B:712:PRO:HD3   | 1.76                     | 0.97              |
| 3:A:1116:LEU:H    | 3:A:1308:THR:HB   | 1.24                     | 0.97              |
| 5:C:258:ILE:HD11  | 11:K:42:LEU:HD21  | 1.45                     | 0.97              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:106:GLU:C    | 8:H:108:SER:H     | 1.57                     | 0.97              |
| 3:A:134:ARG:HD3  | 3:A:221:SER:O     | 1.63                     | 0.97              |
| 3:A:609:ASP:O    | 3:A:611:GLN:N     | 1.98                     | 0.97              |
| 4:B:274:PRO:O    | 4:B:276:ILE:N     | 1.97                     | 0.97              |
| 5:C:260:LEU:O    | 5:C:264:GLN:HG3   | 1.64                     | 0.97              |
| 8:H:81:PRO:HB2   | 8:H:82:PRO:CD     | 1.94                     | 0.97              |
| 3:A:528:LEU:HA   | 3:A:531:ILE:HG22  | 1.42                     | 0.97              |
| 4:B:698:GLU:O    | 4:B:701:ILE:HD12  | 1.63                     | 0.97              |
| 4:B:846:ILE:HG23 | 4:B:974:PRO:HG2   | 1.43                     | 0.97              |
| 3:A:889:SER:HB2  | 3:A:892:ALA:H     | 1.28                     | 0.96              |
| 4:B:549:THR:HG22 | 4:B:550:ASP:N     | 1.77                     | 0.96              |
| 5:C:194:GLU:O    | 5:C:195:GLN:HG3   | 1.64                     | 0.96              |
| 3:A:406:ILE:HD12 | 3:A:406:ILE:H     | 1.28                     | 0.96              |
| 4:B:977:GLY:CA   | 4:B:1099:VAL:HG21 | 1.95                     | 0.96              |
| 3:A:55:ASP:HA    | 3:A:58:LEU:HB2    | 1.46                     | 0.96              |
| 2:T:5:DT:H2''    | 2:T:6:DC:H5'      | 1.44                     | 0.96              |
| 4:B:780:VAL:HG21 | 10:J:56:LEU:CD1   | 1.95                     | 0.96              |
| 3:A:709:THR:HG22 | 3:A:711:ARG:H     | 1.27                     | 0.96              |
| 4:B:521:LEU:CD2  | 4:B:635:ARG:HG2   | 1.95                     | 0.96              |
| 2:T:2:DC:H2'     | 2:T:3:DG:H8       | 1.25                     | 0.96              |
| 3:A:1228:TRP:HB3 | 3:A:1238:ILE:HD13 | 1.47                     | 0.96              |
| 3:A:528:LEU:HD12 | 3:A:528:LEU:O     | 1.65                     | 0.96              |
| 3:A:794:PRO:HG2  | 3:A:795:GLU:HG2   | 1.47                     | 0.96              |
| 4:B:899:ILE:HD11 | 4:B:911:ILE:HG12  | 1.47                     | 0.96              |
| 6:E:126:SER:O    | 6:E:128:PRO:HD3   | 1.66                     | 0.96              |
| 3:A:321:PRO:O    | 3:A:322:VAL:HG13  | 1.66                     | 0.96              |
| 3:A:452:LYS:HB2  | 4:B:1141:HIS:HE1  | 1.28                     | 0.96              |
| 3:A:7:SER:CB     | 4:B:1193:GLN:NE2  | 2.29                     | 0.95              |
| 3:A:148:CYS:O    | 3:A:149:GLU:O     | 1.84                     | 0.95              |
| 3:A:321:PRO:O    | 3:A:322:VAL:CG2   | 2.13                     | 0.95              |
| 4:B:912:ILE:HD11 | 4:B:966:VAL:HG23  | 1.45                     | 0.95              |
| 3:A:320:ARG:HB2  | 3:A:321:PRO:CB    | 1.96                     | 0.95              |
| 3:A:1392:SER:O   | 3:A:1393:ASN:ND2  | 1.97                     | 0.95              |
| 3:A:55:ASP:O     | 3:A:57:ARG:N      | 1.99                     | 0.95              |
| 4:B:635:ARG:CD   | 4:B:636:PRO:HD3   | 1.96                     | 0.95              |
| 3:A:213:HIS:O    | 3:A:214:ILE:O     | 1.84                     | 0.95              |
| 3:A:14:VAL:H     | 3:A:1432:GLN:HE22 | 1.04                     | 0.95              |
| 3:A:605:MET:HA   | 3:A:605:MET:HE3   | 1.46                     | 0.95              |
| 3:A:894:GLU:C    | 3:A:896:ARG:H     | 1.73                     | 0.95              |
| 4:B:477:ALA:HB3  | 4:B:479:VAL:CG2   | 1.97                     | 0.94              |
| 3:A:326:ARG:HG2  | 3:A:1406:VAL:HG21 | 1.49                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:58:PHE:HE2   | 11:K:74:ARG:HE    | 0.98                     | 0.94              |
| 3:A:58:LEU:HD22   | 3:A:243:PRO:HB3   | 1.49                     | 0.94              |
| 3:A:1161:THR:HG22 | 3:A:1163:ILE:N    | 1.81                     | 0.94              |
| 3:A:886:ILE:HG12  | 3:A:943:LEU:HD12  | 1.49                     | 0.94              |
| 3:A:899:VAL:HG12  | 3:A:929:LEU:CD1   | 1.97                     | 0.94              |
| 7:F:81:THR:CG2    | 7:F:136:ARG:HD3   | 1.96                     | 0.94              |
| 8:H:82:PRO:O      | 8:H:83:GLN:HB2    | 1.67                     | 0.94              |
| 3:A:208:LEU:O     | 3:A:209:ASN:O     | 1.85                     | 0.94              |
| 3:A:805:LEU:C     | 3:A:805:LEU:HD12  | 1.91                     | 0.94              |
| 4:B:167:ILE:HG23  | 4:B:424:LEU:CD1   | 1.97                     | 0.94              |
| 3:A:90:VAL:HG12   | 3:A:297:GLN:HE21  | 1.32                     | 0.94              |
| 3:A:90:VAL:HG13   | 3:A:297:GLN:HB2   | 1.48                     | 0.94              |
| 3:A:320:ARG:H     | 3:A:320:ARG:CD    | 1.81                     | 0.94              |
| 3:A:547:LEU:HD22  | 11:K:58:PHE:HD1   | 1.32                     | 0.94              |
| 4:B:345:LYS:O     | 4:B:347:LYS:N     | 2.01                     | 0.94              |
| 3:A:351:THR:CG2   | 4:B:1103:ILE:HD12 | 1.96                     | 0.94              |
| 3:A:528:LEU:C     | 3:A:530:GLY:H     | 1.70                     | 0.94              |
| 3:A:58:LEU:CD2    | 3:A:243:PRO:HB3   | 1.98                     | 0.94              |
| 3:A:265:LYS:HE3   | 3:A:323:LYS:HG3   | 1.48                     | 0.93              |
| 3:A:1116:LEU:HD22 | 3:A:1311:VAL:HG22 | 1.49                     | 0.93              |
| 3:A:99:ILE:HA     | 3:A:102:VAL:HG23  | 1.46                     | 0.93              |
| 2:T:1:DA:N3       | 2:T:1:DA:H2'      | 1.81                     | 0.93              |
| 3:A:1171:GLN:HB2  | 3:A:1172:LEU:HD23 | 1.51                     | 0.93              |
| 4:B:473:MET:C     | 4:B:475:SER:N     | 2.19                     | 0.93              |
| 4:B:780:VAL:HG21  | 10:J:56:LEU:HD11  | 1.48                     | 0.93              |
| 4:B:796:LEU:HB3   | 4:B:799:PRO:HD3   | 1.46                     | 0.93              |
| 5:C:57:VAL:CG1    | 10:J:60:PHE:HB2   | 1.98                     | 0.93              |
| 4:B:550:ASP:OD1   | 4:B:551:PRO:HD2   | 1.67                     | 0.93              |
| 5:C:36:VAL:HG23   | 11:K:41:THR:HG21  | 1.50                     | 0.93              |
| 3:A:1362:TYR:CD1  | 3:A:1363:VAL:N    | 2.36                     | 0.93              |
| 4:B:477:ALA:CB    | 4:B:479:VAL:HG22  | 1.99                     | 0.93              |
| 11:K:32:VAL:HG23  | 11:K:74:ARG:HG3   | 1.49                     | 0.93              |
| 3:A:312:PRO:O     | 3:A:313:GLN:CG    | 2.17                     | 0.93              |
| 9:I:10:CYS:SG     | 9:I:31:THR:HG22   | 2.08                     | 0.93              |
| 3:A:58:LEU:O      | 3:A:59:GLY:O      | 1.86                     | 0.93              |
| 4:B:1051:THR:HG22 | 4:B:1053:GLU:N    | 1.84                     | 0.93              |
| 4:B:1081:LEU:O    | 5:C:189:THR:HG23  | 1.69                     | 0.93              |
| 4:B:1106:ARG:HH21 | 4:B:1109:GLY:H    | 1.14                     | 0.93              |
| 10:J:44:TYR:HA    | 10:J:47:ARG:HB2   | 1.48                     | 0.93              |
| 3:A:855:THR:HG21  | 3:A:857:ARG:NE    | 1.83                     | 0.92              |
| 3:A:908:LEU:HD11  | 3:A:983:ILE:HD11  | 1.49                     | 0.92              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:737:THR:HG21 | 9:I:66:PRO:O      | 1.70                     | 0.92              |
| 5:C:134:ILE:CD1  | 5:C:141:GLY:HA3   | 1.99                     | 0.92              |
| 6:E:52:ARG:CB    | 6:E:53:PRO:HD2    | 1.95                     | 0.92              |
| 4:B:708:GLU:HG3  | 4:B:709:ASP:H     | 1.34                     | 0.92              |
| 5:C:115:SER:HB3  | 5:C:141:GLY:O     | 1.69                     | 0.92              |
| 6:E:168:TYR:C    | 6:E:169:ARG:HG2   | 1.92                     | 0.92              |
| 4:B:102:VAL:HG21 | 4:B:112:LEU:HD22  | 1.48                     | 0.92              |
| 9:I:29:CYS:SG    | 9:I:31:THR:HB     | 2.10                     | 0.92              |
| 3:A:1053:PHE:O   | 3:A:1055:ARG:N    | 2.02                     | 0.92              |
| 4:B:737:THR:HG23 | 9:I:66:PRO:CB     | 1.99                     | 0.92              |
| 6:E:28:TYR:CE1   | 6:E:78:LEU:HD13   | 2.04                     | 0.92              |
| 3:A:391:LEU:HD13 | 3:A:400:PRO:O     | 1.70                     | 0.92              |
| 3:A:590:ARG:HB3  | 3:A:605:MET:H     | 1.31                     | 0.92              |
| 3:A:1362:TYR:HD1 | 3:A:1363:VAL:H    | 1.05                     | 0.92              |
| 4:B:234:ILE:H    | 4:B:234:ILE:HD13  | 1.33                     | 0.92              |
| 5:C:45:ALA:HA    | 5:C:72:LEU:HD12   | 1.51                     | 0.92              |
| 3:A:332:LYS:HG3  | 3:A:333:GLU:HG2   | 1.51                     | 0.92              |
| 4:B:977:GLY:HA3  | 4:B:1099:VAL:CG2  | 1.99                     | 0.92              |
| 8:H:108:SER:O    | 8:H:109:LYS:HB2   | 1.65                     | 0.92              |
| 3:A:718:VAL:O    | 3:A:722:LEU:HD12  | 1.70                     | 0.91              |
| 4:B:701:ILE:CB   | 4:B:740:HIS:HE1   | 1.82                     | 0.91              |
| 4:B:955:THR:CG2  | 4:B:956:THR:H     | 1.81                     | 0.91              |
| 3:A:107:CYS:HB3  | 3:A:114:LEU:HD22  | 1.48                     | 0.91              |
| 3:A:1277:GLU:HG3 | 3:A:1278:ASN:ND2  | 1.83                     | 0.91              |
| 4:B:112:LEU:HD12 | 4:B:113:TYR:H     | 1.33                     | 0.91              |
| 4:B:727:LYS:HD3  | 4:B:1049:ASP:OD1  | 1.69                     | 0.91              |
| 4:B:102:VAL:CG2  | 4:B:112:LEU:HD22  | 2.00                     | 0.91              |
| 3:A:530:GLY:C    | 3:A:532:ARG:H     | 1.58                     | 0.91              |
| 4:B:549:THR:CG2  | 4:B:550:ASP:H     | 1.84                     | 0.91              |
| 4:B:912:ILE:HD11 | 4:B:966:VAL:CG2   | 2.00                     | 0.91              |
| 3:A:830:LYS:HE3  | 3:A:1098:VAL:HG21 | 1.53                     | 0.91              |
| 3:A:133:LYS:O    | 3:A:137:ALA:HB2   | 1.71                     | 0.91              |
| 3:A:399:HIS:HB3  | 3:A:400:PRO:HD3   | 1.50                     | 0.91              |
| 4:B:25:ILE:HD12  | 4:B:651:LEU:HD12  | 1.50                     | 0.91              |
| 8:H:113:ALA:HA   | 8:H:125:LEU:O     | 1.71                     | 0.91              |
| 11:K:49:GLU:HG3  | 11:K:94:ILE:CD1   | 2.00                     | 0.91              |
| 3:A:185:TRP:O    | 3:A:186:LYS:HB2   | 1.69                     | 0.90              |
| 3:A:1434:ALA:HB1 | 3:A:1436:ILE:HD12 | 1.50                     | 0.90              |
| 8:H:97:MET:HB2   | 8:H:118:PHE:CD2   | 2.06                     | 0.90              |
| 8:H:84:ALA:C     | 8:H:86:ASP:H      | 1.79                     | 0.90              |
| 9:I:99:LEU:HB2   | 9:I:112:SER:HB3   | 1.49                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:57:LEU:HD12  | 11:K:76:GLN:CG    | 2.01                     | 0.90              |
| 3:A:261:ASP:CB    | 3:A:323:LYS:HD2   | 2.01                     | 0.90              |
| 3:A:666:ILE:HD11  | 4:B:1030:LEU:HD13 | 1.52                     | 0.90              |
| 4:B:984:HIS:HD2   | 4:B:1024:ALA:HB3  | 1.36                     | 0.90              |
| 11:K:57:LEU:HD12  | 11:K:76:GLN:HG3   | 1.53                     | 0.90              |
| 4:B:827:ILE:HG12  | 4:B:1012:ILE:HD11 | 1.54                     | 0.90              |
| 5:C:51:VAL:HG22   | 5:C:155:LEU:CD2   | 2.02                     | 0.90              |
| 3:A:406:ILE:HD12  | 3:A:406:ILE:N     | 1.86                     | 0.90              |
| 3:A:20:GLY:O      | 3:A:21:LEU:HD23   | 1.72                     | 0.90              |
| 4:B:701:ILE:HB    | 4:B:740:HIS:CE1   | 2.07                     | 0.90              |
| 7:F:101:ILE:HD11  | 7:F:121:ALA:HB2   | 1.54                     | 0.90              |
| 3:A:944:ARG:HG2   | 3:A:1298:TYR:OH   | 1.72                     | 0.89              |
| 12:L:55:ILE:O     | 12:L:56:LEU:HB2   | 1.72                     | 0.89              |
| 3:A:33:ALA:HB2    | 3:A:82:GLY:HA2    | 1.53                     | 0.89              |
| 4:B:293:PRO:HG2   | 4:B:296:GLU:HB2   | 1.54                     | 0.89              |
| 3:A:858:ASN:C     | 3:A:858:ASN:HD22  | 1.79                     | 0.89              |
| 3:A:888:GLY:O     | 3:A:889:SER:O     | 1.90                     | 0.89              |
| 4:B:1162:ILE:HD13 | 4:B:1168:LEU:C    | 1.97                     | 0.89              |
| 6:E:112:TYR:CE1   | 6:E:136:ASN:HB2   | 2.07                     | 0.89              |
| 4:B:25:ILE:HD11   | 4:B:653:VAL:HB    | 1.52                     | 0.89              |
| 4:B:332:ASP:O     | 4:B:334:ILE:N     | 2.05                     | 0.89              |
| 4:B:479:VAL:O     | 4:B:480:SER:HB3   | 1.69                     | 0.89              |
| 6:E:111:VAL:O     | 6:E:111:VAL:HG12  | 1.72                     | 0.89              |
| 3:A:90:VAL:HG11   | 3:A:297:GLN:CA    | 2.01                     | 0.89              |
| 3:A:353:ILE:HD13  | 3:A:487:MET:CE    | 2.02                     | 0.89              |
| 4:B:114:PRO:HD3   | 4:B:124:TYR:CE1   | 2.07                     | 0.89              |
| 4:B:1106:ARG:HD2  | 4:B:1126:GLY:O    | 1.72                     | 0.89              |
| 7:F:98:ALA:HA     | 7:F:101:ILE:HD12  | 1.54                     | 0.89              |
| 4:B:322:PHE:CZ    | 9:I:30:ARG:HD2    | 2.07                     | 0.89              |
| 4:B:788:ARG:CB    | 4:B:788:ARG:HH11  | 1.86                     | 0.89              |
| 6:E:131:THR:HG22  | 6:E:132:ILE:H     | 1.35                     | 0.89              |
| 4:B:471:LYS:O     | 4:B:473:MET:N     | 2.06                     | 0.89              |
| 5:C:3:GLU:HG3     | 5:C:4:GLU:N       | 1.74                     | 0.88              |
| 6:E:54:GLN:O      | 6:E:57:MET:HB3    | 1.71                     | 0.88              |
| 10:J:5:VAL:HG12   | 10:J:6:ARG:HG3    | 1.54                     | 0.88              |
| 10:J:9:SER:OG     | 10:J:45:CYS:HB2   | 1.73                     | 0.88              |
| 3:A:531:ILE:HD13  | 3:A:622:VAL:HG21  | 1.54                     | 0.88              |
| 3:A:523:ILE:HD13  | 3:A:622:VAL:HG22  | 1.55                     | 0.88              |
| 3:A:535:THR:HG21  | 3:A:617:VAL:H     | 1.36                     | 0.88              |
| 6:E:124:VAL:HG22  | 6:E:132:ILE:CG2   | 2.03                     | 0.88              |
| 4:B:129:PHE:CE2   | 4:B:166:PHE:HB2   | 2.09                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:106:GLU:C     | 8:H:108:SER:N     | 2.29                     | 0.88              |
| 6:E:23:VAL:HG13   | 6:E:28:TYR:HD1    | 1.38                     | 0.88              |
| 11:K:65:HIS:HD2   | 11:K:67:PHE:H     | 1.20                     | 0.88              |
| 2:T:6:DC:H2''     | 2:T:7:DC:C5'      | 2.03                     | 0.88              |
| 4:B:278:GLN:HG2   | 4:B:279:ASP:H     | 1.37                     | 0.88              |
| 3:A:809:THR:HG23  | 3:A:812:GLU:OE1   | 1.72                     | 0.88              |
| 3:A:868:TYR:HE1   | 3:A:1064:VAL:CG1  | 1.86                     | 0.88              |
| 3:A:1173:HIS:CD2  | 3:A:1227:ILE:HG23 | 2.07                     | 0.88              |
| 3:A:1291:VAL:HG13 | 3:A:1292:PRO:HD2  | 1.52                     | 0.88              |
| 3:A:1355:VAL:HG12 | 3:A:1356:ILE:N    | 1.89                     | 0.88              |
| 4:B:798:TYR:HD2   | 10:J:4:PRO:HG3    | 1.39                     | 0.88              |
| 9:I:25:LEU:HD12   | 9:I:26:LEU:H      | 1.36                     | 0.88              |
| 3:A:169:ASN:H     | 3:A:169:ASN:HD22  | 0.89                     | 0.88              |
| 3:A:925:LEU:C     | 3:A:927:VAL:H     | 1.78                     | 0.88              |
| 3:A:1364:ASN:HD21 | 3:A:1366:ARG:HG2  | 1.32                     | 0.88              |
| 4:B:1002:THR:CG2  | 4:B:1006:ILE:HB   | 2.04                     | 0.88              |
| 5:C:44:LEU:CB     | 5:C:77:ILE:HD11   | 1.99                     | 0.88              |
| 9:I:10:CYS:SG     | 9:I:31:THR:CG2    | 2.62                     | 0.88              |
| 3:A:322:VAL:CB    | 3:A:323:LYS:HD3   | 2.04                     | 0.88              |
| 5:C:71:PRO:HB2    | 5:C:133:ILE:HD12  | 1.53                     | 0.88              |
| 3:A:261:ASP:HB3   | 3:A:323:LYS:HD2   | 1.50                     | 0.88              |
| 4:B:316:PRO:HA    | 4:B:319:GLU:HG3   | 1.54                     | 0.88              |
| 4:B:329:THR:CA    | 4:B:332:ASP:HB2   | 2.03                     | 0.88              |
| 5:C:46:ILE:HG21   | 5:C:157:CYS:HB3   | 1.56                     | 0.88              |
| 3:A:590:ARG:HB3   | 3:A:605:MET:N     | 1.89                     | 0.87              |
| 3:A:1373:ASP:O    | 3:A:1377:THR:HG23 | 1.73                     | 0.87              |
| 5:C:258:ILE:CD1   | 11:K:42:LEU:HD21  | 2.04                     | 0.87              |
| 6:E:37:LEU:O      | 6:E:38:PRO:O      | 1.92                     | 0.87              |
| 9:I:17:ARG:CG     | 9:I:18:GLU:H      | 1.86                     | 0.87              |
| 3:A:1404:GLU:O    | 3:A:1408:ILE:HG12 | 1.72                     | 0.87              |
| 4:B:469:GLN:O     | 4:B:471:LYS:N     | 2.05                     | 0.87              |
| 4:B:788:ARG:HB3   | 4:B:788:ARG:NH1   | 1.89                     | 0.87              |
| 3:A:265:LYS:NZ    | 3:A:322:VAL:CG2   | 2.36                     | 0.87              |
| 3:A:455:MET:O     | 3:A:456:MET:HG2   | 1.74                     | 0.87              |
| 3:A:793:SER:HB2   | 3:A:794:PRO:HD2   | 1.57                     | 0.87              |
| 3:A:894:GLU:O     | 3:A:896:ARG:N     | 2.07                     | 0.87              |
| 3:A:504:LEU:HD11  | 7:F:91:ALA:CB     | 2.05                     | 0.87              |
| 3:A:925:LEU:C     | 3:A:927:VAL:N     | 2.26                     | 0.87              |
| 4:B:130:VAL:HG12  | 4:B:132:VAL:HG23  | 1.56                     | 0.87              |
| 4:B:200:GLY:HA2   | 4:B:202:TYR:CE2   | 2.09                     | 0.87              |
| 5:C:18:VAL:HG23   | 5:C:240:VAL:CG1   | 2.04                     | 0.87              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:103:CYS:C     | 3:A:105:CYS:H    | 1.77                     | 0.87              |
| 4:B:1177:HIS:O    | 4:B:1179:GLN:N   | 2.06                     | 0.87              |
| 5:C:70:ILE:CD1    | 5:C:144:ILE:HD11 | 2.05                     | 0.87              |
| 4:B:1107:ALA:O    | 4:B:1108:ARG:HB3 | 1.75                     | 0.87              |
| 3:A:115:LEU:HB2   | 3:A:122:MET:HE3  | 1.56                     | 0.86              |
| 5:C:46:ILE:HD11   | 5:C:72:LEU:HD11  | 1.57                     | 0.86              |
| 4:B:230:ALA:HB3   | 4:B:231:PRO:HD3  | 1.56                     | 0.86              |
| 5:C:114:TYR:CD2   | 5:C:140:ASN:HB2  | 2.10                     | 0.86              |
| 3:A:72:GLU:OE1    | 3:A:72:GLU:HA    | 1.73                     | 0.86              |
| 4:B:299:GLU:OE1   | 4:B:572:HIS:HB3  | 1.75                     | 0.86              |
| 3:A:679:ILE:HG23  | 3:A:729:ALA:HB1  | 1.57                     | 0.86              |
| 5:C:133:ILE:HD11  | 5:C:237:SER:HA   | 1.57                     | 0.86              |
| 3:A:262:LEU:O     | 3:A:266:LEU:HB2  | 1.75                     | 0.86              |
| 3:A:401:GLY:H     | 3:A:435:HIS:HD2  | 1.23                     | 0.86              |
| 3:A:565:ILE:HG23  | 3:A:567:LYS:CE   | 2.06                     | 0.86              |
| 4:B:955:THR:OG1   | 12:L:55:ILE:HA   | 1.74                     | 0.86              |
| 4:B:957:ASN:HB3   | 4:B:961:LEU:HD12 | 1.57                     | 0.86              |
| 4:B:1156:ASP:HB3  | 4:B:1198:TYR:H   | 1.39                     | 0.86              |
| 5:C:70:ILE:HD12   | 5:C:144:ILE:HD11 | 1.56                     | 0.86              |
| 3:A:68:GLN:C      | 3:A:70:CYS:H     | 1.79                     | 0.86              |
| 4:B:955:THR:HG23  | 12:L:54:ARG:O    | 1.74                     | 0.86              |
| 10:J:64:ASN:CB    | 10:J:65:PRO:HD3  | 2.00                     | 0.86              |
| 3:A:583:PRO:O     | 3:A:610:GLY:HA3  | 1.75                     | 0.86              |
| 3:A:1015:VAL:CG1  | 3:A:1019:CYS:SG  | 2.64                     | 0.86              |
| 6:E:187:TYR:HD2   | 6:E:188:LEU:HD23 | 1.40                     | 0.86              |
| 3:A:1127:ASP:HB2  | 3:A:1130:GLN:HB3 | 1.58                     | 0.86              |
| 4:B:120:ARG:CD    | 4:B:955:THR:HG21 | 2.05                     | 0.86              |
| 3:A:897:TYR:HD2   | 3:A:936:LEU:HD13 | 1.40                     | 0.85              |
| 4:B:322:PHE:CD1   | 4:B:322:PHE:O    | 2.29                     | 0.85              |
| 4:B:363:HIS:O     | 4:B:364:ILE:HB   | 1.75                     | 0.85              |
| 4:B:996:ARG:NH2   | 5:C:38:ILE:HD12  | 1.91                     | 0.85              |
| 6:E:65:THR:C      | 6:E:67:GLU:H     | 1.81                     | 0.85              |
| 8:H:139:ASN:O     | 8:H:140:ALA:HB2  | 1.75                     | 0.85              |
| 4:B:91:SER:OG     | 4:B:133:LYS:HB2  | 1.75                     | 0.85              |
| 4:B:860:MET:HG2   | 4:B:861:ASP:N    | 1.91                     | 0.85              |
| 3:A:90:VAL:CG1    | 3:A:297:GLN:HB2  | 2.06                     | 0.85              |
| 3:A:630:ILE:HD12  | 3:A:630:ILE:N    | 1.90                     | 0.85              |
| 3:A:1256:GLU:O    | 3:A:1258:HIS:N   | 2.09                     | 0.85              |
| 3:A:1445:ILE:HD12 | 3:A:1445:ILE:N   | 1.90                     | 0.85              |
| 4:B:474:SER:CA    | 4:B:476:ARG:HG3  | 2.04                     | 0.85              |
| 5:C:10:ILE:HD13   | 5:C:20:PHE:HB3   | 1.58                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:229:TYR:N     | 5:C:229:TYR:CD1   | 2.36                     | 0.85              |
| 3:A:1319:VAL:HG13 | 3:A:1320:PRO:HD2  | 1.55                     | 0.85              |
| 4:B:577:ALA:HB1   | 4:B:589:VAL:CG1   | 2.06                     | 0.85              |
| 8:H:89:LEU:C      | 8:H:91:ASP:H      | 1.81                     | 0.85              |
| 10:J:10:CYS:SG    | 10:J:43:ARG:CD    | 2.64                     | 0.85              |
| 3:A:898:ARG:HB2   | 3:A:933:TYR:HE1   | 1.42                     | 0.85              |
| 3:A:1410:PHE:CD2  | 4:B:1212:ILE:HD11 | 2.12                     | 0.85              |
| 3:A:130:ASP:O     | 3:A:131:SER:C     | 2.18                     | 0.85              |
| 4:B:466:TRP:N     | 4:B:475:SER:OG    | 2.08                     | 0.85              |
| 7:F:147:SER:OG    | 7:F:150:GLU:HG3   | 1.76                     | 0.85              |
| 9:I:25:LEU:HD12   | 9:I:26:LEU:N      | 1.89                     | 0.85              |
| 3:A:179:LEU:CD1   | 3:A:297:GLN:HG2   | 2.07                     | 0.85              |
| 3:A:898:ARG:HB2   | 3:A:933:TYR:CE1   | 2.12                     | 0.85              |
| 5:C:44:LEU:HD12   | 5:C:160:LYS:O     | 1.76                     | 0.85              |
| 4:B:129:PHE:CE2   | 4:B:166:PHE:CB    | 2.60                     | 0.85              |
| 4:B:634:TYR:CE1   | 4:B:692:TYR:CD1   | 2.64                     | 0.85              |
| 4:B:798:TYR:CD2   | 10:J:4:PRO:HG3    | 2.11                     | 0.85              |
| 3:A:320:ARG:NH2   | 4:B:469:GLN:O     | 2.08                     | 0.85              |
| 4:B:902:GLY:O     | 12:L:65:VAL:HG11  | 1.77                     | 0.85              |
| 4:B:1099:VAL:CG1  | 4:B:1103:ILE:HD11 | 2.06                     | 0.85              |
| 5:C:3:GLU:CG      | 5:C:4:GLU:H       | 1.88                     | 0.85              |
| 3:A:91:PHE:CD2    | 3:A:297:GLN:OE1   | 2.29                     | 0.84              |
| 4:B:230:ALA:N     | 4:B:231:PRO:HD2   | 1.91                     | 0.84              |
| 8:H:3:ASN:CG      | 8:H:4:THR:H       | 1.81                     | 0.84              |
| 11:K:12:LEU:H     | 11:K:12:LEU:HD12  | 1.38                     | 0.84              |
| 3:A:12:ARG:HD3    | 4:B:1192:TYR:HE2  | 1.40                     | 0.84              |
| 3:A:1319:VAL:HB   | 3:A:1322:ILE:HD12 | 1.59                     | 0.84              |
| 4:B:65:GLU:CG     | 4:B:66:ASP:N      | 2.33                     | 0.84              |
| 4:B:475:SER:O     | 4:B:477:ALA:N     | 2.10                     | 0.84              |
| 4:B:1072:MET:HE3  | 4:B:1085:ILE:HG21 | 1.57                     | 0.84              |
| 5:C:98:VAL:C      | 5:C:99:LEU:HD23   | 2.01                     | 0.84              |
| 3:A:261:ASP:CG    | 3:A:323:LYS:HD2   | 2.02                     | 0.84              |
| 4:B:29:ASP:HB3    | 4:B:658:ILE:HD13  | 1.57                     | 0.84              |
| 4:B:736:THR:O     | 4:B:736:THR:HG22  | 1.77                     | 0.84              |
| 3:A:929:LEU:HD21  | 3:A:983:ILE:CG2   | 2.07                     | 0.84              |
| 4:B:236:HIS:HD2   | 4:B:389:ALA:HB2   | 1.42                     | 0.84              |
| 4:B:801:LYS:HG2   | 10:J:52:THR:HG23  | 1.58                     | 0.84              |
| 3:A:779:PHE:CE1   | 3:A:785:PRO:HD3   | 2.13                     | 0.84              |
| 3:A:1362:TYR:HD1  | 3:A:1363:VAL:N    | 1.72                     | 0.84              |
| 4:B:256:VAL:HG11  | 4:B:382:ILE:HD11  | 1.57                     | 0.84              |
| 3:A:635:ARG:NH2   | 3:A:877:HIS:ND1   | 2.26                     | 0.84              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:B:431:TYR:CE1   | 4:B:447:ALA:HB2  | 2.13                     | 0.84              |
| 11:K:92:ASN:HA    | 11:K:95:ILE:HD12 | 1.56                     | 0.84              |
| 3:A:919:ILE:O     | 3:A:920:LEU:C    | 2.20                     | 0.84              |
| 3:A:1422:ARG:HH21 | 4:B:1220:ARG:CD  | 1.90                     | 0.84              |
| 4:B:62:ILE:HD12   | 4:B:418:LYS:HE2  | 1.59                     | 0.84              |
| 3:A:380:VAL:HG21  | 3:A:430:TRP:N    | 1.93                     | 0.84              |
| 3:A:322:VAL:HB    | 3:A:323:LYS:HD3  | 1.58                     | 0.84              |
| 3:A:522:GLY:C     | 3:A:523:ILE:HD12 | 2.01                     | 0.84              |
| 3:A:922:ASP:OD1   | 3:A:923:LEU:N    | 2.09                     | 0.84              |
| 9:I:7:CYS:N       | 9:I:14:LEU:HD21  | 1.93                     | 0.84              |
| 3:A:821:ARG:O     | 3:A:825:ILE:HG12 | 1.78                     | 0.84              |
| 3:A:981:LEU:CD2   | 3:A:1039:LYS:HA  | 2.08                     | 0.84              |
| 3:A:151:ASP:OD1   | 3:A:163:SER:HA   | 1.78                     | 0.83              |
| 3:A:955:PRO:O     | 3:A:956:LEU:HG   | 1.78                     | 0.83              |
| 8:H:81:PRO:CB     | 8:H:82:PRO:HD2   | 2.04                     | 0.83              |
| 9:I:15:TYR:HB3    | 9:I:16:PRO:CD    | 2.08                     | 0.83              |
| 3:A:1200:ALA:O    | 3:A:1203:ASN:N   | 2.09                     | 0.83              |
| 4:B:577:ALA:HB1   | 4:B:589:VAL:HG13 | 1.59                     | 0.83              |
| 4:B:708:GLU:O     | 4:B:710:LEU:N    | 2.10                     | 0.83              |
| 3:A:322:VAL:HG12  | 3:A:323:LYS:HD3  | 1.59                     | 0.83              |
| 3:A:1291:VAL:CG1  | 3:A:1292:PRO:HD2 | 2.07                     | 0.83              |
| 6:E:116:ILE:O     | 6:E:118:PRO:HD3  | 1.77                     | 0.83              |
| 3:A:59:GLY:CA     | 3:A:67:CYS:SG    | 2.67                     | 0.83              |
| 4:B:474:SER:O     | 4:B:476:ARG:HB2  | 1.79                     | 0.83              |
| 4:B:707:PRO:HB3   | 4:B:741:CYS:SG   | 2.18                     | 0.83              |
| 4:B:744:HIS:HD2   | 4:B:746:SER:OG   | 1.59                     | 0.83              |
| 3:A:265:LYS:HE3   | 3:A:323:LYS:CG   | 2.08                     | 0.83              |
| 3:A:343:LYS:NZ    | 4:B:1197:PRO:HB3 | 1.93                     | 0.83              |
| 4:B:474:SER:HA    | 4:B:476:ARG:CG   | 2.07                     | 0.83              |
| 4:B:635:ARG:CB    | 4:B:636:PRO:CD   | 2.40                     | 0.83              |
| 4:B:744:HIS:CD2   | 4:B:746:SER:OG   | 2.31                     | 0.83              |
| 4:B:1104:HIS:HB2  | 4:B:1122:ARG:HB2 | 1.60                     | 0.83              |
| 8:H:84:ALA:CA     | 8:H:87:ARG:HB2   | 2.08                     | 0.83              |
| 5:C:242:GLN:HE21  | 5:C:246:ARG:HE   | 1.25                     | 0.83              |
| 8:H:84:ALA:HA     | 8:H:87:ARG:HB2   | 1.61                     | 0.83              |
| 10:J:7:CYS:HA     | 10:J:49:MET:HE3  | 1.61                     | 0.83              |
| 3:A:451:HIS:O     | 4:B:1137:CYS:SG  | 2.36                     | 0.83              |
| 3:A:888:GLY:O     | 3:A:940:ARG:NH2  | 2.10                     | 0.83              |
| 3:A:1322:ILE:O    | 3:A:1324:PRO:HD3 | 1.78                     | 0.83              |
| 4:B:474:SER:C     | 4:B:476:ARG:N    | 2.26                     | 0.83              |
| 4:B:1076:HIS:ND1  | 11:K:40:HIS:HD2  | 1.76                     | 0.83              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:E:64:PRO:HG3    | 6:E:76:GLY:HA2   | 1.59                     | 0.83              |
| 7:F:111:LEU:O     | 7:F:113:GLY:N    | 2.10                     | 0.83              |
| 8:H:84:ALA:CB     | 8:H:87:ARG:HB2   | 2.09                     | 0.83              |
| 4:B:555:ILE:HD11  | 4:B:582:VAL:HG11 | 1.61                     | 0.83              |
| 7:F:155:LEU:HD23  | 7:F:155:LEU:N    | 1.84                     | 0.83              |
| 6:E:124:VAL:HG22  | 6:E:132:ILE:HG21 | 1.59                     | 0.83              |
| 9:I:50:THR:CG2    | 9:I:52:ILE:HG22  | 2.09                     | 0.83              |
| 3:A:321:PRO:HD2   | 3:A:322:VAL:HA   | 1.58                     | 0.82              |
| 7:F:111:LEU:C     | 7:F:113:GLY:H    | 1.86                     | 0.82              |
| 3:A:1342:GLU:HG2  | 6:E:212:ARG:NH1  | 1.93                     | 0.82              |
| 3:A:207:ILE:HA    | 3:A:210:ILE:HG13 | 1.61                     | 0.82              |
| 3:A:765:VAL:HG22  | 3:A:802:ASN:O    | 1.79                     | 0.82              |
| 4:B:640:VAL:HG23  | 4:B:740:HIS:CA   | 2.08                     | 0.82              |
| 4:B:682:SER:O     | 4:B:686:ASN:ND2  | 2.12                     | 0.82              |
| 3:A:302:THR:CG2   | 3:A:313:GLN:HE22 | 1.93                     | 0.82              |
| 5:C:46:ILE:CG2    | 5:C:157:CYS:HB3  | 2.09                     | 0.82              |
| 8:H:40:LEU:CD1    | 8:H:123:MET:HE3  | 2.09                     | 0.82              |
| 3:A:1441:PHE:CZ   | 7:F:89:GLU:HA    | 2.15                     | 0.82              |
| 4:B:1099:VAL:HG12 | 4:B:1103:ILE:CD1 | 2.09                     | 0.82              |
| 4:B:1104:HIS:HB2  | 4:B:1122:ARG:HD2 | 1.60                     | 0.82              |
| 3:A:458:HIS:CE1   | 3:A:507:VAL:HG21 | 2.14                     | 0.82              |
| 3:A:996:ASN:O     | 3:A:998:LEU:HB2  | 1.79                     | 0.82              |
| 4:B:797:TYR:HB3   | 4:B:798:TYR:CD1  | 2.14                     | 0.82              |
| 5:C:22:LEU:HD21   | 5:C:25:VAL:HG21  | 1.59                     | 0.82              |
| 3:A:30:ILE:HG13   | 4:B:1183:LYS:HZ1 | 1.45                     | 0.82              |
| 3:A:779:PHE:CZ    | 3:A:785:PRO:HD3  | 2.15                     | 0.82              |
| 3:A:1161:THR:HG22 | 3:A:1162:VAL:N   | 1.92                     | 0.82              |
| 4:B:168:GLY:CA    | 4:B:454:THR:OG1  | 2.28                     | 0.82              |
| 9:I:7:CYS:HB2     | 9:I:14:LEU:CD2   | 2.09                     | 0.82              |
| 6:E:161:LYS:O     | 6:E:163:GLU:N    | 2.12                     | 0.82              |
| 7:F:155:LEU:H     | 7:F:155:LEU:CD2  | 1.84                     | 0.82              |
| 8:H:32:THR:HG22   | 8:H:33:GLN:CG    | 2.09                     | 0.82              |
| 4:B:65:GLU:HG2    | 4:B:66:ASP:H     | 0.73                     | 0.82              |
| 8:H:12:VAL:HG13   | 8:H:28:ALA:HB2   | 1.62                     | 0.82              |
| 11:K:46:ILE:HG23  | 11:K:50:LEU:HD12 | 1.60                     | 0.82              |
| 12:L:43:THR:CG2   | 12:L:43:THR:O    | 2.27                     | 0.81              |
| 3:A:590:ARG:HG3   | 3:A:590:ARG:HH11 | 1.45                     | 0.81              |
| 7:F:132:LEU:O     | 7:F:148:VAL:HG23 | 1.80                     | 0.81              |
| 9:I:25:LEU:HB3    | 9:I:38:ALA:HB2   | 1.62                     | 0.81              |
| 3:A:219:PHE:O     | 3:A:222:LEU:HD12 | 1.78                     | 0.81              |
| 3:A:567:LYS:HB2   | 3:A:568:PRO:CD   | 2.03                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:834:THR:HG21  | 3:A:1077:THR:CA   | 2.10                     | 0.81              |
| 3:A:907:THR:HG22  | 3:A:908:LEU:H     | 1.45                     | 0.81              |
| 3:A:1161:THR:CG2  | 3:A:1163:ILE:H    | 1.86                     | 0.81              |
| 3:A:1394:THR:CG2  | 3:A:1398:MET:HE3  | 2.10                     | 0.81              |
| 4:B:472:ALA:O     | 4:B:474:SER:N     | 2.13                     | 0.81              |
| 4:B:563:MET:HA    | 4:B:589:VAL:O     | 1.81                     | 0.81              |
| 4:B:756:ILE:HG21  | 4:B:759:PRO:HB3   | 1.60                     | 0.81              |
| 4:B:1077:THR:HG22 | 4:B:1079:LYS:H    | 1.42                     | 0.81              |
| 5:C:39:ALA:HA     | 5:C:164:ALA:HB3   | 1.62                     | 0.81              |
| 6:E:113:GLN:HB3   | 6:E:137:GLU:OE1   | 1.80                     | 0.81              |
| 11:K:57:LEU:HB2   | 11:K:76:GLN:HG2   | 1.62                     | 0.81              |
| 11:K:90:ALA:O     | 11:K:94:ILE:HD13  | 1.80                     | 0.81              |
| 2:T:2:DC:C2'      | 2:T:3:DG:H8       | 1.92                     | 0.81              |
| 3:A:265:LYS:CE    | 3:A:323:LYS:HE2   | 2.10                     | 0.81              |
| 4:B:882:THR:CG2   | 4:B:935:ARG:HA    | 2.08                     | 0.81              |
| 5:C:58:LEU:HD21   | 10:J:57:ILE:HD13  | 1.60                     | 0.81              |
| 10:J:51:LEU:O     | 10:J:51:LEU:HD12  | 1.81                     | 0.81              |
| 12:L:43:THR:O     | 12:L:43:THR:HG22  | 1.79                     | 0.81              |
| 3:A:492:PRO:C     | 3:A:493:GLN:HE21  | 1.87                     | 0.81              |
| 3:A:898:ARG:HD2   | 3:A:899:VAL:N     | 1.96                     | 0.81              |
| 3:A:1042:PHE:CE2  | 3:A:1046:LEU:HD12 | 2.15                     | 0.81              |
| 8:H:93:TYR:CD1    | 8:H:143:LEU:HB2   | 2.15                     | 0.81              |
| 8:H:142:LEU:HD12  | 8:H:143:LEU:N     | 1.96                     | 0.81              |
| 3:A:1101:LEU:HG   | 3:A:1105:LEU:CD1  | 2.11                     | 0.81              |
| 4:B:737:THR:CG2   | 9:I:66:PRO:HB2    | 2.10                     | 0.81              |
| 4:B:737:THR:CG2   | 9:I:66:PRO:CB     | 2.58                     | 0.81              |
| 4:B:986:GLN:OE1   | 4:B:986:GLN:HA    | 1.80                     | 0.81              |
| 9:I:78:CYS:SG     | 9:I:103:CYS:SG    | 2.78                     | 0.81              |
| 3:A:119:ASN:O     | 3:A:122:MET:HB3   | 1.81                     | 0.81              |
| 3:A:278:THR:O     | 3:A:278:THR:CG2   | 2.24                     | 0.81              |
| 3:A:1173:HIS:HD2  | 3:A:1227:ILE:HG23 | 1.45                     | 0.81              |
| 5:C:66:ARG:NH2    | 10:J:3:VAL:O      | 2.14                     | 0.81              |
| 6:E:43:LYS:O      | 6:E:47:CYS:HB2    | 1.81                     | 0.81              |
| 9:I:47:GLU:OE1    | 9:I:50:THR:HG23   | 1.81                     | 0.81              |
| 3:A:58:LEU:CD2    | 3:A:80:HIS:O      | 2.29                     | 0.81              |
| 4:B:423:LYS:HZ3   | 4:B:423:LYS:HB2   | 1.44                     | 0.81              |
| 4:B:830:TYR:CE1   | 4:B:1000:PRO:HB3  | 2.16                     | 0.81              |
| 6:E:171:LYS:HB2   | 6:E:174:GLN:HG3   | 1.63                     | 0.81              |
| 7:F:86:THR:OG1    | 7:F:89:GLU:HG3    | 1.81                     | 0.81              |
| 3:A:13:THR:HB     | 3:A:15:LYS:NZ     | 1.96                     | 0.81              |
| 3:A:1242:VAL:HG12 | 3:A:1243:VAL:N    | 1.96                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:175:ARG:HG2   | 4:B:175:ARG:HH11  | 1.44                     | 0.81              |
| 5:C:134:ILE:HD12  | 5:C:141:GLY:CA    | 2.11                     | 0.81              |
| 3:A:546:VAL:HG12  | 3:A:550:LEU:CD2   | 2.11                     | 0.81              |
| 3:A:705:LYS:HG3   | 3:A:713:SER:HB3   | 1.62                     | 0.81              |
| 3:A:1052:GLN:O    | 3:A:1053:PHE:O    | 1.97                     | 0.81              |
| 3:A:1342:GLU:HG2  | 6:E:212:ARG:HH12  | 1.45                     | 0.81              |
| 11:K:49:GLU:CG    | 11:K:94:ILE:HD11  | 2.11                     | 0.81              |
| 3:A:901:LEU:HA    | 3:A:907:THR:CG2   | 2.11                     | 0.80              |
| 3:A:1076:ALA:HA   | 3:A:1079:MET:HE2  | 1.61                     | 0.80              |
| 4:B:519:TRP:CZ2   | 4:B:705:MET:HE1   | 2.17                     | 0.80              |
| 4:B:984:HIS:CD2   | 4:B:1024:ALA:HB3  | 2.15                     | 0.80              |
| 4:B:1077:THR:CG2  | 4:B:1079:LYS:H    | 1.94                     | 0.80              |
| 7:F:75:PRO:O      | 7:F:79:ARG:HD2    | 1.81                     | 0.80              |
| 7:F:109:VAL:HG12  | 7:F:110:ASP:H     | 1.42                     | 0.80              |
| 3:A:65:LEU:HD23   | 3:A:65:LEU:N      | 1.96                     | 0.80              |
| 9:I:10:CYS:HB3    | 9:I:31:THR:CG2    | 2.05                     | 0.80              |
| 11:K:50:LEU:HD21  | 11:K:75:ILE:HD13  | 1.63                     | 0.80              |
| 3:A:14:VAL:H      | 3:A:1432:GLN:NE2  | 1.80                     | 0.80              |
| 3:A:908:LEU:O     | 3:A:909:ASP:O     | 1.98                     | 0.80              |
| 3:A:1101:LEU:O    | 3:A:1105:LEU:HD12 | 1.80                     | 0.80              |
| 8:H:139:ASN:O     | 8:H:140:ALA:CB    | 2.28                     | 0.80              |
| 2:T:4:DA:H5'      | 3:A:832:ALA:HA    | 1.64                     | 0.80              |
| 3:A:445:ASN:ND2   | 3:A:446:ARG:N     | 2.30                     | 0.80              |
| 3:A:783:THR:O     | 3:A:784:LEU:HD23  | 1.82                     | 0.80              |
| 4:B:737:THR:HG23  | 9:I:66:PRO:HB3    | 1.63                     | 0.80              |
| 3:A:649:ILE:O     | 3:A:653:VAL:CG2   | 2.30                     | 0.80              |
| 3:A:1409:LEU:HD13 | 4:B:1207:LEU:HD21 | 1.63                     | 0.80              |
| 5:C:52:GLU:OE2    | 5:C:154:LYS:HG2   | 1.81                     | 0.80              |
| 5:C:173:ALA:O     | 5:C:174:ALA:HB3   | 1.81                     | 0.80              |
| 12:L:68:GLU:OE1   | 12:L:68:GLU:O     | 2.00                     | 0.80              |
| 3:A:146:MET:O     | 3:A:170:THR:CG2   | 2.29                     | 0.80              |
| 3:A:239:LEU:HD12  | 3:A:240:PRO:O     | 1.82                     | 0.80              |
| 10:J:64:ASN:HB3   | 10:J:65:PRO:CD    | 2.11                     | 0.80              |
| 4:B:108:VAL:HG12  | 4:B:109:THR:N     | 1.94                     | 0.80              |
| 10:J:36:LEU:HD12  | 10:J:47:ARG:HG2   | 1.64                     | 0.80              |
| 3:A:886:ILE:HD11  | 3:A:943:LEU:HB2   | 1.64                     | 0.80              |
| 4:B:521:LEU:HD23  | 4:B:635:ARG:HG2   | 1.64                     | 0.80              |
| 4:B:794:ASN:HD22  | 4:B:794:ASN:N     | 1.80                     | 0.80              |
| 3:A:697:ALA:HB2   | 3:A:702:LEU:HG    | 1.62                     | 0.79              |
| 3:A:305:ASP:OD1   | 3:A:306:ASN:N     | 2.15                     | 0.79              |
| 3:A:1319:VAL:CG1  | 3:A:1320:PRO:HD2  | 2.11                     | 0.79              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:640:VAL:HG23 | 4:B:740:HIS:HA    | 1.62                     | 0.79              |
| 4:B:788:ARG:CB   | 4:B:788:ARG:NH1   | 2.45                     | 0.79              |
| 4:B:1175:LEU:O   | 4:B:1176:ASN:CB   | 2.27                     | 0.79              |
| 11:K:65:HIS:CD2  | 11:K:67:PHE:H     | 1.99                     | 0.79              |
| 3:A:313:GLN:O    | 3:A:314:ALA:HB2   | 1.80                     | 0.79              |
| 3:A:322:VAL:HB   | 3:A:323:LYS:HG2   | 1.63                     | 0.79              |
| 3:A:1284:MET:HA  | 3:A:1306:LEU:HD23 | 1.64                     | 0.79              |
| 4:B:806:THR:HG22 | 4:B:808:ALA:H     | 1.48                     | 0.79              |
| 3:A:504:LEU:HD11 | 7:F:91:ALA:HB2    | 1.64                     | 0.79              |
| 3:A:547:LEU:HD22 | 11:K:58:PHE:CD1   | 2.16                     | 0.79              |
| 3:A:785:PRO:HB2  | 4:B:701:ILE:HD11  | 1.64                     | 0.79              |
| 4:B:846:ILE:CG2  | 4:B:974:PRO:HG2   | 2.12                     | 0.79              |
| 4:B:1182:CYS:O   | 4:B:1183:LYS:O    | 2.01                     | 0.79              |
| 8:H:41:ASP:O     | 8:H:42:ILE:HD13   | 1.82                     | 0.79              |
| 3:A:569:LYS:HG2  | 3:A:571:LEU:HD11  | 1.64                     | 0.79              |
| 3:A:575:LYS:HD3  | 3:A:612:ILE:HD11  | 1.65                     | 0.79              |
| 4:B:800:GLN:HG2  | 10:J:52:THR:HG21  | 1.63                     | 0.79              |
| 3:A:7:SER:HB3    | 4:B:1193:GLN:HE22 | 1.44                     | 0.79              |
| 4:B:68:THR:O     | 4:B:69:LEU:HD23   | 1.82                     | 0.79              |
| 4:B:999:MET:HG3  | 4:B:1000:PRO:HD2  | 1.65                     | 0.79              |
| 6:E:170:LEU:HD13 | 6:E:175:LEU:CD2   | 2.12                     | 0.79              |
| 9:I:17:ARG:CG    | 9:I:18:GLU:N      | 2.45                     | 0.79              |
| 3:A:58:LEU:HD22  | 3:A:243:PRO:CB    | 2.11                     | 0.79              |
| 3:A:531:ILE:CG1  | 3:A:622:VAL:HG11  | 2.11                     | 0.79              |
| 4:B:62:ILE:HG23  | 4:B:418:LYS:HG2   | 1.63                     | 0.79              |
| 4:B:428:ILE:C    | 4:B:430:ARG:N     | 2.35                     | 0.79              |
| 5:C:182:PRO:HB2  | 5:C:207:CYS:SG    | 2.22                     | 0.79              |
| 6:E:164:LEU:HD13 | 6:E:211:TYR:CE2   | 2.18                     | 0.79              |
| 8:H:47:PHE:HB3   | 8:H:95:TYR:HD1    | 1.46                     | 0.79              |
| 3:A:343:LYS:HZ3  | 4:B:1197:PRO:HB3  | 1.48                     | 0.79              |
| 3:A:598:LEU:HD13 | 8:H:25:ARG:NH1    | 1.97                     | 0.79              |
| 4:B:124:TYR:OH   | 4:B:179:CYS:HA    | 1.83                     | 0.79              |
| 9:I:10:CYS:SG    | 9:I:32:CYS:SG     | 2.80                     | 0.79              |
| 3:A:58:LEU:HD21  | 3:A:80:HIS:O      | 1.83                     | 0.79              |
| 3:A:68:GLN:NE2   | 3:A:80:HIS:NE2    | 2.31                     | 0.79              |
| 3:A:120:GLU:HG2  | 3:A:120:GLU:O     | 1.81                     | 0.79              |
| 3:A:567:LYS:CB   | 8:H:96:VAL:H      | 1.96                     | 0.79              |
| 4:B:815:ARG:HH11 | 4:B:815:ARG:HG3   | 1.48                     | 0.78              |
| 4:B:1076:HIS:ND1 | 11:K:40:HIS:CD2   | 2.51                     | 0.78              |
| 5:C:93:ASP:O     | 5:C:127:ARG:NH2   | 2.16                     | 0.78              |
| 9:I:33:SER:O     | 9:I:34:TYR:O      | 2.01                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:114:LEU:HD13  | 3:A:171:GLN:NE2   | 1.97                     | 0.78              |
| 3:A:1004:ASN:C    | 3:A:1004:ASN:OD1  | 2.27                     | 0.78              |
| 4:B:174:LEU:CD2   | 4:B:204:ILE:HD11  | 2.10                     | 0.78              |
| 11:K:7:PHE:HA     | 11:K:10:PHE:CZ    | 2.18                     | 0.78              |
| 3:A:676:MET:SD    | 3:A:679:ILE:HD12  | 2.22                     | 0.78              |
| 3:A:714:PHE:CG    | 9:I:97:MET:HE1    | 2.19                     | 0.78              |
| 3:A:868:TYR:CE1   | 3:A:1064:VAL:HG21 | 2.18                     | 0.78              |
| 5:C:92:CYS:SG     | 5:C:94:LYS:CB     | 2.72                     | 0.78              |
| 5:C:244:VAL:O     | 5:C:248:ILE:HG13  | 1.83                     | 0.78              |
| 6:E:30:ILE:HG23   | 6:E:34:GLU:OE1    | 1.83                     | 0.78              |
| 3:A:12:ARG:HD3    | 4:B:1192:TYR:CE2  | 2.18                     | 0.78              |
| 3:A:1228:TRP:HB3  | 3:A:1238:ILE:CD1  | 2.13                     | 0.78              |
| 4:B:167:ILE:HD12  | 4:B:424:LEU:HD11  | 1.65                     | 0.78              |
| 6:E:96:PHE:O      | 6:E:98:ILE:N      | 2.17                     | 0.78              |
| 2:T:2:DC:C2'      | 2:T:3:DG:C8       | 2.65                     | 0.78              |
| 4:B:834:ASN:O     | 4:B:1013:ASN:HB2  | 1.82                     | 0.78              |
| 3:A:107:CYS:CB    | 3:A:114:LEU:HD22  | 2.13                     | 0.78              |
| 3:A:265:LYS:HZ3   | 3:A:322:VAL:HG21  | 1.47                     | 0.78              |
| 3:A:326:ARG:CG    | 3:A:1406:VAL:HG21 | 2.14                     | 0.78              |
| 7:F:135:ARG:HG2   | 7:F:137:TYR:CE1   | 2.19                     | 0.78              |
| 8:H:40:LEU:HD13   | 8:H:123:MET:HE3   | 1.65                     | 0.78              |
| 11:K:40:HIS:CE1   | 11:K:63:VAL:HG11  | 2.18                     | 0.78              |
| 4:B:129:PHE:CD2   | 4:B:166:PHE:HB2   | 2.19                     | 0.78              |
| 8:H:5:LEU:HD22    | 8:H:133:ASN:O     | 1.84                     | 0.78              |
| 8:H:42:ILE:HD12   | 8:H:95:TYR:CZ     | 2.19                     | 0.78              |
| 9:I:19:ASP:O      | 9:I:23:ASN:HA     | 1.84                     | 0.78              |
| 9:I:42:LEU:HD12   | 9:I:43:VAL:N      | 1.98                     | 0.78              |
| 3:A:463:ILE:HB    | 3:A:464:PRO:HD2   | 1.66                     | 0.78              |
| 3:A:1222:ASN:O    | 3:A:1223:ASP:HB3  | 1.81                     | 0.78              |
| 3:A:1273:LEU:O    | 3:A:1274:ARG:HB3  | 1.82                     | 0.78              |
| 3:A:1437:GLY:HA3  | 7:F:88:TYR:CD2    | 2.18                     | 0.78              |
| 5:C:134:ILE:HD11  | 5:C:141:GLY:HA3   | 1.62                     | 0.78              |
| 3:A:1279:ILE:HG22 | 3:A:1279:ILE:O    | 1.81                     | 0.78              |
| 4:B:365:THR:HG23  | 4:B:367:LEU:H     | 1.49                     | 0.78              |
| 4:B:1171:VAL:CG1  | 4:B:1172:ILE:H    | 1.96                     | 0.78              |
| 5:C:196:ASP:O     | 5:C:200:GLU:HB2   | 1.84                     | 0.78              |
| 4:B:806:THR:N     | 4:B:809:MET:HE3   | 1.99                     | 0.78              |
| 9:I:7:CYS:CA      | 9:I:14:LEU:HD21   | 2.13                     | 0.78              |
| 11:K:93:SER:O     | 11:K:97:LYS:HG3   | 1.83                     | 0.78              |
| 3:A:958:VAL:HG22  | 3:A:1052:GLN:HB3  | 1.64                     | 0.77              |
| 4:B:273:LEU:HB2   | 4:B:276:ILE:HD12  | 1.64                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:711:GLU:N     | 4:B:712:PRO:CD    | 2.47                     | 0.77              |
| 4:B:954:VAL:O     | 12:L:55:ILE:O     | 2.01                     | 0.77              |
| 3:A:852:TYR:CE1   | 7:F:136:ARG:HG2   | 2.19                     | 0.77              |
| 3:A:913:LEU:HD12  | 3:A:915:SER:H     | 1.48                     | 0.77              |
| 3:A:1189:SER:OG   | 3:A:1190:PRO:HD2  | 1.84                     | 0.77              |
| 4:B:169:ARG:HB2   | 4:B:454:THR:CG2   | 2.14                     | 0.77              |
| 4:B:770:GLN:HG2   | 4:B:983:ARG:O     | 1.84                     | 0.77              |
| 4:B:1116:ARG:HG3  | 4:B:1198:TYR:CD2  | 2.19                     | 0.77              |
| 6:E:162:ARG:HH21  | 6:E:166:LYS:HZ3   | 1.30                     | 0.77              |
| 10:J:43:ARG:CG    | 10:J:46:CYS:HB2   | 2.12                     | 0.77              |
| 3:A:1150:SER:OG   | 3:A:1264:GLU:OE1  | 2.02                     | 0.77              |
| 3:A:1329:THR:HG22 | 3:A:1331:SER:H    | 1.50                     | 0.77              |
| 9:I:42:LEU:HD12   | 9:I:43:VAL:H      | 1.47                     | 0.77              |
| 9:I:68:LEU:HB3    | 9:I:84:VAL:HG22   | 1.67                     | 0.77              |
| 3:A:320:ARG:N     | 3:A:320:ARG:CD    | 2.41                     | 0.77              |
| 5:C:227:THR:HG22  | 5:C:229:TYR:CE1   | 2.18                     | 0.77              |
| 9:I:6:PHE:HB3     | 9:I:12:ASN:O      | 1.84                     | 0.77              |
| 3:A:1120:LEU:HD23 | 3:A:1125:ALA:O    | 1.85                     | 0.77              |
| 3:A:1155:ASP:OD2  | 3:A:1162:VAL:HG23 | 1.84                     | 0.77              |
| 4:B:708:GLU:C     | 4:B:710:LEU:H     | 1.91                     | 0.77              |
| 12:L:48:CYS:HB3   | 12:L:51:CYS:O     | 1.85                     | 0.77              |
| 4:B:112:LEU:HD12  | 4:B:113:TYR:N     | 1.99                     | 0.77              |
| 4:B:645:SER:O     | 4:B:647:GLY:N     | 2.16                     | 0.77              |
| 4:B:759:PRO:HD2   | 4:B:1046:PRO:HG3  | 1.67                     | 0.77              |
| 6:E:64:PRO:HG2    | 6:E:76:GLY:HA2    | 1.67                     | 0.77              |
| 4:B:911:ILE:HG22  | 4:B:912:ILE:HG13  | 1.65                     | 0.77              |
| 5:C:56:THR:HG21   | 5:C:145:CYS:SG    | 2.24                     | 0.77              |
| 3:A:445:ASN:HB3   | 3:A:455:MET:HE2   | 1.67                     | 0.77              |
| 4:B:635:ARG:CG    | 4:B:636:PRO:HD3   | 2.13                     | 0.77              |
| 5:C:4:GLU:HG3     | 5:C:5:GLY:H       | 1.50                     | 0.77              |
| 5:C:46:ILE:CD1    | 5:C:72:LEU:HD11   | 2.15                     | 0.77              |
| 9:I:19:ASP:HB2    | 9:I:24:ARG:HG3    | 1.67                     | 0.77              |
| 3:A:660:ASN:C     | 3:A:660:ASN:HD22  | 1.92                     | 0.77              |
| 4:B:1084:GLN:OE1  | 4:B:1084:GLN:N    | 2.18                     | 0.77              |
| 7:F:81:THR:HG22   | 7:F:136:ARG:HH11  | 1.50                     | 0.77              |
| 3:A:247:ARG:HH11  | 3:A:263:THR:HG23  | 1.49                     | 0.77              |
| 3:A:528:LEU:C     | 3:A:530:GLY:N     | 2.38                     | 0.77              |
| 4:B:166:PHE:C     | 4:B:166:PHE:CD2   | 2.61                     | 0.77              |
| 4:B:635:ARG:HD2   | 4:B:636:PRO:CD    | 2.14                     | 0.77              |
| 4:B:640:VAL:O     | 4:B:650:GLU:O     | 2.03                     | 0.77              |
| 4:B:956:THR:OG1   | 4:B:961:LEU:O     | 2.02                     | 0.77              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:630:ILE:H     | 3:A:630:ILE:CD1  | 1.92                     | 0.76              |
| 3:A:852:TYR:CE2   | 3:A:1060:PRO:HB2 | 2.20                     | 0.76              |
| 4:B:56:ASP:C      | 4:B:57:TYR:HD1   | 1.93                     | 0.76              |
| 4:B:474:SER:O     | 4:B:475:SER:C    | 2.28                     | 0.76              |
| 5:C:227:THR:HG22  | 5:C:229:TYR:HE1  | 1.51                     | 0.76              |
| 5:C:229:TYR:HD1   | 5:C:229:TYR:H    | 1.33                     | 0.76              |
| 3:A:855:THR:CG2   | 3:A:857:ARG:HE   | 1.94                     | 0.76              |
| 7:F:99:LEU:HD11   | 7:F:103:MET:HE3  | 1.68                     | 0.76              |
| 3:A:26:GLU:O      | 3:A:29:ALA:N     | 2.17                     | 0.76              |
| 3:A:588:LEU:HD12  | 3:A:589:GLN:H    | 1.51                     | 0.76              |
| 3:A:898:ARG:HA    | 3:A:933:TYR:CD1  | 2.21                     | 0.76              |
| 4:B:1184:GLY:O    | 4:B:1186:ASP:N   | 2.18                     | 0.76              |
| 6:E:127:ILE:O     | 6:E:127:ILE:HG12 | 1.84                     | 0.76              |
| 3:A:96:ILE:HG22   | 3:A:97:ALA:N     | 2.00                     | 0.76              |
| 3:A:672:ASP:CB    | 3:A:736:ASN:OD1  | 2.33                     | 0.76              |
| 3:A:1171:GLN:HB2  | 3:A:1172:LEU:CD2 | 2.16                     | 0.76              |
| 3:A:1193:LEU:HD12 | 3:A:1194:ARG:N   | 2.00                     | 0.76              |
| 7:F:135:ARG:HG2   | 7:F:137:TYR:HE1  | 1.50                     | 0.76              |
| 8:H:51:ALA:O      | 8:H:52:GLN:C     | 2.28                     | 0.76              |
| 8:H:89:LEU:O      | 8:H:91:ASP:N     | 2.18                     | 0.76              |
| 3:A:1168:GLU:O    | 3:A:1170:ILE:N   | 2.19                     | 0.76              |
| 4:B:46:GLN:HG3    | 4:B:47:GLN:H     | 1.50                     | 0.76              |
| 4:B:1106:ARG:HH21 | 4:B:1109:GLY:N   | 1.83                     | 0.76              |
| 3:A:868:TYR:CE2   | 3:A:1366:ARG:HD3 | 2.21                     | 0.76              |
| 4:B:427:ASP:HA    | 4:B:430:ARG:HH11 | 1.50                     | 0.76              |
| 4:B:751:VAL:HG12  | 4:B:752:ALA:N    | 1.99                     | 0.76              |
| 5:C:99:LEU:HD23   | 5:C:99:LEU:N     | 2.01                     | 0.76              |
| 3:A:1237:ILE:CG2  | 3:A:1238:ILE:N   | 2.48                     | 0.76              |
| 4:B:723:VAL:O     | 4:B:724:ASP:C    | 2.29                     | 0.76              |
| 3:A:530:GLY:O     | 3:A:531:ILE:C    | 2.29                     | 0.76              |
| 3:A:573:SER:O     | 3:A:576:GLN:HB2  | 1.85                     | 0.76              |
| 5:C:242:GLN:O     | 5:C:246:ARG:HG3  | 1.85                     | 0.76              |
| 11:K:12:LEU:HD12  | 11:K:12:LEU:N    | 2.00                     | 0.76              |
| 11:K:46:ILE:CG2   | 11:K:50:LEU:HD12 | 2.16                     | 0.76              |
| 3:A:84:ILE:HG22   | 3:A:241:VAL:CG2  | 2.16                     | 0.76              |
| 7:F:107:VAL:HG11  | 7:F:111:LEU:HD11 | 1.66                     | 0.76              |
| 8:H:134:ASN:O     | 8:H:135:LEU:O    | 2.04                     | 0.76              |
| 3:A:106:VAL:CG1   | 3:A:107:CYS:N    | 2.49                     | 0.76              |
| 3:A:107:CYS:SG    | 3:A:108:MET:N    | 2.58                     | 0.76              |
| 4:B:859:TYR:OH    | 4:B:941:LEU:HD22 | 1.86                     | 0.76              |
| 3:A:902:LEU:HD11  | 3:A:926:GLN:HG3  | 1.67                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1154:TYR:HE1  | 9:I:18:GLU:HG2    | 1.50                     | 0.75              |
| 4:B:521:LEU:HD21  | 4:B:635:ARG:HG2   | 1.67                     | 0.75              |
| 9:I:29:CYS:SG     | 9:I:31:THR:CB     | 2.74                     | 0.75              |
| 3:A:896:ARG:HD2   | 3:A:897:TYR:HE1   | 1.51                     | 0.75              |
| 3:A:901:LEU:O     | 3:A:903:ASN:N     | 2.20                     | 0.75              |
| 4:B:1072:MET:CE   | 4:B:1085:ILE:HG21 | 2.17                     | 0.75              |
| 10:J:10:CYS:HB2   | 10:J:45:CYS:SG    | 2.25                     | 0.75              |
| 3:A:546:VAL:HG12  | 3:A:550:LEU:HD21  | 1.68                     | 0.75              |
| 3:A:608:ILE:O     | 3:A:609:ASP:O     | 2.04                     | 0.75              |
| 3:A:1120:LEU:HB3  | 3:A:1124:HIS:O    | 1.86                     | 0.75              |
| 3:A:1242:VAL:CG1  | 3:A:1243:VAL:H    | 1.92                     | 0.75              |
| 6:E:39:LEU:O      | 6:E:40:GLU:C      | 2.28                     | 0.75              |
| 6:E:198:ILE:HD11  | 6:E:212:ARG:HG3   | 1.68                     | 0.75              |
| 3:A:804:TYR:CE1   | 4:B:1021:MET:HE3  | 2.20                     | 0.75              |
| 3:A:868:TYR:CD1   | 3:A:1064:VAL:HG21 | 2.22                     | 0.75              |
| 3:A:1206:ASP:O    | 3:A:1274:ARG:NH1  | 2.19                     | 0.75              |
| 4:B:27:ALA:O      | 4:B:28:GLU:C      | 2.26                     | 0.75              |
| 4:B:640:VAL:HG23  | 4:B:740:HIS:N     | 2.00                     | 0.75              |
| 3:A:352:VAL:HG12  | 3:A:353:ILE:N     | 2.00                     | 0.75              |
| 4:B:99:LYS:HB3    | 4:B:180:TYR:CE2   | 2.21                     | 0.75              |
| 5:C:5:GLY:O       | 5:C:7:GLN:HG2     | 1.87                     | 0.75              |
| 5:C:51:VAL:HG22   | 5:C:155:LEU:HD22  | 1.66                     | 0.75              |
| 6:E:13:TRP:CE3    | 6:E:39:LEU:HD13   | 2.22                     | 0.75              |
| 12:L:48:CYS:CB    | 12:L:51:CYS:O     | 2.34                     | 0.75              |
| 3:A:265:LYS:HZ2   | 3:A:322:VAL:CG2   | 1.96                     | 0.75              |
| 3:A:444:PHE:HB3   | 3:A:458:HIS:HD2   | 1.50                     | 0.75              |
| 3:A:1394:THR:HG22 | 3:A:1395:GLY:N    | 2.01                     | 0.75              |
| 3:A:1444:MET:HB2  | 7:F:133:VAL:HG12  | 1.67                     | 0.75              |
| 4:B:385:LEU:O     | 4:B:385:LEU:HG    | 1.86                     | 0.75              |
| 4:B:556:THR:HG22  | 4:B:557:PHE:N     | 2.02                     | 0.75              |
| 4:B:806:THR:HG22  | 4:B:808:ALA:N     | 2.00                     | 0.75              |
| 4:B:1024:ALA:HA   | 4:B:1027:ILE:HD12 | 1.67                     | 0.75              |
| 7:F:125:LEU:HB2   | 7:F:130:ILE:HD12  | 1.69                     | 0.75              |
| 5:C:131:HIS:O     | 5:C:132:PRO:C     | 2.28                     | 0.75              |
| 3:A:321:PRO:O     | 3:A:322:VAL:CG1   | 2.33                     | 0.75              |
| 4:B:994:TYR:HB2   | 4:B:999:MET:HE1   | 1.69                     | 0.75              |
| 8:H:109:LYS:HB3   | 8:H:110:ASP:CG    | 2.10                     | 0.75              |
| 3:A:886:ILE:HG12  | 3:A:943:LEU:CD1   | 2.16                     | 0.75              |
| 3:A:1208:THR:OG1  | 3:A:1211:GLN:OE1  | 2.03                     | 0.75              |
| 3:A:1212:VAL:O    | 3:A:1216:ILE:HG13 | 1.87                     | 0.75              |
| 4:B:46:GLN:HE22   | 4:B:496:ARG:HA    | 1.52                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:123:ASN:HD22  | 5:C:125:MET:HG2   | 1.51                     | 0.75              |
| 6:E:111:VAL:O     | 6:E:111:VAL:CG1   | 2.35                     | 0.75              |
| 3:A:445:ASN:HD22  | 3:A:446:ARG:N     | 1.85                     | 0.74              |
| 3:A:648:ASN:O     | 3:A:652:VAL:HG23  | 1.86                     | 0.74              |
| 3:A:1101:LEU:HG   | 3:A:1105:LEU:HD11 | 1.69                     | 0.74              |
| 4:B:482:VAL:O     | 4:B:482:VAL:HG23  | 1.87                     | 0.74              |
| 4:B:1066:SER:O    | 4:B:1067:ARG:HD3  | 1.87                     | 0.74              |
| 8:H:7:ASP:O       | 8:H:8:ASP:HB2     | 1.87                     | 0.74              |
| 9:I:111:THR:HG22  | 9:I:113:ASP:H     | 1.52                     | 0.74              |
| 3:A:399:HIS:O     | 3:A:435:HIS:CD2   | 2.40                     | 0.74              |
| 3:A:1364:ASN:ND2  | 3:A:1366:ARG:HH11 | 1.84                     | 0.74              |
| 4:B:421:PHE:O     | 4:B:425:THR:HB    | 1.86                     | 0.74              |
| 11:K:33:ILE:HD12  | 11:K:73:LEU:HD23  | 1.67                     | 0.74              |
| 3:A:90:VAL:CG1    | 3:A:297:GLN:NE2   | 2.41                     | 0.74              |
| 4:B:899:ILE:HD11  | 4:B:911:ILE:CG1   | 2.18                     | 0.74              |
| 10:J:3:VAL:HG21   | 10:J:18:TRP:CB    | 2.17                     | 0.74              |
| 3:A:152:VAL:O     | 3:A:162:VAL:HG23  | 1.87                     | 0.74              |
| 3:A:680:THR:HG22  | 3:A:681:GLU:N     | 2.00                     | 0.74              |
| 4:B:96:TYR:N      | 4:B:129:PHE:O     | 2.21                     | 0.74              |
| 4:B:542:MET:HE3   | 4:B:747:MET:HG3   | 1.68                     | 0.74              |
| 4:B:546:SER:OG    | 4:B:631:GLY:N     | 2.19                     | 0.74              |
| 4:B:955:THR:CG2   | 4:B:956:THR:N     | 2.44                     | 0.74              |
| 4:B:977:GLY:CA    | 4:B:1099:VAL:CG2  | 2.63                     | 0.74              |
| 9:I:50:THR:HG22   | 9:I:52:ILE:H      | 1.52                     | 0.74              |
| 11:K:40:HIS:CE1   | 11:K:63:VAL:CG1   | 2.70                     | 0.74              |
| 11:K:87:LEU:O     | 11:K:90:ALA:HB3   | 1.86                     | 0.74              |
| 3:A:1025:ARG:HH11 | 3:A:1025:ARG:CG   | 2.00                     | 0.74              |
| 4:B:986:GLN:HE21  | 4:B:1016:ALA:HB1  | 1.51                     | 0.74              |
| 5:C:241:ASP:O     | 5:C:245:VAL:HG23  | 1.87                     | 0.74              |
| 3:A:742:ASN:HA    | 3:A:745:GLN:HB2   | 1.70                     | 0.74              |
| 4:B:464:GLY:CA    | 4:B:478:GLY:HA2   | 2.15                     | 0.74              |
| 3:A:4:GLN:HE22    | 4:B:1159:ARG:H    | 1.33                     | 0.74              |
| 3:A:37:PHE:H      | 3:A:52:GLY:HA2    | 1.53                     | 0.74              |
| 3:A:401:GLY:N     | 3:A:435:HIS:HD2   | 1.84                     | 0.74              |
| 3:A:1025:ARG:HA   | 3:A:1030:ARG:NH1  | 2.03                     | 0.74              |
| 3:A:1028:THR:O    | 3:A:1029:ARG:C    | 2.31                     | 0.74              |
| 4:B:128:LEU:HB3   | 4:B:167:ILE:O     | 1.87                     | 0.74              |
| 4:B:174:LEU:HD12  | 4:B:179:CYS:SG    | 2.28                     | 0.74              |
| 4:B:247:GLY:O     | 4:B:248:SER:HB2   | 1.86                     | 0.74              |
| 4:B:1165:ILE:CG2  | 4:B:1166:CYS:N    | 2.48                     | 0.74              |
| 5:C:58:LEU:HD23   | 5:C:58:LEU:N      | 2.03                     | 0.74              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:E:115:ASN:C     | 6:E:116:ILE:HG12 | 2.13                     | 0.74              |
| 9:I:31:THR:HG22   | 9:I:32:CYS:N     | 2.03                     | 0.74              |
| 11:K:27:ALA:HB1   | 11:K:28:PRO:CD   | 2.17                     | 0.74              |
| 3:A:794:PRO:HG2   | 3:A:795:GLU:H    | 1.52                     | 0.74              |
| 1:R:8:G:O2'       | 1:R:9:G:H5'      | 1.87                     | 0.74              |
| 3:A:90:VAL:CG1    | 3:A:297:GLN:CB   | 2.66                     | 0.74              |
| 3:A:635:ARG:HH21  | 3:A:877:HIS:HA   | 1.53                     | 0.74              |
| 3:A:868:TYR:CE1   | 3:A:1064:VAL:CG1 | 2.68                     | 0.74              |
| 4:B:247:GLY:O     | 4:B:248:SER:CB   | 2.36                     | 0.74              |
| 10:J:52:THR:O     | 10:J:53:HIS:C    | 2.31                     | 0.74              |
| 1:R:9:G:C4'       | 4:B:1097:HIS:NE2 | 2.51                     | 0.74              |
| 3:A:569:LYS:HG2   | 3:A:571:LEU:CD1  | 2.17                     | 0.74              |
| 3:A:902:LEU:O     | 3:A:903:ASN:HB2  | 1.88                     | 0.74              |
| 3:A:1363:VAL:HB   | 3:A:1368:MET:HE2 | 1.70                     | 0.74              |
| 5:C:145:CYS:HA    | 10:J:2:ILE:HD11  | 1.67                     | 0.74              |
| 8:H:84:ALA:HB1    | 8:H:87:ARG:HB2   | 1.70                     | 0.74              |
| 8:H:104:PHE:CZ    | 8:H:136:LYS:HA   | 2.23                     | 0.74              |
| 9:I:2:THR:O       | 9:I:3:THR:C      | 2.30                     | 0.74              |
| 1:R:10:A:H8       | 1:R:10:A:OP2     | 1.70                     | 0.73              |
| 3:A:1355:VAL:CG1  | 3:A:1356:ILE:N   | 2.51                     | 0.73              |
| 4:B:291:ILE:CG2   | 4:B:297:ILE:HD13 | 2.18                     | 0.73              |
| 5:C:58:LEU:HD11   | 10:J:2:ILE:HD12  | 1.70                     | 0.73              |
| 3:A:43:GLU:O      | 3:A:46:THR:HB    | 1.87                     | 0.73              |
| 3:A:151:ASP:OD1   | 3:A:163:SER:CA   | 2.36                     | 0.73              |
| 3:A:1237:ILE:HG22 | 3:A:1238:ILE:N   | 2.01                     | 0.73              |
| 4:B:862:GLN:O     | 4:B:914:LYS:NZ   | 2.20                     | 0.73              |
| 5:C:37:MET:SD     | 5:C:232:VAL:HG21 | 2.27                     | 0.73              |
| 12:L:46:VAL:O     | 12:L:47:ARG:HB2  | 1.87                     | 0.73              |
| 1:R:9:G:H4'       | 4:B:1097:HIS:NE2 | 2.04                     | 0.73              |
| 3:A:320:ARG:HH21  | 4:B:471:LYS:CB   | 2.01                     | 0.73              |
| 3:A:523:ILE:HD13  | 3:A:622:VAL:CG2  | 2.18                     | 0.73              |
| 3:A:828:ALA:CB    | 4:B:530:GLY:HA2  | 2.18                     | 0.73              |
| 3:A:1355:VAL:HG12 | 3:A:1356:ILE:H   | 1.51                     | 0.73              |
| 4:B:310:MET:O     | 4:B:313:MET:HB2  | 1.88                     | 0.73              |
| 4:B:784:ASN:ND2   | 4:B:788:ARG:HD2  | 2.02                     | 0.73              |
| 6:E:7:ARG:C       | 6:E:9:ILE:H      | 1.95                     | 0.73              |
| 8:H:108:SER:O     | 8:H:109:LYS:CB   | 2.36                     | 0.73              |
| 3:A:179:LEU:HD13  | 3:A:297:GLN:HG2  | 1.71                     | 0.73              |
| 4:B:843:GLN:HA    | 4:B:846:ILE:HD12 | 1.68                     | 0.73              |
| 9:I:99:LEU:HB2    | 9:I:112:SER:CB   | 2.17                     | 0.73              |
| 11:K:40:HIS:HE1   | 11:K:63:VAL:CG1  | 2.01                     | 0.73              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 12:L:29:TYR:HB3   | 12:L:56:LEU:HD22 | 1.70                     | 0.73              |
| 3:A:92:HIS:HB2    | 3:A:236:LEU:CD1  | 2.19                     | 0.73              |
| 3:A:599:SER:O     | 3:A:601:LYS:N    | 2.22                     | 0.73              |
| 3:A:1377:THR:C    | 3:A:1379:GLY:H   | 1.95                     | 0.73              |
| 4:B:451:LYS:O     | 4:B:452:THR:C    | 2.31                     | 0.73              |
| 6:E:194:GLU:O     | 6:E:213:ILE:HD12 | 1.88                     | 0.73              |
| 3:A:541:ILE:HG22  | 3:A:546:VAL:HG22 | 1.70                     | 0.73              |
| 5:C:69:LEU:O      | 10:J:6:ARG:HD2   | 1.87                     | 0.73              |
| 5:C:120:ILE:HD11  | 5:C:130:GLY:O    | 1.88                     | 0.73              |
| 8:H:42:ILE:O      | 8:H:44:VAL:HG23  | 1.89                     | 0.73              |
| 10:J:45:CYS:O     | 10:J:48:ARG:HG3  | 1.88                     | 0.73              |
| 11:K:58:PHE:HE2   | 11:K:74:ARG:NE   | 1.82                     | 0.73              |
| 9:I:96:SER:HB2    | 9:I:98:VAL:HG23  | 1.69                     | 0.73              |
| 3:A:901:LEU:O     | 3:A:902:LEU:C    | 2.31                     | 0.73              |
| 3:A:1067:LEU:HD21 | 3:A:1367:HIS:CE1 | 2.15                     | 0.73              |
| 4:B:369:GLY:O     | 4:B:370:PHE:HD1  | 1.71                     | 0.73              |
| 4:B:1171:VAL:HG12 | 4:B:1172:ILE:N   | 1.95                     | 0.73              |
| 6:E:162:ARG:NH2   | 6:E:166:LYS:NZ   | 2.36                     | 0.73              |
| 3:A:421:ALA:HA    | 3:A:424:ILE:HD11 | 1.70                     | 0.73              |
| 3:A:475:THR:HG22  | 3:A:476:SER:H    | 1.53                     | 0.73              |
| 3:A:849:MET:HE1   | 3:A:1061:GLY:HA2 | 1.71                     | 0.73              |
| 4:B:63:ILE:HA     | 4:B:421:PHE:CE2  | 2.24                     | 0.73              |
| 4:B:287:ARG:CG    | 4:B:292:ILE:HD13 | 2.16                     | 0.73              |
| 4:B:698:GLU:O     | 4:B:701:ILE:CD1  | 2.37                     | 0.73              |
| 4:B:1152:MET:O    | 4:B:1157:ALA:HB2 | 1.88                     | 0.73              |
| 6:E:23:VAL:HG13   | 6:E:28:TYR:CD1   | 2.24                     | 0.73              |
| 6:E:179:GLN:HB2   | 6:E:182:ASP:HB2  | 1.68                     | 0.73              |
| 8:H:11:GLN:N      | 8:H:29:ALA:O     | 2.21                     | 0.73              |
| 8:H:142:LEU:C     | 8:H:143:LEU:HG   | 2.13                     | 0.73              |
| 3:A:170:THR:HG22  | 3:A:171:GLN:H    | 1.53                     | 0.73              |
| 3:A:929:LEU:HD21  | 3:A:983:ILE:HG23 | 1.70                     | 0.73              |
| 3:A:1422:ARG:NH2  | 4:B:1220:ARG:HD3 | 1.99                     | 0.73              |
| 3:A:1428:VAL:HG13 | 4:B:1151:LEU:CD2 | 2.19                     | 0.73              |
| 4:B:195:CYS:HB3   | 4:B:782:LEU:HD22 | 1.69                     | 0.73              |
| 4:B:882:THR:HG22  | 4:B:883:LEU:N    | 2.02                     | 0.73              |
| 4:B:1165:ILE:HG22 | 4:B:1166:CYS:H   | 1.50                     | 0.73              |
| 3:A:35:ILE:HG22   | 3:A:270:LEU:HD13 | 1.71                     | 0.72              |
| 3:A:1161:THR:HG22 | 3:A:1162:VAL:H   | 1.54                     | 0.72              |
| 4:B:227:LYS:N     | 4:B:395:GLN:OE1  | 2.21                     | 0.72              |
| 3:A:20:GLY:C      | 3:A:21:LEU:HD23  | 2.14                     | 0.72              |
| 3:A:144:THR:O     | 3:A:146:MET:HE2  | 1.88                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1154:TYR:CE2  | 3:A:1156:PRO:HB3  | 2.23                     | 0.72              |
| 3:A:553:VAL:HG13  | 3:A:648:ASN:HB3   | 1.70                     | 0.72              |
| 3:A:605:MET:HE1   | 3:A:615:GLY:O     | 1.89                     | 0.72              |
| 3:A:1067:LEU:CD2  | 3:A:1367:HIS:HE1  | 2.00                     | 0.72              |
| 3:A:1169:ILE:HD12 | 3:A:1169:ILE:N    | 2.00                     | 0.72              |
| 4:B:783:THR:HG22  | 10:J:63:TYR:HE1   | 1.54                     | 0.72              |
| 4:B:1203:LEU:CD1  | 4:B:1207:LEU:HG   | 2.19                     | 0.72              |
| 3:A:675:THR:O     | 3:A:679:ILE:HG13  | 1.90                     | 0.72              |
| 3:A:873:MET:HG2   | 3:A:957:PRO:CG    | 2.19                     | 0.72              |
| 3:A:1364:ASN:HD21 | 3:A:1366:ARG:HH11 | 1.37                     | 0.72              |
| 4:B:55:VAL:HG12   | 4:B:56:ASP:N      | 2.02                     | 0.72              |
| 4:B:751:VAL:HG12  | 4:B:752:ALA:H     | 1.54                     | 0.72              |
| 8:H:93:TYR:CD1    | 8:H:143:LEU:CB    | 2.72                     | 0.72              |
| 9:I:33:SER:O      | 9:I:35:VAL:HG23   | 1.89                     | 0.72              |
| 3:A:1156:PRO:O    | 3:A:1158:PRO:HD3  | 1.90                     | 0.72              |
| 3:A:1397:LEU:O    | 3:A:1400:CYS:HB2  | 1.90                     | 0.72              |
| 4:B:708:GLU:HG3   | 4:B:709:ASP:N     | 2.04                     | 0.72              |
| 4:B:817:LEU:N     | 4:B:818:PRO:HD3   | 2.02                     | 0.72              |
| 4:B:868:MET:O     | 4:B:869:SER:OG    | 2.04                     | 0.72              |
| 9:I:103:CYS:O     | 9:I:104:LEU:HD23  | 1.89                     | 0.72              |
| 3:A:225:ASN:O     | 3:A:226:GLU:C     | 2.32                     | 0.72              |
| 3:A:444:PHE:CE2   | 3:A:470:LEU:HD23  | 2.24                     | 0.72              |
| 3:A:1154:TYR:CE1  | 9:I:18:GLU:HG2    | 2.25                     | 0.72              |
| 3:A:1209:MET:SD   | 3:A:1236:LEU:HD22 | 2.29                     | 0.72              |
| 4:B:123:THR:HG22  | 4:B:125:SER:HB3   | 1.70                     | 0.72              |
| 4:B:129:PHE:CE2   | 4:B:166:PHE:HB3   | 2.24                     | 0.72              |
| 6:E:124:VAL:H     | 6:E:125:PRO:HD2   | 1.54                     | 0.72              |
| 6:E:178:ILE:HG12  | 6:E:179:GLN:N     | 2.03                     | 0.72              |
| 9:I:19:ASP:CB     | 9:I:24:ARG:HG3    | 2.20                     | 0.72              |
| 3:A:1018:PHE:O    | 3:A:1021:LEU:HB3  | 1.88                     | 0.72              |
| 3:A:1434:ALA:O    | 3:A:1436:ILE:N    | 2.21                     | 0.72              |
| 3:A:378:GLU:OE1   | 3:A:434:ARG:NH1   | 2.22                     | 0.72              |
| 3:A:805:LEU:C     | 3:A:805:LEU:CD1   | 2.60                     | 0.72              |
| 4:B:98:THR:O      | 4:B:126:SER:CB    | 2.38                     | 0.72              |
| 4:B:830:TYR:HE1   | 4:B:1000:PRO:HB3  | 1.53                     | 0.72              |
| 5:C:57:VAL:HB     | 5:C:58:LEU:HD23   | 1.70                     | 0.72              |
| 3:A:185:TRP:HH2   | 3:A:200:ARG:HD3   | 1.55                     | 0.72              |
| 3:A:1394:THR:HG21 | 3:A:1398:MET:HE3  | 1.71                     | 0.72              |
| 4:B:597:MET:O     | 4:B:598:GLU:C     | 2.30                     | 0.72              |
| 4:B:638:PHE:CD1   | 4:B:743:ILE:HD13  | 2.24                     | 0.72              |
| 6:E:37:LEU:O      | 6:E:37:LEU:HG     | 1.88                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:41:PRO:O      | 9:I:43:VAL:HG23   | 1.89                     | 0.72              |
| 10:J:52:THR:O     | 10:J:54:VAL:HG23  | 1.90                     | 0.72              |
| 3:A:1193:LEU:HD12 | 3:A:1193:LEU:C    | 2.15                     | 0.72              |
| 4:B:112:LEU:O     | 4:B:180:TYR:HE1   | 1.73                     | 0.72              |
| 4:B:1065:GLN:HE21 | 4:B:1067:ARG:H    | 1.38                     | 0.72              |
| 6:E:46:TYR:CD2    | 6:E:58:MET:HE3    | 2.25                     | 0.72              |
| 10:J:2:ILE:C      | 10:J:53:HIS:NE2   | 2.47                     | 0.72              |
| 10:J:21:TYR:HB2   | 10:J:39:LEU:HD11  | 1.72                     | 0.72              |
| 3:A:351:THR:HG23  | 4:B:1103:ILE:CD1  | 2.14                     | 0.71              |
| 4:B:36:ALA:C      | 4:B:37:PHE:O      | 2.21                     | 0.71              |
| 4:B:1196:ILE:HB   | 4:B:1197:PRO:HD2  | 1.72                     | 0.71              |
| 3:A:90:VAL:CG1    | 3:A:297:GLN:HA    | 2.10                     | 0.71              |
| 3:A:401:GLY:C     | 3:A:435:HIS:CD2   | 2.68                     | 0.71              |
| 3:A:1424:VAL:HG22 | 3:A:1436:ILE:HD11 | 1.71                     | 0.71              |
| 4:B:356:LEU:N     | 4:B:356:LEU:HD23  | 2.04                     | 0.71              |
| 4:B:426:LYS:O     | 4:B:430:ARG:HD2   | 1.91                     | 0.71              |
| 4:B:796:LEU:HB3   | 4:B:799:PRO:CD    | 2.19                     | 0.71              |
| 3:A:253:ASN:CG    | 3:A:254:GLU:N     | 2.47                     | 0.71              |
| 4:B:63:ILE:CD1    | 4:B:95:ILE:HD12   | 2.21                     | 0.71              |
| 4:B:291:ILE:HG22  | 4:B:297:ILE:HD13  | 1.73                     | 0.71              |
| 4:B:957:ASN:O     | 4:B:958:GLN:C     | 2.32                     | 0.71              |
| 9:I:15:TYR:O      | 9:I:27:PHE:HD2    | 1.73                     | 0.71              |
| 10:J:3:VAL:HG21   | 10:J:18:TRP:HB2   | 1.72                     | 0.71              |
| 11:K:61:TYR:CD1   | 11:K:61:TYR:C     | 2.68                     | 0.71              |
| 4:B:527:THR:OG1   | 4:B:528:PRO:HD2   | 1.90                     | 0.71              |
| 3:A:403:LYS:HB2   | 3:A:404:TYR:CD1   | 2.26                     | 0.71              |
| 3:A:417:TYR:O     | 3:A:418:SER:HB3   | 1.90                     | 0.71              |
| 3:A:1194:ARG:NH2  | 3:A:1237:ILE:CD1  | 2.54                     | 0.71              |
| 3:A:1436:ILE:O    | 3:A:1439:GLY:N    | 2.24                     | 0.71              |
| 4:B:1006:ILE:HD11 | 10:J:45:CYS:SG    | 2.30                     | 0.71              |
| 4:B:1060:ARG:C    | 4:B:1062:HIS:H    | 1.99                     | 0.71              |
| 3:A:244:PRO:O     | 3:A:247:ARG:N     | 2.23                     | 0.71              |
| 3:A:785:PRO:HG2   | 4:B:703:ILE:HD12  | 1.72                     | 0.71              |
| 3:A:1116:LEU:N    | 3:A:1308:THR:HB   | 2.03                     | 0.71              |
| 3:A:1227:ILE:HG22 | 3:A:1228:TRP:H    | 1.53                     | 0.71              |
| 11:K:102:LYS:O    | 11:K:106:GLU:HG3  | 1.90                     | 0.71              |
| 3:A:475:THR:HG22  | 3:A:476:SER:N     | 2.05                     | 0.71              |
| 3:A:984:LYS:O     | 3:A:988:LEU:HB2   | 1.89                     | 0.71              |
| 4:B:287:ARG:NH1   | 4:B:324:ILE:O     | 2.24                     | 0.71              |
| 4:B:952:VAL:HG22  | 4:B:966:VAL:HG13  | 1.73                     | 0.71              |
| 3:A:68:GLN:O      | 3:A:70:CYS:N      | 2.24                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:265:LYS:HE2   | 3:A:323:LYS:CE    | 2.18                     | 0.71              |
| 3:A:869:GLY:O     | 3:A:870:GLU:HB2   | 1.88                     | 0.71              |
| 4:B:37:PHE:O      | 4:B:39:ARG:N      | 2.23                     | 0.71              |
| 4:B:34:ILE:HD11   | 4:B:743:ILE:HG22  | 1.72                     | 0.71              |
| 4:B:63:ILE:HD13   | 4:B:95:ILE:HD12   | 1.71                     | 0.71              |
| 4:B:1155:SER:OG   | 4:B:1156:ASP:N    | 2.21                     | 0.71              |
| 3:A:970:THR:O     | 3:A:970:THR:HG22  | 1.89                     | 0.71              |
| 3:A:1007:ILE:O    | 3:A:1010:ALA:N    | 2.22                     | 0.71              |
| 4:B:352:ALA:C     | 4:B:354:ASP:H     | 1.97                     | 0.71              |
| 4:B:788:ARG:HH11  | 4:B:788:ARG:HB2   | 1.56                     | 0.71              |
| 11:K:53:ASP:O     | 11:K:56:VAL:CG2   | 2.35                     | 0.71              |
| 2:T:4:DA:H2'      | 2:T:5:DT:H72      | 1.73                     | 0.70              |
| 3:A:255:SER:HB3   | 4:B:918:ILE:HG23  | 1.73                     | 0.70              |
| 3:A:530:GLY:O     | 3:A:532:ARG:N     | 2.22                     | 0.70              |
| 5:C:143:LEU:C     | 5:C:143:LEU:HD12  | 2.13                     | 0.70              |
| 6:E:39:LEU:O      | 6:E:41:ASP:N      | 2.24                     | 0.70              |
| 10:J:7:CYS:CA     | 10:J:49:MET:HE3   | 2.21                     | 0.70              |
| 3:A:614:PHE:CD1   | 3:A:614:PHE:C     | 2.69                     | 0.70              |
| 3:A:736:ASN:O     | 3:A:737:LEU:C     | 2.34                     | 0.70              |
| 3:A:1227:ILE:HG22 | 3:A:1228:TRP:N    | 2.06                     | 0.70              |
| 7:F:83:PRO:HG2    | 7:F:84:TYR:HD1    | 1.55                     | 0.70              |
| 11:K:33:ILE:HD13  | 11:K:87:LEU:HD22  | 1.72                     | 0.70              |
| 11:K:91:CYS:O     | 11:K:94:ILE:HB    | 1.91                     | 0.70              |
| 3:A:92:HIS:O      | 3:A:95:PHE:HB2    | 1.91                     | 0.70              |
| 3:A:106:VAL:HG12  | 3:A:107:CYS:N     | 2.05                     | 0.70              |
| 3:A:242:PRO:O     | 3:A:247:ARG:NH2   | 2.20                     | 0.70              |
| 3:A:423:ASP:C     | 3:A:424:ILE:HG13  | 2.14                     | 0.70              |
| 3:A:1161:THR:CG2  | 3:A:1162:VAL:H    | 2.04                     | 0.70              |
| 4:B:179:CYS:SG    | 4:B:181:LEU:HD12  | 2.30                     | 0.70              |
| 4:B:857:ARG:NH2   | 4:B:942:ARG:NH1   | 2.38                     | 0.70              |
| 4:B:1060:ARG:C    | 4:B:1062:HIS:N    | 2.48                     | 0.70              |
| 4:B:1060:ARG:O    | 4:B:1063:GLY:N    | 2.24                     | 0.70              |
| 8:H:44:VAL:O      | 8:H:44:VAL:HG12   | 1.92                     | 0.70              |
| 3:A:14:VAL:N      | 3:A:1432:GLN:HE22 | 1.85                     | 0.70              |
| 3:A:107:CYS:N     | 3:A:114:LEU:HD21  | 2.06                     | 0.70              |
| 3:A:302:THR:OG1   | 3:A:313:GLN:NE2   | 2.24                     | 0.70              |
| 3:A:322:VAL:HB    | 3:A:323:LYS:CD    | 2.20                     | 0.70              |
| 3:A:381:THR:HG22  | 3:A:383:TYR:HB2   | 1.72                     | 0.70              |
| 6:E:98:ILE:O      | 6:E:99:HIS:C      | 2.31                     | 0.70              |
| 3:A:39:GLU:O      | 3:A:53:LEU:HB2    | 1.91                     | 0.70              |
| 3:A:1041:ALA:O    | 3:A:1044:TRP:HB3  | 1.91                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1436:ILE:O    | 3:A:1437:GLY:C    | 2.34                     | 0.70              |
| 4:B:44:VAL:O      | 4:B:45:SER:C      | 2.33                     | 0.70              |
| 4:B:1106:ARG:NH2  | 4:B:1109:GLY:C    | 2.48                     | 0.70              |
| 5:C:237:SER:O     | 5:C:238:ILE:HG13  | 1.89                     | 0.70              |
| 7:F:98:ALA:CA     | 7:F:101:ILE:HD12  | 2.21                     | 0.70              |
| 3:A:40:THR:O      | 3:A:41:MET:HG3    | 1.90                     | 0.70              |
| 3:A:70:CYS:C      | 3:A:71:GLN:HG3    | 2.15                     | 0.70              |
| 3:A:875:ALA:HA    | 3:A:878:ILE:HD12  | 1.71                     | 0.70              |
| 3:A:971:PHE:HB2   | 3:A:973:ILE:HD13  | 1.72                     | 0.70              |
| 3:A:1428:VAL:HG13 | 4:B:1151:LEU:HD23 | 1.72                     | 0.70              |
| 4:B:115:GLN:O     | 4:B:119:LEU:HD12  | 1.91                     | 0.70              |
| 3:A:834:THR:HG21  | 3:A:1077:THR:CB   | 2.21                     | 0.70              |
| 3:A:901:LEU:HD23  | 3:A:907:THR:HG21  | 1.71                     | 0.70              |
| 3:A:1285:MET:HG2  | 3:A:1307:GLU:OE2  | 1.91                     | 0.70              |
| 4:B:274:PRO:O     | 4:B:276:ILE:HG13  | 1.92                     | 0.70              |
| 4:B:1060:ARG:O    | 4:B:1062:HIS:N    | 2.25                     | 0.70              |
| 6:E:168:TYR:C     | 6:E:169:ARG:CG    | 2.63                     | 0.70              |
| 3:A:120:GLU:HG3   | 3:A:123:ARG:HD3   | 1.74                     | 0.70              |
| 3:A:179:LEU:HD12  | 3:A:297:GLN:HG2   | 1.73                     | 0.70              |
| 3:A:1143:LEU:O    | 3:A:1146:VAL:HG23 | 1.91                     | 0.70              |
| 3:A:1213:GLY:HA2  | 3:A:1216:ILE:HD12 | 1.74                     | 0.70              |
| 4:B:1084:GLN:HG2  | 5:C:201:TRP:CH2   | 2.27                     | 0.70              |
| 5:C:11:ARG:HE     | 5:C:21:ILE:HD11   | 1.56                     | 0.70              |
| 2:T:6:DC:C2'      | 2:T:7:DC:H5'      | 2.18                     | 0.70              |
| 3:A:115:LEU:HD12  | 3:A:122:MET:HE2   | 1.74                     | 0.70              |
| 3:A:247:ARG:CG    | 3:A:247:ARG:O     | 2.39                     | 0.70              |
| 3:A:1006:ILE:HD11 | 6:E:163:GLU:OE2   | 1.92                     | 0.70              |
| 3:A:1017:LEU:HB2  | 6:E:205:SER:HA    | 1.74                     | 0.70              |
| 6:E:113:GLN:O     | 6:E:114:ASN:ND2   | 2.25                     | 0.70              |
| 7:F:72:LYS:O      | 7:F:73:ALA:HB2    | 1.90                     | 0.70              |
| 8:H:89:LEU:HB2    | 8:H:91:ASP:CG     | 2.17                     | 0.70              |
| 3:A:261:ASP:HB3   | 3:A:323:LYS:CG    | 2.22                     | 0.70              |
| 3:A:322:VAL:HB    | 3:A:323:LYS:CG    | 2.21                     | 0.70              |
| 3:A:325:ILE:O     | 3:A:329:LEU:HG    | 1.92                     | 0.70              |
| 3:A:599:SER:HB3   | 3:A:603:ASN:H     | 1.57                     | 0.70              |
| 3:A:607:ILE:HG12  | 3:A:612:ILE:HA    | 1.72                     | 0.70              |
| 3:A:894:GLU:C     | 3:A:896:ARG:N     | 2.43                     | 0.70              |
| 3:A:1152:ILE:O    | 3:A:1152:ILE:HG22 | 1.90                     | 0.70              |
| 4:B:471:LYS:O     | 4:B:472:ALA:C     | 2.35                     | 0.70              |
| 4:B:992:ILE:CD1   | 11:K:67:PHE:HE2   | 2.04                     | 0.70              |
| 4:B:1203:LEU:C    | 4:B:1203:LEU:HD12 | 2.17                     | 0.70              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:E:29:PHE:O     | 6:E:30:ILE:HG13   | 1.91                     | 0.70              |
| 3:A:472:LEU:HD11 | 4:B:835:GLN:NE2   | 2.06                     | 0.69              |
| 3:A:590:ARG:NH2  | 3:A:620:LYS:O     | 2.25                     | 0.69              |
| 4:B:634:TYR:CE1  | 4:B:692:TYR:HD1   | 2.09                     | 0.69              |
| 4:B:642:ASP:O    | 4:B:644:GLU:N     | 2.25                     | 0.69              |
| 4:B:739:THR:OG1  | 4:B:740:HIS:CE1   | 2.44                     | 0.69              |
| 9:I:119:THR:C    | 9:I:120:GLN:HG2   | 2.17                     | 0.69              |
| 12:L:29:TYR:O    | 12:L:30:ILE:HG13  | 1.91                     | 0.69              |
| 3:A:1200:ALA:O   | 3:A:1202:MET:N    | 2.25                     | 0.69              |
| 4:B:501:PRO:O    | 4:B:502:ILE:HB    | 1.92                     | 0.69              |
| 6:E:198:ILE:CD1  | 6:E:212:ARG:HG3   | 2.22                     | 0.69              |
| 8:H:3:ASN:CG     | 8:H:4:THR:N       | 2.50                     | 0.69              |
| 8:H:131:ASN:C    | 8:H:133:ASN:H     | 2.00                     | 0.69              |
| 11:K:51:LEU:HD13 | 11:K:59:ALA:HB3   | 1.73                     | 0.69              |
| 3:A:818:MET:O    | 3:A:819:GLY:O     | 2.10                     | 0.69              |
| 4:B:428:ILE:C    | 4:B:430:ARG:H     | 1.99                     | 0.69              |
| 4:B:840:ILE:HG12 | 4:B:992:ILE:HG22  | 1.74                     | 0.69              |
| 4:B:893:LEU:HD21 | 4:B:913:GLY:N     | 2.07                     | 0.69              |
| 6:E:131:THR:CG2  | 6:E:132:ILE:H     | 1.90                     | 0.69              |
| 9:I:119:THR:C    | 9:I:120:GLN:CG    | 2.64                     | 0.69              |
| 3:A:302:THR:CG2  | 3:A:313:GLN:NE2   | 2.54                     | 0.69              |
| 3:A:321:PRO:O    | 3:A:322:VAL:CB    | 2.40                     | 0.69              |
| 3:A:450:LEU:H    | 3:A:450:LEU:HD12  | 1.58                     | 0.69              |
| 4:B:30:SER:O     | 4:B:34:ILE:HD13   | 1.91                     | 0.69              |
| 4:B:313:MET:HG3  | 4:B:390:LEU:HD21  | 1.74                     | 0.69              |
| 4:B:373:ARG:HA   | 4:B:566:LEU:HD23  | 1.74                     | 0.69              |
| 4:B:882:THR:HG21 | 4:B:935:ARG:CA    | 2.17                     | 0.69              |
| 4:B:1103:ILE:N   | 4:B:1103:ILE:CD1  | 2.42                     | 0.69              |
| 5:C:110:THR:O    | 5:C:110:THR:HG22  | 1.91                     | 0.69              |
| 3:A:901:LEU:HB2  | 3:A:926:GLN:HG2   | 1.75                     | 0.69              |
| 3:A:1126:ALA:O   | 3:A:1128:GLN:N    | 2.25                     | 0.69              |
| 4:B:899:ILE:HD11 | 4:B:911:ILE:HG23  | 1.74                     | 0.69              |
| 6:E:35:VAL:O     | 6:E:37:LEU:N      | 2.25                     | 0.69              |
| 3:A:341:MET:HE1  | 3:A:843:LYS:NZ    | 2.08                     | 0.69              |
| 3:A:380:VAL:CG2  | 3:A:430:TRP:N     | 2.50                     | 0.69              |
| 3:A:964:ILE:HD12 | 3:A:1037:LEU:HD21 | 1.75                     | 0.69              |
| 3:A:1097:GLY:C   | 3:A:1099:PRO:HD2  | 2.18                     | 0.69              |
| 4:B:65:GLU:C     | 4:B:67:SER:H      | 1.99                     | 0.69              |
| 4:B:475:SER:C    | 4:B:477:ALA:H     | 2.01                     | 0.69              |
| 4:B:1104:HIS:CG  | 4:B:1122:ARG:HB2  | 2.28                     | 0.69              |
| 5:C:148:ARG:NH1  | 10:J:64:ASN:HA    | 2.06                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:E:60:PHE:CE2    | 6:E:80:VAL:HG21   | 2.27                     | 0.69              |
| 3:A:1113:THR:O    | 3:A:1113:THR:HG22 | 1.92                     | 0.69              |
| 3:A:1148:ILE:HD11 | 3:A:1198:ASP:HB2  | 1.75                     | 0.69              |
| 4:B:46:GLN:HE21   | 4:B:496:ARG:HG2   | 1.57                     | 0.69              |
| 4:B:175:ARG:HH11  | 4:B:175:ARG:CG    | 2.05                     | 0.69              |
| 4:B:284:ILE:O     | 4:B:287:ARG:N     | 2.26                     | 0.69              |
| 4:B:446:LEU:O     | 4:B:447:ALA:HB3   | 1.92                     | 0.69              |
| 10:J:45:CYS:SG    | 10:J:46:CYS:N     | 2.65                     | 0.69              |
| 3:A:68:GLN:C      | 3:A:70:CYS:N      | 2.50                     | 0.69              |
| 3:A:129:LYS:O     | 3:A:130:ASP:HB2   | 1.91                     | 0.69              |
| 3:A:445:ASN:CB    | 3:A:455:MET:HE2   | 2.23                     | 0.69              |
| 3:A:451:HIS:CE1   | 3:A:1074:GLU:HG3  | 2.28                     | 0.69              |
| 3:A:582:ILE:HG22  | 3:A:610:GLY:HA2   | 1.74                     | 0.69              |
| 3:A:622:VAL:HG22  | 3:A:622:VAL:O     | 1.93                     | 0.69              |
| 3:A:1161:THR:CG2  | 3:A:1162:VAL:N    | 2.56                     | 0.69              |
| 3:A:1169:ILE:H    | 3:A:1169:ILE:CD1  | 1.90                     | 0.69              |
| 4:B:98:THR:O      | 4:B:126:SER:HB2   | 1.92                     | 0.69              |
| 4:B:365:THR:HG23  | 4:B:366:GLN:N     | 2.06                     | 0.69              |
| 4:B:420:LEU:HD21  | 4:B:468:GLU:OE2   | 1.92                     | 0.69              |
| 4:B:429:PHE:O     | 4:B:433:GLN:OE1   | 2.11                     | 0.69              |
| 4:B:778:MET:HE3   | 4:B:853:SER:CB    | 2.23                     | 0.69              |
| 4:B:800:GLN:CG    | 10:J:52:THR:HG21  | 2.23                     | 0.69              |
| 10:J:9:SER:HG     | 10:J:45:CYS:HB2   | 1.57                     | 0.69              |
| 3:A:98:LYS:O      | 3:A:100:LYS:N     | 2.25                     | 0.69              |
| 3:A:261:ASP:CB    | 3:A:323:LYS:CD    | 2.63                     | 0.69              |
| 3:A:751:SER:HB2   | 4:B:1015:HIS:HE1  | 1.57                     | 0.69              |
| 3:A:946:VAL:HG22  | 6:E:201:LYS:HB3   | 1.75                     | 0.69              |
| 3:A:1116:LEU:HD21 | 3:A:1312:ASN:H    | 1.58                     | 0.69              |
| 4:B:993:THR:O     | 4:B:994:TYR:HD2   | 1.76                     | 0.69              |
| 4:B:1084:GLN:NE2  | 5:C:191:TYR:CA    | 2.55                     | 0.69              |
| 3:A:115:LEU:HD11  | 3:A:142:CYS:HB3   | 1.74                     | 0.69              |
| 4:B:236:HIS:CD2   | 4:B:389:ALA:HB2   | 2.26                     | 0.69              |
| 4:B:1184:GLY:O    | 4:B:1185:CYS:C    | 2.36                     | 0.69              |
| 5:C:46:ILE:HA     | 5:C:159:ALA:HA    | 1.75                     | 0.69              |
| 8:H:113:ALA:CA    | 8:H:125:LEU:O     | 2.41                     | 0.69              |
| 10:J:59:LYS:O     | 10:J:62:ARG:HB2   | 1.93                     | 0.69              |
| 3:A:151:ASP:OD1   | 3:A:162:VAL:O     | 2.10                     | 0.68              |
| 3:A:321:PRO:HD2   | 3:A:322:VAL:CA    | 2.17                     | 0.68              |
| 3:A:456:MET:HG3   | 3:A:478:TYR:OH    | 1.94                     | 0.68              |
| 3:A:874:ASP:OD1   | 3:A:876:ALA:N     | 2.27                     | 0.68              |
| 3:A:886:ILE:CD1   | 3:A:943:LEU:HB2   | 2.22                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:93:GLY:O      | 4:B:94:LYS:C      | 2.36                     | 0.68              |
| 4:B:121:ASN:N     | 4:B:121:ASN:HD22  | 1.90                     | 0.68              |
| 5:C:173:ALA:O     | 5:C:174:ALA:CB    | 2.40                     | 0.68              |
| 7:F:120:ILE:O     | 7:F:123:LYS:N     | 2.25                     | 0.68              |
| 9:I:34:TYR:CD2    | 9:I:35:VAL:N      | 2.62                     | 0.68              |
| 9:I:55:THR:HG23   | 9:I:58:VAL:CG2    | 2.23                     | 0.68              |
| 3:A:893:PHE:C     | 3:A:893:PHE:CD2   | 2.70                     | 0.68              |
| 3:A:1336:MET:HE3  | 3:A:1381:LEU:HG   | 1.76                     | 0.68              |
| 4:B:114:PRO:CG    | 4:B:181:LEU:HD11  | 2.24                     | 0.68              |
| 3:A:26:GLU:HA     | 3:A:29:ALA:HB3    | 1.74                     | 0.68              |
| 3:A:471:ASN:O     | 3:A:474:VAL:HG12  | 1.94                     | 0.68              |
| 3:A:532:ARG:HG2   | 3:A:533:LYS:N     | 2.07                     | 0.68              |
| 3:A:804:TYR:HE1   | 4:B:1021:MET:HE3  | 1.58                     | 0.68              |
| 4:B:751:VAL:CG1   | 4:B:752:ALA:N     | 2.56                     | 0.68              |
| 4:B:1147:LEU:HD22 | 4:B:1151:LEU:HD22 | 1.76                     | 0.68              |
| 6:E:102:GLU:C     | 6:E:104:ASN:H     | 2.02                     | 0.68              |
| 3:A:49:LYS:O      | 3:A:50:ILE:CG1    | 2.38                     | 0.68              |
| 3:A:262:LEU:HG    | 3:A:328:ARG:NH2   | 2.09                     | 0.68              |
| 3:A:535:THR:CG2   | 3:A:616:VAL:HA    | 2.23                     | 0.68              |
| 4:B:205:ILE:HG22  | 4:B:206:ASN:ND2   | 2.09                     | 0.68              |
| 4:B:355:ILE:C     | 4:B:356:LEU:HD23  | 2.18                     | 0.68              |
| 5:C:92:CYS:SG     | 5:C:94:LYS:HB2    | 2.33                     | 0.68              |
| 5:C:163:ILE:HD12  | 5:C:166:GLU:HB2   | 1.76                     | 0.68              |
| 6:E:156:LEU:CD2   | 6:E:197:LYS:HB2   | 2.23                     | 0.68              |
| 3:A:123:ARG:O     | 3:A:124:GLN:C     | 2.36                     | 0.68              |
| 3:A:401:GLY:H     | 3:A:435:HIS:CD2   | 2.10                     | 0.68              |
| 3:A:765:VAL:HG21  | 3:A:800:VAL:HG11  | 1.74                     | 0.68              |
| 3:A:783:THR:CG2   | 3:A:815:PHE:CE2   | 2.77                     | 0.68              |
| 3:A:809:THR:HB    | 3:A:810:PRO:HD2   | 1.74                     | 0.68              |
| 3:A:852:TYR:CD2   | 3:A:1060:PRO:CB   | 2.77                     | 0.68              |
| 3:A:873:MET:HG2   | 3:A:957:PRO:HG3   | 1.74                     | 0.68              |
| 3:A:1041:ALA:O    | 3:A:1044:TRP:N    | 2.23                     | 0.68              |
| 3:A:1254:ALA:O    | 3:A:1255:GLU:HB2  | 1.91                     | 0.68              |
| 4:B:350:GLN:O     | 4:B:352:ALA:N     | 2.27                     | 0.68              |
| 5:C:141:GLY:O     | 5:C:142:VAL:HB    | 1.91                     | 0.68              |
| 7:F:120:ILE:HG22  | 7:F:121:ALA:N     | 2.07                     | 0.68              |
| 9:I:75:CYS:SG     | 9:I:78:CYS:HB3    | 2.34                     | 0.68              |
| 11:K:7:PHE:C      | 11:K:9:LEU:H      | 2.01                     | 0.68              |
| 4:B:781:PHE:O     | 4:B:782:LEU:HG    | 1.93                     | 0.68              |
| 4:B:847:ASP:HB3   | 5:C:167:HIS:CD2   | 2.28                     | 0.68              |
| 4:B:994:TYR:HB2   | 4:B:999:MET:CE    | 2.23                     | 0.68              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:C:39:ALA:HA     | 5:C:164:ALA:CB   | 2.24                     | 0.68              |
| 3:A:444:PHE:HE2   | 3:A:470:LEU:HD23 | 1.56                     | 0.68              |
| 3:A:497:THR:HG23  | 4:B:1146:PHE:HD1 | 1.59                     | 0.68              |
| 3:A:777:PHE:HD2   | 3:A:782:ARG:C    | 2.02                     | 0.68              |
| 3:A:858:ASN:ND2   | 3:A:860:LEU:H    | 1.92                     | 0.68              |
| 4:B:114:PRO:HG3   | 4:B:181:LEU:CD1  | 2.24                     | 0.68              |
| 4:B:363:HIS:O     | 4:B:364:ILE:CB   | 2.42                     | 0.68              |
| 4:B:640:VAL:O     | 4:B:641:GLU:C    | 2.37                     | 0.68              |
| 4:B:899:ILE:CD1   | 4:B:911:ILE:HG23 | 2.24                     | 0.68              |
| 12:L:58:LYS:O     | 12:L:59:ALA:HB3  | 1.94                     | 0.68              |
| 3:A:179:LEU:HD13  | 3:A:297:GLN:CG   | 2.24                     | 0.68              |
| 3:A:219:PHE:O     | 3:A:222:LEU:O    | 2.12                     | 0.68              |
| 3:A:504:LEU:HD11  | 7:F:91:ALA:HB1   | 1.76                     | 0.68              |
| 3:A:575:LYS:HB3   | 3:A:612:ILE:HG12 | 1.76                     | 0.68              |
| 3:A:780:VAL:O     | 3:A:782:ARG:HG2  | 1.94                     | 0.68              |
| 3:A:1095:THR:OG1  | 3:A:1113:THR:HB  | 1.94                     | 0.68              |
| 3:A:1121:GLU:O    | 3:A:1124:HIS:O   | 2.12                     | 0.68              |
| 3:A:1308:THR:HG22 | 3:A:1309:ASP:N   | 2.07                     | 0.68              |
| 4:B:256:VAL:HG11  | 4:B:382:ILE:HD13 | 1.73                     | 0.68              |
| 4:B:541:LEU:HB2   | 4:B:747:MET:HE3  | 1.73                     | 0.68              |
| 4:B:758:PHE:CE2   | 4:B:1044:ALA:HA  | 2.29                     | 0.68              |
| 4:B:815:ARG:HG3   | 4:B:815:ARG:NH1  | 2.08                     | 0.68              |
| 11:K:32:VAL:HG23  | 11:K:74:ARG:CG   | 2.23                     | 0.68              |
| 3:A:10:PRO:O      | 4:B:1193:GLN:HB3 | 1.94                     | 0.68              |
| 3:A:40:THR:HG22   | 3:A:41:MET:CE    | 2.23                     | 0.68              |
| 3:A:710:LEU:H     | 3:A:710:LEU:HD12 | 1.59                     | 0.68              |
| 3:A:1308:THR:HG22 | 3:A:1310:GLY:N   | 2.09                     | 0.68              |
| 3:A:1339:LEU:HD13 | 6:E:147:HIS:HD2  | 1.59                     | 0.68              |
| 4:B:369:GLY:O     | 4:B:370:PHE:CD1  | 2.47                     | 0.68              |
| 4:B:1095:LEU:C    | 4:B:1096:ARG:O   | 2.27                     | 0.68              |
| 8:H:93:TYR:CD2    | 8:H:145:ARG:HD3  | 2.29                     | 0.68              |
| 3:A:356:ASP:HB2   | 3:A:469:ARG:NH1  | 2.09                     | 0.68              |
| 4:B:34:ILE:HD13   | 4:B:34:ILE:H     | 1.59                     | 0.68              |
| 4:B:575:PRO:C     | 4:B:577:ALA:H    | 2.02                     | 0.68              |
| 4:B:918:ILE:O     | 4:B:933:SER:N    | 2.27                     | 0.68              |
| 6:E:7:ARG:C       | 6:E:9:ILE:N      | 2.50                     | 0.68              |
| 8:H:126:GLU:C     | 8:H:130:ARG:NH1  | 2.52                     | 0.68              |
| 9:I:117:LYS:O     | 9:I:118:ARG:HG2  | 1.94                     | 0.68              |
| 11:K:47:ARG:HH11  | 11:K:47:ARG:C    | 2.02                     | 0.68              |
| 11:K:47:ARG:HH11  | 11:K:47:ARG:CG   | 2.07                     | 0.68              |
| 3:A:30:ILE:HD11   | 4:B:1170:THR:OG1 | 1.94                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:211:PHE:O     | 3:A:213:HIS:N     | 2.27                     | 0.67              |
| 3:A:534:LEU:O     | 3:A:539:THR:HG21  | 1.94                     | 0.67              |
| 5:C:33:LEU:CD1    | 5:C:37:MET:HE2    | 2.25                     | 0.67              |
| 5:C:33:LEU:HD12   | 5:C:37:MET:HE2    | 1.76                     | 0.67              |
| 10:J:32:GLU:CD    | 10:J:32:GLU:H     | 2.01                     | 0.67              |
| 11:K:7:PHE:HA     | 11:K:10:PHE:CE2   | 2.29                     | 0.67              |
| 3:A:444:PHE:HB3   | 3:A:458:HIS:CD2   | 2.30                     | 0.67              |
| 3:A:856:THR:O     | 3:A:856:THR:HG22  | 1.94                     | 0.67              |
| 3:A:868:TYR:CZ    | 3:A:1366:ARG:HD3  | 2.29                     | 0.67              |
| 4:B:519:TRP:C     | 4:B:519:TRP:CD1   | 2.72                     | 0.67              |
| 4:B:1024:ALA:HA   | 4:B:1027:ILE:CD1  | 2.23                     | 0.67              |
| 5:C:115:SER:CB    | 5:C:141:GLY:O     | 2.40                     | 0.67              |
| 5:C:245:VAL:HA    | 5:C:248:ILE:HD12  | 1.76                     | 0.67              |
| 3:A:807:GLY:O     | 4:B:728:ARG:HD3   | 1.94                     | 0.67              |
| 3:A:913:LEU:HD11  | 3:A:981:LEU:O     | 1.95                     | 0.67              |
| 4:B:423:LYS:HB2   | 4:B:423:LYS:NZ    | 2.07                     | 0.67              |
| 4:B:817:LEU:N     | 4:B:818:PRO:CD    | 2.57                     | 0.67              |
| 4:B:1156:ASP:HB3  | 4:B:1198:TYR:N    | 2.09                     | 0.67              |
| 5:C:32:SER:HA     | 5:C:35:ARG:HG3    | 1.74                     | 0.67              |
| 9:I:8:ARG:O       | 9:I:9:ASP:C       | 2.37                     | 0.67              |
| 3:A:901:LEU:HG    | 3:A:926:GLN:NE2   | 1.99                     | 0.67              |
| 3:A:914:GLU:C     | 3:A:916:GLY:H     | 2.02                     | 0.67              |
| 8:H:47:PHE:CD2    | 8:H:95:TYR:HB2    | 2.29                     | 0.67              |
| 3:A:375:THR:OG1   | 3:A:434:ARG:N     | 2.27                     | 0.67              |
| 3:A:1036:ARG:HG3  | 3:A:1036:ARG:HH11 | 1.60                     | 0.67              |
| 4:B:641:GLU:C     | 4:B:643:ASP:H     | 2.01                     | 0.67              |
| 5:C:145:CYS:HA    | 10:J:2:ILE:CD1    | 2.23                     | 0.67              |
| 6:E:57:MET:HG2    | 6:E:57:MET:O      | 1.95                     | 0.67              |
| 6:E:112:TYR:CZ    | 6:E:136:ASN:HB2   | 2.29                     | 0.67              |
| 6:E:161:LYS:O     | 6:E:162:ARG:C     | 2.37                     | 0.67              |
| 8:H:128:ASN:OD1   | 8:H:128:ASN:O     | 2.13                     | 0.67              |
| 9:I:7:CYS:HB2     | 9:I:14:LEU:HD21   | 1.76                     | 0.67              |
| 3:A:455:MET:C     | 3:A:456:MET:HG2   | 2.19                     | 0.67              |
| 3:A:582:ILE:CG2   | 3:A:610:GLY:HA2   | 2.25                     | 0.67              |
| 3:A:1136:SER:HB3  | 3:A:1206:ASP:OD2  | 1.95                     | 0.67              |
| 3:A:1299:VAL:HG12 | 3:A:1300:LYS:N    | 2.01                     | 0.67              |
| 3:A:1422:ARG:NH2  | 4:B:1220:ARG:CD   | 2.56                     | 0.67              |
| 4:B:641:GLU:O     | 4:B:643:ASP:N     | 2.28                     | 0.67              |
| 11:K:47:ARG:HH11  | 11:K:47:ARG:CB    | 2.07                     | 0.67              |
| 1:R:5:A:H2'       | 1:R:6:G:C8        | 2.30                     | 0.67              |
| 3:A:96:ILE:HG22   | 3:A:97:ALA:H      | 1.58                     | 0.67              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:131:SER:O     | 3:A:134:ARG:HB3  | 1.93                     | 0.67              |
| 3:A:267:ALA:C     | 3:A:269:ILE:N    | 2.45                     | 0.67              |
| 3:A:535:THR:HG21  | 3:A:617:VAL:N    | 2.07                     | 0.67              |
| 4:B:59:LEU:HD11   | 4:B:417:PHE:CE2  | 2.30                     | 0.67              |
| 4:B:200:GLY:HA2   | 4:B:202:TYR:HE2  | 1.56                     | 0.67              |
| 4:B:1084:GLN:HE22 | 5:C:191:TYR:C    | 2.03                     | 0.67              |
| 5:C:74:SER:HB3    | 5:C:77:ILE:HG13  | 1.77                     | 0.67              |
| 3:A:289:ILE:O     | 3:A:291:GLU:N    | 2.28                     | 0.67              |
| 3:A:391:LEU:O     | 3:A:394:ASN:N    | 2.28                     | 0.67              |
| 3:A:751:SER:HB2   | 4:B:1015:HIS:CE1 | 2.30                     | 0.67              |
| 3:A:852:TYR:CD2   | 3:A:1060:PRO:HB2 | 2.29                     | 0.67              |
| 3:A:889:SER:O     | 3:A:940:ARG:NH2  | 2.27                     | 0.67              |
| 3:A:1228:TRP:HA   | 3:A:1237:ILE:O   | 1.94                     | 0.67              |
| 4:B:986:GLN:NE2   | 4:B:1016:ALA:HB1 | 2.09                     | 0.67              |
| 4:B:1069:PHE:HA   | 4:B:1085:ILE:O   | 1.94                     | 0.67              |
| 4:B:1104:HIS:CB   | 4:B:1122:ARG:HB2 | 2.24                     | 0.67              |
| 4:B:1180:PHE:O    | 4:B:1181:GLU:O   | 2.12                     | 0.67              |
| 5:C:18:VAL:CG2    | 5:C:240:VAL:CG1  | 2.73                     | 0.67              |
| 6:E:190:LEU:N     | 6:E:190:LEU:HD23 | 2.09                     | 0.67              |
| 3:A:99:ILE:CA     | 3:A:102:VAL:HG23 | 2.24                     | 0.67              |
| 3:A:115:LEU:HD12  | 3:A:122:MET:CE   | 2.25                     | 0.67              |
| 3:A:166:GLY:O     | 3:A:167:CYS:HB3  | 1.94                     | 0.67              |
| 3:A:1099:PRO:HG2  | 3:A:1100:ARG:H   | 1.59                     | 0.67              |
| 4:B:34:ILE:HD12   | 4:B:542:MET:HE1  | 1.75                     | 0.67              |
| 4:B:321:GLY:O     | 4:B:323:VAL:N    | 2.25                     | 0.67              |
| 5:C:186:LEU:HB3   | 5:C:188:HIS:HD2  | 1.60                     | 0.67              |
| 6:E:156:LEU:HG    | 6:E:195:VAL:O    | 1.94                     | 0.67              |
| 8:H:128:ASN:OD1   | 8:H:131:ASN:ND2  | 2.28                     | 0.67              |
| 3:A:114:LEU:C     | 3:A:115:LEU:HD23 | 2.19                     | 0.67              |
| 4:B:562:GLY:HA3   | 4:B:590:HIS:CE1  | 2.30                     | 0.67              |
| 5:C:226:ASP:O     | 5:C:227:THR:HB   | 1.95                     | 0.67              |
| 7:F:111:LEU:HD13  | 7:F:111:LEU:H    | 1.59                     | 0.67              |
| 11:K:10:PHE:CE1   | 11:K:11:LEU:HD13 | 2.30                     | 0.67              |
| 3:A:267:ALA:O     | 3:A:269:ILE:N    | 2.28                     | 0.66              |
| 3:A:546:VAL:O     | 3:A:550:LEU:HD23 | 1.94                     | 0.66              |
| 3:A:689:LYS:HB3   | 3:A:721:PHE:CD1  | 2.30                     | 0.66              |
| 3:A:892:ALA:HA    | 3:A:895:LYS:CB   | 2.13                     | 0.66              |
| 4:B:118:ARG:HH22  | 4:B:194:GLU:CD   | 2.03                     | 0.66              |
| 4:B:376:PHE:CE2   | 4:B:569:TYR:HD2  | 2.13                     | 0.66              |
| 4:B:797:TYR:O     | 4:B:799:PRO:HD2  | 1.94                     | 0.66              |
| 5:C:240:VAL:O     | 5:C:243:VAL:N    | 2.28                     | 0.66              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:E:79:TRP:N      | 6:E:107:THR:O    | 2.28                     | 0.66              |
| 3:A:103:CYS:C     | 3:A:105:CYS:N    | 2.44                     | 0.66              |
| 3:A:542:GLU:O     | 3:A:546:VAL:HG23 | 1.95                     | 0.66              |
| 3:A:783:THR:CG2   | 3:A:815:PHE:HE2  | 2.07                     | 0.66              |
| 4:B:778:MET:CE    | 4:B:853:SER:HB3  | 2.25                     | 0.66              |
| 4:B:1120:GLU:O    | 4:B:1124:ARG:NH1 | 2.28                     | 0.66              |
| 4:B:1203:LEU:HD12 | 4:B:1207:LEU:HG  | 1.78                     | 0.66              |
| 5:C:249:ASP:OD1   | 5:C:253:LYS:HE3  | 1.95                     | 0.66              |
| 3:A:185:TRP:CH2   | 3:A:200:ARG:HD3  | 2.30                     | 0.66              |
| 3:A:313:GLN:O     | 3:A:314:ALA:CB   | 2.44                     | 0.66              |
| 8:H:76:THR:O      | 8:H:77:ARG:O     | 2.12                     | 0.66              |
| 10:J:53:HIS:HE1   | 10:J:55:ASP:OD1  | 1.79                     | 0.66              |
| 3:A:875:ALA:HB2   | 3:A:1366:ARG:HD2 | 1.77                     | 0.66              |
| 4:B:46:GLN:NE2    | 4:B:496:ARG:HG2  | 2.09                     | 0.66              |
| 4:B:128:LEU:HB2   | 4:B:168:GLY:O    | 1.95                     | 0.66              |
| 4:B:179:CYS:SG    | 4:B:181:LEU:HB2  | 2.35                     | 0.66              |
| 4:B:314:LEU:C     | 4:B:316:PRO:HD2  | 2.21                     | 0.66              |
| 3:A:108:MET:N     | 3:A:108:MET:SD   | 2.68                     | 0.66              |
| 3:A:445:ASN:HB2   | 3:A:454:SER:O    | 1.96                     | 0.66              |
| 3:A:523:ILE:HG22  | 3:A:528:LEU:HB2  | 1.77                     | 0.66              |
| 3:A:814:PHE:O     | 3:A:817:ALA:HB3  | 1.94                     | 0.66              |
| 3:A:1168:GLU:C    | 3:A:1170:ILE:H   | 2.03                     | 0.66              |
| 3:A:1398:MET:HB2  | 3:A:1426:GLU:OE2 | 1.96                     | 0.66              |
| 4:B:166:PHE:C     | 4:B:166:PHE:HD2  | 2.03                     | 0.66              |
| 3:A:261:ASP:HB3   | 3:A:323:LYS:CE   | 2.25                     | 0.66              |
| 3:A:364:VAL:HG12  | 3:A:458:HIS:HB3  | 1.77                     | 0.66              |
| 3:A:582:ILE:HD11  | 3:A:629:LEU:HD11 | 1.76                     | 0.66              |
| 3:A:744:LYS:HE2   | 3:A:748:MET:HE2  | 1.77                     | 0.66              |
| 3:A:902:LEU:CD1   | 3:A:926:GLN:HG3  | 2.25                     | 0.66              |
| 3:A:925:LEU:O     | 3:A:927:VAL:N    | 2.28                     | 0.66              |
| 3:A:990:VAL:HG21  | 3:A:1026:LEU:O   | 1.95                     | 0.66              |
| 4:B:108:VAL:CG1   | 4:B:109:THR:H    | 2.04                     | 0.66              |
| 4:B:227:LYS:HB2   | 4:B:395:GLN:OE1  | 1.96                     | 0.66              |
| 4:B:648:HIS:NE2   | 4:B:650:GLU:OE1  | 2.28                     | 0.66              |
| 3:A:380:VAL:HG22  | 3:A:430:TRP:O    | 1.95                     | 0.66              |
| 3:A:449:SER:OG    | 4:B:1134:GLU:OE2 | 2.14                     | 0.66              |
| 3:A:601:LYS:HB3   | 3:A:603:ASN:OD1  | 1.95                     | 0.66              |
| 4:B:93:GLY:O      | 4:B:94:LYS:O     | 2.13                     | 0.66              |
| 4:B:449:ASN:O     | 4:B:450:ALA:C    | 2.39                     | 0.66              |
| 8:H:84:ALA:C      | 8:H:86:ASP:N     | 2.48                     | 0.66              |
| 3:A:743:VAL:O     | 3:A:747:VAL:HG23 | 1.96                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:849:MET:HG3   | 3:A:849:MET:O     | 1.95                     | 0.66              |
| 3:A:1341:ILE:HG23 | 3:A:1342:GLU:N    | 2.10                     | 0.66              |
| 4:B:947:GLY:C     | 4:B:948:ILE:HG13  | 2.21                     | 0.66              |
| 10:J:8:PHE:H      | 10:J:49:MET:HE3   | 1.59                     | 0.66              |
| 11:K:53:ASP:OD1   | 11:K:56:VAL:HG22  | 1.95                     | 0.66              |
| 3:A:71:GLN:C      | 3:A:73:GLY:H      | 1.97                     | 0.66              |
| 3:A:81:PHE:CE1    | 4:B:1208:MET:HE2  | 2.31                     | 0.66              |
| 3:A:374:LEU:HB2   | 3:A:436:ILE:CD1   | 2.25                     | 0.66              |
| 3:A:838:GLN:OE1   | 3:A:838:GLN:O     | 2.14                     | 0.66              |
| 3:A:1277:GLU:HG3  | 3:A:1278:ASN:HD22 | 1.58                     | 0.66              |
| 3:A:1308:THR:HG21 | 3:A:1310:GLY:O    | 1.95                     | 0.66              |
| 4:B:168:GLY:HA2   | 4:B:454:THR:HG1   | 1.59                     | 0.66              |
| 4:B:449:ASN:OD1   | 4:B:451:LYS:HB3   | 1.96                     | 0.66              |
| 4:B:662:MET:O     | 4:B:665:GLU:N     | 2.19                     | 0.66              |
| 4:B:1149:GLU:HA   | 4:B:1153:GLU:OE2  | 1.96                     | 0.66              |
| 4:B:797:TYR:C     | 4:B:799:PRO:HD2   | 2.20                     | 0.66              |
| 7:F:101:ILE:CD1   | 7:F:121:ALA:HB2   | 2.26                     | 0.66              |
| 10:J:3:VAL:HG21   | 10:J:18:TRP:CG    | 2.31                     | 0.66              |
| 3:A:273:ASN:OD1   | 3:A:296:LEU:HD21  | 1.96                     | 0.65              |
| 3:A:321:PRO:CG    | 3:A:322:VAL:N     | 2.54                     | 0.65              |
| 3:A:567:LYS:NZ    | 8:H:95:TYR:CZ     | 2.64                     | 0.65              |
| 3:A:650:GLN:O     | 3:A:654:ASN:HB2   | 1.97                     | 0.65              |
| 3:A:1172:LEU:HD23 | 3:A:1172:LEU:N    | 2.10                     | 0.65              |
| 3:A:1364:ASN:HD21 | 3:A:1366:ARG:NH1  | 1.94                     | 0.65              |
| 5:C:63:ILE:O      | 5:C:64:ALA:C      | 2.39                     | 0.65              |
| 6:E:116:ILE:HG21  | 6:E:121:MET:HG2   | 1.78                     | 0.65              |
| 7:F:101:ILE:HD13  | 7:F:117:PRO:O     | 1.97                     | 0.65              |
| 10:J:57:ILE:HA    | 10:J:60:PHE:CD2   | 2.31                     | 0.65              |
| 4:B:46:GLN:HG3    | 4:B:47:GLN:N      | 2.11                     | 0.65              |
| 4:B:199:MET:O     | 4:B:200:GLY:O     | 2.14                     | 0.65              |
| 4:B:295:GLY:HA2   | 4:B:298:LEU:HG    | 1.78                     | 0.65              |
| 4:B:383:ASN:HD22  | 4:B:384:ARG:HH11  | 1.44                     | 0.65              |
| 8:H:102:TYR:N     | 8:H:102:TYR:CD2   | 2.64                     | 0.65              |
| 2:T:8:DT:H2'      | 2:T:9:DC:H6       | 1.61                     | 0.65              |
| 3:A:374:LEU:HB2   | 3:A:436:ILE:HD12  | 1.79                     | 0.65              |
| 3:A:993:LEU:HD11  | 3:A:997:LEU:HD21  | 1.77                     | 0.65              |
| 3:A:1283:VAL:HG12 | 3:A:1284:MET:N    | 2.10                     | 0.65              |
| 4:B:291:ILE:HD12  | 4:B:291:ILE:N     | 2.11                     | 0.65              |
| 4:B:563:MET:HE2   | 4:B:588:GLY:HA3   | 1.78                     | 0.65              |
| 4:B:977:GLY:C     | 4:B:1099:VAL:CG2  | 2.68                     | 0.65              |
| 8:H:77:ARG:HB2    | 8:H:77:ARG:HH11   | 1.59                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:79:TRP:C      | 8:H:80:ARG:O      | 2.32                     | 0.65              |
| 3:A:208:LEU:O     | 3:A:209:ASN:C     | 2.39                     | 0.65              |
| 3:A:399:HIS:CB    | 3:A:400:PRO:HD3   | 2.24                     | 0.65              |
| 3:A:548:ASN:HD21  | 11:K:47:ARG:HE    | 1.44                     | 0.65              |
| 3:A:568:PRO:CB    | 5:C:221:TYR:CE1   | 2.79                     | 0.65              |
| 3:A:645:LEU:O     | 3:A:649:ILE:HG13  | 1.96                     | 0.65              |
| 3:A:1138:ILE:O    | 3:A:1276:VAL:HG23 | 1.97                     | 0.65              |
| 4:B:957:ASN:O     | 4:B:959:ASP:N     | 2.29                     | 0.65              |
| 11:K:63:VAL:HG23  | 11:K:63:VAL:O     | 1.96                     | 0.65              |
| 2:T:11:DC:H2'     | 2:T:12:DG:H8      | 1.61                     | 0.65              |
| 3:A:90:VAL:HG12   | 3:A:297:GLN:CD    | 2.21                     | 0.65              |
| 3:A:606:LEU:HB2   | 3:A:614:PHE:CZ    | 2.32                     | 0.65              |
| 3:A:777:PHE:CE2   | 3:A:782:ARG:HA    | 2.31                     | 0.65              |
| 3:A:1052:GLN:C    | 3:A:1053:PHE:O    | 2.35                     | 0.65              |
| 4:B:1034:VAL:HG12 | 4:B:1035:ALA:N    | 2.10                     | 0.65              |
| 6:E:77:SER:HB3    | 6:E:105:PHE:HD2   | 1.61                     | 0.65              |
| 6:E:178:ILE:HB    | 6:E:212:ARG:HD3   | 1.77                     | 0.65              |
| 11:K:22:ASP:HB3   | 11:K:23:PRO:HD2   | 1.79                     | 0.65              |
| 3:A:1102:LYS:O    | 3:A:1106:ASN:ND2  | 2.30                     | 0.65              |
| 3:A:1194:ARG:NH2  | 3:A:1237:ILE:HD13 | 2.11                     | 0.65              |
| 4:B:392:ARG:O     | 4:B:393:LYS:HE3   | 1.97                     | 0.65              |
| 8:H:93:TYR:CE2    | 8:H:145:ARG:HD3   | 2.31                     | 0.65              |
| 3:A:219:PHE:HE2   | 3:A:231:PRO:HD2   | 1.60                     | 0.65              |
| 3:A:265:LYS:CE    | 3:A:323:LYS:CG    | 2.74                     | 0.65              |
| 4:B:882:THR:OG1   | 4:B:935:ARG:HG3   | 1.96                     | 0.65              |
| 4:B:1072:MET:O    | 4:B:1081:LEU:HB2  | 1.96                     | 0.65              |
| 5:C:137:LYS:HG2   | 5:C:138:GLU:N     | 2.11                     | 0.65              |
| 11:K:12:LEU:H     | 11:K:12:LEU:CD1   | 2.09                     | 0.65              |
| 3:A:76:GLU:OE1    | 4:B:1159:ARG:NH1  | 2.28                     | 0.65              |
| 3:A:756:ILE:HG22  | 3:A:757:ASN:N     | 2.10                     | 0.65              |
| 3:A:997:LEU:N     | 3:A:997:LEU:HD23  | 2.10                     | 0.65              |
| 3:A:1154:TYR:HB2  | 3:A:1191:TRP:CZ3  | 2.32                     | 0.65              |
| 4:B:352:ALA:O     | 4:B:356:LEU:HG    | 1.97                     | 0.65              |
| 4:B:637:LEU:HA    | 4:B:743:ILE:HD11  | 1.79                     | 0.65              |
| 4:B:778:MET:CE    | 4:B:853:SER:CB    | 2.74                     | 0.65              |
| 5:C:74:SER:HA     | 5:C:77:ILE:HG12   | 1.77                     | 0.65              |
| 6:E:102:GLU:O     | 6:E:104:ASN:N     | 2.30                     | 0.65              |
| 3:A:51:GLY:HA2    | 3:A:56:PRO:HG2    | 1.79                     | 0.65              |
| 3:A:279:LEU:O     | 3:A:282:ASN:O     | 2.14                     | 0.65              |
| 3:A:475:THR:CG2   | 3:A:476:SER:N     | 2.60                     | 0.65              |
| 3:A:505:CYS:SG    | 4:B:1141:HIS:HD2  | 2.20                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:94:LYS:HD3    | 4:B:95:ILE:O      | 1.96                     | 0.65              |
| 4:B:638:PHE:CE1   | 4:B:743:ILE:HA    | 2.31                     | 0.65              |
| 4:B:1006:ILE:HG21 | 4:B:1087:PHE:HE2  | 1.61                     | 0.65              |
| 3:A:168:GLY:C     | 3:A:169:ASN:O     | 2.39                     | 0.65              |
| 3:A:169:ASN:ND2   | 3:A:169:ASN:N     | 2.11                     | 0.65              |
| 4:B:815:ARG:HH11  | 4:B:815:ARG:CG    | 2.09                     | 0.65              |
| 8:H:3:ASN:OD1     | 8:H:4:THR:N       | 2.30                     | 0.65              |
| 3:A:96:ILE:CG2    | 3:A:97:ALA:N      | 2.59                     | 0.64              |
| 3:A:718:VAL:HG12  | 3:A:722:LEU:HD11  | 1.78                     | 0.64              |
| 3:A:1194:ARG:CZ   | 3:A:1237:ILE:HD13 | 2.27                     | 0.64              |
| 4:B:62:ILE:CD1    | 4:B:418:LYS:HE2   | 2.26                     | 0.64              |
| 4:B:556:THR:HG22  | 4:B:557:PHE:H     | 1.58                     | 0.64              |
| 4:B:556:THR:CG2   | 4:B:557:PHE:N     | 2.59                     | 0.64              |
| 2:T:4:DA:H2''     | 2:T:5:DT:C6       | 2.31                     | 0.64              |
| 3:A:51:GLY:HA2    | 3:A:56:PRO:CG     | 2.28                     | 0.64              |
| 3:A:871:ASP:HB3   | 6:E:204:THR:HG23  | 1.79                     | 0.64              |
| 3:A:1134:ILE:HA   | 3:A:1137:ALA:HB3  | 1.80                     | 0.64              |
| 4:B:211:VAL:O     | 4:B:480:SER:HA    | 1.97                     | 0.64              |
| 4:B:361:LEU:N     | 4:B:362:PRO:CD    | 2.60                     | 0.64              |
| 4:B:435:THR:O     | 4:B:437:GLU:N     | 2.29                     | 0.64              |
| 4:B:589:VAL:HG12  | 4:B:590:HIS:N     | 2.11                     | 0.64              |
| 4:B:827:ILE:O     | 4:B:828:ALA:HB2   | 1.97                     | 0.64              |
| 5:C:57:VAL:HG21   | 10:J:57:ILE:HD11  | 1.78                     | 0.64              |
| 3:A:419:LYS:HG3   | 3:A:420:ARG:HG3   | 1.77                     | 0.64              |
| 3:A:834:THR:HB    | 3:A:1077:THR:HG23 | 1.79                     | 0.64              |
| 3:A:980:ASP:O     | 3:A:980:ASP:OD2   | 2.15                     | 0.64              |
| 3:A:1229:SER:HB3  | 3:A:1233:ASP:OD2  | 1.97                     | 0.64              |
| 4:B:976:ILE:HD11  | 4:B:992:ILE:HD12  | 1.79                     | 0.64              |
| 5:C:114:TYR:CD2   | 5:C:140:ASN:CB    | 2.80                     | 0.64              |
| 12:L:53:HIS:O     | 12:L:55:ILE:N     | 2.30                     | 0.64              |
| 1:R:8:G:O3'       | 4:B:776:GLN:NE2   | 2.31                     | 0.64              |
| 2:T:13:DA:H2''    | 2:T:14:DT:C5'     | 2.27                     | 0.64              |
| 3:A:528:LEU:O     | 3:A:530:GLY:N     | 2.31                     | 0.64              |
| 3:A:528:LEU:CA    | 3:A:531:ILE:HG22  | 2.24                     | 0.64              |
| 3:A:541:ILE:CD1   | 3:A:574:GLY:HA2   | 2.28                     | 0.64              |
| 3:A:567:LYS:CB    | 3:A:568:PRO:CD    | 2.69                     | 0.64              |
| 3:A:1166:ASP:O    | 3:A:1170:ILE:HG12 | 1.97                     | 0.64              |
| 3:A:1224:LEU:HD11 | 3:A:1240:CYS:HB3  | 1.78                     | 0.64              |
| 4:B:114:PRO:HG3   | 4:B:181:LEU:HD11  | 1.79                     | 0.64              |
| 4:B:913:GLY:HA2   | 4:B:938:SER:HB3   | 1.78                     | 0.64              |
| 6:E:195:VAL:HG22  | 6:E:213:ILE:HD13  | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:109:ILE:HD12  | 9:I:109:ILE:N     | 2.12                     | 0.64              |
| 3:A:209:ASN:O     | 3:A:212:LYS:N     | 2.31                     | 0.64              |
| 3:A:870:GLU:CB    | 6:E:204:THR:HG21  | 2.27                     | 0.64              |
| 3:A:1193:LEU:HD11 | 3:A:1195:LEU:HD21 | 1.78                     | 0.64              |
| 4:B:773:MET:O     | 4:B:776:GLN:N     | 2.31                     | 0.64              |
| 4:B:1115:THR:HG22 | 4:B:1117:GLN:HG3  | 1.80                     | 0.64              |
| 6:E:136:ASN:C     | 6:E:136:ASN:OD1   | 2.40                     | 0.64              |
| 11:K:7:PHE:C      | 11:K:9:LEU:N      | 2.55                     | 0.64              |
| 11:K:27:ALA:HB1   | 11:K:28:PRO:HD3   | 1.78                     | 0.64              |
| 3:A:666:ILE:O     | 3:A:667:GLY:C     | 2.41                     | 0.64              |
| 3:A:900:ASP:O     | 3:A:907:THR:HG23  | 1.98                     | 0.64              |
| 9:I:15:TYR:N      | 9:I:15:TYR:CD1    | 2.65                     | 0.64              |
| 3:A:211:PHE:C     | 3:A:213:HIS:N     | 2.54                     | 0.64              |
| 3:A:681:GLU:O     | 3:A:684:ALA:HB3   | 1.98                     | 0.64              |
| 3:A:913:LEU:CD1   | 3:A:914:GLU:N     | 2.39                     | 0.64              |
| 4:B:431:TYR:CD1   | 4:B:447:ALA:HB2   | 2.32                     | 0.64              |
| 4:B:550:ASP:OD1   | 4:B:551:PRO:CD    | 2.45                     | 0.64              |
| 4:B:1006:ILE:CG2  | 4:B:1007:VAL:N    | 2.61                     | 0.64              |
| 5:C:184:ASN:O     | 5:C:187:LYS:N     | 2.28                     | 0.64              |
| 8:H:59:ILE:O      | 8:H:60:ALA:HB3    | 1.97                     | 0.64              |
| 3:A:904:THR:O     | 3:A:905:ASP:C     | 2.40                     | 0.64              |
| 3:A:1011:GLN:NE2  | 3:A:1015:VAL:HG21 | 2.12                     | 0.64              |
| 4:B:617:ARG:NE    | 4:B:619:ILE:HD13  | 2.13                     | 0.64              |
| 4:B:701:ILE:HG12  | 4:B:702:LEU:N     | 2.11                     | 0.64              |
| 4:B:846:ILE:HG23  | 4:B:974:PRO:CG    | 2.22                     | 0.64              |
| 4:B:984:HIS:ND1   | 4:B:984:HIS:N     | 2.45                     | 0.64              |
| 4:B:995:ARG:HB3   | 4:B:997:GLU:OE2   | 1.98                     | 0.64              |
| 5:C:39:ALA:CA     | 5:C:164:ALA:HB3   | 2.27                     | 0.64              |
| 5:C:93:ASP:OD1    | 5:C:122:SER:HB2   | 1.98                     | 0.64              |
| 3:A:13:THR:HB     | 3:A:15:LYS:HZ2    | 1.59                     | 0.64              |
| 3:A:1141:THR:HG21 | 3:A:1205:LYS:HD2  | 1.78                     | 0.64              |
| 3:A:1308:THR:HG22 | 3:A:1310:GLY:H    | 1.61                     | 0.64              |
| 3:A:1331:SER:OG   | 3:A:1333:ILE:HG22 | 1.98                     | 0.64              |
| 4:B:60:GLN:OE1    | 4:B:94:LYS:HA     | 1.97                     | 0.64              |
| 4:B:485:ARG:HH11  | 4:B:485:ARG:HG3   | 1.62                     | 0.64              |
| 4:B:1084:GLN:NE2  | 5:C:192:TRP:N     | 2.45                     | 0.64              |
| 5:C:41:ILE:HD11   | 5:C:172:PRO:HG3   | 1.79                     | 0.64              |
| 5:C:241:ASP:CG    | 5:C:242:GLN:N     | 2.54                     | 0.64              |
| 6:E:162:ARG:NH2   | 6:E:166:LYS:HZ3   | 1.94                     | 0.64              |
| 7:F:81:THR:O      | 7:F:82:THR:C      | 2.40                     | 0.64              |
| 3:A:380:VAL:CG2   | 3:A:430:TRP:O     | 2.45                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:590:ARG:HH21 | 3:A:621:THR:HA    | 1.63                     | 0.64              |
| 3:A:780:VAL:HG23 | 4:B:699:GLU:OE1   | 1.97                     | 0.64              |
| 3:A:1344:GLY:O   | 3:A:1345:ARG:C    | 2.39                     | 0.64              |
| 4:B:230:ALA:HB3  | 4:B:231:PRO:CD    | 2.25                     | 0.64              |
| 4:B:616:ILE:HD12 | 4:B:616:ILE:N     | 2.12                     | 0.64              |
| 6:E:211:TYR:N    | 6:E:211:TYR:CD1   | 2.65                     | 0.64              |
| 9:I:55:THR:HG23  | 9:I:58:VAL:HG23   | 1.78                     | 0.64              |
| 3:A:76:GLU:O     | 3:A:78:PRO:HD3    | 1.98                     | 0.63              |
| 3:A:89:PRO:C     | 3:A:204:THR:HG21  | 2.22                     | 0.63              |
| 3:A:1410:PHE:O   | 3:A:1413:GLY:N    | 2.32                     | 0.63              |
| 4:B:816:GLU:N    | 4:B:816:GLU:CD    | 2.56                     | 0.63              |
| 4:B:1103:ILE:H   | 4:B:1103:ILE:CD1  | 1.93                     | 0.63              |
| 6:E:55:ARG:O     | 6:E:58:MET:HB2    | 1.97                     | 0.63              |
| 8:H:12:VAL:HA    | 8:H:28:ALA:CB     | 2.29                     | 0.63              |
| 9:I:27:PHE:O     | 9:I:28:GLU:HB3    | 1.98                     | 0.63              |
| 9:I:29:CYS:SG    | 9:I:32:CYS:N      | 2.68                     | 0.63              |
| 10:J:10:CYS:SG   | 10:J:43:ARG:NE    | 2.71                     | 0.63              |
| 3:A:58:LEU:HD21  | 3:A:243:PRO:HB3   | 1.77                     | 0.63              |
| 3:A:70:CYS:O     | 3:A:71:GLN:OE1    | 2.16                     | 0.63              |
| 3:A:352:VAL:CG1  | 3:A:353:ILE:N     | 2.61                     | 0.63              |
| 3:A:855:THR:HG23 | 3:A:857:ARG:HG2   | 1.80                     | 0.63              |
| 3:A:1155:ASP:OD2 | 3:A:1161:THR:HG23 | 1.98                     | 0.63              |
| 4:B:628:THR:O    | 4:B:628:THR:HG22  | 1.97                     | 0.63              |
| 9:I:15:TYR:HB3   | 9:I:16:PRO:HD3    | 1.77                     | 0.63              |
| 3:A:668:ASP:CG   | 3:A:742:ASN:HD22  | 2.04                     | 0.63              |
| 4:B:256:VAL:O    | 4:B:385:LEU:HD13  | 1.98                     | 0.63              |
| 4:B:805:THR:HA   | 4:B:809:MET:HE1   | 1.80                     | 0.63              |
| 2:T:11:DC:H2''   | 2:T:12:DG:H5'     | 1.80                     | 0.63              |
| 3:A:7:SER:HB3    | 4:B:1193:GLN:CD   | 2.24                     | 0.63              |
| 3:A:381:THR:O    | 3:A:382:PRO:C     | 2.42                     | 0.63              |
| 3:A:1105:LEU:HB3 | 3:A:1384:VAL:HG21 | 1.80                     | 0.63              |
| 3:A:1219:THR:CG2 | 3:A:1271:ILE:HD11 | 2.29                     | 0.63              |
| 3:A:1308:THR:CG2 | 3:A:1309:ASP:N    | 2.61                     | 0.63              |
| 3:A:1341:ILE:CG2 | 3:A:1342:GLU:N    | 2.61                     | 0.63              |
| 3:A:1434:ALA:CB  | 3:A:1436:ILE:HD12 | 2.24                     | 0.63              |
| 4:B:957:ASN:ND2  | 4:B:958:GLN:N     | 2.45                     | 0.63              |
| 5:C:74:SER:O     | 5:C:77:ILE:HB     | 1.98                     | 0.63              |
| 6:E:65:THR:C     | 6:E:67:GLU:N      | 2.52                     | 0.63              |
| 8:H:31:THR:O     | 8:H:32:THR:CB     | 2.45                     | 0.63              |
| 10:J:1:MET:H1    | 10:J:56:LEU:HB2   | 1.62                     | 0.63              |
| 3:A:95:PHE:CD1   | 3:A:234:MET:HG2   | 2.33                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:644:GLU:HG3  | 4:B:654:ARG:HH22  | 1.64                     | 0.63              |
| 8:H:58:THR:HG22  | 8:H:59:ILE:N      | 2.13                     | 0.63              |
| 3:A:90:VAL:CG1   | 3:A:297:GLN:HE21  | 2.07                     | 0.63              |
| 3:A:96:ILE:HG21  | 3:A:176:LYS:HE3   | 1.79                     | 0.63              |
| 3:A:666:ILE:CD1  | 4:B:1030:LEU:HD13 | 2.27                     | 0.63              |
| 3:A:785:PRO:HG3  | 4:B:698:GLU:HG2   | 1.81                     | 0.63              |
| 4:B:219:ALA:HB3  | 4:B:222:ILE:HD11  | 1.81                     | 0.63              |
| 4:B:843:GLN:HA   | 4:B:846:ILE:CD1   | 2.28                     | 0.63              |
| 4:B:1096:ARG:O   | 4:B:1097:HIS:HB2  | 1.99                     | 0.63              |
| 5:C:77:ILE:HD13  | 5:C:129:ILE:HD11  | 1.80                     | 0.63              |
| 6:E:187:TYR:CD2  | 6:E:187:TYR:O     | 2.51                     | 0.63              |
| 6:E:204:THR:HG22 | 6:E:205:SER:N     | 2.14                     | 0.63              |
| 3:A:219:PHE:CE2  | 3:A:231:PRO:HD2   | 2.33                     | 0.63              |
| 3:A:308:ILE:H    | 3:A:308:ILE:HD12  | 1.62                     | 0.63              |
| 3:A:1136:SER:CB  | 3:A:1206:ASP:OD2  | 2.47                     | 0.63              |
| 4:B:52:ASN:O     | 4:B:56:ASP:HB2    | 1.98                     | 0.63              |
| 4:B:280:ILE:HG21 | 4:B:285:ILE:CG1   | 2.24                     | 0.63              |
| 4:B:352:ALA:C    | 4:B:354:ASP:N     | 2.55                     | 0.63              |
| 4:B:585:VAL:HG12 | 4:B:587:HIS:CD2   | 2.33                     | 0.63              |
| 2:T:13:DA:H2''   | 2:T:14:DT:H5'     | 1.79                     | 0.63              |
| 3:A:30:ILE:HG13  | 4:B:1170:THR:HG23 | 1.81                     | 0.63              |
| 3:A:321:PRO:C    | 3:A:322:VAL:HG22  | 2.22                     | 0.63              |
| 3:A:335:ARG:O    | 3:A:336:ILE:C     | 2.41                     | 0.63              |
| 3:A:376:TYR:C    | 3:A:376:TYR:CD2   | 2.76                     | 0.63              |
| 3:A:777:PHE:CD2  | 3:A:782:ARG:C     | 2.77                     | 0.63              |
| 4:B:377:PHE:O    | 4:B:380:TYR:N     | 2.31                     | 0.63              |
| 4:B:546:SER:HA   | 4:B:612:GLU:OE2   | 1.99                     | 0.63              |
| 4:B:597:MET:O    | 4:B:600:LEU:N     | 2.32                     | 0.63              |
| 4:B:900:ALA:O    | 4:B:903:VAL:HG23  | 1.98                     | 0.63              |
| 4:B:1219:ASP:O   | 4:B:1220:ARG:C    | 2.42                     | 0.63              |
| 5:C:148:ARG:H    | 5:C:151:GLN:HG3   | 1.64                     | 0.63              |
| 3:A:33:ALA:C     | 3:A:34:LYS:HG3    | 2.23                     | 0.63              |
| 3:A:518:LYS:HG3  | 3:A:519:PRO:O     | 1.98                     | 0.63              |
| 5:C:43:THR:CG2   | 5:C:44:LEU:N      | 2.61                     | 0.63              |
| 6:E:121:MET:C    | 6:E:123:LEU:H     | 2.07                     | 0.63              |
| 6:E:131:THR:HG22 | 6:E:132:ILE:N     | 2.12                     | 0.63              |
| 9:I:101:PHE:N    | 9:I:101:PHE:CD1   | 2.66                     | 0.63              |
| 11:K:7:PHE:O     | 11:K:9:LEU:N      | 2.32                     | 0.63              |
| 11:K:10:PHE:CD1  | 11:K:11:LEU:HD13  | 2.34                     | 0.63              |
| 3:A:706:HIS:HD2  | 3:A:1282:VAL:O    | 1.82                     | 0.62              |
| 3:A:1057:VAL:CG1 | 3:A:1058:VAL:N    | 2.62                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:34:ILE:HD13   | 4:B:34:ILE:N      | 2.14                     | 0.62              |
| 4:B:485:ARG:HH11  | 4:B:485:ARG:CG    | 2.11                     | 0.62              |
| 4:B:634:TYR:O     | 4:B:635:ARG:HB3   | 1.99                     | 0.62              |
| 4:B:637:LEU:HD13  | 4:B:740:HIS:HB2   | 1.81                     | 0.62              |
| 3:A:265:LYS:CE    | 3:A:323:LYS:HG3   | 2.27                     | 0.62              |
| 3:A:445:ASN:HD22  | 3:A:446:ARG:H     | 1.45                     | 0.62              |
| 4:B:189:LEU:O     | 4:B:190:TYR:C     | 2.40                     | 0.62              |
| 4:B:263:GLY:O     | 4:B:264:SER:C     | 2.40                     | 0.62              |
| 4:B:801:LYS:H     | 10:J:52:THR:CG2   | 2.11                     | 0.62              |
| 6:E:124:VAL:HG22  | 6:E:132:ILE:HG22  | 1.80                     | 0.62              |
| 3:A:375:THR:HA    | 3:A:434:ARG:O     | 1.98                     | 0.62              |
| 3:A:432:VAL:O     | 3:A:433:GLU:C     | 2.42                     | 0.62              |
| 3:A:476:SER:O     | 3:A:479:ASN:N     | 2.32                     | 0.62              |
| 3:A:657:LEU:O     | 3:A:658:LEU:C     | 2.42                     | 0.62              |
| 3:A:904:THR:HG22  | 3:A:905:ASP:H     | 1.64                     | 0.62              |
| 4:B:227:LYS:CB    | 4:B:395:GLN:OE1   | 2.47                     | 0.62              |
| 4:B:329:THR:HG22  | 4:B:332:ASP:OD2   | 1.99                     | 0.62              |
| 4:B:1059:LEU:HD11 | 4:B:1064:TYR:HB2  | 1.81                     | 0.62              |
| 4:B:1192:TYR:CE2  | 4:B:1218:THR:HG21 | 2.34                     | 0.62              |
| 5:C:262:LEU:HD21  | 11:K:19:LEU:HD12  | 1.81                     | 0.62              |
| 3:A:265:LYS:HZ1   | 3:A:322:VAL:HG11  | 1.64                     | 0.62              |
| 3:A:793:SER:CB    | 3:A:794:PRO:HD2   | 2.25                     | 0.62              |
| 4:B:35:SER:O      | 4:B:37:PHE:O      | 2.18                     | 0.62              |
| 4:B:471:LYS:CG    | 4:B:472:ALA:N     | 2.49                     | 0.62              |
| 4:B:492:LEU:HB3   | 4:B:751:VAL:HG21  | 1.79                     | 0.62              |
| 5:C:134:ILE:CD1   | 5:C:141:GLY:CA    | 2.70                     | 0.62              |
| 7:F:123:LYS:HG2   | 7:F:123:LYS:O     | 1.98                     | 0.62              |
| 12:L:42:ARG:O     | 12:L:43:THR:HB    | 1.98                     | 0.62              |
| 2:T:11:DC:H2'     | 2:T:12:DG:C8      | 2.35                     | 0.62              |
| 3:A:272:ALA:HB3   | 3:A:296:LEU:HD12  | 1.82                     | 0.62              |
| 4:B:102:VAL:CG2   | 4:B:112:LEU:HB2   | 2.29                     | 0.62              |
| 4:B:129:PHE:HE2   | 4:B:166:PHE:HB3   | 1.63                     | 0.62              |
| 4:B:287:ARG:HA    | 4:B:291:ILE:O     | 1.99                     | 0.62              |
| 4:B:788:ARG:NH1   | 4:B:790:ASP:OD1   | 2.24                     | 0.62              |
| 4:B:957:ASN:ND2   | 4:B:958:GLN:HB2   | 2.14                     | 0.62              |
| 8:H:116:TYR:HB2   | 8:H:123:MET:CB    | 2.25                     | 0.62              |
| 9:I:33:SER:C      | 9:I:34:TYR:O      | 2.40                     | 0.62              |
| 2:T:8:DT:H2''     | 2:T:9:DC:O5'      | 1.98                     | 0.62              |
| 3:A:98:LYS:O      | 3:A:101:LYS:N     | 2.32                     | 0.62              |
| 3:A:599:SER:C     | 3:A:601:LYS:H     | 2.08                     | 0.62              |
| 3:A:622:VAL:HA    | 3:A:630:ILE:HD11  | 1.80                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:996:ASN:HA    | 3:A:998:LEU:HD23  | 1.81                     | 0.62              |
| 3:A:1057:VAL:HG12 | 3:A:1058:VAL:N    | 2.13                     | 0.62              |
| 4:B:435:THR:O     | 4:B:436:VAL:HG23  | 2.00                     | 0.62              |
| 4:B:1096:ARG:CG   | 4:B:1096:ARG:HH11 | 2.12                     | 0.62              |
| 11:K:51:LEU:HD12  | 11:K:59:ALA:HB3   | 1.79                     | 0.62              |
| 12:L:58:LYS:O     | 12:L:59:ALA:CB    | 2.47                     | 0.62              |
| 2:T:4:DA:H2'      | 2:T:5:DT:C7       | 2.29                     | 0.62              |
| 3:A:7:SER:HB2     | 4:B:1193:GLN:NE2  | 2.11                     | 0.62              |
| 3:A:27:VAL:HG11   | 3:A:238:CYS:SG    | 2.39                     | 0.62              |
| 3:A:129:LYS:O     | 3:A:130:ASP:CB    | 2.48                     | 0.62              |
| 3:A:897:TYR:N     | 3:A:897:TYR:HD1   | 1.97                     | 0.62              |
| 3:A:1192:LEU:HD22 | 3:A:1239:ARG:NH2  | 2.14                     | 0.62              |
| 4:B:25:ILE:HG22   | 4:B:26:THR:H      | 1.64                     | 0.62              |
| 4:B:114:PRO:O     | 4:B:115:GLN:C     | 2.40                     | 0.62              |
| 4:B:333:PHE:CD1   | 4:B:333:PHE:O     | 2.52                     | 0.62              |
| 4:B:449:ASN:OD1   | 4:B:451:LYS:HD2   | 1.99                     | 0.62              |
| 4:B:1033:LYS:HB2  | 4:B:1089:PRO:HD2  | 1.81                     | 0.62              |
| 4:B:1184:GLY:O    | 4:B:1186:ASP:OD2  | 2.17                     | 0.62              |
| 6:E:211:TYR:N     | 6:E:211:TYR:HD1   | 1.97                     | 0.62              |
| 11:K:40:HIS:HE1   | 11:K:63:VAL:HG13  | 1.62                     | 0.62              |
| 3:A:89:PRO:O      | 3:A:204:THR:CG2   | 2.38                     | 0.62              |
| 3:A:265:LYS:NZ    | 3:A:322:VAL:CB    | 2.62                     | 0.62              |
| 3:A:531:ILE:CD1   | 3:A:622:VAL:HG21  | 2.29                     | 0.62              |
| 3:A:567:LYS:HD3   | 8:H:95:TYR:CG     | 2.34                     | 0.62              |
| 3:A:768:GLN:CG    | 3:A:816:HIS:HA    | 2.30                     | 0.62              |
| 4:B:739:THR:HG1   | 4:B:740:HIS:CE1   | 2.18                     | 0.62              |
| 4:B:1173:ALA:C    | 4:B:1175:LEU:H    | 2.07                     | 0.62              |
| 9:I:10:CYS:CB     | 9:I:31:THR:CG2    | 2.70                     | 0.62              |
| 9:I:103:CYS:SG    | 9:I:104:LEU:N     | 2.73                     | 0.62              |
| 3:A:267:ALA:O     | 3:A:271:LYS:N     | 2.32                     | 0.62              |
| 3:A:609:ASP:O     | 3:A:610:GLY:C     | 2.40                     | 0.62              |
| 3:A:705:LYS:O     | 3:A:706:HIS:C     | 2.41                     | 0.62              |
| 4:B:773:MET:O     | 4:B:775:LYS:N     | 2.33                     | 0.62              |
| 4:B:1196:ILE:HB   | 4:B:1197:PRO:CD   | 2.29                     | 0.62              |
| 5:C:26:ASP:O      | 5:C:27:LEU:C      | 2.42                     | 0.62              |
| 6:E:118:PRO:O     | 6:E:122:LYS:HD2   | 1.99                     | 0.62              |
| 7:F:81:THR:OG1    | 7:F:144:GLU:OE1   | 2.18                     | 0.62              |
| 10:J:21:TYR:HB2   | 10:J:39:LEU:CD1   | 2.29                     | 0.62              |
| 3:A:587:HIS:CE1   | 3:A:969:GLN:HG2   | 2.35                     | 0.62              |
| 4:B:48:LEU:O      | 4:B:49:ASP:C      | 2.42                     | 0.62              |
| 4:B:291:ILE:HG22  | 4:B:297:ILE:CD1   | 2.29                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:313:MET:CG    | 4:B:390:LEU:HD21  | 2.28                     | 0.62              |
| 4:B:638:PHE:CD2   | 4:B:653:VAL:HG21  | 2.35                     | 0.62              |
| 4:B:1191:ILE:HG23 | 4:B:1192:TYR:N    | 2.15                     | 0.62              |
| 5:C:136:ASP:OD2   | 5:C:140:ASN:O     | 2.18                     | 0.62              |
| 8:H:2:SER:O       | 8:H:3:ASN:HB2     | 1.99                     | 0.62              |
| 8:H:42:ILE:HD12   | 8:H:95:TYR:CE2    | 2.35                     | 0.62              |
| 3:A:320:ARG:NH2   | 4:B:471:LYS:HB3   | 2.06                     | 0.61              |
| 3:A:356:ASP:C     | 3:A:356:ASP:OD1   | 2.43                     | 0.61              |
| 3:A:714:PHE:CD2   | 9:I:97:MET:HE1    | 2.34                     | 0.61              |
| 3:A:1389:PHE:CE1  | 3:A:1390:ASN:OD1  | 2.53                     | 0.61              |
| 4:B:653:VAL:HG22  | 4:B:689:LEU:HB3   | 1.82                     | 0.61              |
| 4:B:1056:SER:HB3  | 4:B:1066:SER:O    | 2.00                     | 0.61              |
| 5:C:133:ILE:HD13  | 5:C:236:GLY:C     | 2.25                     | 0.61              |
| 6:E:89:GLY:HA3    | 6:E:117:THR:OG1   | 2.00                     | 0.61              |
| 3:A:134:ARG:O     | 3:A:137:ALA:HB3   | 2.00                     | 0.61              |
| 3:A:598:LEU:HD13  | 8:H:25:ARG:HH12   | 1.65                     | 0.61              |
| 3:A:668:ASP:HB3   | 3:A:743:VAL:HG23  | 1.82                     | 0.61              |
| 3:A:693:VAL:HG13  | 3:A:702:LEU:HD21  | 1.81                     | 0.61              |
| 3:A:897:TYR:HD2   | 3:A:936:LEU:CD1   | 2.11                     | 0.61              |
| 3:A:1224:LEU:HD12 | 3:A:1241:ARG:O    | 1.99                     | 0.61              |
| 4:B:36:ALA:O      | 4:B:37:PHE:O      | 2.17                     | 0.61              |
| 4:B:350:GLN:O     | 4:B:351:TYR:C     | 2.43                     | 0.61              |
| 7:F:75:PRO:C      | 7:F:77:ASP:N      | 2.55                     | 0.61              |
| 8:H:101:ALA:HB2   | 8:H:116:TYR:CE2   | 2.35                     | 0.61              |
| 10:J:32:GLU:CD    | 10:J:32:GLU:N     | 2.58                     | 0.61              |
| 3:A:588:LEU:HD12  | 3:A:589:GLN:N     | 2.14                     | 0.61              |
| 4:B:203:PHE:HE1   | 4:B:212:LEU:HD12  | 1.65                     | 0.61              |
| 4:B:258:LEU:HD13  | 4:B:269:ILE:HG12  | 1.82                     | 0.61              |
| 4:B:638:PHE:O     | 4:B:740:HIS:CB    | 2.48                     | 0.61              |
| 5:C:80:LEU:CD1    | 5:C:95:CYS:HA     | 2.30                     | 0.61              |
| 3:A:33:ALA:CB     | 3:A:82:GLY:HA2    | 2.29                     | 0.61              |
| 3:A:321:PRO:HG2   | 3:A:322:VAL:N     | 2.15                     | 0.61              |
| 3:A:577:ILE:O     | 3:A:580:VAL:N     | 2.29                     | 0.61              |
| 3:A:896:ARG:HD2   | 3:A:897:TYR:CE1   | 2.35                     | 0.61              |
| 3:A:1105:LEU:HB3  | 3:A:1384:VAL:CG2  | 2.31                     | 0.61              |
| 3:A:1137:ALA:C    | 3:A:1138:ILE:HD13 | 2.25                     | 0.61              |
| 3:A:1140:HIS:HB2  | 3:A:1276:VAL:O    | 1.99                     | 0.61              |
| 3:A:1313:LEU:O    | 3:A:1315:GLU:N    | 2.33                     | 0.61              |
| 3:A:1338:VAL:HG12 | 3:A:1339:LEU:N    | 2.15                     | 0.61              |
| 4:B:102:VAL:HG22  | 4:B:112:LEU:HD22  | 1.82                     | 0.61              |
| 4:B:195:CYS:CB    | 4:B:782:LEU:HD22  | 2.30                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:420:LEU:O     | 4:B:423:LYS:N     | 2.34                     | 0.61              |
| 10:J:3:VAL:HA     | 10:J:53:HIS:CG    | 2.35                     | 0.61              |
| 10:J:57:ILE:HA    | 10:J:60:PHE:HD2   | 1.66                     | 0.61              |
| 3:A:552:TRP:NE1   | 3:A:655:PHE:CD1   | 2.68                     | 0.61              |
| 3:A:645:LEU:O     | 3:A:645:LEU:HD12  | 2.01                     | 0.61              |
| 3:A:899:VAL:HG21  | 3:A:1029:ARG:HG2  | 1.83                     | 0.61              |
| 3:A:1193:LEU:HD11 | 3:A:1195:LEU:CD2  | 2.31                     | 0.61              |
| 4:B:326:ASP:OD1   | 4:B:329:THR:OG1   | 2.18                     | 0.61              |
| 4:B:986:GLN:OE1   | 4:B:986:GLN:CA    | 2.46                     | 0.61              |
| 12:L:38:LEU:HD21  | 12:L:48:CYS:HA    | 1.81                     | 0.61              |
| 3:A:18:GLN:HE21   | 3:A:1418:LEU:CD1  | 2.13                     | 0.61              |
| 3:A:1426:GLU:HA   | 3:A:1429:ILE:HD12 | 1.83                     | 0.61              |
| 4:B:681:TRP:O     | 4:B:684:LEU:HB2   | 2.01                     | 0.61              |
| 6:E:2:ASP:O       | 6:E:3:GLN:HB3     | 1.99                     | 0.61              |
| 6:E:113:GLN:CA    | 6:E:137:GLU:HG3   | 2.28                     | 0.61              |
| 8:H:112:ILE:O     | 8:H:126:GLU:HA    | 2.00                     | 0.61              |
| 3:A:100:LYS:HB3   | 3:A:100:LYS:NZ    | 2.15                     | 0.61              |
| 3:A:106:VAL:C     | 3:A:114:LEU:HD21  | 2.25                     | 0.61              |
| 3:A:492:PRO:O     | 3:A:493:GLN:NE2   | 2.33                     | 0.61              |
| 3:A:1347:ALA:O    | 3:A:1348:LEU:C    | 2.38                     | 0.61              |
| 4:B:40:GLU:OE1    | 4:B:682:SER:HB2   | 2.01                     | 0.61              |
| 4:B:248:SER:O     | 4:B:249:ARG:HB2   | 2.00                     | 0.61              |
| 4:B:1096:ARG:NH1  | 4:B:1096:ARG:HG2  | 2.16                     | 0.61              |
| 5:C:34:ARG:HA     | 5:C:37:MET:HE3    | 1.82                     | 0.61              |
| 6:E:7:ARG:O       | 6:E:9:ILE:N       | 2.34                     | 0.61              |
| 6:E:28:TYR:HE1    | 6:E:78:LEU:CD1    | 2.04                     | 0.61              |
| 6:E:114:ASN:O     | 6:E:115:ASN:HB3   | 2.00                     | 0.61              |
| 8:H:47:PHE:HD2    | 8:H:95:TYR:CD1    | 2.19                     | 0.61              |
| 8:H:101:ALA:HB2   | 8:H:116:TYR:CD2   | 2.35                     | 0.61              |
| 3:A:68:GLN:NE2    | 3:A:70:CYS:HB3    | 2.16                     | 0.61              |
| 3:A:254:GLU:O     | 4:B:918:ILE:HG13  | 2.00                     | 0.61              |
| 3:A:255:SER:CB    | 4:B:918:ILE:HG23  | 2.30                     | 0.61              |
| 3:A:276:LEU:HD11  | 3:A:292:ALA:O     | 2.01                     | 0.61              |
| 3:A:1049:ILE:O    | 3:A:1050:GLU:C    | 2.43                     | 0.61              |
| 3:A:1345:ARG:HD2  | 3:A:1373:ASP:OD1  | 2.01                     | 0.61              |
| 3:A:1389:PHE:CD1  | 3:A:1389:PHE:C    | 2.78                     | 0.61              |
| 4:B:427:ASP:O     | 4:B:430:ARG:HB2   | 2.00                     | 0.61              |
| 4:B:869:SER:O     | 4:B:870:ILE:HG13  | 2.00                     | 0.61              |
| 8:H:26:ILE:O      | 8:H:39:THR:HA     | 1.99                     | 0.61              |
| 8:H:142:LEU:HD12  | 8:H:143:LEU:H     | 1.64                     | 0.61              |
| 3:A:332:LYS:H     | 3:A:337:ARG:CB    | 2.13                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:367:PRO:HB3  | 3:A:465:TYR:O     | 2.01                     | 0.61              |
| 3:A:858:ASN:C    | 3:A:858:ASN:ND2   | 2.46                     | 0.61              |
| 3:A:1209:MET:HB2 | 3:A:1231:ASP:OD2  | 2.01                     | 0.61              |
| 3:A:1339:LEU:CD1 | 6:E:147:HIS:CD2   | 2.84                     | 0.61              |
| 4:B:431:TYR:CD1  | 4:B:447:ALA:CB    | 2.83                     | 0.61              |
| 4:B:1131:GLY:O   | 4:B:1132:GLU:C    | 2.43                     | 0.61              |
| 6:E:116:ILE:O    | 6:E:118:PRO:CD    | 2.48                     | 0.61              |
| 6:E:178:ILE:CD1  | 6:E:185:ALA:HB2   | 2.31                     | 0.61              |
| 7:F:111:LEU:CD1  | 7:F:111:LEU:N     | 2.64                     | 0.61              |
| 7:F:127:GLU:O    | 7:F:129:LYS:N     | 2.33                     | 0.61              |
| 3:A:337:ARG:NH1  | 3:A:839:ARG:NH1   | 2.48                     | 0.61              |
| 3:A:805:LEU:HD12 | 3:A:805:LEU:O     | 2.00                     | 0.61              |
| 3:A:901:LEU:N    | 3:A:926:GLN:NE2   | 2.48                     | 0.61              |
| 3:A:902:LEU:O    | 3:A:903:ASN:CB    | 2.48                     | 0.61              |
| 4:B:233:PRO:HG2  | 4:B:234:ILE:HD13  | 1.82                     | 0.61              |
| 6:E:58:MET:O     | 6:E:60:PHE:N      | 2.34                     | 0.61              |
| 6:E:178:ILE:HG23 | 6:E:214:CYS:HA    | 1.82                     | 0.61              |
| 7:F:89:GLU:O     | 7:F:93:ILE:HD13   | 2.01                     | 0.61              |
| 8:H:76:THR:O     | 8:H:76:THR:HG22   | 2.00                     | 0.61              |
| 12:L:45:ALA:O    | 12:L:46:VAL:CG2   | 2.49                     | 0.61              |
| 12:L:46:VAL:HG13 | 12:L:56:LEU:HD12  | 1.83                     | 0.61              |
| 2:T:6:DC:H4'     | 3:A:447:GLN:CD    | 2.25                     | 0.60              |
| 3:A:918:GLU:O    | 3:A:919:ILE:HD13  | 2.00                     | 0.60              |
| 3:A:964:ILE:CD1  | 3:A:1037:LEU:HD21 | 2.31                     | 0.60              |
| 3:A:1017:LEU:HB2 | 6:E:205:SER:CA    | 2.30                     | 0.60              |
| 4:B:604:ARG:NH2  | 4:B:614:SER:HA    | 2.15                     | 0.60              |
| 4:B:1065:GLN:NE2 | 4:B:1067:ARG:H    | 1.98                     | 0.60              |
| 4:B:1074:ASN:C   | 4:B:1074:ASN:OD1  | 2.42                     | 0.60              |
| 9:I:7:CYS:CB     | 9:I:14:LEU:HD21   | 2.31                     | 0.60              |
| 3:A:40:THR:C     | 3:A:41:MET:HG3    | 2.26                     | 0.60              |
| 3:A:92:HIS:HB2   | 3:A:236:LEU:HD11  | 1.82                     | 0.60              |
| 3:A:714:PHE:O    | 3:A:718:VAL:HG23  | 2.01                     | 0.60              |
| 3:A:929:LEU:HD21 | 3:A:983:ILE:HG21  | 1.83                     | 0.60              |
| 3:A:1386:ARG:HA  | 3:A:1390:ASN:HB2  | 1.82                     | 0.60              |
| 4:B:704:ALA:HB3  | 4:B:741:CYS:HB2   | 1.82                     | 0.60              |
| 4:B:797:TYR:HB3  | 4:B:798:TYR:HD1   | 1.63                     | 0.60              |
| 5:C:69:LEU:O     | 10:J:6:ARG:NH1    | 2.34                     | 0.60              |
| 5:C:241:ASP:CG   | 5:C:242:GLN:H     | 2.08                     | 0.60              |
| 8:H:25:ARG:O     | 8:H:26:ILE:HD12   | 2.01                     | 0.60              |
| 9:I:96:SER:C     | 9:I:98:VAL:H      | 2.08                     | 0.60              |
| 10:J:8:PHE:H     | 10:J:49:MET:CE    | 2.14                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:185:TRP:O     | 3:A:186:LYS:CB    | 2.48                     | 0.60              |
| 3:A:1170:ILE:O    | 3:A:1171:GLN:C    | 2.44                     | 0.60              |
| 4:B:22:SER:O      | 4:B:23:ALA:O      | 2.19                     | 0.60              |
| 4:B:273:LEU:HB2   | 4:B:276:ILE:CD1   | 2.30                     | 0.60              |
| 4:B:322:PHE:CE2   | 9:I:30:ARG:HD2    | 2.36                     | 0.60              |
| 4:B:1017:ILE:HB   | 4:B:1018:PRO:HD3  | 1.83                     | 0.60              |
| 5:C:5:GLY:O       | 5:C:7:GLN:CG      | 2.48                     | 0.60              |
| 5:C:167:HIS:CE1   | 12:L:70:ARG:HA    | 2.37                     | 0.60              |
| 6:E:173:SER:O     | 6:E:175:LEU:N     | 2.34                     | 0.60              |
| 7:F:128:LYS:NZ    | 7:F:149:GLU:O     | 2.29                     | 0.60              |
| 3:A:321:PRO:HG2   | 3:A:322:VAL:H     | 1.65                     | 0.60              |
| 3:A:380:VAL:HB    | 3:A:428:TYR:HA    | 1.83                     | 0.60              |
| 3:A:898:ARG:HA    | 3:A:933:TYR:HD1   | 1.64                     | 0.60              |
| 3:A:1051:ALA:O    | 3:A:1054:LEU:HB2  | 2.01                     | 0.60              |
| 3:A:1132:LYS:O    | 3:A:1133:LEU:C    | 2.44                     | 0.60              |
| 4:B:701:ILE:CB    | 4:B:740:HIS:CE1   | 2.74                     | 0.60              |
| 4:B:773:MET:C     | 4:B:775:LYS:H     | 2.09                     | 0.60              |
| 4:B:992:ILE:HD11  | 11:K:67:PHE:HE2   | 1.65                     | 0.60              |
| 5:C:243:VAL:O     | 5:C:244:VAL:C     | 2.43                     | 0.60              |
| 6:E:36:GLU:O      | 6:E:38:PRO:HD3    | 2.01                     | 0.60              |
| 6:E:135:PHE:HB3   | 6:E:140:LEU:CD1   | 2.24                     | 0.60              |
| 6:E:162:ARG:HH21  | 6:E:166:LYS:NZ    | 1.92                     | 0.60              |
| 8:H:49:VAL:CG1    | 8:H:50:ALA:N      | 2.64                     | 0.60              |
| 8:H:96:VAL:HG22   | 8:H:143:LEU:HA    | 1.83                     | 0.60              |
| 9:I:52:ILE:HG13   | 9:I:52:ILE:O      | 2.01                     | 0.60              |
| 10:J:8:PHE:N      | 10:J:49:MET:HE3   | 2.16                     | 0.60              |
| 5:C:116:LYS:HB2   | 5:C:140:ASN:HA    | 1.84                     | 0.60              |
| 6:E:178:ILE:CG1   | 6:E:179:GLN:N     | 2.64                     | 0.60              |
| 8:H:15:VAL:O      | 8:H:15:VAL:CG1    | 2.49                     | 0.60              |
| 3:A:527:THR:O     | 3:A:531:ILE:N     | 2.35                     | 0.60              |
| 3:A:608:ILE:O     | 3:A:611:GLN:HB2   | 2.02                     | 0.60              |
| 3:A:714:PHE:CB    | 9:I:97:MET:HE1    | 2.30                     | 0.60              |
| 3:A:853:ASP:OD1   | 3:A:853:ASP:O     | 2.19                     | 0.60              |
| 3:A:1107:VAL:HG11 | 3:A:1381:LEU:HB3  | 1.84                     | 0.60              |
| 3:A:1168:GLU:HB3  | 3:A:1169:ILE:HD12 | 1.83                     | 0.60              |
| 3:A:1349:TYR:HB2  | 3:A:1372:VAL:HG21 | 1.84                     | 0.60              |
| 4:B:293:PRO:O     | 4:B:295:GLY:N     | 2.33                     | 0.60              |
| 4:B:461:LEU:CD1   | 4:B:466:TRP:CH2   | 2.85                     | 0.60              |
| 4:B:593:PRO:HG2   | 4:B:617:ARG:NH1   | 2.16                     | 0.60              |
| 4:B:976:ILE:HG22  | 4:B:977:GLY:N     | 2.16                     | 0.60              |
| 4:B:1067:ARG:O    | 4:B:1086:PHE:HE1  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:22:LEU:CD2   | 5:C:25:VAL:CG2    | 2.70                     | 0.60              |
| 3:A:351:THR:HG22 | 3:A:352:VAL:N     | 2.09                     | 0.60              |
| 3:A:596:THR:O    | 3:A:598:LEU:N     | 2.35                     | 0.60              |
| 3:A:733:ALA:C    | 3:A:735:VAL:N     | 2.57                     | 0.60              |
| 3:A:886:ILE:HD11 | 3:A:943:LEU:CB    | 2.32                     | 0.60              |
| 3:A:898:ARG:CB   | 3:A:933:TYR:CE1   | 2.83                     | 0.60              |
| 3:A:1154:TYR:HE1 | 9:I:18:GLU:CG     | 2.14                     | 0.60              |
| 3:A:1293:SER:OG  | 3:A:1295:THR:HG23 | 2.01                     | 0.60              |
| 3:A:1349:TYR:C   | 3:A:1349:TYR:CD2  | 2.79                     | 0.60              |
| 4:B:461:LEU:HD12 | 4:B:466:TRP:CZ3   | 2.35                     | 0.60              |
| 11:K:49:GLU:CB   | 11:K:94:ILE:HD11  | 2.31                     | 0.60              |
| 3:A:419:LYS:NZ   | 3:A:419:LYS:HB3   | 2.16                     | 0.60              |
| 3:A:566:ILE:O    | 3:A:567:LYS:O     | 2.19                     | 0.60              |
| 3:A:909:ASP:CG   | 3:A:910:PRO:CD    | 2.75                     | 0.60              |
| 3:A:1044:TRP:O   | 3:A:1045:VAL:C    | 2.44                     | 0.60              |
| 3:A:1120:LEU:CD2 | 3:A:1125:ALA:O    | 2.49                     | 0.60              |
| 3:A:1444:MET:HB3 | 3:A:1445:ILE:HD12 | 1.83                     | 0.60              |
| 4:B:723:VAL:O    | 4:B:725:PRO:N     | 2.35                     | 0.60              |
| 4:B:802:PRO:HB3  | 4:B:1091:TYR:CD1  | 2.36                     | 0.60              |
| 4:B:863:GLU:OE2  | 4:B:873:THR:HA    | 2.01                     | 0.60              |
| 4:B:1138:MET:HA  | 4:B:1138:MET:HE3  | 1.84                     | 0.60              |
| 5:C:29:MET:HB2   | 11:K:45:LEU:HD11  | 1.84                     | 0.60              |
| 5:C:145:CYS:SG   | 5:C:146:LYS:N     | 2.74                     | 0.60              |
| 11:K:88:LYS:O    | 11:K:89:ASN:C     | 2.43                     | 0.60              |
| 3:A:304:MET:HG3  | 4:B:1210:MET:HG3  | 1.84                     | 0.60              |
| 3:A:380:VAL:HG23 | 3:A:430:TRP:H     | 1.61                     | 0.60              |
| 3:A:1100:ARG:O   | 3:A:1101:LEU:C    | 2.44                     | 0.60              |
| 3:A:1256:GLU:C   | 3:A:1258:HIS:H    | 2.10                     | 0.60              |
| 4:B:64:CYS:O     | 4:B:65:GLU:CB     | 2.48                     | 0.60              |
| 5:C:123:ASN:ND2  | 5:C:125:MET:HG2   | 2.17                     | 0.60              |
| 5:C:244:VAL:HG21 | 11:K:105:PHE:CZ   | 2.36                     | 0.60              |
| 8:H:88:SER:C     | 8:H:89:LEU:HG     | 2.27                     | 0.60              |
| 10:J:34:THR:O    | 10:J:35:ALA:C     | 2.43                     | 0.60              |
| 3:A:13:THR:HB    | 3:A:15:LYS:HZ1    | 1.65                     | 0.60              |
| 3:A:40:THR:HG21  | 3:A:259:GLU:OE2   | 2.02                     | 0.60              |
| 3:A:267:ALA:C    | 3:A:269:ILE:H     | 2.09                     | 0.60              |
| 3:A:381:THR:O    | 3:A:384:ASN:N     | 2.34                     | 0.60              |
| 3:A:809:THR:HB   | 3:A:810:PRO:CD    | 2.31                     | 0.60              |
| 3:A:921:GLY:O    | 3:A:922:ASP:O     | 2.18                     | 0.60              |
| 3:A:1339:LEU:CD1 | 6:E:147:HIS:HD2   | 2.14                     | 0.60              |
| 4:B:293:PRO:HG2  | 4:B:296:GLU:CB    | 2.31                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:1170:THR:CG2  | 4:B:1183:LYS:NZ   | 2.64                     | 0.60              |
| 6:E:61:GLN:CG     | 6:E:62:ALA:N      | 2.64                     | 0.60              |
| 6:E:78:LEU:HD12   | 6:E:107:THR:HG21  | 1.84                     | 0.60              |
| 11:K:47:ARG:NH1   | 11:K:47:ARG:HB3   | 2.17                     | 0.60              |
| 3:A:304:MET:CG    | 4:B:1210:MET:HG3  | 2.31                     | 0.59              |
| 3:A:832:ALA:O     | 3:A:833:GLU:C     | 2.45                     | 0.59              |
| 4:B:325:GLN:NE2   | 9:I:12:ASN:OD1    | 2.34                     | 0.59              |
| 4:B:349:ILE:O     | 4:B:350:GLN:C     | 2.45                     | 0.59              |
| 6:E:29:PHE:C      | 6:E:30:ILE:HG13   | 2.27                     | 0.59              |
| 7:F:97:ARG:NE     | 7:F:124:GLU:OE2   | 2.35                     | 0.59              |
| 8:H:25:ARG:HA     | 8:H:40:LEU:O      | 2.02                     | 0.59              |
| 9:I:50:THR:HG22   | 9:I:52:ILE:HG22   | 1.81                     | 0.59              |
| 9:I:103:CYS:C     | 9:I:104:LEU:HD23  | 2.27                     | 0.59              |
| 3:A:31:SER:CB     | 3:A:83:HIS:HB3    | 2.32                     | 0.59              |
| 3:A:135:PHE:HD1   | 3:A:222:LEU:HB2   | 1.67                     | 0.59              |
| 3:A:1283:VAL:O    | 3:A:1306:LEU:HA   | 2.01                     | 0.59              |
| 4:B:408:LEU:O     | 4:B:412:LEU:HD12  | 2.01                     | 0.59              |
| 4:B:801:LYS:H     | 10:J:52:THR:HG22  | 1.66                     | 0.59              |
| 4:B:1202:LEU:HD13 | 4:B:1206:GLU:OE2  | 2.02                     | 0.59              |
| 10:J:53:HIS:CE1   | 10:J:55:ASP:OD1   | 2.54                     | 0.59              |
| 3:A:472:LEU:HD11  | 4:B:835:GLN:HE22  | 1.66                     | 0.59              |
| 3:A:574:GLY:O     | 3:A:575:LYS:C     | 2.44                     | 0.59              |
| 3:A:648:ASN:N     | 3:A:648:ASN:OD1   | 2.34                     | 0.59              |
| 3:A:993:LEU:CD1   | 3:A:997:LEU:HD21  | 2.32                     | 0.59              |
| 3:A:1127:ASP:C    | 3:A:1129:GLU:N    | 2.60                     | 0.59              |
| 4:B:20:ASP:N      | 4:B:655:LYS:HZ3   | 2.00                     | 0.59              |
| 4:B:547:VAL:N     | 4:B:612:GLU:OE2   | 2.36                     | 0.59              |
| 4:B:1170:THR:O    | 4:B:1170:THR:HG22 | 2.03                     | 0.59              |
| 10:J:58:GLU:HA    | 10:J:61:LEU:HD12  | 1.84                     | 0.59              |
| 11:K:6:ARG:O      | 11:K:8:GLU:N      | 2.36                     | 0.59              |
| 3:A:91:PHE:N      | 3:A:297:GLN:HE22  | 2.00                     | 0.59              |
| 3:A:331:GLY:O     | 3:A:332:LYS:HB3   | 2.02                     | 0.59              |
| 3:A:614:PHE:C     | 3:A:614:PHE:HD1   | 2.09                     | 0.59              |
| 4:B:1065:GLN:HE21 | 4:B:1067:ARG:N    | 1.98                     | 0.59              |
| 5:C:4:GLU:HG3     | 5:C:5:GLY:N       | 2.17                     | 0.59              |
| 7:F:97:ARG:HD3    | 7:F:100:GLN:OE1   | 2.02                     | 0.59              |
| 7:F:135:ARG:HG2   | 7:F:135:ARG:O     | 2.02                     | 0.59              |
| 8:H:58:THR:HB     | 8:H:143:LEU:HD12  | 1.83                     | 0.59              |
| 9:I:7:CYS:C       | 9:I:8:ARG:O       | 2.34                     | 0.59              |
| 9:I:59:VAL:O      | 9:I:60:GLN:C      | 2.45                     | 0.59              |
| 3:A:150:THR:O     | 3:A:151:ASP:OD2   | 2.21                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:206:GLU:O     | 3:A:209:ASN:HB2   | 2.02                     | 0.59              |
| 3:A:493:GLN:HE21  | 3:A:493:GLN:N     | 2.01                     | 0.59              |
| 3:A:559:VAL:O     | 3:A:560:ILE:C     | 2.44                     | 0.59              |
| 3:A:1120:LEU:O    | 3:A:1323:ASP:CB   | 2.50                     | 0.59              |
| 3:A:1441:PHE:HZ   | 7:F:88:TYR:O      | 1.84                     | 0.59              |
| 4:B:269:ILE:HD11  | 4:B:386:LEU:HD21  | 1.85                     | 0.59              |
| 5:C:240:VAL:O     | 5:C:241:ASP:C     | 2.45                     | 0.59              |
| 6:E:81:GLU:HB3    | 6:E:96:PHE:HE1    | 1.66                     | 0.59              |
| 9:I:75:CYS:HB3    | 9:I:103:CYS:HB2   | 1.85                     | 0.59              |
| 10:J:16:ASP:OD1   | 10:J:17:LYS:HG3   | 2.03                     | 0.59              |
| 3:A:23:SER:HB2    | 3:A:25:GLU:HB2    | 1.84                     | 0.59              |
| 3:A:49:LYS:NZ     | 3:A:60:SER:HA     | 2.18                     | 0.59              |
| 3:A:494:SER:O     | 3:A:498:ARG:HG3   | 2.03                     | 0.59              |
| 3:A:1011:GLN:HE22 | 3:A:1015:VAL:HG21 | 1.67                     | 0.59              |
| 3:A:1120:LEU:O    | 3:A:1323:ASP:HB3  | 2.01                     | 0.59              |
| 4:B:102:VAL:HG23  | 4:B:112:LEU:HB2   | 1.84                     | 0.59              |
| 4:B:851:PHE:O     | 4:B:974:PRO:HD3   | 2.01                     | 0.59              |
| 5:C:16:ASP:HA     | 5:C:240:VAL:HG22  | 1.85                     | 0.59              |
| 3:A:427:GLN:O     | 3:A:428:TYR:C     | 2.46                     | 0.59              |
| 3:A:541:ILE:HD11  | 3:A:574:GLY:HA2   | 1.83                     | 0.59              |
| 3:A:997:LEU:O     | 3:A:998:LEU:O     | 2.20                     | 0.59              |
| 4:B:178:ASN:O     | 4:B:179:CYS:C     | 2.45                     | 0.59              |
| 4:B:300:HIS:HE1   | 4:B:376:PHE:CE1   | 2.20                     | 0.59              |
| 4:B:744:HIS:CG    | 4:B:745:PRO:HD2   | 2.38                     | 0.59              |
| 5:C:92:CYS:SG     | 5:C:94:LYS:HB3    | 2.42                     | 0.59              |
| 5:C:116:LYS:HE2   | 5:C:117:ASP:OD1   | 2.03                     | 0.59              |
| 5:C:146:LYS:NZ    | 10:J:58:GLU:OE2   | 2.30                     | 0.59              |
| 12:L:47:ARG:HG3   | 12:L:52:GLY:O     | 2.02                     | 0.59              |
| 3:A:99:ILE:HG12   | 3:A:234:MET:SD    | 2.43                     | 0.59              |
| 3:A:495:GLU:HA    | 3:A:498:ARG:HG3   | 1.85                     | 0.59              |
| 3:A:658:LEU:C     | 3:A:658:LEU:HD12  | 2.28                     | 0.59              |
| 3:A:878:ILE:HG22  | 3:A:879:GLU:N     | 2.17                     | 0.59              |
| 4:B:431:TYR:CZ    | 4:B:447:ALA:HB2   | 2.37                     | 0.59              |
| 5:C:22:LEU:HD22   | 5:C:25:VAL:HG21   | 1.78                     | 0.59              |
| 6:E:83:CYS:SG     | 6:E:85:GLU:HB2    | 2.43                     | 0.59              |
| 8:H:32:THR:HG22   | 8:H:33:GLN:H      | 1.68                     | 0.59              |
| 11:K:63:VAL:O     | 11:K:63:VAL:CG2   | 2.50                     | 0.59              |
| 3:A:14:VAL:HG23   | 3:A:1432:GLN:NE2  | 2.18                     | 0.59              |
| 3:A:302:THR:HA    | 3:A:305:ASP:O     | 2.03                     | 0.59              |
| 3:A:576:GLN:O     | 3:A:579:SER:HB2   | 2.02                     | 0.59              |
| 3:A:715:GLU:O     | 3:A:719:VAL:HG23  | 2.02                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:834:THR:CB    | 3:A:1077:THR:HG23 | 2.33                     | 0.59              |
| 4:B:871:THR:O     | 4:B:872:GLU:C     | 2.46                     | 0.59              |
| 8:H:77:ARG:O      | 8:H:78:SER:C      | 2.46                     | 0.59              |
| 12:L:29:TYR:C     | 12:L:30:ILE:HG13  | 2.27                     | 0.59              |
| 12:L:34:CYS:O     | 12:L:35:SER:HB2   | 2.03                     | 0.59              |
| 3:A:93:VAL:CG2    | 3:A:301:ALA:HA    | 2.33                     | 0.59              |
| 3:A:306:ASN:HD21  | 3:A:324:SER:HB3   | 1.68                     | 0.59              |
| 3:A:565:ILE:HG12  | 3:A:567:LYS:HZ1   | 1.67                     | 0.59              |
| 3:A:1009:ASN:O    | 3:A:1013:ASP:OD2  | 2.21                     | 0.59              |
| 3:A:1156:PRO:CD   | 3:A:1157:ASP:H    | 2.16                     | 0.59              |
| 3:A:1192:LEU:HD11 | 3:A:1239:ARG:HB3  | 1.84                     | 0.59              |
| 4:B:53:GLN:HG3    | 4:B:53:GLN:O      | 2.03                     | 0.59              |
| 4:B:276:ILE:HG22  | 4:B:277:LYS:N     | 2.18                     | 0.59              |
| 4:B:286:PHE:HB3   | 4:B:297:ILE:CD1   | 2.33                     | 0.59              |
| 4:B:461:LEU:CD1   | 4:B:466:TRP:HH2   | 2.16                     | 0.59              |
| 4:B:515:HIS:HD2   | 4:B:517:THR:OG1   | 1.84                     | 0.59              |
| 4:B:578:THR:OG1   | 4:B:593:PRO:HG3   | 2.03                     | 0.59              |
| 4:B:642:ASP:OD1   | 4:B:642:ASP:N     | 2.36                     | 0.59              |
| 4:B:1067:ARG:O    | 4:B:1086:PHE:CE1  | 2.56                     | 0.59              |
| 4:B:1184:GLY:C    | 4:B:1186:ASP:N    | 2.60                     | 0.59              |
| 5:C:226:ASP:O     | 5:C:227:THR:CB    | 2.47                     | 0.59              |
| 6:E:20:LYS:HE2    | 6:E:60:PHE:CZ     | 2.36                     | 0.59              |
| 6:E:94:LYS:HE2    | 6:E:98:ILE:HG12   | 1.84                     | 0.59              |
| 11:K:22:ASP:HB3   | 11:K:23:PRO:CD    | 2.33                     | 0.59              |
| 12:L:32:ALA:HB3   | 12:L:55:ILE:HD12  | 1.84                     | 0.59              |
| 12:L:53:HIS:O     | 12:L:55:ILE:HG12  | 2.03                     | 0.59              |
| 2:T:11:DC:H2''    | 2:T:12:DG:C5'     | 2.33                     | 0.58              |
| 3:A:101:LYS:HA    | 3:A:139:TRP:HE1   | 1.66                     | 0.58              |
| 3:A:384:ASN:OD1   | 3:A:385:ILE:N     | 2.36                     | 0.58              |
| 3:A:416:ARG:HG3   | 3:A:417:TYR:CE2   | 2.38                     | 0.58              |
| 3:A:783:THR:HG21  | 3:A:815:PHE:CZ    | 2.38                     | 0.58              |
| 4:B:278:GLN:HG2   | 4:B:279:ASP:N     | 2.14                     | 0.58              |
| 4:B:428:ILE:O     | 4:B:429:PHE:C     | 2.45                     | 0.58              |
| 4:B:557:PHE:C     | 4:B:557:PHE:CD2   | 2.81                     | 0.58              |
| 4:B:773:MET:C     | 4:B:775:LYS:N     | 2.59                     | 0.58              |
| 4:B:1172:ILE:HG22 | 4:B:1172:ILE:O    | 2.02                     | 0.58              |
| 4:B:1197:PRO:O    | 4:B:1200:ALA:HB3  | 2.03                     | 0.58              |
| 6:E:109:ILE:O     | 6:E:109:ILE:HG22  | 2.02                     | 0.58              |
| 7:F:83:PRO:CD     | 7:F:84:TYR:H      | 2.15                     | 0.58              |
| 3:A:89:PRO:C      | 3:A:90:VAL:CG2    | 2.77                     | 0.58              |
| 3:A:635:ARG:NH2   | 3:A:877:HIS:HA    | 2.16                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1208:THR:HB   | 3:A:1211:GLN:HB2  | 1.83                     | 0.58              |
| 4:B:329:THR:C     | 4:B:332:ASP:HB2   | 2.27                     | 0.58              |
| 8:H:24:CYS:HB2    | 8:H:44:VAL:HG21   | 1.86                     | 0.58              |
| 8:H:58:THR:O      | 8:H:59:ILE:HD13   | 2.03                     | 0.58              |
| 3:A:322:VAL:O     | 3:A:323:LYS:CD    | 2.52                     | 0.58              |
| 3:A:933:TYR:O     | 3:A:937:VAL:HG23  | 2.03                     | 0.58              |
| 3:A:963:ILE:CG2   | 3:A:1045:VAL:HG13 | 2.33                     | 0.58              |
| 3:A:1198:ASP:OD1  | 3:A:1199:ARG:N    | 2.37                     | 0.58              |
| 3:A:1236:LEU:C    | 3:A:1237:ILE:HG13 | 2.29                     | 0.58              |
| 4:B:166:PHE:HD2   | 4:B:166:PHE:O     | 1.86                     | 0.58              |
| 4:B:314:LEU:O     | 4:B:315:LYS:C     | 2.46                     | 0.58              |
| 4:B:650:GLU:HG3   | 4:B:651:LEU:H     | 1.67                     | 0.58              |
| 4:B:806:THR:H     | 4:B:809:MET:HE3   | 1.67                     | 0.58              |
| 4:B:1084:GLN:HG2  | 5:C:201:TRP:CZ2   | 2.38                     | 0.58              |
| 6:E:81:GLU:HB3    | 6:E:96:PHE:CE1    | 2.38                     | 0.58              |
| 6:E:173:SER:C     | 6:E:175:LEU:H     | 2.11                     | 0.58              |
| 10:J:21:TYR:CE1   | 10:J:25:LEU:HD21  | 2.38                     | 0.58              |
| 3:A:112:LYS:HG2   | 3:A:113:LEU:H     | 1.68                     | 0.58              |
| 3:A:244:PRO:HG2   | 3:A:245:PRO:HD2   | 1.83                     | 0.58              |
| 3:A:356:ASP:HB2   | 3:A:469:ARG:HH11  | 1.68                     | 0.58              |
| 3:A:436:ILE:HD11  | 3:A:491:VAL:HG21  | 1.86                     | 0.58              |
| 3:A:1364:ASN:HD22 | 3:A:1366:ARG:HG2  | 1.64                     | 0.58              |
| 4:B:411:PRO:HA    | 4:B:414:ALA:HB3   | 1.83                     | 0.58              |
| 4:B:412:LEU:O     | 4:B:413:LEU:C     | 2.46                     | 0.58              |
| 4:B:784:ASN:CG    | 4:B:788:ARG:HD2   | 2.27                     | 0.58              |
| 6:E:86:PRO:O      | 6:E:114:ASN:HB2   | 2.03                     | 0.58              |
| 6:E:113:GLN:HB3   | 6:E:137:GLU:CD    | 2.27                     | 0.58              |
| 11:K:71:PHE:CD1   | 11:K:71:PHE:C     | 2.82                     | 0.58              |
| 2:T:5:DT:C2'      | 2:T:6:DC:H5'      | 2.28                     | 0.58              |
| 3:A:294:SER:O     | 3:A:298:PHE:HB3   | 2.04                     | 0.58              |
| 3:A:760:GLN:OE1   | 4:B:1021:MET:HE1  | 2.03                     | 0.58              |
| 3:A:1208:THR:O    | 3:A:1212:VAL:HG23 | 2.04                     | 0.58              |
| 3:A:1342:GLU:CG   | 6:E:212:ARG:HH12  | 2.16                     | 0.58              |
| 4:B:787:VAL:O     | 4:B:787:VAL:HG12  | 2.02                     | 0.58              |
| 5:C:22:LEU:HD23   | 5:C:22:LEU:C      | 2.28                     | 0.58              |
| 5:C:66:ARG:CZ     | 10:J:2:ILE:CG2    | 2.82                     | 0.58              |
| 5:C:146:LYS:O     | 5:C:147:LEU:HD23  | 2.03                     | 0.58              |
| 6:E:61:GLN:HG2    | 6:E:62:ALA:N      | 2.10                     | 0.58              |
| 3:A:35:ILE:O      | 3:A:270:LEU:HD11  | 2.03                     | 0.58              |
| 3:A:58:LEU:HD23   | 3:A:80:HIS:O      | 2.01                     | 0.58              |
| 3:A:541:ILE:HG22  | 3:A:546:VAL:CG2   | 2.33                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:751:SER:CB   | 4:B:1015:HIS:HE1  | 2.16                     | 0.58              |
| 3:A:929:LEU:N    | 3:A:929:LEU:HD23  | 2.18                     | 0.58              |
| 3:A:1203:ASN:O   | 3:A:1204:ASP:C    | 2.47                     | 0.58              |
| 4:B:282:ILE:HG13 | 4:B:283:VAL:N     | 2.19                     | 0.58              |
| 4:B:482:VAL:O    | 4:B:483:LEU:C     | 2.47                     | 0.58              |
| 4:B:912:ILE:HD11 | 4:B:966:VAL:HG21  | 1.86                     | 0.58              |
| 4:B:1080:LYS:HG3 | 5:C:180:TYR:CE2   | 2.38                     | 0.58              |
| 1:R:9:G:H4'      | 4:B:1097:HIS:CD2  | 2.39                     | 0.58              |
| 3:A:89:PRO:C     | 3:A:204:THR:CG2   | 2.77                     | 0.58              |
| 3:A:338:GLY:HA2  | 4:B:1129:ARG:HH22 | 1.69                     | 0.58              |
| 3:A:444:PHE:HE2  | 3:A:470:LEU:CD2   | 2.16                     | 0.58              |
| 3:A:528:LEU:HD13 | 3:A:531:ILE:CG2   | 2.34                     | 0.58              |
| 3:A:577:ILE:O    | 3:A:578:LEU:C     | 2.46                     | 0.58              |
| 3:A:614:PHE:CD1  | 3:A:614:PHE:O     | 2.56                     | 0.58              |
| 4:B:230:ALA:N    | 4:B:231:PRO:CD    | 2.65                     | 0.58              |
| 4:B:635:ARG:NH2  | 4:B:698:GLU:OE2   | 2.37                     | 0.58              |
| 6:E:65:THR:OG1   | 6:E:68:SER:N      | 2.31                     | 0.58              |
| 9:I:96:SER:CB    | 9:I:98:VAL:HG23   | 2.34                     | 0.58              |
| 3:A:496:GLU:O    | 3:A:499:ALA:N     | 2.35                     | 0.58              |
| 3:A:709:THR:HB   | 3:A:712:GLU:HG3   | 1.86                     | 0.58              |
| 3:A:1074:GLU:O   | 3:A:1078:GLN:HG2  | 2.04                     | 0.58              |
| 3:A:1292:PRO:HD3 | 3:A:1298:TYR:CE2  | 2.39                     | 0.58              |
| 4:B:236:HIS:HD2  | 4:B:389:ALA:CB    | 2.15                     | 0.58              |
| 4:B:273:LEU:O    | 4:B:274:PRO:O     | 2.22                     | 0.58              |
| 4:B:760:ASP:OD1  | 4:B:760:ASP:N     | 2.30                     | 0.58              |
| 6:E:204:THR:CG2  | 6:E:205:SER:N     | 2.66                     | 0.58              |
| 7:F:109:VAL:CG2  | 7:F:124:GLU:HG3   | 2.34                     | 0.58              |
| 8:H:138:GLU:C    | 8:H:139:ASN:O     | 2.46                     | 0.58              |
| 10:J:1:MET:N     | 10:J:56:LEU:N     | 2.52                     | 0.58              |
| 11:K:47:ARG:O    | 11:K:47:ARG:HG2   | 2.02                     | 0.58              |
| 3:A:908:LEU:CD1  | 3:A:983:ILE:HD11  | 2.27                     | 0.58              |
| 3:A:1273:LEU:O   | 3:A:1274:ARG:CB   | 2.50                     | 0.58              |
| 4:B:778:MET:HE3  | 4:B:853:SER:HB2   | 1.83                     | 0.58              |
| 3:A:482:PHE:O    | 4:B:989:THR:HG23  | 2.04                     | 0.58              |
| 3:A:743:VAL:HG11 | 3:A:758:ILE:CD1   | 2.34                     | 0.58              |
| 3:A:834:THR:O    | 3:A:837:ILE:HB    | 2.03                     | 0.58              |
| 3:A:1364:ASN:ND2 | 3:A:1364:ASN:C    | 2.62                     | 0.58              |
| 4:B:287:ARG:NH2  | 4:B:294:ASP:OD2   | 2.37                     | 0.58              |
| 4:B:519:TRP:HZ2  | 4:B:705:MET:HE1   | 1.67                     | 0.58              |
| 5:C:11:ARG:HG3   | 5:C:19:ASP:O      | 2.04                     | 0.58              |
| 12:L:53:HIS:C    | 12:L:55:ILE:H     | 2.11                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:68:GLN:NE2   | 3:A:80:HIS:CE1    | 2.72                     | 0.57              |
| 3:A:828:ALA:HB2  | 4:B:530:GLY:HA2   | 1.86                     | 0.57              |
| 3:A:953:ASN:C    | 3:A:954:TRP:CD1   | 2.82                     | 0.57              |
| 4:B:326:ASP:CG   | 4:B:329:THR:OG1   | 2.47                     | 0.57              |
| 4:B:1024:ALA:O   | 4:B:1025:HIS:C    | 2.46                     | 0.57              |
| 4:B:1104:HIS:HB2 | 4:B:1122:ARG:CD   | 2.33                     | 0.57              |
| 5:C:56:THR:HG22  | 5:C:57:VAL:H      | 1.69                     | 0.57              |
| 3:A:8:SER:OG     | 4:B:1180:PHE:HE1  | 1.87                     | 0.57              |
| 3:A:57:ARG:O     | 3:A:68:GLN:HG3    | 2.04                     | 0.57              |
| 3:A:387:ARG:O    | 3:A:391:LEU:HD23  | 2.04                     | 0.57              |
| 3:A:530:GLY:HA2  | 3:A:533:LYS:H     | 1.69                     | 0.57              |
| 3:A:898:ARG:HD2  | 3:A:898:ARG:C     | 2.28                     | 0.57              |
| 3:A:898:ARG:CB   | 3:A:933:TYR:HE1   | 2.16                     | 0.57              |
| 3:A:1039:LYS:HG3 | 3:A:1040:GLN:N    | 2.18                     | 0.57              |
| 3:A:1134:ILE:O   | 3:A:1135:ARG:C    | 2.47                     | 0.57              |
| 3:A:1150:SER:HB2 | 3:A:1195:LEU:HD22 | 1.86                     | 0.57              |
| 3:A:1265:ASN:O   | 3:A:1266:THR:C    | 2.47                     | 0.57              |
| 4:B:282:ILE:HG13 | 4:B:283:VAL:H     | 1.67                     | 0.57              |
| 5:C:4:GLU:CG     | 5:C:5:GLY:H       | 2.14                     | 0.57              |
| 5:C:133:ILE:HD11 | 5:C:237:SER:CA    | 2.33                     | 0.57              |
| 6:E:75:MET:CG    | 6:E:76:GLY:N      | 2.67                     | 0.57              |
| 6:E:113:GLN:C    | 6:E:114:ASN:HD22  | 2.11                     | 0.57              |
| 6:E:161:LYS:O    | 6:E:164:LEU:N     | 2.38                     | 0.57              |
| 9:I:98:VAL:HG12  | 9:I:99:LEU:N      | 2.19                     | 0.57              |
| 11:K:43:GLY:HA2  | 11:K:71:PHE:CZ    | 2.39                     | 0.57              |
| 3:A:148:CYS:HB3  | 3:A:167:CYS:O     | 2.05                     | 0.57              |
| 3:A:314:ALA:C    | 3:A:319:GLY:O     | 2.47                     | 0.57              |
| 3:A:780:VAL:HG23 | 4:B:699:GLU:CD    | 2.29                     | 0.57              |
| 3:A:845:LEU:O    | 3:A:848:ILE:HG12  | 2.04                     | 0.57              |
| 3:A:1042:PHE:CE2 | 3:A:1046:LEU:CD1  | 2.88                     | 0.57              |
| 3:A:1368:MET:O   | 3:A:1371:LEU:HB3  | 2.04                     | 0.57              |
| 4:B:616:ILE:HD12 | 4:B:616:ILE:H     | 1.69                     | 0.57              |
| 8:H:89:LEU:HD22  | 8:H:91:ASP:OD2    | 2.04                     | 0.57              |
| 11:K:50:LEU:O    | 11:K:56:VAL:HG11  | 2.05                     | 0.57              |
| 3:A:300:VAL:O    | 3:A:300:VAL:HG12  | 2.02                     | 0.57              |
| 3:A:897:TYR:N    | 3:A:897:TYR:CD1   | 2.70                     | 0.57              |
| 6:E:40:GLU:O     | 6:E:43:LYS:HB3    | 2.04                     | 0.57              |
| 6:E:164:LEU:HD22 | 6:E:211:TYR:HD2   | 1.69                     | 0.57              |
| 3:A:103:CYS:O    | 3:A:105:CYS:N     | 2.37                     | 0.57              |
| 3:A:455:MET:HE3  | 4:B:1134:GLU:HG3  | 1.86                     | 0.57              |
| 3:A:564:ALA:O    | 8:H:97:MET:HB3    | 2.04                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:738:LYS:NZ    | 5:C:194:GLU:HA   | 2.19                     | 0.57              |
| 3:A:979:SER:OG    | 3:A:981:LEU:HD12 | 2.04                     | 0.57              |
| 3:A:1007:ILE:O    | 3:A:1010:ALA:HB3 | 2.04                     | 0.57              |
| 3:A:1256:GLU:O    | 3:A:1259:MET:N   | 2.37                     | 0.57              |
| 4:B:205:ILE:CG2   | 4:B:206:ASN:ND2  | 2.67                     | 0.57              |
| 4:B:796:LEU:HB3   | 4:B:799:PRO:HG3  | 1.86                     | 0.57              |
| 4:B:1077:THR:HG22 | 4:B:1079:LYS:N   | 2.18                     | 0.57              |
| 4:B:1219:ASP:O    | 4:B:1221:SER:N   | 2.37                     | 0.57              |
| 5:C:73:GLN:HG3    | 5:C:74:SER:N     | 2.18                     | 0.57              |
| 6:E:88:VAL:O      | 6:E:116:ILE:HA   | 2.05                     | 0.57              |
| 6:E:97:VAL:HG13   | 6:E:127:ILE:HG21 | 1.86                     | 0.57              |
| 6:E:197:LYS:C     | 6:E:198:ILE:HG13 | 2.28                     | 0.57              |
| 11:K:70:ARG:O     | 11:K:71:PHE:HB3  | 2.02                     | 0.57              |
| 12:L:60:ARG:HD2   | 12:L:61:THR:H    | 1.70                     | 0.57              |
| 3:A:18:GLN:HB3    | 4:B:1215:ARG:HG3 | 1.86                     | 0.57              |
| 3:A:41:MET:HB3    | 3:A:48:ALA:O     | 2.04                     | 0.57              |
| 3:A:115:LEU:CD1   | 3:A:142:CYS:HB3  | 2.34                     | 0.57              |
| 3:A:582:ILE:CD1   | 3:A:629:LEU:HD11 | 2.34                     | 0.57              |
| 3:A:808:LEU:O     | 4:B:728:ARG:NH1  | 2.37                     | 0.57              |
| 3:A:1154:TYR:HD1  | 3:A:1191:TRP:CH2 | 2.21                     | 0.57              |
| 3:A:1195:LEU:HD11 | 3:A:1267:MET:CE  | 2.34                     | 0.57              |
| 4:B:952:VAL:HB    | 12:L:58:LYS:HB2  | 1.86                     | 0.57              |
| 4:B:1006:ILE:CD1  | 10:J:45:CYS:SG   | 2.93                     | 0.57              |
| 5:C:36:VAL:HG23   | 11:K:41:THR:CG2  | 2.29                     | 0.57              |
| 6:E:127:ILE:HD13  | 6:E:127:ILE:H    | 1.70                     | 0.57              |
| 11:K:100:ALA:O    | 11:K:103:THR:HB  | 2.04                     | 0.57              |
| 3:A:22:PHE:HB2    | 4:B:1211:ASN:OD1 | 2.04                     | 0.57              |
| 3:A:224:PHE:CZ    | 3:A:231:PRO:HG3  | 2.39                     | 0.57              |
| 3:A:396:PRO:C     | 3:A:397:ASN:OD1  | 2.48                     | 0.57              |
| 3:A:442:VAL:O     | 3:A:457:ALA:HA   | 2.04                     | 0.57              |
| 3:A:1376:THR:HG23 | 3:A:1376:THR:O   | 2.03                     | 0.57              |
| 4:B:23:ALA:HB1    | 4:B:24:PRO:HD2   | 1.86                     | 0.57              |
| 4:B:33:VAL:O      | 4:B:36:ALA:HB3   | 2.05                     | 0.57              |
| 4:B:744:HIS:O     | 4:B:747:MET:HG2  | 2.04                     | 0.57              |
| 4:B:754:SER:O     | 4:B:806:THR:HG21 | 2.04                     | 0.57              |
| 4:B:913:GLY:HA2   | 4:B:938:SER:CB   | 2.35                     | 0.57              |
| 6:E:35:VAL:C      | 6:E:37:LEU:H     | 2.13                     | 0.57              |
| 7:F:82:THR:HG22   | 7:F:83:PRO:HD2   | 1.87                     | 0.57              |
| 2:T:5:DT:H1'      | 3:A:448:PRO:HB3  | 1.87                     | 0.57              |
| 3:A:247:ARG:O     | 3:A:247:ARG:HG3  | 2.05                     | 0.57              |
| 3:A:396:PRO:C     | 3:A:397:ASN:CG   | 2.73                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1035:TYR:O    | 3:A:1037:LEU:N    | 2.37                     | 0.57              |
| 3:A:1349:TYR:HD2  | 3:A:1350:LYS:N    | 2.02                     | 0.57              |
| 4:B:295:GLY:C     | 4:B:297:ILE:N     | 2.55                     | 0.57              |
| 4:B:361:LEU:O     | 4:B:363:HIS:O     | 2.23                     | 0.57              |
| 4:B:839:MET:HG3   | 4:B:1010:LEU:HD11 | 1.87                     | 0.57              |
| 4:B:1035:ALA:O    | 4:B:1036:ALA:C    | 2.46                     | 0.57              |
| 6:E:161:LYS:HD2   | 6:E:195:VAL:HG23  | 1.85                     | 0.57              |
| 11:K:49:GLU:C     | 11:K:51:LEU:H     | 2.11                     | 0.57              |
| 3:A:511:ILE:HG12  | 3:A:521:MET:HE3   | 1.87                     | 0.57              |
| 3:A:540:PHE:HD2   | 3:A:572:TRP:O     | 1.87                     | 0.57              |
| 3:A:546:VAL:O     | 3:A:550:LEU:CD2   | 2.53                     | 0.57              |
| 3:A:783:THR:HG21  | 3:A:815:PHE:CE2   | 2.40                     | 0.57              |
| 4:B:644:GLU:CG    | 4:B:654:ARG:HH22  | 2.18                     | 0.57              |
| 4:B:708:GLU:CG    | 4:B:709:ASP:H     | 2.04                     | 0.57              |
| 3:A:35:ILE:HG22   | 3:A:35:ILE:O      | 2.05                     | 0.57              |
| 3:A:95:PHE:O      | 3:A:96:ILE:C      | 2.48                     | 0.57              |
| 3:A:255:SER:HB3   | 4:B:918:ILE:CG2   | 2.35                     | 0.57              |
| 3:A:348:SER:HB2   | 4:B:1128:LEU:HD12 | 1.86                     | 0.57              |
| 3:A:403:LYS:HB2   | 3:A:404:TYR:HD1   | 1.67                     | 0.57              |
| 3:A:1391:ARG:HG2  | 3:A:1391:ARG:HH11 | 1.70                     | 0.57              |
| 4:B:28:GLU:O      | 4:B:30:SER:N      | 2.37                     | 0.57              |
| 4:B:519:TRP:CH2   | 4:B:705:MET:HE1   | 2.39                     | 0.57              |
| 4:B:797:TYR:HB3   | 4:B:798:TYR:CE1   | 2.40                     | 0.57              |
| 6:E:164:LEU:HD22  | 6:E:211:TYR:CD2   | 2.40                     | 0.57              |
| 7:F:111:LEU:C     | 7:F:113:GLY:N     | 2.54                     | 0.57              |
| 3:A:47:ARG:HH21   | 3:A:255:SER:HA    | 1.70                     | 0.56              |
| 3:A:55:ASP:O      | 3:A:58:LEU:N      | 2.25                     | 0.56              |
| 3:A:591:PHE:CD2   | 3:A:595:THR:HG22  | 2.40                     | 0.56              |
| 3:A:1076:ALA:C    | 3:A:1078:GLN:H    | 2.12                     | 0.56              |
| 3:A:1116:LEU:CD2  | 3:A:1311:VAL:HA   | 2.35                     | 0.56              |
| 3:A:1238:ILE:HG22 | 3:A:1240:CYS:SG   | 2.45                     | 0.56              |
| 4:B:708:GLU:C     | 4:B:710:LEU:N     | 2.60                     | 0.56              |
| 4:B:798:TYR:CD1   | 4:B:798:TYR:N     | 2.71                     | 0.56              |
| 7:F:147:SER:OG    | 7:F:150:GLU:CG    | 2.48                     | 0.56              |
| 8:H:36:CYS:CB     | 8:H:130:ARG:HH22  | 2.17                     | 0.56              |
| 11:K:56:VAL:HA    | 11:K:77:THR:HG22  | 1.87                     | 0.56              |
| 3:A:18:GLN:HB3    | 4:B:1215:ARG:HB2  | 1.86                     | 0.56              |
| 3:A:31:SER:HB2    | 3:A:83:HIS:HB3    | 1.87                     | 0.56              |
| 3:A:726:ARG:HG2   | 3:A:727:ASP:N     | 2.19                     | 0.56              |
| 3:A:765:VAL:CG2   | 3:A:800:VAL:CG1   | 2.83                     | 0.56              |
| 3:A:857:ARG:HB3   | 3:A:863:VAL:HA    | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:64:CYS:O     | 4:B:65:GLU:HB3   | 2.04                     | 0.56              |
| 4:B:361:LEU:CD2  | 4:B:377:PHE:HD2  | 2.18                     | 0.56              |
| 4:B:365:THR:CG2  | 4:B:366:GLN:N    | 2.68                     | 0.56              |
| 4:B:666:TYR:O    | 4:B:668:ASP:N    | 2.33                     | 0.56              |
| 4:B:800:GLN:CG   | 10:J:52:THR:CG2  | 2.82                     | 0.56              |
| 8:H:129:TYR:CD2  | 8:H:129:TYR:N    | 2.73                     | 0.56              |
| 9:I:106:CYS:O    | 9:I:107:SER:C    | 2.46                     | 0.56              |
| 3:A:18:GLN:NE2   | 3:A:1418:LEU:HB2 | 2.20                     | 0.56              |
| 3:A:67:CYS:O     | 3:A:70:CYS:CB    | 2.32                     | 0.56              |
| 3:A:130:ASP:O    | 3:A:132:LYS:N    | 2.38                     | 0.56              |
| 3:A:135:PHE:HD1  | 3:A:222:LEU:CB   | 2.19                     | 0.56              |
| 3:A:211:PHE:C    | 3:A:213:HIS:H    | 2.13                     | 0.56              |
| 3:A:522:GLY:O    | 3:A:523:ILE:HD12 | 2.05                     | 0.56              |
| 3:A:531:ILE:HD12 | 3:A:649:ILE:CG2  | 2.35                     | 0.56              |
| 3:A:565:ILE:HG12 | 3:A:567:LYS:NZ   | 2.20                     | 0.56              |
| 3:A:635:ARG:CZ   | 3:A:877:HIS:ND1  | 2.68                     | 0.56              |
| 3:A:668:ASP:OD2  | 3:A:742:ASN:ND2  | 2.32                     | 0.56              |
| 3:A:706:HIS:CD2  | 3:A:1282:VAL:O   | 2.58                     | 0.56              |
| 3:A:733:ALA:O    | 3:A:734:GLU:C    | 2.45                     | 0.56              |
| 3:A:898:ARG:C    | 3:A:898:ARG:CD   | 2.77                     | 0.56              |
| 3:A:925:LEU:O    | 3:A:928:LEU:N    | 2.39                     | 0.56              |
| 3:A:1068:ALA:O   | 3:A:1069:ALA:C   | 2.47                     | 0.56              |
| 4:B:121:ASN:HD22 | 4:B:121:ASN:H    | 1.53                     | 0.56              |
| 4:B:252:SER:O    | 4:B:252:SER:OG   | 2.20                     | 0.56              |
| 4:B:554:ILE:O    | 4:B:555:ILE:C    | 2.48                     | 0.56              |
| 4:B:640:VAL:CG2  | 4:B:740:HIS:CA   | 2.82                     | 0.56              |
| 4:B:782:LEU:O    | 4:B:783:THR:C    | 2.47                     | 0.56              |
| 4:B:954:VAL:HG21 | 12:L:29:TYR:HE2  | 1.69                     | 0.56              |
| 4:B:955:THR:HG23 | 12:L:54:ARG:C    | 2.30                     | 0.56              |
| 5:C:66:ARG:CZ    | 10:J:2:ILE:HG21  | 2.36                     | 0.56              |
| 5:C:181:ASP:CG   | 5:C:186:LEU:HD13 | 2.29                     | 0.56              |
| 3:A:67:CYS:O     | 3:A:68:GLN:NE2   | 2.38                     | 0.56              |
| 3:A:267:ALA:O    | 3:A:268:ASP:C    | 2.48                     | 0.56              |
| 3:A:947:PHE:CD2  | 3:A:954:TRP:CE2  | 2.94                     | 0.56              |
| 4:B:175:ARG:CG   | 4:B:175:ARG:NH1  | 2.62                     | 0.56              |
| 4:B:412:LEU:HB3  | 4:B:466:TRP:NE1  | 2.19                     | 0.56              |
| 4:B:461:LEU:HD11 | 4:B:466:TRP:HH2  | 1.71                     | 0.56              |
| 4:B:466:TRP:HB2  | 4:B:479:VAL:CG2  | 2.36                     | 0.56              |
| 5:C:162:GLY:HA3  | 5:C:170:TRP:CE2  | 2.41                     | 0.56              |
| 3:A:443:LEU:HD12 | 4:B:1146:PHE:CZ  | 2.41                     | 0.56              |
| 3:A:909:ASP:CG   | 3:A:910:PRO:HD3  | 2.30                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1355:VAL:O    | 3:A:1358:SER:OG   | 2.23                     | 0.56              |
| 4:B:454:THR:HG22  | 4:B:454:THR:O     | 2.05                     | 0.56              |
| 4:B:689:LEU:O     | 4:B:690:VAL:HG23  | 2.04                     | 0.56              |
| 4:B:893:LEU:HD21  | 4:B:913:GLY:H     | 1.71                     | 0.56              |
| 4:B:1202:LEU:O    | 4:B:1203:LEU:C    | 2.48                     | 0.56              |
| 5:C:36:VAL:CG2    | 11:K:41:THR:HG21  | 2.32                     | 0.56              |
| 5:C:169:LYS:NZ    | 12:L:69:ALA:O     | 2.38                     | 0.56              |
| 6:E:27:GLY:O      | 6:E:28:TYR:CD2    | 2.59                     | 0.56              |
| 7:F:111:LEU:H     | 7:F:111:LEU:CD1   | 2.19                     | 0.56              |
| 11:K:33:ILE:CD1   | 11:K:87:LEU:HD22  | 2.36                     | 0.56              |
| 3:A:18:GLN:HG3    | 3:A:228:PHE:CE1   | 2.40                     | 0.56              |
| 3:A:18:GLN:CB     | 4:B:1215:ARG:HB2  | 2.35                     | 0.56              |
| 3:A:209:ASN:O     | 3:A:210:ILE:C     | 2.47                     | 0.56              |
| 3:A:303:TYR:O     | 3:A:325:ILE:HG13  | 2.06                     | 0.56              |
| 3:A:803:SER:C     | 3:A:805:LEU:N     | 2.60                     | 0.56              |
| 3:A:901:LEU:HD23  | 3:A:907:THR:HG22  | 1.83                     | 0.56              |
| 3:A:1116:LEU:HD13 | 3:A:1329:THR:OG1  | 2.05                     | 0.56              |
| 3:A:1322:ILE:H    | 3:A:1322:ILE:HD13 | 1.70                     | 0.56              |
| 4:B:476:ARG:O     | 4:B:478:GLY:N     | 2.39                     | 0.56              |
| 4:B:642:ASP:HA    | 4:B:649:LYS:HA    | 1.87                     | 0.56              |
| 4:B:792:MET:HA    | 4:B:856:PHE:O     | 2.05                     | 0.56              |
| 5:C:77:ILE:HA     | 5:C:129:ILE:HD11  | 1.87                     | 0.56              |
| 6:E:171:LYS:O     | 6:E:172:GLU:C     | 2.48                     | 0.56              |
| 8:H:15:VAL:HG22   | 8:H:26:ILE:HD11   | 1.88                     | 0.56              |
| 8:H:47:PHE:CD2    | 8:H:95:TYR:CB     | 2.89                     | 0.56              |
| 3:A:289:ILE:HG22  | 3:A:290:GLU:N     | 2.21                     | 0.56              |
| 3:A:531:ILE:HD12  | 3:A:649:ILE:HG21  | 1.87                     | 0.56              |
| 3:A:804:TYR:CE2   | 4:B:763:GLN:HA    | 2.40                     | 0.56              |
| 3:A:805:LEU:O     | 4:B:761:HIS:ND1   | 2.38                     | 0.56              |
| 3:A:924:LYS:O     | 3:A:927:VAL:HG12  | 2.06                     | 0.56              |
| 3:A:1340:GLY:N    | 6:E:183:PRO:HG2   | 2.20                     | 0.56              |
| 3:A:1394:THR:CG2  | 3:A:1395:GLY:N    | 2.68                     | 0.56              |
| 4:B:169:ARG:N     | 4:B:454:THR:OG1   | 2.39                     | 0.56              |
| 4:B:560:GLU:O     | 4:B:561:TRP:CD1   | 2.58                     | 0.56              |
| 4:B:686:ASN:C     | 4:B:688:GLY:H     | 2.14                     | 0.56              |
| 4:B:816:GLU:C     | 4:B:818:PRO:HD3   | 2.30                     | 0.56              |
| 4:B:1182:CYS:O    | 4:B:1182:CYS:SG   | 2.63                     | 0.56              |
| 4:B:1202:LEU:O    | 4:B:1205:GLN:N    | 2.38                     | 0.56              |
| 5:C:58:LEU:CD2    | 10:J:57:ILE:HD13  | 2.35                     | 0.56              |
| 5:C:244:VAL:CG2   | 5:C:245:VAL:N     | 2.69                     | 0.56              |
| 6:E:182:ASP:O     | 6:E:185:ALA:N     | 2.38                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:F:72:LYS:O      | 7:F:73:ALA:CB     | 2.54                     | 0.56              |
| 8:H:38:LEU:HB2    | 8:H:125:LEU:CD1   | 2.36                     | 0.56              |
| 9:I:56:ALA:O      | 9:I:57:GLY:C      | 2.44                     | 0.56              |
| 3:A:463:ILE:CB    | 3:A:464:PRO:HD2   | 2.30                     | 0.56              |
| 3:A:868:TYR:CE1   | 3:A:1064:VAL:CG2  | 2.89                     | 0.56              |
| 3:A:962:ARG:HA    | 3:A:965:GLN:HE21  | 1.71                     | 0.56              |
| 4:B:1017:ILE:H    | 4:B:1018:PRO:CD   | 2.19                     | 0.56              |
| 11:K:83:PRO:HA    | 11:K:86:ALA:HB3   | 1.87                     | 0.56              |
| 3:A:765:VAL:HG23  | 3:A:800:VAL:HB    | 1.87                     | 0.56              |
| 3:A:1001:ARG:HD2  | 7:F:80:ALA:O      | 2.05                     | 0.56              |
| 4:B:236:HIS:CD2   | 4:B:389:ALA:CB    | 2.88                     | 0.56              |
| 4:B:362:PRO:C     | 4:B:363:HIS:O     | 2.40                     | 0.56              |
| 4:B:469:GLN:HG3   | 4:B:470:LYS:H     | 1.70                     | 0.56              |
| 4:B:789:MET:HE1   | 4:B:965:LYS:O     | 2.06                     | 0.56              |
| 5:C:22:LEU:HD23   | 5:C:25:VAL:HG21   | 1.84                     | 0.56              |
| 3:A:346:ASP:HB2   | 4:B:1154:ALA:HB1  | 1.88                     | 0.56              |
| 3:A:531:ILE:CD1   | 3:A:622:VAL:HG11  | 2.34                     | 0.56              |
| 3:A:599:SER:C     | 3:A:601:LYS:N     | 2.64                     | 0.56              |
| 3:A:672:ASP:CG    | 3:A:674:PRO:HD2   | 2.31                     | 0.56              |
| 4:B:298:LEU:N     | 4:B:298:LEU:HD23  | 2.20                     | 0.56              |
| 4:B:323:VAL:O     | 4:B:323:VAL:HG12  | 2.06                     | 0.56              |
| 5:C:194:GLU:C     | 5:C:195:GLN:HG3   | 2.30                     | 0.56              |
| 6:E:63:ASN:HB3    | 6:E:64:PRO:HD2    | 1.88                     | 0.56              |
| 11:K:32:VAL:CG2   | 11:K:74:ARG:HG3   | 2.32                     | 0.56              |
| 3:A:365:GLY:HA3   | 3:A:469:ARG:HB2   | 1.87                     | 0.55              |
| 3:A:496:GLU:O     | 3:A:499:ALA:HB3   | 2.06                     | 0.55              |
| 3:A:711:ARG:HH12  | 9:I:95:THR:HB     | 1.70                     | 0.55              |
| 3:A:818:MET:O     | 3:A:819:GLY:C     | 2.49                     | 0.55              |
| 3:A:841:LEU:O     | 3:A:845:LEU:HG    | 2.05                     | 0.55              |
| 3:A:1325:THR:HG22 | 3:A:1326:ARG:HG3  | 1.87                     | 0.55              |
| 3:A:1410:PHE:HD2  | 4:B:1212:ILE:HD11 | 1.64                     | 0.55              |
| 4:B:361:LEU:HD23  | 4:B:377:PHE:HD2   | 1.70                     | 0.55              |
| 5:C:74:SER:CA     | 5:C:77:ILE:HG12   | 2.35                     | 0.55              |
| 5:C:80:LEU:HD11   | 5:C:95:CYS:C      | 2.31                     | 0.55              |
| 7:F:75:PRO:C      | 7:F:77:ASP:H      | 2.14                     | 0.55              |
| 7:F:97:ARG:O      | 7:F:98:ALA:C      | 2.49                     | 0.55              |
| 8:H:99:GLY:O      | 8:H:138:GLU:O     | 2.24                     | 0.55              |
| 9:I:33:SER:O      | 9:I:34:TYR:C      | 2.48                     | 0.55              |
| 3:A:23:SER:HB3    | 3:A:233:TRP:CZ2   | 2.41                     | 0.55              |
| 3:A:116:ASP:C     | 3:A:118:HIS:N     | 2.58                     | 0.55              |
| 3:A:247:ARG:NH1   | 3:A:263:THR:HG23  | 2.19                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:709:THR:HB    | 3:A:712:GLU:H     | 1.71                     | 0.55              |
| 3:A:1117:THR:N    | 3:A:1328:TYR:O    | 2.35                     | 0.55              |
| 4:B:130:VAL:HG12  | 4:B:132:VAL:CG2   | 2.33                     | 0.55              |
| 4:B:694:ASP:O     | 4:B:695:ALA:C     | 2.50                     | 0.55              |
| 4:B:899:ILE:CD1   | 4:B:911:ILE:HG12  | 2.30                     | 0.55              |
| 6:E:164:LEU:CD1   | 6:E:211:TYR:CE2   | 2.88                     | 0.55              |
| 6:E:187:TYR:HD2   | 6:E:188:LEU:CD2   | 2.17                     | 0.55              |
| 11:K:28:PRO:O     | 11:K:29:ASN:C     | 2.49                     | 0.55              |
| 3:A:397:ASN:OD1   | 3:A:397:ASN:N     | 2.39                     | 0.55              |
| 3:A:414:ASP:C     | 3:A:414:ASP:OD1   | 2.48                     | 0.55              |
| 3:A:590:ARG:HH11  | 3:A:590:ARG:CG    | 2.15                     | 0.55              |
| 3:A:690:VAL:CG2   | 3:A:718:VAL:HG13  | 2.36                     | 0.55              |
| 3:A:873:MET:HG2   | 3:A:957:PRO:HG2   | 1.88                     | 0.55              |
| 3:A:1100:ARG:CZ   | 3:A:1104:ILE:HD11 | 2.37                     | 0.55              |
| 3:A:1319:VAL:CG1  | 3:A:1320:PRO:CD   | 2.84                     | 0.55              |
| 3:A:1410:PHE:CE2  | 4:B:1212:ILE:HD11 | 2.40                     | 0.55              |
| 4:B:130:VAL:CG1   | 4:B:132:VAL:HG23  | 2.31                     | 0.55              |
| 4:B:286:PHE:HB3   | 4:B:297:ILE:HD11  | 1.88                     | 0.55              |
| 4:B:365:THR:HG23  | 4:B:367:LEU:N     | 2.19                     | 0.55              |
| 4:B:613:VAL:HG12  | 4:B:627:PHE:O     | 2.06                     | 0.55              |
| 4:B:627:PHE:HB3   | 4:B:632:ARG:HH11  | 1.70                     | 0.55              |
| 4:B:653:VAL:O     | 4:B:654:ARG:CD    | 2.55                     | 0.55              |
| 4:B:778:MET:O     | 4:B:819:ALA:HB1   | 2.07                     | 0.55              |
| 4:B:1159:ARG:NE   | 4:B:1193:GLN:HG3  | 2.21                     | 0.55              |
| 5:C:98:VAL:C      | 5:C:99:LEU:CD2    | 2.77                     | 0.55              |
| 5:C:258:ILE:HD11  | 11:K:42:LEU:CD2   | 2.29                     | 0.55              |
| 6:E:100:ILE:HG22  | 6:E:101:GLN:N     | 2.21                     | 0.55              |
| 7:F:133:VAL:HG23  | 7:F:147:SER:HA    | 1.88                     | 0.55              |
| 8:H:102:TYR:N     | 8:H:102:TYR:HD2   | 2.05                     | 0.55              |
| 3:A:152:VAL:HG12  | 3:A:153:PRO:N     | 2.22                     | 0.55              |
| 3:A:407:ARG:HD3   | 3:A:413:ILE:HD13  | 1.87                     | 0.55              |
| 3:A:494:SER:N     | 4:B:1149:GLU:OE2  | 2.39                     | 0.55              |
| 4:B:26:THR:O      | 4:B:29:ASP:HB2    | 2.07                     | 0.55              |
| 4:B:315:LYS:HG2   | 9:I:13:MET:HE1    | 1.88                     | 0.55              |
| 4:B:911:ILE:CD1   | 4:B:941:LEU:HD23  | 2.36                     | 0.55              |
| 4:B:979:LYS:C     | 4:B:980:PHE:CD1   | 2.84                     | 0.55              |
| 4:B:1203:LEU:HD11 | 4:B:1207:LEU:HG   | 1.88                     | 0.55              |
| 5:C:8:VAL:HA      | 5:C:21:ILE:O      | 2.06                     | 0.55              |
| 9:I:62:ILE:CG2    | 9:I:63:GLY:N      | 2.69                     | 0.55              |
| 3:A:1392:SER:C    | 3:A:1393:ASN:ND2  | 2.65                     | 0.55              |
| 4:B:203:PHE:CD1   | 4:B:461:LEU:HD21  | 2.41                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:976:ILE:O     | 4:B:990:ILE:HB    | 2.07                     | 0.55              |
| 4:B:1168:LEU:C    | 4:B:1170:THR:H    | 2.13                     | 0.55              |
| 5:C:80:LEU:HD11   | 5:C:95:CYS:HA     | 1.88                     | 0.55              |
| 8:H:12:VAL:HG13   | 8:H:26:ILE:HG23   | 1.88                     | 0.55              |
| 3:A:896:ARG:C     | 3:A:897:TYR:HD1   | 2.15                     | 0.55              |
| 3:A:942:PHE:C     | 3:A:942:PHE:CD2   | 2.85                     | 0.55              |
| 4:B:658:ILE:O     | 4:B:661:LEU:HB2   | 2.07                     | 0.55              |
| 4:B:665:GLU:O     | 4:B:668:ASP:HB2   | 2.07                     | 0.55              |
| 4:B:766:ARG:O     | 4:B:769:TYR:N     | 2.38                     | 0.55              |
| 4:B:897:GLY:O     | 4:B:898:LEU:HD23  | 2.06                     | 0.55              |
| 4:B:900:ALA:HB1   | 12:L:61:THR:OG1   | 2.06                     | 0.55              |
| 4:B:1017:ILE:H    | 4:B:1018:PRO:HD2  | 1.71                     | 0.55              |
| 4:B:1208:MET:HA   | 4:B:1212:ILE:O    | 2.07                     | 0.55              |
| 5:C:172:PRO:CD    | 5:C:173:ALA:N     | 2.69                     | 0.55              |
| 6:E:75:MET:HG2    | 6:E:76:GLY:N      | 2.21                     | 0.55              |
| 3:A:607:ILE:CG1   | 3:A:612:ILE:HA    | 2.37                     | 0.55              |
| 3:A:955:PRO:C     | 3:A:956:LEU:HG    | 2.31                     | 0.55              |
| 3:A:963:ILE:HG22  | 3:A:1045:VAL:HG13 | 1.89                     | 0.55              |
| 3:A:1377:THR:C    | 3:A:1379:GLY:N    | 2.64                     | 0.55              |
| 3:A:1436:ILE:CG2  | 3:A:1437:GLY:N    | 2.70                     | 0.55              |
| 4:B:234:ILE:H     | 4:B:234:ILE:CD1   | 2.12                     | 0.55              |
| 11:K:21:ILE:HG13  | 11:K:33:ILE:HG23  | 1.89                     | 0.55              |
| 3:A:93:VAL:C      | 3:A:95:PHE:H      | 2.15                     | 0.55              |
| 3:A:528:LEU:HD12  | 3:A:528:LEU:C     | 2.31                     | 0.55              |
| 3:A:590:ARG:HH21  | 3:A:620:LYS:C     | 2.14                     | 0.55              |
| 3:A:642:CYS:O     | 3:A:645:LEU:HB3   | 2.06                     | 0.55              |
| 3:A:1338:VAL:HG12 | 3:A:1339:LEU:HG   | 1.88                     | 0.55              |
| 3:A:1342:GLU:CG   | 6:E:212:ARG:NH1   | 2.69                     | 0.55              |
| 4:B:110:HIS:CD2   | 4:B:111:ALA:H     | 2.25                     | 0.55              |
| 4:B:170:LEU:HD12  | 4:B:171:PRO:HD2   | 1.88                     | 0.55              |
| 4:B:760:ASP:O     | 4:B:762:ASN:N     | 2.36                     | 0.55              |
| 4:B:795:ILE:HD12  | 4:B:795:ILE:N     | 2.21                     | 0.55              |
| 4:B:1106:ARG:NH2  | 4:B:1109:GLY:N    | 2.54                     | 0.55              |
| 6:E:16:PHE:O      | 6:E:17:ARG:C      | 2.49                     | 0.55              |
| 3:A:24:PRO:CB     | 3:A:237:THR:HG21  | 2.37                     | 0.55              |
| 4:B:69:LEU:HD22   | 4:B:429:PHE:CE1   | 2.42                     | 0.55              |
| 4:B:400:HIS:CE1   | 4:B:517:THR:HG21  | 2.42                     | 0.55              |
| 4:B:449:ASN:O     | 4:B:451:LYS:N     | 2.40                     | 0.55              |
| 4:B:1051:THR:HG21 | 4:B:1053:GLU:HB2  | 1.89                     | 0.55              |
| 5:C:47:ASP:O      | 5:C:48:SER:HB2    | 2.06                     | 0.55              |
| 9:I:28:GLU:OE2    | 9:I:28:GLU:C      | 2.50                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:7:SER:HA     | 4:B:1175:LEU:HD21 | 1.89                     | 0.55              |
| 3:A:179:LEU:CD1  | 3:A:297:GLN:CG    | 2.81                     | 0.55              |
| 3:A:335:ARG:HH11 | 4:B:1202:LEU:HD12 | 1.72                     | 0.55              |
| 3:A:474:VAL:HG22 | 3:A:474:VAL:O     | 2.07                     | 0.55              |
| 3:A:569:LYS:HD2  | 5:C:221:TYR:O     | 2.06                     | 0.55              |
| 3:A:596:THR:O    | 3:A:597:LEU:C     | 2.46                     | 0.55              |
| 3:A:1127:ASP:C   | 3:A:1129:GLU:H    | 2.13                     | 0.55              |
| 4:B:114:PRO:HG2  | 4:B:181:LEU:HD11  | 1.88                     | 0.55              |
| 4:B:446:LEU:O    | 4:B:446:LEU:HD23  | 2.07                     | 0.55              |
| 4:B:566:LEU:O    | 4:B:567:GLU:C     | 2.50                     | 0.55              |
| 4:B:724:ASP:C    | 4:B:724:ASP:OD1   | 2.50                     | 0.55              |
| 8:H:36:CYS:HB2   | 8:H:126:GLU:O     | 2.06                     | 0.55              |
| 3:A:265:LYS:C    | 3:A:267:ALA:H     | 2.15                     | 0.54              |
| 3:A:618:GLU:C    | 3:A:618:GLU:CD    | 2.75                     | 0.54              |
| 3:A:639:PRO:HG2  | 3:A:640:GLN:H     | 1.72                     | 0.54              |
| 3:A:845:LEU:HB3  | 3:A:1065:GLY:O    | 2.07                     | 0.54              |
| 3:A:853:ASP:OD1  | 3:A:853:ASP:C     | 2.50                     | 0.54              |
| 3:A:937:VAL:O    | 3:A:938:LYS:C     | 2.49                     | 0.54              |
| 4:B:22:SER:O     | 4:B:654:ARG:HD2   | 2.07                     | 0.54              |
| 4:B:70:ILE:O     | 4:B:70:ILE:HG22   | 2.06                     | 0.54              |
| 4:B:118:ARG:HA   | 4:B:207:GLY:HA2   | 1.89                     | 0.54              |
| 4:B:223:VAL:CG1  | 4:B:223:VAL:O     | 2.54                     | 0.54              |
| 4:B:356:LEU:N    | 4:B:356:LEU:CD2   | 2.66                     | 0.54              |
| 4:B:542:MET:HE2  | 4:B:747:MET:HE2   | 1.88                     | 0.54              |
| 4:B:640:VAL:CG2  | 4:B:740:HIS:N     | 2.70                     | 0.54              |
| 4:B:662:MET:C    | 4:B:664:THR:N     | 2.63                     | 0.54              |
| 4:B:899:ILE:HD11 | 4:B:911:ILE:CB    | 2.37                     | 0.54              |
| 4:B:975:GLN:HG2  | 4:B:976:ILE:H     | 1.71                     | 0.54              |
| 4:B:1076:HIS:CG  | 11:K:40:HIS:HD2   | 2.24                     | 0.54              |
| 5:C:43:THR:HG23  | 5:C:44:LEU:H      | 1.72                     | 0.54              |
| 6:E:147:HIS:O    | 6:E:148:GLU:C     | 2.50                     | 0.54              |
| 2:T:8:DT:H2'     | 2:T:9:DC:C6       | 2.41                     | 0.54              |
| 3:A:321:PRO:C    | 3:A:322:VAL:HG13  | 2.32                     | 0.54              |
| 3:A:568:PRO:HB2  | 5:C:221:TYR:CE1   | 2.43                     | 0.54              |
| 3:A:608:ILE:C    | 3:A:609:ASP:O     | 2.48                     | 0.54              |
| 3:A:679:ILE:CG2  | 3:A:729:ALA:HB1   | 2.32                     | 0.54              |
| 3:A:879:GLU:O    | 3:A:881:GLN:HG3   | 2.07                     | 0.54              |
| 3:A:886:ILE:HG22 | 3:A:887:GLY:N     | 2.22                     | 0.54              |
| 4:B:43:LEU:HD11  | 4:B:811:TYR:O     | 2.08                     | 0.54              |
| 4:B:374:LYS:O    | 4:B:375:ALA:C     | 2.50                     | 0.54              |
| 4:B:1008:PRO:HG2 | 4:B:1011:ILE:HD11 | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:1177:HIS:O    | 4:B:1178:ASN:C    | 2.49                     | 0.54              |
| 9:I:59:VAL:O      | 9:I:61:ASP:N      | 2.40                     | 0.54              |
| 11:K:32:VAL:O     | 11:K:32:VAL:CG1   | 2.55                     | 0.54              |
| 3:A:273:ASN:CA    | 3:A:296:LEU:HD11  | 2.37                     | 0.54              |
| 3:A:1224:LEU:HD11 | 3:A:1240:CYS:CB   | 2.37                     | 0.54              |
| 3:A:1225:PHE:C    | 3:A:1226:VAL:HG23 | 2.32                     | 0.54              |
| 3:A:1400:CYS:SG   | 3:A:1409:LEU:HG   | 2.47                     | 0.54              |
| 4:B:236:HIS:C     | 4:B:237:VAL:HG23  | 2.33                     | 0.54              |
| 4:B:900:ALA:CB    | 12:L:61:THR:OG1   | 2.55                     | 0.54              |
| 5:C:58:LEU:HD21   | 10:J:57:ILE:CD1   | 2.33                     | 0.54              |
| 6:E:190:LEU:N     | 6:E:190:LEU:CD2   | 2.69                     | 0.54              |
| 8:H:4:THR:HG22    | 8:H:5:LEU:N       | 2.23                     | 0.54              |
| 8:H:58:THR:HB     | 8:H:143:LEU:CD1   | 2.37                     | 0.54              |
| 8:H:61:SER:HB3    | 8:H:139:ASN:HB3   | 1.90                     | 0.54              |
| 8:H:81:PRO:CB     | 8:H:82:PRO:CD     | 2.71                     | 0.54              |
| 3:A:181:LEU:O     | 3:A:202:LEU:HD12  | 2.08                     | 0.54              |
| 3:A:261:ASP:HB3   | 3:A:323:LYS:HE3   | 1.88                     | 0.54              |
| 3:A:493:GLN:H     | 4:B:1149:GLU:CD   | 2.16                     | 0.54              |
| 3:A:640:GLN:O     | 3:A:643:ALA:HB3   | 2.07                     | 0.54              |
| 3:A:1410:PHE:O    | 3:A:1411:GLU:C    | 2.50                     | 0.54              |
| 4:B:174:LEU:HD22  | 4:B:204:ILE:CD1   | 2.14                     | 0.54              |
| 4:B:423:LYS:HA    | 4:B:426:LYS:HZ1   | 1.72                     | 0.54              |
| 4:B:893:LEU:CD2   | 4:B:913:GLY:H     | 2.21                     | 0.54              |
| 4:B:1064:TYR:N    | 4:B:1064:TYR:CD1  | 2.75                     | 0.54              |
| 6:E:157:SER:C     | 6:E:159:ASP:N     | 2.61                     | 0.54              |
| 7:F:123:LYS:O     | 7:F:123:LYS:CG    | 2.55                     | 0.54              |
| 2:T:1:DA:C2'      | 2:T:2:DC:O5'      | 2.44                     | 0.54              |
| 3:A:283:GLY:O     | 3:A:285:PRO:HD3   | 2.07                     | 0.54              |
| 3:A:417:TYR:O     | 3:A:418:SER:CB    | 2.56                     | 0.54              |
| 3:A:566:ILE:C     | 3:A:567:LYS:O     | 2.48                     | 0.54              |
| 3:A:756:ILE:O     | 3:A:759:ALA:HB3   | 2.08                     | 0.54              |
| 3:A:909:ASP:OD2   | 3:A:910:PRO:HD3   | 2.07                     | 0.54              |
| 3:A:918:GLU:O     | 3:A:918:GLU:OE1   | 2.25                     | 0.54              |
| 3:A:974:ASP:OD1   | 3:A:974:ASP:N     | 2.40                     | 0.54              |
| 3:A:1291:VAL:CG1  | 3:A:1292:PRO:CD   | 2.84                     | 0.54              |
| 3:A:1436:ILE:CD1  | 4:B:1139:ILE:HG23 | 2.38                     | 0.54              |
| 4:B:34:ILE:N      | 4:B:34:ILE:CD1    | 2.71                     | 0.54              |
| 4:B:230:ALA:CB    | 4:B:231:PRO:CD    | 2.83                     | 0.54              |
| 4:B:589:VAL:CG1   | 4:B:590:HIS:N     | 2.70                     | 0.54              |
| 4:B:1073:TYR:N    | 4:B:1073:TYR:CD1  | 2.74                     | 0.54              |
| 5:C:6:PRO:HG2     | 11:K:97:LYS:HB3   | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:166:GLU:HG3   | 11:K:10:PHE:CZ    | 2.42                     | 0.54              |
| 5:C:242:GLN:HE21  | 5:C:246:ARG:NE    | 2.00                     | 0.54              |
| 6:E:9:ILE:O       | 6:E:10:SER:C      | 2.50                     | 0.54              |
| 6:E:90:VAL:H      | 6:E:120:ALA:HB2   | 1.72                     | 0.54              |
| 6:E:126:SER:C     | 6:E:128:PRO:HD3   | 2.29                     | 0.54              |
| 8:H:103:LYS:HB3   | 8:H:115:TYR:HD1   | 1.73                     | 0.54              |
| 9:I:64:SER:O      | 9:I:65:ASP:C      | 2.50                     | 0.54              |
| 11:K:73:LEU:HD21  | 11:K:75:ILE:HD11  | 1.89                     | 0.54              |
| 2:T:5:DT:H2''     | 2:T:6:DC:C5'      | 2.29                     | 0.54              |
| 3:A:273:ASN:N     | 3:A:296:LEU:CD1   | 2.70                     | 0.54              |
| 3:A:605:MET:HA    | 3:A:605:MET:CE    | 2.28                     | 0.54              |
| 3:A:863:VAL:HG23  | 6:E:170:LEU:HD21  | 1.90                     | 0.54              |
| 3:A:1132:LYS:O    | 3:A:1135:ARG:CB   | 2.55                     | 0.54              |
| 3:A:1191:TRP:HD1  | 3:A:1256:GLU:CD   | 2.16                     | 0.54              |
| 3:A:1219:THR:HG21 | 3:A:1271:ILE:HD11 | 1.90                     | 0.54              |
| 4:B:34:ILE:O      | 4:B:35:SER:C      | 2.50                     | 0.54              |
| 4:B:59:LEU:CD1    | 4:B:417:PHE:CE2   | 2.90                     | 0.54              |
| 4:B:288:ALA:O     | 4:B:327:ARG:NH2   | 2.37                     | 0.54              |
| 4:B:356:LEU:O     | 4:B:357:GLN:HG3   | 2.07                     | 0.54              |
| 4:B:843:GLN:HB2   | 4:B:993:THR:HB    | 1.90                     | 0.54              |
| 4:B:899:ILE:HD11  | 4:B:911:ILE:CG2   | 2.36                     | 0.54              |
| 4:B:1084:GLN:HB3  | 5:C:201:TRP:HH2   | 1.72                     | 0.54              |
| 5:C:92:CYS:SG     | 5:C:94:LYS:N      | 2.80                     | 0.54              |
| 5:C:260:LEU:O     | 5:C:263:THR:HB    | 2.08                     | 0.54              |
| 6:E:156:LEU:HD21  | 6:E:197:LYS:HB2   | 1.88                     | 0.54              |
| 6:E:157:SER:O     | 6:E:159:ASP:N     | 2.41                     | 0.54              |
| 6:E:162:ARG:NH2   | 6:E:166:LYS:HZ2   | 2.04                     | 0.54              |
| 7:F:73:ALA:O      | 7:F:74:ILE:CG1    | 2.45                     | 0.54              |
| 8:H:88:SER:O      | 8:H:89:LEU:HG     | 2.07                     | 0.54              |
| 3:A:341:MET:HE1   | 3:A:843:LYS:HZ3   | 1.71                     | 0.54              |
| 3:A:526:ASP:O     | 3:A:527:THR:C     | 2.50                     | 0.54              |
| 3:A:530:GLY:O     | 3:A:653:VAL:CG1   | 2.56                     | 0.54              |
| 3:A:1351:GLU:O    | 3:A:1352:VAL:C    | 2.49                     | 0.54              |
| 4:B:641:GLU:HB3   | 4:B:643:ASP:OD2   | 2.08                     | 0.54              |
| 4:B:707:PRO:CD    | 4:B:708:GLU:H     | 2.19                     | 0.54              |
| 4:B:750:GLY:O     | 4:B:751:VAL:C     | 2.51                     | 0.54              |
| 4:B:1159:ARG:HE   | 4:B:1193:GLN:HE21 | 1.56                     | 0.54              |
| 5:C:172:PRO:CD    | 5:C:173:ALA:H     | 2.21                     | 0.54              |
| 5:C:193:TYR:H     | 5:C:193:TYR:HD2   | 1.55                     | 0.54              |
| 6:E:37:LEU:O      | 6:E:37:LEU:CG     | 2.56                     | 0.54              |
| 6:E:98:ILE:O      | 6:E:100:ILE:N     | 2.40                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:I:25:LEU:O     | 9:I:26:LEU:HD23   | 2.08                     | 0.54              |
| 3:A:54:ASN:O     | 3:A:55:ASP:CB     | 2.56                     | 0.54              |
| 3:A:168:GLY:O    | 3:A:169:ASN:O     | 2.26                     | 0.54              |
| 3:A:447:GLN:HA   | 3:A:448:PRO:C     | 2.33                     | 0.54              |
| 3:A:537:ARG:HH11 | 3:A:537:ARG:CG    | 2.21                     | 0.54              |
| 3:A:1067:LEU:CD2 | 3:A:1367:HIS:CE1  | 2.84                     | 0.54              |
| 3:A:1220:PHE:O   | 3:A:1222:ASN:N    | 2.40                     | 0.54              |
| 4:B:378:LEU:O    | 4:B:382:ILE:HG12  | 2.08                     | 0.54              |
| 4:B:469:GLN:CG   | 4:B:470:LYS:H     | 2.21                     | 0.54              |
| 4:B:563:MET:CE   | 4:B:588:GLY:HA3   | 2.37                     | 0.54              |
| 4:B:577:ALA:HB1  | 4:B:589:VAL:HG11  | 1.86                     | 0.54              |
| 4:B:1099:VAL:O   | 4:B:1103:ILE:CD1  | 2.56                     | 0.54              |
| 4:B:1102:LYS:HB2 | 4:B:1103:ILE:HD13 | 1.90                     | 0.54              |
| 4:B:1170:THR:CG2 | 4:B:1183:LYS:HZ1  | 2.21                     | 0.54              |
| 5:C:69:LEU:N     | 5:C:69:LEU:CD1    | 2.71                     | 0.54              |
| 5:C:80:LEU:HD11  | 5:C:95:CYS:CA     | 2.38                     | 0.54              |
| 6:E:115:ASN:O    | 6:E:116:ILE:HG12  | 2.08                     | 0.54              |
| 3:A:14:VAL:HG23  | 3:A:1432:GLN:HE22 | 1.72                     | 0.54              |
| 3:A:139:TRP:O    | 3:A:141:LEU:N     | 2.40                     | 0.54              |
| 3:A:216:VAL:O    | 3:A:219:PHE:HB2   | 2.08                     | 0.54              |
| 3:A:306:ASN:N    | 3:A:306:ASN:ND2   | 2.55                     | 0.54              |
| 3:A:492:PRO:C    | 3:A:493:GLN:NE2   | 2.63                     | 0.54              |
| 3:A:856:THR:HB   | 3:A:865:GLN:HB2   | 1.89                     | 0.54              |
| 3:A:863:VAL:HG11 | 3:A:866:PHE:CE2   | 2.43                     | 0.54              |
| 3:A:1261:LYS:C   | 3:A:1263:ILE:N    | 2.63                     | 0.54              |
| 4:B:555:ILE:HD11 | 4:B:582:VAL:CG1   | 2.33                     | 0.54              |
| 6:E:157:SER:O    | 6:E:158:SER:C     | 2.51                     | 0.54              |
| 9:I:50:THR:CG2   | 9:I:52:ILE:CG2    | 2.83                     | 0.54              |
| 3:A:353:ILE:HG21 | 3:A:487:MET:HB2   | 1.89                     | 0.54              |
| 3:A:370:ILE:HG22 | 3:A:374:LEU:HD12  | 1.90                     | 0.54              |
| 3:A:547:LEU:CD2  | 11:K:58:PHE:HD1   | 2.14                     | 0.54              |
| 3:A:1325:THR:O   | 6:E:148:GLU:HB2   | 2.07                     | 0.54              |
| 4:B:57:TYR:CD1   | 4:B:57:TYR:N      | 2.76                     | 0.54              |
| 4:B:123:THR:O    | 4:B:125:SER:N     | 2.41                     | 0.54              |
| 4:B:223:VAL:O    | 4:B:223:VAL:HG12  | 2.08                     | 0.54              |
| 4:B:1160:VAL:O   | 4:B:1194:ILE:HD13 | 2.07                     | 0.54              |
| 5:C:99:LEU:N     | 5:C:99:LEU:CD2    | 2.70                     | 0.54              |
| 8:H:131:ASN:C    | 8:H:133:ASN:N     | 2.66                     | 0.54              |
| 11:K:32:VAL:O    | 11:K:32:VAL:HG12  | 2.07                     | 0.54              |
| 11:K:65:HIS:CD2  | 11:K:66:PRO:N     | 2.76                     | 0.54              |
| 3:A:77:CYS:SG    | 3:A:80:HIS:CE1    | 3.01                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:529:CYS:O     | 3:A:529:CYS:SG    | 2.66                     | 0.53              |
| 3:A:1225:PHE:C    | 3:A:1226:VAL:CG2  | 2.81                     | 0.53              |
| 3:A:1229:SER:CB   | 3:A:1233:ASP:OD2  | 2.56                     | 0.53              |
| 4:B:233:PRO:HG2   | 4:B:234:ILE:H     | 1.73                     | 0.53              |
| 4:B:297:ILE:O     | 4:B:300:HIS:N     | 2.41                     | 0.53              |
| 4:B:426:LYS:O     | 4:B:430:ARG:CZ    | 2.56                     | 0.53              |
| 4:B:590:HIS:CD2   | 4:B:596:LEU:HD22  | 2.43                     | 0.53              |
| 4:B:801:LYS:N     | 10:J:52:THR:CG2   | 2.71                     | 0.53              |
| 5:C:265:MET:HE1   | 11:K:19:LEU:O     | 2.09                     | 0.53              |
| 6:E:55:ARG:C      | 6:E:57:MET:N      | 2.66                     | 0.53              |
| 7:F:76:LYS:O      | 7:F:79:ARG:HD3    | 2.08                     | 0.53              |
| 3:A:16:GLU:HB2    | 4:B:1217:TYR:HB2  | 1.91                     | 0.53              |
| 3:A:401:GLY:CA    | 3:A:435:HIS:HD2   | 2.21                     | 0.53              |
| 3:A:989:GLY:O     | 3:A:990:VAL:C     | 2.51                     | 0.53              |
| 3:A:996:ASN:C     | 3:A:998:LEU:N     | 2.62                     | 0.53              |
| 3:A:1133:LEU:H    | 3:A:1133:LEU:HD23 | 1.71                     | 0.53              |
| 4:B:292:ILE:HD12  | 4:B:326:ASP:HA    | 1.90                     | 0.53              |
| 4:B:1084:GLN:NE2  | 5:C:191:TYR:C     | 2.66                     | 0.53              |
| 4:B:1096:ARG:HH11 | 4:B:1096:ARG:HG2  | 1.72                     | 0.53              |
| 5:C:255:VAL:HG12  | 11:K:91:CYS:HB3   | 1.90                     | 0.53              |
| 8:H:84:ALA:HB1    | 8:H:87:ARG:CB     | 2.38                     | 0.53              |
| 3:A:139:TRP:C     | 3:A:141:LEU:N     | 2.63                     | 0.53              |
| 3:A:273:ASN:N     | 3:A:296:LEU:HD11  | 2.22                     | 0.53              |
| 3:A:805:LEU:HD12  | 3:A:806:ARG:N     | 2.22                     | 0.53              |
| 3:A:889:SER:CB    | 3:A:892:ALA:H     | 2.11                     | 0.53              |
| 3:A:897:TYR:CD2   | 3:A:936:LEU:HD13  | 2.32                     | 0.53              |
| 3:A:1148:ILE:CD1  | 3:A:1198:ASP:HB2  | 2.38                     | 0.53              |
| 3:A:1349:TYR:O    | 3:A:1350:LYS:C    | 2.49                     | 0.53              |
| 3:A:1441:PHE:CZ   | 7:F:88:TYR:C      | 2.87                     | 0.53              |
| 4:B:361:LEU:N     | 4:B:361:LEU:HD12  | 2.22                     | 0.53              |
| 4:B:917:PRO:C     | 4:B:918:ILE:HD13  | 2.33                     | 0.53              |
| 4:B:1219:ASP:C    | 4:B:1221:SER:N    | 2.64                     | 0.53              |
| 5:C:52:GLU:HA     | 12:L:64:LEU:HD22  | 1.91                     | 0.53              |
| 5:C:57:VAL:CG2    | 10:J:57:ILE:HD11  | 2.37                     | 0.53              |
| 5:C:63:ILE:HG22   | 5:C:67:LEU:HD11   | 1.91                     | 0.53              |
| 2:T:1:DA:H2''     | 2:T:2:DC:C5'      | 2.39                     | 0.53              |
| 3:A:26:GLU:O      | 3:A:27:VAL:C      | 2.50                     | 0.53              |
| 3:A:107:CYS:O     | 3:A:111:GLY:HA2   | 2.09                     | 0.53              |
| 3:A:265:LYS:HZ1   | 3:A:322:VAL:CB    | 2.21                     | 0.53              |
| 3:A:577:ILE:C     | 3:A:579:SER:N     | 2.65                     | 0.53              |
| 3:A:857:ARG:NH1   | 7:F:139:PRO:HG2   | 2.24                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:896:ARG:HB3   | 3:A:897:TYR:CD1   | 2.44                     | 0.53              |
| 3:A:913:LEU:HD12  | 3:A:915:SER:N     | 2.21                     | 0.53              |
| 3:A:1098:VAL:O    | 3:A:1099:PRO:C    | 2.51                     | 0.53              |
| 3:A:1227:ILE:O    | 3:A:1238:ILE:HA   | 2.09                     | 0.53              |
| 3:A:1326:ARG:O    | 3:A:1327:ILE:O    | 2.26                     | 0.53              |
| 4:B:638:PHE:HD2   | 4:B:653:VAL:HG21  | 1.71                     | 0.53              |
| 4:B:821:GLN:HB2   | 4:B:851:PHE:CE2   | 2.44                     | 0.53              |
| 4:B:856:PHE:CD1   | 4:B:856:PHE:N     | 2.76                     | 0.53              |
| 4:B:992:ILE:HD13  | 11:K:67:PHE:HE2   | 1.71                     | 0.53              |
| 4:B:1106:ARG:NH1  | 4:B:1118:PRO:HB3  | 2.23                     | 0.53              |
| 5:C:36:VAL:O      | 5:C:37:MET:C      | 2.51                     | 0.53              |
| 6:E:153:HIS:O     | 6:E:154:ILE:HG12  | 2.09                     | 0.53              |
| 9:I:85:PHE:C      | 9:I:86:PHE:CD2    | 2.86                     | 0.53              |
| 11:K:47:ARG:HH11  | 11:K:47:ARG:HG2   | 1.73                     | 0.53              |
| 3:A:24:PRO:HG3    | 3:A:237:THR:HG21  | 1.89                     | 0.53              |
| 3:A:89:PRO:C      | 3:A:90:VAL:HG23   | 2.33                     | 0.53              |
| 3:A:116:ASP:C     | 3:A:118:HIS:H     | 2.15                     | 0.53              |
| 3:A:472:LEU:HD11  | 4:B:835:GLN:CD    | 2.33                     | 0.53              |
| 3:A:543:LEU:CD1   | 3:A:547:LEU:HD11  | 2.39                     | 0.53              |
| 3:A:544:ASP:OD1   | 3:A:545:GLN:N     | 2.40                     | 0.53              |
| 3:A:567:LYS:HG3   | 3:A:568:PRO:HG2   | 1.90                     | 0.53              |
| 3:A:679:ILE:HG23  | 3:A:729:ALA:CB    | 2.34                     | 0.53              |
| 3:A:690:VAL:CG1   | 3:A:718:VAL:HG13  | 2.39                     | 0.53              |
| 3:A:691:LEU:C     | 3:A:691:LEU:HD12  | 2.33                     | 0.53              |
| 3:A:1155:ASP:HB3  | 3:A:1241:ARG:HH21 | 1.73                     | 0.53              |
| 4:B:228:LYS:O     | 4:B:229:ALA:O     | 2.25                     | 0.53              |
| 4:B:487:THR:CG2   | 4:B:488:TYR:N     | 2.71                     | 0.53              |
| 4:B:877:PRO:O     | 4:B:878:GLN:CG    | 2.56                     | 0.53              |
| 4:B:1147:LEU:O    | 4:B:1151:LEU:HB2  | 2.09                     | 0.53              |
| 4:B:1158:PHE:CE2  | 4:B:1160:VAL:HG22 | 2.43                     | 0.53              |
| 11:K:65:HIS:HD2   | 11:K:67:PHE:N     | 1.97                     | 0.53              |
| 3:A:351:THR:HG21  | 3:A:466:SER:O     | 2.08                     | 0.53              |
| 3:A:613:ILE:HD13  | 3:A:613:ILE:N     | 2.23                     | 0.53              |
| 3:A:928:LEU:O     | 3:A:931:GLU:N     | 2.42                     | 0.53              |
| 3:A:947:PHE:HD2   | 3:A:954:TRP:CZ2   | 2.27                     | 0.53              |
| 3:A:1105:LEU:HD23 | 3:A:1384:VAL:HG21 | 1.89                     | 0.53              |
| 3:A:1118:VAL:O    | 3:A:1305:VAL:HG13 | 2.08                     | 0.53              |
| 3:A:1348:LEU:O    | 3:A:1352:VAL:HG23 | 2.09                     | 0.53              |
| 3:A:1408:ILE:O    | 3:A:1412:ALA:HB2  | 2.07                     | 0.53              |
| 4:B:654:ARG:C     | 4:B:656:GLY:N     | 2.65                     | 0.53              |
| 4:B:1096:ARG:HG3  | 4:B:1097:HIS:N    | 2.23                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:C:70:ILE:HD11   | 5:C:144:ILE:HD11 | 1.86                     | 0.53              |
| 7:F:99:LEU:CD1    | 7:F:99:LEU:C     | 2.82                     | 0.53              |
| 12:L:45:ALA:O     | 12:L:46:VAL:HG23 | 2.09                     | 0.53              |
| 3:A:82:GLY:HA3    | 3:A:241:VAL:HB   | 1.91                     | 0.53              |
| 3:A:250:ILE:O     | 3:A:251:SER:HB3  | 2.08                     | 0.53              |
| 3:A:381:THR:HG23  | 3:A:382:PRO:CD   | 2.38                     | 0.53              |
| 3:A:456:MET:HG3   | 3:A:478:TYR:HH   | 1.73                     | 0.53              |
| 3:A:484:GLY:O     | 3:A:485:ASP:C    | 2.51                     | 0.53              |
| 3:A:582:ILE:HG22  | 3:A:610:GLY:CA   | 2.39                     | 0.53              |
| 3:A:755:PHE:O     | 3:A:758:ILE:N    | 2.42                     | 0.53              |
| 3:A:1041:ALA:O    | 3:A:1042:PHE:C   | 2.52                     | 0.53              |
| 3:A:1313:LEU:O    | 3:A:1314:SER:C   | 2.52                     | 0.53              |
| 3:A:1444:MET:CB   | 7:F:133:VAL:HG12 | 2.38                     | 0.53              |
| 4:B:321:GLY:O     | 4:B:324:ILE:N    | 2.41                     | 0.53              |
| 4:B:604:ARG:HH21  | 4:B:614:SER:HA   | 1.74                     | 0.53              |
| 4:B:826:ALA:HB2   | 4:B:1087:PHE:CE1 | 2.43                     | 0.53              |
| 5:C:60:ASP:CB     | 12:L:67:PHE:CE1  | 2.80                     | 0.53              |
| 5:C:67:LEU:O      | 5:C:70:ILE:HB    | 2.08                     | 0.53              |
| 5:C:133:ILE:C     | 5:C:134:ILE:HD13 | 2.32                     | 0.53              |
| 5:C:227:THR:C     | 5:C:228:PHE:CD1  | 2.86                     | 0.53              |
| 7:F:81:THR:CG2    | 7:F:136:ARG:HH11 | 2.19                     | 0.53              |
| 7:F:109:VAL:CG2   | 7:F:124:GLU:CG   | 2.87                     | 0.53              |
| 3:A:104:GLU:O     | 3:A:142:CYS:O    | 2.26                     | 0.53              |
| 3:A:116:ASP:O     | 3:A:118:HIS:N    | 2.41                     | 0.53              |
| 3:A:219:PHE:CZ    | 3:A:230:ARG:HG2  | 2.44                     | 0.53              |
| 3:A:341:MET:HE1   | 3:A:843:LYS:HZ1  | 1.74                     | 0.53              |
| 3:A:382:PRO:HD3   | 3:A:428:TYR:CE2  | 2.44                     | 0.53              |
| 3:A:549:MET:O     | 3:A:550:LEU:C    | 2.50                     | 0.53              |
| 3:A:606:LEU:HD22  | 3:A:614:PHE:CE2  | 2.43                     | 0.53              |
| 4:B:274:PRO:HG2   | 4:B:359:GLU:O    | 2.09                     | 0.53              |
| 4:B:317:CYS:O     | 4:B:320:ASP:N    | 2.33                     | 0.53              |
| 4:B:466:TRP:HB2   | 4:B:479:VAL:HG23 | 1.91                     | 0.53              |
| 4:B:712:PRO:CD    | 4:B:712:PRO:O    | 2.51                     | 0.53              |
| 4:B:901:PRO:HA    | 4:B:949:VAL:HB   | 1.89                     | 0.53              |
| 4:B:957:ASN:HD21  | 4:B:958:GLN:HB2  | 1.73                     | 0.53              |
| 4:B:1007:VAL:HG22 | 4:B:1008:PRO:HD2 | 1.91                     | 0.53              |
| 5:C:74:SER:HB3    | 5:C:77:ILE:CG1   | 2.39                     | 0.53              |
| 6:E:121:MET:C     | 6:E:123:LEU:N    | 2.64                     | 0.53              |
| 7:F:97:ARG:NH2    | 7:F:108:PHE:CE1  | 2.77                     | 0.53              |
| 3:A:555:ASP:O     | 3:A:556:TRP:C    | 2.50                     | 0.53              |
| 3:A:662:PHE:O     | 4:B:828:ALA:HA   | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:675:THR:HG21  | 3:A:736:ASN:HD21  | 1.73                     | 0.53              |
| 3:A:928:LEU:O     | 3:A:929:LEU:C     | 2.52                     | 0.53              |
| 3:A:993:LEU:HB2   | 3:A:1046:LEU:HD21 | 1.91                     | 0.53              |
| 3:A:1064:VAL:O    | 3:A:1065:GLY:C    | 2.51                     | 0.53              |
| 3:A:1209:MET:O    | 3:A:1212:VAL:HB   | 2.09                     | 0.53              |
| 4:B:112:LEU:O     | 4:B:180:TYR:CE1   | 2.59                     | 0.53              |
| 4:B:498:THR:HB    | 4:B:537:LYS:O     | 2.08                     | 0.53              |
| 4:B:800:GLN:HG3   | 10:J:52:THR:HB    | 1.90                     | 0.53              |
| 4:B:805:THR:HA    | 4:B:809:MET:CE    | 2.39                     | 0.53              |
| 4:B:840:ILE:O     | 4:B:1010:LEU:HD12 | 2.09                     | 0.53              |
| 4:B:844:SER:OG    | 4:B:996:ARG:N     | 2.27                     | 0.53              |
| 4:B:885:MET:HA    | 4:B:936:ASP:HB3   | 1.91                     | 0.53              |
| 4:B:942:ARG:HB2   | 4:B:945:GLU:HB2   | 1.91                     | 0.53              |
| 4:B:1172:ILE:O    | 4:B:1172:ILE:CG2  | 2.56                     | 0.53              |
| 9:I:111:THR:CG2   | 9:I:113:ASP:H     | 2.22                     | 0.53              |
| 3:A:112:LYS:HG2   | 3:A:113:LEU:N     | 2.23                     | 0.53              |
| 3:A:122:MET:O     | 3:A:123:ARG:C     | 2.51                     | 0.53              |
| 3:A:550:LEU:HD12  | 3:A:556:TRP:NE1   | 2.24                     | 0.53              |
| 3:A:899:VAL:CG1   | 3:A:929:LEU:CD1   | 2.81                     | 0.53              |
| 3:A:1132:LYS:O    | 3:A:1135:ARG:HB3  | 2.09                     | 0.53              |
| 3:A:1299:VAL:CG1  | 3:A:1300:LYS:H    | 1.99                     | 0.53              |
| 3:A:1362:TYR:CE1  | 3:A:1363:VAL:C    | 2.87                     | 0.53              |
| 3:A:1368:MET:O    | 3:A:1369:ALA:C    | 2.52                     | 0.53              |
| 4:B:203:PHE:CE1   | 4:B:212:LEU:HD12  | 2.44                     | 0.53              |
| 4:B:635:ARG:CD    | 4:B:636:PRO:CD    | 2.78                     | 0.53              |
| 4:B:824:ILE:HD11  | 10:J:45:CYS:HA    | 1.91                     | 0.53              |
| 5:C:41:ILE:CG1    | 5:C:172:PRO:HG3   | 2.39                     | 0.53              |
| 5:C:181:ASP:OD1   | 5:C:183:TRP:O     | 2.26                     | 0.53              |
| 5:C:244:VAL:HG21  | 11:K:105:PHE:CE1  | 2.43                     | 0.53              |
| 8:H:23:VAL:HG12   | 8:H:24:CYS:N      | 2.23                     | 0.53              |
| 3:A:30:ILE:HG13   | 4:B:1170:THR:CG2  | 2.38                     | 0.52              |
| 3:A:50:ILE:C      | 3:A:52:GLY:H      | 2.17                     | 0.52              |
| 3:A:230:ARG:O     | 3:A:233:TRP:HB2   | 2.08                     | 0.52              |
| 3:A:254:GLU:HB3   | 4:B:935:ARG:HH11  | 1.73                     | 0.52              |
| 3:A:472:LEU:O     | 3:A:475:THR:HB    | 2.09                     | 0.52              |
| 3:A:567:LYS:O     | 3:A:569:LYS:N     | 2.40                     | 0.52              |
| 3:A:660:ASN:ND2   | 4:B:1082:MET:HB3  | 2.24                     | 0.52              |
| 3:A:667:GLY:O     | 3:A:669:THR:N     | 2.42                     | 0.52              |
| 3:A:892:ALA:CA    | 3:A:895:LYS:HB2   | 2.15                     | 0.52              |
| 3:A:1148:ILE:HG22 | 3:A:1149:ALA:N    | 2.24                     | 0.52              |
| 4:B:369:GLY:HA2   | 4:B:371:GLU:OE1   | 2.09                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:C:77:ILE:CD1    | 5:C:129:ILE:HD11 | 2.38                     | 0.52              |
| 5:C:193:TYR:N     | 5:C:193:TYR:CD2  | 2.76                     | 0.52              |
| 5:C:244:VAL:HG21  | 11:K:105:PHE:CE2 | 2.45                     | 0.52              |
| 8:H:39:THR:OG1    | 8:H:124:ARG:HB3  | 2.08                     | 0.52              |
| 8:H:114:VAL:N     | 8:H:125:LEU:O    | 2.41                     | 0.52              |
| 3:A:70:CYS:C      | 3:A:71:GLN:CG    | 2.82                     | 0.52              |
| 3:A:184:SER:O     | 3:A:185:TRP:CB   | 2.57                     | 0.52              |
| 3:A:367:PRO:HA    | 3:A:463:ILE:HD12 | 1.91                     | 0.52              |
| 3:A:447:GLN:CB    | 3:A:448:PRO:HA   | 2.39                     | 0.52              |
| 3:A:870:GLU:HG2   | 6:E:208:TYR:CD2  | 2.44                     | 0.52              |
| 3:A:1146:VAL:HG12 | 3:A:1201:ALA:HB3 | 1.91                     | 0.52              |
| 3:A:1200:ALA:C    | 3:A:1202:MET:N   | 2.66                     | 0.52              |
| 4:B:215:GLN:O     | 4:B:406:LEU:HA   | 2.09                     | 0.52              |
| 4:B:278:GLN:CG    | 4:B:279:ASP:H    | 2.17                     | 0.52              |
| 4:B:843:GLN:HB2   | 4:B:993:THR:CB   | 2.39                     | 0.52              |
| 4:B:847:ASP:HB3   | 5:C:167:HIS:HD2  | 1.72                     | 0.52              |
| 4:B:936:ASP:OD2   | 4:B:938:SER:OG   | 2.28                     | 0.52              |
| 6:E:65:THR:OG1    | 6:E:67:GLU:CB    | 2.48                     | 0.52              |
| 6:E:178:ILE:CG2   | 6:E:214:CYS:HA   | 2.39                     | 0.52              |
| 11:K:83:PRO:O     | 11:K:87:LEU:N    | 2.37                     | 0.52              |
| 3:A:60:SER:OG     | 3:A:64:ASN:O     | 2.25                     | 0.52              |
| 3:A:76:GLU:O      | 3:A:76:GLU:HG3   | 2.09                     | 0.52              |
| 3:A:213:HIS:C     | 3:A:214:ILE:O    | 2.51                     | 0.52              |
| 3:A:844:ALA:HB2   | 3:A:1389:PHE:CD2 | 2.45                     | 0.52              |
| 3:A:919:ILE:O     | 3:A:921:GLY:N    | 2.42                     | 0.52              |
| 3:A:964:ILE:HG22  | 3:A:965:GLN:N    | 2.23                     | 0.52              |
| 3:A:1256:GLU:C    | 3:A:1258:HIS:N   | 2.63                     | 0.52              |
| 4:B:59:LEU:CD1    | 4:B:417:PHE:CD2  | 2.92                     | 0.52              |
| 4:B:757:PRO:O     | 4:B:758:PHE:HB2  | 2.08                     | 0.52              |
| 4:B:800:GLN:HG3   | 10:J:52:THR:CG2  | 2.40                     | 0.52              |
| 5:C:135:GLN:C     | 5:C:136:ASP:O    | 2.48                     | 0.52              |
| 11:K:40:HIS:CE1   | 11:K:63:VAL:HG13 | 2.39                     | 0.52              |
| 12:L:34:CYS:SG    | 12:L:35:SER:N    | 2.82                     | 0.52              |
| 3:A:115:LEU:CG    | 3:A:142:CYS:HB3  | 2.40                     | 0.52              |
| 3:A:657:LEU:O     | 3:A:660:ASN:N    | 2.41                     | 0.52              |
| 3:A:665:GLY:HA2   | 4:B:1086:PHE:CD1 | 2.44                     | 0.52              |
| 3:A:878:ILE:C     | 3:A:879:GLU:CG   | 2.82                     | 0.52              |
| 3:A:914:GLU:C     | 3:A:916:GLY:N    | 2.66                     | 0.52              |
| 3:A:1099:PRO:O    | 3:A:1102:LYS:HB3 | 2.10                     | 0.52              |
| 4:B:109:THR:HG22  | 4:B:109:THR:O    | 2.09                     | 0.52              |
| 4:B:803:LEU:H     | 4:B:822:ASN:HD21 | 1.56                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:912:ILE:O     | 4:B:938:SER:HB2   | 2.09                     | 0.52              |
| 4:B:983:ARG:C     | 4:B:984:HIS:ND1   | 2.68                     | 0.52              |
| 5:C:74:SER:CB     | 5:C:77:ILE:HG13   | 2.38                     | 0.52              |
| 5:C:186:LEU:HB3   | 5:C:188:HIS:CD2   | 2.44                     | 0.52              |
| 6:E:15:ALA:O      | 6:E:19:VAL:HG23   | 2.09                     | 0.52              |
| 6:E:134:THR:C     | 6:E:135:PHE:HD1   | 2.17                     | 0.52              |
| 3:A:50:ILE:C      | 3:A:52:GLY:N      | 2.67                     | 0.52              |
| 3:A:827:THR:C     | 3:A:829:VAL:H     | 2.17                     | 0.52              |
| 3:A:933:TYR:O     | 3:A:933:TYR:CD2   | 2.62                     | 0.52              |
| 4:B:25:ILE:HG22   | 4:B:29:ASP:HB2    | 1.91                     | 0.52              |
| 4:B:824:ILE:HG12  | 10:J:48:ARG:HH12  | 1.74                     | 0.52              |
| 4:B:1161:HIS:O    | 4:B:1162:ILE:HG12 | 2.09                     | 0.52              |
| 9:I:32:CYS:O      | 9:I:33:SER:OG     | 2.23                     | 0.52              |
| 3:A:15:LYS:HB3    | 4:B:1220:ARG:HA   | 1.91                     | 0.52              |
| 3:A:224:PHE:CD2   | 3:A:231:PRO:HD3   | 2.45                     | 0.52              |
| 3:A:453:MET:HE3   | 3:A:520:CYS:SG    | 2.49                     | 0.52              |
| 3:A:777:PHE:CD2   | 3:A:782:ARG:CA    | 2.93                     | 0.52              |
| 3:A:900:ASP:HA    | 3:A:926:GLN:CD    | 2.34                     | 0.52              |
| 3:A:904:THR:CG2   | 3:A:905:ASP:H     | 2.22                     | 0.52              |
| 3:A:908:LEU:O     | 3:A:909:ASP:C     | 2.53                     | 0.52              |
| 3:A:1207:LEU:HD22 | 3:A:1208:THR:H    | 1.74                     | 0.52              |
| 3:A:1308:THR:CG2  | 3:A:1310:GLY:O    | 2.57                     | 0.52              |
| 10:J:64:ASN:CB    | 10:J:65:PRO:CD    | 2.75                     | 0.52              |
| 3:A:244:PRO:CG    | 3:A:245:PRO:HD2   | 2.40                     | 0.52              |
| 3:A:406:ILE:HD12  | 3:A:431:LYS:O     | 2.09                     | 0.52              |
| 3:A:660:ASN:C     | 3:A:660:ASN:ND2   | 2.61                     | 0.52              |
| 3:A:874:ASP:OD1   | 3:A:874:ASP:C     | 2.53                     | 0.52              |
| 3:A:1139:GLU:O    | 3:A:1140:HIS:O    | 2.28                     | 0.52              |
| 4:B:647:GLY:O     | 4:B:648:HIS:CG    | 2.63                     | 0.52              |
| 4:B:705:MET:H     | 4:B:710:LEU:CD1   | 2.22                     | 0.52              |
| 4:B:763:GLN:HG2   | 4:B:765:PRO:HD2   | 1.90                     | 0.52              |
| 6:E:90:VAL:N      | 6:E:120:ALA:HB2   | 2.24                     | 0.52              |
| 6:E:113:GLN:CB    | 6:E:137:GLU:CD    | 2.83                     | 0.52              |
| 6:E:187:TYR:CD2   | 6:E:188:LEU:HD23  | 2.32                     | 0.52              |
| 3:A:447:GLN:HB3   | 3:A:448:PRO:HA    | 1.92                     | 0.52              |
| 3:A:595:THR:OG1   | 3:A:603:ASN:HB3   | 2.10                     | 0.52              |
| 3:A:1116:LEU:HD22 | 3:A:1311:VAL:CG2  | 2.31                     | 0.52              |
| 4:B:197:PHE:CG    | 4:B:817:LEU:HD11  | 2.45                     | 0.52              |
| 4:B:686:ASN:ND2   | 4:B:686:ASN:H     | 2.06                     | 0.52              |
| 4:B:858:SER:HA    | 4:B:966:VAL:O     | 2.09                     | 0.52              |
| 4:B:1065:GLN:NE2  | 4:B:1067:ARG:N    | 2.56                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 11:K:6:ARG:O      | 11:K:7:PHE:C     | 2.51                     | 0.52              |
| 11:K:91:CYS:O     | 11:K:95:ILE:HG13 | 2.10                     | 0.52              |
| 3:A:354:SER:HA    | 3:A:482:PHE:CD2  | 2.45                     | 0.52              |
| 3:A:886:ILE:HD11  | 3:A:944:ARG:N    | 2.25                     | 0.52              |
| 3:A:925:LEU:O     | 3:A:926:GLN:C    | 2.49                     | 0.52              |
| 3:A:1138:ILE:HD13 | 3:A:1138:ILE:N   | 2.25                     | 0.52              |
| 4:B:25:ILE:HG22   | 4:B:26:THR:N     | 2.23                     | 0.52              |
| 4:B:45:SER:O      | 4:B:46:GLN:C     | 2.52                     | 0.52              |
| 4:B:130:VAL:CG1   | 4:B:132:VAL:CG2  | 2.88                     | 0.52              |
| 4:B:448:ILE:HG22  | 4:B:450:ALA:H    | 1.75                     | 0.52              |
| 4:B:562:GLY:O     | 4:B:563:MET:C    | 2.53                     | 0.52              |
| 4:B:760:ASP:C     | 4:B:762:ASN:H    | 2.16                     | 0.52              |
| 4:B:807:ARG:HG3   | 4:B:807:ARG:HH11 | 1.74                     | 0.52              |
| 7:F:97:ARG:HE     | 7:F:124:GLU:CD   | 2.18                     | 0.52              |
| 12:L:62:LYS:C     | 12:L:64:LEU:H    | 2.17                     | 0.52              |
| 3:A:225:ASN:O     | 3:A:227:VAL:N    | 2.43                     | 0.52              |
| 3:A:269:ILE:C     | 3:A:271:LYS:N    | 2.67                     | 0.52              |
| 3:A:741:ASN:HD22  | 3:A:744:LYS:H    | 1.58                     | 0.52              |
| 3:A:899:VAL:CG2   | 3:A:1029:ARG:HG2 | 2.39                     | 0.52              |
| 3:A:928:LEU:C     | 3:A:930:ASP:N    | 2.66                     | 0.52              |
| 3:A:930:ASP:O     | 3:A:931:GLU:C    | 2.52                     | 0.52              |
| 4:B:280:ILE:CG2   | 4:B:285:ILE:HG12 | 2.26                     | 0.52              |
| 4:B:364:ILE:O     | 4:B:365:THR:HB   | 2.10                     | 0.52              |
| 4:B:806:THR:CG2   | 4:B:808:ALA:H    | 2.21                     | 0.52              |
| 4:B:957:ASN:HB3   | 4:B:961:LEU:CD1  | 2.35                     | 0.52              |
| 4:B:1029:CYS:O    | 4:B:1030:LEU:C   | 2.53                     | 0.52              |
| 8:H:31:THR:O      | 8:H:32:THR:HB    | 2.09                     | 0.52              |
| 8:H:82:PRO:C      | 8:H:84:ALA:H     | 2.10                     | 0.52              |
| 8:H:129:TYR:C     | 8:H:131:ASN:H    | 2.17                     | 0.52              |
| 10:J:28:ASP:N     | 10:J:28:ASP:OD1  | 2.43                     | 0.52              |
| 11:K:83:PRO:O     | 11:K:86:ALA:HB3  | 2.10                     | 0.52              |
| 3:A:54:ASN:O      | 3:A:55:ASP:HB3   | 2.10                     | 0.51              |
| 3:A:380:VAL:HG21  | 3:A:430:TRP:HB2  | 1.91                     | 0.51              |
| 3:A:738:LYS:HZ1   | 5:C:194:GLU:HA   | 1.75                     | 0.51              |
| 3:A:834:THR:HG21  | 3:A:1077:THR:N   | 2.23                     | 0.51              |
| 3:A:900:ASP:HA    | 3:A:926:GLN:NE2  | 2.25                     | 0.51              |
| 3:A:1267:MET:O    | 3:A:1271:ILE:HB  | 2.10                     | 0.51              |
| 3:A:1339:LEU:HD11 | 6:E:147:HIS:CD2  | 2.45                     | 0.51              |
| 4:B:20:ASP:N      | 4:B:655:LYS:NZ   | 2.58                     | 0.51              |
| 4:B:292:ILE:HD11  | 4:B:327:ARG:N    | 2.25                     | 0.51              |
| 4:B:474:SER:HA    | 4:B:476:ARG:CD   | 2.40                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:B:648:HIS:C     | 4:B:648:HIS:CD2  | 2.88                     | 0.51              |
| 4:B:1130:PHE:HZ   | 4:B:1138:MET:HG2 | 1.75                     | 0.51              |
| 5:C:134:ILE:HD12  | 5:C:141:GLY:HA2  | 1.90                     | 0.51              |
| 6:E:195:VAL:CG2   | 6:E:213:ILE:HD13 | 2.40                     | 0.51              |
| 8:H:11:GLN:HA     | 8:H:53:ASP:O     | 2.10                     | 0.51              |
| 9:I:55:THR:HG23   | 9:I:58:VAL:HG21  | 1.92                     | 0.51              |
| 3:A:107:CYS:HB3   | 3:A:114:LEU:CD2  | 2.32                     | 0.51              |
| 3:A:464:PRO:HG2   | 3:A:465:TYR:HD1  | 1.74                     | 0.51              |
| 3:A:557:ASP:OD2   | 3:A:559:VAL:CG2  | 2.58                     | 0.51              |
| 3:A:565:ILE:HG23  | 3:A:567:LYS:HG2  | 1.91                     | 0.51              |
| 3:A:690:VAL:O     | 3:A:691:LEU:C    | 2.52                     | 0.51              |
| 3:A:1029:ARG:O    | 3:A:1033:GLN:N   | 2.32                     | 0.51              |
| 3:A:1053:PHE:O    | 3:A:1054:LEU:C   | 2.53                     | 0.51              |
| 3:A:1118:VAL:CG2  | 3:A:1306:LEU:HB2 | 2.40                     | 0.51              |
| 3:A:1172:LEU:HD23 | 3:A:1172:LEU:H   | 1.75                     | 0.51              |
| 3:A:1400:CYS:C    | 3:A:1402:PHE:H   | 2.17                     | 0.51              |
| 3:A:1412:ALA:HA   | 3:A:1417:GLU:OE2 | 2.10                     | 0.51              |
| 4:B:1084:GLN:HE22 | 5:C:192:TRP:N    | 2.05                     | 0.51              |
| 4:B:1191:ILE:C    | 4:B:1192:TYR:CD1 | 2.89                     | 0.51              |
| 6:E:20:LYS:HE2    | 6:E:60:PHE:CE1   | 2.45                     | 0.51              |
| 8:H:32:THR:HG22   | 8:H:33:GLN:N     | 2.24                     | 0.51              |
| 8:H:42:ILE:HG23   | 8:H:95:TYR:CE1   | 2.45                     | 0.51              |
| 8:H:102:TYR:HD2   | 8:H:102:TYR:H    | 1.55                     | 0.51              |
| 9:I:59:VAL:O      | 9:I:62:ILE:N     | 2.27                     | 0.51              |
| 11:K:78:THR:HG22  | 11:K:79:GLU:O    | 2.10                     | 0.51              |
| 1:R:10:A:OP2      | 1:R:10:A:C8      | 2.58                     | 0.51              |
| 3:A:322:VAL:O     | 3:A:323:LYS:CG   | 2.58                     | 0.51              |
| 3:A:825:ILE:O     | 3:A:826:ASP:C    | 2.48                     | 0.51              |
| 3:A:913:LEU:CD1   | 3:A:915:SER:H    | 2.19                     | 0.51              |
| 3:A:1100:ARG:NH2  | 3:A:1351:GLU:HG2 | 2.25                     | 0.51              |
| 4:B:245:GLU:OE1   | 4:B:551:PRO:HG2  | 2.09                     | 0.51              |
| 4:B:273:LEU:CD2   | 4:B:360:PHE:HD1  | 2.24                     | 0.51              |
| 4:B:332:ASP:C     | 4:B:334:ILE:H    | 2.16                     | 0.51              |
| 4:B:640:VAL:HG23  | 4:B:739:THR:C    | 2.35                     | 0.51              |
| 4:B:662:MET:O     | 4:B:663:ALA:C    | 2.53                     | 0.51              |
| 4:B:666:TYR:C     | 4:B:668:ASP:H    | 2.17                     | 0.51              |
| 4:B:701:ILE:CG1   | 4:B:740:HIS:HE1  | 2.24                     | 0.51              |
| 4:B:892:LYS:HE2   | 4:B:904:ARG:O    | 2.10                     | 0.51              |
| 6:E:55:ARG:C      | 6:E:57:MET:H     | 2.17                     | 0.51              |
| 8:H:109:LYS:C     | 8:H:111:LEU:H    | 2.16                     | 0.51              |
| 11:K:73:LEU:CD2   | 11:K:75:ILE:HD11 | 2.41                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:K:97:LYS:O    | 11:K:100:ALA:HB3  | 2.09                     | 0.51              |
| 3:A:359:LEU:HD22 | 3:A:363:GLN:HB2   | 1.91                     | 0.51              |
| 3:A:618:GLU:CD   | 3:A:620:LYS:H     | 2.17                     | 0.51              |
| 3:A:666:ILE:HA   | 4:B:1026:LEU:CD1  | 2.41                     | 0.51              |
| 3:A:826:ASP:O    | 3:A:830:LYS:N     | 2.39                     | 0.51              |
| 3:A:849:MET:CE   | 3:A:1061:GLY:HA2  | 2.39                     | 0.51              |
| 4:B:57:TYR:HD1   | 4:B:57:TYR:N      | 2.09                     | 0.51              |
| 4:B:566:LEU:HD11 | 4:B:586:TRP:CD2   | 2.44                     | 0.51              |
| 4:B:1102:LYS:O   | 4:B:1104:HIS:N    | 2.40                     | 0.51              |
| 5:C:242:GLN:NE2  | 5:C:246:ARG:HE    | 2.02                     | 0.51              |
| 9:I:15:TYR:O     | 9:I:27:PHE:CD2    | 2.61                     | 0.51              |
| 11:K:82:ASP:OD2  | 11:K:84:LYS:HD2   | 2.11                     | 0.51              |
| 3:A:92:HIS:C     | 3:A:92:HIS:CD2    | 2.88                     | 0.51              |
| 3:A:324:SER:O    | 3:A:326:ARG:N     | 2.36                     | 0.51              |
| 3:A:694:THR:HA   | 3:A:714:PHE:HE1   | 1.75                     | 0.51              |
| 3:A:737:LEU:HD23 | 3:A:737:LEU:H     | 1.75                     | 0.51              |
| 3:A:756:ILE:CG2  | 3:A:757:ASN:N     | 2.74                     | 0.51              |
| 3:A:848:ILE:HB   | 3:A:1065:GLY:CA   | 2.41                     | 0.51              |
| 3:A:1119:TYR:HD2 | 3:A:1305:VAL:HG22 | 1.76                     | 0.51              |
| 4:B:469:GLN:O    | 4:B:470:LYS:C     | 2.53                     | 0.51              |
| 4:B:793:ALA:C    | 4:B:794:ASN:HD22  | 2.18                     | 0.51              |
| 5:C:116:LYS:O    | 5:C:116:LYS:HG2   | 2.09                     | 0.51              |
| 5:C:167:HIS:CD2  | 5:C:168:ALA:H     | 2.29                     | 0.51              |
| 10:J:3:VAL:HA    | 10:J:53:HIS:CD2   | 2.45                     | 0.51              |
| 3:A:552:TRP:NE1  | 3:A:655:PHE:HD1   | 2.07                     | 0.51              |
| 3:A:552:TRP:CD1  | 3:A:655:PHE:CD1   | 2.99                     | 0.51              |
| 3:A:568:PRO:CB   | 5:C:221:TYR:HE1   | 2.22                     | 0.51              |
| 3:A:743:VAL:CG1  | 3:A:758:ILE:HD11  | 2.41                     | 0.51              |
| 3:A:1261:LYS:C   | 3:A:1263:ILE:H    | 2.18                     | 0.51              |
| 4:B:516:ASN:HD22 | 4:B:516:ASN:H     | 1.58                     | 0.51              |
| 4:B:981:ALA:HA   | 4:B:1092:TYR:CD2  | 2.45                     | 0.51              |
| 4:B:1016:ALA:O   | 4:B:1017:ILE:HD13 | 2.10                     | 0.51              |
| 4:B:1159:ARG:HE  | 4:B:1193:GLN:NE2  | 2.09                     | 0.51              |
| 6:E:143:ASN:OD1  | 6:E:187:TYR:HE1   | 1.93                     | 0.51              |
| 11:K:24:ASP:CG   | 11:K:74:ARG:HH11  | 2.18                     | 0.51              |
| 11:K:28:PRO:C    | 11:K:30:ALA:N     | 2.68                     | 0.51              |
| 12:L:48:CYS:HB3  | 12:L:51:CYS:C     | 2.35                     | 0.51              |
| 1:R:8:G:H2'      | 1:R:9:G:H8        | 1.76                     | 0.51              |
| 3:A:24:PRO:HB3   | 3:A:237:THR:HG21  | 1.92                     | 0.51              |
| 3:A:67:CYS:HB3   | 3:A:68:GLN:NE2    | 2.25                     | 0.51              |
| 3:A:853:ASP:CG   | 3:A:855:THR:HB    | 2.27                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:898:ARG:O    | 3:A:899:VAL:HG23  | 2.11                     | 0.51              |
| 3:A:1105:LEU:O   | 3:A:1384:VAL:HG23 | 2.10                     | 0.51              |
| 3:A:1389:PHE:HE1 | 3:A:1390:ASN:OD1  | 1.93                     | 0.51              |
| 4:B:121:ASN:N    | 4:B:121:ASN:ND2   | 2.57                     | 0.51              |
| 4:B:417:PHE:O    | 4:B:418:LYS:C     | 2.50                     | 0.51              |
| 4:B:471:LYS:CG   | 4:B:472:ALA:H     | 1.91                     | 0.51              |
| 4:B:653:VAL:O    | 4:B:654:ARG:HD3   | 2.10                     | 0.51              |
| 4:B:1159:ARG:HE  | 4:B:1193:GLN:HG3  | 1.75                     | 0.51              |
| 4:B:1187:ASN:OD1 | 4:B:1190:ASP:O    | 2.29                     | 0.51              |
| 4:B:1215:ARG:O   | 4:B:1216:LEU:HD23 | 2.11                     | 0.51              |
| 5:C:96:SER:O     | 5:C:97:VAL:HG23   | 2.11                     | 0.51              |
| 8:H:95:TYR:HE2   | 8:H:97:MET:SD     | 2.33                     | 0.51              |
| 8:H:109:LYS:HB3  | 8:H:110:ASP:OD2   | 2.10                     | 0.51              |
| 9:I:50:THR:HG22  | 9:I:52:ILE:N      | 2.24                     | 0.51              |
| 9:I:83:ASN:ND2   | 9:I:83:ASN:N      | 2.55                     | 0.51              |
| 10:J:18:TRP:CZ2  | 10:J:22:LEU:HD11  | 2.46                     | 0.51              |
| 3:A:403:LYS:O    | 3:A:404:TYR:O     | 2.28                     | 0.51              |
| 3:A:680:THR:O    | 3:A:681:GLU:C     | 2.54                     | 0.51              |
| 3:A:697:ALA:HA   | 3:A:702:LEU:HB2   | 1.93                     | 0.51              |
| 3:A:834:THR:CG2  | 3:A:1077:THR:HG23 | 2.40                     | 0.51              |
| 3:A:855:THR:HG23 | 3:A:857:ARG:CG    | 2.40                     | 0.51              |
| 3:A:970:THR:O    | 3:A:970:THR:CG2   | 2.58                     | 0.51              |
| 3:A:1319:VAL:HB  | 3:A:1322:ILE:CD1  | 2.35                     | 0.51              |
| 4:B:426:LYS:O    | 4:B:430:ARG:NH1   | 2.44                     | 0.51              |
| 4:B:428:ILE:O    | 4:B:432:MET:HE2   | 2.10                     | 0.51              |
| 4:B:600:LEU:C    | 4:B:615:MET:HE1   | 2.35                     | 0.51              |
| 4:B:613:VAL:CG1  | 4:B:627:PHE:O     | 2.57                     | 0.51              |
| 4:B:770:GLN:CG   | 4:B:983:ARG:O     | 2.58                     | 0.51              |
| 6:E:85:GLU:OE2   | 6:E:92:THR:HG21   | 2.11                     | 0.51              |
| 10:J:57:ILE:HG23 | 10:J:58:GLU:N     | 2.25                     | 0.51              |
| 1:R:4:G:H1       | 2:T:11:DC:H42     | 1.59                     | 0.51              |
| 3:A:147:VAL:HB   | 3:A:149:GLU:H     | 1.76                     | 0.51              |
| 3:A:352:VAL:CG1  | 3:A:353:ILE:H     | 2.22                     | 0.51              |
| 3:A:385:ILE:O    | 3:A:386:ASP:C     | 2.53                     | 0.51              |
| 3:A:541:ILE:CG2  | 3:A:546:VAL:HG22  | 2.39                     | 0.51              |
| 3:A:655:PHE:CE2  | 3:A:659:HIS:HD2   | 2.28                     | 0.51              |
| 3:A:908:LEU:C    | 3:A:909:ASP:O     | 2.53                     | 0.51              |
| 4:B:34:ILE:HD11  | 4:B:743:ILE:CG2   | 2.39                     | 0.51              |
| 4:B:364:ILE:HD13 | 4:B:585:VAL:HG22  | 1.93                     | 0.51              |
| 4:B:933:SER:OG   | 4:B:934:LYS:N     | 2.42                     | 0.51              |
| 4:B:1056:SER:HB3 | 4:B:1066:SER:HB2  | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:49:VAL:O      | 8:H:50:ALA:HB2    | 2.10                     | 0.51              |
| 8:H:115:TYR:HA    | 8:H:123:MET:O     | 2.11                     | 0.51              |
| 9:I:115:LYS:O     | 9:I:116:ASN:O     | 2.29                     | 0.51              |
| 12:L:28:LYS:HB2   | 12:L:39:SER:HA    | 1.93                     | 0.51              |
| 3:A:335:ARG:O     | 3:A:338:GLY:N     | 2.43                     | 0.51              |
| 3:A:404:TYR:CD1   | 3:A:404:TYR:N     | 2.78                     | 0.51              |
| 3:A:590:ARG:NH2   | 3:A:620:LYS:C     | 2.68                     | 0.51              |
| 3:A:609:ASP:O     | 3:A:611:GLN:HB2   | 2.10                     | 0.51              |
| 3:A:742:ASN:CA    | 3:A:745:GLN:HB2   | 2.41                     | 0.51              |
| 3:A:889:SER:HB2   | 3:A:892:ALA:N     | 2.12                     | 0.51              |
| 3:A:1074:GLU:HB3  | 3:A:1075:PRO:CD   | 2.41                     | 0.51              |
| 3:A:1101:LEU:HG   | 3:A:1105:LEU:HD12 | 1.93                     | 0.51              |
| 3:A:1118:VAL:HG23 | 3:A:1306:LEU:HB2  | 1.92                     | 0.51              |
| 3:A:1441:PHE:HZ   | 7:F:88:TYR:C      | 2.19                     | 0.51              |
| 4:B:361:LEU:HD23  | 4:B:377:PHE:CD2   | 2.45                     | 0.51              |
| 4:B:760:ASP:C     | 4:B:762:ASN:N     | 2.69                     | 0.51              |
| 4:B:781:PHE:HE2   | 4:B:793:ALA:HB1   | 1.75                     | 0.51              |
| 4:B:796:LEU:HB3   | 4:B:799:PRO:CG    | 2.41                     | 0.51              |
| 5:C:258:ILE:HG22  | 5:C:259:LEU:N     | 2.25                     | 0.51              |
| 7:F:77:ASP:HB3    | 7:F:78:GLN:HG3    | 1.92                     | 0.51              |
| 11:K:27:ALA:CB    | 11:K:28:PRO:HD3   | 2.38                     | 0.51              |
| 3:A:91:PHE:N      | 3:A:297:GLN:NE2   | 2.58                     | 0.50              |
| 3:A:166:GLY:O     | 3:A:167:CYS:CB    | 2.59                     | 0.50              |
| 3:A:455:MET:HE3   | 4:B:1134:GLU:CG   | 2.41                     | 0.50              |
| 3:A:571:LEU:HD22  | 8:H:46:LEU:HD11   | 1.93                     | 0.50              |
| 3:A:823:GLY:O     | 3:A:824:LEU:C     | 2.54                     | 0.50              |
| 3:A:836:TYR:O     | 3:A:837:ILE:C     | 2.54                     | 0.50              |
| 3:A:929:LEU:HD23  | 3:A:929:LEU:H     | 1.76                     | 0.50              |
| 3:A:947:PHE:CE2   | 3:A:954:TRP:CE2   | 2.99                     | 0.50              |
| 3:A:1076:ALA:HA   | 3:A:1079:MET:CE   | 2.38                     | 0.50              |
| 3:A:1127:ASP:CB   | 3:A:1130:GLN:HB3  | 2.38                     | 0.50              |
| 3:A:1168:GLU:C    | 3:A:1170:ILE:N    | 2.68                     | 0.50              |
| 3:A:1197:LEU:HD12 | 3:A:1209:MET:SD   | 2.51                     | 0.50              |
| 3:A:1402:PHE:CD2  | 3:A:1403:GLU:N    | 2.76                     | 0.50              |
| 4:B:110:HIS:NE2   | 12:L:53:HIS:HE1   | 2.09                     | 0.50              |
| 4:B:637:LEU:HD23  | 4:B:742:GLU:OE2   | 2.11                     | 0.50              |
| 4:B:737:THR:HG21  | 9:I:66:PRO:C      | 2.33                     | 0.50              |
| 4:B:785:TYR:CE2   | 10:J:60:PHE:HE1   | 2.29                     | 0.50              |
| 4:B:864:LYS:HG3   | 4:B:865:LYS:N     | 2.25                     | 0.50              |
| 4:B:1024:ALA:O    | 4:B:1027:ILE:N    | 2.44                     | 0.50              |
| 5:C:40:GLU:OE1    | 5:C:254:LYS:NZ    | 2.28                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:80:LEU:HD12   | 5:C:94:LYS:O      | 2.11                     | 0.50              |
| 6:E:147:HIS:HB3   | 6:E:150:VAL:HG23  | 1.93                     | 0.50              |
| 7:F:97:ARG:HG3    | 7:F:101:ILE:HD11  | 1.92                     | 0.50              |
| 9:I:119:THR:O     | 9:I:119:THR:CG2   | 2.59                     | 0.50              |
| 12:L:25:ALA:O     | 12:L:26:THR:OG1   | 2.22                     | 0.50              |
| 3:A:167:CYS:O     | 3:A:167:CYS:SG    | 2.70                     | 0.50              |
| 3:A:590:ARG:O     | 3:A:591:PHE:HB2   | 2.11                     | 0.50              |
| 3:A:691:LEU:O     | 3:A:694:THR:HB    | 2.11                     | 0.50              |
| 3:A:825:ILE:HD13  | 4:B:533:CYS:SG    | 2.52                     | 0.50              |
| 3:A:855:THR:HG23  | 3:A:856:THR:N     | 2.24                     | 0.50              |
| 3:A:1283:VAL:CG1  | 3:A:1284:MET:N    | 2.74                     | 0.50              |
| 3:A:1327:ILE:O    | 3:A:1327:ILE:HG23 | 2.10                     | 0.50              |
| 4:B:472:ALA:C     | 4:B:474:SER:N     | 2.69                     | 0.50              |
| 4:B:827:ILE:HD12  | 4:B:1086:PHE:CD2  | 2.47                     | 0.50              |
| 4:B:996:ARG:NH2   | 5:C:38:ILE:CD1    | 2.70                     | 0.50              |
| 5:C:249:ASP:O     | 5:C:253:LYS:HG3   | 2.11                     | 0.50              |
| 7:F:136:ARG:HD2   | 7:F:146:TRP:CD1   | 2.46                     | 0.50              |
| 8:H:4:THR:CG2     | 8:H:5:LEU:N       | 2.73                     | 0.50              |
| 8:H:7:ASP:O       | 8:H:8:ASP:CB      | 2.59                     | 0.50              |
| 9:I:19:ASP:OD2    | 9:I:24:ARG:NE     | 2.30                     | 0.50              |
| 2:T:4:DA:C2'      | 2:T:5:DT:C6       | 2.93                     | 0.50              |
| 3:A:115:LEU:HB2   | 3:A:122:MET:CE    | 2.35                     | 0.50              |
| 3:A:491:VAL:CG1   | 3:A:492:PRO:HD2   | 2.42                     | 0.50              |
| 3:A:1025:ARG:HG2  | 3:A:1025:ARG:NH1  | 2.02                     | 0.50              |
| 3:A:1118:VAL:HG12 | 3:A:1327:ILE:HG13 | 1.94                     | 0.50              |
| 3:A:1236:LEU:O    | 3:A:1237:ILE:HG13 | 2.11                     | 0.50              |
| 3:A:1412:ALA:HA   | 3:A:1417:GLU:HG3  | 1.92                     | 0.50              |
| 4:B:34:ILE:CD1    | 4:B:542:MET:HE1   | 2.41                     | 0.50              |
| 4:B:426:LYS:O     | 4:B:430:ARG:CD    | 2.60                     | 0.50              |
| 4:B:844:SER:HG    | 4:B:996:ARG:H     | 1.57                     | 0.50              |
| 4:B:901:PRO:O     | 4:B:949:VAL:O     | 2.30                     | 0.50              |
| 5:C:241:ASP:HB3   | 11:K:109:TRP:CE2  | 2.46                     | 0.50              |
| 3:A:218:ASP:O     | 3:A:219:PHE:O     | 2.30                     | 0.50              |
| 3:A:253:ASN:CG    | 3:A:254:GLU:H     | 1.99                     | 0.50              |
| 3:A:334:GLY:O     | 3:A:335:ARG:C     | 2.55                     | 0.50              |
| 3:A:709:THR:C     | 3:A:711:ARG:N     | 2.66                     | 0.50              |
| 3:A:803:SER:C     | 3:A:805:LEU:H     | 2.18                     | 0.50              |
| 3:A:858:ASN:ND2   | 3:A:860:LEU:N     | 2.59                     | 0.50              |
| 3:A:870:GLU:HB3   | 6:E:204:THR:HG21  | 1.94                     | 0.50              |
| 3:A:1118:VAL:HG12 | 3:A:1327:ILE:CD1  | 2.41                     | 0.50              |
| 4:B:51:PHE:O      | 4:B:54:PHE:HB3    | 2.11                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:435:THR:C    | 4:B:437:GLU:N     | 2.70                     | 0.50              |
| 6:E:89:GLY:O     | 6:E:91:LYS:N      | 2.44                     | 0.50              |
| 3:A:113:LEU:HD12 | 3:A:218:ASP:OD1   | 2.11                     | 0.50              |
| 3:A:381:THR:HG23 | 3:A:382:PRO:HD2   | 1.94                     | 0.50              |
| 3:A:568:PRO:HB3  | 5:C:221:TYR:CE1   | 2.46                     | 0.50              |
| 3:A:868:TYR:OH   | 3:A:1366:ARG:HD3  | 2.12                     | 0.50              |
| 3:A:1042:PHE:C   | 3:A:1042:PHE:CD2  | 2.89                     | 0.50              |
| 3:A:1045:VAL:O   | 3:A:1049:ILE:HG13 | 2.12                     | 0.50              |
| 3:A:1171:GLN:O   | 3:A:1174:PHE:CZ   | 2.64                     | 0.50              |
| 4:B:101:MET:C    | 4:B:102:VAL:CG2   | 2.83                     | 0.50              |
| 4:B:113:TYR:O    | 4:B:114:PRO:C     | 2.50                     | 0.50              |
| 4:B:236:HIS:NE2  | 4:B:389:ALA:HA    | 2.26                     | 0.50              |
| 4:B:640:VAL:CG1  | 4:B:650:GLU:O     | 2.60                     | 0.50              |
| 4:B:1106:ARG:CG  | 4:B:1107:ALA:N    | 2.75                     | 0.50              |
| 5:C:23:SER:O     | 5:C:25:VAL:HG22   | 2.11                     | 0.50              |
| 5:C:46:ILE:HG23  | 5:C:157:CYS:HB3   | 1.92                     | 0.50              |
| 5:C:173:ALA:O    | 5:C:233:GLU:O     | 2.28                     | 0.50              |
| 6:E:97:VAL:HG13  | 6:E:127:ILE:CG2   | 2.42                     | 0.50              |
| 8:H:15:VAL:CG2   | 8:H:26:ILE:HD11   | 2.42                     | 0.50              |
| 9:I:55:THR:CG2   | 9:I:56:ALA:N      | 2.74                     | 0.50              |
| 11:K:47:ARG:CB   | 11:K:47:ARG:NH1   | 2.74                     | 0.50              |
| 3:A:139:TRP:O    | 3:A:140:THR:C     | 2.55                     | 0.50              |
| 3:A:296:LEU:O    | 3:A:300:VAL:HG23  | 2.12                     | 0.50              |
| 3:A:298:PHE:C    | 3:A:298:PHE:CD2   | 2.89                     | 0.50              |
| 4:B:288:ALA:HB1  | 4:B:331:LEU:HD13  | 1.93                     | 0.50              |
| 4:B:317:CYS:O    | 4:B:318:VAL:C     | 2.54                     | 0.50              |
| 4:B:1051:THR:HB  | 4:B:1054:GLY:H    | 1.75                     | 0.50              |
| 5:C:62:PHE:C     | 5:C:62:PHE:CD2    | 2.90                     | 0.50              |
| 6:E:96:PHE:O     | 6:E:97:VAL:C      | 2.53                     | 0.50              |
| 6:E:161:LYS:HD2  | 6:E:195:VAL:CG2   | 2.42                     | 0.50              |
| 7:F:90:ARG:HG3   | 7:F:94:LEU:HD12   | 1.94                     | 0.50              |
| 9:I:32:CYS:SG    | 9:I:34:TYR:N      | 2.76                     | 0.50              |
| 9:I:51:ASN:O     | 9:I:54:GLU:HG3    | 2.12                     | 0.50              |
| 10:J:31:ASP:O    | 10:J:33:GLY:N     | 2.44                     | 0.50              |
| 11:K:61:TYR:HD1  | 11:K:62:LYS:N     | 2.10                     | 0.50              |
| 3:A:335:ARG:HD3  | 3:A:339:ASN:HD22  | 1.77                     | 0.50              |
| 3:A:491:VAL:H    | 4:B:1150:ARG:NH2  | 2.09                     | 0.50              |
| 3:A:536:LEU:O    | 3:A:537:ARG:C     | 2.53                     | 0.50              |
| 3:A:707:GLY:HA3  | 3:A:1281:ARG:HD3  | 1.93                     | 0.50              |
| 3:A:815:PHE:C    | 3:A:817:ALA:N     | 2.66                     | 0.50              |
| 3:A:901:LEU:CG   | 3:A:926:GLN:HE21  | 2.04                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:903:ASN:O    | 3:A:904:THR:C     | 2.53                     | 0.50              |
| 3:A:1400:CYS:O   | 3:A:1402:PHE:N    | 2.38                     | 0.50              |
| 4:B:424:LEU:HD12 | 4:B:448:ILE:HG23  | 1.93                     | 0.50              |
| 4:B:465:ASN:O    | 4:B:467:GLY:N     | 2.45                     | 0.50              |
| 4:B:521:LEU:HD23 | 4:B:635:ARG:CG    | 2.38                     | 0.50              |
| 5:C:163:ILE:O    | 5:C:164:ALA:C     | 2.55                     | 0.50              |
| 6:E:178:ILE:HD13 | 6:E:185:ALA:HB2   | 1.94                     | 0.50              |
| 7:F:140:ASP:OD1  | 7:F:141:GLY:N     | 2.45                     | 0.50              |
| 8:H:36:CYS:SG    | 8:H:130:ARG:NH2   | 2.75                     | 0.50              |
| 9:I:7:CYS:SG     | 9:I:34:TYR:HB3    | 2.52                     | 0.50              |
| 10:J:57:ILE:C    | 10:J:59:LYS:N     | 2.67                     | 0.50              |
| 11:K:32:VAL:HG23 | 11:K:74:ARG:CB    | 2.42                     | 0.50              |
| 3:A:56:PRO:O     | 3:A:57:ARG:HG3    | 2.12                     | 0.50              |
| 3:A:91:PHE:HB2   | 3:A:297:GLN:OE1   | 2.11                     | 0.50              |
| 3:A:306:ASN:HD21 | 3:A:324:SER:CB    | 2.25                     | 0.50              |
| 3:A:332:LYS:O    | 3:A:334:GLY:N     | 2.45                     | 0.50              |
| 3:A:344:ARG:C    | 3:A:345:VAL:HG13  | 2.36                     | 0.50              |
| 3:A:830:LYS:CE   | 3:A:1098:VAL:HG21 | 2.35                     | 0.50              |
| 3:A:908:LEU:HD11 | 3:A:983:ILE:CD1   | 2.32                     | 0.50              |
| 4:B:274:PRO:O    | 4:B:275:TYR:C     | 2.53                     | 0.50              |
| 4:B:293:PRO:O    | 4:B:294:ASP:C     | 2.55                     | 0.50              |
| 4:B:380:TYR:HE1  | 4:B:579:ARG:HE    | 1.59                     | 0.50              |
| 4:B:423:LYS:HA   | 4:B:426:LYS:NZ    | 2.27                     | 0.50              |
| 4:B:627:PHE:O    | 4:B:632:ARG:NH1   | 2.43                     | 0.50              |
| 4:B:885:MET:HA   | 4:B:936:ASP:CB    | 2.42                     | 0.50              |
| 5:C:233:GLU:OE2  | 10:J:43:ARG:NH2   | 2.45                     | 0.50              |
| 10:J:36:LEU:CD1  | 10:J:47:ARG:HG2   | 2.39                     | 0.50              |
| 3:A:88:LYS:HD2   | 3:A:293:GLU:OE2   | 2.12                     | 0.50              |
| 3:A:135:PHE:C    | 3:A:135:PHE:CD2   | 2.89                     | 0.50              |
| 3:A:688:LYS:O    | 3:A:691:LEU:HB3   | 2.11                     | 0.50              |
| 3:A:834:THR:HG21 | 3:A:1077:THR:HA   | 1.90                     | 0.50              |
| 3:A:1151:GLU:C   | 3:A:1152:ILE:HD12 | 2.37                     | 0.50              |
| 4:B:476:ARG:O    | 4:B:477:ALA:C     | 2.52                     | 0.50              |
| 4:B:483:LEU:HD22 | 4:B:491:THR:HG23  | 1.94                     | 0.50              |
| 4:B:487:THR:O    | 4:B:488:TYR:C     | 2.55                     | 0.50              |
| 4:B:979:LYS:O    | 4:B:980:PHE:CD1   | 2.65                     | 0.50              |
| 4:B:1173:ALA:C   | 4:B:1175:LEU:N    | 2.70                     | 0.50              |
| 5:C:27:LEU:O     | 5:C:30:ALA:N      | 2.43                     | 0.50              |
| 5:C:41:ILE:O     | 5:C:41:ILE:HG12   | 2.11                     | 0.50              |
| 5:C:74:SER:CB    | 5:C:77:ILE:CG1    | 2.89                     | 0.50              |
| 6:E:136:ASN:O    | 6:E:137:GLU:C     | 2.54                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:F:136:ARG:O    | 7:F:143:PHE:HA    | 2.12                     | 0.50              |
| 3:A:512:VAL:O    | 3:A:512:VAL:CG1   | 2.60                     | 0.49              |
| 3:A:786:HIS:HE1  | 4:B:742:GLU:OE1   | 1.94                     | 0.49              |
| 3:A:870:GLU:C    | 6:E:204:THR:HG21  | 2.37                     | 0.49              |
| 3:A:1105:LEU:CD2 | 3:A:1384:VAL:HG21 | 2.42                     | 0.49              |
| 3:A:1389:PHE:O   | 3:A:1389:PHE:HD1  | 1.94                     | 0.49              |
| 4:B:355:ILE:HG22 | 4:B:356:LEU:HD23  | 1.94                     | 0.49              |
| 4:B:377:PHE:O    | 4:B:380:TYR:HB3   | 2.12                     | 0.49              |
| 4:B:430:ARG:O    | 4:B:431:TYR:O     | 2.30                     | 0.49              |
| 4:B:1106:ARG:NH2 | 4:B:1109:GLY:H    | 1.94                     | 0.49              |
| 5:C:141:GLY:O    | 5:C:142:VAL:O     | 2.29                     | 0.49              |
| 9:I:103:CYS:SG   | 9:I:106:CYS:SG    | 3.09                     | 0.49              |
| 10:J:50:ILE:C    | 10:J:52:THR:N     | 2.67                     | 0.49              |
| 11:K:18:LYS:HE3  | 11:K:38:GLU:OE2   | 2.12                     | 0.49              |
| 3:A:92:HIS:O     | 3:A:92:HIS:CD2    | 2.65                     | 0.49              |
| 3:A:151:ASP:C    | 3:A:152:VAL:CG2   | 2.85                     | 0.49              |
| 3:A:244:PRO:O    | 3:A:246:VAL:N     | 2.45                     | 0.49              |
| 3:A:265:LYS:HZ1  | 3:A:322:VAL:CG1   | 2.24                     | 0.49              |
| 3:A:269:ILE:HG13 | 3:A:299:HIS:HB3   | 1.93                     | 0.49              |
| 3:A:385:ILE:HD11 | 3:A:428:TYR:CE2   | 2.48                     | 0.49              |
| 3:A:568:PRO:O    | 5:C:221:TYR:CE1   | 2.64                     | 0.49              |
| 3:A:714:PHE:HB3  | 9:I:97:MET:HE1    | 1.92                     | 0.49              |
| 3:A:1076:ALA:O   | 3:A:1079:MET:HG3  | 2.12                     | 0.49              |
| 3:A:1098:VAL:N   | 3:A:1099:PRO:HD2  | 2.27                     | 0.49              |
| 3:A:1444:MET:N   | 7:F:133:VAL:O     | 2.45                     | 0.49              |
| 4:B:105:SER:O    | 4:B:106:ASP:C     | 2.54                     | 0.49              |
| 4:B:487:THR:HG22 | 4:B:489:SER:N     | 2.27                     | 0.49              |
| 4:B:525:ALA:O    | 4:B:527:THR:HG22  | 2.13                     | 0.49              |
| 4:B:614:SER:HB3  | 4:B:694:ASP:OD1   | 2.12                     | 0.49              |
| 4:B:882:THR:O    | 4:B:882:THR:HG23  | 2.12                     | 0.49              |
| 4:B:1023:VAL:O   | 4:B:1027:ILE:HG13 | 2.11                     | 0.49              |
| 4:B:1191:ILE:CG2 | 4:B:1192:TYR:N    | 2.74                     | 0.49              |
| 6:E:173:SER:HB2  | 6:E:177:ARG:NH2   | 2.27                     | 0.49              |
| 3:A:27:VAL:CG1   | 3:A:238:CYS:SG    | 3.00                     | 0.49              |
| 3:A:67:CYS:C     | 3:A:68:GLN:NE2    | 2.70                     | 0.49              |
| 3:A:312:PRO:C    | 3:A:313:GLN:HG3   | 2.30                     | 0.49              |
| 3:A:332:LYS:C    | 3:A:334:GLY:N     | 2.69                     | 0.49              |
| 3:A:399:HIS:CB   | 3:A:400:PRO:CD    | 2.90                     | 0.49              |
| 3:A:530:GLY:CA   | 3:A:532:ARG:H     | 2.22                     | 0.49              |
| 3:A:534:LEU:O    | 3:A:539:THR:CG2   | 2.59                     | 0.49              |
| 3:A:852:TYR:CZ   | 7:F:136:ARG:HG2   | 2.48                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1242:VAL:O    | 3:A:1243:VAL:HG23 | 2.12                     | 0.49              |
| 3:A:1258:HIS:O    | 3:A:1261:LYS:HB2  | 2.13                     | 0.49              |
| 5:C:38:ILE:HG12   | 5:C:176:ILE:HD12  | 1.94                     | 0.49              |
| 9:I:19:ASP:O      | 9:I:23:ASN:CA     | 2.58                     | 0.49              |
| 9:I:85:PHE:O      | 9:I:86:PHE:HB3    | 2.12                     | 0.49              |
| 3:A:419:LYS:HB3   | 3:A:419:LYS:HZ2   | 1.78                     | 0.49              |
| 3:A:811:GLN:O     | 3:A:812:GLU:C     | 2.54                     | 0.49              |
| 3:A:820:GLY:HA2   | 3:A:823:GLY:H     | 1.77                     | 0.49              |
| 3:A:853:ASP:C     | 3:A:855:THR:H     | 2.19                     | 0.49              |
| 3:A:901:LEU:H     | 3:A:926:GLN:CD    | 2.21                     | 0.49              |
| 3:A:904:THR:CG2   | 3:A:905:ASP:N     | 2.75                     | 0.49              |
| 3:A:1094:VAL:HG12 | 3:A:1095:THR:N    | 2.27                     | 0.49              |
| 3:A:1156:PRO:HD2  | 3:A:1157:ASP:H    | 1.77                     | 0.49              |
| 3:A:1339:LEU:HD13 | 6:E:147:HIS:CD2   | 2.43                     | 0.49              |
| 4:B:291:ILE:HD12  | 4:B:291:ILE:H     | 1.78                     | 0.49              |
| 3:A:115:LEU:HD11  | 3:A:142:CYS:CB    | 2.43                     | 0.49              |
| 3:A:261:ASP:HB2   | 3:A:323:LYS:HB3   | 1.95                     | 0.49              |
| 3:A:340:LEU:HD22  | 3:A:1429:ILE:HG23 | 1.95                     | 0.49              |
| 3:A:343:LYS:HE3   | 4:B:1151:LEU:O    | 2.13                     | 0.49              |
| 3:A:655:PHE:O     | 3:A:656:TRP:C     | 2.55                     | 0.49              |
| 3:A:709:THR:HG22  | 3:A:711:ARG:N     | 2.11                     | 0.49              |
| 3:A:857:ARG:CZ    | 7:F:139:PRO:HG2   | 2.42                     | 0.49              |
| 3:A:898:ARG:CD    | 3:A:899:VAL:N     | 2.71                     | 0.49              |
| 3:A:903:ASN:O     | 3:A:906:HIS:N     | 2.46                     | 0.49              |
| 4:B:236:HIS:CD2   | 4:B:389:ALA:HA    | 2.48                     | 0.49              |
| 4:B:411:PRO:C     | 4:B:414:ALA:HB3   | 2.37                     | 0.49              |
| 4:B:449:ASN:O     | 4:B:449:ASN:CG    | 2.56                     | 0.49              |
| 4:B:759:PRO:HB2   | 4:B:767:ASN:HD21  | 1.76                     | 0.49              |
| 4:B:785:TYR:CD1   | 4:B:786:ASN:N     | 2.81                     | 0.49              |
| 4:B:1030:LEU:HD11 | 4:B:1067:ARG:C    | 2.37                     | 0.49              |
| 5:C:193:TYR:HD2   | 5:C:193:TYR:N     | 2.11                     | 0.49              |
| 6:E:78:LEU:HD23   | 6:E:78:LEU:C      | 2.37                     | 0.49              |
| 6:E:100:ILE:O     | 6:E:101:GLN:C     | 2.56                     | 0.49              |
| 3:A:381:THR:HG23  | 3:A:382:PRO:HG2   | 1.95                     | 0.49              |
| 3:A:537:ARG:HH11  | 3:A:537:ARG:HG2   | 1.77                     | 0.49              |
| 3:A:1007:ILE:O    | 3:A:1010:ALA:CB   | 2.60                     | 0.49              |
| 3:A:1025:ARG:HA   | 3:A:1030:ARG:HH11 | 1.75                     | 0.49              |
| 3:A:1053:PHE:HD2  | 3:A:1054:LEU:H    | 1.59                     | 0.49              |
| 3:A:1139:GLU:O    | 3:A:1140:HIS:C    | 2.56                     | 0.49              |
| 3:A:1160:SER:HA   | 3:A:1170:ILE:HG21 | 1.94                     | 0.49              |
| 3:A:1166:ASP:OD2  | 3:A:1239:ARG:NE   | 2.36                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1370:LEU:O    | 3:A:1374:VAL:HG23 | 2.12                     | 0.49              |
| 4:B:124:TYR:CB    | 4:B:204:ILE:HD13  | 2.42                     | 0.49              |
| 4:B:191:LYS:C     | 4:B:193:LYS:H     | 2.21                     | 0.49              |
| 4:B:778:MET:HE1   | 4:B:853:SER:HB3   | 1.94                     | 0.49              |
| 4:B:847:ASP:C     | 4:B:849:GLY:N     | 2.71                     | 0.49              |
| 4:B:871:THR:O     | 4:B:872:GLU:O     | 2.31                     | 0.49              |
| 4:B:978:ASP:OD1   | 4:B:1098:MET:HB3  | 2.12                     | 0.49              |
| 4:B:1215:ARG:C    | 4:B:1216:LEU:HD23 | 2.38                     | 0.49              |
| 3:A:35:ILE:HA     | 3:A:52:GLY:O      | 2.12                     | 0.49              |
| 3:A:568:PRO:O     | 5:C:221:TYR:HE1   | 1.96                     | 0.49              |
| 3:A:818:MET:HG3   | 4:B:514:LEU:HD23  | 1.94                     | 0.49              |
| 3:A:862:ASN:HA    | 6:E:174:GLN:HA    | 1.94                     | 0.49              |
| 3:A:896:ARG:HB3   | 3:A:897:TYR:HD1   | 1.78                     | 0.49              |
| 3:A:927:VAL:HG12  | 3:A:928:LEU:N     | 2.28                     | 0.49              |
| 4:B:641:GLU:C     | 4:B:643:ASP:N     | 2.69                     | 0.49              |
| 4:B:653:VAL:C     | 4:B:654:ARG:HG2   | 2.38                     | 0.49              |
| 5:C:191:TYR:N     | 5:C:191:TYR:HD1   | 2.11                     | 0.49              |
| 9:I:4:PHE:CE1     | 9:I:13:MET:HE2    | 2.47                     | 0.49              |
| 9:I:32:CYS:SG     | 9:I:33:SER:N      | 2.82                     | 0.49              |
| 11:K:9:LEU:N      | 11:K:9:LEU:HD23   | 2.27                     | 0.49              |
| 3:A:106:VAL:CG1   | 3:A:107:CYS:H     | 2.24                     | 0.49              |
| 3:A:273:ASN:HA    | 3:A:296:LEU:CD1   | 2.43                     | 0.49              |
| 3:A:452:LYS:CB    | 4:B:1141:HIS:HE1  | 2.13                     | 0.49              |
| 3:A:543:LEU:HD11  | 3:A:547:LEU:HD11  | 1.94                     | 0.49              |
| 3:A:705:LYS:CG    | 3:A:713:SER:HB3   | 2.40                     | 0.49              |
| 3:A:902:LEU:HG    | 3:A:926:GLN:HG3   | 1.95                     | 0.49              |
| 3:A:1116:LEU:CD1  | 3:A:1329:THR:OG1  | 2.60                     | 0.49              |
| 3:A:1166:ASP:OD1  | 3:A:1194:ARG:NH2  | 2.41                     | 0.49              |
| 3:A:1308:THR:CG2  | 3:A:1309:ASP:H    | 2.24                     | 0.49              |
| 3:A:1399:ARG:NH2  | 3:A:1417:GLU:OE1  | 2.45                     | 0.49              |
| 4:B:173:MET:N     | 4:B:203:PHE:HE2   | 2.11                     | 0.49              |
| 4:B:1135:ARG:O    | 4:B:1136:ASP:C    | 2.53                     | 0.49              |
| 4:B:1158:PHE:CD2  | 4:B:1198:TYR:HD1  | 2.30                     | 0.49              |
| 6:E:114:ASN:O     | 6:E:115:ASN:CB    | 2.61                     | 0.49              |
| 11:K:53:ASP:OD1   | 11:K:56:VAL:CG2   | 2.61                     | 0.49              |
| 1:R:10:A:O3'      | 3:A:485:ASP:OD1   | 2.31                     | 0.49              |
| 3:A:84:ILE:HG22   | 3:A:241:VAL:HG22  | 1.92                     | 0.49              |
| 3:A:351:THR:CG2   | 3:A:352:VAL:H     | 2.01                     | 0.49              |
| 3:A:452:LYS:CB    | 4:B:1141:HIS:CE1  | 2.82                     | 0.49              |
| 3:A:1017:LEU:O    | 3:A:1017:LEU:HD23 | 2.13                     | 0.49              |
| 3:A:1169:ILE:HG22 | 3:A:1169:ILE:O    | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1354:ASN:O    | 3:A:1355:VAL:C    | 2.55                     | 0.49              |
| 4:B:515:HIS:CD2   | 4:B:517:THR:H     | 2.31                     | 0.49              |
| 4:B:614:SER:OG    | 4:B:627:PHE:HB2   | 2.12                     | 0.49              |
| 4:B:778:MET:HE1   | 4:B:853:SER:CB    | 2.43                     | 0.49              |
| 4:B:826:ALA:HB2   | 4:B:1087:PHE:CD1  | 2.48                     | 0.49              |
| 4:B:842:ASN:HB3   | 4:B:845:SER:OG    | 2.13                     | 0.49              |
| 4:B:957:ASN:ND2   | 4:B:957:ASN:C     | 2.71                     | 0.49              |
| 5:C:41:ILE:CD1    | 5:C:172:PRO:HG3   | 2.41                     | 0.49              |
| 5:C:100:THR:HB    | 5:C:119:VAL:HG12  | 1.93                     | 0.49              |
| 6:E:39:LEU:O      | 6:E:42:PHE:N      | 2.38                     | 0.49              |
| 6:E:64:PRO:HG2    | 6:E:76:GLY:CA     | 2.37                     | 0.49              |
| 6:E:98:ILE:C      | 6:E:100:ILE:N     | 2.71                     | 0.49              |
| 6:E:177:ARG:HD3   | 6:E:215:MET:SD    | 2.53                     | 0.49              |
| 6:E:178:ILE:CG1   | 6:E:179:GLN:H     | 2.25                     | 0.49              |
| 8:H:129:TYR:C     | 8:H:131:ASN:N     | 2.71                     | 0.49              |
| 3:A:361:LEU:N     | 3:A:471:ASN:HD22  | 2.10                     | 0.49              |
| 3:A:401:GLY:O     | 3:A:435:HIS:HB2   | 2.12                     | 0.49              |
| 3:A:567:LYS:HB2   | 8:H:95:TYR:HA     | 1.95                     | 0.49              |
| 3:A:612:ILE:C     | 3:A:613:ILE:HD13  | 2.38                     | 0.49              |
| 3:A:699:ALA:C     | 3:A:701:LEU:H     | 2.21                     | 0.49              |
| 3:A:1116:LEU:HB2  | 3:A:1308:THR:CB   | 2.43                     | 0.49              |
| 3:A:1130:GLN:O    | 3:A:1134:ILE:HG13 | 2.13                     | 0.49              |
| 3:A:1265:ASN:O    | 3:A:1268:LEU:N    | 2.46                     | 0.49              |
| 4:B:224:GLN:O     | 4:B:238:ALA:HA    | 2.13                     | 0.49              |
| 4:B:317:CYS:O     | 4:B:319:GLU:N     | 2.46                     | 0.49              |
| 4:B:563:MET:O     | 4:B:563:MET:CG    | 2.45                     | 0.49              |
| 4:B:841:MET:O     | 4:B:993:THR:HA    | 2.11                     | 0.49              |
| 4:B:1106:ARG:HH21 | 4:B:1109:GLY:C    | 2.19                     | 0.49              |
| 5:C:37:MET:HG2    | 5:C:243:VAL:HG12  | 1.95                     | 0.49              |
| 5:C:62:PHE:HD2    | 5:C:62:PHE:O      | 1.96                     | 0.49              |
| 7:F:74:ILE:HG23   | 7:F:75:PRO:HD2    | 1.93                     | 0.49              |
| 8:H:134:ASN:O     | 8:H:135:LEU:C     | 2.55                     | 0.49              |
| 3:A:294:SER:O     | 3:A:298:PHE:CB    | 2.60                     | 0.48              |
| 3:A:474:VAL:O     | 3:A:474:VAL:HG13  | 2.13                     | 0.48              |
| 3:A:531:ILE:CD1   | 3:A:649:ILE:HG21  | 2.42                     | 0.48              |
| 3:A:538:ASP:OD1   | 8:H:22:LYS:HB2    | 2.13                     | 0.48              |
| 3:A:942:PHE:O     | 3:A:945:GLU:HB3   | 2.13                     | 0.48              |
| 3:A:1154:TYR:HB2  | 3:A:1191:TRP:HZ3  | 1.76                     | 0.48              |
| 3:A:1348:LEU:HD21 | 3:A:1375:MET:SD   | 2.53                     | 0.48              |
| 4:B:51:PHE:O      | 4:B:54:PHE:N      | 2.42                     | 0.48              |
| 4:B:291:ILE:HG21  | 4:B:297:ILE:HD13  | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:313:MET:HE2   | 4:B:386:LEU:HD22  | 1.94                     | 0.48              |
| 4:B:321:GLY:C     | 4:B:323:VAL:N     | 2.71                     | 0.48              |
| 4:B:352:ALA:O     | 4:B:354:ASP:N     | 2.46                     | 0.48              |
| 4:B:780:VAL:CG1   | 4:B:817:LEU:HD23  | 2.43                     | 0.48              |
| 4:B:1096:ARG:O    | 4:B:1097:HIS:CB   | 2.60                     | 0.48              |
| 4:B:1147:LEU:CD2  | 4:B:1151:LEU:HD22 | 2.42                     | 0.48              |
| 6:E:66:GLU:HA     | 6:E:69:ILE:HB     | 1.94                     | 0.48              |
| 11:K:47:ARG:NH1   | 11:K:48:ALA:N     | 2.61                     | 0.48              |
| 3:A:107:CYS:N     | 3:A:114:LEU:CD2   | 2.75                     | 0.48              |
| 3:A:138:ILE:O     | 3:A:139:TRP:C     | 2.55                     | 0.48              |
| 3:A:335:ARG:HD3   | 3:A:335:ARG:HA    | 1.63                     | 0.48              |
| 3:A:493:GLN:NE2   | 3:A:493:GLN:HA    | 2.28                     | 0.48              |
| 3:A:882:SER:HA    | 3:A:952:ALA:O     | 2.13                     | 0.48              |
| 3:A:1141:THR:CG2  | 3:A:1205:LYS:HD2  | 2.43                     | 0.48              |
| 4:B:42:GLY:C      | 4:B:43:LEU:HD23   | 2.38                     | 0.48              |
| 4:B:660:LYS:O     | 4:B:663:ALA:HB3   | 2.14                     | 0.48              |
| 4:B:689:LEU:C     | 4:B:690:VAL:HG23  | 2.38                     | 0.48              |
| 4:B:839:MET:CG    | 4:B:1010:LEU:HD11 | 2.43                     | 0.48              |
| 4:B:843:GLN:HG3   | 4:B:843:GLN:O     | 2.12                     | 0.48              |
| 4:B:1031:LEU:HD13 | 4:B:1055:ILE:HD12 | 1.95                     | 0.48              |
| 7:F:136:ARG:O     | 7:F:143:PHE:HB2   | 2.12                     | 0.48              |
| 8:H:5:LEU:CD2     | 8:H:133:ASN:O     | 2.58                     | 0.48              |
| 9:I:15:TYR:O      | 9:I:27:PHE:HA     | 2.13                     | 0.48              |
| 9:I:113:ASP:OD2   | 9:I:116:ASN:HB2   | 2.12                     | 0.48              |
| 3:A:322:VAL:O     | 3:A:323:LYS:CB    | 2.60                     | 0.48              |
| 3:A:809:THR:CB    | 3:A:810:PRO:CD    | 2.91                     | 0.48              |
| 3:A:897:TYR:HB3   | 3:A:936:LEU:HD12  | 1.95                     | 0.48              |
| 3:A:1109:LYS:O    | 3:A:1111:MET:N    | 2.43                     | 0.48              |
| 3:A:1311:VAL:HG21 | 3:A:1329:THR:CG2  | 2.44                     | 0.48              |
| 3:A:1441:PHE:CE1  | 7:F:89:GLU:HA     | 2.49                     | 0.48              |
| 4:B:293:PRO:HA    | 9:I:12:ASN:HD21   | 1.78                     | 0.48              |
| 4:B:461:LEU:HD12  | 4:B:466:TRP:HZ3   | 1.77                     | 0.48              |
| 4:B:640:VAL:HG12  | 4:B:650:GLU:O     | 2.13                     | 0.48              |
| 4:B:847:ASP:OD2   | 11:K:6:ARG:NH2    | 2.40                     | 0.48              |
| 4:B:861:ASP:OD1   | 4:B:914:LYS:NZ    | 2.41                     | 0.48              |
| 4:B:976:ILE:HD11  | 4:B:992:ILE:CD1   | 2.42                     | 0.48              |
| 6:E:187:TYR:CD2   | 6:E:187:TYR:C     | 2.92                     | 0.48              |
| 8:H:76:THR:HG23   | 8:H:77:ARG:NH2    | 2.27                     | 0.48              |
| 10:J:14:VAL:C     | 10:J:16:ASP:H     | 2.22                     | 0.48              |
| 10:J:59:LYS:O     | 10:J:62:ARG:CB    | 2.60                     | 0.48              |
| 3:A:78:PRO:O      | 3:A:79:GLY:C      | 2.56                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:241:VAL:HG13 | 3:A:266:LEU:CD1  | 2.43                     | 0.48              |
| 3:A:445:ASN:ND2  | 3:A:446:ARG:C    | 2.72                     | 0.48              |
| 3:A:706:HIS:NE2  | 3:A:1139:GLU:OE2 | 2.45                     | 0.48              |
| 3:A:840:ARG:O    | 3:A:841:LEU:C    | 2.55                     | 0.48              |
| 4:B:34:ILE:CD1   | 4:B:743:ILE:CG2  | 2.91                     | 0.48              |
| 4:B:179:CYS:O    | 4:B:181:LEU:N    | 2.47                     | 0.48              |
| 4:B:195:CYS:SG   | 4:B:196:PRO:HD2  | 2.54                     | 0.48              |
| 4:B:300:HIS:CE1  | 4:B:376:PHE:CZ   | 3.01                     | 0.48              |
| 4:B:628:THR:O    | 4:B:628:THR:CG2  | 2.60                     | 0.48              |
| 4:B:893:LEU:HD23 | 4:B:897:GLY:C    | 2.39                     | 0.48              |
| 5:C:237:SER:C    | 5:C:238:ILE:HG13 | 2.38                     | 0.48              |
| 6:E:59:SER:CB    | 6:E:81:GLU:HA    | 2.43                     | 0.48              |
| 7:F:80:ALA:O     | 7:F:81:THR:C     | 2.57                     | 0.48              |
| 7:F:109:VAL:HG21 | 7:F:124:GLU:HG3  | 1.94                     | 0.48              |
| 10:J:3:VAL:CG2   | 10:J:18:TRP:CG   | 2.96                     | 0.48              |
| 3:A:44:THR:O     | 3:A:45:GLN:HB2   | 2.13                     | 0.48              |
| 3:A:68:GLN:NE2   | 3:A:70:CYS:CB    | 2.76                     | 0.48              |
| 3:A:492:PRO:CB   | 3:A:497:THR:HG22 | 2.43                     | 0.48              |
| 3:A:590:ARG:HG2  | 3:A:591:PHE:N    | 2.29                     | 0.48              |
| 3:A:808:LEU:HD12 | 3:A:808:LEU:N    | 2.29                     | 0.48              |
| 3:A:898:ARG:CA   | 3:A:933:TYR:CE1  | 2.97                     | 0.48              |
| 3:A:947:PHE:CD2  | 3:A:954:TRP:CZ2  | 3.01                     | 0.48              |
| 3:A:1398:MET:O   | 3:A:1399:ARG:C   | 2.56                     | 0.48              |
| 4:B:54:PHE:O     | 4:B:55:VAL:C     | 2.56                     | 0.48              |
| 4:B:230:ALA:O    | 4:B:232:SER:N    | 2.44                     | 0.48              |
| 4:B:1033:LYS:HE3 | 4:B:1087:PHE:O   | 2.13                     | 0.48              |
| 6:E:13:TRP:CD2   | 6:E:39:LEU:HD13  | 2.48                     | 0.48              |
| 8:H:138:GLU:O    | 8:H:139:ASN:O    | 2.31                     | 0.48              |
| 11:K:29:ASN:ND2  | 11:K:78:THR:O    | 2.46                     | 0.48              |
| 12:L:61:THR:HG22 | 12:L:62:LYS:H    | 1.78                     | 0.48              |
| 3:A:43:GLU:O     | 3:A:46:THR:CB    | 2.60                     | 0.48              |
| 3:A:381:THR:CG2  | 3:A:383:TYR:HB2  | 2.42                     | 0.48              |
| 3:A:507:VAL:HG13 | 3:A:521:MET:HE1  | 1.95                     | 0.48              |
| 3:A:783:THR:HB   | 3:A:787:PHE:HD1  | 1.78                     | 0.48              |
| 3:A:901:LEU:HD23 | 3:A:907:THR:HG23 | 1.89                     | 0.48              |
| 3:A:935:GLN:C    | 3:A:937:VAL:N    | 2.66                     | 0.48              |
| 3:A:941:LYS:O    | 3:A:942:PHE:C    | 2.56                     | 0.48              |
| 4:B:124:TYR:HB3  | 4:B:204:ILE:HD13 | 1.95                     | 0.48              |
| 4:B:170:LEU:HD13 | 4:B:457:LEU:HD13 | 1.96                     | 0.48              |
| 4:B:190:TYR:CZ   | 10:J:62:ARG:HG2  | 2.48                     | 0.48              |
| 4:B:653:VAL:O    | 4:B:654:ARG:HG2  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:796:LEU:CB   | 4:B:799:PRO:HD3   | 2.32                     | 0.48              |
| 4:B:864:LYS:N    | 4:B:872:GLU:OE1   | 2.40                     | 0.48              |
| 4:B:1072:MET:HE3 | 4:B:1085:ILE:CG2  | 2.35                     | 0.48              |
| 11:K:4:PRO:O     | 11:K:5:ASP:C      | 2.56                     | 0.48              |
| 3:A:114:LEU:H    | 3:A:114:LEU:HG    | 1.48                     | 0.48              |
| 3:A:137:ALA:O    | 3:A:138:ILE:O     | 2.32                     | 0.48              |
| 3:A:251:SER:OG   | 3:A:252:PHE:N     | 2.47                     | 0.48              |
| 3:A:618:GLU:CD   | 3:A:619:LYS:N     | 2.70                     | 0.48              |
| 3:A:893:PHE:C    | 3:A:893:PHE:HD2   | 2.19                     | 0.48              |
| 3:A:983:ILE:HD12 | 3:A:1028:THR:HG21 | 1.96                     | 0.48              |
| 3:A:1021:LEU:O   | 3:A:1022:LEU:C    | 2.56                     | 0.48              |
| 3:A:1044:TRP:C   | 3:A:1046:LEU:N    | 2.69                     | 0.48              |
| 4:B:55:VAL:O     | 4:B:56:ASP:C      | 2.56                     | 0.48              |
| 4:B:118:ARG:NH2  | 4:B:194:GLU:OE1   | 2.47                     | 0.48              |
| 4:B:234:ILE:HA   | 4:B:259:TYR:HA    | 1.95                     | 0.48              |
| 4:B:463:THR:HG21 | 4:B:465:ASN:ND2   | 2.28                     | 0.48              |
| 4:B:598:GLU:O    | 4:B:599:THR:C     | 2.57                     | 0.48              |
| 4:B:652:LYS:O    | 4:B:653:VAL:O     | 2.31                     | 0.48              |
| 6:E:26:ARG:NH2   | 6:E:109:ILE:HD11  | 2.28                     | 0.48              |
| 6:E:39:LEU:C     | 6:E:41:ASP:N      | 2.71                     | 0.48              |
| 8:H:93:TYR:CD1   | 8:H:143:LEU:HB3   | 2.48                     | 0.48              |
| 12:L:60:ARG:HG3  | 12:L:61:THR:O     | 2.13                     | 0.48              |
| 3:A:18:GLN:HE21  | 3:A:1418:LEU:HD13 | 1.78                     | 0.48              |
| 3:A:148:CYS:HB3  | 3:A:167:CYS:C     | 2.38                     | 0.48              |
| 3:A:465:TYR:CD2  | 4:B:976:ILE:HD12  | 2.49                     | 0.48              |
| 3:A:768:GLN:HG3  | 3:A:816:HIS:HA    | 1.94                     | 0.48              |
| 3:A:839:ARG:O    | 3:A:843:LYS:N     | 2.41                     | 0.48              |
| 3:A:901:LEU:H    | 3:A:926:GLN:CG    | 2.27                     | 0.48              |
| 3:A:1120:LEU:O   | 3:A:1323:ASP:HB2  | 2.13                     | 0.48              |
| 4:B:666:TYR:C    | 4:B:668:ASP:N     | 2.72                     | 0.48              |
| 4:B:1081:LEU:HA  | 4:B:1081:LEU:HD23 | 1.75                     | 0.48              |
| 4:B:1152:MET:O   | 4:B:1156:ASP:O    | 2.31                     | 0.48              |
| 5:C:164:ALA:O    | 5:C:166:GLU:N     | 2.47                     | 0.48              |
| 6:E:20:LYS:O     | 6:E:21:GLU:C      | 2.57                     | 0.48              |
| 6:E:100:ILE:HD11 | 6:E:108:GLY:HA2   | 1.94                     | 0.48              |
| 6:E:182:ASP:HA   | 6:E:183:PRO:HD2   | 1.57                     | 0.48              |
| 7:F:98:ALA:O     | 7:F:117:PRO:HB2   | 2.13                     | 0.48              |
| 11:K:49:GLU:C    | 11:K:51:LEU:N     | 2.71                     | 0.48              |
| 3:A:76:GLU:O     | 3:A:76:GLU:CG     | 2.61                     | 0.48              |
| 3:A:399:HIS:O    | 3:A:401:GLY:N     | 2.41                     | 0.48              |
| 3:A:567:LYS:HD3  | 8:H:95:TYR:HA     | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:648:ASN:O     | 3:A:649:ILE:C     | 2.56                     | 0.48              |
| 3:A:910:PRO:HB3   | 3:A:916:GLY:CA    | 2.44                     | 0.48              |
| 3:A:1254:ALA:O    | 3:A:1255:GLU:CB   | 2.60                     | 0.48              |
| 4:B:431:TYR:CG    | 4:B:447:ALA:HB1   | 2.49                     | 0.48              |
| 4:B:780:VAL:HG12  | 4:B:817:LEU:CD2   | 2.44                     | 0.48              |
| 4:B:826:ALA:O     | 4:B:1011:ILE:HG23 | 2.14                     | 0.48              |
| 4:B:1006:ILE:HG22 | 4:B:1007:VAL:N    | 2.28                     | 0.48              |
| 4:B:1076:HIS:CE1  | 11:K:40:HIS:CD2   | 3.02                     | 0.48              |
| 5:C:49:VAL:HG12   | 5:C:155:LEU:HD22  | 1.96                     | 0.48              |
| 5:C:104:PHE:HB2   | 5:C:152:GLU:HG2   | 1.96                     | 0.48              |
| 6:E:36:GLU:O      | 6:E:38:PRO:CD     | 2.62                     | 0.48              |
| 6:E:78:LEU:HG     | 6:E:79:TRP:N      | 2.28                     | 0.48              |
| 6:E:178:ILE:HD11  | 6:E:185:ALA:HB2   | 1.95                     | 0.48              |
| 7:F:75:PRO:O      | 7:F:77:ASP:N      | 2.47                     | 0.48              |
| 7:F:95:GLY:O      | 7:F:98:ALA:HB3    | 2.13                     | 0.48              |
| 7:F:101:ILE:HD13  | 7:F:120:ILE:HG22  | 1.95                     | 0.48              |
| 7:F:111:LEU:HD13  | 7:F:111:LEU:N     | 2.26                     | 0.48              |
| 11:K:17:SER:O     | 11:K:18:LYS:C     | 2.55                     | 0.48              |
| 11:K:64:GLU:OE1   | 11:K:72:LYS:HE3   | 2.14                     | 0.48              |
| 2:T:1:DA:C2       | 2:T:2:DC:H5       | 2.32                     | 0.48              |
| 3:A:12:ARG:CB     | 4:B:1218:THR:CG2  | 2.92                     | 0.48              |
| 3:A:24:PRO:CD     | 3:A:25:GLU:H      | 2.27                     | 0.48              |
| 3:A:144:THR:O     | 3:A:146:MET:HG3   | 2.14                     | 0.48              |
| 3:A:300:VAL:O     | 3:A:304:MET:HE2   | 2.14                     | 0.48              |
| 3:A:389:THR:OG1   | 3:A:426:LEU:HD12  | 2.14                     | 0.48              |
| 3:A:416:ARG:HG3   | 3:A:417:TYR:CD2   | 2.49                     | 0.48              |
| 3:A:530:GLY:C     | 3:A:653:VAL:HG11  | 2.39                     | 0.48              |
| 3:A:583:PRO:O     | 3:A:610:GLY:CA    | 2.54                     | 0.48              |
| 3:A:947:PHE:CE2   | 3:A:954:TRP:CD2   | 3.02                     | 0.48              |
| 3:A:1041:ALA:O    | 3:A:1044:TRP:CB   | 2.60                     | 0.48              |
| 4:B:129:PHE:CD2   | 4:B:166:PHE:CB    | 2.89                     | 0.48              |
| 4:B:1013:ASN:OD1  | 4:B:1015:HIS:HB2  | 2.14                     | 0.48              |
| 5:C:194:GLU:HB2   | 5:C:200:GLU:OE2   | 2.14                     | 0.48              |
| 6:E:157:SER:OG    | 6:E:160:GLU:HB2   | 2.14                     | 0.48              |
| 6:E:173:SER:C     | 6:E:175:LEU:N     | 2.69                     | 0.48              |
| 7:F:155:LEU:N     | 7:F:155:LEU:CD2   | 2.53                     | 0.48              |
| 8:H:143:LEU:C     | 8:H:144:ILE:HG13  | 2.39                     | 0.48              |
| 3:A:89:PRO:O      | 3:A:90:VAL:HG22   | 2.14                     | 0.47              |
| 3:A:209:ASN:HB3   | 3:A:210:ILE:H     | 1.43                     | 0.47              |
| 3:A:351:THR:HG23  | 4:B:1103:ILE:HG23 | 1.94                     | 0.47              |
| 3:A:1195:LEU:HD11 | 3:A:1267:MET:HE3  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:B:63:ILE:HD12   | 4:B:95:ILE:HD12  | 1.96                     | 0.47              |
| 4:B:1159:ARG:HH21 | 4:B:1193:GLN:NE2 | 2.12                     | 0.47              |
| 5:C:5:GLY:O       | 5:C:6:PRO:C      | 2.56                     | 0.47              |
| 6:E:13:TRP:O      | 6:E:16:PHE:HB3   | 2.13                     | 0.47              |
| 7:F:125:LEU:HB2   | 7:F:130:ILE:CD1  | 2.41                     | 0.47              |
| 8:H:12:VAL:HG13   | 8:H:26:ILE:CG2   | 2.44                     | 0.47              |
| 10:J:57:ILE:CG2   | 10:J:58:GLU:N    | 2.77                     | 0.47              |
| 11:K:94:ILE:N     | 11:K:94:ILE:HD12 | 2.27                     | 0.47              |
| 2:T:1:DA:C2       | 2:T:2:DC:C5      | 3.01                     | 0.47              |
| 3:A:33:ALA:HB3    | 3:A:83:HIS:N     | 2.29                     | 0.47              |
| 3:A:99:ILE:C      | 3:A:102:VAL:HG23 | 2.39                     | 0.47              |
| 3:A:322:VAL:HG11  | 3:A:323:LYS:HD3  | 1.85                     | 0.47              |
| 3:A:493:GLN:NE2   | 3:A:493:GLN:CA   | 2.77                     | 0.47              |
| 3:A:551:TYR:CD1   | 3:A:551:TYR:C    | 2.89                     | 0.47              |
| 3:A:591:PHE:HA    | 3:A:595:THR:HG21 | 1.96                     | 0.47              |
| 3:A:741:ASN:ND2   | 3:A:743:VAL:HB   | 2.29                     | 0.47              |
| 3:A:919:ILE:CG2   | 3:A:922:ASP:HB2  | 2.44                     | 0.47              |
| 4:B:128:LEU:HD12  | 4:B:128:LEU:HA   | 1.50                     | 0.47              |
| 4:B:186:GLU:O     | 4:B:189:LEU:HB2  | 2.14                     | 0.47              |
| 4:B:1077:THR:CG2  | 4:B:1079:LYS:CB  | 2.92                     | 0.47              |
| 6:E:80:VAL:HA     | 6:E:109:ILE:CG2  | 2.44                     | 0.47              |
| 8:H:135:LEU:CD2   | 8:H:136:LYS:HD2  | 2.43                     | 0.47              |
| 9:I:34:TYR:O      | 9:I:35:VAL:HG23  | 2.13                     | 0.47              |
| 1:R:5:A:H2'       | 1:R:6:G:H8       | 1.79                     | 0.47              |
| 3:A:144:THR:O     | 3:A:146:MET:CE   | 2.59                     | 0.47              |
| 3:A:244:PRO:CB    | 3:A:245:PRO:CD   | 2.92                     | 0.47              |
| 3:A:512:VAL:HA    | 3:A:519:PRO:HA   | 1.96                     | 0.47              |
| 3:A:921:GLY:C     | 3:A:922:ASP:O    | 2.57                     | 0.47              |
| 3:A:1300:LYS:O    | 3:A:1302:PRO:HD3 | 2.14                     | 0.47              |
| 4:B:26:THR:O      | 4:B:27:ALA:C     | 2.57                     | 0.47              |
| 4:B:174:LEU:O     | 4:B:175:ARG:CB   | 2.62                     | 0.47              |
| 4:B:254:LEU:HD22  | 4:B:361:LEU:CD1  | 2.27                     | 0.47              |
| 4:B:364:ILE:O     | 4:B:365:THR:CB   | 2.62                     | 0.47              |
| 4:B:464:GLY:HA2   | 4:B:479:VAL:O    | 2.14                     | 0.47              |
| 4:B:518:HIS:O     | 4:B:519:TRP:C    | 2.55                     | 0.47              |
| 4:B:600:LEU:HB3   | 4:B:615:MET:HE1  | 1.97                     | 0.47              |
| 4:B:803:LEU:N     | 4:B:822:ASN:HD21 | 2.13                     | 0.47              |
| 4:B:976:ILE:HA    | 4:B:990:ILE:CG2  | 2.45                     | 0.47              |
| 4:B:995:ARG:HB2   | 4:B:995:ARG:CZ   | 2.44                     | 0.47              |
| 5:C:29:MET:HB2    | 11:K:45:LEU:CD1  | 2.44                     | 0.47              |
| 5:C:191:TYR:N     | 5:C:191:TYR:CD1  | 2.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:E:136:ASN:OD1   | 6:E:137:GLU:N     | 2.46                     | 0.47              |
| 11:K:32:VAL:HG23  | 11:K:74:ARG:HA    | 1.95                     | 0.47              |
| 11:K:42:LEU:O     | 11:K:43:GLY:C     | 2.58                     | 0.47              |
| 3:A:61:ILE:O      | 3:A:62:ASP:C      | 2.50                     | 0.47              |
| 3:A:247:ARG:O     | 3:A:247:ARG:HG2   | 2.15                     | 0.47              |
| 3:A:785:PRO:HB2   | 4:B:701:ILE:CD1   | 2.40                     | 0.47              |
| 3:A:900:ASP:CA    | 3:A:926:GLN:NE2   | 2.77                     | 0.47              |
| 3:A:901:LEU:CB    | 3:A:926:GLN:HG2   | 2.42                     | 0.47              |
| 3:A:902:LEU:CG    | 3:A:926:GLN:HG3   | 2.44                     | 0.47              |
| 3:A:982:THR:HB    | 3:A:985:ASP:H     | 1.80                     | 0.47              |
| 3:A:1394:THR:HG22 | 3:A:1395:GLY:H    | 1.76                     | 0.47              |
| 3:A:1424:VAL:HG12 | 3:A:1425:SER:N    | 2.30                     | 0.47              |
| 4:B:121:ASN:O     | 4:B:206:ASN:HA    | 2.13                     | 0.47              |
| 4:B:165:VAL:CG1   | 4:B:166:PHE:N     | 2.72                     | 0.47              |
| 4:B:879:ARG:HB3   | 4:B:883:LEU:HD22  | 1.97                     | 0.47              |
| 4:B:917:PRO:O     | 4:B:918:ILE:HD13  | 2.13                     | 0.47              |
| 4:B:992:ILE:HD11  | 11:K:67:PHE:CE2   | 2.49                     | 0.47              |
| 4:B:1131:GLY:C    | 4:B:1133:MET:N    | 2.71                     | 0.47              |
| 4:B:1159:ARG:HE   | 4:B:1193:GLN:CG   | 2.26                     | 0.47              |
| 4:B:1168:LEU:HB3  | 4:B:1170:THR:OG1  | 2.15                     | 0.47              |
| 4:B:1183:LYS:O    | 4:B:1185:CYS:N    | 2.47                     | 0.47              |
| 6:E:127:ILE:HD11  | 6:E:132:ILE:HD12  | 1.95                     | 0.47              |
| 11:K:47:ARG:C     | 11:K:47:ARG:NH1   | 2.71                     | 0.47              |
| 3:A:135:PHE:CD2   | 3:A:135:PHE:O     | 2.67                     | 0.47              |
| 3:A:464:PRO:O     | 3:A:465:TYR:HB2   | 2.14                     | 0.47              |
| 3:A:671:ALA:O     | 3:A:672:ASP:C     | 2.56                     | 0.47              |
| 3:A:943:LEU:C     | 3:A:945:GLU:N     | 2.69                     | 0.47              |
| 3:A:1152:ILE:CG1  | 3:A:1260:LEU:HD23 | 2.44                     | 0.47              |
| 3:A:1193:LEU:C    | 3:A:1193:LEU:CD1  | 2.86                     | 0.47              |
| 3:A:1423:GLY:O    | 3:A:1424:VAL:C    | 2.56                     | 0.47              |
| 4:B:98:THR:OG1    | 4:B:127:GLY:HA3   | 2.14                     | 0.47              |
| 4:B:258:LEU:O     | 4:B:259:TYR:C     | 2.56                     | 0.47              |
| 4:B:294:ASP:N     | 9:I:12:ASN:ND2    | 2.63                     | 0.47              |
| 4:B:660:LYS:HE2   | 4:B:679:TYR:CE2   | 2.50                     | 0.47              |
| 4:B:816:GLU:N     | 4:B:816:GLU:OE1   | 2.48                     | 0.47              |
| 4:B:1203:LEU:HD12 | 4:B:1203:LEU:O    | 2.14                     | 0.47              |
| 5:C:204:SER:O     | 5:C:205:LYS:C     | 2.55                     | 0.47              |
| 6:E:153:HIS:N     | 6:E:153:HIS:HD1   | 2.13                     | 0.47              |
| 6:E:188:LEU:HB2   | 6:E:190:LEU:HD21  | 1.95                     | 0.47              |
| 8:H:77:ARG:HB2    | 8:H:77:ARG:NH1    | 2.28                     | 0.47              |
| 3:A:51:GLY:HA2    | 3:A:56:PRO:HG3    | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:733:ALA:O     | 3:A:735:VAL:N     | 2.47                     | 0.47              |
| 3:A:935:GLN:HE21  | 3:A:1023:ARG:NH1  | 2.13                     | 0.47              |
| 3:A:997:LEU:O     | 3:A:1053:PHE:CE2  | 2.67                     | 0.47              |
| 3:A:1097:GLY:O    | 3:A:1098:VAL:C    | 2.57                     | 0.47              |
| 3:A:1332:PHE:CE1  | 3:A:1348:LEU:HD13 | 2.49                     | 0.47              |
| 4:B:298:LEU:HD23  | 4:B:298:LEU:H     | 1.78                     | 0.47              |
| 4:B:1084:GLN:N    | 4:B:1084:GLN:CD   | 2.68                     | 0.47              |
| 5:C:119:VAL:HG12  | 5:C:119:VAL:O     | 2.14                     | 0.47              |
| 6:E:204:THR:HG22  | 6:E:205:SER:H     | 1.78                     | 0.47              |
| 1:R:5:A:C2        | 1:R:6:G:C5        | 3.03                     | 0.47              |
| 1:R:9:G:O4'       | 4:B:1097:HIS:CE1  | 2.68                     | 0.47              |
| 2:T:4:DA:C5       | 3:A:831:THR:HG21  | 2.50                     | 0.47              |
| 3:A:100:LYS:NZ    | 3:A:100:LYS:CB    | 2.78                     | 0.47              |
| 3:A:210:ILE:O     | 3:A:213:HIS:N     | 2.44                     | 0.47              |
| 3:A:306:ASN:N     | 3:A:306:ASN:HD22  | 2.12                     | 0.47              |
| 3:A:320:ARG:NH2   | 4:B:470:LYS:C     | 2.73                     | 0.47              |
| 3:A:352:VAL:HG12  | 3:A:353:ILE:H     | 1.76                     | 0.47              |
| 3:A:570:PRO:O     | 3:A:572:TRP:CZ3   | 2.67                     | 0.47              |
| 3:A:723:ASN:O     | 3:A:724:GLU:C     | 2.56                     | 0.47              |
| 3:A:765:VAL:HG21  | 3:A:800:VAL:CG1   | 2.40                     | 0.47              |
| 3:A:834:THR:HG21  | 3:A:1077:THR:HG23 | 1.96                     | 0.47              |
| 3:A:1079:MET:C    | 3:A:1080:THR:OG1  | 2.53                     | 0.47              |
| 3:A:1436:ILE:HD13 | 4:B:1139:ILE:HG23 | 1.97                     | 0.47              |
| 3:A:1445:ILE:H    | 3:A:1445:ILE:CD1  | 2.06                     | 0.47              |
| 4:B:174:LEU:O     | 4:B:175:ARG:HB2   | 2.14                     | 0.47              |
| 4:B:198:ASP:OD1   | 4:B:485:ARG:NH2   | 2.45                     | 0.47              |
| 4:B:202:TYR:CD2   | 4:B:202:TYR:N     | 2.82                     | 0.47              |
| 4:B:204:ILE:N     | 4:B:204:ILE:HD12  | 2.30                     | 0.47              |
| 4:B:291:ILE:CG2   | 4:B:297:ILE:CD1   | 2.90                     | 0.47              |
| 4:B:324:ILE:O     | 4:B:324:ILE:HG22  | 2.12                     | 0.47              |
| 4:B:384:ARG:HH22  | 4:B:621:GLU:HG3   | 1.79                     | 0.47              |
| 4:B:446:LEU:O     | 4:B:447:ALA:CB    | 2.60                     | 0.47              |
| 4:B:579:ARG:HB2   | 4:B:586:TRP:NE1   | 2.29                     | 0.47              |
| 4:B:653:VAL:O     | 4:B:654:ARG:CG    | 2.63                     | 0.47              |
| 4:B:830:TYR:HB3   | 4:B:831:SER:H     | 1.46                     | 0.47              |
| 4:B:890:TYR:CE2   | 4:B:910:VAL:HG21  | 2.50                     | 0.47              |
| 4:B:1065:GLN:HG3  | 4:B:1065:GLN:O    | 2.14                     | 0.47              |
| 5:C:11:ARG:HE     | 5:C:21:ILE:CD1    | 2.26                     | 0.47              |
| 5:C:18:VAL:O      | 5:C:231:ASN:HA    | 2.15                     | 0.47              |
| 5:C:57:VAL:CG1    | 10:J:60:PHE:CB    | 2.82                     | 0.47              |
| 5:C:62:PHE:C      | 5:C:62:PHE:HD2    | 2.22                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 8:H:47:PHE:CG     | 8:H:47:PHE:O     | 2.67                     | 0.47              |
| 8:H:142:LEU:HD12  | 8:H:142:LEU:C    | 2.36                     | 0.47              |
| 3:A:182:VAL:HG22  | 3:A:201:VAL:HG13 | 1.96                     | 0.47              |
| 3:A:210:ILE:HB    | 3:A:211:PHE:H    | 1.16                     | 0.47              |
| 3:A:332:LYS:C     | 3:A:334:GLY:H    | 2.23                     | 0.47              |
| 3:A:475:THR:O     | 3:A:476:SER:C    | 2.58                     | 0.47              |
| 3:A:476:SER:O     | 3:A:478:TYR:N    | 2.48                     | 0.47              |
| 3:A:518:LYS:CB    | 3:A:519:PRO:HD2  | 2.45                     | 0.47              |
| 3:A:635:ARG:HH21  | 3:A:877:HIS:CA   | 2.24                     | 0.47              |
| 3:A:715:GLU:OE2   | 3:A:774:ARG:NH1  | 2.46                     | 0.47              |
| 3:A:744:LYS:O     | 3:A:747:VAL:HB   | 2.15                     | 0.47              |
| 3:A:809:THR:CG2   | 3:A:812:GLU:OE1  | 2.55                     | 0.47              |
| 3:A:889:SER:HB3   | 3:A:891:ALA:HB3  | 1.97                     | 0.47              |
| 3:A:1017:LEU:CB   | 6:E:205:SER:HA   | 2.44                     | 0.47              |
| 3:A:1061:GLY:O    | 3:A:1062:GLU:C   | 2.57                     | 0.47              |
| 3:A:1227:ILE:C    | 3:A:1228:TRP:CE3 | 2.93                     | 0.47              |
| 3:A:1353:TYR:O    | 3:A:1354:ASN:C   | 2.55                     | 0.47              |
| 4:B:128:LEU:CB    | 4:B:167:ILE:O    | 2.61                     | 0.47              |
| 4:B:363:HIS:ND1   | 4:B:363:HIS:N    | 2.63                     | 0.47              |
| 4:B:474:SER:CA    | 4:B:476:ARG:CG   | 2.82                     | 0.47              |
| 4:B:1051:THR:HG22 | 4:B:1052:VAL:N   | 2.29                     | 0.47              |
| 5:C:17:ASN:OD1    | 5:C:233:GLU:HG2  | 2.15                     | 0.47              |
| 5:C:44:LEU:HD22   | 5:C:129:ILE:HG13 | 1.97                     | 0.47              |
| 7:F:135:ARG:O     | 7:F:135:ARG:CG   | 2.61                     | 0.47              |
| 9:I:4:PHE:CD2     | 9:I:4:PHE:N      | 2.81                     | 0.47              |
| 2:T:6:DC:C4       | 2:T:7:DC:C5      | 3.03                     | 0.47              |
| 3:A:65:LEU:N      | 3:A:65:LEU:CD2   | 2.67                     | 0.47              |
| 3:A:123:ARG:O     | 3:A:126:LEU:HG   | 2.14                     | 0.47              |
| 3:A:1048:ASN:O    | 3:A:1051:ALA:HB3 | 2.15                     | 0.47              |
| 3:A:1192:LEU:CD2  | 3:A:1239:ARG:NH2 | 2.76                     | 0.47              |
| 3:A:1334:ASP:O    | 3:A:1335:ILE:C   | 2.57                     | 0.47              |
| 3:A:1364:ASN:OD1  | 3:A:1366:ARG:NH1 | 2.48                     | 0.47              |
| 4:B:173:MET:N     | 4:B:203:PHE:CE2  | 2.82                     | 0.47              |
| 4:B:216:GLU:OE1   | 4:B:500:THR:OG1  | 2.33                     | 0.47              |
| 4:B:286:PHE:O     | 4:B:291:ILE:O    | 2.33                     | 0.47              |
| 4:B:360:PHE:C     | 4:B:362:PRO:HD3  | 2.40                     | 0.47              |
| 4:B:393:LYS:NZ    | 9:I:89:GLN:HB3   | 2.30                     | 0.47              |
| 4:B:530:GLY:O     | 4:B:533:CYS:HB2  | 2.15                     | 0.47              |
| 4:B:821:GLN:CD    | 4:B:851:PHE:H    | 2.22                     | 0.47              |
| 4:B:951:GLN:CG    | 12:L:57:LEU:HD22 | 2.45                     | 0.47              |
| 4:B:1023:VAL:O    | 4:B:1024:ALA:C   | 2.57                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:1106:ARG:NH2 | 4:B:1109:GLY:CA   | 2.78                     | 0.47              |
| 4:B:1165:ILE:CG2 | 4:B:1166:CYS:H    | 2.20                     | 0.47              |
| 6:E:12:LEU:HB2   | 6:E:55:ARG:NH2    | 2.29                     | 0.47              |
| 6:E:131:THR:CG2  | 6:E:132:ILE:N     | 2.65                     | 0.47              |
| 6:E:164:LEU:HD13 | 6:E:211:TYR:HE2   | 1.74                     | 0.47              |
| 8:H:42:ILE:O     | 8:H:44:VAL:N      | 2.48                     | 0.47              |
| 8:H:44:VAL:O     | 8:H:44:VAL:CG1    | 2.62                     | 0.47              |
| 10:J:5:VAL:O     | 10:J:6:ARG:O      | 2.32                     | 0.47              |
| 3:A:17:VAL:HB    | 3:A:1419:ASP:HB3  | 1.96                     | 0.47              |
| 3:A:265:LYS:CE   | 3:A:323:LYS:CE    | 2.88                     | 0.47              |
| 3:A:505:CYS:SG   | 4:B:1141:HIS:CD2  | 3.06                     | 0.47              |
| 3:A:1151:GLU:O   | 3:A:1152:ILE:HD12 | 2.15                     | 0.47              |
| 3:A:1167:GLU:O   | 3:A:1168:GLU:C    | 2.57                     | 0.47              |
| 3:A:1189:SER:O   | 3:A:1241:ARG:HD3  | 2.14                     | 0.47              |
| 3:A:1271:ILE:HA  | 3:A:1271:ILE:HD13 | 1.62                     | 0.47              |
| 3:A:1407:GLU:O   | 3:A:1411:GLU:HG2  | 2.15                     | 0.47              |
| 4:B:224:GLN:O    | 4:B:239:GLU:N     | 2.47                     | 0.47              |
| 4:B:236:HIS:O    | 4:B:237:VAL:CG2   | 2.64                     | 0.47              |
| 4:B:515:HIS:CD2  | 4:B:517:THR:OG1   | 2.66                     | 0.47              |
| 4:B:737:THR:O    | 4:B:738:PHE:C     | 2.58                     | 0.47              |
| 4:B:778:MET:HB3  | 4:B:796:LEU:HD13  | 1.96                     | 0.47              |
| 4:B:906:SER:O    | 4:B:909:ASP:CG    | 2.58                     | 0.47              |
| 4:B:1032:SER:C   | 4:B:1089:PRO:HG2  | 2.40                     | 0.47              |
| 5:C:253:LYS:O    | 5:C:256:ALA:HB3   | 2.15                     | 0.47              |
| 8:H:11:GLN:HG3   | 8:H:53:ASP:O      | 2.14                     | 0.47              |
| 8:H:89:LEU:HD13  | 8:H:91:ASP:OD1    | 2.14                     | 0.47              |
| 3:A:32:VAL:HA    | 3:A:57:ARG:HH11   | 1.79                     | 0.46              |
| 3:A:93:VAL:HG21  | 3:A:301:ALA:HA    | 1.97                     | 0.46              |
| 3:A:382:PRO:HD3  | 3:A:428:TYR:CD2   | 2.49                     | 0.46              |
| 3:A:455:MET:C    | 3:A:456:MET:CG    | 2.87                     | 0.46              |
| 3:A:795:GLU:HG2  | 3:A:795:GLU:H     | 1.12                     | 0.46              |
| 3:A:898:ARG:HA   | 3:A:933:TYR:CE1   | 2.49                     | 0.46              |
| 3:A:1227:ILE:CG2 | 3:A:1228:TRP:N    | 2.77                     | 0.46              |
| 3:A:1298:TYR:O   | 3:A:1299:VAL:HG22 | 2.14                     | 0.46              |
| 3:A:1345:ARG:HG3 | 3:A:1372:VAL:HG12 | 1.97                     | 0.46              |
| 3:A:1364:ASN:CG  | 3:A:1366:ARG:HH11 | 2.23                     | 0.46              |
| 4:B:189:LEU:C    | 4:B:191:LYS:N     | 2.69                     | 0.46              |
| 4:B:230:ALA:C    | 4:B:232:SER:H     | 2.22                     | 0.46              |
| 4:B:827:ILE:O    | 4:B:828:ALA:CB    | 2.63                     | 0.46              |
| 4:B:956:THR:HA   | 4:B:963:PHE:HB2   | 1.96                     | 0.46              |
| 4:B:1034:VAL:O   | 4:B:1037:LEU:HB2  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:162:GLY:HA3   | 5:C:170:TRP:CD2   | 2.51                     | 0.46              |
| 8:H:25:ARG:C      | 8:H:26:ILE:HD12   | 2.40                     | 0.46              |
| 9:I:68:LEU:HD23   | 9:I:68:LEU:HA     | 1.67                     | 0.46              |
| 3:A:68:GLN:HE22   | 3:A:70:CYS:CB     | 2.27                     | 0.46              |
| 3:A:885:THR:HG22  | 3:A:940:ARG:HG3   | 1.97                     | 0.46              |
| 3:A:921:GLY:O     | 3:A:922:ASP:C     | 2.58                     | 0.46              |
| 3:A:928:LEU:HA    | 3:A:928:LEU:HD23  | 1.56                     | 0.46              |
| 3:A:1274:ARG:HG3  | 3:A:1274:ARG:O    | 2.14                     | 0.46              |
| 3:A:1422:ARG:NH2  | 4:B:1220:ARG:HD2  | 2.28                     | 0.46              |
| 4:B:38:PHE:CE2    | 4:B:43:LEU:HD21   | 2.51                     | 0.46              |
| 4:B:199:MET:SD    | 4:B:199:MET:N     | 2.78                     | 0.46              |
| 4:B:202:TYR:CD1   | 4:B:209:GLU:HB3   | 2.51                     | 0.46              |
| 4:B:486:TYR:HE2   | 4:B:778:MET:HG3   | 1.81                     | 0.46              |
| 4:B:911:ILE:HD12  | 4:B:941:LEU:HD23  | 1.97                     | 0.46              |
| 6:E:143:ASN:OD1   | 6:E:187:TYR:CE1   | 2.68                     | 0.46              |
| 11:K:94:ILE:CD1   | 11:K:94:ILE:N     | 2.78                     | 0.46              |
| 3:A:26:GLU:HA     | 3:A:29:ALA:CB     | 2.45                     | 0.46              |
| 3:A:69:THR:HB     | 4:B:1174:LYS:HE3  | 1.97                     | 0.46              |
| 3:A:91:PHE:C      | 3:A:297:GLN:HE22  | 2.24                     | 0.46              |
| 3:A:106:VAL:HG13  | 3:A:107:CYS:H     | 1.81                     | 0.46              |
| 3:A:207:ILE:H     | 3:A:207:ILE:HG13  | 1.13                     | 0.46              |
| 3:A:220:THR:O     | 3:A:221:SER:C     | 2.58                     | 0.46              |
| 3:A:254:GLU:HB3   | 4:B:935:ARG:NH1   | 2.30                     | 0.46              |
| 3:A:959:ASN:C     | 3:A:959:ASN:OD1   | 2.58                     | 0.46              |
| 3:A:1009:ASN:ND2  | 3:A:1012:ARG:HH12 | 2.12                     | 0.46              |
| 3:A:1100:ARG:O    | 3:A:1103:GLU:N    | 2.48                     | 0.46              |
| 3:A:1389:PHE:C    | 3:A:1389:PHE:HD1  | 2.22                     | 0.46              |
| 3:A:1424:VAL:HG11 | 4:B:1139:ILE:HD13 | 1.97                     | 0.46              |
| 4:B:300:HIS:CE1   | 4:B:376:PHE:CE1   | 3.03                     | 0.46              |
| 5:C:77:ILE:HA     | 5:C:129:ILE:CD1   | 2.45                     | 0.46              |
| 6:E:170:LEU:HD13  | 6:E:175:LEU:HD22  | 1.93                     | 0.46              |
| 8:H:128:ASN:O     | 8:H:128:ASN:CG    | 2.57                     | 0.46              |
| 3:A:30:ILE:HA     | 4:B:1183:LYS:NZ   | 2.30                     | 0.46              |
| 3:A:361:LEU:HA    | 3:A:471:ASN:ND2   | 2.30                     | 0.46              |
| 3:A:779:PHE:CE1   | 3:A:784:LEU:HA    | 2.50                     | 0.46              |
| 3:A:802:ASN:OD1   | 4:B:729:ILE:N     | 2.48                     | 0.46              |
| 3:A:1271:ILE:O    | 3:A:1271:ILE:HG22 | 2.14                     | 0.46              |
| 4:B:40:GLU:OE2    | 4:B:681:TRP:HB3   | 2.15                     | 0.46              |
| 4:B:282:ILE:HD12  | 4:B:286:PHE:HD1   | 1.81                     | 0.46              |
| 4:B:486:TYR:CE2   | 4:B:778:MET:HG3   | 2.50                     | 0.46              |
| 4:B:1056:SER:O    | 4:B:1066:SER:HB2  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:1076:HIS:CG  | 11:K:40:HIS:CD2   | 3.02                     | 0.46              |
| 5:C:58:LEU:N     | 5:C:58:LEU:CD2    | 2.72                     | 0.46              |
| 5:C:141:GLY:C    | 5:C:142:VAL:O     | 2.56                     | 0.46              |
| 5:C:258:ILE:HD12 | 11:K:42:LEU:HD21  | 1.95                     | 0.46              |
| 6:E:53:PRO:HB2   | 6:E:55:ARG:NH1    | 2.31                     | 0.46              |
| 6:E:100:ILE:HD13 | 6:E:108:GLY:HA3   | 1.97                     | 0.46              |
| 9:I:2:THR:O      | 9:I:2:THR:HG22    | 2.16                     | 0.46              |
| 9:I:115:LYS:O    | 9:I:116:ASN:C     | 2.59                     | 0.46              |
| 11:K:46:ILE:O    | 11:K:50:LEU:HB2   | 2.15                     | 0.46              |
| 11:K:49:GLU:HA   | 11:K:49:GLU:OE1   | 2.14                     | 0.46              |
| 12:L:27:LEU:O    | 12:L:28:LYS:HG2   | 2.15                     | 0.46              |
| 3:A:8:SER:OG     | 4:B:1180:PHE:CE1  | 2.67                     | 0.46              |
| 3:A:257:ARG:CG   | 3:A:258:GLY:H     | 2.29                     | 0.46              |
| 3:A:894:GLU:HG3  | 3:A:898:ARG:HB2   | 1.96                     | 0.46              |
| 3:A:1004:ASN:ND2 | 6:E:167:ARG:CD    | 2.52                     | 0.46              |
| 4:B:179:CYS:C    | 4:B:181:LEU:N     | 2.74                     | 0.46              |
| 4:B:589:VAL:HG12 | 4:B:590:HIS:H     | 1.79                     | 0.46              |
| 4:B:653:VAL:HG12 | 4:B:654:ARG:N     | 2.31                     | 0.46              |
| 5:C:43:THR:CG2   | 5:C:44:LEU:H      | 2.28                     | 0.46              |
| 7:F:120:ILE:CG2  | 7:F:121:ALA:N     | 2.77                     | 0.46              |
| 8:H:32:THR:CG2   | 8:H:33:GLN:CG     | 2.88                     | 0.46              |
| 8:H:112:ILE:HG23 | 8:H:113:ALA:N     | 2.30                     | 0.46              |
| 1:R:9:G:P        | 4:B:776:GLN:HE22  | 2.38                     | 0.46              |
| 3:A:90:VAL:CG1   | 3:A:297:GLN:CA    | 2.78                     | 0.46              |
| 3:A:147:VAL:C    | 3:A:149:GLU:H     | 2.23                     | 0.46              |
| 3:A:182:VAL:CG2  | 3:A:201:VAL:HG13  | 2.45                     | 0.46              |
| 3:A:491:VAL:HA   | 3:A:492:PRO:HD2   | 1.62                     | 0.46              |
| 3:A:782:ARG:NH1  | 3:A:785:PRO:HA    | 2.31                     | 0.46              |
| 3:A:783:THR:HB   | 3:A:787:PHE:CD1   | 2.50                     | 0.46              |
| 3:A:809:THR:H    | 3:A:812:GLU:HB2   | 1.80                     | 0.46              |
| 3:A:899:VAL:HG11 | 3:A:908:LEU:HD21  | 1.98                     | 0.46              |
| 3:A:1402:PHE:CG  | 3:A:1403:GLU:N    | 2.79                     | 0.46              |
| 4:B:63:ILE:HG12  | 4:B:421:PHE:CZ    | 2.51                     | 0.46              |
| 4:B:769:TYR:C    | 4:B:771:SER:N     | 2.73                     | 0.46              |
| 4:B:984:HIS:CD2  | 4:B:1025:HIS:N    | 2.84                     | 0.46              |
| 6:E:63:ASN:HA    | 6:E:64:PRO:HD3    | 1.64                     | 0.46              |
| 6:E:96:PHE:C     | 6:E:98:ILE:N      | 2.72                     | 0.46              |
| 3:A:30:ILE:CG1   | 4:B:1170:THR:HG23 | 2.46                     | 0.46              |
| 3:A:57:ARG:O     | 3:A:68:GLN:CG     | 2.64                     | 0.46              |
| 3:A:92:HIS:HB2   | 3:A:236:LEU:HD12  | 1.95                     | 0.46              |
| 3:A:553:VAL:HG22 | 3:A:652:VAL:HG22  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:821:ARG:O     | 3:A:822:GLU:C     | 2.58                     | 0.46              |
| 3:A:910:PRO:HA    | 3:A:916:GLY:HA2   | 1.96                     | 0.46              |
| 3:A:1015:VAL:O    | 3:A:1018:PHE:N    | 2.49                     | 0.46              |
| 4:B:195:CYS:HB2   | 4:B:784:ASN:OD1   | 2.15                     | 0.46              |
| 4:B:563:MET:O     | 4:B:564:GLU:C     | 2.57                     | 0.46              |
| 4:B:854:LEU:HA    | 4:B:854:LEU:HD23  | 1.47                     | 0.46              |
| 5:C:181:ASP:OD2   | 5:C:186:LEU:HD13  | 2.14                     | 0.46              |
| 5:C:231:ASN:ND2   | 5:C:231:ASN:C     | 2.74                     | 0.46              |
| 9:I:14:LEU:HB3    | 9:I:28:GLU:C      | 2.41                     | 0.46              |
| 3:A:215:SER:OG    | 3:A:216:VAL:N     | 2.49                     | 0.46              |
| 3:A:336:ILE:HG22  | 3:A:337:ARG:N     | 2.30                     | 0.46              |
| 3:A:550:LEU:O     | 3:A:551:TYR:C     | 2.58                     | 0.46              |
| 3:A:573:SER:O     | 3:A:574:GLY:C     | 2.59                     | 0.46              |
| 3:A:590:ARG:NH2   | 3:A:621:THR:HA    | 2.30                     | 0.46              |
| 3:A:666:ILE:HA    | 4:B:1026:LEU:HD13 | 1.97                     | 0.46              |
| 3:A:777:PHE:CE2   | 3:A:782:ARG:CA    | 2.99                     | 0.46              |
| 3:A:816:HIS:O     | 3:A:816:HIS:ND1   | 2.49                     | 0.46              |
| 3:A:837:ILE:C     | 3:A:839:ARG:H     | 2.22                     | 0.46              |
| 3:A:878:ILE:CG2   | 3:A:879:GLU:N     | 2.79                     | 0.46              |
| 3:A:985:ASP:O     | 3:A:986:ILE:C     | 2.58                     | 0.46              |
| 3:A:1152:ILE:HG13 | 3:A:1260:LEU:HD23 | 1.97                     | 0.46              |
| 3:A:1171:GLN:CB   | 3:A:1172:LEU:HD23 | 2.32                     | 0.46              |
| 3:A:1210:GLY:O    | 3:A:1211:GLN:C    | 2.57                     | 0.46              |
| 4:B:737:THR:O     | 4:B:738:PHE:O     | 2.33                     | 0.46              |
| 4:B:1084:GLN:HE22 | 5:C:191:TYR:CA    | 2.21                     | 0.46              |
| 5:C:124:LEU:O     | 5:C:125:MET:HB2   | 2.16                     | 0.46              |
| 6:E:144:ILE:CG1   | 6:E:145:THR:N     | 2.79                     | 0.46              |
| 6:E:171:LYS:O     | 6:E:173:SER:N     | 2.49                     | 0.46              |
| 9:I:15:TYR:N      | 9:I:15:TYR:HD1    | 2.11                     | 0.46              |
| 11:K:61:TYR:HA    | 11:K:72:LYS:O     | 2.16                     | 0.46              |
| 3:A:211:PHE:O     | 3:A:212:LYS:C     | 2.59                     | 0.46              |
| 3:A:414:ASP:O     | 3:A:416:ARG:N     | 2.49                     | 0.46              |
| 3:A:476:SER:HB2   | 3:A:477:PRO:CD    | 2.46                     | 0.46              |
| 3:A:873:MET:HE3   | 3:A:957:PRO:HG2   | 1.98                     | 0.46              |
| 3:A:1211:GLN:O    | 3:A:1215:ARG:HB2  | 2.16                     | 0.46              |
| 4:B:478:GLY:C     | 4:B:479:VAL:O     | 2.45                     | 0.46              |
| 4:B:620:ARG:H     | 4:B:620:ARG:HG3   | 1.48                     | 0.46              |
| 4:B:779:GLY:HA2   | 4:B:796:LEU:HB2   | 1.98                     | 0.46              |
| 4:B:1213:THR:HA   | 4:B:1214:PRO:HD3  | 1.68                     | 0.46              |
| 6:E:103:LYS:O     | 6:E:104:ASN:C     | 2.59                     | 0.46              |
| 6:E:153:HIS:C     | 6:E:154:ILE:HG12  | 2.41                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:49:VAL:HG13   | 8:H:50:ALA:N      | 2.30                     | 0.46              |
| 9:I:92:ARG:HG2    | 9:I:94:ASP:OD2    | 2.15                     | 0.46              |
| 3:A:181:LEU:HB2   | 3:A:202:LEU:HB2   | 1.98                     | 0.46              |
| 3:A:596:THR:C     | 3:A:598:LEU:N     | 2.73                     | 0.46              |
| 3:A:841:LEU:HD23  | 3:A:841:LEU:HA    | 1.66                     | 0.46              |
| 3:A:1147:THR:HG21 | 3:A:1268:LEU:HD21 | 1.98                     | 0.46              |
| 3:A:1163:ILE:HA   | 3:A:1164:PRO:HD2  | 1.56                     | 0.46              |
| 3:A:1441:PHE:CZ   | 7:F:89:GLU:CA     | 2.92                     | 0.46              |
| 4:B:59:LEU:HG     | 4:B:95:ILE:HD13   | 1.97                     | 0.46              |
| 4:B:179:CYS:C     | 4:B:181:LEU:H     | 2.24                     | 0.46              |
| 4:B:361:LEU:N     | 4:B:361:LEU:CD1   | 2.78                     | 0.46              |
| 4:B:421:PHE:HA    | 4:B:453:ILE:HD11  | 1.97                     | 0.46              |
| 4:B:780:VAL:HG12  | 4:B:817:LEU:HD23  | 1.96                     | 0.46              |
| 4:B:856:PHE:HA    | 4:B:968:VAL:O     | 2.16                     | 0.46              |
| 4:B:898:LEU:O     | 4:B:899:ILE:C     | 2.59                     | 0.46              |
| 4:B:1060:ARG:O    | 4:B:1061:GLU:C    | 2.59                     | 0.46              |
| 4:B:1161:HIS:CD2  | 4:B:1173:ALA:HB2  | 2.51                     | 0.46              |
| 4:B:1184:GLY:O    | 4:B:1186:ASP:CG   | 2.59                     | 0.46              |
| 5:C:167:HIS:CD2   | 5:C:168:ALA:N     | 2.84                     | 0.46              |
| 6:E:202:SER:C     | 6:E:204:THR:H     | 2.24                     | 0.46              |
| 7:F:77:ASP:O      | 7:F:78:GLN:C      | 2.59                     | 0.46              |
| 8:H:50:ALA:O      | 8:H:53:ASP:HB2    | 2.16                     | 0.46              |
| 8:H:59:ILE:O      | 8:H:60:ALA:CB     | 2.61                     | 0.46              |
| 9:I:98:VAL:CG1    | 9:I:99:LEU:N      | 2.79                     | 0.46              |
| 10:J:23:ASN:O     | 10:J:27:GLU:HB2   | 2.15                     | 0.46              |
| 1:R:8:G:N2        | 2:T:8:DT:N3       | 2.64                     | 0.45              |
| 1:R:9:G:C5'       | 4:B:1097:HIS:NE2  | 2.80                     | 0.45              |
| 3:A:335:ARG:NH1   | 4:B:1202:LEU:HD12 | 2.31                     | 0.45              |
| 3:A:549:MET:HE1   | 3:A:656:TRP:HD1   | 1.82                     | 0.45              |
| 3:A:683:ILE:HD13  | 3:A:725:ALA:HB1   | 1.99                     | 0.45              |
| 3:A:892:ALA:HB2   | 3:A:895:LYS:HD2   | 1.98                     | 0.45              |
| 3:A:1005:GLU:O    | 3:A:1005:GLU:HG3  | 2.16                     | 0.45              |
| 3:A:1155:ASP:CG   | 3:A:1162:VAL:HG23 | 2.41                     | 0.45              |
| 3:A:1305:VAL:HG12 | 3:A:1306:LEU:N    | 2.30                     | 0.45              |
| 3:A:1340:GLY:CA   | 6:E:183:PRO:HG2   | 2.46                     | 0.45              |
| 3:A:1349:TYR:CD2  | 3:A:1350:LYS:N    | 2.83                     | 0.45              |
| 4:B:877:PRO:O     | 4:B:878:GLN:HG2   | 2.16                     | 0.45              |
| 4:B:957:ASN:C     | 4:B:957:ASN:HD22  | 2.24                     | 0.45              |
| 4:B:1027:ILE:O    | 4:B:1028:GLU:C    | 2.59                     | 0.45              |
| 4:B:1064:TYR:N    | 4:B:1064:TYR:HD1  | 2.14                     | 0.45              |
| 5:C:41:ILE:HA     | 5:C:42:PRO:HD3    | 1.49                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:245:VAL:C     | 5:C:247:GLY:N     | 2.73                     | 0.45              |
| 6:E:82:PHE:CD1    | 6:E:82:PHE:N      | 2.84                     | 0.45              |
| 7:F:81:THR:CG2    | 7:F:136:ARG:CD    | 2.84                     | 0.45              |
| 8:H:5:LEU:HB3     | 8:H:133:ASN:O     | 2.16                     | 0.45              |
| 3:A:320:ARG:CB    | 3:A:321:PRO:CB    | 2.74                     | 0.45              |
| 3:A:376:TYR:CD2   | 3:A:376:TYR:O     | 2.69                     | 0.45              |
| 3:A:601:LYS:HB3   | 3:A:603:ASN:CG    | 2.41                     | 0.45              |
| 3:A:785:PRO:CG    | 4:B:703:ILE:HD12  | 2.45                     | 0.45              |
| 3:A:867:ILE:HG22  | 3:A:872:GLY:N     | 2.32                     | 0.45              |
| 3:A:1032:LEU:O    | 3:A:1036:ARG:HG2  | 2.17                     | 0.45              |
| 3:A:1101:LEU:HD13 | 3:A:1355:VAL:HG11 | 1.99                     | 0.45              |
| 3:A:1399:ARG:O    | 3:A:1400:CYS:C    | 2.59                     | 0.45              |
| 3:A:1410:PHE:C    | 3:A:1412:ALA:N    | 2.71                     | 0.45              |
| 4:B:331:LEU:O     | 4:B:332:ASP:O     | 2.34                     | 0.45              |
| 4:B:472:ALA:O     | 4:B:473:MET:C     | 2.59                     | 0.45              |
| 4:B:476:ARG:C     | 4:B:478:GLY:N     | 2.73                     | 0.45              |
| 4:B:545:ILE:C     | 4:B:634:TYR:HE2   | 2.25                     | 0.45              |
| 4:B:550:ASP:HA    | 4:B:551:PRO:HD3   | 1.61                     | 0.45              |
| 4:B:610:ASN:O     | 4:B:613:VAL:HG23  | 2.15                     | 0.45              |
| 4:B:744:HIS:HA    | 4:B:745:PRO:HD3   | 1.50                     | 0.45              |
| 4:B:780:VAL:HA    | 4:B:795:ILE:HG23  | 1.98                     | 0.45              |
| 4:B:848:ARG:HH22  | 4:B:996:ARG:NH1   | 2.14                     | 0.45              |
| 4:B:953:LEU:HD22  | 4:B:965:LYS:HB2   | 1.97                     | 0.45              |
| 4:B:953:LEU:HD23  | 4:B:953:LEU:C     | 2.42                     | 0.45              |
| 4:B:999:MET:HG2   | 4:B:1008:PRO:HD2  | 1.97                     | 0.45              |
| 4:B:1159:ARG:NE   | 4:B:1193:GLN:HE21 | 2.15                     | 0.45              |
| 5:C:31:ASN:C      | 5:C:33:LEU:N      | 2.74                     | 0.45              |
| 6:E:32:GLN:HG3    | 6:E:32:GLN:O      | 2.16                     | 0.45              |
| 9:I:42:LEU:C      | 9:I:43:VAL:HG23   | 2.41                     | 0.45              |
| 10:J:50:ILE:C     | 10:J:52:THR:H     | 2.25                     | 0.45              |
| 12:L:30:ILE:HD11  | 12:L:59:ALA:HA    | 1.98                     | 0.45              |
| 12:L:45:ALA:O     | 12:L:46:VAL:HG22  | 2.16                     | 0.45              |
| 3:A:353:ILE:CG2   | 3:A:487:MET:HB2   | 2.46                     | 0.45              |
| 3:A:406:ILE:CD1   | 3:A:406:ILE:N     | 2.58                     | 0.45              |
| 3:A:682:THR:HA    | 3:A:685:GLU:OE2   | 2.16                     | 0.45              |
| 3:A:695:LYS:O     | 3:A:696:GLU:C     | 2.58                     | 0.45              |
| 3:A:715:GLU:O     | 3:A:716:ASP:C     | 2.57                     | 0.45              |
| 3:A:980:ASP:OD2   | 3:A:980:ASP:C     | 2.58                     | 0.45              |
| 3:A:1073:GLY:O    | 3:A:1076:ALA:HB3  | 2.17                     | 0.45              |
| 3:A:1159:ARG:H    | 3:A:1159:ARG:HG2  | 1.56                     | 0.45              |
| 3:A:1364:ASN:ND2  | 3:A:1366:ARG:NH1  | 2.55                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:25:ILE:HD12  | 4:B:651:LEU:CD1   | 2.34                     | 0.45              |
| 4:B:501:PRO:O    | 4:B:502:ILE:CB    | 2.64                     | 0.45              |
| 5:C:118:LEU:HB2  | 5:C:132:PRO:HG3   | 1.97                     | 0.45              |
| 5:C:120:ILE:HG21 | 5:C:124:LEU:HD21  | 1.98                     | 0.45              |
| 6:E:102:GLU:C    | 6:E:104:ASN:N     | 2.69                     | 0.45              |
| 7:F:133:VAL:HG22 | 7:F:146:TRP:C     | 2.42                     | 0.45              |
| 8:H:58:THR:HG22  | 8:H:59:ILE:H      | 1.80                     | 0.45              |
| 9:I:20:LYS:HB2   | 9:I:21:GLU:H      | 1.37                     | 0.45              |
| 2:T:14:DT:H2''   | 3:A:317:LYS:HG2   | 1.97                     | 0.45              |
| 3:A:58:LEU:O     | 3:A:59:GLY:C      | 2.55                     | 0.45              |
| 3:A:71:GLN:C     | 3:A:73:GLY:N      | 2.61                     | 0.45              |
| 3:A:269:ILE:C    | 3:A:271:LYS:H     | 2.24                     | 0.45              |
| 3:A:356:ASP:HA   | 3:A:357:PRO:HD2   | 1.79                     | 0.45              |
| 3:A:518:LYS:HG3  | 3:A:519:PRO:HD2   | 1.99                     | 0.45              |
| 3:A:642:CYS:O    | 3:A:643:ALA:C     | 2.58                     | 0.45              |
| 3:A:792:TYR:N    | 3:A:792:TYR:CD1   | 2.85                     | 0.45              |
| 3:A:1189:SER:OG  | 3:A:1190:PRO:CD   | 2.62                     | 0.45              |
| 4:B:350:GLN:O    | 4:B:353:LYS:N     | 2.50                     | 0.45              |
| 4:B:430:ARG:C    | 4:B:431:TYR:O     | 2.55                     | 0.45              |
| 4:B:562:GLY:HA3  | 4:B:590:HIS:HE1   | 1.78                     | 0.45              |
| 4:B:589:VAL:CG1  | 4:B:590:HIS:H     | 2.28                     | 0.45              |
| 4:B:1072:MET:CE  | 4:B:1085:ILE:CG2  | 2.92                     | 0.45              |
| 6:E:3:GLN:HG3    | 6:E:4:GLU:N       | 2.30                     | 0.45              |
| 8:H:106:GLU:HG3  | 8:H:112:ILE:HD11  | 1.98                     | 0.45              |
| 9:I:83:ASN:HA    | 9:I:102:VAL:O     | 2.16                     | 0.45              |
| 9:I:85:PHE:O     | 9:I:86:PHE:CB     | 2.65                     | 0.45              |
| 1:R:8:G:HO2'     | 1:R:9:G:H5'       | 1.79                     | 0.45              |
| 3:A:35:ILE:O     | 3:A:270:LEU:CD1   | 2.65                     | 0.45              |
| 3:A:128:ILE:CG2  | 3:A:128:ILE:O     | 2.65                     | 0.45              |
| 3:A:966:ASN:O    | 3:A:1044:TRP:CH2  | 2.70                     | 0.45              |
| 3:A:1205:LYS:O   | 3:A:1207:LEU:N    | 2.50                     | 0.45              |
| 3:A:1437:GLY:C   | 7:F:88:TYR:HB3    | 2.42                     | 0.45              |
| 4:B:647:GLY:O    | 4:B:648:HIS:CD2   | 2.69                     | 0.45              |
| 4:B:732:SER:HB3  | 4:B:734:HIS:CD2   | 2.51                     | 0.45              |
| 4:B:848:ARG:NH1  | 10:J:8:PHE:O      | 2.49                     | 0.45              |
| 4:B:1099:VAL:O   | 4:B:1103:ILE:HD11 | 2.16                     | 0.45              |
| 5:C:27:LEU:O     | 5:C:29:MET:N      | 2.49                     | 0.45              |
| 5:C:142:VAL:CG1  | 5:C:143:LEU:N     | 2.80                     | 0.45              |
| 9:I:58:VAL:C     | 9:I:59:VAL:HG23   | 2.41                     | 0.45              |
| 11:K:24:ASP:CG   | 11:K:74:ARG:NH1   | 2.74                     | 0.45              |
| 3:A:91:PHE:CA    | 3:A:297:GLN:HE22  | 2.29                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:535:THR:HG22  | 3:A:616:VAL:HA   | 1.96                     | 0.45              |
| 3:A:853:ASP:C     | 3:A:855:THR:N    | 2.75                     | 0.45              |
| 3:A:1210:GLY:O    | 3:A:1214:GLU:N   | 2.44                     | 0.45              |
| 4:B:27:ALA:O      | 4:B:30:SER:OG    | 2.34                     | 0.45              |
| 4:B:369:GLY:C     | 4:B:370:PHE:HD1  | 2.24                     | 0.45              |
| 4:B:408:LEU:HD12  | 4:B:408:LEU:HA   | 1.57                     | 0.45              |
| 4:B:428:ILE:HG13  | 4:B:448:ILE:HD13 | 1.97                     | 0.45              |
| 4:B:429:PHE:C     | 4:B:433:GLN:OE1  | 2.60                     | 0.45              |
| 4:B:523:CYS:SG    | 4:B:524:PRO:HD2  | 2.56                     | 0.45              |
| 4:B:569:TYR:CE1   | 4:B:589:VAL:HG21 | 2.52                     | 0.45              |
| 4:B:802:PRO:HB3   | 4:B:1091:TYR:CG  | 2.51                     | 0.45              |
| 5:C:3:GLU:CG      | 5:C:4:GLU:N      | 2.55                     | 0.45              |
| 5:C:196:ASP:C     | 5:C:198:ALA:N    | 2.74                     | 0.45              |
| 7:F:83:PRO:CD     | 7:F:84:TYR:N     | 2.79                     | 0.45              |
| 8:H:107:VAL:C     | 8:H:108:SER:O    | 2.57                     | 0.45              |
| 9:I:4:PHE:CE1     | 9:I:13:MET:CE    | 3.00                     | 0.45              |
| 9:I:99:LEU:HD23   | 9:I:99:LEU:HA    | 1.72                     | 0.45              |
| 11:K:27:ALA:CB    | 11:K:28:PRO:CD   | 2.83                     | 0.45              |
| 12:L:53:HIS:C     | 12:L:55:ILE:N    | 2.73                     | 0.45              |
| 3:A:315:LEU:CD1   | 3:A:319:GLY:HA2  | 2.27                     | 0.45              |
| 3:A:642:CYS:O     | 3:A:645:LEU:N    | 2.49                     | 0.45              |
| 3:A:1198:ASP:O    | 3:A:1202:MET:HG2 | 2.17                     | 0.45              |
| 4:B:357:GLN:O     | 4:B:366:GLN:HA   | 2.17                     | 0.45              |
| 4:B:579:ARG:HB2   | 4:B:586:TRP:HE1  | 1.82                     | 0.45              |
| 4:B:782:LEU:HB3   | 4:B:784:ASN:OD1  | 2.17                     | 0.45              |
| 4:B:860:MET:CG    | 4:B:861:ASP:N    | 2.72                     | 0.45              |
| 4:B:899:ILE:HG22  | 4:B:900:ALA:N    | 2.32                     | 0.45              |
| 4:B:1096:ARG:HH11 | 4:B:1096:ARG:CB  | 2.30                     | 0.45              |
| 4:B:1148:LYS:O    | 4:B:1152:MET:N   | 2.50                     | 0.45              |
| 6:E:82:PHE:N      | 6:E:82:PHE:HD1   | 2.15                     | 0.45              |
| 3:A:18:GLN:HE22   | 3:A:1418:LEU:HB2 | 1.81                     | 0.45              |
| 3:A:62:ASP:O      | 3:A:63:ARG:C     | 2.60                     | 0.45              |
| 3:A:543:LEU:O     | 3:A:544:ASP:C    | 2.58                     | 0.45              |
| 3:A:694:THR:HA    | 3:A:714:PHE:CE1  | 2.51                     | 0.45              |
| 3:A:800:VAL:HA    | 3:A:812:GLU:HG2  | 1.98                     | 0.45              |
| 3:A:884:ASP:OD2   | 3:A:884:ASP:N    | 2.49                     | 0.45              |
| 3:A:1127:ASP:HB3  | 3:A:1130:GLN:H   | 1.82                     | 0.45              |
| 3:A:1166:ASP:O    | 3:A:1170:ILE:CG1 | 2.62                     | 0.45              |
| 3:A:1215:ARG:HA   | 3:A:1215:ARG:HD2 | 1.49                     | 0.45              |
| 3:A:1329:THR:C    | 3:A:1331:SER:N   | 2.75                     | 0.45              |
| 4:B:270:LYS:HE3   | 4:B:281:PRO:HG3  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:B:282:ILE:CG1   | 4:B:283:VAL:N    | 2.79                     | 0.45              |
| 4:B:292:ILE:HD11  | 4:B:327:ARG:H    | 1.82                     | 0.45              |
| 4:B:469:GLN:C     | 4:B:471:LYS:H    | 2.25                     | 0.45              |
| 4:B:521:LEU:CD2   | 4:B:635:ARG:CG   | 2.84                     | 0.45              |
| 4:B:542:MET:HE1   | 4:B:743:ILE:HG21 | 1.97                     | 0.45              |
| 4:B:574:SER:HB3   | 4:B:591:ARG:HH21 | 1.82                     | 0.45              |
| 4:B:847:ASP:C     | 4:B:849:GLY:H    | 2.25                     | 0.45              |
| 4:B:1051:THR:CG2  | 4:B:1053:GLU:HB2 | 2.46                     | 0.45              |
| 5:C:41:ILE:HD11   | 5:C:172:PRO:CG   | 2.47                     | 0.45              |
| 5:C:66:ARG:HH21   | 10:J:4:PRO:HA    | 1.82                     | 0.45              |
| 5:C:183:TRP:C     | 5:C:185:LYS:H    | 2.25                     | 0.45              |
| 5:C:183:TRP:CZ2   | 5:C:207:CYS:HB3  | 2.51                     | 0.45              |
| 6:E:63:ASN:HB3    | 6:E:64:PRO:CD    | 2.46                     | 0.45              |
| 6:E:195:VAL:HG22  | 6:E:213:ILE:CD1  | 2.47                     | 0.45              |
| 7:F:81:THR:CG2    | 7:F:136:ARG:NH1  | 2.64                     | 0.45              |
| 10:J:16:ASP:OD1   | 10:J:16:ASP:C    | 2.60                     | 0.45              |
| 10:J:25:LEU:HB2   | 10:J:26:GLN:H    | 1.66                     | 0.45              |
| 10:J:48:ARG:HD2   | 10:J:48:ARG:C    | 2.42                     | 0.45              |
| 11:K:40:HIS:O     | 11:K:41:THR:C    | 2.57                     | 0.45              |
| 11:K:99:GLY:O     | 11:K:100:ALA:C   | 2.60                     | 0.45              |
| 11:K:101:LEU:O    | 11:K:102:LYS:C   | 2.60                     | 0.45              |
| 3:A:202:LEU:HD12  | 3:A:202:LEU:N    | 2.32                     | 0.45              |
| 3:A:351:THR:O     | 3:A:486:GLU:HG2  | 2.16                     | 0.45              |
| 3:A:764:CYS:HB2   | 3:A:801:GLU:O    | 2.17                     | 0.45              |
| 3:A:886:ILE:CD1   | 3:A:944:ARG:HG3  | 2.47                     | 0.45              |
| 3:A:1051:ALA:O    | 3:A:1052:GLN:C   | 2.59                     | 0.45              |
| 3:A:1213:GLY:HA2  | 3:A:1216:ILE:CD1 | 2.46                     | 0.45              |
| 3:A:1313:LEU:O    | 3:A:1316:VAL:N   | 2.39                     | 0.45              |
| 3:A:1382:THR:HG22 | 3:A:1388:GLY:CA  | 2.46                     | 0.45              |
| 4:B:213:ILE:O     | 4:B:214:ALA:C    | 2.60                     | 0.45              |
| 4:B:226:PHE:O     | 4:B:236:HIS:HA   | 2.16                     | 0.45              |
| 4:B:284:ILE:O     | 4:B:285:ILE:C    | 2.60                     | 0.45              |
| 4:B:744:HIS:CG    | 4:B:745:PRO:CD   | 3.00                     | 0.45              |
| 4:B:796:LEU:O     | 4:B:799:PRO:HD2  | 2.17                     | 0.45              |
| 4:B:797:TYR:CE2   | 5:C:62:PHE:HA    | 2.52                     | 0.45              |
| 4:B:821:GLN:OE1   | 4:B:851:PHE:N    | 2.45                     | 0.45              |
| 4:B:1082:MET:HA   | 5:C:189:THR:HA   | 1.98                     | 0.45              |
| 4:B:1115:THR:O    | 4:B:1116:ARG:CB  | 2.65                     | 0.45              |
| 4:B:1177:HIS:C    | 4:B:1179:GLN:N   | 2.75                     | 0.45              |
| 5:C:101:LEU:HB3   | 5:C:155:LEU:HB2  | 1.98                     | 0.45              |
| 5:C:183:TRP:O     | 5:C:185:LYS:N    | 2.49                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:C:231:ASN:C     | 5:C:231:ASN:HD22 | 2.24                     | 0.45              |
| 5:C:246:ARG:O     | 5:C:250:THR:OG1  | 2.33                     | 0.45              |
| 10:J:36:LEU:O     | 10:J:37:SER:C    | 2.58                     | 0.45              |
| 3:A:244:PRO:O     | 3:A:245:PRO:C    | 2.60                     | 0.45              |
| 3:A:786:HIS:N     | 3:A:786:HIS:CD2  | 2.85                     | 0.45              |
| 3:A:901:LEU:CA    | 3:A:907:THR:HG23 | 2.32                     | 0.45              |
| 3:A:1237:ILE:CG2  | 3:A:1238:ILE:H   | 2.25                     | 0.45              |
| 3:A:1319:VAL:HG12 | 3:A:1320:PRO:N   | 2.32                     | 0.45              |
| 3:A:1338:VAL:O    | 6:E:183:PRO:CB   | 2.64                     | 0.45              |
| 4:B:38:PHE:CE2    | 4:B:43:LEU:CD2   | 3.01                     | 0.45              |
| 4:B:62:ILE:CG2    | 4:B:418:LYS:HG2  | 2.39                     | 0.45              |
| 4:B:359:GLU:C     | 4:B:362:PRO:HD3  | 2.42                     | 0.45              |
| 4:B:712:PRO:O     | 4:B:712:PRO:HD2  | 2.17                     | 0.45              |
| 5:C:146:LYS:C     | 5:C:147:LEU:HD23 | 2.42                     | 0.45              |
| 5:C:261:ALA:HA    | 5:C:264:GLN:CD   | 2.43                     | 0.45              |
| 6:E:23:VAL:CG1    | 6:E:28:TYR:HB2   | 2.47                     | 0.45              |
| 8:H:84:ALA:CB     | 8:H:87:ARG:CB    | 2.90                     | 0.45              |
| 9:I:65:ASP:HA     | 9:I:66:PRO:HD3   | 1.71                     | 0.45              |
| 3:A:32:VAL:HG12   | 3:A:57:ARG:HD2   | 1.99                     | 0.44              |
| 3:A:273:ASN:HA    | 3:A:296:LEU:HD13 | 1.98                     | 0.44              |
| 3:A:878:ILE:C     | 3:A:879:GLU:HG3  | 2.41                     | 0.44              |
| 3:A:1019:CYS:O    | 3:A:1020:CYS:C   | 2.60                     | 0.44              |
| 3:A:1039:LYS:CD   | 3:A:1039:LYS:C   | 2.90                     | 0.44              |
| 3:A:1290:LYS:HA   | 3:A:1299:VAL:O   | 2.17                     | 0.44              |
| 3:A:1326:ARG:O    | 3:A:1327:ILE:C   | 2.59                     | 0.44              |
| 3:A:1365:TYR:O    | 3:A:1366:ARG:C   | 2.58                     | 0.44              |
| 4:B:170:LEU:CD1   | 4:B:457:LEU:HD13 | 2.46                     | 0.44              |
| 4:B:360:PHE:CE1   | 4:B:361:LEU:HD13 | 2.52                     | 0.44              |
| 4:B:428:ILE:O     | 4:B:430:ARG:N    | 2.50                     | 0.44              |
| 4:B:451:LYS:O     | 4:B:453:ILE:N    | 2.50                     | 0.44              |
| 4:B:573:GLN:O     | 4:B:573:GLN:HG2  | 2.16                     | 0.44              |
| 4:B:859:TYR:OH    | 4:B:941:LEU:CD2  | 2.61                     | 0.44              |
| 6:E:43:LYS:O      | 6:E:44:ALA:C     | 2.59                     | 0.44              |
| 6:E:210:SER:C     | 6:E:211:TYR:CD1  | 2.95                     | 0.44              |
| 11:K:43:GLY:CA    | 11:K:71:PHE:CZ   | 3.01                     | 0.44              |
| 3:A:22:PHE:HB2    | 4:B:1211:ASN:CG  | 2.42                     | 0.44              |
| 3:A:855:THR:CG2   | 3:A:857:ARG:CG   | 2.95                     | 0.44              |
| 3:A:947:PHE:C     | 3:A:949:ASP:N    | 2.73                     | 0.44              |
| 3:A:1067:LEU:HG   | 3:A:1067:LEU:O   | 1.97                     | 0.44              |
| 3:A:1384:VAL:O    | 3:A:1389:PHE:CE2 | 2.70                     | 0.44              |
| 4:B:101:MET:C     | 4:B:102:VAL:HG23 | 2.42                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:213:ILE:O     | 4:B:215:GLN:HG2   | 2.17                     | 0.44              |
| 4:B:234:ILE:HD13  | 4:B:234:ILE:N     | 2.17                     | 0.44              |
| 4:B:356:LEU:HA    | 4:B:360:PHE:HB3   | 1.98                     | 0.44              |
| 4:B:420:LEU:CD2   | 4:B:468:GLU:OE2   | 2.65                     | 0.44              |
| 4:B:461:LEU:HD12  | 4:B:461:LEU:HA    | 1.68                     | 0.44              |
| 4:B:894:ASP:OD2   | 12:L:58:LYS:NZ    | 2.48                     | 0.44              |
| 4:B:992:ILE:HG13  | 4:B:993:THR:H     | 1.81                     | 0.44              |
| 5:C:17:ASN:C      | 5:C:18:VAL:HG23   | 2.42                     | 0.44              |
| 5:C:80:LEU:HD12   | 5:C:95:CYS:HA     | 1.99                     | 0.44              |
| 6:E:53:PRO:CB     | 6:E:55:ARG:NH1    | 2.81                     | 0.44              |
| 3:A:61:ILE:C      | 3:A:63:ARG:N      | 2.66                     | 0.44              |
| 3:A:167:CYS:O     | 3:A:169:ASN:ND2   | 2.51                     | 0.44              |
| 3:A:379:VAL:O     | 3:A:384:ASN:ND2   | 2.48                     | 0.44              |
| 3:A:445:ASN:HB2   | 3:A:455:MET:HG2   | 1.98                     | 0.44              |
| 3:A:537:ARG:C     | 3:A:539:THR:H     | 2.23                     | 0.44              |
| 3:A:551:TYR:CE2   | 11:K:74:ARG:HB2   | 2.52                     | 0.44              |
| 3:A:808:LEU:HD21  | 3:A:816:HIS:HD2   | 1.82                     | 0.44              |
| 3:A:961:ARG:O     | 3:A:965:GLN:HG3   | 2.16                     | 0.44              |
| 3:A:1074:GLU:HB3  | 3:A:1075:PRO:HD3  | 1.99                     | 0.44              |
| 3:A:1200:ALA:O    | 3:A:1201:ALA:C    | 2.59                     | 0.44              |
| 3:A:1313:LEU:HD23 | 3:A:1338:VAL:HG21 | 1.98                     | 0.44              |
| 3:A:1387:HIS:O    | 3:A:1388:GLY:O    | 2.36                     | 0.44              |
| 4:B:107:GLY:C     | 4:B:108:VAL:O     | 2.57                     | 0.44              |
| 4:B:383:ASN:ND2   | 4:B:384:ARG:HH11  | 2.11                     | 0.44              |
| 4:B:412:LEU:HB3   | 4:B:466:TRP:CE2   | 2.52                     | 0.44              |
| 4:B:801:LYS:O     | 10:J:52:THR:HG21  | 2.17                     | 0.44              |
| 4:B:839:MET:HE1   | 4:B:980:PHE:HB2   | 2.00                     | 0.44              |
| 4:B:900:ALA:C     | 4:B:903:VAL:HG23  | 2.43                     | 0.44              |
| 4:B:912:ILE:O     | 4:B:938:SER:CB    | 2.65                     | 0.44              |
| 4:B:1079:LYS:HE3  | 5:C:188:HIS:ND1   | 2.32                     | 0.44              |
| 5:C:144:ILE:HD13  | 5:C:144:ILE:HA    | 1.82                     | 0.44              |
| 6:E:11:ARG:O      | 6:E:12:LEU:C      | 2.57                     | 0.44              |
| 9:I:101:PHE:O     | 9:I:109:ILE:HA    | 2.17                     | 0.44              |
| 10:J:1:MET:HE2    | 10:J:1:MET:HB2    | 1.60                     | 0.44              |
| 11:K:92:ASN:O     | 11:K:96:ASN:ND2   | 2.51                     | 0.44              |
| 3:A:209:ASN:O     | 3:A:212:LYS:HB2   | 2.18                     | 0.44              |
| 3:A:493:GLN:HE21  | 3:A:493:GLN:CA    | 2.30                     | 0.44              |
| 3:A:943:LEU:O     | 3:A:944:ARG:C     | 2.59                     | 0.44              |
| 3:A:1066:VAL:O    | 3:A:1067:LEU:C    | 2.60                     | 0.44              |
| 3:A:1434:ALA:C    | 3:A:1436:ILE:N    | 2.75                     | 0.44              |
| 4:B:636:PRO:HB2   | 4:B:637:LEU:H     | 1.09                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:708:GLU:CG    | 4:B:709:ASP:N     | 2.73                     | 0.44              |
| 4:B:745:PRO:HB2   | 4:B:1047:PHE:CD1  | 2.52                     | 0.44              |
| 4:B:981:ALA:O     | 4:B:982:SER:O     | 2.36                     | 0.44              |
| 4:B:1084:GLN:NE2  | 5:C:192:TRP:H     | 2.14                     | 0.44              |
| 4:B:1106:ARG:CD   | 4:B:1126:GLY:O    | 2.57                     | 0.44              |
| 5:C:44:LEU:HD12   | 5:C:44:LEU:HA     | 1.73                     | 0.44              |
| 5:C:69:LEU:N      | 5:C:69:LEU:HD13   | 2.33                     | 0.44              |
| 7:F:116:ASP:O     | 7:F:117:PRO:C     | 2.60                     | 0.44              |
| 7:F:121:ALA:HA    | 7:F:124:GLU:HB2   | 2.00                     | 0.44              |
| 12:L:45:ALA:C     | 12:L:46:VAL:HG23  | 2.42                     | 0.44              |
| 3:A:7:SER:CB      | 4:B:1193:GLN:HE22 | 2.12                     | 0.44              |
| 3:A:24:PRO:CG     | 3:A:237:THR:HG21  | 2.47                     | 0.44              |
| 3:A:273:ASN:CA    | 3:A:296:LEU:CD1   | 2.95                     | 0.44              |
| 3:A:657:LEU:HD12  | 3:A:657:LEU:C     | 2.43                     | 0.44              |
| 3:A:894:GLU:HG3   | 3:A:898:ARG:CB    | 2.48                     | 0.44              |
| 3:A:954:TRP:CD1   | 3:A:954:TRP:N     | 2.84                     | 0.44              |
| 3:A:1153:TYR:CD2  | 3:A:1163:ILE:HD11 | 2.52                     | 0.44              |
| 3:A:1343:ALA:O    | 3:A:1346:ALA:HB3  | 2.18                     | 0.44              |
| 4:B:31:TRP:CD2    | 4:B:807:ARG:HD2   | 2.53                     | 0.44              |
| 4:B:759:PRO:HB2   | 4:B:767:ASN:ND2   | 2.32                     | 0.44              |
| 4:B:766:ARG:HD3   | 4:B:766:ARG:HA    | 1.83                     | 0.44              |
| 4:B:996:ARG:CZ    | 5:C:38:ILE:HD12   | 2.47                     | 0.44              |
| 4:B:1002:THR:HG22 | 4:B:1006:ILE:O    | 2.17                     | 0.44              |
| 4:B:1031:LEU:HD13 | 4:B:1055:ILE:CD1  | 2.47                     | 0.44              |
| 4:B:1033:LYS:HA   | 4:B:1089:PRO:CG   | 2.47                     | 0.44              |
| 4:B:1202:LEU:HD22 | 4:B:1202:LEU:HA   | 1.45                     | 0.44              |
| 4:B:1208:MET:C    | 4:B:1210:MET:H    | 2.26                     | 0.44              |
| 5:C:167:HIS:HD2   | 5:C:168:ALA:H     | 1.64                     | 0.44              |
| 8:H:30:SER:C      | 8:H:31:THR:O      | 2.55                     | 0.44              |
| 8:H:95:TYR:CE2    | 8:H:97:MET:SD     | 3.10                     | 0.44              |
| 8:H:98:TYR:N      | 8:H:118:PHE:HD2   | 2.16                     | 0.44              |
| 9:I:85:PHE:C      | 9:I:85:PHE:CD1    | 2.95                     | 0.44              |
| 10:J:1:MET:N      | 10:J:56:LEU:HB2   | 2.32                     | 0.44              |
| 11:K:29:ASN:CG    | 11:K:77:THR:O     | 2.61                     | 0.44              |
| 3:A:67:CYS:O      | 3:A:68:GLN:CD     | 2.61                     | 0.44              |
| 3:A:504:LEU:CD1   | 7:F:91:ALA:HB1    | 2.47                     | 0.44              |
| 3:A:537:ARG:CG    | 3:A:537:ARG:NH1   | 2.77                     | 0.44              |
| 3:A:567:LYS:CD    | 8:H:96:VAL:H      | 2.30                     | 0.44              |
| 3:A:834:THR:HG21  | 3:A:1077:THR:CG2  | 2.47                     | 0.44              |
| 3:A:901:LEU:HD12  | 3:A:926:GLN:HG2   | 1.97                     | 0.44              |
| 3:A:946:VAL:HG12  | 3:A:947:PHE:CD1   | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1017:LEU:HB2  | 6:E:206:GLY:H     | 1.82                     | 0.44              |
| 3:A:1228:TRP:CA   | 3:A:1237:ILE:O    | 2.63                     | 0.44              |
| 4:B:189:LEU:O     | 4:B:192:LEU:N     | 2.51                     | 0.44              |
| 4:B:197:PHE:CD1   | 4:B:817:LEU:HD11  | 2.53                     | 0.44              |
| 4:B:361:LEU:N     | 4:B:362:PRO:HD3   | 2.31                     | 0.44              |
| 4:B:724:ASP:OD1   | 4:B:724:ASP:O     | 2.35                     | 0.44              |
| 4:B:756:ILE:CG2   | 4:B:759:PRO:HB3   | 2.38                     | 0.44              |
| 4:B:1077:THR:HG23 | 4:B:1079:LYS:H    | 1.77                     | 0.44              |
| 4:B:1101:ASP:C    | 4:B:1122:ARG:NH2  | 2.75                     | 0.44              |
| 4:B:1197:PRO:O    | 4:B:1200:ALA:CB   | 2.64                     | 0.44              |
| 6:E:12:LEU:HD12   | 6:E:12:LEU:O      | 2.18                     | 0.44              |
| 7:F:97:ARG:CD     | 7:F:100:GLN:OE1   | 2.66                     | 0.44              |
| 8:H:7:ASP:OD1     | 8:H:8:ASP:N       | 2.50                     | 0.44              |
| 8:H:126:GLU:O     | 8:H:130:ARG:NH1   | 2.47                     | 0.44              |
| 3:A:23:SER:C      | 3:A:25:GLU:N      | 2.73                     | 0.44              |
| 3:A:71:GLN:HB2    | 3:A:72:GLU:H      | 1.23                     | 0.44              |
| 3:A:375:THR:OG1   | 3:A:433:GLU:C     | 2.61                     | 0.44              |
| 3:A:590:ARG:CG    | 3:A:590:ARG:NH1   | 2.78                     | 0.44              |
| 3:A:963:ILE:HG21  | 3:A:1045:VAL:HG13 | 1.98                     | 0.44              |
| 4:B:272:THR:C     | 4:B:273:LEU:HG    | 2.43                     | 0.44              |
| 4:B:626:ILE:HD12  | 4:B:626:ILE:N     | 2.33                     | 0.44              |
| 4:B:761:HIS:H     | 4:B:761:HIS:CD2   | 2.35                     | 0.44              |
| 4:B:1053:GLU:O    | 4:B:1054:GLY:C    | 2.58                     | 0.44              |
| 4:B:1095:LEU:O    | 4:B:1096:ARG:C    | 2.61                     | 0.44              |
| 4:B:1144:ALA:O    | 4:B:1147:LEU:N    | 2.47                     | 0.44              |
| 6:E:59:SER:OG     | 6:E:81:GLU:HG3    | 2.17                     | 0.44              |
| 7:F:86:THR:OG1    | 7:F:89:GLU:CG     | 2.60                     | 0.44              |
| 10:J:35:ALA:O     | 10:J:36:LEU:C     | 2.60                     | 0.44              |
| 12:L:61:THR:HG22  | 12:L:62:LYS:N     | 2.32                     | 0.44              |
| 2:T:5:DT:C1'      | 3:A:448:PRO:HB3   | 2.47                     | 0.44              |
| 3:A:51:GLY:CA     | 3:A:56:PRO:HG2    | 2.45                     | 0.44              |
| 3:A:98:LYS:O      | 3:A:99:ILE:C      | 2.61                     | 0.44              |
| 3:A:129:LYS:O     | 3:A:130:ASP:OD2   | 2.36                     | 0.44              |
| 3:A:264:PHE:O     | 3:A:267:ALA:HB3   | 2.18                     | 0.44              |
| 3:A:441:PRO:O     | 3:A:441:PRO:HG2   | 2.18                     | 0.44              |
| 3:A:657:LEU:O     | 3:A:657:LEU:HD12  | 2.18                     | 0.44              |
| 3:A:1079:MET:C    | 3:A:1080:THR:HG1  | 2.19                     | 0.44              |
| 3:A:1096:SER:O    | 3:A:1099:PRO:CG   | 2.66                     | 0.44              |
| 3:A:1200:ALA:C    | 3:A:1202:MET:H    | 2.26                     | 0.44              |
| 3:A:1209:MET:HA   | 3:A:1212:VAL:CG2  | 2.48                     | 0.44              |
| 3:A:1215:ARG:O    | 3:A:1219:THR:OG1  | 2.36                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1284:MET:HG2  | 3:A:1306:LEU:HD21 | 1.99                     | 0.44              |
| 3:A:1441:PHE:CZ   | 7:F:88:TYR:O      | 2.69                     | 0.44              |
| 4:B:61:ASP:N      | 4:B:61:ASP:OD1    | 2.51                     | 0.44              |
| 4:B:120:ARG:HD2   | 4:B:955:THR:CG2   | 2.16                     | 0.44              |
| 4:B:624:LEU:C     | 4:B:624:LEU:HD12  | 2.41                     | 0.44              |
| 4:B:751:VAL:HG22  | 4:B:812:LEU:HD11  | 1.98                     | 0.44              |
| 5:C:164:ALA:C     | 5:C:166:GLU:N     | 2.76                     | 0.44              |
| 6:E:17:ARG:O      | 6:E:20:LYS:HB2    | 2.17                     | 0.44              |
| 7:F:134:ILE:HG22  | 7:F:135:ARG:N     | 2.32                     | 0.44              |
| 11:K:63:VAL:O     | 11:K:64:GLU:C     | 2.57                     | 0.44              |
| 3:A:151:ASP:OD1   | 3:A:163:SER:CB    | 2.66                     | 0.44              |
| 3:A:528:LEU:HA    | 3:A:531:ILE:H     | 1.82                     | 0.44              |
| 3:A:658:LEU:HD12  | 3:A:658:LEU:O     | 2.18                     | 0.44              |
| 3:A:690:VAL:HG22  | 3:A:718:VAL:HG13  | 1.98                     | 0.44              |
| 3:A:935:GLN:O     | 3:A:936:LEU:C     | 2.60                     | 0.44              |
| 3:A:1009:ASN:O    | 3:A:1013:ASP:CG   | 2.61                     | 0.44              |
| 3:A:1256:GLU:O    | 3:A:1257:ASP:C    | 2.60                     | 0.44              |
| 3:A:1352:VAL:O    | 3:A:1353:TYR:C    | 2.60                     | 0.44              |
| 3:A:1376:THR:O    | 3:A:1376:THR:CG2  | 2.66                     | 0.44              |
| 4:B:286:PHE:CG    | 4:B:297:ILE:HD12  | 2.52                     | 0.44              |
| 4:B:456:GLY:HA3   | 4:B:468:GLU:OE2   | 2.18                     | 0.44              |
| 4:B:868:MET:O     | 4:B:869:SER:CB    | 2.66                     | 0.44              |
| 4:B:1012:ILE:C    | 4:B:1012:ILE:HD12 | 2.42                     | 0.44              |
| 4:B:1159:ARG:HH21 | 4:B:1193:GLN:HE21 | 1.66                     | 0.44              |
| 6:E:61:GLN:HB2    | 6:E:78:LEU:O      | 2.17                     | 0.44              |
| 9:I:84:VAL:O      | 9:I:84:VAL:HG12   | 2.17                     | 0.44              |
| 12:L:62:LYS:O     | 12:L:64:LEU:HG    | 2.18                     | 0.44              |
| 3:A:54:ASN:O      | 3:A:54:ASN:OD1    | 2.36                     | 0.43              |
| 3:A:268:ASP:HB3   | 3:A:299:HIS:CD2   | 2.53                     | 0.43              |
| 3:A:332:LYS:H     | 3:A:337:ARG:HB2   | 1.82                     | 0.43              |
| 3:A:667:GLY:C     | 3:A:669:THR:H     | 2.25                     | 0.43              |
| 3:A:919:ILE:HG23  | 3:A:922:ASP:HB2   | 1.99                     | 0.43              |
| 3:A:1017:LEU:HB2  | 6:E:206:GLY:N     | 2.33                     | 0.43              |
| 4:B:273:LEU:HD21  | 4:B:360:PHE:HD1   | 1.82                     | 0.43              |
| 4:B:427:ASP:HA    | 4:B:430:ARG:HD2   | 2.00                     | 0.43              |
| 4:B:834:ASN:HB2   | 4:B:839:MET:HA    | 2.00                     | 0.43              |
| 4:B:986:GLN:OE1   | 4:B:986:GLN:C     | 2.61                     | 0.43              |
| 4:B:1183:LYS:O    | 4:B:1183:LYS:CE   | 2.66                     | 0.43              |
| 5:C:69:LEU:C      | 10:J:6:ARG:HH11   | 2.26                     | 0.43              |
| 8:H:12:VAL:HA     | 8:H:28:ALA:HB1    | 2.00                     | 0.43              |
| 8:H:134:ASN:C     | 8:H:135:LEU:O     | 2.60                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:89:PRO:O     | 3:A:90:VAL:CG2    | 2.66                     | 0.43              |
| 3:A:134:ARG:CD   | 3:A:221:SER:O     | 2.49                     | 0.43              |
| 3:A:451:HIS:HB3  | 3:A:453:MET:H     | 1.82                     | 0.43              |
| 3:A:691:LEU:HD11 | 3:A:695:LYS:HD2   | 2.00                     | 0.43              |
| 3:A:878:ILE:HG23 | 3:A:956:LEU:C     | 2.43                     | 0.43              |
| 3:A:1135:ARG:C   | 3:A:1137:ALA:H    | 2.26                     | 0.43              |
| 3:A:1276:VAL:HB  | 3:A:1279:ILE:HD13 | 2.00                     | 0.43              |
| 4:B:25:ILE:H     | 4:B:25:ILE:HG13   | 1.64                     | 0.43              |
| 4:B:100:PRO:O    | 4:B:180:TYR:OH    | 2.37                     | 0.43              |
| 4:B:107:GLY:O    | 4:B:108:VAL:O     | 2.37                     | 0.43              |
| 4:B:376:PHE:CZ   | 4:B:569:TYR:HB3   | 2.52                     | 0.43              |
| 4:B:483:LEU:HB3  | 4:B:484:ASN:H     | 1.60                     | 0.43              |
| 4:B:884:ARG:O    | 4:B:936:ASP:HB3   | 2.17                     | 0.43              |
| 4:B:951:GLN:HG2  | 12:L:57:LEU:HD22  | 2.00                     | 0.43              |
| 4:B:1072:MET:HB2 | 4:B:1085:ILE:CD1  | 2.49                     | 0.43              |
| 7:F:101:ILE:CD1  | 7:F:120:ILE:HG22  | 2.48                     | 0.43              |
| 8:H:76:THR:O     | 8:H:76:THR:CG2    | 2.66                     | 0.43              |
| 9:I:7:CYS:SG     | 9:I:8:ARG:O       | 2.77                     | 0.43              |
| 9:I:84:VAL:O     | 9:I:84:VAL:CG1    | 2.65                     | 0.43              |
| 11:K:65:HIS:CD2  | 11:K:65:HIS:C     | 2.95                     | 0.43              |
| 2:T:6:DC:H4'     | 3:A:447:GLN:OE1   | 2.18                     | 0.43              |
| 3:A:88:LYS:HA    | 3:A:89:PRO:HD2    | 1.70                     | 0.43              |
| 3:A:152:VAL:CG1  | 3:A:153:PRO:HD2   | 2.48                     | 0.43              |
| 3:A:179:LEU:HD11 | 3:A:298:PHE:HA    | 1.99                     | 0.43              |
| 3:A:361:LEU:N    | 3:A:471:ASN:ND2   | 2.67                     | 0.43              |
| 3:A:389:THR:C    | 3:A:391:LEU:N     | 2.77                     | 0.43              |
| 3:A:547:LEU:CD2  | 11:K:58:PHE:CD1   | 2.96                     | 0.43              |
| 3:A:548:ASN:HD21 | 11:K:47:ARG:NE    | 2.15                     | 0.43              |
| 3:A:583:PRO:HG2  | 3:A:586:ILE:HG13  | 2.00                     | 0.43              |
| 3:A:599:SER:O    | 3:A:602:ASP:N     | 2.32                     | 0.43              |
| 3:A:690:VAL:HG13 | 3:A:718:VAL:HG22  | 2.00                     | 0.43              |
| 3:A:946:VAL:CG2  | 6:E:201:LYS:HB3   | 2.47                     | 0.43              |
| 3:A:1189:SER:HG  | 3:A:1190:PRO:HD2  | 1.81                     | 0.43              |
| 3:A:1284:MET:HB3 | 3:A:1284:MET:HE3  | 1.59                     | 0.43              |
| 4:B:63:ILE:CG1   | 4:B:421:PHE:CZ    | 3.01                     | 0.43              |
| 4:B:634:TYR:CD1  | 4:B:692:TYR:HB3   | 2.53                     | 0.43              |
| 4:B:744:HIS:CD2  | 4:B:745:PRO:HD2   | 2.53                     | 0.43              |
| 4:B:890:TYR:O    | 4:B:892:LYS:N     | 2.50                     | 0.43              |
| 4:B:996:ARG:NH2  | 5:C:174:ALA:O     | 2.51                     | 0.43              |
| 4:B:1001:PHE:CD2 | 5:C:34:ARG:NH2    | 2.86                     | 0.43              |
| 5:C:27:LEU:HA    | 5:C:228:PHE:CZ    | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:F:117:PRO:O     | 7:F:120:ILE:HB    | 2.18                     | 0.43              |
| 8:H:93:TYR:HD2    | 8:H:145:ARG:HB3   | 1.83                     | 0.43              |
| 11:K:92:ASN:O     | 11:K:93:SER:C     | 2.60                     | 0.43              |
| 2:T:10:DT:OP1     | 4:B:857:ARG:NH2   | 2.51                     | 0.43              |
| 3:A:7:SER:OG      | 3:A:9:ALA:HB3     | 2.17                     | 0.43              |
| 3:A:244:PRO:C     | 3:A:246:VAL:N     | 2.76                     | 0.43              |
| 3:A:326:ARG:O     | 3:A:330:LYS:N     | 2.51                     | 0.43              |
| 3:A:867:ILE:HG22  | 3:A:872:GLY:CA    | 2.49                     | 0.43              |
| 3:A:909:ASP:OD1   | 3:A:911:SER:HB3   | 2.17                     | 0.43              |
| 3:A:1146:VAL:HG11 | 3:A:1202:MET:SD   | 2.59                     | 0.43              |
| 3:A:1156:PRO:CD   | 3:A:1157:ASP:N    | 2.81                     | 0.43              |
| 3:A:1207:LEU:HD11 | 3:A:1273:LEU:HD23 | 2.01                     | 0.43              |
| 3:A:1219:THR:HG23 | 3:A:1271:ILE:HD11 | 2.00                     | 0.43              |
| 4:B:112:LEU:HD12  | 4:B:112:LEU:HA    | 1.62                     | 0.43              |
| 4:B:173:MET:O     | 4:B:176:SER:CB    | 2.66                     | 0.43              |
| 4:B:359:GLU:HA    | 4:B:362:PRO:HG3   | 2.01                     | 0.43              |
| 4:B:420:LEU:C     | 4:B:423:LYS:H     | 2.26                     | 0.43              |
| 4:B:458:LYS:O     | 4:B:462:ALA:N     | 2.52                     | 0.43              |
| 4:B:572:HIS:CD2   | 4:B:572:HIS:C     | 2.96                     | 0.43              |
| 4:B:705:MET:H     | 4:B:710:LEU:HD12  | 1.82                     | 0.43              |
| 4:B:841:MET:SD    | 4:B:990:ILE:HD11  | 2.58                     | 0.43              |
| 4:B:872:GLU:HG3   | 4:B:916:THR:OG1   | 2.19                     | 0.43              |
| 4:B:1099:VAL:C    | 4:B:1103:ILE:HD11 | 2.44                     | 0.43              |
| 4:B:1170:THR:CG2  | 4:B:1183:LYS:HZ3  | 2.32                     | 0.43              |
| 4:B:1197:PRO:O    | 4:B:1200:ALA:N    | 2.50                     | 0.43              |
| 5:C:41:ILE:HG12   | 5:C:172:PRO:HG3   | 2.00                     | 0.43              |
| 7:F:81:THR:CB     | 7:F:144:GLU:OE1   | 2.67                     | 0.43              |
| 11:K:47:ARG:HD3   | 11:K:60:ALA:HA    | 1.99                     | 0.43              |
| 3:A:235:ILE:H     | 3:A:235:ILE:HD12  | 1.83                     | 0.43              |
| 3:A:325:ILE:HG22  | 4:B:1210:MET:SD   | 2.59                     | 0.43              |
| 3:A:427:GLN:O     | 3:A:428:TYR:O     | 2.36                     | 0.43              |
| 3:A:453:MET:C     | 3:A:455:MET:H     | 2.27                     | 0.43              |
| 4:B:54:PHE:HB3    | 4:B:55:VAL:H      | 1.58                     | 0.43              |
| 4:B:125:SER:HB2   | 4:B:171:PRO:N     | 2.33                     | 0.43              |
| 4:B:170:LEU:O     | 4:B:171:PRO:C     | 2.60                     | 0.43              |
| 4:B:236:HIS:C     | 4:B:237:VAL:CG2   | 2.92                     | 0.43              |
| 4:B:474:SER:O     | 4:B:476:ARG:N     | 2.47                     | 0.43              |
| 4:B:488:TYR:HE2   | 4:B:813:LYS:HB2   | 1.83                     | 0.43              |
| 4:B:640:VAL:CG2   | 4:B:740:HIS:HA    | 2.39                     | 0.43              |
| 4:B:701:ILE:HG12  | 4:B:703:ILE:HG13  | 2.01                     | 0.43              |
| 4:B:701:ILE:C     | 4:B:701:ILE:HD13  | 2.43                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:835:GLN:O     | 4:B:836:GLU:C     | 2.62                     | 0.43              |
| 4:B:1159:ARG:CD   | 4:B:1193:GLN:HG3  | 2.48                     | 0.43              |
| 5:C:137:LYS:HD3   | 5:C:138:GLU:HG2   | 2.00                     | 0.43              |
| 7:F:75:PRO:O      | 7:F:76:LYS:C      | 2.62                     | 0.43              |
| 7:F:93:ILE:HD11   | 7:F:134:ILE:HD11  | 2.00                     | 0.43              |
| 8:H:91:ASP:CG     | 8:H:91:ASP:O      | 2.60                     | 0.43              |
| 3:A:138:ILE:HG22  | 3:A:139:TRP:N     | 2.33                     | 0.43              |
| 3:A:139:TRP:C     | 3:A:141:LEU:H     | 2.26                     | 0.43              |
| 3:A:367:PRO:CB    | 3:A:466:SER:HA    | 2.49                     | 0.43              |
| 3:A:470:LEU:HD21  | 3:A:487:MET:HE1   | 2.00                     | 0.43              |
| 3:A:787:PHE:CE1   | 3:A:796:SER:HA    | 2.53                     | 0.43              |
| 3:A:986:ILE:HD13  | 3:A:1032:LEU:HD11 | 2.01                     | 0.43              |
| 3:A:1035:TYR:O    | 3:A:1037:LEU:HD23 | 2.19                     | 0.43              |
| 3:A:1044:TRP:O    | 3:A:1046:LEU:N    | 2.52                     | 0.43              |
| 3:A:1362:TYR:CE1  | 3:A:1363:VAL:O    | 2.71                     | 0.43              |
| 3:A:1418:LEU:HD21 | 4:B:1222:ARG:HG3  | 2.00                     | 0.43              |
| 3:A:1430:LEU:N    | 3:A:1430:LEU:HD23 | 2.33                     | 0.43              |
| 4:B:52:ASN:C      | 4:B:54:PHE:H      | 2.26                     | 0.43              |
| 4:B:176:SER:O     | 4:B:182:SER:HB3   | 2.18                     | 0.43              |
| 4:B:317:CYS:C     | 4:B:319:GLU:N     | 2.77                     | 0.43              |
| 4:B:430:ARG:HB3   | 4:B:434:ARG:NH1   | 2.34                     | 0.43              |
| 4:B:535:LEU:HD23  | 4:B:535:LEU:HA    | 1.71                     | 0.43              |
| 4:B:1022:THR:HG23 | 4:B:1022:THR:O    | 2.18                     | 0.43              |
| 6:E:128:PRO:HA    | 6:E:129:PRO:HA    | 1.72                     | 0.43              |
| 12:L:43:THR:O     | 12:L:43:THR:HG23  | 2.17                     | 0.43              |
| 2:T:8:DT:OP2      | 2:T:8:DT:H73      | 2.18                     | 0.43              |
| 3:A:12:ARG:HB2    | 4:B:1218:THR:CG2  | 2.48                     | 0.43              |
| 3:A:491:VAL:O     | 3:A:493:GLN:NE2   | 2.52                     | 0.43              |
| 3:A:873:MET:HE1   | 3:A:1053:PHE:CZ   | 2.53                     | 0.43              |
| 3:A:1016:THR:O    | 3:A:1017:LEU:C    | 2.58                     | 0.43              |
| 3:A:1168:GLU:O    | 3:A:1171:GLN:N    | 2.51                     | 0.43              |
| 4:B:113:TYR:O     | 4:B:116:GLU:N     | 2.52                     | 0.43              |
| 4:B:170:LEU:HD12  | 4:B:171:PRO:CD    | 2.48                     | 0.43              |
| 4:B:211:VAL:CG2   | 4:B:483:LEU:HG    | 2.48                     | 0.43              |
| 4:B:233:PRO:HG2   | 4:B:234:ILE:N     | 2.33                     | 0.43              |
| 4:B:254:LEU:HD12  | 4:B:272:THR:O     | 2.19                     | 0.43              |
| 4:B:365:THR:HG21  | 4:B:367:LEU:HD12  | 2.01                     | 0.43              |
| 4:B:377:PHE:C     | 4:B:379:GLY:N     | 2.76                     | 0.43              |
| 4:B:423:LYS:NZ    | 4:B:423:LYS:CB    | 2.76                     | 0.43              |
| 4:B:710:LEU:O     | 4:B:711:GLU:HB3   | 2.19                     | 0.43              |
| 4:B:789:MET:HE3   | 4:B:965:LYS:HB3   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:842:ASN:O     | 4:B:846:ILE:HG13  | 2.18                     | 0.43              |
| 4:B:1058:LEU:HA   | 4:B:1058:LEU:HD23 | 1.73                     | 0.43              |
| 4:B:1095:LEU:O    | 4:B:1096:ARG:O    | 2.35                     | 0.43              |
| 6:E:71:LYS:HD3    | 6:E:160:GLU:OE2   | 2.18                     | 0.43              |
| 6:E:127:ILE:H     | 6:E:127:ILE:CD1   | 2.31                     | 0.43              |
| 3:A:152:VAL:HG13  | 3:A:153:PRO:HD2   | 2.00                     | 0.43              |
| 3:A:793:SER:OG    | 3:A:795:GLU:HG3   | 2.18                     | 0.43              |
| 3:A:1382:THR:HG22 | 3:A:1388:GLY:HA3  | 2.00                     | 0.43              |
| 3:A:1387:HIS:ND1  | 3:A:1387:HIS:N    | 2.67                     | 0.43              |
| 4:B:169:ARG:HD2   | 4:B:454:THR:HG21  | 2.01                     | 0.43              |
| 4:B:273:LEU:C     | 4:B:274:PRO:O     | 2.61                     | 0.43              |
| 4:B:368:GLU:HB3   | 4:B:369:GLY:H     | 1.71                     | 0.43              |
| 4:B:541:LEU:CB    | 4:B:747:MET:HE3   | 2.45                     | 0.43              |
| 4:B:554:ILE:O     | 4:B:557:PHE:N     | 2.52                     | 0.43              |
| 4:B:1098:MET:HE3  | 4:B:1098:MET:HB2  | 1.53                     | 0.43              |
| 4:B:1132:GLU:O    | 4:B:1135:ARG:HB3  | 2.18                     | 0.43              |
| 5:C:184:ASN:O     | 5:C:185:LYS:C     | 2.61                     | 0.43              |
| 5:C:260:LEU:O     | 5:C:264:GLN:CG    | 2.52                     | 0.43              |
| 6:E:186:LEU:HD23  | 6:E:186:LEU:HA    | 1.91                     | 0.43              |
| 8:H:15:VAL:O      | 8:H:15:VAL:HG12   | 2.17                     | 0.43              |
| 8:H:62:SER:HB2    | 8:H:63:LEU:H      | 1.29                     | 0.43              |
| 11:K:82:ASP:HA    | 11:K:83:PRO:HD2   | 1.61                     | 0.43              |
| 3:A:33:ALA:O      | 3:A:34:LYS:HG3    | 2.19                     | 0.43              |
| 3:A:174:ILE:HG22  | 3:A:175:ARG:N     | 2.32                     | 0.43              |
| 3:A:407:ARG:HB3   | 3:A:430:TRP:CZ2   | 2.54                     | 0.43              |
| 3:A:458:HIS:CE1   | 3:A:507:VAL:CG2   | 2.95                     | 0.43              |
| 3:A:511:ILE:HA    | 3:A:521:MET:HE2   | 1.99                     | 0.43              |
| 3:A:699:ALA:O     | 3:A:701:LEU:HG    | 2.18                     | 0.43              |
| 3:A:707:GLY:O     | 3:A:1281:ARG:HD3  | 2.18                     | 0.43              |
| 3:A:778:GLY:HA3   | 4:B:516:ASN:HB2   | 2.01                     | 0.43              |
| 3:A:902:LEU:HG    | 3:A:902:LEU:H     | 1.31                     | 0.43              |
| 3:A:929:LEU:N     | 3:A:929:LEU:CD2   | 2.77                     | 0.43              |
| 3:A:989:GLY:O     | 3:A:992:ASP:N     | 2.34                     | 0.43              |
| 3:A:1076:ALA:C    | 3:A:1078:GLN:N    | 2.77                     | 0.43              |
| 3:A:1325:THR:O    | 6:E:147:HIS:ND1   | 2.52                     | 0.43              |
| 3:A:1331:SER:HG   | 3:A:1333:ILE:HG22 | 1.84                     | 0.43              |
| 3:A:1349:TYR:O    | 3:A:1351:GLU:N    | 2.52                     | 0.43              |
| 4:B:46:GLN:NE2    | 4:B:496:ARG:HA    | 2.27                     | 0.43              |
| 4:B:100:PRO:HG2   | 4:B:124:TYR:CZ    | 2.54                     | 0.43              |
| 4:B:174:LEU:HD23  | 4:B:202:TYR:CE1   | 2.54                     | 0.43              |
| 4:B:566:LEU:O     | 4:B:569:TYR:HB2   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:B:639:ILE:HD11  | 4:B:691:GLU:HG3  | 2.01                     | 0.43              |
| 4:B:1007:VAL:HG13 | 4:B:1008:PRO:N   | 2.33                     | 0.43              |
| 5:C:73:GLN:HE21   | 5:C:75:MET:HB2   | 1.83                     | 0.43              |
| 6:E:95:THR:HG22   | 6:E:95:THR:O     | 2.17                     | 0.43              |
| 6:E:117:THR:O     | 6:E:120:ALA:HB3  | 2.18                     | 0.43              |
| 3:A:76:GLU:O      | 3:A:76:GLU:OE2   | 2.37                     | 0.43              |
| 3:A:254:GLU:C     | 4:B:918:ILE:HG21 | 2.43                     | 0.43              |
| 3:A:271:LYS:O     | 3:A:272:ALA:C    | 2.61                     | 0.43              |
| 3:A:391:LEU:O     | 3:A:392:VAL:C    | 2.60                     | 0.43              |
| 3:A:401:GLY:CA    | 3:A:435:HIS:CD2  | 3.01                     | 0.43              |
| 3:A:420:ARG:O     | 3:A:424:ILE:CG1  | 2.66                     | 0.43              |
| 3:A:473:SER:O     | 3:A:521:MET:HB3  | 2.19                     | 0.43              |
| 3:A:518:LYS:HB2   | 3:A:519:PRO:HD2  | 2.01                     | 0.43              |
| 3:A:533:LYS:O     | 3:A:534:LEU:C    | 2.61                     | 0.43              |
| 3:A:742:ASN:C     | 3:A:745:GLN:HB2  | 2.44                     | 0.43              |
| 3:A:743:VAL:HG11  | 3:A:758:ILE:HD11 | 2.01                     | 0.43              |
| 3:A:928:LEU:O     | 3:A:930:ASP:N    | 2.51                     | 0.43              |
| 4:B:360:PHE:CD1   | 4:B:361:LEU:HD13 | 2.54                     | 0.43              |
| 4:B:554:ILE:HG22  | 4:B:555:ILE:N    | 2.33                     | 0.43              |
| 4:B:638:PHE:O     | 4:B:740:HIS:HB2  | 2.18                     | 0.43              |
| 4:B:1196:ILE:HD13 | 4:B:1196:ILE:N   | 2.33                     | 0.43              |
| 5:C:35:ARG:HB2    | 5:C:36:VAL:H     | 1.67                     | 0.43              |
| 6:E:79:TRP:CE3    | 6:E:79:TRP:HA    | 2.53                     | 0.43              |
| 7:F:97:ARG:NH2    | 7:F:124:GLU:OE2  | 2.52                     | 0.43              |
| 11:K:61:TYR:CD1   | 11:K:62:LYS:N    | 2.86                     | 0.43              |
| 11:K:83:PRO:O     | 11:K:84:LYS:C    | 2.62                     | 0.43              |
| 3:A:185:TRP:HB3   | 3:A:186:LYS:H    | 1.69                     | 0.42              |
| 3:A:376:TYR:CE2   | 3:A:377:PRO:O    | 2.71                     | 0.42              |
| 3:A:463:ILE:CB    | 3:A:464:PRO:CD   | 2.97                     | 0.42              |
| 3:A:494:SER:HB2   | 3:A:496:GLU:HG3  | 2.01                     | 0.42              |
| 3:A:518:LYS:HG3   | 3:A:519:PRO:CD   | 2.49                     | 0.42              |
| 3:A:562:THR:HA    | 3:A:563:PRO:HD3  | 1.73                     | 0.42              |
| 3:A:838:GLN:O     | 3:A:842:VAL:HG23 | 2.19                     | 0.42              |
| 3:A:924:LYS:HE3   | 3:A:924:LYS:HB2  | 1.57                     | 0.42              |
| 3:A:1000:LEU:HD23 | 3:A:1000:LEU:HA  | 1.71                     | 0.42              |
| 3:A:1127:ASP:O    | 3:A:1129:GLU:N   | 2.52                     | 0.42              |
| 4:B:294:ASP:H     | 9:I:12:ASN:HD21  | 1.67                     | 0.42              |
| 4:B:308:TRP:CG    | 4:B:309:GLN:N    | 2.86                     | 0.42              |
| 4:B:453:ILE:C     | 4:B:455:SER:N    | 2.75                     | 0.42              |
| 4:B:911:ILE:HD11  | 4:B:941:LEU:HG   | 2.00                     | 0.42              |
| 4:B:914:LYS:H     | 4:B:938:SER:HB3  | 1.83                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:C:196:ASP:C    | 5:C:198:ALA:H     | 2.26                     | 0.42              |
| 8:H:47:PHE:CD2   | 8:H:95:TYR:CD1    | 3.04                     | 0.42              |
| 8:H:47:PHE:CD1   | 8:H:47:PHE:C      | 2.97                     | 0.42              |
| 9:I:7:CYS:SG     | 9:I:34:TYR:CB     | 3.07                     | 0.42              |
| 11:K:44:ASN:HA   | 11:K:61:TYR:HE2   | 1.84                     | 0.42              |
| 3:A:35:ILE:HG22  | 3:A:270:LEU:CD1   | 2.44                     | 0.42              |
| 3:A:320:ARG:NH2  | 4:B:471:LYS:N     | 2.67                     | 0.42              |
| 3:A:587:HIS:HE1  | 3:A:969:GLN:HG2   | 1.83                     | 0.42              |
| 3:A:754:SER:OG   | 3:A:757:ASN:ND2   | 2.51                     | 0.42              |
| 3:A:806:ARG:HH11 | 3:A:806:ARG:HD2   | 1.68                     | 0.42              |
| 3:A:900:ASP:C    | 3:A:926:GLN:NE2   | 2.77                     | 0.42              |
| 4:B:53:GLN:O     | 4:B:53:GLN:CG     | 2.67                     | 0.42              |
| 4:B:124:TYR:OH   | 4:B:179:CYS:CA    | 2.62                     | 0.42              |
| 4:B:376:PHE:CE2  | 4:B:569:TYR:CD2   | 3.01                     | 0.42              |
| 4:B:410:GLY:O    | 4:B:412:LEU:N     | 2.52                     | 0.42              |
| 4:B:653:VAL:HG12 | 4:B:654:ARG:H     | 1.84                     | 0.42              |
| 4:B:936:ASP:CG   | 4:B:937:ALA:N     | 2.77                     | 0.42              |
| 4:B:970:THR:HG22 | 4:B:971:THR:N     | 2.34                     | 0.42              |
| 4:B:1084:GLN:CB  | 5:C:201:TRP:HH2   | 2.32                     | 0.42              |
| 4:B:1116:ARG:HG3 | 4:B:1198:TYR:CG   | 2.52                     | 0.42              |
| 4:B:1203:LEU:CD1 | 4:B:1203:LEU:C    | 2.88                     | 0.42              |
| 7:F:77:ASP:HB3   | 7:F:78:GLN:H      | 1.60                     | 0.42              |
| 9:I:85:PHE:CD1   | 9:I:86:PHE:N      | 2.87                     | 0.42              |
| 3:A:535:THR:HG21 | 3:A:616:VAL:HA    | 2.00                     | 0.42              |
| 3:A:622:VAL:CG2  | 3:A:622:VAL:O     | 2.61                     | 0.42              |
| 3:A:1074:GLU:C   | 3:A:1076:ALA:N    | 2.76                     | 0.42              |
| 3:A:1135:ARG:HB3 | 3:A:1136:SER:H    | 1.48                     | 0.42              |
| 3:A:1147:THR:HA  | 3:A:1197:LEU:HD23 | 2.01                     | 0.42              |
| 3:A:1193:LEU:HB2 | 3:A:1260:LEU:HD21 | 2.01                     | 0.42              |
| 4:B:449:ASN:HD21 | 4:B:451:LYS:CD    | 2.33                     | 0.42              |
| 4:B:702:LEU:HA   | 4:B:702:LEU:HD12  | 1.46                     | 0.42              |
| 4:B:816:GLU:C    | 4:B:818:PRO:CD    | 2.91                     | 0.42              |
| 4:B:952:VAL:O    | 12:L:57:LEU:HD23  | 2.19                     | 0.42              |
| 4:B:1033:LYS:O   | 4:B:1034:VAL:C    | 2.61                     | 0.42              |
| 4:B:1099:VAL:O   | 4:B:1101:ASP:N    | 2.52                     | 0.42              |
| 4:B:1219:ASP:C   | 4:B:1221:SER:H    | 2.27                     | 0.42              |
| 5:C:166:GLU:HG3  | 11:K:10:PHE:HZ    | 1.82                     | 0.42              |
| 6:E:175:LEU:HB3  | 6:E:213:ILE:HG22  | 2.01                     | 0.42              |
| 9:I:106:CYS:SG   | 9:I:108:HIS:CB    | 3.08                     | 0.42              |
| 9:I:117:LYS:C    | 9:I:118:ARG:HG2   | 2.44                     | 0.42              |
| 12:L:34:CYS:O    | 12:L:35:SER:CB    | 2.67                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:343:LYS:HD3   | 4:B:1155:SER:OG   | 2.19                     | 0.42              |
| 3:A:587:HIS:HA    | 3:A:607:ILE:O     | 2.19                     | 0.42              |
| 3:A:691:LEU:C     | 3:A:691:LEU:CD1   | 2.92                     | 0.42              |
| 3:A:722:LEU:HD12  | 3:A:722:LEU:H     | 1.84                     | 0.42              |
| 3:A:857:ARG:HB3   | 3:A:862:ASN:O     | 2.20                     | 0.42              |
| 3:A:910:PRO:HB3   | 3:A:916:GLY:HA3   | 2.01                     | 0.42              |
| 3:A:1195:LEU:HD11 | 3:A:1267:MET:HE1  | 2.02                     | 0.42              |
| 3:A:1347:ALA:C    | 3:A:1349:TYR:N    | 2.77                     | 0.42              |
| 3:A:1354:ASN:HA   | 3:A:1357:ALA:HB3  | 2.01                     | 0.42              |
| 3:A:1398:MET:HB2  | 3:A:1398:MET:HE2  | 1.70                     | 0.42              |
| 4:B:92:PHE:HD2    | 4:B:130:VAL:HG11  | 1.84                     | 0.42              |
| 4:B:165:VAL:HG13  | 4:B:166:PHE:N     | 2.35                     | 0.42              |
| 4:B:515:HIS:O     | 4:B:516:ASN:C     | 2.62                     | 0.42              |
| 4:B:745:PRO:O     | 4:B:748:ILE:HG12  | 2.20                     | 0.42              |
| 4:B:773:MET:O     | 4:B:774:GLY:C     | 2.61                     | 0.42              |
| 4:B:1059:LEU:CD1  | 4:B:1064:TYR:HB2  | 2.49                     | 0.42              |
| 4:B:1084:GLN:CD   | 4:B:1084:GLN:H    | 2.26                     | 0.42              |
| 4:B:1099:VAL:H    | 4:B:1099:VAL:HG23 | 1.50                     | 0.42              |
| 4:B:1148:LYS:O    | 4:B:1149:GLU:C    | 2.62                     | 0.42              |
| 5:C:46:ILE:CD1    | 5:C:159:ALA:HB2   | 2.30                     | 0.42              |
| 5:C:134:ILE:HD12  | 5:C:141:GLY:HA3   | 1.72                     | 0.42              |
| 6:E:135:PHE:CB    | 6:E:140:LEU:HD11  | 2.27                     | 0.42              |
| 7:F:93:ILE:O      | 7:F:94:LEU:C      | 2.60                     | 0.42              |
| 8:H:40:LEU:HD12   | 8:H:40:LEU:HA     | 1.86                     | 0.42              |
| 10:J:7:CYS:SG     | 10:J:10:CYS:N     | 2.90                     | 0.42              |
| 3:A:137:ALA:O     | 3:A:138:ILE:C     | 2.62                     | 0.42              |
| 3:A:226:GLU:HB3   | 3:A:227:VAL:H     | 1.68                     | 0.42              |
| 3:A:402:ALA:HB1   | 3:A:433:GLU:O     | 2.19                     | 0.42              |
| 3:A:542:GLU:C     | 3:A:546:VAL:HG23  | 2.44                     | 0.42              |
| 3:A:655:PHE:O     | 3:A:658:LEU:HB3   | 2.19                     | 0.42              |
| 3:A:941:LYS:O     | 3:A:943:LEU:N     | 2.52                     | 0.42              |
| 3:A:1099:PRO:O    | 3:A:1100:ARG:C    | 2.63                     | 0.42              |
| 4:B:190:TYR:CE1   | 10:J:62:ARG:HG2   | 2.54                     | 0.42              |
| 4:B:297:ILE:O     | 4:B:299:GLU:N     | 2.52                     | 0.42              |
| 4:B:417:PHE:O     | 4:B:418:LYS:O     | 2.37                     | 0.42              |
| 4:B:783:THR:HG22  | 10:J:63:TYR:CE1   | 2.45                     | 0.42              |
| 4:B:834:ASN:O     | 4:B:834:ASN:CG    | 2.62                     | 0.42              |
| 4:B:1059:LEU:HD23 | 4:B:1066:SER:HA   | 2.02                     | 0.42              |
| 5:C:59:ALA:O      | 5:C:60:ASP:C      | 2.62                     | 0.42              |
| 5:C:69:LEU:HD12   | 5:C:169:LYS:HB3   | 2.01                     | 0.42              |
| 5:C:213:PRO:O     | 5:C:214:ASN:C     | 2.61                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:C:261:ALA:HA    | 5:C:264:GLN:HG3   | 2.01                     | 0.42              |
| 6:E:46:TYR:CD2    | 6:E:57:MET:O      | 2.72                     | 0.42              |
| 6:E:85:GLU:HB3    | 6:E:87:SER:O      | 2.20                     | 0.42              |
| 7:F:135:ARG:CG    | 7:F:137:TYR:HE1   | 2.26                     | 0.42              |
| 8:H:40:LEU:HD13   | 8:H:123:MET:CE    | 2.43                     | 0.42              |
| 8:H:138:GLU:O     | 8:H:139:ASN:C     | 2.61                     | 0.42              |
| 11:K:45:LEU:HA    | 11:K:45:LEU:HD12  | 1.61                     | 0.42              |
| 3:A:314:ALA:O     | 3:A:319:GLY:O     | 2.37                     | 0.42              |
| 3:A:463:ILE:HB    | 3:A:464:PRO:CD    | 2.43                     | 0.42              |
| 3:A:1026:LEU:HD23 | 3:A:1026:LEU:HA   | 1.71                     | 0.42              |
| 3:A:1319:VAL:HG12 | 3:A:1320:PRO:CD   | 2.50                     | 0.42              |
| 4:B:110:HIS:CD2   | 4:B:111:ALA:N     | 2.88                     | 0.42              |
| 4:B:167:ILE:CG2   | 4:B:424:LEU:CD1   | 2.76                     | 0.42              |
| 4:B:420:LEU:C     | 4:B:422:LYS:N     | 2.74                     | 0.42              |
| 4:B:527:THR:OG1   | 4:B:528:PRO:CD    | 2.65                     | 0.42              |
| 4:B:591:ARG:O     | 4:B:592:ASN:C     | 2.63                     | 0.42              |
| 4:B:606:LYS:HB2   | 4:B:606:LYS:HE3   | 1.88                     | 0.42              |
| 4:B:759:PRO:CD    | 4:B:1046:PRO:HG3  | 2.43                     | 0.42              |
| 4:B:781:PHE:CE1   | 4:B:782:LEU:HD12  | 2.54                     | 0.42              |
| 4:B:785:TYR:CD1   | 4:B:785:TYR:C     | 2.97                     | 0.42              |
| 4:B:802:PRO:CB    | 4:B:1091:TYR:CD1  | 3.03                     | 0.42              |
| 4:B:803:LEU:O     | 4:B:1042:GLY:HA3  | 2.19                     | 0.42              |
| 4:B:954:VAL:HA    | 4:B:963:PHE:O     | 2.20                     | 0.42              |
| 4:B:957:ASN:HD22  | 4:B:958:GLN:N     | 2.16                     | 0.42              |
| 4:B:1053:GLU:O    | 4:B:1055:ILE:N    | 2.53                     | 0.42              |
| 4:B:1139:ILE:H    | 4:B:1139:ILE:HG13 | 1.61                     | 0.42              |
| 7:F:81:THR:HG22   | 7:F:136:ARG:CZ    | 2.45                     | 0.42              |
| 8:H:32:THR:CG2    | 8:H:33:GLN:H      | 2.26                     | 0.42              |
| 8:H:89:LEU:HB2    | 8:H:91:ASP:CB     | 2.49                     | 0.42              |
| 8:H:93:TYR:HD2    | 8:H:145:ARG:HD3   | 1.82                     | 0.42              |
| 9:I:75:CYS:CB     | 9:I:103:CYS:HB2   | 2.49                     | 0.42              |
| 11:K:18:LYS:C     | 11:K:19:LEU:HD23  | 2.44                     | 0.42              |
| 3:A:50:ILE:HB     | 3:A:52:GLY:H      | 1.85                     | 0.42              |
| 3:A:151:ASP:OD1   | 3:A:163:SER:HB3   | 2.19                     | 0.42              |
| 3:A:290:GLU:H     | 3:A:290:GLU:HG3   | 1.44                     | 0.42              |
| 3:A:423:ASP:HB3   | 3:A:424:ILE:H     | 1.49                     | 0.42              |
| 3:A:834:THR:HG21  | 3:A:1077:THR:OG1  | 2.18                     | 0.42              |
| 3:A:877:HIS:CD2   | 3:A:1056:SER:HA   | 2.54                     | 0.42              |
| 3:A:939:ASP:HA    | 3:A:942:PHE:HB3   | 2.01                     | 0.42              |
| 4:B:102:VAL:CG2   | 4:B:112:LEU:CD2   | 2.88                     | 0.42              |
| 4:B:114:PRO:HG3   | 4:B:181:LEU:HD12  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:541:LEU:HD12  | 4:B:747:MET:HE1   | 2.01                     | 0.42              |
| 4:B:724:ASP:HA    | 4:B:725:PRO:HD2   | 1.88                     | 0.42              |
| 4:B:815:ARG:H     | 4:B:815:ARG:HG2   | 1.63                     | 0.42              |
| 4:B:911:ILE:HD11  | 4:B:941:LEU:CG    | 2.50                     | 0.42              |
| 5:C:37:MET:SD     | 5:C:232:VAL:CG2   | 3.04                     | 0.42              |
| 6:E:215:MET:HB3   | 6:E:215:MET:HE3   | 1.33                     | 0.42              |
| 7:F:120:ILE:HG22  | 7:F:121:ALA:H     | 1.81                     | 0.42              |
| 9:I:29:CYS:SG     | 9:I:31:THR:CG2    | 3.08                     | 0.42              |
| 9:I:111:THR:CG2   | 9:I:112:SER:N     | 2.82                     | 0.42              |
| 10:J:54:VAL:O     | 10:J:56:LEU:N     | 2.49                     | 0.42              |
| 3:A:112:LYS:O     | 3:A:114:LEU:HD23  | 2.19                     | 0.42              |
| 3:A:325:ILE:CG2   | 4:B:1210:MET:SD   | 3.08                     | 0.42              |
| 3:A:923:LEU:HD23  | 3:A:923:LEU:HA    | 1.84                     | 0.42              |
| 3:A:1230:GLU:N    | 3:A:1233:ASP:OD2  | 2.52                     | 0.42              |
| 3:A:1336:MET:CE   | 3:A:1381:LEU:HG   | 2.47                     | 0.42              |
| 3:A:1362:TYR:CE1  | 3:A:1364:ASN:HA   | 2.54                     | 0.42              |
| 4:B:170:LEU:HA    | 4:B:171:PRO:HD2   | 1.50                     | 0.42              |
| 4:B:227:LYS:H     | 4:B:395:GLN:CD    | 2.23                     | 0.42              |
| 4:B:276:ILE:CG2   | 4:B:277:LYS:N     | 2.81                     | 0.42              |
| 4:B:453:ILE:C     | 4:B:455:SER:H     | 2.28                     | 0.42              |
| 4:B:469:GLN:C     | 4:B:471:LYS:N     | 2.76                     | 0.42              |
| 4:B:594:ALA:O     | 4:B:595:ARG:C     | 2.62                     | 0.42              |
| 4:B:722:ASP:OD1   | 4:B:722:ASP:N     | 2.51                     | 0.42              |
| 4:B:796:LEU:O     | 4:B:799:PRO:CD    | 2.68                     | 0.42              |
| 4:B:1006:ILE:HG23 | 4:B:1007:VAL:N    | 2.34                     | 0.42              |
| 4:B:1162:ILE:HD13 | 4:B:1168:LEU:O    | 2.20                     | 0.42              |
| 5:C:31:ASN:O      | 5:C:34:ARG:N      | 2.53                     | 0.42              |
| 5:C:61:GLU:O      | 5:C:64:ALA:HB3    | 2.20                     | 0.42              |
| 5:C:66:ARG:NH1    | 10:J:2:ILE:HG21   | 2.35                     | 0.42              |
| 6:E:25:ASP:C      | 6:E:27:GLY:N      | 2.74                     | 0.42              |
| 11:K:83:PRO:O     | 11:K:86:ALA:N     | 2.52                     | 0.42              |
| 3:A:384:ASN:O     | 3:A:385:ILE:C     | 2.63                     | 0.42              |
| 3:A:453:MET:HB3   | 3:A:477:PRO:CB    | 2.50                     | 0.42              |
| 3:A:943:LEU:O     | 3:A:946:VAL:N     | 2.53                     | 0.42              |
| 3:A:1100:ARG:NH1  | 3:A:1104:ILE:HD11 | 2.34                     | 0.42              |
| 3:A:1237:ILE:HG23 | 3:A:1238:ILE:H    | 1.85                     | 0.42              |
| 3:A:1381:LEU:HD23 | 3:A:1381:LEU:HA   | 1.48                     | 0.42              |
| 4:B:314:LEU:C     | 4:B:316:PRO:CD    | 2.93                     | 0.42              |
| 4:B:349:ILE:O     | 4:B:352:ALA:N     | 2.49                     | 0.42              |
| 4:B:361:LEU:N     | 4:B:362:PRO:HD2   | 2.33                     | 0.42              |
| 4:B:482:VAL:O     | 4:B:482:VAL:CG2   | 2.58                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:581:PHE:CB    | 4:B:625:LYS:HG2   | 2.50                     | 0.42              |
| 4:B:638:PHE:HE1   | 4:B:743:ILE:HA    | 1.81                     | 0.42              |
| 4:B:769:TYR:C     | 4:B:771:SER:H     | 2.27                     | 0.42              |
| 4:B:890:TYR:C     | 4:B:892:LYS:H     | 2.28                     | 0.42              |
| 4:B:1106:ARG:HE   | 4:B:1109:GLY:N    | 2.18                     | 0.42              |
| 4:B:1138:MET:HA   | 4:B:1138:MET:CE   | 2.40                     | 0.42              |
| 4:B:1170:THR:HG23 | 4:B:1183:LYS:HZ1  | 1.84                     | 0.42              |
| 4:B:1192:TYR:CD2  | 4:B:1218:THR:HG21 | 2.55                     | 0.42              |
| 5:C:153:LEU:HD13  | 5:C:153:LEU:HA    | 1.72                     | 0.42              |
| 6:E:78:LEU:HD23   | 6:E:78:LEU:O      | 2.20                     | 0.42              |
| 8:H:104:PHE:CE2   | 8:H:136:LYS:HA    | 2.54                     | 0.42              |
| 9:I:34:TYR:C      | 9:I:35:VAL:HG23   | 2.45                     | 0.42              |
| 11:K:103:THR:O    | 11:K:106:GLU:HB2  | 2.19                     | 0.42              |
| 12:L:47:ARG:CG    | 12:L:52:GLY:O     | 2.68                     | 0.42              |
| 2:T:11:DC:C2'     | 2:T:12:DG:H8      | 2.31                     | 0.42              |
| 3:A:60:SER:HB2    | 3:A:61:ILE:H      | 1.44                     | 0.42              |
| 3:A:211:PHE:CG    | 3:A:231:PRO:HB2   | 2.55                     | 0.42              |
| 3:A:214:ILE:HG22  | 3:A:215:SER:N     | 2.35                     | 0.42              |
| 3:A:265:LYS:NZ    | 3:A:322:VAL:HB    | 2.35                     | 0.42              |
| 3:A:380:VAL:HG22  | 3:A:430:TRP:C     | 2.45                     | 0.42              |
| 3:A:531:ILE:HG12  | 3:A:622:VAL:CG1   | 2.27                     | 0.42              |
| 3:A:540:PHE:CE1   | 8:H:43:ASN:ND2    | 2.88                     | 0.42              |
| 3:A:878:ILE:CG2   | 3:A:956:LEU:N     | 2.83                     | 0.42              |
| 3:A:898:ARG:HD3   | 3:A:933:TYR:CD1   | 2.55                     | 0.42              |
| 3:A:939:ASP:O     | 3:A:940:ARG:C     | 2.60                     | 0.42              |
| 3:A:1119:TYR:CD2  | 3:A:1305:VAL:HG22 | 2.54                     | 0.42              |
| 3:A:1408:ILE:O    | 3:A:1412:ALA:CB   | 2.68                     | 0.42              |
| 3:A:1441:PHE:HB2  | 7:F:134:ILE:HG23  | 2.01                     | 0.42              |
| 3:A:1444:MET:HB3  | 3:A:1445:ILE:H    | 1.60                     | 0.42              |
| 4:B:95:ILE:HA     | 4:B:129:PHE:O     | 2.19                     | 0.42              |
| 4:B:166:PHE:HE2   | 4:B:450:ALA:CB    | 2.33                     | 0.42              |
| 4:B:563:MET:CE    | 4:B:588:GLY:CA    | 2.98                     | 0.42              |
| 4:B:620:ARG:NH2   | 9:I:89:GLN:NE2    | 2.67                     | 0.42              |
| 4:B:806:THR:HB    | 4:B:809:MET:HE3   | 2.02                     | 0.42              |
| 5:C:38:ILE:HG12   | 5:C:176:ILE:CD1   | 2.50                     | 0.42              |
| 5:C:43:THR:HG22   | 5:C:44:LEU:N      | 2.34                     | 0.42              |
| 5:C:206:ASN:ND2   | 5:C:229:TYR:CD2   | 2.88                     | 0.42              |
| 6:E:47:CYS:HA     | 6:E:52:ARG:O      | 2.19                     | 0.42              |
| 7:F:109:VAL:HG12  | 7:F:110:ASP:N     | 2.21                     | 0.42              |
| 8:H:93:TYR:HA     | 8:H:145:ARG:HB3   | 2.01                     | 0.42              |
| 11:K:39:ASP:OD1   | 11:K:39:ASP:C     | 2.63                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:37:PHE:N      | 3:A:37:PHE:CD1   | 2.88                     | 0.41              |
| 3:A:184:SER:OG    | 3:A:185:TRP:N    | 2.52                     | 0.41              |
| 3:A:341:MET:HB3   | 3:A:341:MET:HE3  | 1.51                     | 0.41              |
| 3:A:569:LYS:CD    | 5:C:221:TYR:O    | 2.68                     | 0.41              |
| 3:A:588:LEU:HD12  | 3:A:588:LEU:HA   | 1.44                     | 0.41              |
| 3:A:662:PHE:CE1   | 3:A:742:ASN:HB3  | 2.55                     | 0.41              |
| 3:A:787:PHE:CZ    | 3:A:796:SER:HA   | 2.54                     | 0.41              |
| 3:A:1057:VAL:HG12 | 3:A:1058:VAL:O   | 2.19                     | 0.41              |
| 3:A:1204:ASP:C    | 3:A:1204:ASP:OD1 | 2.63                     | 0.41              |
| 3:A:1227:ILE:CG2  | 3:A:1228:TRP:H   | 2.28                     | 0.41              |
| 3:A:1291:VAL:HG12 | 3:A:1292:PRO:HD2 | 1.97                     | 0.41              |
| 3:A:1340:GLY:HA2  | 6:E:183:PRO:HG2  | 2.01                     | 0.41              |
| 4:B:286:PHE:C     | 4:B:291:ILE:O    | 2.63                     | 0.41              |
| 4:B:686:ASN:C     | 4:B:688:GLY:N    | 2.78                     | 0.41              |
| 4:B:753:ALA:O     | 4:B:755:ILE:N    | 2.53                     | 0.41              |
| 4:B:844:SER:O     | 4:B:847:ASP:HB2  | 2.20                     | 0.41              |
| 4:B:848:ARG:NH2   | 4:B:996:ARG:NH1  | 2.68                     | 0.41              |
| 4:B:882:THR:HB    | 4:B:934:LYS:C    | 2.44                     | 0.41              |
| 5:C:24:ASN:C      | 5:C:25:VAL:HG22  | 2.45                     | 0.41              |
| 5:C:27:LEU:HA     | 5:C:228:PHE:CE2  | 2.54                     | 0.41              |
| 5:C:37:MET:HE3    | 5:C:37:MET:HB2   | 1.82                     | 0.41              |
| 6:E:187:TYR:C     | 6:E:188:LEU:HD23 | 2.45                     | 0.41              |
| 9:I:26:LEU:HD23   | 9:I:26:LEU:HA    | 1.65                     | 0.41              |
| 10:J:21:TYR:CD2   | 10:J:22:LEU:HD12 | 2.54                     | 0.41              |
| 11:K:5:ASP:HB3    | 11:K:7:PHE:CE2   | 2.55                     | 0.41              |
| 3:A:265:LYS:HE3   | 3:A:323:LYS:HG2  | 1.97                     | 0.41              |
| 3:A:324:SER:O     | 3:A:325:ILE:HB   | 2.19                     | 0.41              |
| 3:A:582:ILE:HD11  | 3:A:629:LEU:CD1  | 2.47                     | 0.41              |
| 3:A:633:VAL:HG11  | 3:A:645:LEU:HD22 | 2.02                     | 0.41              |
| 3:A:770:VAL:HG13  | 3:A:822:GLU:OE1  | 2.20                     | 0.41              |
| 3:A:997:LEU:O     | 3:A:1053:PHE:CD2 | 2.73                     | 0.41              |
| 3:A:1156:PRO:CG   | 3:A:1157:ASP:N   | 2.84                     | 0.41              |
| 4:B:51:PHE:O      | 4:B:54:PHE:CB    | 2.68                     | 0.41              |
| 4:B:291:ILE:N     | 4:B:291:ILE:CD1  | 2.80                     | 0.41              |
| 4:B:369:GLY:HA2   | 4:B:371:GLU:CD   | 2.45                     | 0.41              |
| 4:B:403:LYS:C     | 4:B:404:LYS:HG2  | 2.45                     | 0.41              |
| 4:B:431:TYR:CD1   | 4:B:447:ALA:HB1  | 2.54                     | 0.41              |
| 4:B:664:THR:O     | 4:B:664:THR:HG22 | 2.20                     | 0.41              |
| 4:B:843:GLN:HB2   | 4:B:993:THR:OG1  | 2.20                     | 0.41              |
| 4:B:991:GLY:O     | 4:B:992:ILE:HB   | 2.18                     | 0.41              |
| 4:B:1058:LEU:O    | 4:B:1059:LEU:C   | 2.63                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:1085:ILE:CG2  | 4:B:1086:PHE:N    | 2.83                     | 0.41              |
| 4:B:1106:ARG:HH21 | 4:B:1109:GLY:CA   | 2.33                     | 0.41              |
| 6:E:53:PRO:O      | 6:E:55:ARG:N      | 2.52                     | 0.41              |
| 7:F:94:LEU:HD23   | 7:F:94:LEU:HA     | 1.69                     | 0.41              |
| 9:I:40:SER:HB2    | 9:I:41:PRO:HD3    | 2.02                     | 0.41              |
| 11:K:3:ALA:HA     | 11:K:4:PRO:HD3    | 1.76                     | 0.41              |
| 11:K:28:PRO:O     | 11:K:28:PRO:HD2   | 2.20                     | 0.41              |
| 1:R:9:G:H5'       | 4:B:1097:HIS:NE2  | 2.35                     | 0.41              |
| 3:A:38:PRO:N      | 3:A:270:LEU:HD22  | 2.35                     | 0.41              |
| 3:A:95:PHE:O      | 3:A:99:ILE:HG13   | 2.20                     | 0.41              |
| 3:A:100:LYS:HB3   | 3:A:100:LYS:HZ2   | 1.83                     | 0.41              |
| 3:A:147:VAL:HB    | 3:A:149:GLU:N     | 2.36                     | 0.41              |
| 3:A:208:LEU:HD22  | 3:A:212:LYS:HG3   | 2.02                     | 0.41              |
| 3:A:381:THR:CB    | 3:A:382:PRO:HD2   | 2.49                     | 0.41              |
| 3:A:603:ASN:O     | 3:A:604:GLY:C     | 2.63                     | 0.41              |
| 3:A:606:LEU:HD12  | 3:A:606:LEU:HA    | 1.68                     | 0.41              |
| 3:A:783:THR:HG23  | 3:A:815:PHE:HE2   | 1.84                     | 0.41              |
| 3:A:1004:ASN:ND2  | 6:E:167:ARG:CG    | 2.84                     | 0.41              |
| 3:A:1348:LEU:HD12 | 3:A:1348:LEU:HA   | 1.73                     | 0.41              |
| 4:B:297:ILE:O     | 4:B:298:LEU:C     | 2.63                     | 0.41              |
| 4:B:474:SER:HA    | 4:B:476:ARG:NE    | 2.35                     | 0.41              |
| 4:B:982:SER:HB2   | 4:B:983:ARG:H     | 1.56                     | 0.41              |
| 5:C:29:MET:C      | 5:C:31:ASN:N      | 2.77                     | 0.41              |
| 5:C:35:ARG:O      | 5:C:38:ILE:HB     | 2.21                     | 0.41              |
| 5:C:238:ILE:CG2   | 5:C:242:GLN:HB2   | 2.49                     | 0.41              |
| 6:E:26:ARG:HH22   | 6:E:109:ILE:HD11  | 1.84                     | 0.41              |
| 6:E:78:LEU:CG     | 6:E:107:THR:HG22  | 2.51                     | 0.41              |
| 6:E:198:ILE:N     | 6:E:210:SER:O     | 2.42                     | 0.41              |
| 7:F:74:ILE:CG2    | 7:F:75:PRO:HD2    | 2.50                     | 0.41              |
| 8:H:58:THR:CG2    | 8:H:59:ILE:N      | 2.81                     | 0.41              |
| 3:A:548:ASN:OD1   | 11:K:60:ALA:HB1   | 2.20                     | 0.41              |
| 3:A:588:LEU:HB3   | 3:A:607:ILE:HB    | 2.02                     | 0.41              |
| 3:A:608:ILE:HG12  | 3:A:613:ILE:CG1   | 2.50                     | 0.41              |
| 3:A:903:ASN:HD22  | 3:A:906:HIS:HB2   | 1.85                     | 0.41              |
| 3:A:947:PHE:HE2   | 3:A:954:TRP:CE3   | 2.39                     | 0.41              |
| 3:A:1212:VAL:O    | 3:A:1215:ARG:CB   | 2.69                     | 0.41              |
| 3:A:1286:LYS:HB2  | 3:A:1304:TRP:CH2  | 2.55                     | 0.41              |
| 3:A:1289:ARG:HG2  | 3:A:1291:VAL:HG23 | 2.01                     | 0.41              |
| 3:A:1375:MET:HE2  | 3:A:1375:MET:HB3  | 1.83                     | 0.41              |
| 4:B:225:VAL:HG11  | 4:B:385:LEU:HA    | 2.02                     | 0.41              |
| 4:B:427:ASP:CA    | 4:B:430:ARG:HD2   | 2.50                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:B:431:TYR:CG    | 4:B:447:ALA:CB   | 3.03                     | 0.41              |
| 4:B:594:ALA:C     | 4:B:596:LEU:N    | 2.78                     | 0.41              |
| 4:B:746:SER:O     | 4:B:749:LEU:HB2  | 2.20                     | 0.41              |
| 4:B:1027:ILE:HG13 | 4:B:1027:ILE:H   | 1.54                     | 0.41              |
| 4:B:1035:ALA:O    | 4:B:1039:GLY:N   | 2.44                     | 0.41              |
| 4:B:1106:ARG:HG3  | 4:B:1107:ALA:N   | 2.35                     | 0.41              |
| 6:E:149:LEU:O     | 6:E:151:PRO:HD3  | 2.21                     | 0.41              |
| 7:F:81:THR:O      | 7:F:82:THR:O     | 2.38                     | 0.41              |
| 8:H:25:ARG:HE     | 8:H:25:ARG:HB2   | 1.29                     | 0.41              |
| 8:H:40:LEU:HD11   | 8:H:123:MET:HE3  | 1.95                     | 0.41              |
| 10:J:43:ARG:HD2   | 10:J:45:CYS:SG   | 2.60                     | 0.41              |
| 12:L:27:LEU:H     | 12:L:27:LEU:HD23 | 1.86                     | 0.41              |
| 12:L:46:VAL:HG12  | 12:L:47:ARG:N    | 2.35                     | 0.41              |
| 3:A:368:LYS:HA    | 3:A:462:VAL:CG1  | 2.51                     | 0.41              |
| 3:A:476:SER:O     | 3:A:477:PRO:C    | 2.63                     | 0.41              |
| 3:A:491:VAL:HG13  | 3:A:492:PRO:HD2  | 2.02                     | 0.41              |
| 3:A:751:SER:O     | 3:A:752:LYS:HG2  | 2.21                     | 0.41              |
| 3:A:824:LEU:HA    | 3:A:824:LEU:HD23 | 1.73                     | 0.41              |
| 3:A:1000:LEU:HD23 | 3:A:1001:ARG:H   | 1.86                     | 0.41              |
| 3:A:1050:GLU:O    | 3:A:1051:ALA:C   | 2.64                     | 0.41              |
| 3:A:1139:GLU:O    | 3:A:1139:GLU:CG  | 2.67                     | 0.41              |
| 3:A:1282:VAL:HG13 | 3:A:1283:VAL:N   | 2.34                     | 0.41              |
| 3:A:1364:ASN:HD22 | 3:A:1364:ASN:C   | 2.28                     | 0.41              |
| 4:B:349:ILE:O     | 4:B:350:GLN:O    | 2.37                     | 0.41              |
| 4:B:393:LYS:HE3   | 9:I:89:GLN:O     | 2.20                     | 0.41              |
| 4:B:544:CYS:C     | 4:B:545:ILE:HD12 | 2.45                     | 0.41              |
| 4:B:685:LEU:HD13  | 4:B:690:VAL:HG12 | 2.03                     | 0.41              |
| 4:B:879:ARG:HB2   | 4:B:880:THR:H    | 1.02                     | 0.41              |
| 5:C:51:VAL:HG13   | 5:C:155:LEU:HD23 | 2.03                     | 0.41              |
| 6:E:35:VAL:HG12   | 6:E:36:GLU:N     | 2.36                     | 0.41              |
| 6:E:168:TYR:HD2   | 6:E:168:TYR:HA   | 1.67                     | 0.41              |
| 7:F:99:LEU:C      | 7:F:99:LEU:HD12  | 2.46                     | 0.41              |
| 8:H:18:GLY:O      | 8:H:19:ARG:O     | 2.39                     | 0.41              |
| 8:H:89:LEU:HB2    | 8:H:91:ASP:OD1   | 2.21                     | 0.41              |
| 9:I:9:ASP:OD1     | 9:I:9:ASP:N      | 2.52                     | 0.41              |
| 9:I:54:GLU:C      | 9:I:55:THR:O     | 2.56                     | 0.41              |
| 10:J:1:MET:N      | 10:J:56:LEU:H    | 2.18                     | 0.41              |
| 10:J:5:VAL:HG12   | 10:J:6:ARG:CG    | 2.38                     | 0.41              |
| 10:J:14:VAL:O     | 10:J:16:ASP:N    | 2.54                     | 0.41              |
| 10:J:37:SER:OG    | 10:J:47:ARG:NH2  | 2.53                     | 0.41              |
| 3:A:265:LYS:HZ2   | 3:A:322:VAL:CB   | 2.28                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:302:THR:CB    | 3:A:313:GLN:NE2   | 2.83                     | 0.41              |
| 3:A:336:ILE:HA    | 3:A:340:LEU:HB2   | 2.01                     | 0.41              |
| 3:A:518:LYS:HG3   | 3:A:519:PRO:N     | 2.35                     | 0.41              |
| 3:A:709:THR:O     | 3:A:712:GLU:N     | 2.54                     | 0.41              |
| 3:A:818:MET:HA    | 4:B:514:LEU:HB3   | 2.01                     | 0.41              |
| 3:A:1096:SER:O    | 3:A:1099:PRO:HG2  | 2.20                     | 0.41              |
| 3:A:1154:TYR:H    | 9:I:41:PRO:HB2    | 1.85                     | 0.41              |
| 3:A:1274:ARG:HE   | 3:A:1274:ARG:HB2  | 1.44                     | 0.41              |
| 3:A:1345:ARG:CG   | 3:A:1372:VAL:CG1  | 2.99                     | 0.41              |
| 4:B:236:HIS:CD2   | 4:B:389:ALA:CA    | 3.04                     | 0.41              |
| 4:B:322:PHE:CZ    | 9:I:30:ARG:CD     | 2.92                     | 0.41              |
| 4:B:685:LEU:CD1   | 4:B:690:VAL:HG12  | 2.50                     | 0.41              |
| 4:B:1135:ARG:O    | 4:B:1139:ILE:HG13 | 2.20                     | 0.41              |
| 4:B:1196:ILE:CB   | 4:B:1197:PRO:CD   | 2.96                     | 0.41              |
| 5:C:104:PHE:HA    | 5:C:151:GLN:O     | 2.20                     | 0.41              |
| 5:C:181:ASP:CB    | 5:C:186:LEU:HD13  | 2.50                     | 0.41              |
| 5:C:260:LEU:HD11  | 5:C:264:GLN:HE21  | 1.86                     | 0.41              |
| 6:E:39:LEU:HA     | 6:E:39:LEU:HD12   | 1.80                     | 0.41              |
| 6:E:124:VAL:HG12  | 6:E:125:PRO:N     | 2.35                     | 0.41              |
| 6:E:161:LYS:C     | 6:E:163:GLU:N     | 2.74                     | 0.41              |
| 7:F:128:LYS:HD3   | 7:F:148:VAL:O     | 2.21                     | 0.41              |
| 8:H:36:CYS:HB2    | 8:H:130:ARG:HH22  | 1.86                     | 0.41              |
| 8:H:100:THR:HG22  | 8:H:101:ALA:N     | 2.35                     | 0.41              |
| 9:I:58:VAL:C      | 9:I:59:VAL:CG2    | 2.94                     | 0.41              |
| 9:I:61:ASP:O      | 9:I:62:ILE:C      | 2.63                     | 0.41              |
| 11:K:34:THR:CG2   | 11:K:35:PHE:N     | 2.83                     | 0.41              |
| 11:K:92:ASN:C     | 11:K:94:ILE:N     | 2.78                     | 0.41              |
| 3:A:99:ILE:CG1    | 3:A:234:MET:SD    | 3.09                     | 0.41              |
| 3:A:335:ARG:CD    | 3:A:339:ASN:HD22  | 2.33                     | 0.41              |
| 3:A:567:LYS:HD3   | 8:H:96:VAL:H      | 1.86                     | 0.41              |
| 3:A:1239:ARG:HH12 | 3:A:1241:ARG:HH12 | 1.68                     | 0.41              |
| 4:B:272:THR:O     | 4:B:273:LEU:HG    | 2.19                     | 0.41              |
| 4:B:294:ASP:N     | 9:I:12:ASN:HD21   | 2.18                     | 0.41              |
| 4:B:311:LEU:HA    | 4:B:311:LEU:HD23  | 1.78                     | 0.41              |
| 4:B:473:MET:O     | 4:B:475:SER:N     | 2.51                     | 0.41              |
| 4:B:737:THR:CG2   | 9:I:66:PRO:CA     | 2.98                     | 0.41              |
| 4:B:781:PHE:CD1   | 4:B:782:LEU:HD12  | 2.55                     | 0.41              |
| 4:B:806:THR:CB    | 4:B:809:MET:HE3   | 2.51                     | 0.41              |
| 5:C:239:PRO:O     | 5:C:240:VAL:C     | 2.64                     | 0.41              |
| 5:C:244:VAL:HG23  | 5:C:245:VAL:N     | 2.35                     | 0.41              |
| 8:H:19:ARG:O      | 8:H:20:TYR:CG     | 2.74                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:135:LEU:HD13 | 8:H:137:GLN:NE2   | 2.36                     | 0.41              |
| 11:K:50:LEU:CD1  | 11:K:73:LEU:HD21  | 2.51                     | 0.41              |
| 12:L:46:VAL:O    | 12:L:47:ARG:CB    | 2.63                     | 0.41              |
| 3:A:23:SER:O     | 3:A:27:VAL:HG23   | 2.20                     | 0.41              |
| 3:A:203:SER:O    | 3:A:204:THR:C     | 2.64                     | 0.41              |
| 3:A:233:TRP:C    | 3:A:235:ILE:N     | 2.76                     | 0.41              |
| 3:A:381:THR:HG23 | 3:A:382:PRO:CG    | 2.51                     | 0.41              |
| 3:A:606:LEU:HB2  | 3:A:614:PHE:CE1   | 2.56                     | 0.41              |
| 3:A:660:ASN:O    | 4:B:1081:LEU:HD22 | 2.20                     | 0.41              |
| 3:A:946:VAL:HG12 | 3:A:947:PHE:N     | 2.35                     | 0.41              |
| 3:A:947:PHE:CD1  | 3:A:947:PHE:N     | 2.89                     | 0.41              |
| 3:A:1172:LEU:CD2 | 3:A:1172:LEU:N    | 2.78                     | 0.41              |
| 4:B:44:VAL:HG11  | 4:B:495:LEU:HD13  | 2.02                     | 0.41              |
| 4:B:487:THR:HG22 | 4:B:489:SER:H     | 1.84                     | 0.41              |
| 4:B:766:ARG:O    | 4:B:767:ASN:C     | 2.63                     | 0.41              |
| 4:B:1084:GLN:CG  | 5:C:201:TRP:CH2   | 3.02                     | 0.41              |
| 4:B:1177:HIS:O   | 4:B:1179:GLN:HG3  | 2.21                     | 0.41              |
| 5:C:117:ASP:OD1  | 5:C:117:ASP:N     | 2.53                     | 0.41              |
| 5:C:129:ILE:O    | 5:C:131:HIS:HD2   | 2.03                     | 0.41              |
| 6:E:78:LEU:HG    | 6:E:107:THR:HG22  | 2.03                     | 0.41              |
| 6:E:118:PRO:O    | 6:E:122:LYS:CD    | 2.68                     | 0.41              |
| 6:E:151:PRO:O    | 6:E:153:HIS:ND1   | 2.53                     | 0.41              |
| 6:E:164:LEU:CD2  | 6:E:211:TYR:CD2   | 3.04                     | 0.41              |
| 7:F:101:ILE:HG21 | 7:F:120:ILE:HG21  | 2.02                     | 0.41              |
| 8:H:5:LEU:HD22   | 8:H:133:ASN:C     | 2.45                     | 0.41              |
| 9:I:62:ILE:HG22  | 9:I:63:GLY:N      | 2.34                     | 0.41              |
| 3:A:49:LYS:HZ2   | 3:A:60:SER:HA     | 1.85                     | 0.41              |
| 3:A:50:ILE:O     | 3:A:52:GLY:N      | 2.54                     | 0.41              |
| 3:A:62:ASP:O     | 3:A:64:ASN:N      | 2.54                     | 0.41              |
| 3:A:92:HIS:CG    | 3:A:236:LEU:HD11  | 2.55                     | 0.41              |
| 3:A:151:ASP:C    | 3:A:152:VAL:HG23  | 2.46                     | 0.41              |
| 3:A:218:ASP:O    | 3:A:219:PHE:C     | 2.64                     | 0.41              |
| 3:A:306:ASN:OD1  | 3:A:313:GLN:NE2   | 2.54                     | 0.41              |
| 3:A:359:LEU:HD22 | 3:A:363:GLN:CB    | 2.51                     | 0.41              |
| 3:A:453:MET:HB3  | 3:A:477:PRO:HB2   | 2.03                     | 0.41              |
| 3:A:496:GLU:O    | 3:A:497:THR:C     | 2.63                     | 0.41              |
| 3:A:528:LEU:CD1  | 3:A:531:ILE:CG2   | 2.99                     | 0.41              |
| 3:A:591:PHE:CD2  | 3:A:595:THR:CG2   | 3.04                     | 0.41              |
| 3:A:603:ASN:O    | 3:A:604:GLY:O     | 2.39                     | 0.41              |
| 3:A:639:PRO:HG2  | 3:A:640:GLN:N     | 2.34                     | 0.41              |
| 3:A:655:PHE:CD2  | 3:A:655:PHE:C     | 2.99                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:A:692:ASP:O     | 3:A:693:VAL:C    | 2.59                     | 0.41              |
| 3:A:701:LEU:O     | 3:A:702:LEU:C    | 2.63                     | 0.41              |
| 3:A:728:LYS:O     | 3:A:729:ALA:C    | 2.64                     | 0.41              |
| 3:A:786:HIS:CE1   | 4:B:742:GLU:OE1  | 2.74                     | 0.41              |
| 3:A:789:LYS:CE    | 9:I:67:THR:OG1   | 2.69                     | 0.41              |
| 3:A:791:ASP:OD1   | 3:A:791:ASP:C    | 2.64                     | 0.41              |
| 3:A:982:THR:O     | 3:A:983:ILE:C    | 2.64                     | 0.41              |
| 3:A:990:VAL:HG12  | 3:A:991:LYS:N    | 2.36                     | 0.41              |
| 3:A:997:LEU:HD22  | 3:A:997:LEU:HA   | 1.72                     | 0.41              |
| 3:A:1015:VAL:O    | 3:A:1016:THR:C   | 2.63                     | 0.41              |
| 3:A:1191:TRP:CZ2  | 3:A:1257:ASP:OD1 | 2.74                     | 0.41              |
| 3:A:1198:ASP:O    | 3:A:1199:ARG:C   | 2.64                     | 0.41              |
| 3:A:1279:ILE:HD12 | 3:A:1279:ILE:N   | 2.35                     | 0.41              |
| 3:A:1334:ASP:HA   | 3:A:1337:GLU:OE1 | 2.21                     | 0.41              |
| 3:A:1362:TYR:HE1  | 3:A:1363:VAL:O   | 2.04                     | 0.41              |
| 4:B:36:ALA:HB2    | 4:B:661:LEU:HD22 | 2.03                     | 0.41              |
| 4:B:43:LEU:HD23   | 4:B:43:LEU:HA    | 1.64                     | 0.41              |
| 4:B:281:PRO:HG2   | 4:B:320:ASP:OD2  | 2.21                     | 0.41              |
| 4:B:474:SER:HA    | 4:B:476:ARG:HE   | 1.86                     | 0.41              |
| 4:B:485:ARG:CG    | 4:B:485:ARG:NH1  | 2.76                     | 0.41              |
| 4:B:575:PRO:C     | 4:B:577:ALA:N    | 2.71                     | 0.41              |
| 4:B:586:TRP:CD1   | 4:B:588:GLY:H    | 2.39                     | 0.41              |
| 4:B:701:ILE:CG1   | 4:B:703:ILE:HG13 | 2.51                     | 0.41              |
| 4:B:705:MET:H     | 4:B:710:LEU:HD11 | 1.86                     | 0.41              |
| 4:B:733:HIS:O     | 4:B:734:HIS:C    | 2.63                     | 0.41              |
| 4:B:737:THR:HG21  | 9:I:66:PRO:CA    | 2.51                     | 0.41              |
| 4:B:792:MET:O     | 4:B:793:ALA:HB2  | 2.21                     | 0.41              |
| 4:B:893:LEU:HD23  | 4:B:897:GLY:O    | 2.21                     | 0.41              |
| 4:B:953:LEU:O     | 4:B:964:VAL:HA   | 2.21                     | 0.41              |
| 4:B:1067:ARG:HB2  | 4:B:1069:PHE:CD1 | 2.56                     | 0.41              |
| 4:B:1104:HIS:HB2  | 4:B:1122:ARG:CB  | 2.41                     | 0.41              |
| 4:B:1170:THR:HG23 | 4:B:1183:LYS:NZ  | 2.35                     | 0.41              |
| 4:B:1210:MET:HB2  | 4:B:1210:MET:HE2 | 1.77                     | 0.41              |
| 4:B:1217:TYR:N    | 4:B:1217:TYR:CD1 | 2.89                     | 0.41              |
| 5:C:6:PRO:O       | 5:C:7:GLN:HG2    | 2.20                     | 0.41              |
| 5:C:245:VAL:O     | 5:C:247:GLY:N    | 2.53                     | 0.41              |
| 6:E:32:GLN:O      | 6:E:32:GLN:CG    | 2.69                     | 0.41              |
| 6:E:43:LYS:HA     | 6:E:47:CYS:SG    | 2.61                     | 0.41              |
| 6:E:65:THR:HG1    | 6:E:68:SER:H     | 1.61                     | 0.41              |
| 6:E:124:VAL:H     | 6:E:125:PRO:CD   | 2.29                     | 0.41              |
| 9:I:5:ARG:HD3     | 9:I:36:GLU:OE2   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:K:50:LEU:CD2  | 11:K:75:ILE:HD13  | 2.44                     | 0.41              |
| 11:K:86:ALA:O    | 11:K:90:ALA:HB2   | 2.21                     | 0.41              |
| 3:A:141:LEU:HD23 | 3:A:141:LEU:HA    | 1.79                     | 0.41              |
| 3:A:379:VAL:HG13 | 3:A:380:VAL:HG23  | 2.03                     | 0.41              |
| 3:A:391:LEU:O    | 3:A:394:ASN:HB2   | 2.21                     | 0.41              |
| 3:A:660:ASN:ND2  | 4:B:1082:MET:CB   | 2.84                     | 0.41              |
| 3:A:746:MET:HB3  | 3:A:751:SER:OG    | 2.21                     | 0.41              |
| 3:A:808:LEU:CD2  | 3:A:816:HIS:HD2   | 2.34                     | 0.41              |
| 3:A:856:THR:O    | 3:A:864:ILE:HB    | 2.21                     | 0.41              |
| 3:A:986:ILE:CD1  | 3:A:1032:LEU:HD11 | 2.51                     | 0.41              |
| 3:A:1131:ALA:O   | 3:A:1132:LYS:C    | 2.63                     | 0.41              |
| 3:A:1420:ASP:C   | 3:A:1421:CYS:SG   | 3.04                     | 0.41              |
| 3:A:1437:GLY:CA  | 7:F:88:TYR:CD2    | 2.99                     | 0.41              |
| 4:B:393:LYS:HZ1  | 9:I:89:GLN:HB3    | 1.86                     | 0.41              |
| 4:B:457:LEU:HD23 | 4:B:457:LEU:HA    | 1.71                     | 0.41              |
| 4:B:488:TYR:CE2  | 4:B:813:LYS:HB2   | 2.56                     | 0.41              |
| 4:B:554:ILE:HD13 | 4:B:554:ILE:HA    | 1.86                     | 0.41              |
| 4:B:789:MET:CE   | 4:B:965:LYS:HB3   | 2.51                     | 0.41              |
| 4:B:802:PRO:HA   | 4:B:1091:TYR:CD1  | 2.55                     | 0.41              |
| 4:B:992:ILE:HG13 | 4:B:993:THR:N     | 2.35                     | 0.41              |
| 5:C:63:ILE:O     | 5:C:66:ARG:N      | 2.46                     | 0.41              |
| 6:E:147:HIS:O    | 6:E:150:VAL:N     | 2.38                     | 0.41              |
| 7:F:109:VAL:HG11 | 7:F:123:LYS:HG2   | 2.03                     | 0.41              |
| 9:I:20:LYS:O     | 9:I:21:GLU:O      | 2.38                     | 0.41              |
| 11:K:31:VAL:HG13 | 11:K:32:VAL:N     | 2.35                     | 0.41              |
| 11:K:83:PRO:HA   | 11:K:86:ALA:CB    | 2.50                     | 0.41              |
| 11:K:111:LEU:N   | 11:K:111:LEU:HD23 | 2.36                     | 0.41              |
| 3:A:382:PRO:HG2  | 3:A:383:TYR:H     | 1.85                     | 0.40              |
| 3:A:515:GLN:HG2  | 3:A:516:SER:OG    | 2.21                     | 0.40              |
| 3:A:599:SER:O    | 3:A:600:PRO:C     | 2.56                     | 0.40              |
| 3:A:709:THR:C    | 3:A:711:ARG:H     | 2.29                     | 0.40              |
| 3:A:804:TYR:O    | 4:B:761:HIS:HB3   | 2.21                     | 0.40              |
| 3:A:827:THR:C    | 3:A:829:VAL:N     | 2.78                     | 0.40              |
| 3:A:875:ALA:HA   | 3:A:878:ILE:CD1   | 2.48                     | 0.40              |
| 4:B:113:TYR:HA   | 4:B:114:PRO:HD2   | 1.98                     | 0.40              |
| 4:B:121:ASN:C    | 4:B:206:ASN:HA    | 2.46                     | 0.40              |
| 4:B:225:VAL:O    | 4:B:226:PHE:CD2   | 2.74                     | 0.40              |
| 4:B:230:ALA:O    | 4:B:261:ARG:HD2   | 2.21                     | 0.40              |
| 4:B:254:LEU:HD23 | 4:B:381:MET:HE1   | 2.03                     | 0.40              |
| 4:B:297:ILE:HD13 | 4:B:297:ILE:HA    | 1.70                     | 0.40              |
| 4:B:461:LEU:HD11 | 4:B:466:TRP:CH2   | 2.52                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:582:VAL:HG22 | 4:B:626:ILE:HB   | 2.03                     | 0.40              |
| 4:B:789:MET:HE3  | 4:B:789:MET:HB3  | 1.89                     | 0.40              |
| 4:B:956:THR:HA   | 4:B:961:LEU:O    | 2.22                     | 0.40              |
| 6:E:24:LYS:HG2   | 6:E:25:ASP:N     | 2.34                     | 0.40              |
| 7:F:83:PRO:HD2   | 7:F:84:TYR:H     | 1.84                     | 0.40              |
| 10:J:3:VAL:N     | 10:J:53:HIS:CE1  | 2.89                     | 0.40              |
| 10:J:57:ILE:O    | 10:J:59:LYS:N    | 2.54                     | 0.40              |
| 2:T:4:DA:P       | 2:T:4:DA:H3'     | 2.60                     | 0.40              |
| 3:A:369:SER:CB   | 11:K:2:ASN:OD1   | 2.69                     | 0.40              |
| 3:A:445:ASN:ND2  | 3:A:445:ASN:C    | 2.79                     | 0.40              |
| 3:A:557:ASP:OD2  | 3:A:559:VAL:HG23 | 2.21                     | 0.40              |
| 3:A:598:LEU:O    | 3:A:600:PRO:N    | 2.54                     | 0.40              |
| 3:A:837:ILE:C    | 3:A:839:ARG:N    | 2.79                     | 0.40              |
| 3:A:904:THR:O    | 3:A:906:HIS:N    | 2.54                     | 0.40              |
| 3:A:1057:VAL:CG1 | 3:A:1058:VAL:H   | 2.32                     | 0.40              |
| 3:A:1077:THR:O   | 3:A:1078:GLN:NE2 | 2.54                     | 0.40              |
| 4:B:110:HIS:CG   | 4:B:111:ALA:H    | 2.39                     | 0.40              |
| 4:B:435:THR:C    | 4:B:436:VAL:CG2  | 2.94                     | 0.40              |
| 4:B:493:SER:HB2  | 4:B:751:VAL:HG11 | 2.02                     | 0.40              |
| 4:B:499:ASN:OD1  | 4:B:500:THR:N    | 2.54                     | 0.40              |
| 4:B:694:ASP:O    | 4:B:697:GLU:N    | 2.54                     | 0.40              |
| 4:B:791:THR:O    | 4:B:792:MET:O    | 2.38                     | 0.40              |
| 4:B:800:GLN:HG3  | 10:J:52:THR:CB   | 2.52                     | 0.40              |
| 4:B:1131:GLY:O   | 4:B:1134:GLU:N   | 2.53                     | 0.40              |
| 5:C:16:ASP:O     | 5:C:233:GLU:HA   | 2.21                     | 0.40              |
| 5:C:164:ALA:O    | 5:C:165:LYS:C    | 2.64                     | 0.40              |
| 5:C:186:LEU:HD12 | 5:C:186:LEU:N    | 2.36                     | 0.40              |
| 6:E:63:ASN:CB    | 6:E:64:PRO:CD    | 2.98                     | 0.40              |
| 6:E:117:THR:O    | 6:E:119:SER:N    | 2.55                     | 0.40              |
| 6:E:122:LYS:C    | 6:E:123:LEU:HD23 | 2.46                     | 0.40              |
| 9:I:111:THR:HG22 | 9:I:113:ASP:HB3  | 2.04                     | 0.40              |
| 10:J:43:ARG:O    | 10:J:47:ARG:N    | 2.54                     | 0.40              |
| 3:A:90:VAL:O     | 3:A:235:ILE:HG22 | 2.22                     | 0.40              |
| 3:A:567:LYS:CB   | 8:H:95:TYR:HA    | 2.52                     | 0.40              |
| 3:A:567:LYS:HD3  | 8:H:95:TYR:CA    | 2.51                     | 0.40              |
| 3:A:690:VAL:HG13 | 3:A:718:VAL:HG13 | 2.03                     | 0.40              |
| 3:A:794:PRO:CG   | 3:A:795:GLU:H    | 2.26                     | 0.40              |
| 3:A:815:PHE:O    | 3:A:818:MET:N    | 2.54                     | 0.40              |
| 3:A:849:MET:HE3  | 3:A:1061:GLY:C   | 2.46                     | 0.40              |
| 3:A:886:ILE:HA   | 3:A:886:ILE:HD13 | 1.85                     | 0.40              |
| 3:A:1119:TYR:CD2 | 3:A:1326:ARG:NH2 | 2.90                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:461:LEU:HD12  | 4:B:466:TRP:CH2   | 2.54                     | 0.40              |
| 4:B:512:ARG:HB3   | 4:B:533:CYS:O     | 2.21                     | 0.40              |
| 4:B:847:ASP:O     | 5:C:65:HIS:HE1    | 2.04                     | 0.40              |
| 6:E:12:LEU:HD21   | 6:E:58:MET:HE1    | 2.02                     | 0.40              |
| 6:E:79:TRP:HA     | 6:E:79:TRP:HE3    | 1.85                     | 0.40              |
| 6:E:210:SER:C     | 6:E:211:TYR:HD1   | 2.29                     | 0.40              |
| 7:F:100:GLN:O     | 7:F:101:ILE:C     | 2.63                     | 0.40              |
| 8:H:16:ASP:HA     | 8:H:17:PRO:HD2    | 1.75                     | 0.40              |
| 8:H:25:ARG:HB2    | 8:H:41:ASP:OD1    | 2.20                     | 0.40              |
| 10:J:57:ILE:C     | 10:J:59:LYS:H     | 2.28                     | 0.40              |
| 11:K:58:PHE:CE2   | 11:K:74:ARG:NE    | 2.61                     | 0.40              |
| 11:K:107:THR:O    | 11:K:111:LEU:HD23 | 2.22                     | 0.40              |
| 3:A:67:CYS:C      | 3:A:68:GLN:CD     | 2.89                     | 0.40              |
| 3:A:376:TYR:HA    | 3:A:377:PRO:HD2   | 1.85                     | 0.40              |
| 3:A:789:LYS:HD2   | 9:I:67:THR:OG1    | 2.22                     | 0.40              |
| 3:A:826:ASP:O     | 3:A:827:THR:C     | 2.65                     | 0.40              |
| 3:A:857:ARG:HD3   | 3:A:861:GLY:O     | 2.21                     | 0.40              |
| 3:A:1017:LEU:O    | 3:A:1018:PHE:C    | 2.62                     | 0.40              |
| 3:A:1017:LEU:HD23 | 3:A:1017:LEU:HA   | 1.76                     | 0.40              |
| 3:A:1284:MET:HE2  | 3:A:1284:MET:HB2  | 1.72                     | 0.40              |
| 4:B:212:LEU:HA    | 4:B:212:LEU:HD23  | 1.70                     | 0.40              |
| 4:B:422:LYS:O     | 4:B:425:THR:HG22  | 2.21                     | 0.40              |
| 4:B:514:LEU:HD12  | 4:B:518:HIS:HD2   | 1.86                     | 0.40              |
| 4:B:529:GLU:H     | 4:B:529:GLU:HG3   | 1.64                     | 0.40              |
| 4:B:583:ASN:OD1   | 4:B:628:THR:HB    | 2.21                     | 0.40              |
| 4:B:654:ARG:O     | 4:B:655:LYS:C     | 2.63                     | 0.40              |
| 4:B:792:MET:H     | 4:B:857:ARG:HA    | 1.86                     | 0.40              |
| 4:B:831:SER:CB    | 4:B:994:TYR:OH    | 2.70                     | 0.40              |
| 4:B:869:SER:C     | 4:B:870:ILE:HG13  | 2.46                     | 0.40              |
| 4:B:871:THR:C     | 4:B:872:GLU:O     | 2.64                     | 0.40              |
| 5:C:31:ASN:C      | 5:C:33:LEU:H      | 2.30                     | 0.40              |
| 6:E:77:SER:HB3    | 6:E:105:PHE:CD2   | 2.50                     | 0.40              |
| 7:F:132:LEU:HA    | 7:F:132:LEU:HD23  | 1.82                     | 0.40              |
| 8:H:15:VAL:O      | 8:H:15:VAL:HG13   | 2.19                     | 0.40              |
| 8:H:82:PRO:O      | 8:H:83:GLN:CB     | 2.51                     | 0.40              |
| 9:I:32:CYS:SG     | 9:I:34:TYR:CB     | 3.09                     | 0.40              |
| 11:K:47:ARG:CD    | 11:K:60:ALA:HA    | 2.51                     | 0.40              |
| 12:L:57:LEU:HD23  | 12:L:57:LEU:HA    | 1.89                     | 0.40              |
| 3:A:93:VAL:C      | 3:A:95:PHE:N      | 2.79                     | 0.40              |
| 3:A:266:LEU:HD22  | 3:A:266:LEU:HA    | 1.63                     | 0.40              |
| 3:A:343:LYS:HZ3   | 4:B:1197:PRO:CB   | 2.27                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:404:TYR:HB2  | 3:A:433:GLU:HG3  | 2.04                     | 0.40              |
| 3:A:605:MET:CE   | 3:A:614:PHE:O    | 2.69                     | 0.40              |
| 3:A:688:LYS:O    | 3:A:689:LYS:C    | 2.65                     | 0.40              |
| 3:A:899:VAL:CG2  | 3:A:1029:ARG:NH1 | 2.85                     | 0.40              |
| 3:A:993:LEU:HB2  | 3:A:1046:LEU:CD2 | 2.51                     | 0.40              |
| 3:A:1036:ARG:HG3 | 3:A:1036:ARG:NH1 | 2.32                     | 0.40              |
| 3:A:1284:MET:HA  | 3:A:1306:LEU:CD2 | 2.44                     | 0.40              |
| 4:B:58:THR:O     | 4:B:59:LEU:C     | 2.64                     | 0.40              |
| 4:B:188:ASP:O    | 4:B:192:LEU:HG   | 2.21                     | 0.40              |
| 4:B:213:ILE:C    | 4:B:214:ALA:O    | 2.62                     | 0.40              |
| 4:B:297:ILE:C    | 4:B:299:GLU:N    | 2.79                     | 0.40              |
| 4:B:300:HIS:HE1  | 4:B:376:PHE:CZ   | 2.38                     | 0.40              |
| 4:B:435:THR:HG22 | 4:B:437:GLU:C    | 2.46                     | 0.40              |
| 4:B:515:HIS:H    | 4:B:518:HIS:CD2  | 2.40                     | 0.40              |
| 4:B:755:ILE:HD13 | 4:B:755:ILE:HA   | 1.85                     | 0.40              |
| 4:B:755:ILE:O    | 4:B:755:ILE:CG2  | 2.69                     | 0.40              |
| 4:B:802:PRO:HB3  | 4:B:1091:TYR:CE1 | 2.55                     | 0.40              |
| 4:B:1051:THR:CG2 | 4:B:1052:VAL:N   | 2.84                     | 0.40              |
| 5:C:248:ILE:HG13 | 5:C:248:ILE:H    | 1.51                     | 0.40              |
| 6:E:79:TRP:CD1   | 6:E:100:ILE:HG13 | 2.55                     | 0.40              |
| 6:E:163:GLU:O    | 6:E:164:LEU:C    | 2.65                     | 0.40              |
| 8:H:126:GLU:C    | 8:H:130:ARG:HH12 | 2.24                     | 0.40              |
| 8:H:135:LEU:HD22 | 8:H:136:LYS:CD   | 2.52                     | 0.40              |
| 10:J:8:PHE:N     | 10:J:49:MET:CE   | 2.80                     | 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       |
|-----|-------|-----------------|-----------|-----------|-----------|-------------------|
| 3   | A     | 1383/1733 (80%) | 851 (62%) | 315 (23%) | 217 (16%) | <b>0</b> <b>2</b> |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers  | Percentiles |   |
|-----|-------|-----------------|------------|-----------|-----------|-------------|---|
| 4   | B     | 1088/1224 (89%) | 730 (67%)  | 214 (20%) | 144 (13%) | 0           | 3 |
| 5   | C     | 264/318 (83%)   | 187 (71%)  | 49 (19%)  | 28 (11%)  | 0           | 4 |
| 6   | E     | 212/215 (99%)   | 142 (67%)  | 41 (19%)  | 29 (14%)  | 0           | 2 |
| 7   | F     | 82/155 (53%)    | 49 (60%)   | 26 (32%)  | 7 (8%)    | 0           | 6 |
| 8   | H     | 129/146 (88%)   | 87 (67%)   | 16 (12%)  | 26 (20%)  | 0           | 1 |
| 9   | I     | 117/122 (96%)   | 74 (63%)   | 24 (20%)  | 19 (16%)  | 0           | 2 |
| 10  | J     | 63/70 (90%)     | 42 (67%)   | 11 (18%)  | 10 (16%)  | 0           | 2 |
| 11  | K     | 112/120 (93%)   | 81 (72%)   | 20 (18%)  | 11 (10%)  | 0           | 5 |
| 12  | L     | 44/70 (63%)     | 20 (46%)   | 10 (23%)  | 14 (32%)  | 0           | 0 |
| All | All   | 3494/4173 (84%) | 2263 (65%) | 726 (21%) | 505 (14%) | 0           | 2 |

All (505) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 44  | THR  |
| 3   | A     | 50  | ILE  |
| 3   | A     | 55  | ASP  |
| 3   | A     | 56  | PRO  |
| 3   | A     | 57  | ARG  |
| 3   | A     | 59  | GLY  |
| 3   | A     | 62  | ASP  |
| 3   | A     | 63  | ARG  |
| 3   | A     | 69  | THR  |
| 3   | A     | 72  | GLU  |
| 3   | A     | 74  | MET  |
| 3   | A     | 76  | GLU  |
| 3   | A     | 89  | PRO  |
| 3   | A     | 93  | VAL  |
| 3   | A     | 99  | ILE  |
| 3   | A     | 124 | GLN  |
| 3   | A     | 130 | ASP  |
| 3   | A     | 131 | SER  |
| 3   | A     | 132 | LYS  |
| 3   | A     | 138 | ILE  |
| 3   | A     | 149 | GLU  |
| 3   | A     | 167 | CYS  |
| 3   | A     | 169 | ASN  |
| 3   | A     | 185 | TRP  |
| 3   | A     | 209 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 214 | ILE  |
| 3   | A     | 219 | PHE  |
| 3   | A     | 223 | GLY  |
| 3   | A     | 244 | PRO  |
| 3   | A     | 248 | PRO  |
| 3   | A     | 250 | ILE  |
| 3   | A     | 253 | ASN  |
| 3   | A     | 254 | GLU  |
| 3   | A     | 283 | GLY  |
| 3   | A     | 285 | PRO  |
| 3   | A     | 286 | HIS  |
| 3   | A     | 290 | GLU  |
| 3   | A     | 312 | PRO  |
| 3   | A     | 313 | GLN  |
| 3   | A     | 314 | ALA  |
| 3   | A     | 317 | LYS  |
| 3   | A     | 318 | SER  |
| 3   | A     | 320 | ARG  |
| 3   | A     | 321 | PRO  |
| 3   | A     | 322 | VAL  |
| 3   | A     | 323 | LYS  |
| 3   | A     | 331 | GLY  |
| 3   | A     | 335 | ARG  |
| 3   | A     | 336 | ILE  |
| 3   | A     | 385 | ILE  |
| 3   | A     | 399 | HIS  |
| 3   | A     | 404 | TYR  |
| 3   | A     | 415 | LEU  |
| 3   | A     | 476 | SER  |
| 3   | A     | 567 | LYS  |
| 3   | A     | 568 | PRO  |
| 3   | A     | 593 | GLU  |
| 3   | A     | 597 | LEU  |
| 3   | A     | 610 | GLY  |
| 3   | A     | 668 | ASP  |
| 3   | A     | 888 | GLY  |
| 3   | A     | 889 | SER  |
| 3   | A     | 895 | LYS  |
| 3   | A     | 903 | ASN  |
| 3   | A     | 904 | THR  |
| 3   | A     | 909 | ASP  |
| 3   | A     | 922 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 972  | HIS  |
| 3   | A     | 986  | ILE  |
| 3   | A     | 998  | LEU  |
| 3   | A     | 1036 | ARG  |
| 3   | A     | 1053 | PHE  |
| 3   | A     | 1054 | LEU  |
| 3   | A     | 1080 | THR  |
| 3   | A     | 1110 | ASN  |
| 3   | A     | 1139 | GLU  |
| 3   | A     | 1140 | HIS  |
| 3   | A     | 1169 | ILE  |
| 3   | A     | 1200 | ALA  |
| 3   | A     | 1201 | ALA  |
| 3   | A     | 1223 | ASP  |
| 3   | A     | 1255 | GLU  |
| 3   | A     | 1257 | ASP  |
| 3   | A     | 1274 | ARG  |
| 3   | A     | 1280 | GLU  |
| 3   | A     | 1314 | SER  |
| 3   | A     | 1327 | ILE  |
| 3   | A     | 1389 | PHE  |
| 3   | A     | 1392 | SER  |
| 3   | A     | 1394 | THR  |
| 3   | A     | 1401 | SER  |
| 3   | A     | 1425 | SER  |
| 4   | B     | 21   | GLU  |
| 4   | B     | 23   | ALA  |
| 4   | B     | 29   | ASP  |
| 4   | B     | 38   | PHE  |
| 4   | B     | 55   | VAL  |
| 4   | B     | 65   | GLU  |
| 4   | B     | 108  | VAL  |
| 4   | B     | 168  | GLY  |
| 4   | B     | 229  | ALA  |
| 4   | B     | 231  | PRO  |
| 4   | B     | 248  | SER  |
| 4   | B     | 249  | ARG  |
| 4   | B     | 274  | PRO  |
| 4   | B     | 275  | TYR  |
| 4   | B     | 294  | ASP  |
| 4   | B     | 327  | ARG  |
| 4   | B     | 332  | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | B     | 333  | PHE  |
| 4   | B     | 346  | GLU  |
| 4   | B     | 351  | TYR  |
| 4   | B     | 367  | LEU  |
| 4   | B     | 419  | THR  |
| 4   | B     | 432  | MET  |
| 4   | B     | 450  | ALA  |
| 4   | B     | 466  | TRP  |
| 4   | B     | 468  | GLU  |
| 4   | B     | 469  | GLN  |
| 4   | B     | 470  | LYS  |
| 4   | B     | 473  | MET  |
| 4   | B     | 476  | ARG  |
| 4   | B     | 531  | GLN  |
| 4   | B     | 635  | ARG  |
| 4   | B     | 636  | PRO  |
| 4   | B     | 637  | LEU  |
| 4   | B     | 642  | ASP  |
| 4   | B     | 643  | ASP  |
| 4   | B     | 645  | SER  |
| 4   | B     | 646  | LEU  |
| 4   | B     | 653  | VAL  |
| 4   | B     | 708  | GLU  |
| 4   | B     | 709  | ASP  |
| 4   | B     | 723  | VAL  |
| 4   | B     | 734  | HIS  |
| 4   | B     | 738  | PHE  |
| 4   | B     | 869  | SER  |
| 4   | B     | 878  | GLN  |
| 4   | B     | 958  | GLN  |
| 4   | B     | 982  | SER  |
| 4   | B     | 1046 | PRO  |
| 4   | B     | 1061 | GLU  |
| 4   | B     | 1097 | HIS  |
| 4   | B     | 1103 | ILE  |
| 4   | B     | 1167 | GLY  |
| 4   | B     | 1176 | ASN  |
| 4   | B     | 1178 | ASN  |
| 4   | B     | 1181 | GLU  |
| 4   | B     | 1183 | LYS  |
| 4   | B     | 1214 | PRO  |
| 5   | C     | 107  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | C     | 142 | VAL  |
| 5   | C     | 174 | ALA  |
| 5   | C     | 213 | PRO  |
| 5   | C     | 215 | GLU  |
| 5   | C     | 240 | VAL  |
| 6   | E     | 3   | GLN  |
| 6   | E     | 36  | GLU  |
| 6   | E     | 37  | LEU  |
| 6   | E     | 38  | PRO  |
| 6   | E     | 59  | SER  |
| 6   | E     | 77  | SER  |
| 6   | E     | 90  | VAL  |
| 6   | E     | 97  | VAL  |
| 6   | E     | 103 | LYS  |
| 6   | E     | 111 | VAL  |
| 6   | E     | 115 | ASN  |
| 6   | E     | 162 | ARG  |
| 6   | E     | 174 | GLN  |
| 7   | F     | 73  | ALA  |
| 7   | F     | 74  | ILE  |
| 7   | F     | 112 | GLU  |
| 7   | F     | 128 | LYS  |
| 8   | H     | 3   | ASN  |
| 8   | H     | 32  | THR  |
| 8   | H     | 34  | ASP  |
| 8   | H     | 43  | ASN  |
| 8   | H     | 77  | ARG  |
| 8   | H     | 80  | ARG  |
| 8   | H     | 81  | PRO  |
| 8   | H     | 86  | ASP  |
| 8   | H     | 91  | ASP  |
| 8   | H     | 109 | LYS  |
| 8   | H     | 135 | LEU  |
| 8   | H     | 140 | ALA  |
| 9   | I     | 15  | TYR  |
| 9   | I     | 16  | PRO  |
| 9   | I     | 21  | GLU  |
| 9   | I     | 33  | SER  |
| 9   | I     | 34  | TYR  |
| 9   | I     | 79  | HIS  |
| 9   | I     | 116 | ASN  |
| 10  | J     | 2   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 6   | ARG  |
| 10  | J     | 55  | ASP  |
| 10  | J     | 64  | ASN  |
| 11  | K     | 7   | PHE  |
| 11  | K     | 27  | ALA  |
| 11  | K     | 28  | PRO  |
| 12  | L     | 26  | THR  |
| 12  | L     | 35  | SER  |
| 12  | L     | 43  | THR  |
| 12  | L     | 45  | ALA  |
| 12  | L     | 47  | ARG  |
| 12  | L     | 54  | ARG  |
| 12  | L     | 55  | ILE  |
| 12  | L     | 59  | ALA  |
| 12  | L     | 64  | LEU  |
| 3   | A     | 54  | ASN  |
| 3   | A     | 61  | ILE  |
| 3   | A     | 68  | GLN  |
| 3   | A     | 117 | GLU  |
| 3   | A     | 129 | LYS  |
| 3   | A     | 139 | TRP  |
| 3   | A     | 178 | GLY  |
| 3   | A     | 210 | ILE  |
| 3   | A     | 212 | LYS  |
| 3   | A     | 255 | SER  |
| 3   | A     | 257 | ARG  |
| 3   | A     | 315 | LEU  |
| 3   | A     | 409 | SER  |
| 3   | A     | 428 | TYR  |
| 3   | A     | 473 | SER  |
| 3   | A     | 538 | ASP  |
| 3   | A     | 609 | ASP  |
| 3   | A     | 672 | ASP  |
| 3   | A     | 776 | ALA  |
| 3   | A     | 819 | GLY  |
| 3   | A     | 846 | GLU  |
| 3   | A     | 852 | TYR  |
| 3   | A     | 854 | ASN  |
| 3   | A     | 916 | GLY  |
| 3   | A     | 958 | VAL  |
| 3   | A     | 979 | SER  |
| 3   | A     | 980 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 985  | ASP  |
| 3   | A     | 1002 | GLY  |
| 3   | A     | 1028 | THR  |
| 3   | A     | 1135 | ARG  |
| 3   | A     | 1221 | LYS  |
| 3   | A     | 1231 | ASP  |
| 3   | A     | 1386 | ARG  |
| 3   | A     | 1388 | GLY  |
| 3   | A     | 1424 | VAL  |
| 3   | A     | 1437 | GLY  |
| 4   | B     | 27   | ALA  |
| 4   | B     | 37   | PHE  |
| 4   | B     | 94   | LYS  |
| 4   | B     | 124  | TYR  |
| 4   | B     | 132  | VAL  |
| 4   | B     | 200  | GLY  |
| 4   | B     | 266  | ALA  |
| 4   | B     | 318  | VAL  |
| 4   | B     | 350  | GLN  |
| 4   | B     | 365  | THR  |
| 4   | B     | 452  | THR  |
| 4   | B     | 472  | ALA  |
| 4   | B     | 485  | ARG  |
| 4   | B     | 641  | GLU  |
| 4   | B     | 695  | ALA  |
| 4   | B     | 712  | PRO  |
| 4   | B     | 731  | VAL  |
| 4   | B     | 751  | VAL  |
| 4   | B     | 761  | HIS  |
| 4   | B     | 774  | GLY  |
| 4   | B     | 792  | MET  |
| 4   | B     | 793  | ALA  |
| 4   | B     | 872  | GLU  |
| 4   | B     | 891  | ASP  |
| 4   | B     | 942  | ARG  |
| 4   | B     | 959  | ASP  |
| 4   | B     | 1017 | ILE  |
| 4   | B     | 1021 | MET  |
| 4   | B     | 1185 | CYS  |
| 4   | B     | 1202 | LEU  |
| 5   | C     | 5    | GLY  |
| 5   | C     | 28   | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | C     | 46  | ILE  |
| 5   | C     | 110 | THR  |
| 5   | C     | 245 | VAL  |
| 6   | E     | 31  | THR  |
| 6   | E     | 40  | GLU  |
| 6   | E     | 45  | LYS  |
| 6   | E     | 148 | GLU  |
| 6   | E     | 168 | TYR  |
| 6   | E     | 183 | PRO  |
| 8   | H     | 8   | ASP  |
| 8   | H     | 20  | TYR  |
| 8   | H     | 52  | GLN  |
| 8   | H     | 82  | PRO  |
| 8   | H     | 90  | ALA  |
| 8   | H     | 139 | ASN  |
| 9   | I     | 3   | THR  |
| 9   | I     | 10  | CYS  |
| 9   | I     | 11  | ASN  |
| 9   | I     | 23  | ASN  |
| 9   | I     | 60  | GLN  |
| 10  | J     | 8   | PHE  |
| 10  | J     | 32  | GLU  |
| 11  | K     | 5   | ASP  |
| 11  | K     | 13  | GLY  |
| 11  | K     | 78  | THR  |
| 11  | K     | 90  | ALA  |
| 12  | L     | 53  | HIS  |
| 3   | A     | 5   | GLN  |
| 3   | A     | 48  | ALA  |
| 3   | A     | 66  | LYS  |
| 3   | A     | 109 | HIS  |
| 3   | A     | 220 | THR  |
| 3   | A     | 251 | SER  |
| 3   | A     | 259 | GLU  |
| 3   | A     | 268 | ASP  |
| 3   | A     | 306 | ASN  |
| 3   | A     | 333 | GLU  |
| 3   | A     | 517 | ASN  |
| 3   | A     | 529 | CYS  |
| 3   | A     | 556 | TRP  |
| 3   | A     | 600 | PRO  |
| 3   | A     | 604 | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 737  | LEU  |
| 3   | A     | 838  | GLN  |
| 3   | A     | 902  | LEU  |
| 3   | A     | 905  | ASP  |
| 3   | A     | 923  | LEU  |
| 3   | A     | 942  | PHE  |
| 3   | A     | 1037 | LEU  |
| 3   | A     | 1046 | LEU  |
| 3   | A     | 1098 | VAL  |
| 3   | A     | 1115 | SER  |
| 3   | A     | 1133 | LEU  |
| 3   | A     | 1353 | TYR  |
| 3   | A     | 1403 | GLU  |
| 4   | B     | 45   | SER  |
| 4   | B     | 180  | TYR  |
| 4   | B     | 230  | ALA  |
| 4   | B     | 264  | SER  |
| 4   | B     | 265  | SER  |
| 4   | B     | 398  | ARG  |
| 4   | B     | 410  | GLY  |
| 4   | B     | 411  | PRO  |
| 4   | B     | 451  | LYS  |
| 4   | B     | 471  | LYS  |
| 4   | B     | 477  | ALA  |
| 4   | B     | 707  | PRO  |
| 4   | B     | 713  | ALA  |
| 4   | B     | 725  | PRO  |
| 4   | B     | 754  | SER  |
| 4   | B     | 937  | ALA  |
| 4   | B     | 1144 | ALA  |
| 4   | B     | 1220 | ARG  |
| 5   | C     | 4    | GLU  |
| 5   | C     | 6    | PRO  |
| 5   | C     | 48   | SER  |
| 5   | C     | 184  | ASN  |
| 5   | C     | 206  | ASN  |
| 5   | C     | 212  | PRO  |
| 6   | E     | 203  | GLU  |
| 7   | F     | 81   | THR  |
| 7   | F     | 141  | GLY  |
| 8   | H     | 19   | ARG  |
| 9   | I     | 47   | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | I     | 54   | GLU  |
| 9   | I     | 86   | PHE  |
| 10  | J     | 51   | LEU  |
| 10  | J     | 53   | HIS  |
| 11  | K     | 8    | GLU  |
| 11  | K     | 83   | PRO  |
| 3   | A     | 108  | MET  |
| 3   | A     | 140  | THR  |
| 3   | A     | 184  | SER  |
| 3   | A     | 245  | PRO  |
| 3   | A     | 400  | PRO  |
| 3   | A     | 543  | LEU  |
| 3   | A     | 583  | PRO  |
| 3   | A     | 963  | ILE  |
| 3   | A     | 1051 | ALA  |
| 3   | A     | 1077 | THR  |
| 3   | A     | 1168 | GLU  |
| 3   | A     | 1174 | PHE  |
| 3   | A     | 1204 | ASP  |
| 3   | A     | 1206 | ASP  |
| 3   | A     | 1242 | VAL  |
| 3   | A     | 1261 | LYS  |
| 3   | A     | 1287 | TYR  |
| 3   | A     | 1367 | HIS  |
| 3   | A     | 1383 | SER  |
| 3   | A     | 1398 | MET  |
| 4   | B     | 46   | GLN  |
| 4   | B     | 58   | THR  |
| 4   | B     | 179  | CYS  |
| 4   | B     | 298  | LEU  |
| 4   | B     | 394  | ASP  |
| 4   | B     | 464  | GLY  |
| 4   | B     | 598  | GLU  |
| 4   | B     | 711  | GLU  |
| 4   | B     | 828  | ALA  |
| 4   | B     | 865  | LYS  |
| 4   | B     | 879  | ARG  |
| 4   | B     | 1066 | SER  |
| 5   | C     | 165  | LYS  |
| 5   | C     | 202  | PRO  |
| 5   | C     | 214  | ASN  |
| 6   | E     | 16   | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | E     | 124  | VAL  |
| 6   | E     | 137  | GLU  |
| 6   | E     | 161  | LYS  |
| 7   | F     | 96   | THR  |
| 8   | H     | 33   | GLN  |
| 8   | H     | 44   | VAL  |
| 8   | H     | 48   | PRO  |
| 8   | H     | 78   | SER  |
| 8   | H     | 83   | GLN  |
| 8   | H     | 89   | LEU  |
| 9   | I     | 20   | LYS  |
| 9   | I     | 115  | LYS  |
| 12  | L     | 30   | ILE  |
| 3   | A     | 10   | PRO  |
| 3   | A     | 96   | ILE  |
| 3   | A     | 104  | GLU  |
| 3   | A     | 153  | PRO  |
| 3   | A     | 271  | LYS  |
| 3   | A     | 284  | ALA  |
| 3   | A     | 288  | ALA  |
| 3   | A     | 418  | SER  |
| 3   | A     | 424  | ILE  |
| 3   | A     | 526  | ASP  |
| 3   | A     | 599  | SER  |
| 3   | A     | 691  | LEU  |
| 3   | A     | 1050 | GLU  |
| 3   | A     | 1127 | ASP  |
| 3   | A     | 1233 | ASP  |
| 3   | A     | 1270 | ASN  |
| 3   | A     | 1366 | ARG  |
| 3   | A     | 1421 | CYS  |
| 4   | B     | 114  | PRO  |
| 4   | B     | 323  | VAL  |
| 4   | B     | 353  | LYS  |
| 4   | B     | 368  | GLU  |
| 4   | B     | 744  | HIS  |
| 4   | B     | 818  | PRO  |
| 4   | B     | 842  | ASN  |
| 4   | B     | 899  | ILE  |
| 4   | B     | 1108 | ARG  |
| 4   | B     | 1157 | ALA  |
| 5   | C     | 32   | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | C     | 64   | ALA  |
| 5   | C     | 195  | GLN  |
| 5   | C     | 264  | GLN  |
| 8   | H     | 51   | ALA  |
| 9   | I     | 84   | VAL  |
| 9   | I     | 97   | MET  |
| 11  | K     | 4    | PRO  |
| 11  | K     | 88   | LYS  |
| 12  | L     | 56   | LEU  |
| 3   | A     | 51   | GLY  |
| 3   | A     | 316  | GLN  |
| 3   | A     | 625  | SER  |
| 3   | A     | 706  | HIS  |
| 3   | A     | 926  | GLN  |
| 3   | A     | 1049 | ILE  |
| 3   | A     | 1136 | SER  |
| 4   | B     | 28   | GLU  |
| 4   | B     | 324  | ILE  |
| 4   | B     | 418  | LYS  |
| 4   | B     | 724  | ASP  |
| 5   | C     | 136  | ASP  |
| 5   | C     | 185  | LYS  |
| 6   | E     | 8    | ASN  |
| 6   | E     | 172  | GLU  |
| 12  | L     | 48   | CYS  |
| 3   | A     | 477  | PRO  |
| 3   | A     | 756  | ILE  |
| 3   | A     | 1148 | ILE  |
| 4   | B     | 974  | PRO  |
| 4   | B     | 992  | ILE  |
| 5   | C     | 172  | PRO  |
| 6   | E     | 118  | PRO  |
| 3   | A     | 27   | VAL  |
| 3   | A     | 325  | ILE  |
| 3   | A     | 382  | PRO  |
| 3   | A     | 530  | GLY  |
| 3   | A     | 825  | ILE  |
| 3   | A     | 837  | ILE  |
| 4   | B     | 201  | GLY  |
| 4   | B     | 284  | ILE  |
| 4   | B     | 285  | ILE  |
| 4   | B     | 555  | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | J     | 15   | GLY  |
| 12  | L     | 46   | VAL  |
| 3   | A     | 162  | VAL  |
| 3   | A     | 289  | ILE  |
| 4   | B     | 171  | PRO  |
| 5   | C     | 243  | VAL  |
| 10  | J     | 14   | VAL  |
| 3   | A     | 531  | ILE  |
| 3   | A     | 1045 | VAL  |
| 3   | A     | 1335 | ILE  |
| 4   | B     | 247  | GLY  |
| 4   | B     | 292  | ILE  |
| 4   | B     | 870  | ILE  |
| 4   | B     | 877  | PRO  |
| 6   | E     | 127  | ILE  |
| 3   | A     | 639  | PRO  |
| 4   | B     | 467  | GLY  |
| 6   | E     | 76   | 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 |   |
|-----|-------|-----------------|-----------|-----------|-------------|---|
| 3   | A     | 1218/1520 (80%) | 834 (68%) | 384 (32%) | 0           | 2 |
| 4   | B     | 960/1061 (90%)  | 684 (71%) | 276 (29%) | 0           | 2 |
| 5   | C     | 234/274 (85%)   | 168 (72%) | 66 (28%)  | 0           | 2 |
| 6   | E     | 196/197 (100%)  | 134 (68%) | 62 (32%)  | 0           | 2 |
| 7   | F     | 74/137 (54%)    | 53 (72%)  | 21 (28%)  | 0           | 2 |
| 8   | H     | 117/128 (91%)   | 76 (65%)  | 41 (35%)  | 0           | 1 |
| 9   | I     | 113/116 (97%)   | 85 (75%)  | 28 (25%)  | 1           | 4 |
| 10  | J     | 60/65 (92%)     | 42 (70%)  | 18 (30%)  | 0           | 2 |
| 11  | K     | 99/102 (97%)    | 74 (75%)  | 25 (25%)  | 0           | 4 |
| 12  | L     | 40/57 (70%)     | 25 (62%)  | 15 (38%)  | 0           | 0 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles       |
|-----|-------|-----------------|------------|-----------|-------------------|
| All | All   | 3111/3657 (85%) | 2175 (70%) | 936 (30%) | <b>0</b> <b>2</b> |

All (936) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 6   | TYR  |
| 3   | A     | 11  | LEU  |
| 3   | A     | 18  | GLN  |
| 3   | A     | 22  | PHE  |
| 3   | A     | 25  | GLU  |
| 3   | A     | 28  | ARG  |
| 3   | A     | 31  | SER  |
| 3   | A     | 32  | VAL  |
| 3   | A     | 38  | PRO  |
| 3   | A     | 41  | MET  |
| 3   | A     | 47  | ARG  |
| 3   | A     | 49  | LYS  |
| 3   | A     | 50  | ILE  |
| 3   | A     | 53  | LEU  |
| 3   | A     | 56  | PRO  |
| 3   | A     | 60  | SER  |
| 3   | A     | 62  | ASP  |
| 3   | A     | 64  | ASN  |
| 3   | A     | 65  | LEU  |
| 3   | A     | 67  | CYS  |
| 3   | A     | 69  | THR  |
| 3   | A     | 71  | GLN  |
| 3   | A     | 72  | GLU  |
| 3   | A     | 74  | MET  |
| 3   | A     | 80  | HIS  |
| 3   | A     | 83  | HIS  |
| 3   | A     | 84  | ILE  |
| 3   | A     | 93  | VAL  |
| 3   | A     | 96  | ILE  |
| 3   | A     | 98  | LYS  |
| 3   | A     | 100 | LYS  |
| 3   | A     | 102 | VAL  |
| 3   | A     | 105 | CYS  |
| 3   | A     | 106 | VAL  |
| 3   | A     | 113 | LEU  |
| 3   | A     | 114 | LEU  |
| 3   | A     | 115 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 116 | ASP  |
| 3   | A     | 121 | LEU  |
| 3   | A     | 123 | ARG  |
| 3   | A     | 132 | LYS  |
| 3   | A     | 140 | THR  |
| 3   | A     | 142 | CYS  |
| 3   | A     | 143 | LYS  |
| 3   | A     | 147 | VAL  |
| 3   | A     | 150 | THR  |
| 3   | A     | 151 | ASP  |
| 3   | A     | 161 | LEU  |
| 3   | A     | 162 | VAL  |
| 3   | A     | 167 | CYS  |
| 3   | A     | 169 | ASN  |
| 3   | A     | 170 | THR  |
| 3   | A     | 180 | LYS  |
| 3   | A     | 184 | SER  |
| 3   | A     | 185 | TRP  |
| 3   | A     | 186 | LYS  |
| 3   | A     | 207 | ILE  |
| 3   | A     | 208 | LEU  |
| 3   | A     | 215 | SER  |
| 3   | A     | 217 | LYS  |
| 3   | A     | 219 | PHE  |
| 3   | A     | 222 | LEU  |
| 3   | A     | 225 | ASN  |
| 3   | A     | 227 | VAL  |
| 3   | A     | 229 | SER  |
| 3   | A     | 232 | GLU  |
| 3   | A     | 235 | ILE  |
| 3   | A     | 237 | THR  |
| 3   | A     | 238 | CYS  |
| 3   | A     | 239 | LEU  |
| 3   | A     | 240 | PRO  |
| 3   | A     | 247 | ARG  |
| 3   | A     | 248 | PRO  |
| 3   | A     | 249 | SER  |
| 3   | A     | 250 | ILE  |
| 3   | A     | 254 | GLU  |
| 3   | A     | 256 | GLN  |
| 3   | A     | 257 | ARG  |
| 3   | A     | 263 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 265 | LYS  |
| 3   | A     | 266 | LEU  |
| 3   | A     | 271 | LYS  |
| 3   | A     | 275 | SER  |
| 3   | A     | 279 | LEU  |
| 3   | A     | 282 | ASN  |
| 3   | A     | 287 | HIS  |
| 3   | A     | 291 | GLU  |
| 3   | A     | 295 | LEU  |
| 3   | A     | 296 | LEU  |
| 3   | A     | 297 | GLN  |
| 3   | A     | 302 | THR  |
| 3   | A     | 304 | MET  |
| 3   | A     | 306 | ASN  |
| 3   | A     | 307 | ASP  |
| 3   | A     | 308 | ILE  |
| 3   | A     | 315 | LEU  |
| 3   | A     | 318 | SER  |
| 3   | A     | 320 | ARG  |
| 3   | A     | 321 | PRO  |
| 3   | A     | 323 | LYS  |
| 3   | A     | 324 | SER  |
| 3   | A     | 325 | ILE  |
| 3   | A     | 333 | GLU  |
| 3   | A     | 335 | ARG  |
| 3   | A     | 337 | ARG  |
| 3   | A     | 341 | MET  |
| 3   | A     | 348 | SER  |
| 3   | A     | 356 | ASP  |
| 3   | A     | 359 | LEU  |
| 3   | A     | 364 | VAL  |
| 3   | A     | 380 | VAL  |
| 3   | A     | 381 | THR  |
| 3   | A     | 388 | LEU  |
| 3   | A     | 391 | LEU  |
| 3   | A     | 397 | ASN  |
| 3   | A     | 398 | GLU  |
| 3   | A     | 403 | LYS  |
| 3   | A     | 404 | TYR  |
| 3   | A     | 406 | ILE  |
| 3   | A     | 407 | ARG  |
| 3   | A     | 419 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 424 | ILE  |
| 3   | A     | 433 | GLU  |
| 3   | A     | 434 | ARG  |
| 3   | A     | 437 | MET  |
| 3   | A     | 441 | PRO  |
| 3   | A     | 443 | LEU  |
| 3   | A     | 445 | ASN  |
| 3   | A     | 449 | SER  |
| 3   | A     | 450 | LEU  |
| 3   | A     | 452 | LYS  |
| 3   | A     | 453 | MET  |
| 3   | A     | 455 | MET  |
| 3   | A     | 456 | MET  |
| 3   | A     | 462 | VAL  |
| 3   | A     | 463 | ILE  |
| 3   | A     | 466 | SER  |
| 3   | A     | 475 | THR  |
| 3   | A     | 476 | SER  |
| 3   | A     | 481 | ASP  |
| 3   | A     | 493 | GLN  |
| 3   | A     | 496 | GLU  |
| 3   | A     | 500 | GLU  |
| 3   | A     | 501 | LEU  |
| 3   | A     | 512 | VAL  |
| 3   | A     | 513 | SER  |
| 3   | A     | 514 | PRO  |
| 3   | A     | 516 | SER  |
| 3   | A     | 521 | MET  |
| 3   | A     | 524 | VAL  |
| 3   | A     | 525 | GLN  |
| 3   | A     | 528 | LEU  |
| 3   | A     | 531 | ILE  |
| 3   | A     | 533 | LYS  |
| 3   | A     | 534 | LEU  |
| 3   | A     | 535 | THR  |
| 3   | A     | 539 | THR  |
| 3   | A     | 552 | TRP  |
| 3   | A     | 567 | LYS  |
| 3   | A     | 573 | SER  |
| 3   | A     | 576 | GLN  |
| 3   | A     | 577 | ILE  |
| 3   | A     | 589 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 590 | ARG  |
| 3   | A     | 596 | THR  |
| 3   | A     | 597 | LEU  |
| 3   | A     | 598 | LEU  |
| 3   | A     | 601 | LYS  |
| 3   | A     | 607 | ILE  |
| 3   | A     | 608 | ILE  |
| 3   | A     | 612 | ILE  |
| 3   | A     | 614 | PHE  |
| 3   | A     | 618 | GLU  |
| 3   | A     | 621 | THR  |
| 3   | A     | 625 | SER  |
| 3   | A     | 629 | LEU  |
| 3   | A     | 630 | ILE  |
| 3   | A     | 648 | ASN  |
| 3   | A     | 652 | VAL  |
| 3   | A     | 653 | VAL  |
| 3   | A     | 658 | LEU  |
| 3   | A     | 660 | ASN  |
| 3   | A     | 666 | ILE  |
| 3   | A     | 674 | PRO  |
| 3   | A     | 680 | THR  |
| 3   | A     | 682 | THR  |
| 3   | A     | 685 | GLU  |
| 3   | A     | 687 | LYS  |
| 3   | A     | 691 | LEU  |
| 3   | A     | 695 | LYS  |
| 3   | A     | 702 | LEU  |
| 3   | A     | 710 | LEU  |
| 3   | A     | 711 | ARG  |
| 3   | A     | 713 | SER  |
| 3   | A     | 720 | ARG  |
| 3   | A     | 722 | LEU  |
| 3   | A     | 726 | ARG  |
| 3   | A     | 732 | LEU  |
| 3   | A     | 734 | GLU  |
| 3   | A     | 735 | VAL  |
| 3   | A     | 737 | LEU  |
| 3   | A     | 738 | LYS  |
| 3   | A     | 740 | LEU  |
| 3   | A     | 745 | GLN  |
| 3   | A     | 752 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 754 | SER  |
| 3   | A     | 756 | ILE  |
| 3   | A     | 764 | CYS  |
| 3   | A     | 765 | VAL  |
| 3   | A     | 768 | GLN  |
| 3   | A     | 771 | GLU  |
| 3   | A     | 773 | LYS  |
| 3   | A     | 786 | HIS  |
| 3   | A     | 788 | SER  |
| 3   | A     | 795 | GLU  |
| 3   | A     | 803 | SER  |
| 3   | A     | 805 | LEU  |
| 3   | A     | 821 | ARG  |
| 3   | A     | 826 | ASP  |
| 3   | A     | 829 | VAL  |
| 3   | A     | 830 | LYS  |
| 3   | A     | 831 | THR  |
| 3   | A     | 839 | ARG  |
| 3   | A     | 841 | LEU  |
| 3   | A     | 853 | ASP  |
| 3   | A     | 854 | ASN  |
| 3   | A     | 855 | THR  |
| 3   | A     | 856 | THR  |
| 3   | A     | 857 | ARG  |
| 3   | A     | 858 | ASN  |
| 3   | A     | 879 | GLU  |
| 3   | A     | 882 | SER  |
| 3   | A     | 884 | ASP  |
| 3   | A     | 886 | ILE  |
| 3   | A     | 889 | SER  |
| 3   | A     | 890 | ASP  |
| 3   | A     | 893 | PHE  |
| 3   | A     | 896 | ARG  |
| 3   | A     | 897 | TYR  |
| 3   | A     | 898 | ARG  |
| 3   | A     | 899 | VAL  |
| 3   | A     | 902 | LEU  |
| 3   | A     | 904 | THR  |
| 3   | A     | 905 | ASP  |
| 3   | A     | 907 | THR  |
| 3   | A     | 911 | SER  |
| 3   | A     | 913 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 918  | GLU  |
| 3   | A     | 923  | LEU  |
| 3   | A     | 924  | LYS  |
| 3   | A     | 925  | LEU  |
| 3   | A     | 927  | VAL  |
| 3   | A     | 929  | LEU  |
| 3   | A     | 932  | GLU  |
| 3   | A     | 934  | LYS  |
| 3   | A     | 945  | GLU  |
| 3   | A     | 964  | ILE  |
| 3   | A     | 968  | GLN  |
| 3   | A     | 969  | GLN  |
| 3   | A     | 973  | ILE  |
| 3   | A     | 978  | PRO  |
| 3   | A     | 980  | ASP  |
| 3   | A     | 988  | LEU  |
| 3   | A     | 990  | VAL  |
| 3   | A     | 993  | LEU  |
| 3   | A     | 995  | GLU  |
| 3   | A     | 996  | ASN  |
| 3   | A     | 997  | LEU  |
| 3   | A     | 998  | LEU  |
| 3   | A     | 999  | VAL  |
| 3   | A     | 1001 | ARG  |
| 3   | A     | 1004 | ASN  |
| 3   | A     | 1005 | GLU  |
| 3   | A     | 1006 | ILE  |
| 3   | A     | 1009 | ASN  |
| 3   | A     | 1017 | LEU  |
| 3   | A     | 1019 | CYS  |
| 3   | A     | 1022 | LEU  |
| 3   | A     | 1024 | SER  |
| 3   | A     | 1025 | ARG  |
| 3   | A     | 1029 | ARG  |
| 3   | A     | 1032 | LEU  |
| 3   | A     | 1037 | LEU  |
| 3   | A     | 1046 | LEU  |
| 3   | A     | 1052 | GLN  |
| 3   | A     | 1060 | PRO  |
| 3   | A     | 1064 | VAL  |
| 3   | A     | 1070 | GLN  |
| 3   | A     | 1077 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 1079 | MET  |
| 3   | A     | 1081 | LEU  |
| 3   | A     | 1092 | LYS  |
| 3   | A     | 1095 | THR  |
| 3   | A     | 1098 | VAL  |
| 3   | A     | 1103 | GLU  |
| 3   | A     | 1107 | VAL  |
| 3   | A     | 1112 | LYS  |
| 3   | A     | 1116 | LEU  |
| 3   | A     | 1120 | LEU  |
| 3   | A     | 1122 | PRO  |
| 3   | A     | 1128 | GLN  |
| 3   | A     | 1132 | LYS  |
| 3   | A     | 1133 | LEU  |
| 3   | A     | 1134 | ILE  |
| 3   | A     | 1138 | ILE  |
| 3   | A     | 1146 | VAL  |
| 3   | A     | 1150 | SER  |
| 3   | A     | 1156 | PRO  |
| 3   | A     | 1162 | VAL  |
| 3   | A     | 1163 | ILE  |
| 3   | A     | 1169 | ILE  |
| 3   | A     | 1171 | GLN  |
| 3   | A     | 1172 | LEU  |
| 3   | A     | 1173 | HIS  |
| 3   | A     | 1187 | GLN  |
| 3   | A     | 1190 | PRO  |
| 3   | A     | 1193 | LEU  |
| 3   | A     | 1207 | LEU  |
| 3   | A     | 1208 | THR  |
| 3   | A     | 1215 | ARG  |
| 3   | A     | 1223 | ASP  |
| 3   | A     | 1227 | ILE  |
| 3   | A     | 1230 | GLU  |
| 3   | A     | 1231 | ASP  |
| 3   | A     | 1234 | GLU  |
| 3   | A     | 1235 | LYS  |
| 3   | A     | 1240 | CYS  |
| 3   | A     | 1243 | VAL  |
| 3   | A     | 1258 | HIS  |
| 3   | A     | 1262 | LYS  |
| 3   | A     | 1263 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 1264 | GLU  |
| 3   | A     | 1267 | MET  |
| 3   | A     | 1271 | ILE  |
| 3   | A     | 1272 | THR  |
| 3   | A     | 1273 | LEU  |
| 3   | A     | 1274 | ARG  |
| 3   | A     | 1276 | VAL  |
| 3   | A     | 1277 | GLU  |
| 3   | A     | 1280 | GLU  |
| 3   | A     | 1282 | VAL  |
| 3   | A     | 1285 | MET  |
| 3   | A     | 1290 | LYS  |
| 3   | A     | 1292 | PRO  |
| 3   | A     | 1295 | THR  |
| 3   | A     | 1299 | VAL  |
| 3   | A     | 1300 | LYS  |
| 3   | A     | 1309 | ASP  |
| 3   | A     | 1315 | GLU  |
| 3   | A     | 1318 | THR  |
| 3   | A     | 1322 | ILE  |
| 3   | A     | 1323 | ASP  |
| 3   | A     | 1325 | THR  |
| 3   | A     | 1326 | ARG  |
| 3   | A     | 1333 | ILE  |
| 3   | A     | 1336 | MET  |
| 3   | A     | 1338 | VAL  |
| 3   | A     | 1341 | ILE  |
| 3   | A     | 1349 | TYR  |
| 3   | A     | 1355 | VAL  |
| 3   | A     | 1359 | ASP  |
| 3   | A     | 1362 | TYR  |
| 3   | A     | 1364 | ASN  |
| 3   | A     | 1376 | THR  |
| 3   | A     | 1384 | VAL  |
| 3   | A     | 1385 | THR  |
| 3   | A     | 1389 | PHE  |
| 3   | A     | 1390 | ASN  |
| 3   | A     | 1391 | ARG  |
| 3   | A     | 1393 | ASN  |
| 3   | A     | 1398 | MET  |
| 3   | A     | 1400 | CYS  |
| 3   | A     | 1405 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 1406 | VAL  |
| 3   | A     | 1407 | GLU  |
| 3   | A     | 1411 | GLU  |
| 3   | A     | 1420 | ASP  |
| 3   | A     | 1422 | ARG  |
| 3   | A     | 1425 | SER  |
| 3   | A     | 1428 | VAL  |
| 3   | A     | 1433 | MET  |
| 3   | A     | 1435 | PRO  |
| 3   | A     | 1436 | ILE  |
| 3   | A     | 1445 | ILE  |
| 4   | B     | 24   | PRO  |
| 4   | B     | 28   | GLU  |
| 4   | B     | 30   | SER  |
| 4   | B     | 34   | ILE  |
| 4   | B     | 49   | ASP  |
| 4   | B     | 57   | TYR  |
| 4   | B     | 61   | ASP  |
| 4   | B     | 63   | ILE  |
| 4   | B     | 65   | GLU  |
| 4   | B     | 66   | ASP  |
| 4   | B     | 68   | THR  |
| 4   | B     | 94   | LYS  |
| 4   | B     | 97   | VAL  |
| 4   | B     | 98   | THR  |
| 4   | B     | 104  | GLU  |
| 4   | B     | 109  | THR  |
| 4   | B     | 119  | LEU  |
| 4   | B     | 120  | ARG  |
| 4   | B     | 121  | ASN  |
| 4   | B     | 128  | LEU  |
| 4   | B     | 130  | VAL  |
| 4   | B     | 134  | LYS  |
| 4   | B     | 166  | PHE  |
| 4   | B     | 167  | ILE  |
| 4   | B     | 172  | ILE  |
| 4   | B     | 174  | LEU  |
| 4   | B     | 175  | ARG  |
| 4   | B     | 177  | LYS  |
| 4   | B     | 185  | THR  |
| 4   | B     | 188  | ASP  |
| 4   | B     | 189  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 192 | LEU  |
| 4   | B     | 194 | GLU  |
| 4   | B     | 217 | ARG  |
| 4   | B     | 218 | SER  |
| 4   | B     | 222 | ILE  |
| 4   | B     | 223 | VAL  |
| 4   | B     | 225 | VAL  |
| 4   | B     | 231 | PRO  |
| 4   | B     | 234 | ILE  |
| 4   | B     | 240 | ILE  |
| 4   | B     | 245 | GLU  |
| 4   | B     | 246 | LYS  |
| 4   | B     | 249 | ARG  |
| 4   | B     | 251 | ILE  |
| 4   | B     | 252 | SER  |
| 4   | B     | 253 | THR  |
| 4   | B     | 257 | LYS  |
| 4   | B     | 261 | ARG  |
| 4   | B     | 268 | THR  |
| 4   | B     | 274 | PRO  |
| 4   | B     | 275 | TYR  |
| 4   | B     | 276 | ILE  |
| 4   | B     | 282 | ILE  |
| 4   | B     | 283 | VAL  |
| 4   | B     | 298 | LEU  |
| 4   | B     | 304 | ASP  |
| 4   | B     | 305 | VAL  |
| 4   | B     | 309 | GLN  |
| 4   | B     | 315 | LYS  |
| 4   | B     | 316 | PRO  |
| 4   | B     | 319 | GLU  |
| 4   | B     | 322 | PHE  |
| 4   | B     | 329 | THR  |
| 4   | B     | 331 | LEU  |
| 4   | B     | 346 | GLU  |
| 4   | B     | 347 | LYS  |
| 4   | B     | 350 | GLN  |
| 4   | B     | 356 | LEU  |
| 4   | B     | 359 | GLU  |
| 4   | B     | 362 | PRO  |
| 4   | B     | 365 | THR  |
| 4   | B     | 367 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 372 | SER  |
| 4   | B     | 373 | ARG  |
| 4   | B     | 385 | LEU  |
| 4   | B     | 387 | LEU  |
| 4   | B     | 393 | LYS  |
| 4   | B     | 404 | LYS  |
| 4   | B     | 408 | LEU  |
| 4   | B     | 411 | PRO  |
| 4   | B     | 416 | LEU  |
| 4   | B     | 419 | THR  |
| 4   | B     | 423 | LYS  |
| 4   | B     | 424 | LEU  |
| 4   | B     | 425 | THR  |
| 4   | B     | 426 | LYS  |
| 4   | B     | 431 | TYR  |
| 4   | B     | 433 | GLN  |
| 4   | B     | 436 | VAL  |
| 4   | B     | 451 | LYS  |
| 4   | B     | 458 | LYS  |
| 4   | B     | 461 | LEU  |
| 4   | B     | 469 | GLN  |
| 4   | B     | 471 | LYS  |
| 4   | B     | 474 | SER  |
| 4   | B     | 479 | VAL  |
| 4   | B     | 482 | VAL  |
| 4   | B     | 485 | ARG  |
| 4   | B     | 498 | THR  |
| 4   | B     | 499 | ASN  |
| 4   | B     | 511 | PRO  |
| 4   | B     | 513 | GLN  |
| 4   | B     | 519 | TRP  |
| 4   | B     | 521 | LEU  |
| 4   | B     | 531 | GLN  |
| 4   | B     | 537 | LYS  |
| 4   | B     | 539 | LEU  |
| 4   | B     | 540 | SER  |
| 4   | B     | 542 | MET  |
| 4   | B     | 547 | VAL  |
| 4   | B     | 552 | MET  |
| 4   | B     | 554 | ILE  |
| 4   | B     | 556 | THR  |
| 4   | B     | 563 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 567 | GLU  |
| 4   | B     | 570 | VAL  |
| 4   | B     | 572 | HIS  |
| 4   | B     | 573 | GLN  |
| 4   | B     | 574 | SER  |
| 4   | B     | 582 | VAL  |
| 4   | B     | 585 | VAL  |
| 4   | B     | 592 | ASN  |
| 4   | B     | 598 | GLU  |
| 4   | B     | 604 | ARG  |
| 4   | B     | 613 | VAL  |
| 4   | B     | 616 | ILE  |
| 4   | B     | 617 | ARG  |
| 4   | B     | 623 | GLU  |
| 4   | B     | 624 | LEU  |
| 4   | B     | 635 | ARG  |
| 4   | B     | 638 | PHE  |
| 4   | B     | 640 | VAL  |
| 4   | B     | 641 | GLU  |
| 4   | B     | 642 | ASP  |
| 4   | B     | 644 | GLU  |
| 4   | B     | 646 | LEU  |
| 4   | B     | 648 | HIS  |
| 4   | B     | 658 | ILE  |
| 4   | B     | 667 | GLN  |
| 4   | B     | 679 | TYR  |
| 4   | B     | 682 | SER  |
| 4   | B     | 686 | ASN  |
| 4   | B     | 701 | ILE  |
| 4   | B     | 709 | ASP  |
| 4   | B     | 710 | LEU  |
| 4   | B     | 714 | GLU  |
| 4   | B     | 723 | VAL  |
| 4   | B     | 724 | ASP  |
| 4   | B     | 728 | ARG  |
| 4   | B     | 730 | ARG  |
| 4   | B     | 732 | SER  |
| 4   | B     | 737 | THR  |
| 4   | B     | 740 | HIS  |
| 4   | B     | 741 | CYS  |
| 4   | B     | 748 | ILE  |
| 4   | B     | 751 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 760 | ASP  |
| 4   | B     | 762 | ASN  |
| 4   | B     | 764 | SER  |
| 4   | B     | 766 | ARG  |
| 4   | B     | 778 | MET  |
| 4   | B     | 789 | MET  |
| 4   | B     | 790 | ASP  |
| 4   | B     | 791 | THR  |
| 4   | B     | 792 | MET  |
| 4   | B     | 794 | ASN  |
| 4   | B     | 795 | ILE  |
| 4   | B     | 806 | THR  |
| 4   | B     | 807 | ARG  |
| 4   | B     | 810 | GLU  |
| 4   | B     | 812 | LEU  |
| 4   | B     | 815 | ARG  |
| 4   | B     | 816 | GLU  |
| 4   | B     | 817 | LEU  |
| 4   | B     | 825 | VAL  |
| 4   | B     | 837 | ASP  |
| 4   | B     | 838 | SER  |
| 4   | B     | 856 | PHE  |
| 4   | B     | 858 | SER  |
| 4   | B     | 861 | ASP  |
| 4   | B     | 864 | LYS  |
| 4   | B     | 865 | LYS  |
| 4   | B     | 866 | TYR  |
| 4   | B     | 871 | THR  |
| 4   | B     | 878 | GLN  |
| 4   | B     | 879 | ARG  |
| 4   | B     | 882 | THR  |
| 4   | B     | 883 | LEU  |
| 4   | B     | 886 | LYS  |
| 4   | B     | 889 | THR  |
| 4   | B     | 895 | ASP  |
| 4   | B     | 896 | ASP  |
| 4   | B     | 899 | ILE  |
| 4   | B     | 901 | PRO  |
| 4   | B     | 903 | VAL  |
| 4   | B     | 914 | LYS  |
| 4   | B     | 916 | THR  |
| 4   | B     | 933 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | B     | 938  | SER  |
| 4   | B     | 941  | LEU  |
| 4   | B     | 942  | ARG  |
| 4   | B     | 944  | THR  |
| 4   | B     | 949  | VAL  |
| 4   | B     | 953  | LEU  |
| 4   | B     | 956  | THR  |
| 4   | B     | 957  | ASN  |
| 4   | B     | 958  | GLN  |
| 4   | B     | 962  | LYS  |
| 4   | B     | 966  | VAL  |
| 4   | B     | 968  | VAL  |
| 4   | B     | 971  | THR  |
| 4   | B     | 976  | ILE  |
| 4   | B     | 984  | HIS  |
| 4   | B     | 986  | GLN  |
| 4   | B     | 989  | THR  |
| 4   | B     | 990  | ILE  |
| 4   | B     | 993  | THR  |
| 4   | B     | 995  | ARG  |
| 4   | B     | 996  | ARG  |
| 4   | B     | 997  | GLU  |
| 4   | B     | 999  | MET  |
| 4   | B     | 1007 | VAL  |
| 4   | B     | 1018 | PRO  |
| 4   | B     | 1019 | SER  |
| 4   | B     | 1020 | ARG  |
| 4   | B     | 1021 | MET  |
| 4   | B     | 1027 | ILE  |
| 4   | B     | 1030 | LEU  |
| 4   | B     | 1034 | VAL  |
| 4   | B     | 1048 | THR  |
| 4   | B     | 1049 | ASP  |
| 4   | B     | 1050 | ILE  |
| 4   | B     | 1052 | VAL  |
| 4   | B     | 1064 | TYR  |
| 4   | B     | 1065 | GLN  |
| 4   | B     | 1073 | TYR  |
| 4   | B     | 1074 | ASN  |
| 4   | B     | 1077 | THR  |
| 4   | B     | 1082 | MET  |
| 4   | B     | 1096 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | B     | 1103 | ILE  |
| 4   | B     | 1108 | ARG  |
| 4   | B     | 1111 | MET  |
| 4   | B     | 1113 | VAL  |
| 4   | B     | 1114 | LEU  |
| 4   | B     | 1116 | ARG  |
| 4   | B     | 1119 | VAL  |
| 4   | B     | 1120 | GLU  |
| 4   | B     | 1123 | SER  |
| 4   | B     | 1124 | ARG  |
| 4   | B     | 1138 | MET  |
| 4   | B     | 1145 | SER  |
| 4   | B     | 1147 | LEU  |
| 4   | B     | 1151 | LEU  |
| 4   | B     | 1152 | MET  |
| 4   | B     | 1162 | ILE  |
| 4   | B     | 1171 | VAL  |
| 4   | B     | 1172 | ILE  |
| 4   | B     | 1181 | GLU  |
| 4   | B     | 1183 | LYS  |
| 4   | B     | 1185 | CYS  |
| 4   | B     | 1189 | ILE  |
| 4   | B     | 1190 | ASP  |
| 4   | B     | 1191 | ILE  |
| 4   | B     | 1194 | ILE  |
| 4   | B     | 1195 | HIS  |
| 4   | B     | 1196 | ILE  |
| 4   | B     | 1202 | LEU  |
| 4   | B     | 1203 | LEU  |
| 4   | B     | 1206 | GLU  |
| 4   | B     | 1210 | MET  |
| 4   | B     | 1211 | ASN  |
| 4   | B     | 1218 | THR  |
| 4   | B     | 1219 | ASP  |
| 4   | B     | 1222 | ARG  |
| 5   | C     | 4    | GLU  |
| 5   | C     | 11   | ARG  |
| 5   | C     | 22   | LEU  |
| 5   | C     | 23   | SER  |
| 5   | C     | 25   | VAL  |
| 5   | C     | 26   | ASP  |
| 5   | C     | 27   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | C     | 33  | LEU  |
| 5   | C     | 34  | ARG  |
| 5   | C     | 41  | ILE  |
| 5   | C     | 43  | THR  |
| 5   | C     | 46  | ILE  |
| 5   | C     | 50  | GLU  |
| 5   | C     | 53  | THR  |
| 5   | C     | 55  | THR  |
| 5   | C     | 56  | THR  |
| 5   | C     | 57  | VAL  |
| 5   | C     | 58  | LEU  |
| 5   | C     | 67  | LEU  |
| 5   | C     | 69  | LEU  |
| 5   | C     | 70  | ILE  |
| 5   | C     | 75  | MET  |
| 5   | C     | 77  | ILE  |
| 5   | C     | 89  | GLU  |
| 5   | C     | 91  | HIS  |
| 5   | C     | 99  | LEU  |
| 5   | C     | 110 | THR  |
| 5   | C     | 111 | THR  |
| 5   | C     | 117 | ASP  |
| 5   | C     | 119 | VAL  |
| 5   | C     | 121 | VAL  |
| 5   | C     | 122 | SER  |
| 5   | C     | 135 | GLN  |
| 5   | C     | 137 | LYS  |
| 5   | C     | 138 | GLU  |
| 5   | C     | 140 | ASN  |
| 5   | C     | 143 | LEU  |
| 5   | C     | 145 | CYS  |
| 5   | C     | 151 | GLN  |
| 5   | C     | 153 | LEU  |
| 5   | C     | 154 | LYS  |
| 5   | C     | 163 | ILE  |
| 5   | C     | 166 | GLU  |
| 5   | C     | 172 | PRO  |
| 5   | C     | 178 | PHE  |
| 5   | C     | 189 | THR  |
| 5   | C     | 192 | TRP  |
| 5   | C     | 193 | TYR  |
| 5   | C     | 197 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | C     | 199 | LYS  |
| 5   | C     | 209 | TYR  |
| 5   | C     | 215 | GLU  |
| 5   | C     | 229 | TYR  |
| 5   | C     | 231 | ASN  |
| 5   | C     | 233 | GLU  |
| 5   | C     | 234 | SER  |
| 5   | C     | 240 | VAL  |
| 5   | C     | 244 | VAL  |
| 5   | C     | 249 | ASP  |
| 5   | C     | 250 | THR  |
| 5   | C     | 254 | LYS  |
| 5   | C     | 258 | ILE  |
| 5   | C     | 260 | LEU  |
| 5   | C     | 264 | GLN  |
| 5   | C     | 265 | MET  |
| 5   | C     | 268 | ASP  |
| 6   | E     | 3   | GLN  |
| 6   | E     | 4   | GLU  |
| 6   | E     | 6   | GLU  |
| 6   | E     | 8   | ASN  |
| 6   | E     | 9   | ILE  |
| 6   | E     | 19  | VAL  |
| 6   | E     | 31  | THR  |
| 6   | E     | 35  | VAL  |
| 6   | E     | 37  | LEU  |
| 6   | E     | 38  | PRO  |
| 6   | E     | 40  | GLU  |
| 6   | E     | 56  | LYS  |
| 6   | E     | 58  | MET  |
| 6   | E     | 60  | PHE  |
| 6   | E     | 61  | GLN  |
| 6   | E     | 68  | SER  |
| 6   | E     | 73  | PRO  |
| 6   | E     | 75  | MET  |
| 6   | E     | 77  | SER  |
| 6   | E     | 78  | LEU  |
| 6   | E     | 87  | SER  |
| 6   | E     | 92  | THR  |
| 6   | E     | 94  | LYS  |
| 6   | E     | 98  | ILE  |
| 6   | E     | 100 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | E     | 101 | GLN  |
| 6   | E     | 107 | THR  |
| 6   | E     | 109 | ILE  |
| 6   | E     | 117 | THR  |
| 6   | E     | 121 | MET  |
| 6   | E     | 122 | LYS  |
| 6   | E     | 123 | LEU  |
| 6   | E     | 124 | VAL  |
| 6   | E     | 127 | ILE  |
| 6   | E     | 129 | PRO  |
| 6   | E     | 131 | THR  |
| 6   | E     | 132 | ILE  |
| 6   | E     | 134 | THR  |
| 6   | E     | 136 | ASN  |
| 6   | E     | 142 | VAL  |
| 6   | E     | 144 | ILE  |
| 6   | E     | 145 | THR  |
| 6   | E     | 146 | HIS  |
| 6   | E     | 148 | GLU  |
| 6   | E     | 155 | ARG  |
| 6   | E     | 156 | LEU  |
| 6   | E     | 158 | SER  |
| 6   | E     | 165 | LEU  |
| 6   | E     | 168 | TYR  |
| 6   | E     | 169 | ARG  |
| 6   | E     | 172 | GLU  |
| 6   | E     | 175 | LEU  |
| 6   | E     | 176 | PRO  |
| 6   | E     | 187 | TYR  |
| 6   | E     | 188 | LEU  |
| 6   | E     | 190 | LEU  |
| 6   | E     | 191 | LYS  |
| 6   | E     | 196 | VAL  |
| 6   | E     | 204 | THR  |
| 6   | E     | 211 | TYR  |
| 6   | E     | 212 | ARG  |
| 6   | E     | 215 | MET  |
| 7   | F     | 72  | LYS  |
| 7   | F     | 79  | ARG  |
| 7   | F     | 82  | THR  |
| 7   | F     | 87  | LYS  |
| 7   | F     | 90  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | F     | 92  | ARG  |
| 7   | F     | 99  | LEU  |
| 7   | F     | 104 | ASN  |
| 7   | F     | 107 | VAL  |
| 7   | F     | 110 | ASP  |
| 7   | F     | 111 | LEU  |
| 7   | F     | 115 | THR  |
| 7   | F     | 119 | ARG  |
| 7   | F     | 120 | ILE  |
| 7   | F     | 123 | LYS  |
| 7   | F     | 125 | LEU  |
| 7   | F     | 128 | LYS  |
| 7   | F     | 133 | VAL  |
| 7   | F     | 148 | VAL  |
| 7   | F     | 151 | LEU  |
| 7   | F     | 155 | LEU  |
| 8   | H     | 2   | SER  |
| 8   | H     | 8   | ASP  |
| 8   | H     | 9   | ILE  |
| 8   | H     | 12  | VAL  |
| 8   | H     | 14  | GLU  |
| 8   | H     | 15  | VAL  |
| 8   | H     | 21  | ASN  |
| 8   | H     | 25  | ARG  |
| 8   | H     | 26  | ILE  |
| 8   | H     | 27  | GLU  |
| 8   | H     | 30  | SER  |
| 8   | H     | 31  | THR  |
| 8   | H     | 33  | GLN  |
| 8   | H     | 36  | CYS  |
| 8   | H     | 37  | LYS  |
| 8   | H     | 38  | LEU  |
| 8   | H     | 39  | THR  |
| 8   | H     | 48  | PRO  |
| 8   | H     | 49  | VAL  |
| 8   | H     | 61  | SER  |
| 8   | H     | 63  | LEU  |
| 8   | H     | 76  | THR  |
| 8   | H     | 77  | ARG  |
| 8   | H     | 82  | PRO  |
| 8   | H     | 87  | ARG  |
| 8   | H     | 88  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 89  | LEU  |
| 8   | H     | 97  | MET  |
| 8   | H     | 102 | TYR  |
| 8   | H     | 103 | LYS  |
| 8   | H     | 105 | GLU  |
| 8   | H     | 106 | GLU  |
| 8   | H     | 110 | ASP  |
| 8   | H     | 112 | ILE  |
| 8   | H     | 129 | TYR  |
| 8   | H     | 130 | ARG  |
| 8   | H     | 132 | LEU  |
| 8   | H     | 136 | LYS  |
| 8   | H     | 138 | GLU  |
| 8   | H     | 142 | LEU  |
| 8   | H     | 143 | LEU  |
| 9   | I     | 10  | CYS  |
| 9   | I     | 11  | ASN  |
| 9   | I     | 12  | ASN  |
| 9   | I     | 13  | MET  |
| 9   | I     | 14  | LEU  |
| 9   | I     | 15  | TYR  |
| 9   | I     | 16  | PRO  |
| 9   | I     | 24  | ARG  |
| 9   | I     | 26  | LEU  |
| 9   | I     | 28  | GLU  |
| 9   | I     | 29  | CYS  |
| 9   | I     | 30  | ARG  |
| 9   | I     | 31  | THR  |
| 9   | I     | 34  | TYR  |
| 9   | I     | 42  | LEU  |
| 9   | I     | 49  | ILE  |
| 9   | I     | 55  | THR  |
| 9   | I     | 73  | ARG  |
| 9   | I     | 83  | ASN  |
| 9   | I     | 84  | VAL  |
| 9   | I     | 91  | ARG  |
| 9   | I     | 101 | PHE  |
| 9   | I     | 104 | LEU  |
| 9   | I     | 107 | SER  |
| 9   | I     | 109 | ILE  |
| 9   | I     | 117 | LYS  |
| 9   | I     | 119 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | I     | 120 | GLN  |
| 10  | J     | 1   | MET  |
| 10  | J     | 2   | ILE  |
| 10  | J     | 7   | CYS  |
| 10  | J     | 13  | VAL  |
| 10  | J     | 14  | VAL  |
| 10  | J     | 19  | GLU  |
| 10  | J     | 27  | GLU  |
| 10  | J     | 28  | ASP  |
| 10  | J     | 31  | ASP  |
| 10  | J     | 32  | GLU  |
| 10  | J     | 36  | LEU  |
| 10  | J     | 43  | ARG  |
| 10  | J     | 47  | ARG  |
| 10  | J     | 51  | LEU  |
| 10  | J     | 54  | VAL  |
| 10  | J     | 55  | ASP  |
| 10  | J     | 60  | PHE  |
| 10  | J     | 62  | ARG  |
| 11  | K     | 1   | MET  |
| 11  | K     | 9   | LEU  |
| 11  | K     | 17  | SER  |
| 11  | K     | 18  | LYS  |
| 11  | K     | 21  | ILE  |
| 11  | K     | 25  | THR  |
| 11  | K     | 31  | VAL  |
| 11  | K     | 32  | VAL  |
| 11  | K     | 34  | THR  |
| 11  | K     | 42  | LEU  |
| 11  | K     | 46  | ILE  |
| 11  | K     | 47  | ARG  |
| 11  | K     | 50  | LEU  |
| 11  | K     | 53  | ASP  |
| 11  | K     | 55  | LYS  |
| 11  | K     | 56  | VAL  |
| 11  | K     | 61  | TYR  |
| 11  | K     | 71  | PHE  |
| 11  | K     | 76  | GLN  |
| 11  | K     | 77  | THR  |
| 11  | K     | 101 | LEU  |
| 11  | K     | 108 | GLU  |
| 11  | K     | 111 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | K     | 113 | THR  |
| 11  | K     | 114 | LEU  |
| 12  | L     | 27  | LEU  |
| 12  | L     | 28  | LYS  |
| 12  | L     | 31  | CYS  |
| 12  | L     | 38  | LEU  |
| 12  | L     | 40  | LEU  |
| 12  | L     | 41  | SER  |
| 12  | L     | 42  | ARG  |
| 12  | L     | 50  | ASP  |
| 12  | L     | 54  | ARG  |
| 12  | L     | 55  | ILE  |
| 12  | L     | 58  | LYS  |
| 12  | L     | 63  | ARG  |
| 12  | L     | 65  | VAL  |
| 12  | L     | 66  | GLN  |
| 12  | L     | 68  | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 4   | GLN  |
| 3   | A     | 18  | GLN  |
| 3   | A     | 64  | ASN  |
| 3   | A     | 68  | GLN  |
| 3   | A     | 71  | GLN  |
| 3   | A     | 75  | ASN  |
| 3   | A     | 83  | HIS  |
| 3   | A     | 92  | HIS  |
| 3   | A     | 119 | ASN  |
| 3   | A     | 169 | ASN  |
| 3   | A     | 171 | GLN  |
| 3   | A     | 282 | ASN  |
| 3   | A     | 297 | GLN  |
| 3   | A     | 306 | ASN  |
| 3   | A     | 313 | GLN  |
| 3   | A     | 339 | ASN  |
| 3   | A     | 435 | HIS  |
| 3   | A     | 439 | ASN  |
| 3   | A     | 445 | ASN  |
| 3   | A     | 458 | HIS  |
| 3   | A     | 471 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | A     | 493  | GLN  |
| 3   | A     | 510  | GLN  |
| 3   | A     | 587  | HIS  |
| 3   | A     | 631  | HIS  |
| 3   | A     | 650  | GLN  |
| 3   | A     | 660  | ASN  |
| 3   | A     | 736  | ASN  |
| 3   | A     | 741  | ASN  |
| 3   | A     | 742  | ASN  |
| 3   | A     | 745  | GLN  |
| 3   | A     | 757  | ASN  |
| 3   | A     | 786  | HIS  |
| 3   | A     | 858  | ASN  |
| 3   | A     | 903  | ASN  |
| 3   | A     | 906  | HIS  |
| 3   | A     | 926  | GLN  |
| 3   | A     | 935  | GLN  |
| 3   | A     | 965  | GLN  |
| 3   | A     | 968  | GLN  |
| 3   | A     | 994  | GLN  |
| 3   | A     | 1009 | ASN  |
| 3   | A     | 1070 | GLN  |
| 3   | A     | 1078 | GLN  |
| 3   | A     | 1110 | ASN  |
| 3   | A     | 1171 | GLN  |
| 3   | A     | 1173 | HIS  |
| 3   | A     | 1278 | ASN  |
| 3   | A     | 1364 | ASN  |
| 3   | A     | 1367 | HIS  |
| 3   | A     | 1378 | GLN  |
| 3   | A     | 1390 | ASN  |
| 3   | A     | 1432 | GLN  |
| 4   | B     | 46   | GLN  |
| 4   | B     | 110  | HIS  |
| 4   | B     | 121  | ASN  |
| 4   | B     | 206  | ASN  |
| 4   | B     | 255  | GLN  |
| 4   | B     | 300  | HIS  |
| 4   | B     | 325  | GLN  |
| 4   | B     | 366  | GLN  |
| 4   | B     | 383  | ASN  |
| 4   | B     | 400  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | B     | 415  | GLN  |
| 4   | B     | 433  | GLN  |
| 4   | B     | 465  | ASN  |
| 4   | B     | 515  | HIS  |
| 4   | B     | 516  | ASN  |
| 4   | B     | 518  | HIS  |
| 4   | B     | 538  | ASN  |
| 4   | B     | 572  | HIS  |
| 4   | B     | 657  | HIS  |
| 4   | B     | 686  | ASN  |
| 4   | B     | 733  | HIS  |
| 4   | B     | 734  | HIS  |
| 4   | B     | 740  | HIS  |
| 4   | B     | 744  | HIS  |
| 4   | B     | 786  | ASN  |
| 4   | B     | 794  | ASN  |
| 4   | B     | 822  | ASN  |
| 4   | B     | 842  | ASN  |
| 4   | B     | 957  | ASN  |
| 4   | B     | 975  | GLN  |
| 4   | B     | 1015 | HIS  |
| 4   | B     | 1065 | GLN  |
| 4   | B     | 1117 | GLN  |
| 4   | B     | 1141 | HIS  |
| 4   | B     | 1161 | HIS  |
| 4   | B     | 1193 | GLN  |
| 5   | C     | 65   | HIS  |
| 5   | C     | 73   | GLN  |
| 5   | C     | 112  | ASN  |
| 5   | C     | 123  | ASN  |
| 5   | C     | 131  | HIS  |
| 5   | C     | 140  | ASN  |
| 5   | C     | 167  | HIS  |
| 5   | C     | 188  | HIS  |
| 5   | C     | 206  | ASN  |
| 5   | C     | 242  | GLN  |
| 5   | C     | 264  | GLN  |
| 6   | E     | 5    | ASN  |
| 6   | E     | 63   | ASN  |
| 6   | E     | 99   | HIS  |
| 6   | E     | 104  | ASN  |
| 6   | E     | 113  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | E     | 114 | ASN  |
| 6   | E     | 115 | ASN  |
| 6   | E     | 147 | HIS  |
| 8   | H     | 33  | GLN  |
| 8   | H     | 137 | GLN  |
| 9   | I     | 12  | ASN  |
| 9   | I     | 22  | ASN  |
| 9   | I     | 83  | ASN  |
| 9   | I     | 87  | GLN  |
| 9   | I     | 89  | GLN  |
| 9   | I     | 116 | ASN  |
| 10  | J     | 64  | ASN  |
| 11  | K     | 29  | ASN  |
| 11  | K     | 40  | HIS  |
| 11  | K     | 65  | HIS  |
| 11  | K     | 76  | GLN  |
| 11  | K     | 89  | ASN  |
| 11  | K     | 92  | ASN  |
| 11  | K     | 96  | ASN  |
| 12  | L     | 53  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed   | Backbone Outliers | Pucker Outliers |
|-----|-------|------------|-------------------|-----------------|
| 1   | R     | 9/10 (90%) | 2 (22%)           | 0               |

All (2) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 5   | A    |
| 1   | R     | 10  | A    |

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | R     | 10/10 (100%)    | 4.80   | 10 (100%) 0 0 | 30, 82, 200, 200      | 0     |
| 2   | T     | 14/14 (100%)    | 3.48   | 13 (92%) 0 0  | 30, 106, 200, 200     | 0     |
| 3   | A     | 1395/1733 (80%) | 1.07   | 207 (14%) 5 6 | 30, 32, 134, 200      | 0     |
| 4   | B     | 1106/1224 (90%) | 1.06   | 151 (13%) 6 7 | 30, 30, 118, 198      | 0     |
| 5   | C     | 266/318 (83%)   | 0.81   | 13 (4%) 35 21 | 30, 30, 84, 140       | 0     |
| 6   | E     | 214/215 (99%)   | 1.60   | 65 (30%) 1 1  | 30, 67, 153, 200      | 0     |
| 7   | F     | 84/155 (54%)    | 0.78   | 9 (10%) 11 11 | 30, 31, 93, 141       | 0     |
| 8   | H     | 133/146 (91%)   | 1.25   | 25 (18%) 3 4  | 30, 47, 138, 190      | 0     |
| 9   | I     | 119/122 (97%)   | 1.23   | 17 (14%) 6 7  | 30, 32, 114, 163      | 0     |
| 10  | J     | 65/70 (92%)     | 0.75   | 4 (6%) 26 17  | 30, 30, 96, 141       | 0     |
| 11  | K     | 114/120 (95%)   | 0.66   | 3 (2%) 57 35  | 30, 30, 73, 107       | 0     |
| 12  | L     | 46/70 (65%)     | 1.18   | 7 (15%) 5 6   | 30, 45, 132, 158      | 0     |
| All | All   | 3566/4197 (84%) | 1.09   | 524 (14%) 6 6 | 30, 31, 130, 200      | 0     |

All (524) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | A     | 183 | GLY  | 7.9  |
| 1   | R     | 4   | G    | 7.4  |
| 1   | R     | 3   | C    | 6.7  |
| 4   | B     | 475 | SER  | 6.6  |
| 6   | E     | 93  | MET  | 6.1  |
| 3   | A     | 149 | GLU  | 5.9  |
| 1   | R     | 1   | A    | 5.8  |
| 4   | B     | 715 | ALA  | 5.4  |
| 1   | R     | 2   | U    | 5.2  |
| 6   | E     | 83  | CYS  | 5.1  |
| 4   | B     | 473 | MET  | 5.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | T     | 3    | DG   | 5.0  |
| 1   | R     | 9    | G    | 4.9  |
| 4   | B     | 250  | PHE  | 4.9  |
| 4   | B     | 709  | ASP  | 4.9  |
| 2   | T     | 7    | DC   | 4.8  |
| 4   | B     | 882  | THR  | 4.8  |
| 4   | B     | 469  | GLN  | 4.7  |
| 6   | E     | 124  | VAL  | 4.7  |
| 6   | E     | 55   | ARG  | 4.7  |
| 6   | E     | 56   | LYS  | 4.7  |
| 2   | T     | 1    | DA   | 4.6  |
| 8   | H     | 124  | ARG  | 4.5  |
| 6   | E     | 82   | PHE  | 4.5  |
| 3   | A     | 975  | HIS  | 4.4  |
| 1   | R     | 8    | G    | 4.4  |
| 3   | A     | 320  | ARG  | 4.4  |
| 6   | E     | 127  | ILE  | 4.4  |
| 4   | B     | 241  | ARG  | 4.4  |
| 4   | B     | 277  | LYS  | 4.4  |
| 3   | A     | 1431 | GLY  | 4.4  |
| 4   | B     | 531  | GLN  | 4.4  |
| 6   | E     | 88   | VAL  | 4.3  |
| 3   | A     | 223  | GLY  | 4.3  |
| 6   | E     | 79   | TRP  | 4.3  |
| 2   | T     | 14   | DT   | 4.2  |
| 1   | R     | 7    | A    | 4.2  |
| 3   | A     | 313  | GLN  | 4.2  |
| 8   | H     | 129  | TYR  | 4.2  |
| 3   | A     | 173  | THR  | 4.2  |
| 3   | A     | 277  | GLU  | 4.2  |
| 4   | B     | 1217 | TYR  | 4.2  |
| 3   | A     | 109  | HIS  | 4.2  |
| 4   | B     | 245  | GLU  | 4.1  |
| 3   | A     | 1173 | HIS  | 4.1  |
| 4   | B     | 643  | ASP  | 4.1  |
| 2   | T     | 5    | DT   | 4.1  |
| 3   | A     | 311  | GLN  | 4.1  |
| 6   | E     | 123  | LEU  | 4.1  |
| 3   | A     | 66   | LYS  | 4.1  |
| 3   | A     | 840  | ARG  | 4.1  |
| 3   | A     | 628  | GLY  | 4.0  |
| 2   | T     | 13   | DA   | 4.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 12  | L     | 27   | LEU  | 4.0  |
| 9   | I     | 107  | SER  | 4.0  |
| 2   | T     | 4    | DA   | 4.0  |
| 8   | H     | 139  | ASN  | 4.0  |
| 6   | E     | 112  | TYR  | 3.9  |
| 3   | A     | 200  | ARG  | 3.9  |
| 1   | R     | 6    | G    | 3.9  |
| 6   | E     | 100  | ILE  | 3.9  |
| 3   | A     | 26   | GLU  | 3.9  |
| 4   | B     | 429  | PHE  | 3.8  |
| 3   | A     | 139  | TRP  | 3.8  |
| 8   | H     | 134  | ASN  | 3.8  |
| 3   | A     | 92   | HIS  | 3.8  |
| 10  | J     | 53   | HIS  | 3.8  |
| 3   | A     | 5    | GLN  | 3.7  |
| 12  | L     | 42   | ARG  | 3.7  |
| 4   | B     | 468  | GLU  | 3.7  |
| 3   | A     | 247  | ARG  | 3.7  |
| 4   | B     | 945  | GLU  | 3.7  |
| 10  | J     | 65   | PRO  | 3.7  |
| 4   | B     | 467  | GLY  | 3.7  |
| 6   | E     | 11   | ARG  | 3.7  |
| 8   | H     | 35   | GLN  | 3.7  |
| 6   | E     | 96   | PHE  | 3.7  |
| 3   | A     | 252  | PHE  | 3.7  |
| 4   | B     | 275  | TYR  | 3.7  |
| 5   | C     | 47   | ASP  | 3.7  |
| 3   | A     | 663  | SER  | 3.6  |
| 4   | B     | 688  | GLY  | 3.6  |
| 4   | B     | 879  | ARG  | 3.6  |
| 3   | A     | 59   | GLY  | 3.6  |
| 9   | I     | 91   | ARG  | 3.6  |
| 4   | B     | 1224 | PHE  | 3.6  |
| 4   | B     | 636  | PRO  | 3.6  |
| 3   | A     | 38   | PRO  | 3.6  |
| 3   | A     | 96   | ILE  | 3.6  |
| 3   | A     | 1315 | GLU  | 3.6  |
| 3   | A     | 69   | THR  | 3.6  |
| 4   | B     | 474  | SER  | 3.6  |
| 6   | E     | 139  | ALA  | 3.5  |
| 3   | A     | 79   | GLY  | 3.5  |
| 6   | E     | 163  | GLU  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | A     | 211  | PHE  | 3.5  |
| 6   | E     | 63   | ASN  | 3.5  |
| 3   | A     | 1258 | HIS  | 3.5  |
| 2   | T     | 2    | DC   | 3.4  |
| 3   | A     | 1433 | MET  | 3.4  |
| 4   | B     | 883  | LEU  | 3.4  |
| 4   | B     | 267  | ARG  | 3.4  |
| 3   | A     | 739  | ASP  | 3.4  |
| 6   | E     | 131  | THR  | 3.4  |
| 6   | E     | 48   | ASP  | 3.4  |
| 4   | B     | 1220 | ARG  | 3.4  |
| 3   | A     | 972  | HIS  | 3.4  |
| 4   | B     | 648  | HIS  | 3.4  |
| 3   | A     | 72   | GLU  | 3.4  |
| 3   | A     | 65   | LEU  | 3.4  |
| 6   | E     | 46   | TYR  | 3.4  |
| 5   | C     | 50   | GLU  | 3.4  |
| 6   | E     | 16   | PHE  | 3.4  |
| 6   | E     | 102  | GLU  | 3.4  |
| 9   | I     | 37   | GLU  | 3.4  |
| 6   | E     | 109  | ILE  | 3.4  |
| 3   | A     | 44   | THR  | 3.3  |
| 6   | E     | 90   | VAL  | 3.3  |
| 3   | A     | 57   | ARG  | 3.3  |
| 4   | B     | 934  | LYS  | 3.3  |
| 3   | A     | 259  | GLU  | 3.3  |
| 9   | I     | 9    | ASP  | 3.3  |
| 3   | A     | 1165 | GLU  | 3.3  |
| 4   | B     | 868  | MET  | 3.3  |
| 3   | A     | 260  | ASP  | 3.3  |
| 4   | B     | 1049 | ASP  | 3.3  |
| 4   | B     | 1222 | ARG  | 3.3  |
| 3   | A     | 1196 | GLU  | 3.3  |
| 4   | B     | 1188 | LYS  | 3.3  |
| 3   | A     | 130  | ASP  | 3.3  |
| 6   | E     | 86   | PRO  | 3.3  |
| 6   | E     | 103  | LYS  | 3.3  |
| 3   | A     | 28   | ARG  | 3.3  |
| 4   | B     | 304  | ASP  | 3.3  |
| 4   | B     | 1126 | GLY  | 3.3  |
| 8   | H     | 126  | GLU  | 3.3  |
| 3   | A     | 590  | ARG  | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | A     | 1175 | SER  | 3.2  |
| 3   | A     | 1303 | GLU  | 3.2  |
| 3   | A     | 481  | ASP  | 3.2  |
| 3   | A     | 781  | ASP  | 3.2  |
| 4   | B     | 345  | LYS  | 3.2  |
| 6   | E     | 84   | ASP  | 3.2  |
| 6   | E     | 77   | SER  | 3.2  |
| 3   | A     | 1304 | TRP  | 3.2  |
| 8   | H     | 137  | GLN  | 3.2  |
| 3   | A     | 164  | ARG  | 3.2  |
| 3   | A     | 112  | LYS  | 3.2  |
| 6   | E     | 126  | SER  | 3.2  |
| 4   | B     | 476  | ARG  | 3.2  |
| 4   | B     | 866  | TYR  | 3.2  |
| 3   | A     | 165  | GLY  | 3.1  |
| 4   | B     | 134  | LYS  | 3.1  |
| 3   | A     | 136  | ALA  | 3.1  |
| 3   | A     | 1176 | LEU  | 3.1  |
| 6   | E     | 87   | SER  | 3.1  |
| 3   | A     | 56   | PRO  | 3.1  |
| 4   | B     | 247  | GLY  | 3.1  |
| 3   | A     | 140  | THR  | 3.1  |
| 6   | E     | 215  | MET  | 3.1  |
| 4   | B     | 1167 | GLY  | 3.1  |
| 3   | A     | 1127 | ASP  | 3.1  |
| 9   | I     | 93   | LYS  | 3.0  |
| 4   | B     | 20   | ASP  | 3.0  |
| 3   | A     | 705  | LYS  | 3.0  |
| 3   | A     | 240  | PRO  | 3.0  |
| 3   | A     | 167  | CYS  | 3.0  |
| 3   | A     | 1254 | ALA  | 3.0  |
| 3   | A     | 36   | ARG  | 3.0  |
| 3   | A     | 1005 | GLU  | 3.0  |
| 3   | A     | 1301 | GLU  | 3.0  |
| 4   | B     | 869  | SER  | 3.0  |
| 6   | E     | 110  | PHE  | 3.0  |
| 4   | B     | 887  | HIS  | 3.0  |
| 4   | B     | 935  | ARG  | 3.0  |
| 9   | I     | 32   | CYS  | 3.0  |
| 6   | E     | 125  | PRO  | 3.0  |
| 3   | A     | 976  | THR  | 3.0  |
| 3   | A     | 171  | GLN  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | B     | 878  | GLN  | 3.0  |
| 5   | C     | 138  | GLU  | 2.9  |
| 2   | T     | 6    | DC   | 2.9  |
| 5   | C     | 26   | ASP  | 2.9  |
| 3   | A     | 830  | LYS  | 2.9  |
| 3   | A     | 1259 | MET  | 2.9  |
| 3   | A     | 42   | ASP  | 2.9  |
| 3   | A     | 305  | ASP  | 2.9  |
| 8   | H     | 86   | ASP  | 2.9  |
| 8   | H     | 14   | GLU  | 2.9  |
| 3   | A     | 147  | VAL  | 2.9  |
| 4   | B     | 369  | GLY  | 2.9  |
| 3   | A     | 1202 | MET  | 2.9  |
| 9   | I     | 23   | ASN  | 2.9  |
| 4   | B     | 1085 | ILE  | 2.9  |
| 1   | R     | 10   | A    | 2.9  |
| 3   | A     | 117  | GLU  | 2.9  |
| 9   | I     | 75   | CYS  | 2.9  |
| 4   | B     | 959  | ASP  | 2.8  |
| 3   | A     | 753  | GLY  | 2.8  |
| 4   | B     | 647  | GLY  | 2.8  |
| 6   | E     | 35   | VAL  | 2.8  |
| 3   | A     | 121  | LEU  | 2.8  |
| 2   | T     | 9    | DC   | 2.8  |
| 3   | A     | 146  | MET  | 2.8  |
| 4   | B     | 1169 | MET  | 2.8  |
| 3   | A     | 1256 | GLU  | 2.8  |
| 9   | I     | 57   | GLY  | 2.8  |
| 3   | A     | 898  | ARG  | 2.8  |
| 3   | A     | 961  | ARG  | 2.8  |
| 3   | A     | 1261 | LYS  | 2.8  |
| 6   | E     | 20   | LYS  | 2.8  |
| 6   | E     | 53   | PRO  | 2.8  |
| 4   | B     | 65   | GLU  | 2.8  |
| 3   | A     | 592  | ASP  | 2.8  |
| 3   | A     | 176  | LYS  | 2.8  |
| 6   | E     | 122  | LYS  | 2.8  |
| 4   | B     | 431  | TYR  | 2.8  |
| 4   | B     | 484  | ASN  | 2.8  |
| 6   | E     | 2    | ASP  | 2.8  |
| 6   | E     | 47   | CYS  | 2.8  |
| 7   | F     | 154  | ASP  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | A     | 647  | GLY  | 2.8  |
| 4   | B     | 621  | GLU  | 2.8  |
| 3   | A     | 107  | CYS  | 2.8  |
| 6   | E     | 186  | LEU  | 2.8  |
| 3   | A     | 290  | GLU  | 2.8  |
| 6   | E     | 194  | GLU  | 2.8  |
| 3   | A     | 113  | LEU  | 2.7  |
| 4   | B     | 618  | ASP  | 2.7  |
| 8   | H     | 112  | ILE  | 2.7  |
| 3   | A     | 133  | LYS  | 2.7  |
| 3   | A     | 1403 | GLU  | 2.7  |
| 6   | E     | 6    | GLU  | 2.7  |
| 3   | A     | 1013 | ASP  | 2.7  |
| 3   | A     | 1373 | ASP  | 2.7  |
| 3   | A     | 132  | LYS  | 2.7  |
| 4   | B     | 960  | GLY  | 2.7  |
| 4   | B     | 216  | GLU  | 2.7  |
| 6   | E     | 36   | GLU  | 2.7  |
| 3   | A     | 218  | ASP  | 2.7  |
| 3   | A     | 1257 | ASP  | 2.7  |
| 4   | B     | 106  | ASP  | 2.7  |
| 12  | L     | 31   | CYS  | 2.7  |
| 3   | A     | 678  | GLU  | 2.7  |
| 3   | A     | 932  | GLU  | 2.7  |
| 3   | A     | 1199 | ARG  | 2.7  |
| 4   | B     | 266  | ALA  | 2.7  |
| 12  | L     | 45   | ALA  | 2.7  |
| 6   | E     | 66   | GLU  | 2.7  |
| 5   | C     | 200  | GLU  | 2.7  |
| 8   | H     | 27   | GLU  | 2.7  |
| 8   | H     | 76   | THR  | 2.7  |
| 3   | A     | 1174 | PHE  | 2.7  |
| 3   | A     | 250  | ILE  | 2.7  |
| 4   | B     | 870  | ILE  | 2.7  |
| 4   | B     | 986  | GLN  | 2.7  |
| 8   | H     | 83   | GLN  | 2.7  |
| 4   | B     | 1192 | TYR  | 2.7  |
| 4   | B     | 734  | HIS  | 2.6  |
| 8   | H     | 40   | LEU  | 2.6  |
| 4   | B     | 330  | ALA  | 2.6  |
| 4   | B     | 477  | ALA  | 2.6  |
| 4   | B     | 957  | ASN  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | E     | 143  | ASN  | 2.6  |
| 1   | R     | 5    | A    | 2.6  |
| 6   | E     | 106  | GLN  | 2.6  |
| 3   | A     | 144  | THR  | 2.6  |
| 3   | A     | 356  | ASP  | 2.6  |
| 4   | B     | 296  | GLU  | 2.6  |
| 2   | T     | 12   | DG   | 2.6  |
| 3   | A     | 704  | ALA  | 2.6  |
| 3   | A     | 1108 | ALA  | 2.6  |
| 6   | E     | 29   | PHE  | 2.6  |
| 3   | A     | 995  | GLU  | 2.6  |
| 4   | B     | 641  | GLU  | 2.6  |
| 4   | B     | 1219 | ASP  | 2.6  |
| 9   | I     | 82   | GLU  | 2.6  |
| 4   | B     | 1189 | ILE  | 2.6  |
| 9   | I     | 116  | ASN  | 2.6  |
| 2   | T     | 10   | DT   | 2.6  |
| 3   | A     | 231  | PRO  | 2.6  |
| 5   | C     | 268  | ASP  | 2.6  |
| 3   | A     | 91   | PHE  | 2.6  |
| 3   | A     | 685  | GLU  | 2.5  |
| 7   | F     | 76   | LYS  | 2.5  |
| 8   | H     | 37   | LYS  | 2.5  |
| 4   | B     | 211  | VAL  | 2.5  |
| 4   | B     | 881  | ASN  | 2.5  |
| 4   | B     | 278  | GLN  | 2.5  |
| 3   | A     | 1161 | THR  | 2.5  |
| 4   | B     | 1170 | THR  | 2.5  |
| 4   | B     | 1183 | LYS  | 2.5  |
| 4   | B     | 1221 | SER  | 2.5  |
| 3   | A     | 25   | GLU  | 2.5  |
| 3   | A     | 833  | GLU  | 2.5  |
| 4   | B     | 962  | LYS  | 2.5  |
| 3   | A     | 41   | MET  | 2.5  |
| 7   | F     | 123  | LYS  | 2.5  |
| 3   | A     | 85   | ASP  | 2.5  |
| 3   | A     | 1003 | LYS  | 2.5  |
| 4   | B     | 795  | ILE  | 2.5  |
| 3   | A     | 820  | GLY  | 2.5  |
| 3   | A     | 795  | GLU  | 2.5  |
| 4   | B     | 810  | GLU  | 2.5  |
| 4   | B     | 987  | LYS  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | A     | 531  | ILE  | 2.5  |
| 4   | B     | 1046 | PRO  | 2.5  |
| 3   | A     | 178  | GLY  | 2.5  |
| 4   | B     | 861  | ASP  | 2.5  |
| 3   | A     | 587  | HIS  | 2.4  |
| 4   | B     | 1175 | LEU  | 2.4  |
| 3   | A     | 412  | ARG  | 2.4  |
| 4   | B     | 261  | ARG  | 2.4  |
| 4   | B     | 326  | ASP  | 2.4  |
| 3   | A     | 221  | SER  | 2.4  |
| 6   | E     | 121  | MET  | 2.4  |
| 5   | C     | 18   | VAL  | 2.4  |
| 6   | E     | 80   | VAL  | 2.4  |
| 3   | A     | 253  | ASN  | 2.4  |
| 4   | B     | 808  | ALA  | 2.4  |
| 4   | B     | 348  | ARG  | 2.4  |
| 4   | B     | 867  | GLY  | 2.4  |
| 4   | B     | 1206 | GLU  | 2.4  |
| 7   | F     | 155  | LEU  | 2.4  |
| 8   | H     | 63   | LEU  | 2.4  |
| 3   | A     | 185  | TRP  | 2.4  |
| 9   | I     | 73   | ARG  | 2.4  |
| 4   | B     | 820  | GLY  | 2.4  |
| 8   | H     | 85   | GLY  | 2.4  |
| 4   | B     | 903  | VAL  | 2.4  |
| 3   | A     | 1274 | ARG  | 2.4  |
| 3   | A     | 135  | PHE  | 2.4  |
| 6   | E     | 182  | ASP  | 2.4  |
| 4   | B     | 39   | ARG  | 2.4  |
| 4   | B     | 598  | GLU  | 2.4  |
| 3   | A     | 122  | MET  | 2.4  |
| 4   | B     | 64   | CYS  | 2.4  |
| 4   | B     | 572  | HIS  | 2.4  |
| 4   | B     | 436  | VAL  | 2.4  |
| 4   | B     | 111  | ALA  | 2.4  |
| 3   | A     | 312  | PRO  | 2.3  |
| 3   | A     | 154  | SER  | 2.3  |
| 4   | B     | 1131 | GLY  | 2.3  |
| 3   | A     | 162  | VAL  | 2.3  |
| 6   | E     | 28   | TYR  | 2.3  |
| 3   | A     | 177  | ASP  | 2.3  |
| 3   | A     | 1407 | GLU  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | B     | 1164 | GLY  | 2.3  |
| 3   | A     | 524  | VAL  | 2.3  |
| 4   | B     | 1119 | VAL  | 2.3  |
| 4   | B     | 1213 | THR  | 2.3  |
| 3   | A     | 1131 | ALA  | 2.3  |
| 10  | J     | 35   | ALA  | 2.3  |
| 3   | A     | 181  | LEU  | 2.3  |
| 3   | A     | 213  | HIS  | 2.3  |
| 8   | H     | 131  | ASN  | 2.3  |
| 3   | A     | 703  | THR  | 2.3  |
| 4   | B     | 865  | LYS  | 2.3  |
| 3   | A     | 256  | GLN  | 2.3  |
| 6   | E     | 105  | PHE  | 2.3  |
| 9   | I     | 120  | GLN  | 2.3  |
| 3   | A     | 152  | VAL  | 2.3  |
| 3   | A     | 47   | ARG  | 2.3  |
| 3   | A     | 88   | LYS  | 2.3  |
| 6   | E     | 132  | ILE  | 2.3  |
| 8   | H     | 29   | ALA  | 2.3  |
| 3   | A     | 280  | GLU  | 2.3  |
| 3   | A     | 610  | GLY  | 2.3  |
| 4   | B     | 290  | GLY  | 2.3  |
| 5   | C     | 132  | PRO  | 2.3  |
| 3   | A     | 1438 | THR  | 2.3  |
| 11  | K     | 54   | ARG  | 2.3  |
| 3   | A     | 1081 | LEU  | 2.3  |
| 11  | K     | 114  | LEU  | 2.3  |
| 4   | B     | 248  | SER  | 2.3  |
| 3   | A     | 49   | LYS  | 2.3  |
| 3   | A     | 63   | ARG  | 2.3  |
| 3   | A     | 1223 | ASP  | 2.3  |
| 3   | A     | 966  | ASN  | 2.2  |
| 3   | A     | 298  | PHE  | 2.2  |
| 4   | B     | 462  | ALA  | 2.2  |
| 4   | B     | 433  | GLN  | 2.2  |
| 7   | F     | 72   | LYS  | 2.2  |
| 3   | A     | 76   | GLU  | 2.2  |
| 3   | A     | 1342 | GLU  | 2.2  |
| 6   | E     | 133  | GLU  | 2.2  |
| 3   | A     | 665  | GLY  | 2.2  |
| 5   | C     | 249  | ASP  | 2.2  |
| 4   | B     | 529  | GLU  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | B     | 644  | GLU  | 2.2  |
| 4   | B     | 816  | GLU  | 2.2  |
| 6   | E     | 7    | ARG  | 2.2  |
| 6   | E     | 203  | GLU  | 2.2  |
| 4   | B     | 1127 | GLY  | 2.2  |
| 3   | A     | 148  | CYS  | 2.2  |
| 3   | A     | 116  | ASP  | 2.2  |
| 4   | B     | 307  | ASP  | 2.2  |
| 6   | E     | 115  | ASN  | 2.2  |
| 3   | A     | 316  | GLN  | 2.2  |
| 3   | A     | 1011 | GLN  | 2.2  |
| 3   | A     | 929  | LEU  | 2.2  |
| 3   | A     | 1118 | VAL  | 2.2  |
| 4   | B     | 183  | GLU  | 2.2  |
| 8   | H     | 114  | VAL  | 2.2  |
| 4   | B     | 534  | GLY  | 2.2  |
| 3   | A     | 50   | ILE  | 2.2  |
| 3   | A     | 1322 | ILE  | 2.2  |
| 4   | B     | 213  | ILE  | 2.2  |
| 3   | A     | 790  | ASP  | 2.2  |
| 4   | B     | 1174 | LYS  | 2.2  |
| 7   | F     | 140  | ASP  | 2.2  |
| 12  | L     | 44   | ASP  | 2.2  |
| 2   | T     | 11   | DC   | 2.2  |
| 9   | I     | 56   | ALA  | 2.2  |
| 3   | A     | 74   | MET  | 2.2  |
| 3   | A     | 1123 | GLY  | 2.2  |
| 3   | A     | 1417 | GLU  | 2.2  |
| 6   | E     | 116  | ILE  | 2.2  |
| 3   | A     | 1080 | THR  | 2.2  |
| 3   | A     | 1225 | PHE  | 2.2  |
| 3   | A     | 895  | LYS  | 2.2  |
| 4   | B     | 663  | ALA  | 2.2  |
| 3   | A     | 731  | ARG  | 2.2  |
| 6   | E     | 192  | ARG  | 2.2  |
| 3   | A     | 1119 | TYR  | 2.2  |
| 8   | H     | 116  | TYR  | 2.2  |
| 4   | B     | 908  | GLU  | 2.2  |
| 7   | F     | 149  | GLU  | 2.2  |
| 4   | B     | 655  | LYS  | 2.2  |
| 3   | A     | 141  | LEU  | 2.2  |
| 3   | A     | 1281 | ARG  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 8   | H     | 80   | ARG  | 2.1  |
| 10  | J     | 28   | ASP  | 2.1  |
| 3   | A     | 3    | GLY  | 2.1  |
| 3   | A     | 264  | PHE  | 2.1  |
| 6   | E     | 117  | THR  | 2.1  |
| 4   | B     | 432  | MET  | 2.1  |
| 6   | E     | 180  | ARG  | 2.1  |
| 3   | A     | 1008 | GLN  | 2.1  |
| 12  | L     | 66   | GLN  | 2.1  |
| 3   | A     | 1206 | ASP  | 2.1  |
| 8   | H     | 92   | ASP  | 2.1  |
| 3   | A     | 233  | TRP  | 2.1  |
| 4   | B     | 1171 | VAL  | 2.1  |
| 3   | A     | 1388 | GLY  | 2.1  |
| 3   | A     | 232  | GLU  | 2.1  |
| 3   | A     | 309  | ALA  | 2.1  |
| 4   | B     | 786  | ASN  | 2.1  |
| 3   | A     | 768  | GLN  | 2.1  |
| 3   | A     | 1130 | GLN  | 2.1  |
| 3   | A     | 98   | LYS  | 2.1  |
| 6   | E     | 111  | VAL  | 2.1  |
| 9   | I     | 61   | ASP  | 2.1  |
| 4   | B     | 1075 | GLY  | 2.1  |
| 3   | A     | 161  | LEU  | 2.1  |
| 6   | E     | 40   | GLU  | 2.1  |
| 3   | A     | 145  | LYS  | 2.1  |
| 3   | A     | 1300 | LYS  | 2.1  |
| 4   | B     | 309  | GLN  | 2.1  |
| 3   | A     | 81   | PHE  | 2.1  |
| 9   | I     | 35   | VAL  | 2.1  |
| 9   | I     | 43   | VAL  | 2.1  |
| 3   | A     | 1387 | HIS  | 2.1  |
| 3   | A     | 939  | ASP  | 2.1  |
| 3   | A     | 888  | GLY  | 2.1  |
| 3   | A     | 245  | PRO  | 2.1  |
| 3   | A     | 1156 | PRO  | 2.1  |
| 3   | A     | 105  | CYS  | 2.1  |
| 4   | B     | 523  | CYS  | 2.1  |
| 12  | L     | 61   | THR  | 2.1  |
| 4   | B     | 1017 | ILE  | 2.1  |
| 4   | B     | 105  | SER  | 2.1  |
| 4   | B     | 886  | LYS  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | F     | 104  | ASN  | 2.1  |
| 5   | C     | 97   | VAL  | 2.1  |
| 4   | B     | 413  | LEU  | 2.1  |
| 3   | A     | 771  | GLU  | 2.1  |
| 3   | A     | 1307 | GLU  | 2.1  |
| 5   | C     | 40   | GLU  | 2.1  |
| 8   | H     | 100  | THR  | 2.1  |
| 4   | B     | 884  | ARG  | 2.1  |
| 6   | E     | 152  | LYS  | 2.1  |
| 3   | A     | 272  | ALA  | 2.1  |
| 3   | A     | 1389 | PHE  | 2.1  |
| 7   | F     | 78   | GLN  | 2.1  |
| 3   | A     | 53   | LEU  | 2.1  |
| 6   | E     | 184  | VAL  | 2.1  |
| 4   | B     | 1111 | MET  | 2.1  |
| 4   | B     | 733  | HIS  | 2.0  |
| 4   | B     | 698  | GLU  | 2.0  |
| 4   | B     | 989  | THR  | 2.0  |
| 8   | H     | 110  | ASP  | 2.0  |
| 3   | A     | 104  | GLU  | 2.0  |
| 3   | A     | 265  | LYS  | 2.0  |
| 4   | B     | 472  | ALA  | 2.0  |
| 4   | B     | 713  | ALA  | 2.0  |
| 4   | B     | 283  | VAL  | 2.0  |
| 5   | C     | 224  | GLN  | 2.0  |
| 3   | A     | 1390 | ASN  | 2.0  |
| 3   | A     | 286  | HIS  | 2.0  |
| 3   | A     | 706  | HIS  | 2.0  |
| 4   | B     | 113  | TYR  | 2.0  |
| 4   | B     | 918  | ILE  | 2.0  |
| 4   | B     | 1124 | ARG  | 2.0  |
| 4   | B     | 939  | THR  | 2.0  |
| 3   | A     | 1198 | ASP  | 2.0  |
| 4   | B     | 356  | LEU  | 2.0  |
| 4   | B     | 509  | ALA  | 2.0  |
| 4   | B     | 853  | SER  | 2.0  |
| 3   | A     | 1393 | ASN  | 2.0  |
| 4   | B     | 784  | ASN  | 2.0  |
| 3   | A     | 101  | LYS  | 2.0  |
| 11  | K     | 55   | LYS  | 2.0  |
| 3   | A     | 1329 | THR  | 2.0  |
| 4   | B     | 110  | HIS  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | C     | 53   | THR  | 2.0  |
| 3   | A     | 39   | GLU  | 2.0  |
| 4   | B     | 1004 | GLU  | 2.0  |
| 4   | B     | 629  | ASP  | 2.0  |
| 4   | B     | 819  | ALA  | 2.0  |
| 4   | B     | 895  | ASP  | 2.0  |
| 4   | B     | 900  | ALA  | 2.0  |
| 4   | B     | 933  | SER  | 2.0  |
| 3   | A     | 345  | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 13  | ZN   | A     | 1734 | 1/1   | 0.91 | 0.28 | 22,22,22,22                 | 0     |
| 13  | ZN   | B     | 1307 | 1/1   | 0.93 | 0.18 | 22,22,22,22                 | 0     |
| 14  | MG   | A     | 2000 | 1/1   | 0.93 | 0.10 | 22,22,22,22                 | 0     |
| 13  | ZN   | I     | 204  | 1/1   | 0.94 | 0.18 | 22,22,22,22                 | 0     |
| 13  | ZN   | I     | 203  | 1/1   | 0.94 | 0.23 | 22,22,22,22                 | 0     |
| 13  | ZN   | A     | 1735 | 1/1   | 0.96 | 0.15 | 22,22,22,22                 | 0     |
| 13  | ZN   | L     | 105  | 1/1   | 0.99 | 0.07 | 22,22,22,22                 | 0     |
| 13  | ZN   | J     | 101  | 1/1   | 0.99 | 0.04 | 22,22,22,22                 | 0     |
| 13  | ZN   | C     | 319  | 1/1   | 1.00 | 0.02 | 22,22,22,22                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.