

Dataset S1

COMPND ?

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|------|----|-----|-----|---|--------|---------|-------|------|------|
| ATOM | 1 | N | LYS | 1 | -3.184 | -20.450 | 7.531 | 1.00 | 0.00 |
| ATOM | 2 | CA | LYS | 1 | -1.939 | -19.919 | 7.013 | 1.00 | 0.00 |
| ATOM | 3 | C | LYS | 1 | -2.031 | -18.557 | 6.359 | 1.00 | 0.00 |
| ATOM | 4 | O | LYS | 1 | -1.244 | -17.662 | 6.666 | 1.00 | 0.00 |
| ATOM | 5 | CB | LYS | 1 | -1.373 | -20.967 | 6.008 | 1.00 | 0.00 |
| ATOM | 6 | CG | LYS | 1 | -0.884 | -22.284 | 6.678 | 1.00 | 0.00 |
| ATOM | 7 | CD | LYS | 1 | -0.285 | -23.324 | 5.722 | 1.00 | 0.00 |
| ATOM | 8 | CE | LYS | 1 | 0.154 | -24.568 | 6.520 | 1.00 | 0.00 |
| ATOM | 9 | NZ | LYS | 1 | 0.734 | -25.572 | 5.585 | 1.00 | 0.00 |
| ATOM | 10 | N | LEU | 2 | -2.989 | -18.391 | 5.456 | 1.00 | 0.00 |
| ATOM | 11 | CA | LEU | 2 | -3.139 | -17.120 | 4.769 | 1.00 | 0.00 |
| ATOM | 12 | C | LEU | 2 | -3.324 | -15.953 | 5.723 | 1.00 | 0.00 |
| ATOM | 13 | O | LEU | 2 | -2.708 | -14.901 | 5.543 | 1.00 | 0.00 |
| ATOM | 14 | CB | LEU | 2 | -4.306 | -17.173 | 3.786 | 1.00 | 0.00 |
| ATOM | 15 | CG | LEU | 2 | -4.113 | -18.153 | 2.629 | 1.00 | 0.00 |
| ATOM | 16 | CD1 | LEU | 2 | -5.371 | -18.192 | 1.777 | 1.00 | 0.00 |
| ATOM | 17 | CD2 | LEU | 2 | -2.920 | -17.728 | 1.802 | 1.00 | 0.00 |
| ATOM | 18 | N | ASP | 3 | -4.161 | -16.133 | 6.739 | 1.00 | 0.00 |
| ATOM | 19 | CA | ASP | 3 | -4.398 | -15.064 | 7.704 | 1.00 | 0.00 |
| ATOM | 20 | C | ASP | 3 | -3.089 | -14.594 | 8.333 | 1.00 | 0.00 |
| ATOM | 21 | O | ASP | 3 | -2.888 | -13.399 | 8.563 | 1.00 | 0.00 |

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|------|----|-----|-----|---|--------|---------|--------|------|------|
| ATOM | 22 | CB | ASP | 3 | -5.395 | -15.550 | 8.793 | 1.00 | 0.00 |
| ATOM | 23 | CG | ASP | 3 | -6.834 | -15.789 | 8.312 | 1.00 | 0.00 |
| ATOM | 24 | OD1 | ASP | 3 | -7.253 | -15.167 | 7.314 | 1.00 | 0.00 |
| ATOM | 25 | OD2 | ASP | 3 | -7.559 | -16.570 | 8.963 | 1.00 | 0.00 |
| ATOM | 26 | N | ARG | 4 | -2.205 | -15.544 | 8.612 | 1.00 | 0.00 |
| ATOM | 27 | CA | ARG | 4 | -0.915 | -15.228 | 9.201 | 1.00 | 0.00 |
| ATOM | 28 | C | ARG | 4 | -0.106 | -14.418 | 8.190 | 1.00 | 0.00 |
| ATOM | 29 | O | ARG | 4 | 0.471 | -13.382 | 8.526 | 1.00 | 0.00 |
| ATOM | 30 | CB | ARG | 4 | -0.180 | -16.541 | 9.595 | 1.00 | 0.00 |
| ATOM | 31 | CG | ARG | 4 | -0.688 | -17.226 | 10.895 | 1.00 | 0.00 |
| ATOM | 32 | CD | ARG | 4 | -2.203 | -17.489 | 10.858 | 1.00 | 0.00 |
| ATOM | 33 | NE | ARG | 4 | -2.630 | -18.146 | 12.128 | 1.00 | 0.00 |
| ATOM | 34 | CZ | ARG | 4 | -3.875 | -18.510 | 12.423 | 1.00 | 0.00 |
| ATOM | 35 | NH1 | ARG | 4 | -4.887 | -18.338 | 11.620 | 1.00 | 0.00 |
| ATOM | 36 | NH2 | ARG | 4 | -4.095 | -19.066 | 13.572 | 1.00 | 0.00 |
| ATOM | 37 | N | TYR | 5 | -0.082 | -14.896 | 6.950 | 1.00 | 0.00 |
| ATOM | 38 | CA | TYR | 5 | 0.644 | -14.224 | 5.881 | 1.00 | 0.00 |
| ATOM | 39 | C | TYR | 5 | 0.123 | -12.805 | 5.689 | 1.00 | 0.00 |
| ATOM | 40 | O | TYR | 5 | 0.885 | -11.883 | 5.391 | 1.00 | 0.00 |
| ATOM | 41 | CB | TYR | 5 | 0.479 | -14.984 | 4.533 | 1.00 | 0.00 |
| ATOM | 42 | CG | TYR | 5 | 1.125 | -16.371 | 4.441 | 1.00 | 0.00 |
| ATOM | 43 | CD1 | TYR | 5 | 1.842 | -16.898 | 5.520 | 1.00 | 0.00 |
| ATOM | 44 | CD2 | TYR | 5 | 0.991 | -17.123 | 3.270 | 1.00 | 0.00 |
| ATOM | 45 | CE1 | TYR | 5 | 2.411 | -18.166 | 5.428 | 1.00 | 0.00 |
| ATOM | 46 | CE2 | TYR | 5 | 1.562 | -18.390 | 3.180 | 1.00 | 0.00 |

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|------|----|-----|-----|---|--------|---------|--------|------|------|
| ATOM | 47 | CZ | TYR | 5 | 2.271 | -18.909 | 4.260 | 1.00 | 0.00 |
| ATOM | 48 | OH | TYR | 5 | 2.829 | -20.154 | 4.176 | 1.00 | 0.00 |
| ATOM | 49 | N | SER | 6 | -1.180 | -12.634 | 5.866 | 1.00 | 0.00 |
| ATOM | 50 | CA | SER | 6 | -1.776 | -11.323 | 5.698 | 1.00 | 0.00 |
| ATOM | 51 | C | SER | 6 | -1.443 | -10.371 | 6.827 | 1.00 | 0.00 |
| ATOM | 52 | O | SER | 6 | -1.010 | -9.242 | 6.590 | 1.00 | 0.00 |
| ATOM | 53 | CB | SER | 6 | -3.307 | -11.466 | 5.507 | 1.00 | 0.00 |
| ATOM | 54 | OG | SER | 6 | -3.955 | -10.217 | 5.245 | 1.00 | 0.00 |
| ATOM | 55 | N | GLU | 7 | -1.648 | -10.827 | 8.059 | 1.00 | 0.00 |
| ATOM | 56 | CA | GLU | 7 | -1.373 | -10.001 | 9.228 | 1.00 | 0.00 |
| ATOM | 57 | C | GLU | 7 | 0.079 | -9.549 | 9.268 | 1.00 | 0.00 |
| ATOM | 58 | O | GLU | 7 | 0.383 | -8.446 | 9.730 | 1.00 | 0.00 |
| ATOM | 59 | CB | GLU | 7 | -1.737 | -10.770 | 10.529 | 1.00 | 0.00 |
| ATOM | 60 | CG | GLU | 7 | -3.263 | -11.005 | 10.774 | 1.00 | 0.00 |
| ATOM | 61 | CD | GLU | 7 | -3.690 | -11.693 | 12.058 | 1.00 | 0.00 |
| ATOM | 62 | OE1 | GLU | 7 | -2.854 | -12.248 | 12.796 | 1.00 | 0.00 |
| ATOM | 63 | OE2 | GLU | 7 | -4.908 | -11.654 | 12.331 | 1.00 | 0.00 |
| ATOM | 64 | N | TYR | 8 | 0.972 | -10.405 | 8.778 | 1.00 | 0.00 |
| ATOM | 65 | CA | TYR | 8 | 2.394 | -10.084 | 8.751 | 1.00 | 0.00 |
| ATOM | 66 | C | TYR | 8 | 2.674 | -9.002 | 7.712 | 1.00 | 0.00 |
| ATOM | 67 | O | TYR | 8 | 3.498 | -8.110 | 7.934 | 1.00 | 0.00 |
| ATOM | 68 | CB | TYR | 8 | 3.263 | -11.327 | 8.397 | 1.00 | 0.00 |
| ATOM | 69 | CG | TYR | 8 | 3.283 | -12.467 | 9.422 | 1.00 | 0.00 |
| ATOM | 70 | CD1 | TYR | 8 | 2.439 | -13.572 | 9.277 | 1.00 | 0.00 |
| ATOM | 71 | CD2 | TYR | 8 | 4.160 | -12.407 | 10.510 | 1.00 | 0.00 |

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|------|----|---------|----|--------|---------|--------|------|------|
| ATOM | 72 | CE1 TYR | 8 | 2.479 | -14.608 | 10.207 | 1.00 | 0.00 |
| ATOM | 73 | CE2 TYR | 8 | 4.197 | -13.443 | 11.438 | 1.00 | 0.00 |
| ATOM | 74 | CZ TYR | 8 | 3.357 | -14.542 | 11.286 | 1.00 | 0.00 |
| ATOM | 75 | OH TYR | 8 | 3.394 | -15.562 | 12.194 | 1.00 | 0.00 |
| ATOM | 76 | N GLY | 9 | 2.140 | -9.104 | 6.463 | 1.00 | 0.00 |
| ATOM | 77 | CA GLY | 9 | 2.268 | -8.045 | 5.421 | 1.00 | 0.00 |
| ATOM | 78 | C GLY | 9 | 1.593 | -6.677 | 5.687 | 1.00 | 0.00 |
| ATOM | 79 | O GLY | 9 | 2.135 | -5.652 | 5.276 | 1.00 | 0.00 |
| ATOM | 80 | N ALA | 10 | 0.451 | -6.649 | 6.393 | 1.00 | 0.00 |
| ATOM | 81 | CA ALA | 10 | -0.052 | -5.422 | 7.065 | 1.00 | 0.00 |
| ATOM | 82 | C ALA | 10 | 0.868 | -4.857 | 8.205 | 1.00 | 0.00 |
| ATOM | 83 | O ALA | 10 | 1.196 | -3.667 | 8.176 | 1.00 | 0.00 |
| ATOM | 84 | CB ALA | 10 | -1.479 | -5.747 | 7.549 | 1.00 | 0.00 |
| ATOM | 85 | N ALA | 11 | 1.317 | -5.685 | 9.173 | 1.00 | 0.00 |
| ATOM | 86 | CA ALA | 11 | 2.263 | -5.258 | 10.239 | 1.00 | 0.00 |
| ATOM | 87 | C ALA | 11 | 3.691 | -4.821 | 9.768 | 1.00 | 0.00 |
| ATOM | 88 | O ALA | 11 | 4.116 | -3.721 | 10.130 | 1.00 | 0.00 |
| ATOM | 89 | CB ALA | 11 | 2.297 | -6.382 | 11.288 | 1.00 | 0.00 |
| ATOM | 90 | N VAL | 12 | 4.413 | -5.615 | 8.945 | 1.00 | 0.00 |
| ATOM | 91 | CA VAL | 12 | 5.659 | -5.134 | 8.256 | 1.00 | 0.00 |
| ATOM | 92 | C VAL | 12 | 5.419 | -4.577 | 6.804 | 1.00 | 0.00 |
| ATOM | 93 | O VAL | 12 | 6.274 | -4.720 | 5.922 | 1.00 | 0.00 |
| ATOM | 94 | CB VAL | 12 | 6.855 | -6.146 | 8.360 | 1.00 | 0.00 |
| ATOM | 95 | CG1 VAL | 12 | 7.250 | -6.525 | 9.803 | 1.00 | 0.00 |
| ATOM | 96 | CG2 VAL | 12 | 6.751 | -7.412 | 7.482 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|--------|-------|------|------|
| ATOM | 97 | N | LEU | 13 | 4.335 | -3.805 | 6.577 | 1.00 | 0.00 |
| ATOM | 98 | CA | LEU | 13 | 4.154 | -2.992 | 5.334 | 1.00 | 0.00 |
| ATOM | 99 | C | LEU | 13 | 5.302 | -1.965 | 5.025 | 1.00 | 0.00 |
| ATOM | 100 | O | LEU | 13 | 5.637 | -1.750 | 3.860 | 1.00 | 0.00 |
| ATOM | 101 | CB | LEU | 13 | 2.747 | -2.332 | 5.406 | 1.00 | 0.00 |
| ATOM | 102 | CG | LEU | 13 | 2.227 | -1.635 | 4.119 | 1.00 | 0.00 |
| ATOM | 103 | CD1 | LEU | 13 | 1.974 | -2.628 | 2.969 | 1.00 | 0.00 |
| ATOM | 104 | CD2 | LEU | 13 | 0.928 | -0.871 | 4.424 | 1.00 | 0.00 |
| ATOM | 105 | N | PHE | 14 | 5.949 | -1.400 | 6.062 | 1.00 | 0.00 |
| ATOM | 106 | CA | PHE | 14 | 7.104 | -0.513 | 5.956 | 1.00 | 0.00 |
| ATOM | 107 | C | PHE | 14 | 8.353 | -1.303 | 5.572 | 1.00 | 0.00 |
| ATOM | 108 | O | PHE | 14 | 9.229 | -0.791 | 4.878 | 1.00 | 0.00 |
| ATOM | 109 | CB | PHE | 14 | 7.366 | 0.218 | 7.307 | 1.00 | 0.00 |
| ATOM | 110 | CG | PHE | 14 | 6.293 | 1.219 | 7.762 | 1.00 | 0.00 |
| ATOM | 111 | CD1 | PHE | 14 | 5.282 | 0.800 | 8.635 | 1.00 | 0.00 |
| ATOM | 112 | CD2 | PHE | 14 | 6.277 | 2.525 | 7.268 | 1.00 | 0.00 |
| ATOM | 113 | CE1 | PHE | 14 | 4.258 | 1.670 | 8.993 | 1.00 | 0.00 |
| ATOM | 114 | CE2 | PHE | 14 | 5.257 | 3.399 | 7.636 | 1.00 | 0.00 |
| ATOM | 115 | CZ | PHE | 14 | 4.247 | 2.971 | 8.496 | 1.00 | 0.00 |
| ATOM | 116 | N | LEU | 15 | 8.561 | -2.590 | 5.939 | 1.00 | 0.00 |
| ATOM | 117 | CA | LEU | 15 | 9.681 | -3.424 | 5.390 | 1.00 | 0.00 |
| ATOM | 118 | C | LEU | 15 | 9.416 | -4.011 | 3.953 | 1.00 | 0.00 |
| ATOM | 119 | O | LEU | 15 | 10.352 | -4.100 | 3.150 | 1.00 | 0.00 |
| ATOM | 120 | CB | LEU | 15 | 10.119 | -4.481 | 6.437 | 1.00 | 0.00 |
| ATOM | 121 | CG | LEU | 15 | 10.734 | -4.012 | 7.794 | 1.00 | 0.00 |

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| ATOM | 122 | CD1 | LEU | 15 | 12.023 | -3.190 | 7.606 | 1.00 | 0.00 |
| ATOM | 123 | CD2 | LEU | 15 | 9.787 | -3.273 | 8.757 | 1.00 | 0.00 |
| ATOM | 124 | N | LEU | 16 | 8.157 | -4.314 | 3.572 | 1.00 | 0.00 |
| ATOM | 125 | CA | LEU | 16 | 7.728 | -4.349 | 2.137 | 1.00 | 0.00 |
| ATOM | 126 | C | LEU | 16 | 7.957 | -3.014 | 1.332 | 1.00 | 0.00 |
| ATOM | 127 | O | LEU | 16 | 8.422 | -3.067 | 0.192 | 1.00 | 0.00 |
| ATOM | 128 | CB | LEU | 16 | 6.247 | -4.816 | 2.035 | 1.00 | 0.00 |
| ATOM | 129 | CG | LEU | 16 | 5.892 | -6.238 | 2.551 | 1.00 | 0.00 |
| ATOM | 130 | CD1 | LEU | 16 | 4.368 | -6.445 | 2.519 | 1.00 | 0.00 |
| ATOM | 131 | CD2 | LEU | 16 | 6.574 | -7.356 | 1.740 | 1.00 | 0.00 |
| ATOM | 132 | N | MET | 17 | 7.711 | -1.824 | 1.915 | 1.00 | 0.00 |
| ATOM | 133 | CA | MET | 17 | 8.108 | -0.511 | 1.323 | 1.00 | 0.00 |
| ATOM | 134 | C | MET | 17 | 9.634 | -0.344 | 0.998 | 1.00 | 0.00 |
| ATOM | 135 | O | MET | 17 | 9.946 | 0.117 | -0.096 | 1.00 | 0.00 |
| ATOM | 136 | CB | MET | 17 | 7.557 | 0.609 | 2.244 | 1.00 | 0.00 |
| ATOM | 137 | CG | MET | 17 | 7.482 | 2.015 | 1.617 | 1.00 | 0.00 |
| ATOM | 138 | SD | MET | 17 | 7.018 | 3.243 | 2.863 | 1.00 | 0.00 |
| ATOM | 139 | CE | MET | 17 | 5.258 | 2.914 | 3.080 | 1.00 | 0.00 |
| ATOM | 140 | N | CYS | 18 | 10.574 | -0.756 | 1.872 | 1.00 | 0.00 |
| ATOM | 141 | CA | CYS | 18 | 12.022 | -0.906 | 1.513 | 1.00 | 0.00 |
| ATOM | 142 | C | CYS | 18 | 12.426 | -2.072 | 0.563 | 1.00 | 0.00 |
| ATOM | 143 | O | CYS | 18 | 13.458 | -1.960 | -0.104 | 1.00 | 0.00 |
| ATOM | 144 | CB | CYS | 18 | 12.752 | -1.002 | 2.872 | 1.00 | 0.00 |
| ATOM | 145 | SG | CYS | 18 | 14.566 | -0.996 | 2.654 | 1.00 | 0.00 |
| ATOM | 146 | N | THR | 19 | 11.604 | -3.132 | 0.416 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|--------|--------|------|------|
| ATOM | 147 | CA | THR | 19 | 11.632 | -3.994 | -0.809 | 1.00 | 0.00 |
| ATOM | 148 | C | THR | 19 | 11.413 | -3.138 | -2.107 | 1.00 | 0.00 |
| ATOM | 149 | O | THR | 19 | 12.308 | -3.080 | -2.948 | 1.00 | 0.00 |
| ATOM | 150 | CB | THR | 19 | 10.641 | -5.199 | -0.694 | 1.00 | 0.00 |
| ATOM | 151 | OG1 | THR | 19 | 10.675 | -5.796 | 0.599 | 1.00 | 0.00 |
| ATOM | 152 | CG2 | THR | 19 | 10.912 | -6.330 | -1.696 | 1.00 | 0.00 |
| ATOM | 153 | N | PHE | 20 | 10.300 | -2.383 | -2.200 | 1.00 | 0.00 |
| ATOM | 154 | CA | PHE | 20 | 10.068 | -1.392 | -3.291 | 1.00 | 0.00 |
| ATOM | 155 | C | PHE | 20 | 11.006 | -0.129 | -3.346 | 1.00 | 0.00 |
| ATOM | 156 | O | PHE | 20 | 11.181 | 0.391 | -4.444 | 1.00 | 0.00 |
| ATOM | 157 | CB | PHE | 20 | 8.560 | -1.001 | -3.309 | 1.00 | 0.00 |
| ATOM | 158 | CG | PHE | 20 | 7.573 | -2.152 | -3.612 | 1.00 | 0.00 |
| ATOM | 159 | CD1 | PHE | 20 | 6.763 | -2.674 | -2.598 | 1.00 | 0.00 |
| ATOM | 160 | CD2 | PHE | 20 | 7.526 | -2.727 | -4.889 | 1.00 | 0.00 |
| ATOM | 161 | CE1 | PHE | 20 | 5.936 | -3.767 | -2.849 | 1.00 | 0.00 |
| ATOM | 162 | CE2 | PHE | 20 | 6.698 | -3.819 | -5.139 | 1.00 | 0.00 |
| ATOM | 163 | CZ | PHE | 20 | 5.905 | -4.339 | -4.118 | 1.00 | 0.00 |
| ATOM | 164 | N | ALA | 21 | 11.612 | 0.370 | -2.247 | 1.00 | 0.00 |
| ATOM | 165 | CA | ALA | 21 | 12.552 | 1.533 | -2.274 | 1.00 | 0.00 |
| ATOM | 166 | C | ALA | 21 | 14.052 | 1.199 | -2.580 | 1.00 | 0.00 |
| ATOM | 167 | O | ALA | 21 | 14.670 | 1.902 | -3.386 | 1.00 | 0.00 |
| ATOM | 168 | CB | ALA | 21 | 12.391 | 2.330 | -0.967 | 1.00 | 0.00 |
| ATOM | 169 | N | LEU | 22 | 14.637 | 0.111 | -2.027 | 1.00 | 0.00 |
| ATOM | 170 | CA | LEU | 22 | 15.859 | -0.524 | -2.619 | 1.00 | 0.00 |
| ATOM | 171 | C | LEU | 22 | 15.614 | -1.009 | -4.094 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|--------|--------|------|------|
| ATOM | 172 | O | LEU | 22 | 16.452 | -0.690 | -4.929 | 1.00 | 0.00 |
| ATOM | 173 | CB | LEU | 22 | 16.365 | -1.687 | -1.717 | 1.00 | 0.00 |
| ATOM | 174 | CG | LEU | 22 | 16.866 | -1.335 | -0.291 | 1.00 | 0.00 |
| ATOM | 175 | CD1 | LEU | 22 | 17.119 | -2.624 | 0.512 | 1.00 | 0.00 |
| ATOM | 176 | CD2 | LEU | 22 | 18.152 | -0.488 | -0.301 | 1.00 | 0.00 |
| ATOM | 177 | N | ILE | 23 | 14.477 | -1.657 | -4.462 | 1.00 | 0.00 |
| ATOM | 178 | CA | ILE | 23 | 14.064 | -1.836 | -5.900 | 1.00 | 0.00 |
| ATOM | 179 | C | ILE | 23 | 13.822 | -0.489 | -6.684 | 1.00 | 0.00 |
| ATOM | 180 | O | ILE | 23 | 14.142 | -0.470 | -7.864 | 1.00 | 0.00 |
| ATOM | 181 | CB | ILE | 23 | 12.915 | -2.904 | -6.072 | 1.00 | 0.00 |
| ATOM | 182 | CG1 | ILE | 23 | 13.339 | -4.333 | -5.610 | 1.00 | 0.00 |
| ATOM | 183 | CG2 | ILE | 23 | 12.366 | -3.022 | -7.522 | 1.00 | 0.00 |
| ATOM | 184 | CD1 | ILE | 23 | 12.183 | -5.319 | -5.356 | 1.00 | 0.00 |
| ATOM | 185 | N | ALA | 24 | 13.352 | 0.644 | -6.122 | 1.00 | 0.00 |
| ATOM | 186 | CA | ALA | 24 | 13.402 | 1.971 | -6.817 | 1.00 | 0.00 |
| ATOM | 187 | C | ALA | 24 | 14.824 | 2.490 | -7.237 | 1.00 | 0.00 |
| ATOM | 188 | O | ALA | 24 | 14.969 | 3.101 | -8.299 | 1.00 | 0.00 |
| ATOM | 189 | CB | ALA | 24 | 12.649 | 3.003 | -5.959 | 1.00 | 0.00 |
| ATOM | 190 | N | HIS | 25 | 15.870 | 2.205 | -6.443 | 1.00 | 0.00 |
| ATOM | 191 | CA | HIS | 25 | 17.293 | 2.301 | -6.888 | 1.00 | 0.00 |
| ATOM | 192 | C | HIS | 25 | 17.933 | 1.022 | -7.552 | 1.00 | 0.00 |
| ATOM | 193 | O | HIS | 25 | 19.024 | 1.137 | -8.119 | 1.00 | 0.00 |
| ATOM | 194 | CB | HIS | 25 | 18.037 | 2.715 | -5.580 | 1.00 | 0.00 |
| ATOM | 195 | CG | HIS | 25 | 19.509 | 3.094 | -5.732 | 1.00 | 0.00 |
| ATOM | 196 | ND1 | HIS | 25 | 20.544 | 2.210 | -5.490 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|--------|---------|------|------|
| ATOM | 197 | CD2 | HIS | 25 | 20.020 | 4.318 | -6.202 | 1.00 | 0.00 |
| ATOM | 198 | CE1 | HIS | 25 | 21.621 | 2.964 | -5.872 | 1.00 | 0.00 |
| ATOM | 199 | NE2 | HIS | 25 | 21.407 | 4.252 | -6.299 | 1.00 | 0.00 |
| ATOM | 200 | N | TRP | 26 | 17.244 | -0.119 | -7.540 | 1.00 | 0.00 |
| ATOM | 201 | CA | TRP | 26 | 17.695 | -1.370 | -8.194 | 1.00 | 0.00 |
| ATOM | 202 | C | TRP | 26 | 16.487 | -2.053 | -8.911 | 1.00 | 0.00 |
| ATOM | 203 | O | TRP | 26 | 16.178 | -3.201 | -8.614 | 1.00 | 0.00 |
| ATOM | 204 | CB | TRP | 26 | 18.330 | -2.316 | -7.134 | 1.00 | 0.00 |
| ATOM | 205 | CG | TRP | 26 | 19.381 | -1.806 | -6.120 | 1.00 | 0.00 |
| ATOM | 206 | CD1 | TRP | 26 | 19.293 | -1.938 | -4.784 | 1.00 | 0.00 |
| ATOM | 207 | CD2 | TRP | 26 | 20.654 | -1.323 | -6.364 | 1.00 | 0.00 |
| ATOM | 208 | NE1 | TRP | 26 | 20.433 | -1.560 | -4.195 | 1.00 | 0.00 |
| ATOM | 209 | CE2 | TRP | 26 | 21.291 | -1.149 | -5.137 | 1.00 | 0.00 |
| ATOM | 210 | CE3 | TRP | 26 | 21.351 | -1.047 | -7.531 | 1.00 | 0.00 |
| ATOM | 211 | CZ2 | TRP | 26 | 22.587 | -0.677 | -5.071 | 1.00 | 0.00 |
| ATOM | 212 | CZ3 | TRP | 26 | 22.671 | -0.623 | -7.476 | 1.00 | 0.00 |
| ATOM | 213 | CH2 | TRP | 26 | 23.290 | -0.426 | -6.245 | 1.00 | 0.00 |
| ATOM | 214 | N | LEU | 27 | 15.787 | -1.510 | -9.923 | 1.00 | 0.00 |
| ATOM | 215 | CA | LEU | 27 | 15.954 | -0.336 | -10.822 | 1.00 | 0.00 |
| ATOM | 216 | C | LEU | 27 | 17.097 | 0.683 | -10.660 | 1.00 | 0.00 |
| ATOM | 217 | O | LEU | 27 | 18.223 | 0.203 | -10.727 | 1.00 | 0.00 |
| ATOM | 218 | CB | LEU | 27 | 14.629 | 0.197 | -11.416 | 1.00 | 0.00 |
| ATOM | 219 | CG | LEU | 27 | 13.654 | 1.013 | -10.560 | 1.00 | 0.00 |
| ATOM | 220 | CD1 | LEU | 27 | 13.391 | 2.348 | -11.261 | 1.00 | 0.00 |
| ATOM | 221 | CD2 | LEU | 27 | 12.319 | 0.280 | -10.386 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|--------|---------|------|------|
| ATOM | 222 | N | ALA | 28 | 16.859 | 1.998 | -10.500 | 1.00 | 0.00 |
| ATOM | 223 | CA | ALA | 28 | 17.784 | 3.126 | -10.835 | 1.00 | 0.00 |
| ATOM | 224 | C | ALA | 28 | 19.198 | 3.016 | -11.458 | 1.00 | 0.00 |
| ATOM | 225 | O | ALA | 28 | 19.469 | 3.697 | -12.442 | 1.00 | 0.00 |
| ATOM | 226 | CB | ALA | 28 | 17.887 | 4.141 | -9.696 | 1.00 | 0.00 |
| ATOM | 227 | N | CYS | 29 | 20.025 | 2.085 | -11.002 | 1.00 | 0.00 |
| ATOM | 228 | CA | CYS | 29 | 21.488 | 2.183 | -11.154 | 1.00 | 0.00 |
| ATOM | 229 | C | CYS | 29 | 22.184 | 1.127 | -12.028 | 1.00 | 0.00 |
| ATOM | 230 | O | CYS | 29 | 23.095 | 1.463 | -12.784 | 1.00 | 0.00 |
| ATOM | 231 | CB | CYS | 29 | 22.064 | 2.207 | -9.738 | 1.00 | 0.00 |
| ATOM | 232 | SG | CYS | 29 | 23.866 | 2.497 | -9.679 | 1.00 | 0.00 |
| ATOM | 233 | N | ILE | 30 | 21.761 | -0.133 | -11.926 | 1.00 | 0.00 |
| ATOM | 234 | CA | ILE | 30 | 22.308 | -1.220 | -12.773 | 1.00 | 0.00 |
| ATOM | 235 | C | ILE | 30 | 21.846 | -1.094 | -14.245 | 1.00 | 0.00 |
| ATOM | 236 | O | ILE | 30 | 22.713 | -1.008 | -15.113 | 1.00 | 0.00 |
| ATOM | 237 | CB | ILE | 30 | 22.067 | -2.612 | -12.148 | 1.00 | 0.00 |
| ATOM | 238 | CG1 | ILE | 30 | 22.765 | -2.775 | -10.778 | 1.00 | 0.00 |
| ATOM | 239 | CG2 | ILE | 30 | 22.409 | -3.773 | -13.101 | 1.00 | 0.00 |
| ATOM | 240 | CD1 | ILE | 30 | 24.303 | -2.726 | -10.747 | 1.00 | 0.00 |
| ATOM | 241 | N | TRP | 31 | 20.554 | -0.832 | -14.482 | 1.00 | 0.00 |
| ATOM | 242 | CA | TRP | 31 | 19.984 | -0.675 | -15.841 | 1.00 | 0.00 |
| ATOM | 243 | C | TRP | 31 | 20.561 | 0.516 | -16.637 | 1.00 | 0.00 |
| ATOM | 244 | O | TRP | 31 | 20.413 | 0.613 | -17.853 | 1.00 | 0.00 |
| ATOM | 245 | CB | TRP | 31 | 18.448 | -0.577 | -15.785 | 1.00 | 0.00 |
| ATOM | 246 | CG | TRP | 31 | 17.907 | 0.697 | -15.141 | 1.00 | 0.00 |

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|------|-----|---------|----|--------|-------|---------|------|------|
| ATOM | 247 | CD1 TRP | 31 | 17.681 | 0.883 | -13.840 | 1.00 | 0.00 |
| ATOM | 248 | CD2 TRP | 31 | 17.510 | 1.865 | -15.774 | 1.00 | 0.00 |
| ATOM | 249 | NE1 TRP | 31 | 17.177 | 2.108 | -13.641 | 1.00 | 0.00 |
| ATOM | 250 | CE2 TRP | 31 | 17.043 | 2.736 | -14.800 | 1.00 | 0.00 |
| ATOM | 251 | CE3 TRP | 31 | 17.518 | 2.272 | -17.084 | 1.00 | 0.00 |
| ATOM | 252 | CZ2 TRP | 31 | 16.571 | 4.001 | -15.113 | 1.00 | 0.00 |
| ATOM | 253 | CZ3 TRP | 31 | 17.039 | 3.547 | -17.384 | 1.00 | 0.00 |
| ATOM | 254 | CH2 TRP | 31 | 16.551 | 4.401 | -16.427 | 1.00 | 0.00 |
| ATOM | 255 | N TYR | 32 | 21.258 | 1.387 | -15.913 | 1.00 | 0.00 |
| ATOM | 256 | CA TYR | 32 | 21.921 | 2.579 | -16.465 | 1.00 | 0.00 |
| ATOM | 257 | C TYR | 32 | 23.430 | 2.361 | -16.649 | 1.00 | 0.00 |
| ATOM | 258 | O TYR | 32 | 23.993 | 2.688 | -17.693 | 1.00 | 0.00 |
| ATOM | 259 | CB TYR | 32 | 21.657 | 3.764 | -15.527 | 1.00 | 0.00 |
| ATOM | 260 | CG TYR | 32 | 22.310 | 5.055 | -16.024 | 1.00 | 0.00 |
| ATOM | 261 | CD1 TYR | 32 | 21.760 | 5.737 | -17.101 | 1.00 | 0.00 |
| ATOM | 262 | CD2 TYR | 32 | 23.415 | 5.579 | -15.363 | 1.00 | 0.00 |
| ATOM | 263 | CE1 TYR | 32 | 22.310 | 6.943 | -17.517 | 1.00 | 0.00 |
| ATOM | 264 | CE2 TYR | 32 | 23.962 | 6.790 | -15.771 | 1.00 | 0.00 |
| ATOM | 265 | CZ TYR | 32 | 23.407 | 7.466 | -16.848 | 1.00 | 0.00 |
| ATOM | 266 | OH TYR | 32 | 23.960 | 8.626 | -17.290 | 1.00 | 0.00 |
| ATOM | 267 | N ALA | 33 | 24.047 | 1.695 | -15.682 | 1.00 | 0.00 |
| ATOM | 268 | CA ALA | 33 | 25.487 | 1.424 | -15.697 | 1.00 | 0.00 |
| ATOM | 269 | C ALA | 33 | 25.906 | 0.421 | -16.790 | 1.00 | 0.00 |
| ATOM | 270 | O ALA | 33 | 26.947 | 0.585 | -17.427 | 1.00 | 0.00 |
| ATOM | 271 | CB ALA | 33 | 25.774 | 0.947 | -14.285 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|--------|---------|------|------|
| ATOM | 272 | N | ILE | 34 | 24.978 | -0.470 | -17.145 | 1.00 | 0.00 |
| ATOM | 273 | CA | ILE | 34 | 25.215 | -1.439 | -18.213 | 1.00 | 0.00 |
| ATOM | 274 | C | ILE | 34 | 24.765 | -0.858 | -19.546 | 1.00 | 0.00 |
| ATOM | 275 | O | ILE | 34 | 25.330 | -1.172 | -20.591 | 1.00 | 0.00 |
| ATOM | 276 | CB | ILE | 34 | 24.472 | -2.796 | -17.881 | 1.00 | 0.00 |
| ATOM | 277 | CG1 | ILE | 34 | 22.918 | -2.677 | -17.769 | 1.00 | 0.00 |
| ATOM | 278 | CG2 | ILE | 34 | 25.001 | -3.473 | -16.578 | 1.00 | 0.00 |
| ATOM | 279 | CD1 | ILE | 34 | 22.134 | -4.004 | -17.835 | 1.00 | 0.00 |
| ATOM | 280 | N | GLY | 35 | 23.734 | -0.022 | -19.500 | 1.00 | 0.00 |
| ATOM | 281 | CA | GLY | 35 | 23.203 | 0.619 | -20.699 | 1.00 | 0.00 |
| ATOM | 282 | C | GLY | 35 | 24.275 | 1.452 | -21.412 | 1.00 | 0.00 |
| ATOM | 283 | O | GLY | 35 | 24.311 | 1.494 | -22.642 | 1.00 | 0.00 |
| ATOM | 284 | N | ASN | 36 | 25.146 | 2.099 | -20.635 | 1.00 | 0.00 |
| ATOM | 285 | CA | ASN | 36 | 26.224 | 2.935 | -21.171 | 1.00 | 0.00 |
| ATOM | 286 | C | ASN | 36 | 27.429 | 2.128 | -21.654 | 1.00 | 0.00 |
| ATOM | 287 | O | ASN | 36 | 28.205 | 2.603 | -22.479 | 1.00 | 0.00 |
| ATOM | 288 | CB | ASN | 36 | 26.652 | 3.975 | -20.094 | 1.00 | 0.00 |
| ATOM | 289 | CG | ASN | 36 | 25.716 | 5.168 | -19.870 | 1.00 | 0.00 |
| ATOM | 290 | OD1 | ASN | 36 | 25.515 | 6.009 | -20.734 | 1.00 | 0.00 |
| ATOM | 291 | ND2 | ASN | 36 | 25.134 | 5.301 | -18.709 | 1.00 | 0.00 |
| ATOM | 292 | N | MET | 37 | 27.592 | 0.914 | -21.136 | 1.00 | 0.00 |
| ATOM | 293 | CA | MET | 37 | 28.715 | 0.062 | -21.522 | 1.00 | 0.00 |
| ATOM | 294 | C | MET | 37 | 28.307 | -1.052 | -22.493 | 1.00 | 0.00 |
| ATOM | 295 | O | MET | 37 | 29.144 | -1.569 | -23.230 | 1.00 | 0.00 |
| ATOM | 296 | CB | MET | 37 | 29.380 | -0.529 | -20.248 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|--------|---------|------|------|
| ATOM | 297 | CG | MET | 37 | 30.316 | 0.424 | -19.474 | 1.00 | 0.00 |
| ATOM | 298 | SD | MET | 37 | 31.113 | -0.466 | -18.127 | 1.00 | 0.00 |
| ATOM | 299 | CE | MET | 37 | 32.093 | 0.885 | -17.459 | 1.00 | 0.00 |
| ATOM | 300 | N | GLU | 38 | 27.027 | -1.420 | -22.489 | 1.00 | 0.00 |
| ATOM | 301 | CA | GLU | 38 | 26.513 | -2.468 | -23.376 | 1.00 | 0.00 |
| ATOM | 302 | C | GLU | 38 | 26.215 | -1.919 | -24.773 | 1.00 | 0.00 |
| ATOM | 303 | O | GLU | 38 | 26.382 | -2.626 | -25.773 | 1.00 | 0.00 |
| ATOM | 304 | CB | GLU | 38 | 25.234 | -3.103 | -22.759 | 1.00 | 0.00 |
| ATOM | 305 | CG | GLU | 38 | 24.658 | -4.343 | -23.516 | 1.00 | 0.00 |
| ATOM | 306 | CD | GLU | 38 | 25.436 | -5.646 | -23.463 | 1.00 | 0.00 |
| ATOM | 307 | OE1 | GLU | 38 | 26.355 | -5.810 | -22.637 | 1.00 | 0.00 |
| ATOM | 308 | OE2 | GLU | 38 | 25.093 | -6.532 | -24.272 | 1.00 | 0.00 |
| ATOM | 309 | N | GLN | 39 | 25.767 | -0.662 | -24.830 | 1.00 | 0.00 |
| ATOM | 310 | CA | GLN | 39 | 25.448 | 0.011 | -26.094 | 1.00 | 0.00 |
| ATOM | 311 | C | GLN | 39 | 26.738 | 0.307 | -26.873 | 1.00 | 0.00 |
| ATOM | 312 | O | GLN | 39 | 27.823 | -0.091 | -26.447 | 1.00 | 0.00 |
| ATOM | 313 | CB | GLN | 39 | 24.663 | 1.310 | -25.808 | 1.00 | 0.00 |
| ATOM | 314 | CG | GLN | 39 | 23.231 | 1.134 | -25.204 | 1.00 | 0.00 |
| ATOM | 315 | CD | GLN | 39 | 22.378 | 2.379 | -24.926 | 1.00 | 0.00 |
| ATOM | 316 | OE1 | GLN | 39 | 22.068 | 3.144 | -25.825 | 1.00 | 0.00 |
| ATOM | 317 | NE2 | GLN | 39 | 21.993 | 2.648 | -23.705 | 1.00 | 0.00 |
| ATOM | 318 | N | PRO | 40 | 26.625 | 1.002 | -28.005 | 1.00 | 0.00 |
| ATOM | 319 | CA | PRO | 40 | 27.798 | 1.321 | -28.830 | 1.00 | 0.00 |
| ATOM | 320 | C | PRO | 40 | 28.589 | 0.049 | -29.188 | 1.00 | 0.00 |
| ATOM | 321 | O | PRO | 40 | 29.808 | 0.095 | -29.410 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|--------|---------|------|------|
| ATOM | 322 | CB | PRO | 40 | 28.649 | 2.373 | -28.102 | 1.00 | 0.00 |
| ATOM | 323 | CG | PRO | 40 | 28.466 | 2.022 | -26.617 | 1.00 | 0.00 |
| ATOM | 324 | CD | PRO | 40 | 26.999 | 1.595 | -26.533 | 1.00 | 0.00 |
| ATOM | 325 | N | HIS | 41 | 27.880 | -1.080 | -29.235 | 1.00 | 0.00 |
| ATOM | 326 | CA | HIS | 41 | 28.466 | -2.380 | -29.572 | 1.00 | 0.00 |
| ATOM | 327 | C | HIS | 41 | 27.428 | -3.254 | -30.290 | 1.00 | 0.00 |
| ATOM | 328 | O | HIS | 41 | 26.305 | -3.425 | -29.804 | 1.00 | 0.00 |
| ATOM | 329 | CB | HIS | 41 | 29.006 | -3.055 | -28.269 | 1.00 | 0.00 |
| ATOM | 330 | CG | HIS | 41 | 30.238 | -2.427 | -27.619 | 1.00 | 0.00 |
| ATOM | 331 | ND1 | HIS | 41 | 30.235 | -1.517 | -26.572 | 1.00 | 0.00 |
| ATOM | 332 | CD2 | HIS | 41 | 31.564 | -2.695 | -28.008 | 1.00 | 0.00 |
| ATOM | 333 | CE1 | HIS | 41 | 31.573 | -1.301 | -26.396 | 1.00 | 0.00 |
| ATOM | 334 | NE2 | HIS | 41 | 32.449 | -1.963 | -27.219 | 1.00 | 0.00 |
| ATOM | 335 | N | MET | 42 | 27.808 | -3.793 | -31.448 | 1.00 | 0.00 |
| ATOM | 336 | CA | MET | 42 | 26.920 | -4.644 | -32.237 | 1.00 | 0.00 |
| ATOM | 337 | C | MET | 42 | 26.646 | -5.962 | -31.516 | 1.00 | 0.00 |
| ATOM | 338 | O | MET | 42 | 27.379 | -6.347 | -30.599 | 1.00 | 0.00 |
| ATOM | 339 | CB | MET | 42 | 27.548 | -4.897 | -33.636 | 1.00 | 0.00 |
| ATOM | 340 | CG | MET | 42 | 27.711 | -3.654 | -34.536 | 1.00 | 0.00 |
| ATOM | 341 | SD | MET | 42 | 26.092 | -3.054 | -35.046 | 1.00 | 0.00 |
| ATOM | 342 | CE | MET | 42 | 25.721 | -4.305 | -36.282 | 1.00 | 0.00 |
| ATOM | 343 | N | PRO | 43 | 25.583 | -6.645 | -31.937 | 1.00 | 0.00 |
| ATOM | 344 | CA | PRO | 43 | 25.180 | -7.926 | -31.354 | 1.00 | 0.00 |
| ATOM | 345 | C | PRO | 43 | 24.722 | -7.826 | -29.886 | 1.00 | 0.00 |
| ATOM | 346 | O | PRO | 43 | 24.409 | -8.843 | -29.258 | 1.00 | 0.00 |

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| ATOM | 347 | CB | PRO | 43 | 26.323 | -8.931 | -31.559 | 1.00 | 0.00 |
| ATOM | 348 | CG | PRO | 43 | 27.590 | -8.081 | -31.378 | 1.00 | 0.00 |
| ATOM | 349 | CD | PRO | 43 | 27.215 | -6.747 | -32.028 | 1.00 | 0.00 |
| ATOM | 350 | N | SER | 44 | 24.675 | -6.607 | -29.348 | 1.00 | 0.00 |
| ATOM | 351 | CA | SER | 44 | 24.248 | -6.386 | -27.962 | 1.00 | 0.00 |
| ATOM | 352 | C | SER | 44 | 22.731 | -6.190 | -27.865 | 1.00 | 0.00 |
| ATOM | 353 | O | SER | 44 | 22.173 | -5.291 | -28.500 | 1.00 | 0.00 |
| ATOM | 354 | CB | SER | 44 | 25.018 | -5.174 | -27.381 | 1.00 | 0.00 |
| ATOM | 355 | OG | SER | 44 | 26.409 | -5.444 | -27.175 | 1.00 | 0.00 |
| ATOM | 356 | N | ILE | 45 | 22.075 | -7.032 | -27.066 | 1.00 | 0.00 |
| ATOM | 357 | CA | ILE | 45 | 20.621 | -6.968 | -26.885 | 1.00 | 0.00 |
| ATOM | 358 | C | ILE | 45 | 20.239 | -6.022 | -25.749 | 1.00 | 0.00 |
| ATOM | 359 | O | ILE | 45 | 19.270 | -6.264 | -25.023 | 1.00 | 0.00 |
| ATOM | 360 | CB | ILE | 45 | 20.063 | -8.430 | -26.646 | 1.00 | 0.00 |
| ATOM | 361 | CG1 | ILE | 45 | 18.510 | -8.562 | -26.764 | 1.00 | 0.00 |
| ATOM | 362 | CG2 | ILE | 45 | 20.497 | -9.026 | -25.271 | 1.00 | 0.00 |
| ATOM | 363 | CD1 | ILE | 45 | 17.963 | -10.000 | -26.873 | 1.00 | 0.00 |
| ATOM | 364 | N | LYS | 46 | 21.004 | -4.940 | -25.614 | 1.00 | 0.00 |
| ATOM | 365 | CA | LYS | 46 | 20.772 | -3.942 | -24.574 | 1.00 | 0.00 |
| ATOM | 366 | C | LYS | 46 | 20.697 | -2.500 | -25.110 | 1.00 | 0.00 |
| ATOM | 367 | O | LYS | 46 | 21.324 | -1.589 | -24.550 | 1.00 | 0.00 |
| ATOM | 368 | CB | LYS | 46 | 21.888 | -4.064 | -23.494 | 1.00 | 0.00 |
| ATOM | 369 | CG | LYS | 46 | 21.976 | -5.471 | -22.834 | 1.00 | 0.00 |
| ATOM | 370 | CD | LYS | 46 | 20.870 | -5.790 | -21.818 | 1.00 | 0.00 |
| ATOM | 371 | CE | LYS | 46 | 21.085 | -7.206 | -21.249 | 1.00 | 0.00 |

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| ATOM | 372 | NZ | LYS | 46 | 20.007 | -7.507 | -20.265 | 1.00 | 0.00 |
| ATOM | 373 | N | ASP | 47 | 19.934 | -2.274 | -26.201 | 1.00 | 0.00 |
| ATOM | 374 | CA | ASP | 47 | 19.823 | -0.917 | -26.754 | 1.00 | 0.00 |
| ATOM | 375 | C | ASP | 47 | 19.125 | 0.056 | -25.797 | 1.00 | 0.00 |
| ATOM | 376 | O | ASP | 47 | 19.772 | 0.897 | -25.174 | 1.00 | 0.00 |
| ATOM | 377 | CB | ASP | 47 | 18.990 | -1.113 | -28.052 | 1.00 | 0.00 |
| ATOM | 378 | CG | ASP | 47 | 18.931 | 0.103 | -28.988 | 1.00 | 0.00 |
| ATOM | 379 | OD1 | ASP | 47 | 19.593 | 1.122 | -28.704 | 1.00 | 0.00 |
| ATOM | 380 | OD2 | ASP | 47 | 18.184 | 0.051 | -29.988 | 1.00 | 0.00 |
| ATOM | 381 | N | LYS | 48 | 17.807 | -0.082 | -25.678 | 1.00 | 0.00 |
| ATOM | 382 | CA | LYS | 48 | 17.000 | 0.781 | -24.813 | 1.00 | 0.00 |
| ATOM | 383 | C | LYS | 48 | 17.213 | 0.518 | -23.321 | 1.00 | 0.00 |
| ATOM | 384 | O | LYS | 48 | 17.852 | -0.463 | -22.932 | 1.00 | 0.00 |
| ATOM | 385 | CB | LYS | 48 | 15.496 | 0.621 | -25.185 | 1.00 | 0.00 |
| ATOM | 386 | CG | LYS | 48 | 14.918 | 1.810 | -26.006 | 1.00 | 0.00 |
| ATOM | 387 | CD | LYS | 48 | 15.349 | 1.862 | -27.479 | 1.00 | 0.00 |
| ATOM | 388 | CE | LYS | 48 | 14.705 | 3.084 | -28.163 | 1.00 | 0.00 |
| ATOM | 389 | NZ | LYS | 48 | 15.128 | 3.126 | -29.591 | 1.00 | 0.00 |
| ATOM | 390 | N | TYR | 49 | 16.667 | 1.405 | -22.489 | 1.00 | 0.00 |
| ATOM | 391 | CA | TYR | 49 | 16.777 | 1.283 | -21.036 | 1.00 | 0.00 |
| ATOM | 392 | C | TYR | 49 | 15.635 | 0.447 | -20.457 | 1.00 | 0.00 |
| ATOM | 393 | O | TYR | 49 | 15.855 | -0.370 | -19.566 | 1.00 | 0.00 |
| ATOM | 394 | CB | TYR | 49 | 16.764 | 2.669 | -20.327 | 1.00 | 0.00 |
| ATOM | 395 | CG | TYR | 49 | 17.965 | 3.586 | -20.589 | 1.00 | 0.00 |
| ATOM | 396 | CD1 | TYR | 49 | 17.901 | 4.583 | -21.567 | 1.00 | 0.00 |

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| ATOM | 397 | CD2 | TYR | 49 | 19.134 | 3.431 | -19.837 | 1.00 | 0.00 |
| ATOM | 398 | CE1 | TYR | 49 | 18.994 | 5.420 | -21.783 | 1.00 | 0.00 |
| ATOM | 399 | CE2 | TYR | 49 | 20.224 | 4.268 | -20.056 | 1.00 | 0.00 |
| ATOM | 400 | CZ | TYR | 49 | 20.153 | 5.261 | -21.029 | 1.00 | 0.00 |
| ATOM | 401 | OH | TYR | 49 | 21.221 | 6.086 | -21.243 | 1.00 | 0.00 |
| ATOM | 402 | N | VAL | 50 | 14.396 | 0.652 | -20.946 | 1.00 | 0.00 |
| ATOM | 403 | CA | VAL | 50 | 13.251 | -0.113 | -20.439 | 1.00 | 0.00 |
| ATOM | 404 | C | VAL | 50 | 13.506 | -1.617 | -20.432 | 1.00 | 0.00 |
| ATOM | 405 | O | VAL | 50 | 13.007 | -2.338 | -19.564 | 1.00 | 0.00 |
| ATOM | 406 | CB | VAL | 50 | 12.085 | 0.254 | -21.441 | 1.00 | 0.00 |
| ATOM | 407 | CG1 | VAL | 50 | 10.752 | -0.526 | -21.263 | 1.00 | 0.00 |
| ATOM | 408 | CG2 | VAL | 50 | 11.688 | 1.750 | -21.420 | 1.00 | 0.00 |
| ATOM | 409 | N | THR | 51 | 14.284 | -2.081 | -21.407 | 1.00 | 0.00 |
| ATOM | 410 | CA | THR | 51 | 14.623 | -3.497 | -21.513 | 1.00 | 0.00 |
| ATOM | 411 | C | THR | 51 | 15.750 | -3.840 | -20.534 | 1.00 | 0.00 |
| ATOM | 412 | O | THR | 51 | 15.893 | -4.991 | -20.108 | 1.00 | 0.00 |
| ATOM | 413 | CB | THR | 51 | 15.043 | -3.839 | -22.982 | 1.00 | 0.00 |
| ATOM | 414 | OG1 | THR | 51 | 14.071 | -3.360 | -23.902 | 1.00 | 0.00 |
| ATOM | 415 | CG2 | THR | 51 | 15.190 | -5.338 | -23.321 | 1.00 | 0.00 |
| ATOM | 416 | N | ALA | 52 | 16.727 | -2.969 | -20.187 | 1.00 | 0.00 |
| ATOM | 417 | CA | ALA | 52 | 17.689 | -3.223 | -19.073 | 1.00 | 0.00 |
| ATOM | 418 | C | ALA | 52 | 17.080 | -3.413 | -17.627 | 1.00 | 0.00 |
| ATOM | 419 | O | ALA | 52 | 17.697 | -4.087 | -16.795 | 1.00 | 0.00 |
| ATOM | 420 | CB | ALA | 52 | 18.744 | -2.111 | -19.196 | 1.00 | 0.00 |
| ATOM | 421 | N | LEU | 53 | 15.846 | -2.926 | -17.359 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|--------|---------|------|------|
| ATOM | 422 | CA | LEU | 53 | 14.989 | -3.378 | -16.216 | 1.00 | 0.00 |
| ATOM | 423 | C | LEU | 53 | 14.795 | -4.925 | -16.030 | 1.00 | 0.00 |
| ATOM | 424 | O | LEU | 53 | 14.836 | -5.383 | -14.887 | 1.00 | 0.00 |
| ATOM | 425 | CB | LEU | 53 | 13.621 | -2.644 | -16.353 | 1.00 | 0.00 |
| ATOM | 426 | CG | LEU | 53 | 12.573 | -2.817 | -15.219 | 1.00 | 0.00 |
| ATOM | 427 | CD1 | LEU | 53 | 13.045 | -2.223 | -13.885 | 1.00 | 0.00 |
| ATOM | 428 | CD2 | LEU | 53 | 11.238 | -2.166 | -15.623 | 1.00 | 0.00 |
| ATOM | 429 | N | TYR | 54 | 14.625 | -5.730 | -17.106 | 1.00 | 0.00 |
| ATOM | 430 | CA | TYR | 54 | 14.684 | -7.227 | -17.023 | 1.00 | 0.00 |
| ATOM | 431 | C | TYR | 54 | 15.950 | -7.850 | -16.330 | 1.00 | 0.00 |
| ATOM | 432 | O | TYR | 54 | 15.826 | -8.882 | -15.664 | 1.00 | 0.00 |
| ATOM | 433 | CB | TYR | 54 | 14.503 | -7.842 | -18.448 | 1.00 | 0.00 |
| ATOM | 434 | CG | TYR | 54 | 13.063 | -8.148 | -18.898 | 1.00 | 0.00 |
| ATOM | 435 | CD1 | TYR | 54 | 12.324 | -7.200 | -19.613 | 1.00 | 0.00 |
| ATOM | 436 | CD2 | TYR | 54 | 12.522 | -9.424 | -18.689 | 1.00 | 0.00 |
| ATOM | 437 | CE1 | TYR | 54 | 11.070 | -7.530 | -20.128 | 1.00 | 0.00 |
| ATOM | 438 | CE2 | TYR | 54 | 11.274 | -9.755 | -19.216 | 1.00 | 0.00 |
| ATOM | 439 | CZ | TYR | 54 | 10.553 | -8.810 | -19.941 | 1.00 | 0.00 |
| ATOM | 440 | OH | TYR | 54 | 9.314 | -9.120 | -20.441 | 1.00 | 0.00 |
| ATOM | 441 | N | PHE | 55 | 17.142 | -7.245 | -16.493 | 1.00 | 0.00 |
| ATOM | 442 | CA | PHE | 55 | 18.393 | -7.720 | -15.841 | 1.00 | 0.00 |
| ATOM | 443 | C | PHE | 55 | 18.552 | -7.330 | -14.339 | 1.00 | 0.00 |
| ATOM | 444 | O | PHE | 55 | 18.808 | -8.221 | -13.523 | 1.00 | 0.00 |
| ATOM | 445 | CB | PHE | 55 | 19.586 | -7.280 | -16.726 | 1.00 | 0.00 |
| ATOM | 446 | CG | PHE | 55 | 20.819 | -8.183 | -16.602 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|---------|---------|------|------|
| ATOM | 447 | CD1 | PHE | 55 | 20.780 | -9.494 | -17.094 | 1.00 | 0.00 |
| ATOM | 448 | CD2 | PHE | 55 | 21.975 | -7.722 | -15.968 | 1.00 | 0.00 |
| ATOM | 449 | CE1 | PHE | 55 | 21.879 | -10.333 | -16.949 | 1.00 | 0.00 |
| ATOM | 450 | CE2 | PHE | 55 | 23.071 | -8.566 | -15.818 | 1.00 | 0.00 |
| ATOM | 451 | CZ | PHE | 55 | 23.020 | -9.871 | -16.304 | 1.00 | 0.00 |
| ATOM | 452 | N | THR | 56 | 18.297 | -6.063 | -13.938 | 1.00 | 0.00 |
| ATOM | 453 | CA | THR | 56 | 17.985 | -5.727 | -12.504 | 1.00 | 0.00 |
| ATOM | 454 | C | THR | 56 | 16.541 | -6.156 | -12.034 | 1.00 | 0.00 |
| ATOM | 455 | O | THR | 56 | 15.737 | -5.386 | -11.502 | 1.00 | 0.00 |
| ATOM | 456 | CB | THR | 56 | 18.369 | -4.251 | -12.211 | 1.00 | 0.00 |
| ATOM | 457 | OG1 | THR | 56 | 18.263 | -3.998 | -10.815 | 1.00 | 0.00 |
| ATOM | 458 | CG2 | THR | 56 | 17.552 | -3.170 | -12.929 | 1.00 | 0.00 |
| ATOM | 459 | N | PHE | 57 | 16.294 | -7.455 | -12.212 | 1.00 | 0.00 |
| ATOM | 460 | CA | PHE | 57 | 15.039 | -8.175 | -11.915 | 1.00 | 0.00 |
| ATOM | 461 | C | PHE | 57 | 15.514 | -9.665 | -11.887 | 1.00 | 0.00 |
| ATOM | 462 | O | PHE | 57 | 15.887 | -10.161 | -10.822 | 1.00 | 0.00 |
| ATOM | 463 | CB | PHE | 57 | 13.895 | -7.774 | -12.906 | 1.00 | 0.00 |
| ATOM | 464 | CG | PHE | 57 | 12.666 | -8.699 | -12.963 | 1.00 | 0.00 |
| ATOM | 465 | CD1 | PHE | 57 | 11.889 | -8.914 | -11.822 | 1.00 | 0.00 |
| ATOM | 466 | CD2 | PHE | 57 | 12.360 | -9.391 | -14.142 | 1.00 | 0.00 |
| ATOM | 467 | CE1 | PHE | 57 | 10.856 | -9.846 | -11.844 | 1.00 | 0.00 |
| ATOM | 468 | CE2 | PHE | 57 | 11.302 | -10.297 | -14.170 | 1.00 | 0.00 |
| ATOM | 469 | CZ | PHE | 57 | 10.561 | -10.536 | -13.017 | 1.00 | 0.00 |
| ATOM | 470 | N | SER | 58 | 15.594 | -10.348 | -13.046 | 1.00 | 0.00 |
| ATOM | 471 | CA | SER | 58 | 15.985 | -11.781 | -13.140 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|---------|---------|------|------|
| ATOM | 472 | C | SER | 58 | 17.427 | -12.174 | -12.666 | 1.00 | 0.00 |
| ATOM | 473 | O | SER | 58 | 17.579 | -13.209 | -12.007 | 1.00 | 0.00 |
| ATOM | 474 | CB | SER | 58 | 15.694 | -12.185 | -14.603 | 1.00 | 0.00 |
| ATOM | 475 | OG | SER | 58 | 15.811 | -13.592 | -14.781 | 1.00 | 0.00 |
| ATOM | 476 | N | SER | 59 | 18.464 | -11.367 | -12.971 | 1.00 | 0.00 |
| ATOM | 477 | CA | SER | 59 | 19.847 | -11.590 | -12.451 | 1.00 | 0.00 |
| ATOM | 478 | C | SER | 59 | 20.230 | -10.905 | -11.088 | 1.00 | 0.00 |
| ATOM | 479 | O | SER | 59 | 21.425 | -10.854 | -10.769 | 1.00 | 0.00 |
| ATOM | 480 | CB | SER | 59 | 20.814 | -11.179 | -13.588 | 1.00 | 0.00 |
| ATOM | 481 | OG | SER | 59 | 22.166 | -11.459 | -13.222 | 1.00 | 0.00 |
| ATOM | 482 | N | LEU | 60 | 19.275 | -10.448 | -10.253 | 1.00 | 0.00 |
| ATOM | 483 | CA | LEU | 60 | 19.569 | -9.916 | -8.888 | 1.00 | 0.00 |
| ATOM | 484 | C | LEU | 60 | 20.098 | -11.004 | -7.892 | 1.00 | 0.00 |
| ATOM | 485 | O | LEU | 60 | 21.232 | -10.882 | -7.425 | 1.00 | 0.00 |
| ATOM | 486 | CB | LEU | 60 | 18.329 | -9.122 | -8.373 | 1.00 | 0.00 |
| ATOM | 487 | CG | LEU | 60 | 18.178 | -7.667 | -8.893 | 1.00 | 0.00 |
| ATOM | 488 | CD1 | LEU | 60 | 16.754 | -7.146 | -8.653 | 1.00 | 0.00 |
| ATOM | 489 | CD2 | LEU | 60 | 19.145 | -6.676 | -8.221 | 1.00 | 0.00 |
| ATOM | 490 | N | THR | 61 | 19.343 | -12.081 | -7.608 | 1.00 | 0.00 |
| ATOM | 491 | CA | THR | 61 | 19.867 | -13.261 | -6.835 | 1.00 | 0.00 |
| ATOM | 492 | C | THR | 61 | 20.563 | -14.382 | -7.696 | 1.00 | 0.00 |
| ATOM | 493 | O | THR | 61 | 20.602 | -15.545 | -7.285 | 1.00 | 0.00 |
| ATOM | 494 | CB | THR | 61 | 18.742 | -13.853 | -5.924 | 1.00 | 0.00 |
| ATOM | 495 | OG1 | THR | 61 | 17.612 | -14.274 | -6.683 | 1.00 | 0.00 |
| ATOM | 496 | CG2 | THR | 61 | 18.238 | -12.922 | -4.818 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|---------|---------|------|------|
| ATOM | 497 | N | SER | 62 | 21.140 | -14.060 | -8.877 | 1.00 | 0.00 |
| ATOM | 498 | CA | SER | 62 | 21.749 | -15.057 | -9.817 | 1.00 | 0.00 |
| ATOM | 499 | C | SER | 62 | 20.864 | -16.256 | -10.335 | 1.00 | 0.00 |
| ATOM | 500 | O | SER | 62 | 21.419 | -17.266 | -10.783 | 1.00 | 0.00 |
| ATOM | 501 | CB | SER | 62 | 23.131 | -15.499 | -9.265 | 1.00 | 0.00 |
| ATOM | 502 | OG | SER | 62 | 23.819 | -16.307 | -10.220 | 1.00 | 0.00 |
| ATOM | 503 | N | VAL | 63 | 19.521 | -16.136 | -10.344 | 1.00 | 0.00 |
| ATOM | 504 | CA | VAL | 63 | 18.601 | -17.226 | -10.805 | 1.00 | 0.00 |
| ATOM | 505 | C | VAL | 63 | 18.473 | -17.215 | -12.368 | 1.00 | 0.00 |
| ATOM | 506 | O | VAL | 63 | 18.886 | -18.185 | -13.007 | 1.00 | 0.00 |
| ATOM | 507 | CB | VAL | 63 | 17.241 | -17.202 | -10.015 | 1.00 | 0.00 |
| ATOM | 508 | CG1 | VAL | 63 | 16.263 | -18.318 | -10.455 | 1.00 | 0.00 |
| ATOM | 509 | CG2 | VAL | 63 | 17.403 | -17.346 | -8.481 | 1.00 | 0.00 |
| ATOM | 510 | N | GLY | 64 | 17.942 | -16.138 | -12.984 | 1.00 | 0.00 |
| ATOM | 511 | CA | GLY | 64 | 18.038 | -15.947 | -14.455 | 1.00 | 0.00 |
| ATOM | 512 | C | GLY | 64 | 16.955 | -16.613 | -15.339 | 1.00 | 0.00 |
| ATOM | 513 | O | GLY | 64 | 16.471 | -17.715 | -15.071 | 1.00 | 0.00 |
| ATOM | 514 | N | PHE | 65 | 16.645 | -15.949 | -16.460 | 1.00 | 0.00 |
| ATOM | 515 | CA | PHE | 65 | 15.959 | -16.588 | -17.626 | 1.00 | 0.00 |
| ATOM | 516 | C | PHE | 65 | 16.961 | -16.956 | -18.772 | 1.00 | 0.00 |
| ATOM | 517 | O | PHE | 65 | 16.941 | -18.089 | -19.251 | 1.00 | 0.00 |
| ATOM | 518 | CB | PHE | 65 | 14.807 | -15.690 | -18.172 | 1.00 | 0.00 |
| ATOM | 519 | CG | PHE | 65 | 13.623 | -15.385 | -17.240 | 1.00 | 0.00 |
| ATOM | 520 | CD1 | PHE | 65 | 13.340 | -14.061 | -16.884 | 1.00 | 0.00 |
| ATOM | 521 | CD2 | PHE | 65 | 12.793 | -16.412 | -16.777 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|---------|---------|------|------|
| ATOM | 522 | CE1 | PHE | 65 | 12.255 | -13.771 | -16.063 | 1.00 | 0.00 |
| ATOM | 523 | CE2 | PHE | 65 | 11.713 | -16.119 | -15.947 | 1.00 | 0.00 |
| ATOM | 524 | CZ | PHE | 65 | 11.442 | -14.800 | -15.594 | 1.00 | 0.00 |
| ATOM | 525 | N | GLY | 66 | 17.785 | -16.000 | -19.253 | 1.00 | 0.00 |
| ATOM | 526 | CA | GLY | 66 | 18.674 | -16.179 | -20.384 | 1.00 | 0.00 |
| ATOM | 527 | C | GLY | 66 | 18.174 | -15.455 | -21.622 | 1.00 | 0.00 |
| ATOM | 528 | O | GLY | 66 | 18.723 | -15.638 | -22.710 | 1.00 | 0.00 |
| ATOM | 529 | N | ASN | 67 | 17.129 | -14.641 | -21.463 | 1.00 | 0.00 |
| ATOM | 530 | CA | ASN | 67 | 16.581 | -13.879 | -22.582 | 1.00 | 0.00 |
| ATOM | 531 | C | ASN | 67 | 17.411 | -12.608 | -22.812 | 1.00 | 0.00 |
| ATOM | 532 | O | ASN | 67 | 17.265 | -11.943 | -23.837 | 1.00 | 0.00 |
| ATOM | 533 | CB | ASN | 67 | 15.086 | -13.524 | -22.335 | 1.00 | 0.00 |
| ATOM | 534 | CG | ASN | 67 | 14.766 | -12.698 | -21.085 | 1.00 | 0.00 |
| ATOM | 535 | OD1 | ASN | 67 | 15.431 | -12.778 | -20.063 | 1.00 | 0.00 |
| ATOM | 536 | ND2 | ASN | 67 | 13.733 | -11.899 | -21.106 | 1.00 | 0.00 |
| ATOM | 537 | N | VAL | 68 | 18.293 | -12.290 | -21.861 | 1.00 | 0.00 |
| ATOM | 538 | CA | VAL | 68 | 19.181 | -11.126 | -21.950 | 1.00 | 0.00 |
| ATOM | 539 | C | VAL | 68 | 20.450 | -11.333 | -21.110 | 1.00 | 0.00 |
| ATOM | 540 | O | VAL | 68 | 20.359 | -11.634 | -19.917 | 1.00 | 0.00 |
| ATOM | 541 | CB | VAL | 68 | 18.407 | -9.827 | -21.489 | 1.00 | 0.00 |
| ATOM | 542 | CG1 | VAL | 68 | 17.187 | -9.408 | -22.355 | 1.00 | 0.00 |
| ATOM | 543 | CG2 | VAL | 68 | 17.873 | -9.897 | -20.038 | 1.00 | 0.00 |
| ATOM | 544 | N | SER | 69 | 21.624 | -11.175 | -21.736 | 1.00 | 0.00 |
| ATOM | 545 | CA | SER | 69 | 22.929 | -11.342 | -21.070 | 1.00 | 0.00 |
| ATOM | 546 | C | SER | 69 | 24.027 | -10.434 | -21.666 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|---------|---------|------|------|
| ATOM | 547 | O | SER | 69 | 24.088 | -10.257 | -22.879 | 1.00 | 0.00 |
| ATOM | 548 | CB | SER | 69 | 23.331 | -12.837 | -21.130 | 1.00 | 0.00 |
| ATOM | 549 | OG | SER | 69 | 24.548 | -13.115 | -20.429 | 1.00 | 0.00 |
| ATOM | 550 | N | PRO | 70 | 24.876 | -9.810 | -20.812 | 1.00 | 0.00 |
| ATOM | 551 | CA | PRO | 70 | 25.969 | -8.932 | -21.255 | 1.00 | 0.00 |
| ATOM | 552 | C | PRO | 70 | 26.990 | -9.600 | -22.148 | 1.00 | 0.00 |
| ATOM | 553 | O | PRO | 70 | 27.439 | -10.710 | -21.865 | 1.00 | 0.00 |
| ATOM | 554 | CB | PRO | 70 | 26.621 | -8.504 | -19.949 | 1.00 | 0.00 |
| ATOM | 555 | CG | PRO | 70 | 25.470 | -8.282 | -19.099 | 1.00 | 0.00 |
| ATOM | 556 | CD | PRO | 70 | 24.506 | -9.442 | -19.432 | 1.00 | 0.00 |
| ATOM | 557 | N | ASN | 71 | 27.382 | -8.915 | -23.213 | 1.00 | 0.00 |
| ATOM | 558 | CA | ASN | 71 | 28.381 | -9.475 | -24.098 | 1.00 | 0.00 |
| ATOM | 559 | C | ASN | 71 | 29.649 | -8.644 | -23.994 | 1.00 | 0.00 |
| ATOM | 560 | O | ASN | 71 | 30.752 | -9.156 | -24.182 | 1.00 | 0.00 |
| ATOM | 561 | CB | ASN | 71 | 27.864 | -9.510 | -25.566 | 1.00 | 0.00 |
| ATOM | 562 | CG | ASN | 71 | 26.719 | -10.481 | -25.875 | 1.00 | 0.00 |
| ATOM | 563 | OD1 | ASN | 71 | 26.639 | -11.582 | -25.351 | 1.00 | 0.00 |
| ATOM | 564 | ND2 | ASN | 71 | 25.813 | -10.127 | -26.746 | 1.00 | 0.00 |
| ATOM | 565 | N | THR | 72 | 29.485 | -7.366 | -23.669 | 1.00 | 0.00 |
| ATOM | 566 | CA | THR | 72 | 30.620 | -6.459 | -23.530 | 1.00 | 0.00 |
| ATOM | 567 | C | THR | 72 | 31.320 | -6.642 | -22.178 | 1.00 | 0.00 |
| ATOM | 568 | O | THR | 72 | 30.797 | -7.316 | -21.287 | 1.00 | 0.00 |
| ATOM | 569 | CB | THR | 72 | 30.166 | -4.981 | -23.679 | 1.00 | 0.00 |
| ATOM | 570 | OG1 | THR | 72 | 29.047 | -4.726 | -22.819 | 1.00 | 0.00 |
| ATOM | 571 | CG2 | THR | 72 | 29.759 | -4.696 | -25.120 | 1.00 | 0.00 |

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| ATOM | 572 | N | ASN | 73 | 32.506 | -6.052 | -22.032 | 1.00 | 0.00 |
| ATOM | 573 | CA | ASN | 73 | 33.266 | -6.149 | -20.784 | 1.00 | 0.00 |
| ATOM | 574 | C | ASN | 73 | 32.630 | -5.243 | -19.725 | 1.00 | 0.00 |
| ATOM | 575 | O | ASN | 73 | 32.586 | -5.589 | -18.542 | 1.00 | 0.00 |
| ATOM | 576 | CB | ASN | 73 | 34.754 | -5.760 | -21.020 | 1.00 | 0.00 |
| ATOM | 577 | CG | ASN | 73 | 35.594 | -6.715 | -21.875 | 1.00 | 0.00 |
| ATOM | 578 | OD1 | ASN | 73 | 35.456 | -7.928 | -21.824 | 1.00 | 0.00 |
| ATOM | 579 | ND2 | ASN | 73 | 36.503 | -6.215 | -22.668 | 1.00 | 0.00 |
| ATOM | 580 | N | SER | 74 | 32.128 | -4.089 | -20.163 | 1.00 | 0.00 |
| ATOM | 581 | CA | SER | 74 | 31.498 | -3.146 | -19.250 | 1.00 | 0.00 |
| ATOM | 582 | C | SER | 74 | 30.136 | -3.595 | -18.740 | 1.00 | 0.00 |
| ATOM | 583 | O | SER | 74 | 29.649 | -3.097 | -17.719 | 1.00 | 0.00 |
| ATOM | 584 | CB | SER | 74 | 31.421 | -1.755 | -19.929 | 1.00 | 0.00 |
| ATOM | 585 | OG | SER | 74 | 32.704 | -1.138 | -20.080 | 1.00 | 0.00 |
| ATOM | 586 | N | GLU | 75 | 29.516 | -4.533 | -19.454 | 1.00 | 0.00 |
| ATOM | 587 | CA | GLU | 75 | 28.218 | -5.039 | -19.045 | 1.00 | 0.00 |
| ATOM | 588 | C | GLU | 75 | 28.352 | -6.183 | -18.056 | 1.00 | 0.00 |
| ATOM | 589 | O | GLU | 75 | 27.421 | -6.475 | -17.299 | 1.00 | 0.00 |
| ATOM | 590 | CB | GLU | 75 | 27.444 | -5.504 | -20.311 | 1.00 | 0.00 |
| ATOM | 591 | CG | GLU | 75 | 25.960 | -5.937 | -20.079 | 1.00 | 0.00 |
| ATOM | 592 | CD | GLU | 75 | 24.940 | -4.864 | -19.743 | 1.00 | 0.00 |
| ATOM | 593 | OE1 | GLU | 75 | 25.204 | -3.656 | -19.905 | 1.00 | 0.00 |
| ATOM | 594 | OE2 | GLU | 75 | 23.835 | -5.260 | -19.319 | 1.00 | 0.00 |
| ATOM | 595 | N | LYS | 76 | 29.517 | -6.829 | -18.062 | 1.00 | 0.00 |
| ATOM | 596 | CA | LYS | 76 | 29.794 | -7.950 | -17.167 | 1.00 | 0.00 |

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| ATOM | 597 | C | LYS | 76 | 30.278 | -7.477 | -15.793 | 1.00 | 0.00 |
| ATOM | 598 | O | LYS | 76 | 29.960 | -8.091 | -14.770 | 1.00 | 0.00 |
| ATOM | 599 | CB | LYS | 76 | 30.845 | -8.899 | -17.817 | 1.00 | 0.00 |
| ATOM | 600 | CG | LYS | 76 | 30.314 | -9.671 | -19.060 | 1.00 | 0.00 |
| ATOM | 601 | CD | LYS | 76 | 31.312 | -10.645 | -19.703 | 1.00 | 0.00 |
| ATOM | 602 | CE | LYS | 76 | 30.653 | -11.334 | -20.915 | 1.00 | 0.00 |
| ATOM | 603 | NZ | LYS | 76 | 31.628 | -12.276 | -21.532 | 1.00 | 0.00 |
| ATOM | 604 | N | ILE | 77 | 31.050 | -6.391 | -15.778 | 1.00 | 0.00 |
| ATOM | 605 | CA | ILE | 77 | 31.564 | -5.818 | -14.531 | 1.00 | 0.00 |
| ATOM | 606 | C | ILE | 77 | 30.375 | -5.363 | -13.683 | 1.00 | 0.00 |
| ATOM | 607 | O | ILE | 77 | 30.338 | -5.585 | -12.469 | 1.00 | 0.00 |
| ATOM | 608 | CB | ILE | 77 | 32.487 | -4.585 | -14.796 | 1.00 | 0.00 |
| ATOM | 609 | CG1 | ILE | 77 | 33.699 | -5.001 | -15.636 | 1.00 | 0.00 |
| ATOM | 610 | CG2 | ILE | 77 | 32.955 | -3.980 | -13.475 | 1.00 | 0.00 |
| ATOM | 611 | CD1 | ILE | 77 | 34.511 | -3.824 | -16.175 | 1.00 | 0.00 |
| ATOM | 612 | N | PHE | 78 | 29.405 | -4.725 | -14.335 | 1.00 | 0.00 |
| ATOM | 613 | CA | PHE | 78 | 28.209 | -4.246 | -13.654 | 1.00 | 0.00 |
| ATOM | 614 | C | PHE | 78 | 27.261 | -5.428 | -13.424 | 1.00 | 0.00 |
| ATOM | 615 | O | PHE | 78 | 26.323 | -5.345 | -12.624 | 1.00 | 0.00 |
| ATOM | 616 | CB | PHE | 78 | 27.468 | -3.162 | -14.494 | 1.00 | 0.00 |
| ATOM | 617 | CG | PHE | 78 | 28.206 | -1.830 | -14.696 | 1.00 | 0.00 |
| ATOM | 618 | CD1 | PHE | 78 | 28.977 | -1.635 | -15.848 | 1.00 | 0.00 |
| ATOM | 619 | CD2 | PHE | 78 | 28.169 | -0.835 | -13.717 | 1.00 | 0.00 |
| ATOM | 620 | CE1 | PHE | 78 | 29.715 | -0.468 | -16.009 | 1.00 | 0.00 |
| ATOM | 621 | CE2 | PHE | 78 | 28.900 | 0.338 | -13.884 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|---------|---------|------|------|
| ATOM | 622 | CZ | PHE | 78 | 29.675 | 0.520 | -15.028 | 1.00 | 0.00 |
| ATOM | 623 | N | SER | 79 | 27.522 | -6.528 | -14.131 | 1.00 | 0.00 |
| ATOM | 624 | CA | SER | 79 | 26.713 | -7.727 | -13.988 | 1.00 | 0.00 |
| ATOM | 625 | C | SER | 79 | 27.076 | -8.465 | -12.710 | 1.00 | 0.00 |
| ATOM | 626 | O | SER | 79 | 26.213 | -9.027 | -12.031 | 1.00 | 0.00 |
| ATOM | 627 | CB | SER | 79 | 26.847 | -8.642 | -15.231 | 1.00 | 0.00 |
| ATOM | 628 | OG | SER | 79 | 25.997 | -9.792 | -15.170 | 1.00 | 0.00 |
| ATOM | 629 | N | ILE | 80 | 28.366 | -8.463 | -12.383 | 1.00 | 0.00 |
| ATOM | 630 | CA | ILE | 80 | 28.852 | -9.109 | -11.172 | 1.00 | 0.00 |
| ATOM | 631 | C | ILE | 80 | 28.370 | -8.310 | -9.961 | 1.00 | 0.00 |
| ATOM | 632 | O | ILE | 80 | 27.864 | -8.876 | -8.992 | 1.00 | 0.00 |
| ATOM | 633 | CB | ILE | 80 | 30.431 | -9.201 | -11.227 | 1.00 | 0.00 |
| ATOM | 634 | CG1 | ILE | 80 | 30.995 | -10.020 | -12.432 | 1.00 | 0.00 |
| ATOM | 635 | CG2 | ILE | 80 | 31.048 | -9.780 | -9.916 | 1.00 | 0.00 |
| ATOM | 636 | CD1 | ILE | 80 | 32.506 | -9.867 | -12.702 | 1.00 | 0.00 |
| ATOM | 637 | N | CYS | 81 | 28.527 | -6.991 | -10.025 | 1.00 | 0.00 |
| ATOM | 638 | CA | CYS | 81 | 28.088 | -6.121 | -8.938 | 1.00 | 0.00 |
| ATOM | 639 | C | CYS | 81 | 26.575 | -6.261 | -8.755 | 1.00 | 0.00 |
| ATOM | 640 | O | CYS | 81 | 26.058 | -6.149 | -7.643 | 1.00 | 0.00 |
| ATOM | 641 | CB | CYS | 81 | 28.511 | -4.672 | -9.252 | 1.00 | 0.00 |
| ATOM | 642 | SG | CYS | 81 | 28.000 | -3.555 | -7.927 | 1.00 | 0.00 |
| ATOM | 643 | N | VAL | 82 | 25.687 | -6.469 | -9.797 | 1.00 | 0.00 |
| ATOM | 644 | CA | VAL | 82 | 24.231 | -6.848 | -9.602 | 1.00 | 0.00 |
| ATOM | 645 | C | VAL | 82 | 23.958 | -8.230 | -8.926 | 1.00 | 0.00 |
| ATOM | 646 | O | VAL | 82 | 23.127 | -8.288 | -8.017 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|---------|---------|------|------|
| ATOM | 647 | CB | VAL | 82 | 23.293 | -6.587 | -10.837 | 1.00 | 0.00 |
| ATOM | 648 | CG1 | VAL | 82 | 23.305 | -7.621 | -11.979 | 1.00 | 0.00 |
| ATOM | 649 | CG2 | VAL | 82 | 21.800 | -6.463 | -10.448 | 1.00 | 0.00 |
| ATOM | 650 | N | MET | 83 | 24.633 | -9.324 | -9.325 | 1.00 | 0.00 |
| ATOM | 651 | CA | MET | 83 | 24.579 | -10.621 | -8.577 | 1.00 | 0.00 |
| ATOM | 652 | C | MET | 83 | 25.019 | -10.533 | -7.069 | 1.00 | 0.00 |
| ATOM | 653 | O | MET | 83 | 24.336 | -11.070 | -6.190 | 1.00 | 0.00 |
| ATOM | 654 | CB | MET | 83 | 25.367 | -11.700 | -9.370 | 1.00 | 0.00 |
| ATOM | 655 | CG | MET | 83 | 24.700 | -12.149 | -10.688 | 1.00 | 0.00 |
| ATOM | 656 | SD | MET | 83 | 25.708 | -13.415 | -11.489 | 1.00 | 0.00 |
| ATOM | 657 | CE | MET | 83 | 26.362 | -12.487 | -12.888 | 1.00 | 0.00 |
| ATOM | 658 | N | LEU | 84 | 26.096 | -9.782 | -6.761 | 1.00 | 0.00 |
| ATOM | 659 | CA | LEU | 84 | 26.375 | -9.280 | -5.387 | 1.00 | 0.00 |
| ATOM | 660 | C | LEU | 84 | 25.265 | -8.340 | -4.798 | 1.00 | 0.00 |
| ATOM | 661 | O | LEU | 84 | 24.697 | -8.690 | -3.762 | 1.00 | 0.00 |
| ATOM | 662 | CB | LEU | 84 | 27.802 | -8.658 | -5.405 | 1.00 | 0.00 |
| ATOM | 663 | CG | LEU | 84 | 28.382 | -8.166 | -4.051 | 1.00 | 0.00 |
| ATOM | 664 | CD1 | LEU | 84 | 28.581 | -9.304 | -3.033 | 1.00 | 0.00 |
| ATOM | 665 | CD2 | LEU | 84 | 29.724 | -7.450 | -4.281 | 1.00 | 0.00 |
| ATOM | 666 | N | ILE | 85 | 24.929 | -7.180 | -5.411 | 1.00 | 0.00 |
| ATOM | 667 | CA | ILE | 85 | 23.930 | -6.227 | -4.834 | 1.00 | 0.00 |
| ATOM | 668 | C | ILE | 85 | 22.447 | -6.739 | -4.675 | 1.00 | 0.00 |
| ATOM | 669 | O | ILE | 85 | 21.775 | -6.351 | -3.714 | 1.00 | 0.00 |
| ATOM | 670 | CB | ILE | 85 | 24.034 | -4.706 | -5.230 | 1.00 | 0.00 |
| ATOM | 671 | CG1 | ILE | 85 | 23.604 | -4.242 | -6.647 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|---------|--------|------|------|
| ATOM | 672 | CG2 | ILE | 85 | 25.430 | -4.111 | -4.915 | 1.00 | 0.00 |
| ATOM | 673 | CD1 | ILE | 85 | 22.155 | -4.530 | -7.064 | 1.00 | 0.00 |
| ATOM | 674 | N | GLY | 86 | 21.940 | -7.612 | -5.561 | 1.00 | 0.00 |
| ATOM | 675 | CA | GLY | 86 | 20.599 | -8.242 | -5.417 | 1.00 | 0.00 |
| ATOM | 676 | C | GLY | 86 | 20.452 | -9.394 | -4.402 | 1.00 | 0.00 |
| ATOM | 677 | O | GLY | 86 | 19.504 | -9.390 | -3.614 | 1.00 | 0.00 |
| ATOM | 678 | N | SER | 87 | 21.407 | -10.340 | -4.368 | 1.00 | 0.00 |
| ATOM | 679 | CA | SER | 87 | 21.656 | -11.189 | -3.164 | 1.00 | 0.00 |
| ATOM | 680 | C | SER | 87 | 21.822 | -10.431 | -1.800 | 1.00 | 0.00 |
| ATOM | 681 | O | SER | 87 | 21.216 | -10.841 | -0.804 | 1.00 | 0.00 |
| ATOM | 682 | CB | SER | 87 | 22.805 | -12.179 | -3.467 | 1.00 | 0.00 |
| ATOM | 683 | OG | SER | 87 | 24.058 | -11.528 | -3.693 | 1.00 | 0.00 |
| ATOM | 684 | N | LEU | 88 | 22.536 | -9.286 | -1.774 | 1.00 | 0.00 |
| ATOM | 685 | CA | LEU | 88 | 22.500 | -8.333 | -0.630 | 1.00 | 0.00 |
| ATOM | 686 | C | LEU | 88 | 21.109 | -7.701 | -0.277 | 1.00 | 0.00 |
| ATOM | 687 | O | LEU | 88 | 20.704 | -7.753 | 0.889 | 1.00 | 0.00 |
| ATOM | 688 | CB | LEU | 88 | 23.625 | -7.266 | -0.757 | 1.00 | 0.00 |
| ATOM | 689 | CG | LEU | 88 | 25.093 | -7.758 | -0.606 | 1.00 | 0.00 |
| ATOM | 690 | CD1 | LEU | 88 | 26.075 | -6.662 | -1.053 | 1.00 | 0.00 |
| ATOM | 691 | CD2 | LEU | 88 | 25.436 | -8.179 | 0.836 | 1.00 | 0.00 |
| ATOM | 692 | N | MET | 89 | 20.358 | -7.152 | -1.252 | 1.00 | 0.00 |
| ATOM | 693 | CA | MET | 89 | 18.930 | -6.749 | -1.057 | 1.00 | 0.00 |
| ATOM | 694 | C | MET | 89 | 17.977 | -7.885 | -0.533 | 1.00 | 0.00 |
| ATOM | 695 | O | MET | 89 | 17.305 | -7.681 | 0.486 | 1.00 | 0.00 |
| ATOM | 696 | CB | MET | 89 | 18.472 | -6.082 | -2.382 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|---------|--------|------|------|
| ATOM | 697 | CG | MET | 89 | 17.041 | -5.504 | -2.388 | 1.00 | 0.00 |
| ATOM | 698 | SD | MET | 89 | 16.778 | -4.458 | -3.835 | 1.00 | 0.00 |
| ATOM | 699 | CE | MET | 89 | 16.644 | -5.676 | -5.152 | 1.00 | 0.00 |
| ATOM | 700 | N | TYR | 90 | 17.972 | -9.075 | -1.169 | 1.00 | 0.00 |
| ATOM | 701 | CA | TYR | 90 | 17.295 | -10.299 | -0.649 | 1.00 | 0.00 |
| ATOM | 702 | C | TYR | 90 | 17.553 | -10.670 | 0.855 | 1.00 | 0.00 |
| ATOM | 703 | O | TYR | 90 | 16.584 | -10.824 | 1.608 | 1.00 | 0.00 |
| ATOM | 704 | CB | TYR | 90 | 17.621 | -11.460 | -1.644 | 1.00 | 0.00 |
| ATOM | 705 | CG | TYR | 90 | 17.152 | -12.878 | -1.245 | 1.00 | 0.00 |
| ATOM | 706 | CD1 | TYR | 90 | 15.842 | -13.072 | -0.802 | 1.00 | 0.00 |
| ATOM | 707 | CD2 | TYR | 90 | 18.053 | -13.950 | -1.202 | 1.00 | 0.00 |
| ATOM | 708 | CE1 | TYR | 90 | 15.452 | -14.294 | -0.275 | 1.00 | 0.00 |
| ATOM | 709 | CE2 | TYR | 90 | 17.645 | -15.191 | -0.708 | 1.00 | 0.00 |
| ATOM | 710 | CZ | TYR | 90 | 16.342 | -15.360 | -0.245 | 1.00 | 0.00 |
| ATOM | 711 | OH | TYR | 90 | 15.917 | -16.573 | 0.233 | 1.00 | 0.00 |
| ATOM | 712 | N | ALA | 91 | 18.823 | -10.800 | 1.287 | 1.00 | 0.00 |
| ATOM | 713 | CA | ALA | 91 | 19.176 | -11.016 | 2.721 | 1.00 | 0.00 |
| ATOM | 714 | C | ALA | 91 | 18.553 | -10.039 | 3.781 | 1.00 | 0.00 |
| ATOM | 715 | O | ALA | 91 | 18.215 | -10.472 | 4.886 | 1.00 | 0.00 |
| ATOM | 716 | CB | ALA | 91 | 20.715 | -11.027 | 2.779 | 1.00 | 0.00 |
| ATOM | 717 | N | SER | 92 | 18.347 | -8.757 | 3.427 | 1.00 | 0.00 |
| ATOM | 718 | CA | SER | 92 | 17.572 | -7.792 | 4.255 | 1.00 | 0.00 |
| ATOM | 719 | C | SER | 92 | 16.083 | -8.081 | 4.529 | 1.00 | 0.00 |
| ATOM | 720 | O | SER | 92 | 15.635 | -8.047 | 5.679 | 1.00 | 0.00 |
| ATOM | 721 | CB | SER | 92 | 17.817 | -6.370 | 3.675 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|---------|-------|------|------|
| ATOM | 722 | OG | SER | 92 | 17.085 | -6.095 | 2.474 | 1.00 | 0.00 |
| ATOM | 723 | N | ILE | 93 | 15.325 | -8.380 | 3.474 | 1.00 | 0.00 |
| ATOM | 724 | CA | ILE | 93 | 13.884 | -8.721 | 3.595 | 1.00 | 0.00 |
| ATOM | 725 | C | ILE | 93 | 13.654 | -10.140 | 4.253 | 1.00 | 0.00 |
| ATOM | 726 | O | ILE | 93 | 12.643 | -10.301 | 4.933 | 1.00 | 0.00 |
| ATOM | 727 | CB | ILE | 93 | 13.146 | -8.424 | 2.238 | 1.00 | 0.00 |
| ATOM | 728 | CG1 | ILE | 93 | 13.536 | -7.112 | 1.479 | 1.00 | 0.00 |
| ATOM | 729 | CG2 | ILE | 93 | 11.607 | -8.478 | 2.394 | 1.00 | 0.00 |
| ATOM | 730 | CD1 | ILE | 93 | 13.469 | -5.793 | 2.275 | 1.00 | 0.00 |
| ATOM | 731 | N | PHE | 94 | 14.601 | -11.107 | 4.150 | 1.00 | 0.00 |
| ATOM | 732 | CA | PHE | 94 | 14.598 | -12.415 | 4.876 | 1.00 | 0.00 |
| ATOM | 733 | C | PHE | 94 | 14.249 | -12.371 | 6.411 | 1.00 | 0.00 |
| ATOM | 734 | O | PHE | 94 | 13.198 | -12.894 | 6.778 | 1.00 | 0.00 |
| ATOM | 735 | CB | PHE | 94 | 15.966 | -13.102 | 4.554 | 1.00 | 0.00 |
| ATOM | 736 | CG | PHE | 94 | 16.048 | -14.633 | 4.734 | 1.00 | 0.00 |
| ATOM | 737 | CD1 | PHE | 94 | 16.056 | -15.214 | 6.009 | 1.00 | 0.00 |
| ATOM | 738 | CD2 | PHE | 94 | 16.201 | -15.455 | 3.612 | 1.00 | 0.00 |
| ATOM | 739 | CE1 | PHE | 94 | 16.192 | -16.593 | 6.155 | 1.00 | 0.00 |
| ATOM | 740 | CE2 | PHE | 94 | 16.349 | -16.833 | 3.760 | 1.00 | 0.00 |
| ATOM | 741 | CZ | PHE | 94 | 16.338 | -17.401 | 5.031 | 1.00 | 0.00 |
| ATOM | 742 | N | GLY | 95 | 15.068 | -11.753 | 7.293 | 1.00 | 0.00 |
| ATOM | 743 | CA | GLY | 95 | 14.712 | -11.560 | 8.746 | 1.00 | 0.00 |
| ATOM | 744 | C | GLY | 95 | 13.464 | -10.718 | 9.080 | 1.00 | 0.00 |
| ATOM | 745 | O | GLY | 95 | 12.671 | -11.089 | 9.949 | 1.00 | 0.00 |
| ATOM | 746 | N | ASN | 96 | 13.296 | -9.609 | 8.352 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|---------|--------|------|------|
| ATOM | 747 | CA | ASN | 96 | 12.064 | -8.777 | 8.385 | 1.00 | 0.00 |
| ATOM | 748 | C | ASN | 96 | 10.729 | -9.509 | 8.002 | 1.00 | 0.00 |
| ATOM | 749 | O | ASN | 96 | 9.735 | -9.306 | 8.703 | 1.00 | 0.00 |
| ATOM | 750 | CB | ASN | 96 | 12.340 | -7.518 | 7.523 | 1.00 | 0.00 |
| ATOM | 751 | CG | ASN | 96 | 13.334 | -6.521 | 8.147 | 1.00 | 0.00 |
| ATOM | 752 | OD1 | ASN | 96 | 13.123 | -5.995 | 9.234 | 1.00 | 0.00 |
| ATOM | 753 | ND2 | ASN | 96 | 14.437 | -6.218 | 7.511 | 1.00 | 0.00 |
| ATOM | 754 | N | VAL | 97 | 10.695 | -10.387 | 6.974 | 1.00 | 0.00 |
| ATOM | 755 | CA | VAL | 97 | 9.589 | -11.384 | 6.801 | 1.00 | 0.00 |
| ATOM | 756 | C | VAL | 97 | 9.630 | -12.553 | 7.844 | 1.00 | 0.00 |
| ATOM | 757 | O | VAL | 97 | 8.595 | -12.837 | 8.438 | 1.00 | 0.00 |
| ATOM | 758 | CB | VAL | 97 | 9.345 | -11.872 | 5.328 | 1.00 | 0.00 |
| ATOM | 759 | CG1 | VAL | 97 | 9.000 | -10.719 | 4.361 | 1.00 | 0.00 |
| ATOM | 760 | CG2 | VAL | 97 | 10.419 | -12.789 | 4.700 | 1.00 | 0.00 |
| ATOM | 761 | N | SER | 98 | 10.761 | -13.226 | 8.131 | 1.00 | 0.00 |
| ATOM | 762 | CA | SER | 98 | 10.815 | -14.341 | 9.126 | 1.00 | 0.00 |
| ATOM | 763 | C | SER | 98 | 10.213 | -14.033 | 10.540 | 1.00 | 0.00 |
| ATOM | 764 | O | SER | 98 | 9.307 | -14.728 | 10.980 | 1.00 | 0.00 |
| ATOM | 765 | CB | SER | 98 | 12.267 | -14.875 | 9.190 | 1.00 | 0.00 |
| ATOM | 766 | OG | SER | 98 | 12.329 | -16.169 | 9.792 | 1.00 | 0.00 |
| ATOM | 767 | N | ALA | 99 | 10.615 | -12.952 | 11.224 | 1.00 | 0.00 |
| ATOM | 768 | CA | ALA | 99 | 10.446 | -12.755 | 12.657 | 1.00 | 0.00 |
| ATOM | 769 | C | ALA | 99 | 8.997 | -12.375 | 12.950 | 1.00 | 0.00 |
| ATOM | 770 | O | ALA | 99 | 8.481 | -12.658 | 14.032 | 1.00 | 0.00 |
| ATOM | 771 | CB | ALA | 99 | 11.450 | -11.694 | 13.139 | 1.00 | 0.00 |

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|------|-----|-----|-----|-----|--------|---------|--------|------|------|
| ATOM | 772 | N | ILE | 100 | 8.346 | -11.734 | 11.980 | 1.00 | 0.00 |
| ATOM | 773 | CA | ILE | 100 | 6.952 | -11.331 | 12.135 | 1.00 | 0.00 |
| ATOM | 774 | C | ILE | 100 | 6.054 | -12.533 | 11.872 | 1.00 | 0.00 |
| ATOM | 775 | O | ILE | 100 | 5.125 | -12.811 | 12.632 | 1.00 | 0.00 |
| ATOM | 776 | CB | ILE | 100 | 6.631 | -10.130 | 11.155 | 1.00 | 0.00 |
| ATOM | 777 | CG1 | ILE | 100 | 5.201 | -9.522 | 11.317 | 1.00 | 0.00 |
| ATOM | 778 | CG2 | ILE | 100 | 6.831 | -10.504 | 9.654 | 1.00 | 0.00 |
| ATOM | 779 | CD1 | ILE | 100 | 4.965 | -8.686 | 12.591 | 1.00 | 0.00 |
| ATOM | 780 | N | ILE | 101 | 6.339 | -13.248 | 10.791 | 1.00 | 0.00 |
| ATOM | 781 | CA | ILE | 101 | 5.555 | -14.417 | 10.436 | 1.00 | 0.00 |
| ATOM | 782 | C | ILE | 101 | 5.666 | -15.477 | 11.522 | 1.00 | 0.00 |
| ATOM | 783 | O | ILE | 101 | 4.656 | -15.952 | 12.038 | 1.00 | 0.00 |
| ATOM | 784 | CB | ILE | 101 | 6.044 | -14.959 | 9.032 | 1.00 | 0.00 |
| ATOM | 785 | CG1 | ILE | 101 | 5.886 | -13.947 | 7.852 | 1.00 | 0.00 |
| ATOM | 786 | CG2 | ILE | 101 | 5.348 | -16.293 | 8.622 | 1.00 | 0.00 |
| ATOM | 787 | CD1 | ILE | 101 | 6.594 | -14.332 | 6.536 | 1.00 | 0.00 |
| ATOM | 788 | N | GLN | 102 | 6.899 | -15.842 | 11.862 | 1.00 | 0.00 |
| ATOM | 789 | CA | GLN | 102 | 7.155 | -16.851 | 12.885 | 1.00 | 0.00 |
| ATOM | 790 | C | GLN | 102 | 6.452 | -16.498 | 14.199 | 1.00 | 0.00 |
| ATOM | 791 | O | GLN | 102 | 6.013 | -17.389 | 14.937 | 1.00 | 0.00 |
| ATOM | 792 | CB | GLN | 102 | 8.677 | -17.003 | 13.096 | 1.00 | 0.00 |
| ATOM | 793 | CG | GLN | 102 | 9.485 | -17.597 | 11.895 | 1.00 | 0.00 |
| ATOM | 794 | CD | GLN | 102 | 10.997 | -17.809 | 12.043 | 1.00 | 0.00 |
| ATOM | 795 | OE1 | GLN | 102 | 11.745 | -16.874 | 12.279 | 1.00 | 0.00 |
| ATOM | 796 | NE2 | GLN | 102 | 11.507 | -19.005 | 11.893 | 1.00 | 0.00 |

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|------|-----|-----|-----|-----|-------|---------|--------|------|------|
| ATOM | 797 | N | ARG | 103 | 6.341 | -15.199 | 14.481 | 1.00 | 0.00 |
| ATOM | 798 | CA | ARG | 103 | 5.687 | -14.718 | 15.701 | 1.00 | 0.00 |
| ATOM | 799 | C | ARG | 103 | 4.182 | -14.867 | 15.571 | 1.00 | 0.00 |
| ATOM | 800 | O | ARG | 103 | 3.519 | -15.407 | 16.455 | 1.00 | 0.00 |
| ATOM | 801 | CB | ARG | 103 | 6.090 | -13.238 | 15.959 | 1.00 | 0.00 |
| ATOM | 802 | CG | ARG | 103 | 5.586 | -12.632 | 17.299 | 1.00 | 0.00 |
| ATOM | 803 | CD | ARG | 103 | 5.999 | -11.159 | 17.459 | 1.00 | 0.00 |
| ATOM | 804 | NE | ARG | 103 | 5.489 | -10.633 | 18.760 | 1.00 | 0.00 |
| ATOM | 805 | CZ | ARG | 103 | 5.668 | -9.395 | 19.211 | 1.00 | 0.00 |
| ATOM | 806 | NH1 | ARG | 103 | 6.318 | -8.474 | 18.555 | 1.00 | 0.00 |
| ATOM | 807 | NH2 | ARG | 103 | 5.170 | -9.084 | 20.366 | 1.00 | 0.00 |
| ATOM | 808 | N | LEU | 104 | 3.652 | -14.358 | 14.466 | 1.00 | 0.00 |
| ATOM | 809 | CA | LEU | 104 | 2.226 | -14.436 | 14.187 | 1.00 | 0.00 |
| ATOM | 810 | C | LEU | 104 | 1.789 | -15.891 | 14.053 | 1.00 | 0.00 |
| ATOM | 811 | O | LEU | 104 | 0.649 | -16.242 | 14.363 | 1.00 | 0.00 |
| ATOM | 812 | CB | LEU | 104 | 1.912 | -13.640 | 12.888 | 1.00 | 0.00 |
| ATOM | 813 | CG | LEU | 104 | 1.619 | -12.120 | 13.014 | 1.00 | 0.00 |
| ATOM | 814 | CD1 | LEU | 104 | 0.206 | -11.899 | 13.571 | 1.00 | 0.00 |
| ATOM | 815 | CD2 | LEU | 104 | 2.644 | -11.389 | 13.897 | 1.00 | 0.00 |
| ATOM | 816 | N | TYR | 105 | 2.703 | -16.737 | 13.590 | 1.00 | 0.00 |
| ATOM | 817 | CA | TYR | 105 | 2.419 | -18.156 | 13.426 | 1.00 | 0.00 |
| ATOM | 818 | C | TYR | 105 | 2.401 | -18.862 | 14.780 | 1.00 | 0.00 |
| ATOM | 819 | O | TYR | 105 | 1.439 | -19.554 | 15.119 | 1.00 | 0.00 |
| ATOM | 820 | CB | TYR | 105 | 3.470 | -18.809 | 12.521 | 1.00 | 0.00 |
| ATOM | 821 | CG | TYR | 105 | 3.231 | -20.286 | 12.300 | 1.00 | 0.00 |

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|------|-----|-----|-----|-----|--------|---------|--------|------|------|
| ATOM | 822 | CD1 | TYR | 105 | 2.177 | -20.728 | 11.499 | 1.00 | 0.00 |
| ATOM | 823 | CD2 | TYR | 105 | 4.028 | -21.244 | 12.933 | 1.00 | 0.00 |
| ATOM | 824 | CE1 | TYR | 105 | 1.917 | -22.087 | 11.336 | 1.00 | 0.00 |
| ATOM | 825 | CE2 | TYR | 105 | 3.776 | -22.607 | 12.777 | 1.00 | 0.00 |
| ATOM | 826 | CZ | TYR | 105 | 2.718 | -23.019 | 11.978 | 1.00 | 0.00 |
| ATOM | 827 | OH | TYR | 105 | 2.446 | -24.362 | 11.830 | 1.00 | 0.00 |
| ATOM | 828 | N | SER | 106 | 3.474 | -18.685 | 15.548 | 1.00 | 0.00 |
| ATOM | 829 | CA | SER | 106 | 3.589 | -19.300 | 16.866 | 1.00 | 0.00 |
| ATOM | 830 | C | SER | 106 | 2.539 | -18.755 | 17.843 | 1.00 | 0.00 |
| ATOM | 831 | O | SER | 106 | 1.479 | -18.287 | 17.419 | 1.00 | 0.00 |
| ATOM | 832 | CB | SER | 106 | 5.028 | -19.091 | 17.401 | 1.00 | 0.00 |
| ATOM | 833 | OG | SER | 106 | 5.343 | -17.713 | 17.629 | 1.00 | 0.00 |
| ATOM | 834 | N | LYS | 1B | 22.518 | -39.003 | 9.338 | 1.00 | 0.00 |
| ATOM | 835 | CA | LYS | 1B | 21.924 | -37.810 | 8.768 | 1.00 | 0.00 |
| ATOM | 836 | C | LYS | 1B | 20.488 | -37.949 | 8.309 | 1.00 | 0.00 |
| ATOM | 837 | O | LYS | 1B | 19.641 | -37.123 | 8.648 | 1.00 | 0.00 |
| ATOM | 838 | CB | LYS | 1B | 22.832 | -37.363 | 7.584 | 1.00 | 0.00 |
| ATOM | 839 | CG | LYS | 1B | 24.225 | -36.826 | 8.025 | 1.00 | 0.00 |
| ATOM | 840 | CD | LYS | 1B | 25.133 | -36.340 | 6.886 | 1.00 | 0.00 |
| ATOM | 841 | CE | LYS | 1B | 26.470 | -35.840 | 7.467 | 1.00 | 0.00 |
| ATOM | 842 | NZ | LYS | 1B | 27.343 | -35.372 | 6.356 | 1.00 | 0.00 |
| ATOM | 843 | N | LEU | 2B | 20.206 | -38.991 | 7.538 | 1.00 | 0.00 |
| ATOM | 844 | CA | LEU | 2B | 18.857 | -39.193 | 7.040 | 1.00 | 0.00 |
| ATOM | 845 | C | LEU | 2B | 17.823 | -39.264 | 8.150 | 1.00 | 0.00 |
| ATOM | 846 | O | LEU | 2B | 16.757 | -38.656 | 8.046 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|---------|--------|------|------|
| ATOM | 847 | CB | LEU | 2B | 18.782 | -40.455 | 6.183 | 1.00 | 0.00 |
| ATOM | 848 | CG | LEU | 2B | 19.602 | -40.393 | 4.895 | 1.00 | 0.00 |
| ATOM | 849 | CD1 | LEU | 2B | 19.530 | -41.731 | 4.178 | 1.00 | 0.00 |
| ATOM | 850 | CD2 | LEU | 2B | 19.073 | -39.284 | 4.012 | 1.00 | 0.00 |
| ATOM | 851 | N | ASP | 3B | 18.134 | -39.997 | 9.215 | 1.00 | 0.00 |
| ATOM | 852 | CA | ASP | 3B | 17.199 | -40.120 | 10.329 | 1.00 | 0.00 |
| ATOM | 853 | C | ASP | 3B | 16.815 | -38.748 | 10.877 | 1.00 | 0.00 |
| ATOM | 854 | O | ASP | 3B | 15.661 | -38.508 | 11.238 | 1.00 | 0.00 |
| ATOM | 855 | CB | ASP | 3B | 17.823 | -41.008 | 11.442 | 1.00 | 0.00 |
| ATOM | 856 | CG | ASP | 3B | 17.997 | -42.491 | 11.084 | 1.00 | 0.00 |
| ATOM | 857 | OD1 | ASP | 3B | 17.250 | -43.001 | 10.223 | 1.00 | 0.00 |
| ATOM | 858 | OD2 | ASP | 3B | 18.856 | -43.157 | 11.700 | 1.00 | 0.00 |
| ATOM | 859 | N | ARG | 4B | 17.794 | -37.853 | 10.939 | 1.00 | 0.00 |
| ATOM | 860 | CA | ARG | 4B | 17.557 | -36.506 | 11.428 | 1.00 | 0.00 |
| ATOM | 861 | C | ARG | 4B | 16.623 | -35.792 | 10.454 | 1.00 | 0.00 |
| ATOM | 862 | O | ARG | 4B | 15.640 | -35.171 | 10.860 | 1.00 | 0.00 |
| ATOM | 863 | CB | ARG | 4B | 18.910 | -35.753 | 11.573 | 1.00 | 0.00 |
| ATOM | 864 | CG | ARG | 4B | 19.759 | -36.135 | 12.818 | 1.00 | 0.00 |
| ATOM | 865 | CD | ARG | 4B | 20.014 | -37.650 | 12.902 | 1.00 | 0.00 |
| ATOM | 866 | NE | ARG | 4B | 20.830 | -37.955 | 14.113 | 1.00 | 0.00 |
| ATOM | 867 | CZ | ARG | 4B | 21.229 | -39.168 | 14.485 | 1.00 | 0.00 |
| ATOM | 868 | NH1 | ARG | 4B | 20.955 | -40.254 | 13.819 | 1.00 | 0.00 |
| ATOM | 869 | NH2 | ARG | 4B | 21.930 | -39.279 | 15.569 | 1.00 | 0.00 |
| ATOM | 870 | N | TYR | 5B | 16.936 | -35.901 | 9.166 | 1.00 | 0.00 |
| ATOM | 871 | CA | TYR | 5B | 16.131 | -35.278 | 8.125 | 1.00 | 0.00 |

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|------|-----|-----|-----|----|--------|---------|--------|------|------|
| ATOM | 872 | C | TYR | 5B | 14.698 | -35.797 | 8.172 | 1.00 | 0.00 |
| ATOM | 873 | O | TYR | 5B | 13.746 | -35.056 | 7.919 | 1.00 | 0.00 |
| ATOM | 874 | CB | TYR | 5B | 16.709 | -35.589 | 6.714 | 1.00 | 0.00 |
| ATOM | 875 | CG | TYR | 5B | 18.072 | -34.974 | 6.377 | 1.00 | 0.00 |
| ATOM | 876 | CD1 | TYR | 5B | 18.735 | -34.159 | 7.300 | 1.00 | 0.00 |
| ATOM | 877 | CD2 | TYR | 5B | 18.666 | -35.237 | 5.138 | 1.00 | 0.00 |
| ATOM | 878 | CE1 | TYR | 5B | 19.980 | -33.619 | 6.988 | 1.00 | 0.00 |
| ATOM | 879 | CE2 | TYR | 5B | 19.910 | -34.695 | 4.828 | 1.00 | 0.00 |
| ATOM | 880 | CZ | TYR | 5B | 20.566 | -33.887 | 5.754 | 1.00 | 0.00 |
| ATOM | 881 | OH | TYR | 5B | 21.789 | -33.357 | 5.452 | 1.00 | 0.00 |
| ATOM | 882 | N | SER | 6B | 14.551 | -37.073 | 8.502 | 1.00 | 0.00 |
| ATOM | 883 | CA | SER | 6B | 13.229 | -37.665 | 8.567 | 1.00 | 0.00 |
| ATOM | 884 | C | SER | 6B | 12.433 | -37.207 | 9.769 | 1.00 | 0.00 |
| ATOM | 885 | O | SER | 6B | 11.282 | -36.784 | 9.637 | 1.00 | 0.00 |
| ATOM | 886 | CB | SER | 6B | 13.347 | -39.209 | 8.516 | 1.00 | 0.00 |
| ATOM | 887 | OG | SER | 6B | 12.073 | -39.863 | 8.486 | 1.00 | 0.00 |
| ATOM | 888 | N | GLU | 7B | 13.045 | -37.291 | 10.946 | 1.00 | 0.00 |
| ATOM | 889 | CA | GLU | 7B | 12.378 | -36.888 | 12.178 | 1.00 | 0.00 |
| ATOM | 890 | C | GLU | 7B | 11.936 | -35.434 | 12.127 | 1.00 | 0.00 |
| ATOM | 891 | O | GLU | 7B | 10.901 | -35.070 | 12.694 | 1.00 | 0.00 |
| ATOM | 892 | CB | GLU | 7B | 13.309 | -37.129 | 13.399 | 1.00 | 0.00 |
| ATOM | 893 | CG | GLU | 7B | 13.569 | -38.626 | 13.770 | 1.00 | 0.00 |
| ATOM | 894 | CD | GLU | 7B | 14.417 | -38.929 | 14.991 | 1.00 | 0.00 |
| ATOM | 895 | OE1 | GLU | 7B | 15.067 | -38.031 | 15.559 | 1.00 | 0.00 |
| ATOM | 896 | OE2 | GLU | 7B | 14.410 | -40.111 | 15.394 | 1.00 | 0.00 |

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|------|-----|-----|-----|-----|--------|---------|--------|------|------|
| ATOM | 897 | N | TYR | 8B | 12.720 | -34.606 | 11.442 | 1.00 | 0.00 |
| ATOM | 898 | CA | TYR | 8B | 12.399 | -33.191 | 11.312 | 1.00 | 0.00 |
| ATOM | 899 | C | TYR | 8B | 11.192 | -33.002 | 10.398 | 1.00 | 0.00 |
| ATOM | 900 | O | TYR | 8B | 10.335 | -32.148 | 10.648 | 1.00 | 0.00 |
| ATOM | 901 | CB | TYR | 8B | 13.585 | -32.379 | 10.713 | 1.00 | 0.00 |
| ATOM | 902 | CG | TYR | 8B | 14.849 | -32.270 | 11.575 | 1.00 | 0.00 |
| ATOM | 903 | CD1 | TYR | 8B | 15.925 | -33.139 | 11.375 | 1.00 | 0.00 |
| ATOM | 904 | CD2 | TYR | 8B | 14.931 | -31.286 | 12.565 | 1.00 | 0.00 |
| ATOM | 905 | CE1 | TYR | 8B | 17.074 | -33.020 | 12.154 | 1.00 | 0.00 |
| ATOM | 906 | CE2 | TYR | 8B | 16.079 | -31.169 | 13.343 | 1.00 | 0.00 |
| ATOM | 907 | CZ | TYR | 8B | 17.149 | -32.036 | 13.137 | 1.00 | 0.00 |
| ATOM | 908 | OH | TYR | 8B | 18.279 | -31.921 | 13.897 | 1.00 | 0.00 |
| ATOM | 909 | N | GLY | 9B | 11.126 | -33.808 | 9.343 | 1.00 | 0.00 |
| ATOM | 910 | CA | GLY | 9B | 10.016 | -33.736 | 8.399 | 1.00 | 0.00 |
| ATOM | 911 | C | GLY | 9B | 8.729 | -34.225 | 9.064 | 1.00 | 0.00 |
| ATOM | 912 | O | GLY | 9B | 7.688 | -33.568 | 8.983 | 1.00 | 0.00 |
| ATOM | 913 | N | ALA | 10B | 8.816 | -35.376 | 9.728 | 1.00 | 0.00 |
| ATOM | 914 | CA | ALA | 10B | 7.668 | -35.963 | 10.409 | 1.00 | 0.00 |
| ATOM | 915 | C | ALA | 10B | 7.112 | -35.025 | 11.476 | 1.00 | 0.00 |
| ATOM | 916 | O | ALA | 10B | 5.904 | -34.980 | 11.707 | 1.00 | 0.00 |
| ATOM | 917 | CB | ALA | 10B | 8.088 | -37.329 | 10.976 | 1.00 | 0.00 |
| ATOM | 918 | N | ALA | 11B | 8.000 | -34.273 | 12.119 | 1.00 | 0.00 |
| ATOM | 919 | CA | ALA | 11B | 7.596 | -33.342 | 13.165 | 1.00 | 0.00 |
| ATOM | 920 | C | ALA | 11B | 7.145 | -31.989 | 12.611 | 1.00 | 0.00 |
| ATOM | 921 | O | ALA | 11B | 6.138 | -31.435 | 13.064 | 1.00 | 0.00 |

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|------|-----|-----|-----|-----|--------|---------|--------|------|------|
| ATOM | 922 | CB | ALA | 11B | 8.741 | -33.150 | 14.159 | 1.00 | 0.00 |
| ATOM | 923 | N | VAL | 12B | 7.880 | -31.458 | 11.632 | 1.00 | 0.00 |
| ATOM | 924 | CA | VAL | 12B | 7.534 | -30.161 | 11.045 | 1.00 | 0.00 |
| ATOM | 925 | C | VAL | 12B | 6.701 | -30.304 | 9.773 | 1.00 | 0.00 |
| ATOM | 926 | O | VAL | 12B | 6.856 | -29.523 | 8.830 | 1.00 | 0.00 |
| ATOM | 927 | CB | VAL | 12B | 8.847 | -29.327 | 10.767 | 1.00 | 0.00 |
| ATOM | 928 | CG1 | VAL | 12B | 9.691 | -28.934 | 12.011 | 1.00 | 0.00 |
| ATOM | 929 | CG2 | VAL | 12B | 9.839 | -30.021 | 9.803 | 1.00 | 0.00 |
| ATOM | 930 | N | LEU | 13B | 5.818 | -31.300 | 9.754 | 1.00 | 0.00 |
| ATOM | 931 | CA | LEU | 13B | 4.954 | -31.538 | 8.601 | 1.00 | 0.00 |
| ATOM | 932 | C | LEU | 13B | 4.039 | -30.336 | 8.351 | 1.00 | 0.00 |
| ATOM | 933 | O | LEU | 13B | 3.885 | -29.891 | 7.212 | 1.00 | 0.00 |
| ATOM | 934 | CB | LEU | 13B | 4.122 | -32.834 | 8.819 | 1.00 | 0.00 |
| ATOM | 935 | CG | LEU | 13B | 3.199 | -33.313 | 7.667 | 1.00 | 0.00 |
| ATOM | 936 | CD1 | LEU | 13B | 4.037 | -33.666 | 6.430 | 1.00 | 0.00 |
| ATOM | 937 | CD2 | LEU | 13B | 2.328 | -34.516 | 8.064 | 1.00 | 0.00 |
| ATOM | 938 | N | PHE | 14B | 3.440 | -29.810 | 9.420 | 1.00 | 0.00 |
| ATOM | 939 | CA | PHE | 14B | 2.547 | -28.660 | 9.311 | 1.00 | 0.00 |
| ATOM | 940 | C | PHE | 14B | 3.280 | -27.467 | 8.703 | 1.00 | 0.00 |
| ATOM | 941 | O | PHE | 14B | 2.682 | -26.658 | 7.994 | 1.00 | 0.00 |
| ATOM | 942 | CB | PHE | 14B | 1.998 | -28.252 | 10.711 | 1.00 | 0.00 |
| ATOM | 943 | CG | PHE | 14B | 1.064 | -29.260 | 11.400 | 1.00 | 0.00 |
| ATOM | 944 | CD1 | PHE | 14B | 1.593 | -30.183 | 12.309 | 1.00 | 0.00 |
| ATOM | 945 | CD2 | PHE | 14B | -0.295 | -29.308 | 11.083 | 1.00 | 0.00 |
| ATOM | 946 | CE1 | PHE | 14B | 0.777 | -31.153 | 12.880 | 1.00 | 0.00 |

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|------|-----|-----|-----|-----|--------|---------|--------|------|------|
| ATOM | 947 | CE2 | PHE | 14B | -1.114 | -30.273 | 11.663 | 1.00 | 0.00 |
| ATOM | 948 | CZ | PHE | 14B | -0.578 | -31.197 | 12.559 | 1.00 | 0.00 |
| ATOM | 949 | N | LEU | 15B | 4.577 | -27.370 | 8.982 | 1.00 | 0.00 |
| ATOM | 950 | CA | LEU | 15B | 5.409 | -26.286 | 8.465 | 1.00 | 0.00 |
| ATOM | 951 | C | LEU | 15B | 5.497 | -26.380 | 6.947 | 1.00 | 0.00 |
| ATOM | 952 | O | LEU | 15B | 5.137 | -25.451 | 6.223 | 1.00 | 0.00 |
| ATOM | 953 | CB | LEU | 15B | 6.822 | -26.375 | 9.110 | 1.00 | 0.00 |
| ATOM | 954 | CG | LEU | 15B | 6.913 | -26.586 | 10.645 | 1.00 | 0.00 |
| ATOM | 955 | CD1 | LEU | 15B | 6.097 | -25.511 | 11.376 | 1.00 | 0.00 |
| ATOM | 956 | CD2 | LEU | 15B | 6.439 | -27.982 | 11.082 | 1.00 | 0.00 |
| ATOM | 957 | N | LEU | 16B | 5.987 | -27.520 | 6.474 | 1.00 | 0.00 |
| ATOM | 958 | CA | LEU | 16B | 6.138 | -27.768 | 5.050 | 1.00 | 0.00 |
| ATOM | 959 | C | LEU | 16B | 4.807 | -27.626 | 4.321 | 1.00 | 0.00 |
| ATOM | 960 | O | LEU | 16B | 4.753 | -27.117 | 3.201 | 1.00 | 0.00 |
| ATOM | 961 | CB | LEU | 16B | 6.733 | -29.190 | 4.848 | 1.00 | 0.00 |
| ATOM | 962 | CG | LEU | 16B | 8.170 | -29.462 | 5.368 | 1.00 | 0.00 |
| ATOM | 963 | CD1 | LEU | 16B | 8.535 | -30.939 | 5.166 | 1.00 | 0.00 |
| ATOM | 964 | CD2 | LEU | 16B | 9.225 | -28.571 | 4.692 | 1.00 | 0.00 |
| ATOM | 965 | N | MET | 17B | 3.737 | -28.084 | 4.966 | 1.00 | 0.00 |
| ATOM | 966 | CA | MET | 17B | 2.417 | -28.003 | 4.370 | 1.00 | 0.00 |
| ATOM | 967 | C | MET | 17B | 2.062 | -26.589 | 3.966 | 1.00 | 0.00 |
| ATOM | 968 | O | MET | 17B | 1.295 | -26.373 | 3.033 | 1.00 | 0.00 |
| ATOM | 969 | CB | MET | 17B | 1.370 | -28.575 | 5.365 | 1.00 | 0.00 |
| ATOM | 970 | CG | MET | 17B | -0.099 | -28.539 | 4.890 | 1.00 | 0.00 |
| ATOM | 971 | SD | MET | 17B | -1.164 | -29.264 | 6.148 | 1.00 | 0.00 |

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|------|-----|-----|-----|-----|--------|---------|--------|------|------|
| ATOM | 972 | CE | MET | 17B | -2.741 | -29.068 | 5.306 | 1.00 | 0.00 |
| ATOM | 973 | N | CYS | 18B | 2.622 | -25.619 | 4.677 | 1.00 | 0.00 |
| ATOM | 974 | CA | CYS | 18B | 2.359 | -24.223 | 4.375 | 1.00 | 0.00 |
| ATOM | 975 | C | CYS | 18B | 3.142 | -23.785 | 3.156 | 1.00 | 0.00 |
| ATOM | 976 | O | CYS | 18B | 2.598 | -23.140 | 2.269 | 1.00 | 0.00 |
| ATOM | 977 | CB | CYS | 18B | 2.688 | -23.377 | 5.621 | 1.00 | 0.00 |
| ATOM | 978 | SG | CYS | 18B | 1.534 | -23.740 | 6.964 | 1.00 | 0.00 |
| ATOM | 979 | N | THR | 19B | 4.499 | -23.930 | 3.092 | 1.00 | 0.00 |
| ATOM | 980 | CA | THR | 19B | 5.306 | -23.523 | 1.879 | 1.00 | 0.00 |
| ATOM | 981 | C | THR | 19B | 5.138 | -24.453 | 0.623 | 1.00 | 0.00 |
| ATOM | 982 | O | THR | 19B | 6.078 | -24.722 | -0.135 | 1.00 | 0.00 |
| ATOM | 983 | CB | THR | 19B | 6.794 | -23.252 | 2.256 | 1.00 | 0.00 |
| ATOM | 984 | OG1 | THR | 19B | 7.448 | -22.633 | 1.154 | 1.00 | 0.00 |
| ATOM | 985 | CG2 | THR | 19B | 7.641 | -24.486 | 2.620 | 1.00 | 0.00 |
| ATOM | 986 | N | PHE | 20B | 3.900 | -24.906 | 0.405 | 1.00 | 0.00 |
| ATOM | 987 | CA | PHE | 20B | 3.546 | -25.920 | -0.587 | 1.00 | 0.00 |
| ATOM | 988 | C | PHE | 20B | 2.026 | -25.803 | -0.944 | 1.00 | 0.00 |
| ATOM | 989 | O | PHE | 20B | 1.695 | -25.287 | -2.015 | 1.00 | 0.00 |
| ATOM | 990 | CB | PHE | 20B | 4.025 | -27.338 | -0.135 | 1.00 | 0.00 |
| ATOM | 991 | CG | PHE | 20B | 3.895 | -28.435 | -1.204 | 1.00 | 0.00 |
| ATOM | 992 | CD1 | PHE | 20B | 4.869 | -28.567 | -2.200 | 1.00 | 0.00 |
| ATOM | 993 | CD2 | PHE | 20B | 2.795 | -29.299 | -1.201 | 1.00 | 0.00 |
| ATOM | 994 | CE1 | PHE | 20B | 4.741 | -29.549 | -3.180 | 1.00 | 0.00 |
| ATOM | 995 | CE2 | PHE | 20B | 2.668 | -30.279 | -2.183 | 1.00 | 0.00 |
| ATOM | 996 | CZ | PHE | 20B | 3.642 | -30.404 | -3.171 | 1.00 | 0.00 |

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| ATOM | 997 | N | ALA | 21B | 1.098 | -26.245 | -0.067 | 1.00 | 0.00 |
| ATOM | 998 | CA | ALA | 21B | -0.362 | -26.246 | -0.367 | 1.00 | 0.00 |
| ATOM | 999 | C | ALA | 21B | -1.047 | -24.844 | -0.476 | 1.00 | 0.00 |
| ATOM | 1000 | O | ALA | 21B | -1.794 | -24.610 | -1.429 | 1.00 | 0.00 |
| ATOM | 1001 | CB | ALA | 21B | -1.037 | -27.162 | 0.672 | 1.00 | 0.00 |
| ATOM | 1002 | N | LEU | 22B | -0.790 | -23.910 | 0.461 | 1.00 | 0.00 |
| ATOM | 1003 | CA | LEU | 22B | -1.273 | -22.497 | 0.342 | 1.00 | 0.00 |
| ATOM | 1004 | C | LEU | 22B | -0.261 | -21.450 | -0.252 | 1.00 | 0.00 |
| ATOM | 1005 | O | LEU | 22B | -0.684 | -20.322 | -0.523 | 1.00 | 0.00 |
| ATOM | 1006 | CB | LEU | 22B | -1.966 | -22.081 | 1.675 | 1.00 | 0.00 |
| ATOM | 1007 | CG | LEU | 22B | -3.342 | -22.765 | 1.948 | 1.00 | 0.00 |
| ATOM | 1008 | CD1 | LEU | 22B | -3.811 | -22.542 | 3.394 | 1.00 | 0.00 |
| ATOM | 1009 | CD2 | LEU | 22B | -4.454 | -22.277 | 0.997 | 1.00 | 0.00 |
| ATOM | 1010 | N | ILE | 23B | 0.998 | -21.811 | -0.597 | 1.00 | 0.00 |
| ATOM | 1011 | CA | ILE | 23B | 1.769 | -21.105 | -1.679 | 1.00 | 0.00 |
| ATOM | 1012 | C | ILE | 23B | 1.261 | -21.423 | -3.137 | 1.00 | 0.00 |
| ATOM | 1013 | O | ILE | 23B | 1.205 | -20.500 | -3.955 | 1.00 | 0.00 |
| ATOM | 1014 | CB | ILE | 23B | 3.323 | -21.227 | -1.464 | 1.00 | 0.00 |
| ATOM | 1015 | CG1 | ILE | 23B | 4.097 | -19.971 | -1.962 | 1.00 | 0.00 |
| ATOM | 1016 | CG2 | ILE | 23B | 3.953 | -22.497 | -2.093 | 1.00 | 0.00 |
| ATOM | 1017 | CD1 | ILE | 23B | 5.508 | -19.820 | -1.366 | 1.00 | 0.00 |
| ATOM | 1018 | N | ALA | 24B | 0.826 | -22.673 | -3.447 | 1.00 | 0.00 |
| ATOM | 1019 | CA | ALA | 24B | 0.027 | -22.996 | -4.669 | 1.00 | 0.00 |
| ATOM | 1020 | C | ALA | 24B | -1.216 | -22.078 | -4.950 | 1.00 | 0.00 |
| ATOM | 1021 | O | ALA | 24B | -1.391 | -21.639 | -6.086 | 1.00 | 0.00 |

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| ATOM | 1022 | CB | ALA | 24B | -0.349 | -24.487 | -4.608 | 1.00 | 0.00 |
| ATOM | 1023 | N | HIS | 25B | -2.008 | -21.710 | -3.919 | 1.00 | 0.00 |
| ATOM | 1024 | CA | HIS | 25B | -2.978 | -20.572 | -3.982 | 1.00 | 0.00 |
| ATOM | 1025 | C | HIS | 25B | -2.413 | -19.199 | -4.508 | 1.00 | 0.00 |
| ATOM | 1026 | O | HIS | 25B | -3.020 | -18.605 | -5.403 | 1.00 | 0.00 |
| ATOM | 1027 | CB | HIS | 25B | -3.629 | -20.478 | -2.566 | 1.00 | 0.00 |
| ATOM | 1028 | CG | HIS | 25B | -4.642 | -19.351 | -2.347 | 1.00 | 0.00 |
| ATOM | 1029 | ND1 | HIS | 25B | -5.992 | -19.452 | -2.634 | 1.00 | 0.00 |
| ATOM | 1030 | CD2 | HIS | 25B | -4.334 | -18.040 | -1.924 | 1.00 | 0.00 |
| ATOM | 1031 | CE1 | HIS | 25B | -6.403 | -18.167 | -2.375 | 1.00 | 0.00 |
| ATOM | 1032 | NE2 | HIS | 25B | -5.479 | -17.251 | -1.935 | 1.00 | 0.00 |
| ATOM | 1033 | N | TRP | 26B | -1.297 | -18.692 | -3.947 | 1.00 | 0.00 |
| ATOM | 1034 | CA | TRP | 26B | -0.641 | -17.441 | -4.435 | 1.00 | 0.00 |
| ATOM | 1035 | C | TRP | 26B | -0.110 | -17.512 | -5.899 | 1.00 | 0.00 |
| ATOM | 1036 | O | TRP | 26B | -0.510 | -16.687 | -6.724 | 1.00 | 0.00 |
| ATOM | 1037 | CB | TRP | 26B | 0.472 | -17.002 | -3.439 | 1.00 | 0.00 |
| ATOM | 1038 | CG | TRP | 26B | -0.047 | -16.319 | -2.171 | 1.00 | 0.00 |
| ATOM | 1039 | CD1 | TRP | 26B | -0.082 | -16.875 | -0.877 | 1.00 | 0.00 |
| ATOM | 1040 | CD2 | TRP | 26B | -0.581 | -15.047 | -2.047 | 1.00 | 0.00 |
| ATOM | 1041 | NE1 | TRP | 26B | -0.632 | -15.975 | 0.056 | 1.00 | 0.00 |
| ATOM | 1042 | CE2 | TRP | 26B | -0.932 | -14.851 | -0.691 | 1.00 | 0.00 |
| ATOM | 1043 | CE3 | TRP | 26B | -0.816 | -14.026 | -3.006 | 1.00 | 0.00 |
| ATOM | 1044 | CZ2 | TRP | 26B | -1.523 | -13.636 | -0.277 | 1.00 | 0.00 |
| ATOM | 1045 | CZ3 | TRP | 26B | -1.402 | -12.834 | -2.576 | 1.00 | 0.00 |
| ATOM | 1046 | CH2 | TRP | 26B | -1.750 | -12.641 | -1.232 | 1.00 | 0.00 |

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| ATOM | 1047 | N | LEU | 27B | 0.738 | -18.499 | -6.240 | 1.00 | 0.00 |
| ATOM | 1048 | CA | LEU | 27B | 1.163 | -18.735 | -7.650 | 1.00 | 0.00 |
| ATOM | 1049 | C | LEU | 27B | 0.039 | -19.124 | -8.678 | 1.00 | 0.00 |
| ATOM | 1050 | O | LEU | 27B | 0.164 | -18.734 | -9.836 | 1.00 | 0.00 |
| ATOM | 1051 | CB | LEU | 27B | 2.445 | -19.613 | -7.649 | 1.00 | 0.00 |
| ATOM | 1052 | CG | LEU | 27B | 2.324 | -21.091 | -7.194 | 1.00 | 0.00 |
| ATOM | 1053 | CD1 | LEU | 27B | 2.040 | -22.054 | -8.361 | 1.00 | 0.00 |
| ATOM | 1054 | CD2 | LEU | 27B | 3.591 | -21.547 | -6.450 | 1.00 | 0.00 |
| ATOM | 1055 | N | ALA | 28B | -1.079 | -19.775 | -8.291 | 1.00 | 0.00 |
| ATOM | 1056 | CA | ALA | 28B | -2.313 | -19.849 | -9.131 | 1.00 | 0.00 |
| ATOM | 1057 | C | ALA | 28B | -3.043 | -18.501 | -9.427 | 1.00 | 0.00 |
| ATOM | 1058 | O | ALA | 28B | -3.349 | -18.222 | -10.590 | 1.00 | 0.00 |
| ATOM | 1059 | CB | ALA | 28B | -3.249 | -20.898 | -8.503 | 1.00 | 0.00 |
| ATOM | 1060 | N | CYS | 29B | -3.269 | -17.640 | -8.414 | 1.00 | 0.00 |
| ATOM | 1061 | CA | CYS | 29B | -3.650 | -16.217 | -8.641 | 1.00 | 0.00 |
| ATOM | 1062 | C | CYS | 29B | -2.674 | -15.378 | -9.538 | 1.00 | 0.00 |
| ATOM | 1063 | O | CYS | 29B | -3.142 | -14.651 | -10.420 | 1.00 | 0.00 |
| ATOM | 1064 | CB | CYS | 29B | -3.879 | -15.588 | -7.251 | 1.00 | 0.00 |
| ATOM | 1065 | SG | CYS | 29B | -4.502 | -13.878 | -7.413 | 1.00 | 0.00 |
| ATOM | 1066 | N | ILE | 30B | -1.341 | -15.514 | -9.370 | 1.00 | 0.00 |
| ATOM | 1067 | CA | ILE | 30B | -0.342 | -14.878 | -10.283 | 1.00 | 0.00 |
| ATOM | 1068 | C | ILE | 30B | -0.246 | -15.565 | -11.697 | 1.00 | 0.00 |
| ATOM | 1069 | O | ILE | 30B | -0.192 | -14.811 | -12.670 | 1.00 | 0.00 |
| ATOM | 1070 | CB | ILE | 30B | 1.037 | -14.594 | -9.586 | 1.00 | 0.00 |
| ATOM | 1071 | CG1 | ILE | 30B | 0.973 | -13.895 | -8.188 | 1.00 | 0.00 |

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| ATOM | 1072 | CG2 | ILE | 30B | 1.984 | -13.768 | -10.496 | 1.00 | 0.00 |
| ATOM | 1073 | CD1 | ILE | 30B | 0.338 | -12.491 | -8.130 | 1.00 | 0.00 |
| ATOM | 1074 | N | TRP | 31B | -0.291 | -16.914 | -11.881 | 1.00 | 0.00 |
| ATOM | 1075 | CA | TRP | 31B | -0.542 | -17.522 | -13.233 | 1.00 | 0.00 |
| ATOM | 1076 | C | TRP | 31B | -1.839 | -17.078 | -13.979 | 1.00 | 0.00 |
| ATOM | 1077 | O | TRP | 31B | -1.813 | -16.925 | -15.204 | 1.00 | 0.00 |
| ATOM | 1078 | CB | TRP | 31B | -0.253 | -19.044 | -13.370 | 1.00 | 0.00 |
| ATOM | 1079 | CG | TRP | 31B | -1.009 | -20.183 | -12.659 | 1.00 | 0.00 |
| ATOM | 1080 | CD1 | TRP | 31B | -0.352 | -21.148 | -11.861 | 1.00 | 0.00 |
| ATOM | 1081 | CD2 | TRP | 31B | -2.291 | -20.702 | -12.853 | 1.00 | 0.00 |
| ATOM | 1082 | NE1 | TRP | 31B | -1.180 | -22.240 | -11.544 | 1.00 | 0.00 |
| ATOM | 1083 | CE2 | TRP | 31B | -2.372 | -21.947 | -12.170 | 1.00 | 0.00 |
| ATOM | 1084 | CE3 | TRP | 31B | -3.421 | -20.212 | -13.551 | 1.00 | 0.00 |
| ATOM | 1085 | CZ2 | TRP | 31B | -3.573 | -22.690 | -12.173 | 1.00 | 0.00 |
| ATOM | 1086 | CZ3 | TRP | 31B | -4.603 | -20.953 | -13.530 | 1.00 | 0.00 |
| ATOM | 1087 | CH2 | TRP | 31B | -4.676 | -22.177 | -12.857 | 1.00 | 0.00 |
| ATOM | 1088 | N | TYR | 32B | -2.940 | -16.808 | -13.254 | 1.00 | 0.00 |
| ATOM | 1089 | CA | TYR | 32B | -4.098 | -16.060 | -13.801 | 1.00 | 0.00 |
| ATOM | 1090 | C | TYR | 32B | -3.740 | -14.585 | -14.203 | 1.00 | 0.00 |
| ATOM | 1091 | O | TYR | 32B | -3.840 | -14.248 | -15.385 | 1.00 | 0.00 |
| ATOM | 1092 | CB | TYR | 32B | -5.268 | -16.239 | -12.791 | 1.00 | 0.00 |
| ATOM | 1093 | CG | TYR | 32B | -6.641 | -15.776 | -13.299 | 1.00 | 0.00 |
| ATOM | 1094 | CD1 | TYR | 32B | -7.364 | -16.568 | -14.198 | 1.00 | 0.00 |
| ATOM | 1095 | CD2 | TYR | 32B | -7.185 | -14.564 | -12.860 | 1.00 | 0.00 |
| ATOM | 1096 | CE1 | TYR | 32B | -8.605 | -16.143 | -14.667 | 1.00 | 0.00 |

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| ATOM | 1097 | CE2 | TYR | 32B | -8.430 | -14.145 | -13.325 | 1.00 | 0.00 |
| ATOM | 1098 | CZ | TYR | 32B | -9.136 | -14.933 | -14.231 | 1.00 | 0.00 |
| ATOM | 1099 | OH | TYR | 32B | -10.356 | -14.523 | -14.697 | 1.00 | 0.00 |
| ATOM | 1100 | N | ALA | 33B | -3.272 | -13.734 | -13.270 | 1.00 | 0.00 |
| ATOM | 1101 | CA | ALA | 33B | -2.868 | -12.333 | -13.572 | 1.00 | 0.00 |
| ATOM | 1102 | C | ALA | 33B | -1.775 | -12.099 | -14.676 | 1.00 | 0.00 |
| ATOM | 1103 | O | ALA | 33B | -2.004 | -11.273 | -15.565 | 1.00 | 0.00 |
| ATOM | 1104 | CB | ALA | 33B | -2.508 | -11.687 | -12.225 | 1.00 | 0.00 |
| ATOM | 1105 | N | ILE | 34B | -0.638 | -12.830 | -14.678 | 1.00 | 0.00 |
| ATOM | 1106 | CA | ILE | 34B | 0.341 | -12.805 | -15.821 | 1.00 | 0.00 |
| ATOM | 1107 | C | ILE | 34B | -0.208 | -13.403 | -17.165 | 1.00 | 0.00 |
| ATOM | 1108 | O | ILE | 34B | 0.036 | -12.809 | -18.215 | 1.00 | 0.00 |
| ATOM | 1109 | CB | ILE | 34B | 1.777 | -13.338 | -15.459 | 1.00 | 0.00 |
| ATOM | 1110 | CG1 | ILE | 34B | 1.889 | -14.867 | -15.175 | 1.00 | 0.00 |
| ATOM | 1111 | CG2 | ILE | 34B | 2.448 | -12.534 | -14.320 | 1.00 | 0.00 |
| ATOM | 1112 | CD1 | ILE | 34B | 2.438 | -15.696 | -16.349 | 1.00 | 0.00 |
| ATOM | 1113 | N | GLY | 35B | -0.973 | -14.518 | -17.158 | 1.00 | 0.00 |
| ATOM | 1114 | CA | GLY | 35B | -1.661 | -15.050 | -18.374 | 1.00 | 0.00 |
| ATOM | 1115 | C | GLY | 35B | -2.646 | -14.123 | -19.136 | 1.00 | 0.00 |
| ATOM | 1116 | O | GLY | 35B | -2.583 | -14.027 | -20.357 | 1.00 | 0.00 |
| ATOM | 1117 | N | ASN | 36B | -3.497 | -13.371 | -18.422 | 1.00 | 0.00 |
| ATOM | 1118 | CA | ASN | 36B | -4.395 | -12.343 | -18.953 | 1.00 | 0.00 |
| ATOM | 1119 | C | ASN | 36B | -3.658 | -11.203 | -19.657 | 1.00 | 0.00 |
| ATOM | 1120 | O | ASN | 36B | -4.236 | -10.509 | -20.488 | 1.00 | 0.00 |
| ATOM | 1121 | CB | ASN | 36B | -5.286 | -11.793 | -17.800 | 1.00 | 0.00 |

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|------|------|-----|-----|-----|--------|---------|---------|------|------|
| ATOM | 1122 | CG | ASN | 36B | -6.440 | -12.685 | -17.330 | 1.00 | 0.00 |
| ATOM | 1123 | OD1 | ASN | 36B | -7.387 | -12.962 | -18.052 | 1.00 | 0.00 |
| ATOM | 1124 | ND2 | ASN | 36B | -6.422 | -13.145 | -16.108 | 1.00 | 0.00 |
| ATOM | 1125 | N | MET | 37B | -2.387 | -11.005 | -19.320 | 1.00 | 0.00 |
| ATOM | 1126 | CA | MET | 37B | -1.592 | -9.939 | -19.926 | 1.00 | 0.00 |
| ATOM | 1127 | C | MET | 37B | -0.613 | -10.457 | -20.985 | 1.00 | 0.00 |
| ATOM | 1128 | O | MET | 37B | -0.196 | -9.707 | -21.864 | 1.00 | 0.00 |
| ATOM | 1129 | CB | MET | 37B | -0.841 | -9.156 | -18.813 | 1.00 | 0.00 |
| ATOM | 1130 | CG | MET | 37B | -1.684 | -8.134 | -18.022 | 1.00 | 0.00 |
| ATOM | 1131 | SD | MET | 37B | -0.627 | -7.217 | -16.890 | 1.00 | 0.00 |
| ATOM | 1132 | CE | MET | 37B | -1.879 | -6.155 | -16.157 | 1.00 | 0.00 |
| ATOM | 1133 | N | GLU | 38B | -0.248 | -11.736 | -20.899 | 1.00 | 0.00 |
| ATOM | 1134 | CA | GLU | 38B | 0.675 | -12.352 | -21.857 | 1.00 | 0.00 |
| ATOM | 1135 | C | GLU | 38B | -0.051 | -12.782 | -23.132 | 1.00 | 0.00 |
| ATOM | 1136 | O | GLU | 38B | 0.520 | -12.726 | -24.227 | 1.00 | 0.00 |
| ATOM | 1137 | CB | GLU | 38B | 1.385 | -13.569 | -21.199 | 1.00 | 0.00 |
| ATOM | 1138 | CG | GLU | 38B | 2.516 | -14.236 | -22.047 | 1.00 | 0.00 |
| ATOM | 1139 | CD | GLU | 38B | 3.814 | -13.474 | -22.243 | 1.00 | 0.00 |
| ATOM | 1140 | OE1 | GLU | 38B | 4.084 | -12.479 | -21.544 | 1.00 | 0.00 |
| ATOM | 1141 | OE2 | GLU | 38B | 4.588 | -13.909 | -23.120 | 1.00 | 0.00 |
| ATOM | 1142 | N | GLN | 39B | -1.304 | -13.216 | -22.980 | 1.00 | 0.00 |
| ATOM | 1143 | CA | GLN | 39B | -2.137 | -13.653 | -24.108 | 1.00 | 0.00 |
| ATOM | 1144 | C | GLN | 39B | -2.531 | -12.445 | -24.969 | 1.00 | 0.00 |
| ATOM | 1145 | O | GLN | 39B | -2.080 | -11.327 | -24.712 | 1.00 | 0.00 |
| ATOM | 1146 | CB | GLN | 39B | -3.388 | -14.386 | -23.578 | 1.00 | 0.00 |

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| ATOM | 1147 | CG | GLN | 39B | -3.135 | -15.753 | -22.858 | 1.00 | 0.00 |
| ATOM | 1148 | CD | GLN | 39B | -4.333 | -16.556 | -22.336 | 1.00 | 0.00 |
| ATOM | 1149 | OE1 | GLN | 39B | -5.209 | -16.946 | -23.092 | 1.00 | 0.00 |
| ATOM | 1150 | NE2 | GLN | 39B | -4.441 | -16.812 | -21.057 | 1.00 | 0.00 |
| ATOM | 1151 | N | PRO | 40B | -3.367 | -12.662 | -25.984 | 1.00 | 0.00 |
| ATOM | 1152 | CA | PRO | 40B | -3.791 | -11.575 | -26.877 | 1.00 | 0.00 |
| ATOM | 1153 | C | PRO | 40B | -2.576 | -10.841 | -27.475 | 1.00 | 0.00 |
| ATOM | 1154 | O | PRO | 40B | -2.650 | -9.651 | -27.814 | 1.00 | 0.00 |
| ATOM | 1155 | CB | PRO | 40B | -4.739 | -10.640 | -26.110 | 1.00 | 0.00 |
| ATOM | 1156 | CG | PRO | 40B | -4.198 | -10.676 | -24.672 | 1.00 | 0.00 |
| ATOM | 1157 | CD | PRO | 40B | -3.764 | -12.133 | -24.495 | 1.00 | 0.00 |
| ATOM | 1158 | N | HIS | 41B | -1.462 | -11.566 | -27.595 | 1.00 | 0.00 |
| ATOM | 1159 | CA | HIS | 41B | -0.217 | -11.035 | -28.156 | 1.00 | 0.00 |
| ATOM | 1160 | C | HIS | 41B | 0.555 | -12.152 | -28.871 | 1.00 | 0.00 |
| ATOM | 1161 | O | HIS | 41B | 0.788 | -13.223 | -28.299 | 1.00 | 0.00 |
| ATOM | 1162 | CB | HIS | 41B | 0.622 | -10.375 | -27.013 | 1.00 | 0.00 |
| ATOM | 1163 | CG | HIS | 41B | 0.084 | -9.076 | -26.416 | 1.00 | 0.00 |
| ATOM | 1164 | ND1 | HIS | 41B | -0.683 | -8.960 | -25.266 | 1.00 | 0.00 |
| ATOM | 1165 | CD2 | HIS | 41B | 0.299 | -7.799 | -26.970 | 1.00 | 0.00 |
| ATOM | 1166 | CE1 | HIS | 41B | -0.873 | -7.608 | -25.201 | 1.00 | 0.00 |
| ATOM | 1167 | NE2 | HIS | 41B | -0.324 | -6.829 | -26.188 | 1.00 | 0.00 |
| ATOM | 1168 | N | MET | 42B | 0.939 | -11.899 | -30.122 | 1.00 | 0.00 |
| ATOM | 1169 | CA | MET | 42B | 1.681 | -12.873 | -30.919 | 1.00 | 0.00 |
| ATOM | 1170 | C | MET | 42B | 3.081 | -13.091 | -30.351 | 1.00 | 0.00 |
| ATOM | 1171 | O | MET | 42B | 3.582 | -12.274 | -29.570 | 1.00 | 0.00 |

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| ATOM | 1172 | CB | MET | 42B | 1.750 | -12.394 | -32.395 | 1.00 | 0.00 |
| ATOM | 1173 | CG | MET | 42B | 0.400 | -12.307 | -33.139 | 1.00 | 0.00 |
| ATOM | 1174 | SD | MET | 42B | -0.262 | -13.961 | -33.399 | 1.00 | 0.00 |
| ATOM | 1175 | CE | MET | 42B | 0.818 | -14.472 | -34.743 | 1.00 | 0.00 |
| ATOM | 1176 | N | PRO | 43B | 3.703 | -14.200 | -30.745 | 1.00 | 0.00 |
| ATOM | 1177 | CA | PRO | 43B | 5.049 | -14.559 | -30.294 | 1.00 | 0.00 |
| ATOM | 1178 | C | PRO | 43B | 5.141 | -14.865 | -28.787 | 1.00 | 0.00 |
| ATOM | 1179 | O | PRO | 43B | 6.231 | -15.126 | -28.267 | 1.00 | 0.00 |
| ATOM | 1180 | CB | PRO | 43B | 6.019 | -13.456 | -30.744 | 1.00 | 0.00 |
| ATOM | 1181 | CG | PRO | 43B | 5.200 | -12.166 | -30.585 | 1.00 | 0.00 |
| ATOM | 1182 | CD | PRO | 43B | 3.793 | -12.587 | -31.015 | 1.00 | 0.00 |
| ATOM | 1183 | N | SER | 44B | 4.002 | -14.841 | -28.094 | 1.00 | 0.00 |
| ATOM | 1184 | CA | SER | 44B | 3.963 | -15.122 | -26.655 | 1.00 | 0.00 |
| ATOM | 1185 | C | SER | 44B | 3.781 | -16.618 | -26.379 | 1.00 | 0.00 |
| ATOM | 1186 | O | SER | 44B | 2.807 | -17.226 | -26.832 | 1.00 | 0.00 |
| ATOM | 1187 | CB | SER | 44B | 2.837 | -14.281 | -26.004 | 1.00 | 0.00 |
| ATOM | 1188 | OG | SER | 44B | 3.132 | -12.880 | -25.977 | 1.00 | 0.00 |
| ATOM | 1189 | N | ILE | 45B | 4.720 | -17.202 | -25.632 | 1.00 | 0.00 |
| ATOM | 1190 | CA | ILE | 45B | 4.679 | -18.629 | -25.296 | 1.00 | 0.00 |
| ATOM | 1191 | C | ILE | 45B | 3.889 | -18.881 | -24.015 | 1.00 | 0.00 |
| ATOM | 1192 | O | ILE | 45B | 4.224 | -19.774 | -23.232 | 1.00 | 0.00 |
| ATOM | 1193 | CB | ILE | 45B | 6.160 | -19.179 | -25.193 | 1.00 | 0.00 |
| ATOM | 1194 | CG1 | ILE | 45B | 6.275 | -20.737 | -25.168 | 1.00 | 0.00 |
| ATOM | 1195 | CG2 | ILE | 45B | 6.930 | -18.616 | -23.958 | 1.00 | 0.00 |
| ATOM | 1196 | CD1 | ILE | 45B | 7.687 | -21.312 | -25.405 | 1.00 | 0.00 |

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| ATOM | 1197 | N | LYS | 46B | 2.834 | -18.092 | -23.820 | 1.00 | 0.00 |
| ATOM | 1198 | CA | LYS | 46B | 1.980 | -18.204 | -22.642 | 1.00 | 0.00 |
| ATOM | 1199 | C | LYS | 46B | 0.481 | -18.313 | -22.976 | 1.00 | 0.00 |
| ATOM | 1200 | O | LYS | 46B | -0.350 | -17.620 | -22.370 | 1.00 | 0.00 |
| ATOM | 1201 | CB | LYS | 46B | 2.241 | -16.985 | -21.707 | 1.00 | 0.00 |
| ATOM | 1202 | CG | LYS | 46B | 3.722 | -16.849 | -21.246 | 1.00 | 0.00 |
| ATOM | 1203 | CD | LYS | 46B | 4.170 | -17.851 | -20.172 | 1.00 | 0.00 |
| ATOM | 1204 | CE | LYS | 46B | 5.649 | -17.599 | -19.816 | 1.00 | 0.00 |
| ATOM | 1205 | NZ | LYS | 46B | 6.075 | -18.575 | -18.774 | 1.00 | 0.00 |
| ATOM | 1206 | N | ASP | 47B | 0.114 | -19.180 | -23.945 | 1.00 | 0.00 |
| ATOM | 1207 | CA | ASP | 47B | -1.303 | -19.327 | -24.304 | 1.00 | 0.00 |
| ATOM | 1208 | C | ASP | 47B | -2.143 | -19.911 | -23.162 | 1.00 | 0.00 |
| ATOM | 1209 | O | ASP | 47B | -2.896 | -19.193 | -22.506 | 1.00 | 0.00 |
| ATOM | 1210 | CB | ASP | 47B | -1.278 | -20.290 | -25.524 | 1.00 | 0.00 |
| ATOM | 1211 | CG | ASP | 47B | -2.605 | -20.427 | -26.284 | 1.00 | 0.00 |
| ATOM | 1212 | OD1 | ASP | 47B | -3.579 | -19.726 | -25.940 | 1.00 | 0.00 |
| ATOM | 1213 | OD2 | ASP | 47B | -2.684 | -21.272 | -27.200 | 1.00 | 0.00 |
| ATOM | 1214 | N | LYS | 48B | -1.992 | -21.213 | -22.929 | 1.00 | 0.00 |
| ATOM | 1215 | CA | LYS | 48B | -2.735 | -21.916 | -21.881 | 1.00 | 0.00 |
| ATOM | 1216 | C | LYS | 48B | -2.280 | -21.556 | -20.465 | 1.00 | 0.00 |
| ATOM | 1217 | O | LYS | 48B | -1.256 | -20.895 | -20.274 | 1.00 | 0.00 |
| ATOM | 1218 | CB | LYS | 48B | -2.625 | -23.452 | -22.115 | 1.00 | 0.00 |
| ATOM | 1219 | CG | LYS | 48B | -3.911 | -24.094 | -22.712 | 1.00 | 0.00 |
| ATOM | 1220 | CD | LYS | 48B | -4.153 | -23.814 | -24.202 | 1.00 | 0.00 |
| ATOM | 1221 | CE | LYS | 48B | -5.454 | -24.508 | -24.653 | 1.00 | 0.00 |

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| ATOM | 1222 | NZ | LYS | 48B | -5.681 | -24.231 | -26.099 | 1.00 | 0.00 |
| ATOM | 1223 | N | TYR | 49B | -3.052 | -22.003 | -19.474 | 1.00 | 0.00 |
| ATOM | 1224 | CA | TYR | 49B | -2.742 | -21.749 | -18.068 | 1.00 | 0.00 |
| ATOM | 1225 | C | TYR | 49B | -1.838 | -22.837 | -17.488 | 1.00 | 0.00 |
| ATOM | 1226 | O | TYR | 49B | -0.912 | -22.538 | -16.737 | 1.00 | 0.00 |
| ATOM | 1227 | CB | TYR | 49B | -4.024 | -21.670 | -17.189 | 1.00 | 0.00 |
| ATOM | 1228 | CG | TYR | 49B | -4.967 | -20.490 | -17.451 | 1.00 | 0.00 |
| ATOM | 1229 | CD1 | TYR | 49B | -6.083 | -20.640 | -18.280 | 1.00 | 0.00 |
| ATOM | 1230 | CD2 | TYR | 49B | -4.715 | -19.254 | -16.848 | 1.00 | 0.00 |
| ATOM | 1231 | CE1 | TYR | 49B | -6.940 | -19.563 | -18.497 | 1.00 | 0.00 |
| ATOM | 1232 | CE2 | TYR | 49B | -5.573 | -18.180 | -17.068 | 1.00 | 0.00 |
| ATOM | 1233 | CZ | TYR | 49B | -6.685 | -18.336 | -17.892 | 1.00 | 0.00 |
| ATOM | 1234 | OH | TYR | 49B | -7.530 | -17.284 | -18.106 | 1.00 | 0.00 |
| ATOM | 1235 | N | VAL | 50B | -2.105 | -24.116 | -17.818 | 1.00 | 0.00 |
| ATOM | 1236 | CA | VAL | 50B | -1.280 | -25.215 | -17.299 | 1.00 | 0.00 |
| ATOM | 1237 | C | VAL | 50B | 0.211 | -24.980 | -17.513 | 1.00 | 0.00 |
| ATOM | 1238 | O | VAL | 50B | 1.039 | -25.399 | -16.699 | 1.00 | 0.00 |
| ATOM | 1239 | CB | VAL | 50B | -1.775 | -26.471 | -18.121 | 1.00 | 0.00 |
| ATOM | 1240 | CG1 | VAL | 50B | -0.979 | -27.789 | -17.910 | 1.00 | 0.00 |
| ATOM | 1241 | CG2 | VAL | 50B | -3.256 | -26.843 | -17.867 | 1.00 | 0.00 |
| ATOM | 1242 | N | THR | 51B | 0.545 | -24.311 | -18.614 | 1.00 | 0.00 |
| ATOM | 1243 | CA | THR | 51B | 1.935 | -24.004 | -18.936 | 1.00 | 0.00 |
| ATOM | 1244 | C | THR | 51B | 2.403 | -22.788 | -18.130 | 1.00 | 0.00 |
| ATOM | 1245 | O | THR | 51B | 3.600 | -22.618 | -17.874 | 1.00 | 0.00 |
| ATOM | 1246 | CB | THR | 51B | 2.084 | -23.739 | -20.473 | 1.00 | 0.00 |

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|------|------|-----|-----|-----|--------|---------|---------|------|------|
| ATOM | 1247 | OG1 | THR | 51B | 1.489 | -24.793 | -21.219 | 1.00 | 0.00 |
| ATOM | 1248 | CG2 | THR | 51B | 3.526 | -23.648 | -21.015 | 1.00 | 0.00 |
| ATOM | 1249 | N | ALA | 52B | 1.447 | -21.948 | -17.735 | 1.00 | 0.00 |
| ATOM | 1250 | CA | ALA | 52B | 1.735 | -20.761 | -16.935 | 1.00 | 0.00 |
| ATOM | 1251 | C | ALA | 52B | 2.139 | -21.211 | -15.531 | 1.00 | 0.00 |
| ATOM | 1252 | O | ALA | 52B | 2.838 | -20.492 | -14.812 | 1.00 | 0.00 |
| ATOM | 1253 | CB | ALA | 52B | 0.505 | -19.861 | -16.869 | 1.00 | 0.00 |
| ATOM | 1254 | N | LEU | 53B | 1.683 | -22.408 | -15.156 | 1.00 | 0.00 |
| ATOM | 1255 | CA | LEU | 53B | 1.990 | -23.012 | -13.859 | 1.00 | 0.00 |
| ATOM | 1256 | C | LEU | 53B | 3.473 | -23.332 | -13.765 | 1.00 | 0.00 |
| ATOM | 1257 | O | LEU | 53B | 4.113 | -23.057 | -12.748 | 1.00 | 0.00 |
| ATOM | 1258 | CB | LEU | 53B | 1.131 | -24.294 | -13.667 | 1.00 | 0.00 |
| ATOM | 1259 | CG | LEU | 53B | 1.031 | -24.900 | -12.242 | 1.00 | 0.00 |
| ATOM | 1260 | CD1 | LEU | 53B | -0.075 | -25.964 | -12.197 | 1.00 | 0.00 |
| ATOM | 1261 | CD2 | LEU | 53B | 2.358 | -25.511 | -11.761 | 1.00 | 0.00 |
| ATOM | 1262 | N | TYR | 54B | 4.007 | -23.930 | -14.829 | 1.00 | 0.00 |
| ATOM | 1263 | CA | TYR | 54B | 5.418 | -24.291 | -14.879 | 1.00 | 0.00 |
| ATOM | 1264 | C | TYR | 54B | 6.283 | -23.048 | -14.727 | 1.00 | 0.00 |
| ATOM | 1265 | O | TYR | 54B | 7.198 | -23.014 | -13.906 | 1.00 | 0.00 |
| ATOM | 1266 | CB | TYR | 54B | 5.780 | -24.966 | -16.234 | 1.00 | 0.00 |
| ATOM | 1267 | CG | TYR | 54B | 5.163 | -26.343 | -16.504 | 1.00 | 0.00 |
| ATOM | 1268 | CD1 | TYR | 54B | 4.338 | -26.953 | -15.555 | 1.00 | 0.00 |
| ATOM | 1269 | CD2 | TYR | 54B | 5.439 | -27.004 | -17.706 | 1.00 | 0.00 |
| ATOM | 1270 | CE1 | TYR | 54B | 3.789 | -28.208 | -15.810 | 1.00 | 0.00 |
| ATOM | 1271 | CE2 | TYR | 54B | 4.890 | -28.258 | -17.957 | 1.00 | 0.00 |

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|------|------|-----|-----|-----|-------|---------|---------|------|------|
| ATOM | 1272 | CZ | TYR | 54B | 4.066 | -28.858 | -17.009 | 1.00 | 0.00 |
| ATOM | 1273 | OH | TYR | 54B | 3.523 | -30.088 | -17.256 | 1.00 | 0.00 |
| ATOM | 1274 | N | PHE | 55B | 5.989 | -22.029 | -15.527 | 1.00 | 0.00 |
| ATOM | 1275 | CA | PHE | 55B | 6.733 | -20.785 | -15.461 | 1.00 | 0.00 |
| ATOM | 1276 | C | PHE | 55B | 6.772 | -20.254 | -14.030 | 1.00 | 0.00 |
| ATOM | 1277 | O | PHE | 55B | 7.847 | -19.985 | -13.488 | 1.00 | 0.00 |
| ATOM | 1278 | CB | PHE | 55B | 6.067 | -19.713 | -16.376 | 1.00 | 0.00 |
| ATOM | 1279 | CG | PHE | 55B | 6.566 | -18.269 | -16.213 | 1.00 | 0.00 |
| ATOM | 1280 | CD1 | PHE | 55B | 7.774 | -17.883 | -16.806 | 1.00 | 0.00 |
| ATOM | 1281 | CD2 | PHE | 55B | 5.833 | -17.336 | -15.475 | 1.00 | 0.00 |
| ATOM | 1282 | CE1 | PHE | 55B | 8.252 | -16.587 | -16.646 | 1.00 | 0.00 |
| ATOM | 1283 | CE2 | PHE | 55B | 6.307 | -16.035 | -15.326 | 1.00 | 0.00 |
| ATOM | 1284 | CZ | PHE | 55B | 7.517 | -15.662 | -15.908 | 1.00 | 0.00 |
| ATOM | 1285 | N | THR | 56B | 5.624 | -20.078 | -13.310 | 1.00 | 0.00 |
| ATOM | 1286 | CA | THR | 56B | 5.624 | -19.636 | -11.879 | 1.00 | 0.00 |
| ATOM | 1287 | C | THR | 56B | 5.954 | -20.745 | -10.806 | 1.00 | 0.00 |
| ATOM | 1288 | O | THR | 56B | 5.327 | -20.791 | -9.741 | 1.00 | 0.00 |
| ATOM | 1289 | CB | THR | 56B | 4.355 | -18.788 | -11.566 | 1.00 | 0.00 |
| ATOM | 1290 | OG1 | THR | 56B | 4.507 | -18.203 | -10.280 | 1.00 | 0.00 |
| ATOM | 1291 | CG2 | THR | 56B | 3.024 | -19.546 | -11.525 | 1.00 | 0.00 |
| ATOM | 1292 | N | PHE | 57B | 6.989 | -21.575 | -11.038 | 1.00 | 0.00 |
| ATOM | 1293 | CA | PHE | 57B | 7.454 | -22.601 | -10.062 | 1.00 | 0.00 |
| ATOM | 1294 | C | PHE | 57B | 8.984 | -22.901 | -10.203 | 1.00 | 0.00 |
| ATOM | 1295 | O | PHE | 57B | 9.726 | -22.698 | -9.237 | 1.00 | 0.00 |
| ATOM | 1296 | CB | PHE | 57B | 6.546 | -23.870 | -10.113 | 1.00 | 0.00 |

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|------|------|-----|-----|-----|--------|---------|---------|------|------|
| ATOM | 1297 | CG | PHE | 57B | 6.575 | -24.696 | -8.815 | 1.00 | 0.00 |
| ATOM | 1298 | CD1 | PHE | 57B | 5.660 | -24.416 | -7.795 | 1.00 | 0.00 |
| ATOM | 1299 | CD2 | PHE | 57B | 7.540 | -25.690 | -8.615 | 1.00 | 0.00 |
| ATOM | 1300 | CE1 | PHE | 57B | 5.716 | -25.108 | -6.588 | 1.00 | 0.00 |
| ATOM | 1301 | CE2 | PHE | 57B | 7.594 | -26.383 | -7.407 | 1.00 | 0.00 |
| ATOM | 1302 | CZ | PHE | 57B | 6.684 | -26.090 | -6.394 | 1.00 | 0.00 |
| ATOM | 1303 | N | SER | 58B | 9.472 | -23.387 | -11.365 | 1.00 | 0.00 |
| ATOM | 1304 | CA | SER | 58B | 10.919 | -23.722 | -11.555 | 1.00 | 0.00 |
| ATOM | 1305 | C | SER | 58B | 11.874 | -22.512 | -11.834 | 1.00 | 0.00 |
| ATOM | 1306 | O | SER | 58B | 12.943 | -22.437 | -11.220 | 1.00 | 0.00 |
| ATOM | 1307 | CB | SER | 58B | 11.033 | -24.837 | -12.614 | 1.00 | 0.00 |
| ATOM | 1308 | OG | SER | 58B | 12.366 | -25.343 | -12.658 | 1.00 | 0.00 |
| ATOM | 1309 | N | SER | 59B | 11.497 | -21.537 | -12.687 | 1.00 | 0.00 |
| ATOM | 1310 | CA | SER | 59B | 12.157 | -20.192 | -12.709 | 1.00 | 0.00 |
| ATOM | 1311 | C | SER | 59B | 12.136 | -19.372 | -11.369 | 1.00 | 0.00 |
| ATOM | 1312 | O | SER | 59B | 13.072 | -18.617 | -11.104 | 1.00 | 0.00 |
| ATOM | 1313 | CB | SER | 59B | 11.575 | -19.365 | -13.880 | 1.00 | 0.00 |
| ATOM | 1314 | OG | SER | 59B | 11.920 | -19.923 | -15.150 | 1.00 | 0.00 |
| ATOM | 1315 | N | LEU | 60B | 11.109 | -19.546 | -10.521 | 1.00 | 0.00 |
| ATOM | 1316 | CA | LEU | 60B | 11.110 | -19.073 | -9.108 | 1.00 | 0.00 |
| ATOM | 1317 | C | LEU | 60B | 12.092 | -19.854 | -8.172 | 1.00 | 0.00 |
| ATOM | 1318 | O | LEU | 60B | 12.935 | -19.237 | -7.516 | 1.00 | 0.00 |
| ATOM | 1319 | CB | LEU | 60B | 9.644 | -19.153 | -8.573 | 1.00 | 0.00 |
| ATOM | 1320 | CG | LEU | 60B | 8.689 | -17.971 | -8.860 | 1.00 | 0.00 |
| ATOM | 1321 | CD1 | LEU | 60B | 8.516 | -17.697 | -10.364 | 1.00 | 0.00 |

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|------|------|-----|-----|-----|--------|---------|---------|------|------|
| ATOM | 1322 | CD2 | LEU | 60B | 7.325 | -18.265 | -8.212 | 1.00 | 0.00 |
| ATOM | 1323 | N | THR | 61B | 11.944 | -21.188 | -8.051 | 1.00 | 0.00 |
| ATOM | 1324 | CA | THR | 61B | 12.610 | -22.004 | -6.988 | 1.00 | 0.00 |
| ATOM | 1325 | C | THR | 61B | 14.085 | -22.392 | -7.342 | 1.00 | 0.00 |
| ATOM | 1326 | O | THR | 61B | 14.415 | -23.555 | -7.590 | 1.00 | 0.00 |
| ATOM | 1327 | CB | THR | 61B | 11.710 | -23.227 | -6.602 | 1.00 | 0.00 |
| ATOM | 1328 | OG1 | THR | 61B | 11.358 | -24.015 | -7.737 | 1.00 | 0.00 |
| ATOM | 1329 | CG2 | THR | 61B | 10.400 | -22.870 | -5.878 | 1.00 | 0.00 |
| ATOM | 1330 | N | SER | 62B | 14.984 | -21.386 | -7.337 | 1.00 | 0.00 |
| ATOM | 1331 | CA | SER | 62B | 16.457 | -21.551 | -7.550 | 1.00 | 0.00 |
| ATOM | 1332 | C | SER | 62B | 17.020 | -22.135 | -8.895 | 1.00 | 0.00 |
| ATOM | 1333 | O | SER | 62B | 18.241 | -22.083 | -9.074 | 1.00 | 0.00 |
| ATOM | 1334 | CB | SER | 62B | 17.112 | -22.219 | -6.313 | 1.00 | 0.00 |
| ATOM | 1335 | OG | SER | 62B | 18.536 | -22.111 | -6.377 | 1.00 | 0.00 |
| ATOM | 1336 | N | VAL | 63B | 16.201 | -22.678 | -9.814 | 1.00 | 0.00 |
| ATOM | 1337 | CA | VAL | 63B | 16.696 | -23.334 | -11.067 | 1.00 | 0.00 |
| ATOM | 1338 | C | VAL | 63B | 16.977 | -22.277 | -12.186 | 1.00 | 0.00 |
| ATOM | 1339 | O | VAL | 63B | 18.128 | -22.151 | -12.611 | 1.00 | 0.00 |
| ATOM | 1340 | CB | VAL | 63B | 15.759 | -24.523 | -11.498 | 1.00 | 0.00 |
| ATOM | 1341 | CG1 | VAL | 63B | 16.203 | -25.217 | -12.808 | 1.00 | 0.00 |
| ATOM | 1342 | CG2 | VAL | 63B | 15.630 | -25.638 | -10.431 | 1.00 | 0.00 |
| ATOM | 1343 | N | GLY | 64B | 15.951 | -21.558 | -12.688 | 1.00 | 0.00 |
| ATOM | 1344 | CA | GLY | 64B | 16.143 | -20.571 | -13.789 | 1.00 | 0.00 |
| ATOM | 1345 | C | GLY | 64B | 16.320 | -21.156 | -15.208 | 1.00 | 0.00 |
| ATOM | 1346 | O | GLY | 64B | 17.371 | -20.958 | -15.819 | 1.00 | 0.00 |

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|------|------|-----|-----|-----|--------|---------|---------|------|------|
| ATOM | 1347 | N | PHE | 65B | 15.302 | -21.859 | -15.741 | 1.00 | 0.00 |
| ATOM | 1348 | CA | PHE | 65B | 15.437 | -22.577 | -17.045 | 1.00 | 0.00 |
| ATOM | 1349 | C | PHE | 65B | 15.594 | -21.685 | -18.319 | 1.00 | 0.00 |
| ATOM | 1350 | O | PHE | 65B | 16.572 | -21.873 | -19.047 | 1.00 | 0.00 |
| ATOM | 1351 | CB | PHE | 65B | 14.288 | -23.619 | -17.224 | 1.00 | 0.00 |
| ATOM | 1352 | CG | PHE | 65B | 14.455 | -24.988 | -16.542 | 1.00 | 0.00 |
| ATOM | 1353 | CD1 | PHE | 65B | 13.448 | -25.484 | -15.710 | 1.00 | 0.00 |
| ATOM | 1354 | CD2 | PHE | 65B | 15.554 | -25.804 | -16.844 | 1.00 | 0.00 |
| ATOM | 1355 | CE1 | PHE | 65B | 13.542 | -26.769 | -15.179 | 1.00 | 0.00 |
| ATOM | 1356 | CE2 | PHE | 65B | 15.656 | -27.081 | -16.298 | 1.00 | 0.00 |
| ATOM | 1357 | CZ | PHE | 65B | 14.648 | -27.563 | -15.468 | 1.00 | 0.00 |
| ATOM | 1358 | N | GLY | 66B | 14.626 | -20.798 | -18.647 | 1.00 | 0.00 |
| ATOM | 1359 | CA | GLY | 66B | 14.657 | -20.031 | -19.877 | 1.00 | 0.00 |
| ATOM | 1360 | C | GLY | 66B | 13.778 | -20.644 | -20.953 | 1.00 | 0.00 |
| ATOM | 1361 | O | GLY | 66B | 13.819 | -20.211 | -22.106 | 1.00 | 0.00 |
| ATOM | 1362 | N | ASN | 67B | 12.992 | -21.656 | -20.585 | 1.00 | 0.00 |
| ATOM | 1363 | CA | ASN | 67B | 12.091 | -22.304 | -21.533 | 1.00 | 0.00 |
| ATOM | 1364 | C | ASN | 67B | 10.800 | -21.485 | -21.680 | 1.00 | 0.00 |
| ATOM | 1365 | O | ASN | 67B | 10.008 | -21.725 | -22.591 | 1.00 | 0.00 |
| ATOM | 1366 | CB | ASN | 67B | 11.771 | -23.762 | -21.091 | 1.00 | 0.00 |
| ATOM | 1367 | CG | ASN | 67B | 11.114 | -23.943 | -19.718 | 1.00 | 0.00 |
| ATOM | 1368 | OD1 | ASN | 67B | 11.326 | -23.178 | -18.789 | 1.00 | 0.00 |
| ATOM | 1369 | ND2 | ASN | 67B | 10.319 | -24.962 | -19.530 | 1.00 | 0.00 |
| ATOM | 1370 | N | VAL | 68B | 10.609 | -20.507 | -20.792 | 1.00 | 0.00 |
| ATOM | 1371 | CA | VAL | 68B | 9.444 | -19.617 | -20.819 | 1.00 | 0.00 |

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| ATOM | 1372 | C | VAL | 68B | 9.758 | -18.272 | -20.147 | 1.00 | 0.00 |
| ATOM | 1373 | O | VAL | 68B | 10.212 | -18.246 | -19.001 | 1.00 | 0.00 |
| ATOM | 1374 | CB | VAL | 68B | 8.216 | -20.322 | -20.118 | 1.00 | 0.00 |
| ATOM | 1375 | CG1 | VAL | 68B | 7.687 | -21.618 | -20.793 | 1.00 | 0.00 |
| ATOM | 1376 | CG2 | VAL | 68B | 8.473 | -20.708 | -18.641 | 1.00 | 0.00 |
| ATOM | 1377 | N | SER | 69B | 9.521 | -17.166 | -20.864 | 1.00 | 0.00 |
| ATOM | 1378 | CA | SER | 69B | 9.773 | -15.802 | -20.363 | 1.00 | 0.00 |
| ATOM | 1379 | C | SER | 69B | 8.795 | -14.758 | -20.946 | 1.00 | 0.00 |
| ATOM | 1380 | O | SER | 69B | 8.462 | -14.818 | -22.125 | 1.00 | 0.00 |
| ATOM | 1381 | CB | SER | 69B | 11.248 | -15.429 | -20.657 | 1.00 | 0.00 |
| ATOM | 1382 | OG | SER | 69B | 11.614 | -14.151 | -20.125 | 1.00 | 0.00 |
| ATOM | 1383 | N | PRO | 70B | 8.288 | -13.819 | -20.110 | 1.00 | 0.00 |
| ATOM | 1384 | CA | PRO | 70B | 7.360 | -12.765 | -20.544 | 1.00 | 0.00 |
| ATOM | 1385 | C | PRO | 70B | 7.906 | -11.848 | -21.615 | 1.00 | 0.00 |
| ATOM | 1386 | O | PRO | 70B | 9.044 | -11.388 | -21.526 | 1.00 | 0.00 |
| ATOM | 1387 | CB | PRO | 70B | 7.106 | -11.978 | -19.268 | 1.00 | 0.00 |
| ATOM | 1388 | CG | PRO | 70B | 6.995 | -13.034 | -18.283 | 1.00 | 0.00 |
| ATOM | 1389 | CD | PRO | 70B | 8.103 | -14.042 | -18.663 | 1.00 | 0.00 |
| ATOM | 1390 | N | ASN | 71B | 7.089 | -11.557 | -22.618 | 1.00 | 0.00 |
| ATOM | 1391 | CA | ASN | 71B | 7.529 | -10.661 | -23.665 | 1.00 | 0.00 |
| ATOM | 1392 | C | ASN | 71B | 6.719 | -9.378 | -23.585 | 1.00 | 0.00 |
| ATOM | 1393 | O | ASN | 71B | 7.202 | -8.306 | -23.949 | 1.00 | 0.00 |
| ATOM | 1394 | CB | ASN | 71B | 7.373 | -11.324 | -25.065 | 1.00 | 0.00 |
| ATOM | 1395 | CG | ASN | 71B | 8.295 | -12.507 | -25.378 | 1.00 | 0.00 |
| ATOM | 1396 | OD1 | ASN | 71B | 9.455 | -12.549 | -24.995 | 1.00 | 0.00 |

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|------|------|-----|-----|-----|-------|---------|---------|------|------|
| ATOM | 1397 | ND2 | ASN | 71B | 7.832 | -13.493 | -26.099 | 1.00 | 0.00 |
| ATOM | 1398 | N | THR | 72B | 5.494 | -9.490 | -23.083 | 1.00 | 0.00 |
| ATOM | 1399 | CA | THR | 72B | 4.613 | -8.335 | -22.944 | 1.00 | 0.00 |
| ATOM | 1400 | C | THR | 72B | 4.970 | -7.504 | -21.706 | 1.00 | 0.00 |
| ATOM | 1401 | O | THR | 72B | 5.754 | -7.943 | -20.861 | 1.00 | 0.00 |
| ATOM | 1402 | CB | THR | 72B | 3.129 | -8.782 | -22.853 | 1.00 | 0.00 |
| ATOM | 1403 | OG1 | THR | 72B | 2.933 | -9.590 | -21.685 | 1.00 | 0.00 |
| ATOM | 1404 | CG2 | THR | 72B | 2.744 | -9.592 | -24.086 | 1.00 | 0.00 |
| ATOM | 1405 | N | ASN | 73B | 4.575 | -6.209 | -21.690 | 1.00 | 0.00 |
| ATOM | 1406 | CA | ASN | 73B | 5.139 | -5.205 | -20.727 | 1.00 | 0.00 |
| ATOM | 1407 | C | ASN | 73B | 4.135 | -4.425 | -19.816 | 1.00 | 0.00 |
| ATOM | 1408 | O | ASN | 73B | 4.571 | -3.902 | -18.787 | 1.00 | 0.00 |
| ATOM | 1409 | CB | ASN | 73B | 6.163 | -4.284 | -21.448 | 1.00 | 0.00 |
| ATOM | 1410 | CG | ASN | 73B | 7.528 | -4.952 | -21.680 | 1.00 | 0.00 |
| ATOM | 1411 | OD1 | ASN | 73B | 8.288 | -5.195 | -20.749 | 1.00 | 0.00 |
| ATOM | 1412 | ND2 | ASN | 73B | 7.873 | -5.295 | -22.897 | 1.00 | 0.00 |
| ATOM | 1413 | N | SER | 74B | 2.809 | -4.449 | -20.061 | 1.00 | 0.00 |
| ATOM | 1414 | CA | SER | 74B | 1.807 | -4.354 | -18.945 | 1.00 | 0.00 |
| ATOM | 1415 | C | SER | 74B | 1.928 | -5.465 | -17.835 | 1.00 | 0.00 |
| ATOM | 1416 | O | SER | 74B | 1.744 | -5.177 | -16.650 | 1.00 | 0.00 |
| ATOM | 1417 | CB | SER | 74B | 0.386 | -4.325 | -19.553 | 1.00 | 0.00 |
| ATOM | 1418 | OG | SER | 74B | 0.194 | -3.171 | -20.370 | 1.00 | 0.00 |
| ATOM | 1419 | N | GLU | 75B | 2.308 | -6.702 | -18.220 | 1.00 | 0.00 |
| ATOM | 1420 | CA | GLU | 75B | 2.754 | -7.790 | -17.301 | 1.00 | 0.00 |
| ATOM | 1421 | C | GLU | 75B | 3.855 | -7.454 | -16.223 | 1.00 | 0.00 |

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|------|------|-----|-----|-----|-------|---------|---------|------|------|
| ATOM | 1422 | O | GLU | 75B | 3.845 | -8.081 | -15.160 | 1.00 | 0.00 |
| ATOM | 1423 | CB | GLU | 75B | 3.135 | -8.951 | -18.272 | 1.00 | 0.00 |
| ATOM | 1424 | CG | GLU | 75B | 3.442 | -10.343 | -17.660 | 1.00 | 0.00 |
| ATOM | 1425 | CD | GLU | 75B | 4.807 | -10.534 | -17.018 | 1.00 | 0.00 |
| ATOM | 1426 | OE1 | GLU | 75B | 4.932 | -11.401 | -16.130 | 1.00 | 0.00 |
| ATOM | 1427 | OE2 | GLU | 75B | 5.780 | -9.845 | -17.393 | 1.00 | 0.00 |
| ATOM | 1428 | N | LYS | 76B | 4.760 | -6.470 | -16.438 | 1.00 | 0.00 |
| ATOM | 1429 | CA | LYS | 76B | 5.819 | -6.086 | -15.447 | 1.00 | 0.00 |
| ATOM | 1430 | C | LYS | 76B | 5.379 | -5.738 | -13.984 | 1.00 | 0.00 |
| ATOM | 1431 | O | LYS | 76B | 6.138 | -6.024 | -13.056 | 1.00 | 0.00 |
| ATOM | 1432 | CB | LYS | 76B | 6.737 | -4.964 | -16.014 | 1.00 | 0.00 |
| ATOM | 1433 | CG | LYS | 76B | 7.474 | -5.192 | -17.360 | 1.00 | 0.00 |
| ATOM | 1434 | CD | LYS | 76B | 8.670 | -6.177 | -17.404 | 1.00 | 0.00 |
| ATOM | 1435 | CE | LYS | 76B | 8.396 | -7.694 | -17.317 | 1.00 | 0.00 |
| ATOM | 1436 | NZ | LYS | 76B | 7.510 | -8.195 | -18.403 | 1.00 | 0.00 |
| ATOM | 1437 | N | ILE | 77B | 4.166 | -5.196 | -13.760 | 1.00 | 0.00 |
| ATOM | 1438 | CA | ILE | 77B | 3.546 | -5.083 | -12.395 | 1.00 | 0.00 |
| ATOM | 1439 | C | ILE | 77B | 3.422 | -6.475 | -11.662 | 1.00 | 0.00 |
| ATOM | 1440 | O | ILE | 77B | 3.884 | -6.615 | -10.526 | 1.00 | 0.00 |
| ATOM | 1441 | CB | ILE | 77B | 2.187 | -4.285 | -12.492 | 1.00 | 0.00 |
| ATOM | 1442 | CG1 | ILE | 77B | 2.341 | -2.834 | -13.052 | 1.00 | 0.00 |
| ATOM | 1443 | CG2 | ILE | 77B | 1.430 | -4.206 | -11.137 | 1.00 | 0.00 |
| ATOM | 1444 | CD1 | ILE | 77B | 1.061 | -2.247 | -13.675 | 1.00 | 0.00 |
| ATOM | 1445 | N | PHE | 78B | 2.823 | -7.489 | -12.313 | 1.00 | 0.00 |
| ATOM | 1446 | CA | PHE | 78B | 2.748 | -8.877 | -11.767 | 1.00 | 0.00 |

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|------|------|-----|-----|-----|--------|---------|---------|------|------|
| ATOM | 1447 | C | PHE | 78B | 4.061 | -9.725 | -11.895 | 1.00 | 0.00 |
| ATOM | 1448 | O | PHE | 78B | 4.323 | -10.529 | -10.997 | 1.00 | 0.00 |
| ATOM | 1449 | CB | PHE | 78B | 1.498 | -9.594 | -12.350 | 1.00 | 0.00 |
| ATOM | 1450 | CG | PHE | 78B | 0.141 | -8.996 | -11.926 | 1.00 | 0.00 |
| ATOM | 1451 | CD1 | PHE | 78B | -0.598 | -8.217 | -12.824 | 1.00 | 0.00 |
| ATOM | 1452 | CD2 | PHE | 78B | -0.338 | -9.183 | -10.624 | 1.00 | 0.00 |
| ATOM | 1453 | CE1 | PHE | 78B | -1.794 | -7.626 | -12.420 | 1.00 | 0.00 |
| ATOM | 1454 | CE2 | PHE | 78B | -1.533 | -8.590 | -10.223 | 1.00 | 0.00 |
| ATOM | 1455 | CZ | PHE | 78B | -2.259 | -7.811 | -11.121 | 1.00 | 0.00 |
| ATOM | 1456 | N | SER | 79B | 4.920 | -9.534 | -12.922 | 1.00 | 0.00 |
| ATOM | 1457 | CA | SER | 79B | 6.314 | -10.075 | -12.925 | 1.00 | 0.00 |
| ATOM | 1458 | C | SER | 79B | 7.239 | -9.567 | -11.770 | 1.00 | 0.00 |
| ATOM | 1459 | O | SER | 79B | 7.826 | -10.399 | -11.073 | 1.00 | 0.00 |
| ATOM | 1460 | CB | SER | 79B | 6.984 | -9.908 | -14.312 | 1.00 | 0.00 |
| ATOM | 1461 | OG | SER | 79B | 7.010 | -11.153 | -15.010 | 1.00 | 0.00 |
| ATOM | 1462 | N | ILE | 80B | 7.341 | -8.245 | -11.511 | 1.00 | 0.00 |
| ATOM | 1463 | CA | ILE | 80B | 8.040 | -7.698 | -10.292 | 1.00 | 0.00 |
| ATOM | 1464 | C | ILE | 80B | 7.408 | -8.146 | -8.910 | 1.00 | 0.00 |
| ATOM | 1465 | O | ILE | 80B | 8.112 | -8.120 | -7.899 | 1.00 | 0.00 |
| ATOM | 1466 | CB | ILE | 80B | 8.291 | -6.148 | -10.464 | 1.00 | 0.00 |
| ATOM | 1467 | CG1 | ILE | 80B | 9.194 | -5.805 | -11.697 | 1.00 | 0.00 |
| ATOM | 1468 | CG2 | ILE | 80B | 8.925 | -5.476 | -9.213 | 1.00 | 0.00 |
| ATOM | 1469 | CD1 | ILE | 80B | 9.093 | -4.355 | -12.209 | 1.00 | 0.00 |
| ATOM | 1470 | N | CYS | 81B | 6.148 | -8.618 | -8.852 | 1.00 | 0.00 |
| ATOM | 1471 | CA | CYS | 81B | 5.632 | -9.432 | -7.719 | 1.00 | 0.00 |

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|------|------|-----|-----|-----|--------|---------|---------|------|------|
| ATOM | 1472 | C | CYS | 81B | 6.030 | -10.958 | -7.665 | 1.00 | 0.00 |
| ATOM | 1473 | O | CYS | 81B | 5.874 | -11.552 | -6.596 | 1.00 | 0.00 |
| ATOM | 1474 | CB | CYS | 81B | 4.099 | -9.240 | -7.744 | 1.00 | 0.00 |
| ATOM | 1475 | SG | CYS | 81B | 3.343 | -9.937 | -6.236 | 1.00 | 0.00 |
| ATOM | 1476 | N | VAL | 82B | 6.530 | -11.616 | -8.740 | 1.00 | 0.00 |
| ATOM | 1477 | CA | VAL | 82B | 6.604 | -13.114 | -8.821 | 1.00 | 0.00 |
| ATOM | 1478 | C | VAL | 82B | 7.988 | -13.790 | -8.597 | 1.00 | 0.00 |
| ATOM | 1479 | O | VAL | 82B | 8.062 | -14.711 | -7.784 | 1.00 | 0.00 |
| ATOM | 1480 | CB | VAL | 82B | 5.845 | -13.622 | -10.110 | 1.00 | 0.00 |
| ATOM | 1481 | CG1 | VAL | 82B | 6.640 | -13.670 | -11.438 | 1.00 | 0.00 |
| ATOM | 1482 | CG2 | VAL | 82B | 5.214 | -15.017 | -9.909 | 1.00 | 0.00 |
| ATOM | 1483 | N | MET | 83B | 9.060 | -13.450 | -9.339 | 1.00 | 0.00 |
| ATOM | 1484 | CA | MET | 83B | 10.245 | -14.361 | -9.459 | 1.00 | 0.00 |
| ATOM | 1485 | C | MET | 83B | 11.093 | -14.615 | -8.155 | 1.00 | 0.00 |
| ATOM | 1486 | O | MET | 83B | 11.597 | -15.725 | -7.971 | 1.00 | 0.00 |
| ATOM | 1487 | CB | MET | 83B | 11.026 | -13.985 | -10.743 | 1.00 | 0.00 |
| ATOM | 1488 | CG | MET | 83B | 12.082 | -15.016 | -11.194 | 1.00 | 0.00 |
| ATOM | 1489 | SD | MET | 83B | 12.939 | -14.409 | -12.660 | 1.00 | 0.00 |
| ATOM | 1490 | CE | MET | 83B | 14.028 | -15.806 | -12.990 | 1.00 | 0.00 |
| ATOM | 1491 | N | LEU | 84B | 11.158 | -13.660 | -7.211 | 1.00 | 0.00 |
| ATOM | 1492 | CA | LEU | 84B | 11.622 | -13.919 | -5.813 | 1.00 | 0.00 |
| ATOM | 1493 | C | LEU | 84B | 10.548 | -14.533 | -4.820 | 1.00 | 0.00 |
| ATOM | 1494 | O | LEU | 84B | 10.838 | -14.648 | -3.628 | 1.00 | 0.00 |
| ATOM | 1495 | CB | LEU | 84B | 12.233 | -12.570 | -5.321 | 1.00 | 0.00 |
| ATOM | 1496 | CG | LEU | 84B | 13.258 | -12.580 | -4.158 | 1.00 | 0.00 |

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|------|------|-----|-----|-----|--------|---------|--------|------|------|
| ATOM | 1497 | CD1 | LEU | 84B | 14.640 | -13.108 | -4.578 | 1.00 | 0.00 |
| ATOM | 1498 | CD2 | LEU | 84B | 13.453 | -11.153 | -3.613 | 1.00 | 0.00 |
| ATOM | 1499 | N | ILE | 85B | 9.355 | -15.017 | -5.256 | 1.00 | 0.00 |
| ATOM | 1500 | CA | ILE | 85B | 8.473 | -15.933 | -4.442 | 1.00 | 0.00 |
| ATOM | 1501 | C | ILE | 85B | 9.193 | -17.283 | -4.082 | 1.00 | 0.00 |
| ATOM | 1502 | O | ILE | 85B | 9.184 | -17.662 | -2.906 | 1.00 | 0.00 |
| ATOM | 1503 | CB | ILE | 85B | 7.036 | -16.109 | -5.077 | 1.00 | 0.00 |
| ATOM | 1504 | CG1 | ILE | 85B | 6.217 | -14.783 | -5.037 | 1.00 | 0.00 |
| ATOM | 1505 | CG2 | ILE | 85B | 6.174 | -17.254 | -4.466 | 1.00 | 0.00 |
| ATOM | 1506 | CD1 | ILE | 85B | 4.834 | -14.787 | -5.720 | 1.00 | 0.00 |
| ATOM | 1507 | N | GLY | 86B | 9.888 | -17.954 | -5.027 | 1.00 | 0.00 |
| ATOM | 1508 | CA | GLY | 86B | 10.889 | -19.010 | -4.681 | 1.00 | 0.00 |
| ATOM | 1509 | C | GLY | 86B | 12.224 | -18.555 | -4.036 | 1.00 | 0.00 |
| ATOM | 1510 | O | GLY | 86B | 13.305 | -18.989 | -4.442 | 1.00 | 0.00 |
| ATOM | 1511 | N | SER | 87B | 12.133 | -17.683 | -3.022 | 1.00 | 0.00 |
| ATOM | 1512 | CA | SER | 87B | 13.282 | -17.065 | -2.310 | 1.00 | 0.00 |
| ATOM | 1513 | C | SER | 87B | 12.791 | -16.295 | -1.035 | 1.00 | 0.00 |
| ATOM | 1514 | O | SER | 87B | 13.269 | -16.631 | 0.050 | 1.00 | 0.00 |
| ATOM | 1515 | CB | SER | 87B | 14.144 | -16.195 | -3.257 | 1.00 | 0.00 |
| ATOM | 1516 | OG | SER | 87B | 14.874 | -17.000 | -4.183 | 1.00 | 0.00 |
| ATOM | 1517 | N | LEU | 88B | 11.893 | -15.278 | -1.118 | 1.00 | 0.00 |
| ATOM | 1518 | CA | LEU | 88B | 11.320 | -14.570 | 0.078 | 1.00 | 0.00 |
| ATOM | 1519 | C | LEU | 88B | 10.067 | -15.254 | 0.700 | 1.00 | 0.00 |
| ATOM | 1520 | O | LEU | 88B | 10.089 | -15.578 | 1.891 | 1.00 | 0.00 |
| ATOM | 1521 | CB | LEU | 88B | 11.005 | -13.072 | -0.217 | 1.00 | 0.00 |

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|------|------|-----|-----|-----|--------|---------|--------|------|------|
| ATOM | 1522 | CG | LEU | 88B | 12.190 | -12.082 | -0.231 | 1.00 | 0.00 |
| ATOM | 1523 | CD1 | LEU | 88B | 11.683 | -10.674 | -0.595 | 1.00 | 0.00 |
| ATOM | 1524 | CD2 | LEU | 88B | 12.927 | -11.996 | 1.121 | 1.00 | 0.00 |
| ATOM | 1525 | N | MET | 89B | 8.983 | -15.498 | -0.064 | 1.00 | 0.00 |
| ATOM | 1526 | CA | MET | 89B | 7.877 | -16.401 | 0.390 | 1.00 | 0.00 |
| ATOM | 1527 | C | MET | 89B | 8.361 | -17.852 | 0.750 | 1.00 | 0.00 |
| ATOM | 1528 | O | MET | 89B | 8.024 | -18.352 | 1.829 | 1.00 | 0.00 |
| ATOM | 1529 | CB | MET | 89B | 6.731 | -16.406 | -0.653 | 1.00 | 0.00 |
| ATOM | 1530 | CG | MET | 89B | 5.917 | -15.104 | -0.791 | 1.00 | 0.00 |
| ATOM | 1531 | SD | MET | 89B | 4.877 | -14.856 | 0.667 | 1.00 | 0.00 |
| ATOM | 1532 | CE | MET | 89B | 3.286 | -15.457 | 0.062 | 1.00 | 0.00 |
| ATOM | 1533 | N | TYR | 90B | 9.232 | -18.466 | -0.081 | 1.00 | 0.00 |
| ATOM | 1534 | CA | TYR | 90B | 10.028 | -19.660 | 0.317 | 1.00 | 0.00 |
| ATOM | 1535 | C | TYR | 90B | 11.008 | -19.558 | 1.553 | 1.00 | 0.00 |
| ATOM | 1536 | O | TYR | 90B | 11.251 | -20.588 | 2.189 | 1.00 | 0.00 |
| ATOM | 1537 | CB | TYR | 90B | 10.658 | -20.359 | -0.921 | 1.00 | 0.00 |
| ATOM | 1538 | CG | TYR | 90B | 9.808 | -21.501 | -1.515 | 1.00 | 0.00 |
| ATOM | 1539 | CD1 | TYR | 90B | 8.794 | -21.233 | -2.441 | 1.00 | 0.00 |
| ATOM | 1540 | CD2 | TYR | 90B | 10.029 | -22.822 | -1.107 | 1.00 | 0.00 |
| ATOM | 1541 | CE1 | TYR | 90B | 8.030 | -22.272 | -2.969 | 1.00 | 0.00 |
| ATOM | 1542 | CE2 | TYR | 90B | 9.253 | -23.858 | -1.625 | 1.00 | 0.00 |
| ATOM | 1543 | CZ | TYR | 90B | 8.256 | -23.581 | -2.559 | 1.00 | 0.00 |
| ATOM | 1544 | OH | TYR | 90B | 7.484 | -24.592 | -3.063 | 1.00 | 0.00 |
| ATOM | 1545 | N | ALA | 91B | 11.517 | -18.375 | 1.957 | 1.00 | 0.00 |
| ATOM | 1546 | CA | ALA | 91B | 12.197 | -18.190 | 3.278 | 1.00 | 0.00 |

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| ATOM | 1547 | C | ALA | 91B | 11.329 | -18.349 | 4.574 | 1.00 | 0.00 |
| ATOM | 1548 | O | ALA | 91B | 11.855 | -18.808 | 5.591 | 1.00 | 0.00 |
| ATOM | 1549 | CB | ALA | 91B | 12.877 | -16.809 | 3.282 | 1.00 | 0.00 |
| ATOM | 1550 | N | SER | 92B | 10.032 | -17.981 | 4.541 | 1.00 | 0.00 |
| ATOM | 1551 | CA | SER | 92B | 9.077 | -18.110 | 5.688 | 1.00 | 0.00 |
| ATOM | 1552 | C | SER | 92B | 9.101 | -19.408 | 6.575 | 1.00 | 0.00 |
| ATOM | 1553 | O | SER | 92B | 9.089 | -19.320 | 7.806 | 1.00 | 0.00 |
| ATOM | 1554 | CB | SER | 92B | 7.660 | -17.833 | 5.118 | 1.00 | 0.00 |
| ATOM | 1555 | OG | SER | 92B | 7.223 | -18.841 | 4.197 | 1.00 | 0.00 |
| ATOM | 1556 | N | ILE | 93B | 9.147 | -20.591 | 5.946 | 1.00 | 0.00 |
| ATOM | 1557 | CA | ILE | 93B | 9.201 | -21.918 | 6.647 | 1.00 | 0.00 |
| ATOM | 1558 | C | ILE | 93B | 10.644 | -22.506 | 6.899 | 1.00 | 0.00 |
| ATOM | 1559 | O | ILE | 93B | 10.798 | -23.392 | 7.741 | 1.00 | 0.00 |
| ATOM | 1560 | CB | ILE | 93B | 8.205 | -22.867 | 5.885 | 1.00 | 0.00 |
| ATOM | 1561 | CG1 | ILE | 93B | 6.701 | -22.467 | 6.033 | 1.00 | 0.00 |
| ATOM | 1562 | CG2 | ILE | 93B | 8.385 | -24.377 | 6.168 | 1.00 | 0.00 |
| ATOM | 1563 | CD1 | ILE | 93B | 6.121 | -22.398 | 7.460 | 1.00 | 0.00 |
| ATOM | 1564 | N | PHE | 94B | 11.692 | -22.015 | 6.218 | 1.00 | 0.00 |
| ATOM | 1565 | CA | PHE | 94B | 13.095 | -22.361 | 6.379 | 1.00 | 0.00 |
| ATOM | 1566 | C | PHE | 94B | 13.558 | -22.294 | 7.834 | 1.00 | 0.00 |
| ATOM | 1567 | O | PHE | 94B | 14.009 | -23.296 | 8.400 | 1.00 | 0.00 |
| ATOM | 1568 | CB | PHE | 94B | 13.998 | -21.425 | 5.520 | 1.00 | 0.00 |
| ATOM | 1569 | CG | PHE | 94B | 15.486 | -21.798 | 5.437 | 1.00 | 0.00 |
| ATOM | 1570 | CD1 | PHE | 94B | 15.925 | -22.676 | 4.439 | 1.00 | 0.00 |
| ATOM | 1571 | CD2 | PHE | 94B | 16.397 | -21.321 | 6.383 | 1.00 | 0.00 |

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| ATOM | 1572 | CE1 | PHE | 94B | 17.253 | -23.087 | 4.400 | 1.00 | 0.00 |
| ATOM | 1573 | CE2 | PHE | 94B | 17.729 | -21.725 | 6.336 | 1.00 | 0.00 |
| ATOM | 1574 | CZ | PHE | 94B | 18.156 | -22.609 | 5.347 | 1.00 | 0.00 |
| ATOM | 1575 | N | GLY | 95B | 13.442 | -21.115 | 8.464 | 1.00 | 0.00 |
| ATOM | 1576 | CA | GLY | 95B | 13.864 | -20.958 | 9.857 | 1.00 | 0.00 |
| ATOM | 1577 | C | GLY | 95B | 13.307 | -22.041 | 10.768 | 1.00 | 0.00 |
| ATOM | 1578 | O | GLY | 95B | 13.970 | -22.477 | 11.708 | 1.00 | 0.00 |
| ATOM | 1579 | N | ASN | 96B | 12.086 | -22.478 | 10.483 | 1.00 | 0.00 |
| ATOM | 1580 | CA | ASN | 96B | 11.451 | -23.504 | 11.296 | 1.00 | 0.00 |
| ATOM | 1581 | C | ASN | 96B | 12.113 | -24.856 | 11.097 | 1.00 | 0.00 |
| ATOM | 1582 | O | ASN | 96B | 12.555 | -25.495 | 12.053 | 1.00 | 0.00 |
| ATOM | 1583 | CB | ASN | 96B | 9.931 | -23.580 | 10.968 | 1.00 | 0.00 |
| ATOM | 1584 | CG | ASN | 96B | 9.070 | -22.383 | 11.384 | 1.00 | 0.00 |
| ATOM | 1585 | OD1 | ASN | 96B | 9.268 | -21.766 | 12.420 | 1.00 | 0.00 |
| ATOM | 1586 | ND2 | ASN | 96B | 8.076 | -22.026 | 10.615 | 1.00 | 0.00 |
| ATOM | 1587 | N | VAL | 97B | 12.178 | -25.289 | 9.847 | 1.00 | 0.00 |
| ATOM | 1588 | CA | VAL | 97B | 12.780 | -26.568 | 9.525 | 1.00 | 0.00 |
| ATOM | 1589 | C | VAL | 97B | 14.222 | -26.627 | 10.008 | 1.00 | 0.00 |
| ATOM | 1590 | O | VAL | 97B | 14.686 | -27.661 | 10.492 | 1.00 | 0.00 |
| ATOM | 1591 | CB | VAL | 97B | 12.699 | -26.816 | 7.966 | 1.00 | 0.00 |
| ATOM | 1592 | CG1 | VAL | 97B | 11.273 | -26.931 | 7.360 | 1.00 | 0.00 |
| ATOM | 1593 | CG2 | VAL | 97B | 13.415 | -25.735 | 7.121 | 1.00 | 0.00 |
| ATOM | 1594 | N | SER | 98B | 14.927 | -25.509 | 9.884 | 1.00 | 0.00 |
| ATOM | 1595 | CA | SER | 98B | 16.315 | -25.440 | 10.317 | 1.00 | 0.00 |
| ATOM | 1596 | C | SER | 98B | 16.410 | -25.554 | 11.840 | 1.00 | 0.00 |

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|------|------|-----|-----|------|--------|---------|--------|------|------|
| ATOM | 1597 | O | SER | 98B | 17.232 | -26.311 | 12.368 | 1.00 | 0.00 |
| ATOM | 1598 | CB | SER | 98B | 16.960 | -24.129 | 9.803 | 1.00 | 0.00 |
| ATOM | 1599 | OG | SER | 98B | 18.354 | -24.034 | 10.116 | 1.00 | 0.00 |
| ATOM | 1600 | N | ALA | 99B | 15.566 | -24.801 | 12.540 | 1.00 | 0.00 |
| ATOM | 1601 | CA | ALA | 99B | 15.557 | -24.821 | 13.996 | 1.00 | 0.00 |
| ATOM | 1602 | C | ALA | 99B | 15.217 | -26.228 | 14.483 | 1.00 | 0.00 |
| ATOM | 1603 | O | ALA | 99B | 15.638 | -26.636 | 15.565 | 1.00 | 0.00 |
| ATOM | 1604 | CB | ALA | 99B | 14.567 | -23.759 | 14.506 | 1.00 | 0.00 |
| ATOM | 1605 | N | ILE | 100B | 14.456 | -26.965 | 13.675 | 1.00 | 0.00 |
| ATOM | 1606 | CA | ILE | 100B | 14.076 | -28.330 | 14.022 | 1.00 | 0.00 |
| ATOM | 1607 | C | ILE | 100B | 15.234 | -29.267 | 13.700 | 1.00 | 0.00 |
| ATOM | 1608 | O | ILE | 100B | 15.608 | -30.118 | 14.508 | 1.00 | 0.00 |
| ATOM | 1609 | CB | ILE | 100B | 12.758 | -28.733 | 13.244 | 1.00 | 0.00 |
| ATOM | 1610 | CG1 | ILE | 100B | 12.176 | -30.131 | 13.628 | 1.00 | 0.00 |
| ATOM | 1611 | CG2 | ILE | 100B | 12.934 | -28.691 | 11.694 | 1.00 | 0.00 |
| ATOM | 1612 | CD1 | ILE | 100B | 11.512 | -30.225 | 15.018 | 1.00 | 0.00 |
| ATOM | 1613 | N | ILE | 101B | 15.802 | -29.102 | 12.512 | 1.00 | 0.00 |
| ATOM | 1614 | CA | ILE | 101B | 16.915 | -29.934 | 12.091 | 1.00 | 0.00 |
| ATOM | 1615 | C | ILE | 101B | 18.107 | -29.728 | 13.013 | 1.00 | 0.00 |
| ATOM | 1616 | O | ILE | 101B | 18.645 | -30.686 | 13.564 | 1.00 | 0.00 |
| ATOM | 1617 | CB | ILE | 101B | 17.270 | -29.597 | 10.586 | 1.00 | 0.00 |
| ATOM | 1618 | CG1 | ILE | 101B | 16.113 | -29.860 | 9.568 | 1.00 | 0.00 |
| ATOM | 1619 | CG2 | ILE | 101B | 18.540 | -30.349 | 10.080 | 1.00 | 0.00 |
| ATOM | 1620 | CD1 | ILE | 101B | 16.324 | -29.295 | 8.149 | 1.00 | 0.00 |
| ATOM | 1621 | N | GLN | 102B | 18.514 | -28.471 | 13.175 | 1.00 | 0.00 |

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| ATOM | 1622 | CA | GLN | 102B | 19.647 | -28.127 | 14.028 | 1.00 | 0.00 |
| ATOM | 1623 | C | GLN | 102B | 19.468 | -28.689 | 15.441 | 1.00 | 0.00 |
| ATOM | 1624 | O | GLN | 102B | 20.447 | -29.062 | 16.099 | 1.00 | 0.00 |
| ATOM | 1625 | CB | GLN | 102B | 19.825 | -26.593 | 14.061 | 1.00 | 0.00 |
| ATOM | 1626 | CG | GLN | 102B | 20.258 | -25.919 | 12.717 | 1.00 | 0.00 |
| ATOM | 1627 | CD | GLN | 102B | 20.488 | -24.403 | 12.681 | 1.00 | 0.00 |
| ATOM | 1628 | OE1 | GLN | 102B | 19.592 | -23.622 | 12.957 | 1.00 | 0.00 |
| ATOM | 1629 | NE2 | GLN | 102B | 21.655 | -23.927 | 12.325 | 1.00 | 0.00 |
| ATOM | 1630 | N | ARG | 103B | 18.216 | -28.752 | 15.898 | 1.00 | 0.00 |
| ATOM | 1631 | CA | ARG | 103B | 17.898 | -29.273 | 17.230 | 1.00 | 0.00 |
| ATOM | 1632 | C | ARG | 103B | 18.029 | -30.785 | 17.237 | 1.00 | 0.00 |
| ATOM | 1633 | O | ARG | 103B | 18.679 | -31.363 | 18.107 | 1.00 | 0.00 |
| ATOM | 1634 | CB | ARG | 103B | 16.464 | -28.826 | 17.636 | 1.00 | 0.00 |
| ATOM | 1635 | CG | ARG | 103B | 16.037 | -29.183 | 19.087 | 1.00 | 0.00 |
| ATOM | 1636 | CD | ARG | 103B | 14.598 | -28.737 | 19.394 | 1.00 | 0.00 |
| ATOM | 1637 | NE | ARG | 103B | 14.245 | -29.105 | 20.796 | 1.00 | 0.00 |
| ATOM | 1638 | CZ | ARG | 103B | 13.076 | -28.864 | 21.383 | 1.00 | 0.00 |
| ATOM | 1639 | NH1 | ARG | 103B | 12.079 | -28.272 | 20.789 | 1.00 | 0.00 |
| ATOM | 1640 | NH2 | ARG | 103B | 12.918 | -29.238 | 22.613 | 1.00 | 0.00 |
| ATOM | 1641 | N | LEU | 104B | 17.380 | -31.418 | 16.267 | 1.00 | 0.00 |
| ATOM | 1642 | CA | LEU | 104B | 17.421 | -32.866 | 16.128 | 1.00 | 0.00 |
| ATOM | 1643 | C | LEU | 104B | 18.846 | -33.333 | 15.852 | 1.00 | 0.00 |
| ATOM | 1644 | O | LEU | 104B | 19.234 | -34.441 | 16.229 | 1.00 | 0.00 |
| ATOM | 1645 | CB | LEU | 104B | 16.463 | -33.299 | 14.982 | 1.00 | 0.00 |
| ATOM | 1646 | CG | LEU | 104B | 14.972 | -33.557 | 15.333 | 1.00 | 0.00 |

| | | | | | | | | | |
|--------|------|-----|-----|------|--------|---------|--------|------|------|
| ATOM | 1647 | CD1 | LEU | 104B | 14.825 | -34.903 | 16.055 | 1.00 | 0.00 |
| ATOM | 1648 | CD2 | LEU | 104B | 14.362 | -32.438 | 16.193 | 1.00 | 0.00 |
| ATOM | 1649 | N | TYR | 105B | 19.625 | -32.482 | 15.193 | 1.00 | 0.00 |
| ATOM | 1650 | CA | TYR | 105B | 21.010 | -32.801 | 14.876 | 1.00 | 0.00 |
| ATOM | 1651 | C | TYR | 105B | 21.886 | -32.691 | 16.123 | 1.00 | 0.00 |
| ATOM | 1652 | O | TYR | 105B | 22.616 | -33.623 | 16.465 | 1.00 | 0.00 |
| ATOM | 1653 | CB | TYR | 105B | 21.540 | -31.856 | 13.792 | 1.00 | 0.00 |
| ATOM | 1654 | CG | TYR | 105B | 22.976 | -32.136 | 13.408 | 1.00 | 0.00 |
| ATOM | 1655 | CD1 | TYR | 105B | 23.310 | -33.271 | 12.668 | 1.00 | 0.00 |
| ATOM | 1656 | CD2 | TYR | 105B | 24.008 | -31.292 | 13.826 | 1.00 | 0.00 |
| ATOM | 1657 | CE1 | TYR | 105B | 24.636 | -33.565 | 12.358 | 1.00 | 0.00 |
| ATOM | 1658 | CE2 | TYR | 105B | 25.339 | -31.576 | 13.522 | 1.00 | 0.00 |
| ATOM | 1659 | CZ | TYR | 105B | 25.644 | -32.716 | 12.788 | 1.00 | 0.00 |
| ATOM | 1660 | OH | TYR | 105B | 26.956 | -33.019 | 12.496 | 1.00 | 0.00 |
| ATOM | 1661 | N | SER | 106B | 21.811 | -31.544 | 16.793 | 1.00 | 0.00 |
| ATOM | 1662 | CA | SER | 106B | 22.592 | -31.304 | 18.002 | 1.00 | 0.00 |
| ATOM | 1663 | C | SER | 106B | 22.178 | -32.242 | 19.143 | 1.00 | 0.00 |
| ATOM | 1664 | O | SER | 106B | 22.607 | -33.397 | 19.185 | 1.00 | 0.00 |
| ATOM | 1665 | CB | SER | 106B | 22.455 | -29.815 | 18.409 | 1.00 | 0.00 |
| ATOM | 1666 | OG | SER | 106B | 21.118 | -29.461 | 18.780 | 1.00 | 0.00 |
| HETATM | 1667 | OH | OSP | 1 | 14.703 | -8.402 | -6.527 | 1.00 | 0.00 |
| HETATM | 1668 | HH | OSP | 1 | 13.993 | -8.359 | -7.178 | 1.00 | 0.00 |
| HETATM | 1669 | C1 | ALH | 1G | 15.305 | -9.628 | -6.572 | 1.00 | 0.00 |
| HETATM | 1670 | O2 | ALH | 1G | 16.236 | -9.885 | -5.805 | 1.00 | 0.00 |
| HETATM | 1671 | C1 | BEN | 1F | 15.360 | -12.710 | -8.770 | 1.00 | 0.00 |

| | | | | | | | | | |
|--------|------|-----|-----|----|--------|---------|---------|------|------|
| HETATM | 1672 | C2 | BEN | 1F | 14.273 | -12.522 | -9.603 | 1.00 | 0.00 |
| HETATM | 1673 | C3 | BEN | 1F | 13.445 | -11.419 | -9.436 | 1.00 | 0.00 |
| HETATM | 1674 | C4 | BEN | 1F | 13.682 | -10.492 | -8.416 | 1.00 | 0.00 |
| HETATM | 1675 | C5 | BEN | 1F | 14.837 | -10.638 | -7.600 | 1.00 | 0.00 |
| HETATM | 1676 | C6 | BEN | 1F | 15.642 | -11.778 | -7.782 | 1.00 | 0.00 |
| HETATM | 1677 | H1 | BEN | 1F | 16.006 | -13.566 | -8.909 | 1.00 | 0.00 |
| HETATM | 1678 | H2 | BEN | 1F | 14.096 | -13.219 | -10.406 | 1.00 | 0.00 |
| HETATM | 1679 | H3 | BEN | 1F | 12.626 | -11.272 | -10.120 | 1.00 | 0.00 |
| HETATM | 1680 | H6 | BEN | 1F | 16.520 | -11.939 | -7.177 | 1.00 | 0.00 |
| HETATM | 1681 | N1 | AMD | 1E | 12.731 | -9.378 | -8.302 | 1.00 | 0.00 |
| HETATM | 1682 | H1 | AMD | 1E | 12.240 | -9.436 | -9.201 | 1.00 | 0.00 |
| HETATM | 1683 | C1 | BEN | 1D | 4.824 | -11.772 | -2.171 | 1.00 | 0.00 |
| HETATM | 1684 | CL1 | BEN | 1D | 3.165 | -12.140 | -2.648 | 1.00 | 0.00 |
| HETATM | 1685 | C2 | BEN | 1D | 5.140 | -11.506 | -0.838 | 1.00 | 0.00 |
| HETATM | 1686 | CL2 | BEN | 1D | 3.886 | -11.522 | 0.402 | 1.00 | 0.00 |
| HETATM | 1687 | C3 | BEN | 1D | 6.458 | -11.234 | -0.475 | 1.00 | 0.00 |
| HETATM | 1688 | C4 | BEN | 1D | 7.461 | -11.226 | -1.442 | 1.00 | 0.00 |
| HETATM | 1689 | C5 | BEN | 1D | 7.153 | -11.487 | -2.782 | 1.00 | 0.00 |
| HETATM | 1690 | C6 | BEN | 1D | 5.827 | -11.756 | -3.138 | 1.00 | 0.00 |
| HETATM | 1691 | H3 | BEN | 1D | 6.701 | -11.030 | 0.557 | 1.00 | 0.00 |
| HETATM | 1692 | H4 | BEN | 1D | 8.479 | -11.008 | -1.150 | 1.00 | 0.00 |
| HETATM | 1693 | H6 | BEN | 1D | 5.566 | -11.955 | -4.166 | 1.00 | 0.00 |
| HETATM | 1694 | C1 | ETH | 1C | 8.258 | -11.450 | -3.849 | 1.00 | 0.00 |
| HETATM | 1695 | C2 | ETH | 1C | 8.366 | -10.075 | -4.547 | 1.00 | 0.00 |
| HETATM | 1696 | 1H1 | ETH | 1C | 9.232 | -11.726 | -3.401 | 1.00 | 0.00 |

| | | | | | | | | | |
|-----------------------------|------|-----|-----|----|--------|---------|--------|------|------|
| HETATM | 1697 | 2H1 | ETH | 1C | 8.077 | -12.234 | -4.609 | 1.00 | 0.00 |
| HETATM | 1698 | 1H2 | ETH | 1C | 8.423 | -9.280 | -3.778 | 1.00 | 0.00 |
| HETATM | 1699 | 2H2 | ETH | 1C | 7.422 | -9.856 | -5.081 | 1.00 | 0.00 |
| HETATM | 1700 | C1 | BEN | 1B | 10.546 | -10.376 | -7.691 | 1.00 | 0.00 |
| HETATM | 1701 | C2 | BEN | 1B | 9.513 | -10.575 | -6.776 | 1.00 | 0.00 |
| HETATM | 1702 | C3 | BEN | 1B | 9.538 | -9.941 | -5.530 | 1.00 | 0.00 |
| HETATM | 1703 | C4 | BEN | 1B | 10.626 | -9.132 | -5.199 | 1.00 | 0.00 |
| HETATM | 1704 | C5 | BEN | 1B | 11.675 | -8.964 | -6.097 | 1.00 | 0.00 |
| HETATM | 1705 | C6 | BEN | 1B | 11.657 | -9.599 | -7.342 | 1.00 | 0.00 |
| HETATM | 1706 | H1 | BEN | 1B | 10.486 | -10.851 | -8.660 | 1.00 | 0.00 |
| HETATM | 1707 | H2 | BEN | 1B | 8.684 | -11.210 | -7.041 | 1.00 | 0.00 |
| HETATM | 1708 | H4 | BEN | 1B | 10.661 | -8.623 | -4.247 | 1.00 | 0.00 |
| HETATM | 1709 | H5 | BEN | 1B | 12.477 | -8.312 | -5.805 | 1.00 | 0.00 |
| CONNECT 1667 1668 | | | | | | | | | |
| CONNECT 1669 1670 | | | | | | | | | |
| CONNECT 1671 1672 1676 1677 | | | | | | | | | |
| CONNECT 1672 1673 1678 | | | | | | | | | |
| CONNECT 1673 1674 1679 | | | | | | | | | |
| CONNECT 1674 1675 | | | | | | | | | |
| CONNECT 1675 1676 | | | | | | | | | |
| CONNECT 1676 1680 | | | | | | | | | |
| CONNECT 1681 1682 | | | | | | | | | |
| CONNECT 1683 1684 1685 1690 | | | | | | | | | |
| CONNECT 1685 1686 1687 | | | | | | | | | |
| CONNECT 1687 1688 1691 | | | | | | | | | |

CONNECT 1688 1689 1692
CONNECT 1689 1690
CONNECT 1690 1693
CONNECT 1694 1695 1696 1697
CONNECT 1695 1698 1699
CONNECT 1700 1701 1705 1706
CONNECT 1701 1702 1707
CONNECT 1702 1703
CONNECT 1703 1704 1708
CONNECT 1704 1705 1709

| | | | |
|--------|--------------|--------------|--------------|
| SPDBVT | 1.0000000000 | 0.0000000000 | 0.0000000000 |
| SPDBVT | 0.0000000000 | 1.0000000000 | 0.0000000000 |
| SPDBVT | 0.0000000000 | 0.0000000000 | 1.0000000000 |
| SPDBVT | 0.0000000000 | 0.0000000000 | 0.0000000000 |
| SPDBVT | 0.0000000000 | 0.0000000000 | 0.0000000000 |

SPDBVV default;

| | | | |
|--------|-----------------|-------------------|-----------------|
| SPDBVV | 12.048013832248 | 2546.405537008352 | 20.000000000000 |
| SPDBVV | 0.6433143880 | 0.0689082585 | -0.7624947542 |
| SPDBVV | 0.7643748714 | -0.1141776490 | 0.6345821620 |
| SPDBVV | -0.0433319067 | -0.9910676649 | -0.1261238656 |
| SPDBVV | 13.0734996796 | -17.2654991150 | -6.8344998360 |
| SPDBVV | 0.0000000000 | 0.0000000000 | 0.0000000000 |

SPDBVf 34

SPDBVf 34

SPDBVf 34 34 34 34 34 34 34 34 34 34 34 34 34 34 50 50 59 50 50 59

SPDBVI 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00

SPDBVI 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00

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SPDBVI 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00

SPDBVb 0.00 0.00 0.00

END