## SMALL MOLECULES WITH H2O

HET CL A 501 1

HET EDO A 502 4

HET EDO A 503 4

HET EDO A 504 4

HET EDO A 505 4

HET EDO A 506 4

HET EDO A 507 4

HET CL B 501 1

HET EDO B 502 4

HET EDO B 503 4

HET EDO B 504 4

HET EDO B 505 4

HET EDO B 506 4

HET EDO B 507 4

HET EDO B 508 4

HETNAM CL CHLORIDE ION

HETNAM EDO 1,2-ETHANEDIOL

HETSYN EDO ETHYLENE GLYCOL

FORMUL 3 CL 2(CL 1-)

FORMUL 4 EDO 13(C2 H6 O2)

FORMUL 18 HOH \*745(H2 O)

HETATM 6108 CL CL A 501 64.388 16.714 51.655 1.00 18.08 CL

HETATM 6109 C1 EDO A 502 71.593 26.406 41.821 1.00 42.16 C

HETATM 6110 O1 EDO A 502 71.825 27.757 42.234 1.00 50.47 O

HETATM 6111 C2 EDO A 502 71.346 25.518 43.039 1.00 38.32 C

HETATM 6112 O2 EDO A 502 69.951 25.528 43.381 1.00 30.58 O

HETATM 6113 C1 EDO A 503 70.172 19.732 77.879 1.00 33.95 C

HETATM 6114 O1 EDO A 503 69.004 20.451 77.480 1.00 25.03 O

HETATM 6115 C2 EDO A 503 71.393 20.619 77.695 1.00 37.30 C

HETATM 6116 O2 EDO A 503 71.324 21.758 78.561 1.00 34.00 O

HETATM 6117 C1 EDO A 504 31.989 27.170 45.530 1.00 34.42 C

HETATM 6118 O1 EDO A 504 30.986 26.684 46.421 1.00 37.44 O

HETATM 6119 C2 EDO A 504 31.839 28.671 45.331 1.00 37.34 C

HETATM 6120 O2 EDO A 504 33.008 29.156 44.667 1.00 28.48 O

HETATM 6121 C1 EDO A 505 73.357 15.933 45.861 1.00 43.75 C

HETATM 6122 O1 EDO A 505 73.115 16.638 47.084 1.00 49.06 O

HETATM 6123 C2 EDO A 505 74.588 16.515 45.175 1.00 41.79 C

HETATM 6124 O2 EDO A 505 74.399 17.920 44.976 1.00 41.93 O

HETATM 6125 C1 EDO A 506 69.550 22.580 66.391 1.00 27.32 C

HETATM 6126 O1 EDO A 506 70.043 23.732 65.701 1.00 30.45 O

HETATM 6127 C2 EDO A 506 70.686 21.950 67.196 1.00 26.02 C

HETATM 6128 O2 EDO A 506 71.667 21.424 66.293 1.00 27.83 O

HETATM 6129 C1 EDO A 507 19.708 9.646 57.753 1.00 25.79 C

HETATM 6130 O1 EDO A 507 18.674 8.731 58.121 1.00 27.92 O

HETATM 6131 C2 EDO A 507 19.719 9.810 56.242 1.00 28.02 C

HETATM 6132 O2 EDO A 507 18.540 10.521 55.857 1.00 28.69 O

HETATM 6133 CL CL B 501 32.928 19.682 76.227 1.00 18.43 CL

HETATM 6134 C1 EDO B 502 27.799 23.854 50.449 1.00 27.87 C

HETATM 6135 O1 EDO B 502 29.198 24.098 50.270 1.00 23.44 O

HETATM 6136 C2 EDO B 502 26.992 24.610 49.400 1.00 33.95 C

HETATM 6137 O2 EDO B 502 27.338 26.002 49.424 1.00 30.28 O

HETATM 6138 C1 EDO B 503 13.942 18.923 76.468 1.00 44.19 C

HETATM 6139 O1 EDO B 503 15.211 19.551 76.702 1.00 39.98 O

HETATM 6140 C2 EDO B 503 13.326 19.493 75.198 1.00 46.63 C

HETATM 6141 O2 EDO B 503 13.446 20.924 75.219 1.00 49.22 O

HETATM 6142 C1 EDO B 504 75.596 4.509 71.745 1.00 24.89 C

HETATM 6143 O1 EDO B 504 76.942 4.891 72.072 1.00 24.73 O

HETATM 6144 C2 EDO B 504 75.486 4.304 70.238 1.00 26.94 C

HETATM 6145 O2 EDO B 504 76.411 3.281 69.841 1.00 27.31 O

HETATM 6146 C1 EDO B 505 36.452 30.709 80.463 1.00 37.56 C

HETATM 6147 O1 EDO B 505 37.848 30.582 80.792 1.00 28.33 O

HETATM 6148 C2 EDO B 505 36.253 30.953 78.968 1.00 43.28 C

HETATM 6149 O2 EDO B 505 36.757 32.245 78.595 1.00 47.04 O

HETATM 6150 C1 EDO B 506 27.975 11.929 89.769 1.00 46.31 C

HETATM 6151 O1 EDO B 506 28.431 10.710 90.366 1.00 53.56 O

HETATM 6152 C2 EDO B 506 29.129 12.590 89.025 1.00 39.26 C

HETATM 6153 O2 EDO B 506 30.174 12.910 89.952 1.00 41.11 O

HETATM 6154 C1 EDO B 507 62.719 -2.849 44.698 1.00 32.13 C

HETATM 6155 O1 EDO B 507 61.302 -2.753 44.535 1.00 36.57 O

HETATM 6156 C2 EDO B 507 63.224 -1.524 45.235 1.00 33.94 C

HETATM 6157 O2 EDO B 507 62.933 -0.506 44.270 1.00 42.48 O

HETATM 6158 C1 EDO B 508 29.106 26.507 61.380 1.00 25.61 C

HETATM 6159 O1 EDO B 508 28.854 27.709 62.116 1.00 24.03 O

HETATM 6160 C2 EDO B 508 27.892 26.125 60.532 1.00 25.02 C

HETATM 6161 O2 EDO B 508 26.865 25.591 61.375 1.00 24.23 O

HETATM 6162 O HOH A 601 55.247 37.455 47.887 1.00 44.08 O

HETATM 6163 O HOH A 602 50.935 46.176 58.214 1.00 37.40 O

HETATM 6164 O HOH A 603 36.166 1.287 60.642 1.00 26.64 O

HETATM 6165 O HOH A 604 64.597 8.541 70.761 1.00 31.37 O

HETATM 6166 O HOH A 605 87.099 25.759 41.253 1.00 37.77 O

HETATM 6167 O HOH A 606 94.328 20.573 59.951 1.00 34.62 O

HETATM 6168 O HOH A 607 84.158 25.147 48.726 1.00 36.49 O

HETATM 6169 O HOH A 608 49.477 -0.608 42.396 1.00 41.96 O

HETATM 6170 O HOH A 609 52.951 0.935 44.569 1.00 22.19 O

HETATM 6171 O HOH A 610 65.146 7.002 68.924 1.00 17.44 O

HETATM 6172 O HOH A 611 36.256 3.848 63.571 1.00 19.13 O

HETATM 6173 O HOH A 612 15.074 4.338 64.644 1.00 20.27 O

HETATM 6174 O HOH A 613 14.541 7.574 54.738 1.00 42.76 O

HETATM 6175 O HOH A 614 45.801 23.487 36.738 1.00 20.49 O

HETATM 6176 O HOH A 615 60.123 30.785 46.503 1.00 24.71 O

HETATM 6177 O HOH A 616 39.244 9.104 46.324 1.00 16.15 O

HETATM 6178 O HOH A 617 46.587 2.037 43.300 1.00 22.19 O

HETATM 6179 O HOH A 618 25.667 -8.119 80.629 1.00 29.03 O

HETATM 6180 O HOH A 619 49.835 29.690 34.966 1.00 29.42 O

HETATM 6181 O HOH A 620 86.884 26.905 44.971 1.00 28.71 O

HETATM 6182 O HOH A 621 66.495 8.171 73.112 1.00 19.97 O

HETATM 6183 O HOH A 622 35.079 3.054 54.074 1.00 14.45 O

HETATM 6184 O HOH A 623 53.120 28.385 35.503 1.00 24.51 O

HETATM 6185 O HOH A 624 88.642 25.750 43.584 1.00 28.06 O

HETATM 6186 O HOH A 625 28.755 -0.099 72.147 1.00 14.30 O

HETATM 6187 O HOH A 626 55.518 -3.481 47.553 1.00 23.34 O

HETATM 6188 O HOH A 627 43.939 27.054 36.357 1.00 19.37 O

HETATM 6189 O HOH A 628 45.672 36.781 61.769 1.00 30.06 O

HETATM 6190 O HOH A 629 55.949 40.762 52.670 1.00 40.86 O

HETATM 6191 O HOH A 630 84.997 25.355 51.333 1.00 29.77 O

HETATM 6192 O HOH A 631 29.226 -6.940 74.806 1.00 21.33 O

HETATM 6193 O HOH A 632 34.306 -6.051 77.706 1.00 13.82 O

HETATM 6194 O HOH A 633 27.287 -2.369 69.772 1.00 17.84 O

HETATM 6195 O HOH A 634 38.725 3.011 59.915 1.00 17.11 O

HETATM 6196 O HOH A 635 84.909 26.662 40.727 1.00 30.38 O

HETATM 6197 O HOH A 636 35.572 5.755 42.225 1.00 27.03 O

HETATM 6198 O HOH A 637 20.631 15.350 50.219 1.00 28.38 O

HETATM 6199 O HOH A 638 52.904 -0.547 62.531 1.00 18.30 O

HETATM 6200 O HOH A 639 35.713 8.304 50.141 1.00 12.38 O

HETATM 6201 O HOH A 640 31.777 3.340 56.591 1.00 17.43 O

HETATM 6202 O HOH A 641 96.161 24.766 48.688 1.00 33.16 O

HETATM 6203 O HOH A 642 28.285 1.162 65.326 1.00 23.71 O

HETATM 6204 O HOH A 643 32.036 10.644 55.858 1.00 26.31 O

HETATM 6205 O HOH A 644 34.999 -4.212 81.620 1.00 21.22 O

HETATM 6206 O HOH A 645 30.666 14.475 42.474 1.00 46.39 O

HETATM 6207 O HOH A 646 72.910 39.573 64.562 1.00 32.83 O

HETATM 6208 O HOH A 647 66.793 1.622 66.815 1.00 28.46 O

HETATM 6209 O HOH A 648 52.095 45.662 56.065 1.00 33.17 O

HETATM 6210 O HOH A 649 55.809 0.256 64.033 1.00 39.68 O

HETATM 6211 O HOH A 650 30.023 0.414 68.978 1.00 22.74 O

HETATM 6212 O HOH A 651 84.496 29.239 48.642 1.00 36.45 O

HETATM 6213 O HOH A 652 40.959 29.493 36.668 1.00 41.36 O

HETATM 6214 O HOH A 653 82.395 24.024 53.172 1.00 38.39 O

HETATM 6215 O HOH A 654 45.353 42.074 59.218 1.00 33.11 O

HETATM 6216 O HOH A 655 36.086 3.290 43.589 1.00 28.66 O

HETATM 6217 O HOH A 656 27.945 14.508 48.182 1.00 34.47 O

HETATM 6218 O HOH A 657 38.556 6.443 45.216 1.00 28.05 O

HETATM 6219 O HOH A 658 86.220 26.661 47.664 1.00 25.98 O

HETATM 6220 O HOH A 659 14.031 4.822 59.780 1.00 32.28 O

HETATM 6221 O HOH A 660 39.587 5.713 47.593 1.00 24.65 O

HETATM 6222 O HOH A 661 39.698 0.068 42.233 1.00 38.03 O

HETATM 6223 O HOH A 662 19.600 16.706 48.061 1.00 30.87 O

HETATM 6224 O HOH A 663 31.550 2.952 62.305 1.00 39.84 O

HETATM 6225 O HOH A 664 35.494 -1.570 81.531 1.00 22.51 O

HETATM 6226 O HOH A 665 60.879 31.846 49.088 1.00 41.20 O

HETATM 6227 O HOH A 666 36.247 -5.725 79.716 1.00 20.07 O

HETATM 6228 O HOH A 667 40.907 3.083 61.687 1.00 20.77 O

HETATM 6229 O HOH A 668 60.021 -1.692 56.217 1.00 14.30 O

HETATM 6230 O HOH A 669 98.018 25.601 50.316 1.00 47.92 O

HETATM 6231 O HOH A 670 83.000 31.719 44.080 1.00 46.00 O

HETATM 6232 O HOH A 671 13.210 3.488 66.545 1.00 30.58 O

HETATM 6233 O HOH A 672 57.820 22.904 34.060 1.00 46.59 O

HETATM 6234 O HOH A 673 34.350 0.508 58.977 1.00 16.23 O

HETATM 6235 O HOH A 674 32.007 1.587 67.447 1.00 23.48 O

HETATM 6236 O HOH A 675 34.351 0.250 62.932 1.00 27.47 O

HETATM 6237 O HOH A 676 90.520 28.854 38.723 1.00 56.63 O

HETATM 6238 O HOH A 677 42.385 25.308 37.315 1.00 35.96 O

HETATM 6239 O HOH A 678 92.938 25.317 40.199 1.00 47.64 O

HETATM 6240 O HOH A 679 37.231 25.063 38.677 1.00 48.42 O

HETATM 6241 O HOH A 680 19.935 7.741 52.577 1.00 44.85 O

HETATM 6242 O HOH A 681 70.565 3.164 34.661 1.00 46.79 O

HETATM 6243 O HOH A 682 62.307 18.510 32.030 1.00 50.06 O

HETATM 6244 O HOH A 683 57.085 20.093 38.930 1.00 15.63 O

HETATM 6245 O HOH A 684 79.881 18.820 49.399 1.00 16.56 O

HETATM 6246 O HOH A 685 75.077 12.893 58.512 1.00 15.43 O

HETATM 6247 O HOH A 686 80.851 8.988 55.786 1.00 21.33 O

HETATM 6248 O HOH A 687 64.742 -0.596 51.086 1.00 17.70 O

HETATM 6249 O HOH A 688 79.832 17.923 40.222 1.00 23.79 O

HETATM 6250 O HOH A 689 63.717 17.183 36.944 1.00 18.32 O

HETATM 6251 O HOH A 690 58.918 8.560 65.857 1.00 17.27 O

HETATM 6252 O HOH A 691 74.213 10.055 59.197 1.00 19.09 O

HETATM 6253 O HOH A 692 22.233 0.395 73.787 1.00 20.85 O

HETATM 6254 O HOH A 693 52.075 9.000 49.515 1.00 14.77 O

HETATM 6255 O HOH A 694 22.528 3.133 73.201 1.00 19.15 O

HETATM 6256 O HOH A 695 62.139 1.244 61.732 1.00 21.55 O

HETATM 6257 O HOH A 696 26.673 16.560 54.847 1.00 17.21 O

HETATM 6258 O HOH A 697 64.489 8.770 53.292 1.00 17.27 O

HETATM 6259 O HOH A 698 75.521 -0.999 47.511 1.00 19.39 O

HETATM 6260 O HOH A 699 57.633 8.383 43.329 1.00 24.30 O

HETATM 6261 O HOH A 700 50.819 13.833 68.287 1.00 17.54 O

HETATM 6262 O HOH A 701 32.444 -2.487 80.115 1.00 17.92 O

HETATM 6263 O HOH A 702 81.515 18.777 51.808 1.00 32.41 O

HETATM 6264 O HOH A 703 66.826 19.706 53.607 1.00 22.24 O

HETATM 6265 O HOH A 704 53.283 11.281 58.760 1.00 19.43 O

HETATM 6266 O HOH A 705 29.433 2.756 76.663 1.00 17.75 O

HETATM 6267 O HOH A 706 49.931 13.804 59.179 1.00 22.96 O

HETATM 6268 O HOH A 707 68.632 17.905 49.525 1.00 23.00 O

HETATM 6269 O HOH A 708 85.984 6.733 61.878 1.00 29.66 O

HETATM 6270 O HOH A 709 71.755 12.839 59.218 1.00 24.31 O

HETATM 6271 O HOH A 710 66.651 5.043 50.954 1.00 24.09 O

HETATM 6272 O HOH A 711 89.740 11.370 40.242 1.00 24.43 O

HETATM 6273 O HOH A 712 50.582 6.438 53.310 1.00 26.90 O

HETATM 6274 O HOH A 713 64.098 20.063 36.815 1.00 20.86 O

HETATM 6275 O HOH A 714 65.564 14.891 36.872 1.00 23.48 O

HETATM 6276 O HOH A 715 69.378 14.591 57.724 1.00 29.38 O

HETATM 6277 O HOH A 716 53.926 21.415 63.057 1.00 27.43 O

HETATM 6278 O HOH A 717 74.747 -0.174 51.831 1.00 23.55 O

HETATM 6279 O HOH A 718 88.508 22.003 33.566 1.00 39.52 O

HETATM 6280 O HOH A 719 82.876 2.654 54.809 1.00 29.57 O

HETATM 6281 O HOH A 720 69.433 -5.832 47.143 1.00 24.91 O

HETATM 6282 O HOH A 721 83.033 4.470 63.689 1.00 32.92 O

HETATM 6283 O HOH A 722 68.719 26.515 40.351 1.00 40.50 O

HETATM 6284 O HOH A 723 53.214 14.203 40.737 1.00 31.44 O

HETATM 6285 O HOH A 724 76.994 17.858 33.619 1.00 32.08 O

HETATM 6286 O HOH A 725 75.239 -1.958 49.789 1.00 23.98 O

HETATM 6287 O HOH A 726 68.733 -5.444 44.445 1.00 30.93 O

HETATM 6288 O HOH A 727 69.930 17.603 34.128 1.00 29.38 O

HETATM 6289 O HOH A 728 69.156 4.346 39.296 1.00 26.49 O

HETATM 6290 O HOH A 729 78.073 31.039 42.121 1.00 40.26 O

HETATM 6291 O HOH A 730 69.816 13.019 61.651 1.00 29.90 O

HETATM 6292 O HOH A 731 63.841 13.964 58.420 1.00 29.68 O

HETATM 6293 O HOH A 732 72.972 27.057 38.930 1.00 42.29 O

HETATM 6294 O HOH A 733 83.004 15.858 33.433 1.00 36.44 O

HETATM 6295 O HOH A 734 49.038 8.822 44.208 1.00 35.25 O

HETATM 6296 O HOH A 735 95.304 14.633 56.697 1.00 32.60 O

HETATM 6297 O HOH A 736 79.522 12.962 49.365 1.00 32.48 O

HETATM 6298 O HOH A 737 66.830 13.732 59.373 1.00 36.51 O

HETATM 6299 O HOH A 738 79.659 1.810 54.315 1.00 29.67 O

HETATM 6300 O HOH A 739 75.133 22.920 45.458 1.00 38.34 O

HETATM 6301 O HOH A 740 65.937 26.760 41.838 1.00 31.52 O

HETATM 6302 O HOH A 741 45.422 24.754 65.365 1.00 29.99 O

HETATM 6303 O HOH A 742 74.707 25.462 45.013 1.00 35.37 O

HETATM 6304 O HOH A 743 61.841 16.038 35.230 1.00 33.14 O

HETATM 6305 O HOH A 744 66.061 18.560 34.057 1.00 37.85 O

HETATM 6306 O HOH A 745 79.924 -1.963 50.961 1.00 35.34 O

HETATM 6307 O HOH A 746 70.539 31.392 46.311 1.00 50.23 O

HETATM 6308 O HOH A 747 62.844 9.305 40.611 1.00 32.50 O

HETATM 6309 O HOH A 748 71.016 0.073 38.168 1.00 33.25 O

HETATM 6310 O HOH A 749 32.705 4.405 63.620 1.00 37.85 O

HETATM 6311 O HOH A 750 48.471 -0.037 64.032 1.00 33.90 O

HETATM 6312 O HOH A 751 74.530 -4.405 50.069 1.00 37.06 O

HETATM 6313 O HOH A 752 50.552 0.918 62.224 1.00 31.09 O

HETATM 6314 O HOH A 753 76.800 23.119 34.989 1.00 38.13 O

HETATM 6315 O HOH A 754 70.574 2.775 37.243 1.00 29.59 O

HETATM 6316 O HOH A 755 78.160 0.177 37.911 1.00 37.18 O

HETATM 6317 O HOH A 756 20.960 -0.965 75.633 1.00 38.27 O

HETATM 6318 O HOH A 757 53.428 15.300 38.643 1.00 48.74 O

HETATM 6319 O HOH A 758 43.700 31.656 63.409 1.00 34.86 O

HETATM 6320 O HOH A 759 77.487 10.654 48.161 1.00 31.29 O

HETATM 6321 O HOH A 760 59.687 7.247 42.427 1.00 41.20 O

HETATM 6322 O HOH A 761 63.066 20.178 34.279 1.00 41.84 O

HETATM 6323 O HOH A 762 70.907 -2.855 40.272 1.00 40.00 O

HETATM 6324 O HOH A 763 75.998 -0.171 56.509 1.00 22.21 O

HETATM 6325 O HOH A 764 51.679 12.440 40.698 1.00 43.06 O

HETATM 6326 O HOH A 765 54.300 10.987 41.963 1.00 43.73 O

HETATM 6327 O HOH A 766 73.658 10.589 34.890 1.00 39.15 O

HETATM 6328 O HOH A 767 71.810 17.730 67.821 1.00 31.95 O

HETATM 6329 O HOH A 768 90.796 11.607 42.655 1.00 41.31 O

HETATM 6330 O HOH A 769 93.420 22.501 40.270 1.00 37.87 O

HETATM 6331 O HOH A 770 61.285 23.669 35.606 1.00 37.83 O

HETATM 6332 O HOH A 771 90.193 17.349 37.084 1.00 37.56 O

HETATM 6333 O HOH A 772 67.570 14.383 63.073 1.00 32.69 O

HETATM 6334 O HOH A 773 83.522 25.540 34.058 1.00 44.69 O

HETATM 6335 O HOH A 774 96.100 14.848 59.003 1.00 45.78 O

HETATM 6336 O HOH A 775 81.532 -3.283 43.186 1.00 42.18 O

HETATM 6337 O HOH A 776 68.711 -0.240 40.309 1.00 42.64 O

HETATM 6338 O HOH A 777 84.969 17.707 60.505 1.00 41.98 O

HETATM 6339 O HOH A 778 68.008 2.312 40.452 1.00 39.38 O

HETATM 6340 O HOH A 779 72.013 10.490 36.843 1.00 40.79 O

HETATM 6341 O HOH A 780 76.259 11.317 33.271 1.00 50.69 O

HETATM 6342 O HOH A 781 90.651 16.868 46.089 1.00 31.08 O

HETATM 6343 O HOH A 782 31.964 22.578 46.841 1.00 18.23 O

HETATM 6344 O HOH A 783 65.011 2.304 51.342 1.00 16.76 O

HETATM 6345 O HOH A 784 55.673 29.717 61.903 1.00 19.71 O

HETATM 6346 O HOH A 785 30.671 21.183 49.241 1.00 21.77 O

HETATM 6347 O HOH A 786 59.377 2.366 59.700 1.00 16.04 O

HETATM 6348 O HOH A 787 64.657 6.156 52.458 1.00 13.53 O

HETATM 6349 O HOH A 788 70.029 12.446 72.924 1.00 18.80 O

HETATM 6350 O HOH A 789 61.394 28.051 68.486 1.00 16.00 O

HETATM 6351 O HOH A 790 37.393 23.388 42.887 1.00 23.48 O

HETATM 6352 O HOH A 791 38.122 20.650 55.346 1.00 14.80 O

HETATM 6353 O HOH A 792 27.595 22.198 57.978 1.00 18.54 O

HETATM 6354 O HOH A 793 57.092 2.325 61.622 1.00 19.37 O

HETATM 6355 O HOH A 794 50.627 20.517 38.868 1.00 16.03 O

HETATM 6356 O HOH A 795 43.175 27.772 42.741 1.00 17.89 O

HETATM 6357 O HOH A 796 52.353 36.429 51.701 1.00 16.05 O

HETATM 6358 O HOH A 797 61.715 27.463 64.395 1.00 19.22 O

HETATM 6359 O HOH A 798 49.557 26.921 61.309 1.00 22.54 O

HETATM 6360 O HOH A 799 58.128 23.304 36.839 1.00 21.04 O

HETATM 6361 O HOH A 800 36.859 10.614 62.060 1.00 15.54 O

HETATM 6362 O HOH A 801 62.721 -3.331 48.739 1.00 18.26 O

HETATM 6363 O HOH A 802 55.068 9.941 60.446 1.00 17.78 O

HETATM 6364 O HOH A 803 37.485 33.700 47.832 1.00 24.30 O

HETATM 6365 O HOH A 804 34.479 23.397 42.823 1.00 21.89 O

HETATM 6366 O HOH A 805 67.282 31.377 75.033 1.00 23.89 O

HETATM 6367 O HOH A 806 38.643 21.461 41.246 1.00 21.83 O

HETATM 6368 O HOH A 807 31.995 25.266 48.461 1.00 19.11 O

HETATM 6369 O HOH A 808 28.058 14.279 54.090 1.00 16.53 O

HETATM 6370 O HOH A 809 58.384 8.731 68.570 1.00 15.31 O

HETATM 6371 O HOH A 810 68.932 23.508 78.431 1.00 23.10 O

HETATM 6372 O HOH A 811 48.373 7.403 53.684 1.00 21.96 O

HETATM 6373 O HOH A 812 42.111 23.984 40.511 1.00 27.94 O

HETATM 6374 O HOH A 813 59.252 2.575 47.026 1.00 21.78 O

HETATM 6375 O HOH A 814 59.644 28.027 66.030 1.00 23.22 O

HETATM 6376 O HOH A 815 64.228 19.657 52.687 1.00 20.36 O

HETATM 6377 O HOH A 816 39.212 13.941 40.621 1.00 24.07 O

HETATM 6378 O HOH A 817 59.824 -1.661 46.968 1.00 20.63 O

HETATM 6379 O HOH A 818 41.354 27.889 60.714 1.00 24.21 O

HETATM 6380 O HOH A 819 38.675 20.275 58.329 1.00 17.74 O

HETATM 6381 O HOH A 820 14.964 8.731 65.783 1.00 22.71 O

HETATM 6382 O HOH A 821 47.073 10.995 41.938 1.00 28.21 O

HETATM 6383 O HOH A 822 57.654 4.604 46.276 1.00 26.41 O

HETATM 6384 O HOH A 823 39.961 12.411 56.924 1.00 27.25 O

HETATM 6385 O HOH A 824 56.018 29.565 41.321 1.00 27.81 O

HETATM 6386 O HOH A 825 41.229 21.553 41.197 1.00 26.80 O

HETATM 6387 O HOH A 826 61.544 28.329 46.809 1.00 27.97 O

HETATM 6388 O HOH A 827 47.362 35.557 43.434 1.00 27.45 O

HETATM 6389 O HOH A 828 46.663 33.040 59.729 1.00 21.97 O

HETATM 6390 O HOH A 829 53.124 27.603 60.376 1.00 22.20 O

HETATM 6391 O HOH A 830 45.000 8.692 42.059 1.00 32.25 O

HETATM 6392 O HOH A 831 76.175 27.765 68.333 1.00 27.63 O

HETATM 6393 O HOH A 832 59.356 25.873 37.028 1.00 30.02 O

HETATM 6394 O HOH A 833 57.485 23.686 66.062 1.00 23.72 O

HETATM 6395 O HOH A 834 13.278 13.482 59.947 1.00 26.89 O

HETATM 6396 O HOH A 835 53.220 3.146 63.757 1.00 34.19 O

HETATM 6397 O HOH A 836 58.398 29.355 40.316 1.00 29.25 O

HETATM 6398 O HOH A 837 60.064 32.711 65.283 1.00 25.38 O

HETATM 6399 O HOH A 838 68.794 18.490 52.000 1.00 25.93 O

HETATM 6400 O HOH A 839 61.628 6.532 43.956 1.00 28.94 O

HETATM 6401 O HOH A 840 74.419 21.132 66.425 1.00 29.51 O

HETATM 6402 O HOH A 841 50.881 3.689 61.773 1.00 30.14 O

HETATM 6403 O HOH A 842 58.455 30.652 65.679 1.00 29.29 O

HETATM 6404 O HOH A 843 25.675 20.142 49.037 1.00 28.47 O

HETATM 6405 O HOH A 844 50.055 39.819 51.770 1.00 27.33 O

HETATM 6406 O HOH A 845 68.133 32.746 72.580 1.00 35.23 O

HETATM 6407 O HOH A 846 40.585 34.462 47.948 1.00 30.15 O

HETATM 6408 O HOH A 847 50.816 6.696 45.239 1.00 25.57 O

HETATM 6409 O HOH A 848 46.654 15.243 38.780 1.00 27.22 O

HETATM 6410 O HOH A 849 77.304 23.971 74.178 1.00 38.95 O

HETATM 6411 O HOH A 850 45.555 34.901 40.483 1.00 34.13 O

HETATM 6412 O HOH A 851 28.438 19.812 48.542 1.00 35.72 O

HETATM 6413 O HOH A 852 30.554 18.863 44.599 1.00 28.73 O

HETATM 6414 O HOH A 853 67.090 27.443 48.484 1.00 35.05 O

HETATM 6415 O HOH A 854 49.211 23.898 59.672 1.00 30.80 O

HETATM 6416 O HOH A 855 16.090 16.305 59.676 1.00 30.70 O

HETATM 6417 O HOH A 856 56.099 27.554 65.230 1.00 32.51 O

HETATM 6418 O HOH A 857 52.030 9.089 46.098 1.00 31.19 O

HETATM 6419 O HOH A 858 77.900 19.640 68.288 1.00 30.38 O

HETATM 6420 O HOH A 859 70.993 31.090 59.213 1.00 35.76 O

HETATM 6421 O HOH A 860 63.716 25.576 43.178 1.00 31.53 O

HETATM 6422 O HOH A 861 22.802 19.386 49.179 1.00 32.28 O

HETATM 6423 O HOH A 862 68.054 21.003 62.454 1.00 32.15 O

HETATM 6424 O HOH A 863 59.785 35.258 66.405 1.00 31.32 O

HETATM 6425 O HOH A 864 71.227 29.521 54.549 1.00 34.27 O

HETATM 6426 O HOH A 865 46.323 41.941 52.943 1.00 39.15 O

HETATM 6427 O HOH A 866 62.155 31.830 66.423 1.00 35.15 O

HETATM 6428 O HOH A 867 76.201 24.997 56.229 1.00 35.79 O

HETATM 6429 O HOH A 868 49.306 25.815 63.915 1.00 30.51 O

HETATM 6430 O HOH A 869 51.650 25.223 60.396 1.00 34.18 O

HETATM 6431 O HOH A 870 77.668 25.447 66.239 1.00 33.41 O

HETATM 6432 O HOH A 871 72.091 22.832 51.499 1.00 36.27 O

HETATM 6433 O HOH A 872 73.959 27.672 76.640 1.00 38.87 O

HETATM 6434 O HOH A 873 64.617 35.898 57.657 1.00 39.80 O

HETATM 6435 O HOH A 874 60.672 30.831 51.481 1.00 29.58 O

HETATM 6436 O HOH A 875 62.829 29.866 49.482 1.00 42.78 O

HETATM 6437 O HOH A 876 37.568 35.940 53.270 1.00 37.09 O

HETATM 6438 O HOH A 877 36.993 26.533 40.524 1.00 34.33 O

HETATM 6439 O HOH A 878 71.445 20.929 58.936 1.00 34.87 O

HETATM 6440 O HOH A 879 15.855 19.381 49.824 1.00 35.63 O

HETATM 6441 O HOH A 880 54.896 26.253 62.293 1.00 38.74 O

HETATM 6442 O HOH A 881 71.073 17.136 57.123 1.00 43.43 O

HETATM 6443 O HOH A 882 70.606 18.847 65.896 1.00 43.52 O

HETATM 6444 O HOH A 883 51.844 37.106 45.748 1.00 47.35 O

HETATM 6445 O HOH A 884 69.208 30.063 52.861 1.00 39.64 O

HETATM 6446 O HOH A 885 53.737 30.515 40.475 1.00 35.63 O

HETATM 6447 O HOH A 886 50.014 11.123 42.044 1.00 40.78 O

HETATM 6448 O HOH A 887 37.544 32.246 42.964 1.00 43.25 O

HETATM 6449 O HOH A 888 15.273 18.772 64.193 1.00 39.03 O

HETATM 6450 O HOH A 889 64.116 26.767 45.523 1.00 36.37 O

HETATM 6451 O HOH A 890 46.531 25.209 60.943 1.00 41.35 O

HETATM 6452 O HOH A 891 66.909 6.828 59.638 1.00 33.63 O

HETATM 6453 O HOH A 892 23.247 19.332 64.479 1.00 35.19 O

HETATM 6454 O HOH A 893 14.790 20.541 59.619 1.00 37.58 O

HETATM 6455 O HOH A 894 40.251 31.877 41.869 1.00 37.72 O

HETATM 6456 O HOH A 895 52.345 10.530 43.088 1.00 36.73 O

HETATM 6457 O HOH A 896 47.196 24.773 63.456 1.00 36.09 O

HETATM 6458 O HOH A 897 41.878 20.559 38.567 1.00 42.01 O

HETATM 6459 O HOH A 898 29.911 15.680 44.992 1.00 40.07 O

HETATM 6460 O HOH A 899 73.267 16.816 64.878 1.00 39.70 O

HETATM 6461 O HOH A 900 72.782 16.853 59.278 1.00 40.58 O

HETATM 6462 O HOH A 901 36.705 16.565 38.791 1.00 35.34 O

HETATM 6463 O HOH A 902 37.063 14.413 37.180 1.00 47.23 O

HETATM 6464 O HOH A 903 76.369 21.929 64.954 1.00 38.02 O

HETATM 6465 O HOH A 904 52.563 37.691 59.185 1.00 18.76 O

HETATM 6466 O HOH A 905 19.737 4.000 73.449 1.00 21.44 O

HETATM 6467 O HOH A 906 63.945 36.225 61.583 1.00 27.46 O

HETATM 6468 O HOH A 907 61.815 39.343 59.236 1.00 29.88 O

HETATM 6469 O HOH A 908 62.977 35.800 64.018 1.00 32.00 O

HETATM 6470 O HOH A 909 66.183 35.957 59.666 1.00 41.42 O

HETATM 6471 O HOH A 910 48.598 2.277 41.783 1.00 43.55 O

HETATM 6472 O HOH A 911 70.654 33.879 72.496 1.00 48.60 O

HETATM 6473 O HOH A 912 48.553 16.236 37.813 1.00 39.49 O

HETATM 6474 O HOH A 913 67.005 37.233 67.945 1.00 32.69 O

HETATM 6475 O HOH A 914 28.647 19.505 45.828 1.00 45.64 O

HETATM 6476 O HOH A 915 19.375 27.160 52.949 1.00 50.98 O

HETATM 6477 O HOH A 916 73.168 28.158 53.354 1.00 39.74 O

HETATM 6478 O HOH A 917 53.852 37.806 49.895 1.00 44.97 O

HETATM 6479 O HOH A 918 55.638 3.491 44.345 1.00 43.78 O

HETATM 6480 O HOH A 919 56.328 6.866 44.799 1.00 45.41 O

HETATM 6481 O HOH A 920 52.143 35.092 43.531 1.00 32.90 O

HETATM 6482 O HOH A 921 82.360 20.399 54.241 1.00 43.13 O

HETATM 6483 O HOH A 922 99.359 13.464 51.291 1.00 41.75 O

HETATM 6484 O HOH A 923 38.972 34.409 57.263 1.00 40.98 O

HETATM 6485 O HOH A 924 48.595 16.772 65.262 1.00 42.43 O

HETATM 6486 O HOH A 925 48.327 10.693 60.782 1.00 14.28 O

HETATM 6487 O HOH A 926 55.303 8.620 64.543 1.00 22.88 O

HETATM 6488 O HOH A 927 43.147 34.147 47.210 1.00 24.28 O

HETATM 6489 O HOH A 928 50.318 18.472 37.447 1.00 34.07 O

HETATM 6490 O HOH A 929 44.946 38.663 51.036 1.00 29.83 O

HETATM 6491 O HOH A 930 48.044 13.167 65.098 1.00 40.94 O

HETATM 6492 O HOH A 931 47.853 8.770 63.912 1.00 28.34 O

HETATM 6493 O HOH A 932 51.446 11.623 60.510 1.00 28.20 O

HETATM 6494 O HOH A 933 51.168 37.659 48.087 1.00 39.64 O

HETATM 6495 O HOH A 934 60.459 35.098 52.930 1.00 38.20 O

HETATM 6496 O HOH A 935 50.622 11.006 62.540 1.00 27.24 O

HETATM 6497 O HOH A 936 58.658 24.286 52.303 1.00 12.09 O

HETATM 6498 O HOH A 937 70.053 23.393 37.350 1.00 37.64 O

HETATM 6499 O HOH A 938 63.672 34.276 66.447 1.00 31.69 O

HETATM 6500 O HOH A 939 38.349 18.669 38.122 1.00 41.04 O

HETATM 6501 O HOH A 940 77.188 12.306 50.634 1.00 36.60 O

HETATM 6502 O HOH A 941 43.249 23.194 37.557 1.00 36.51 O

HETATM 6503 O HOH A 942 47.596 12.439 58.817 1.00 13.31 O

HETATM 6504 O HOH A 943 50.043 18.641 69.530 1.00 27.87 O

HETATM 6505 O HOH A 944 83.685 14.253 52.716 1.00 35.97 O

HETATM 6506 O HOH A 945 82.046 12.873 51.176 1.00 33.92 O

HETATM 6507 O HOH A 946 66.187 16.257 59.848 1.00 44.51 O

HETATM 6508 O HOH A 947 13.181 19.370 54.196 1.00 41.97 O

HETATM 6509 O HOH A 948 11.650 11.821 61.775 1.00 50.82 O

HETATM 6510 O HOH A 949 88.010 -1.619 47.685 1.00 45.23 O

HETATM 6511 O HOH A 950 23.144 -2.116 85.246 1.00 46.51 O

HETATM 6512 O HOH A 951 68.148 29.871 48.610 1.00 46.43 O

HETATM 6513 O HOH A 952 76.213 16.701 48.935 1.00 42.98 O

HETATM 6514 O HOH A 953 72.972 26.383 49.275 1.00 43.69 O

HETATM 6515 O HOH A 954 66.716 9.158 38.497 1.00 52.64 O

HETATM 6516 O HOH A 955 85.094 11.538 61.175 1.00 40.88 O

HETATM 6517 O HOH A 956 60.643 8.652 39.861 1.00 46.19 O

HETATM 6518 O HOH A 957 83.076 8.435 32.302 1.00 47.64 O

HETATM 6519 O HOH A 958 55.727 9.178 41.593 1.00 49.20 O

HETATM 6520 O HOH A 959 54.772 10.508 63.027 1.00 24.50 O

HETATM 6521 O HOH A 960 53.077 16.961 37.309 1.00 49.20 O

HETATM 6522 O HOH A 961 64.436 30.551 82.685 1.00 47.39 O

HETATM 6523 O HOH A 962 51.634 20.210 63.237 1.00 45.76 O

HETATM 6524 O HOH A 963 17.523 24.733 52.269 1.00 46.11 O

HETATM 6525 O HOH A 964 43.476 13.702 58.378 1.00 33.30 O

HETATM 6526 O HOH A 965 41.841 33.921 59.478 1.00 44.93 O

HETATM 6527 O HOH A 966 66.584 30.600 77.947 1.00 33.76 O

HETATM 6528 O HOH A 967 68.560 17.634 59.037 1.00 40.91 O

HETATM 6529 O HOH A 968 90.741 14.917 62.815 1.00 46.52 O

HETATM 6530 O HOH A 969 79.549 -3.345 40.125 1.00 47.82 O

HETATM 6531 O HOH A 970 16.317 4.193 72.543 1.00 45.03 O

HETATM 6532 O HOH A 971 71.921 23.128 36.031 1.00 47.68 O

HETATM 6533 O HOH A 972 76.352 26.973 73.659 1.00 44.41 O

HETATM 6534 O HOH A 973 51.527 31.543 38.109 1.00 36.69 O

HETATM 6535 O HOH A 974 18.609 23.481 49.809 1.00 38.55 O

HETATM 6536 O HOH A 975 44.636 37.615 48.251 1.00 44.34 O

HETATM 6537 O HOH A 976 78.143 25.568 71.195 1.00 50.58 O

HETATM 6538 O HOH A 977 40.126 28.608 40.670 1.00 42.35 O

HETATM 6539 O HOH A 978 31.654 23.110 44.038 1.00 50.91 O

HETATM 6540 O HOH A 979 54.408 5.807 43.640 1.00 46.44 O

HETATM 6541 O HOH A 980 70.167 11.895 34.438 1.00 47.73 O

HETATM 6542 O HOH A 981 89.119 26.956 37.127 1.00 53.92 O

HETATM 6543 O HOH A 982 72.843 33.177 70.913 1.00 50.33 O

HETATM 6544 O HOH A 983 43.030 11.680 55.963 1.00 48.17 O

HETATM 6545 O HOH A 984 38.813 32.736 59.166 1.00 28.91 O

HETATM 6546 O HOH A 985 50.282 14.614 61.563 1.00 24.59 O

HETATM 6547 O HOH A 986 47.637 11.006 64.957 1.00 23.12 O

HETATM 6548 O HOH A 987 99.561 19.298 55.966 1.00 39.38 O

HETATM 6549 O HOH A 988 70.438 30.656 68.062 1.00 38.74 O

HETATM 6550 O HOH A 989 21.767 -3.478 79.688 1.00 41.08 O

HETATM 6551 O HOH A 990 82.703 2.333 61.523 1.00 45.78 O

HETATM 6552 O HOH B 601 44.625 0.206 85.316 1.00 37.30 O

HETATM 6553 O HOH B 602 42.784 42.853 74.408 1.00 38.77 O

HETATM 6554 O HOH B 603 35.329 39.169 67.386 1.00 32.57 O

HETATM 6555 O HOH B 604 41.303 37.190 61.575 1.00 36.21 O

HETATM 6556 O HOH B 605 30.403 10.250 58.994 1.00 17.83 O

HETATM 6557 O HOH B 606 52.414 22.936 91.112 1.00 23.75 O

HETATM 6558 O HOH B 607 57.730 -0.842 67.170 1.00 23.59 O

HETATM 6559 O HOH B 608 58.194 1.738 64.269 1.00 17.07 O

HETATM 6560 O HOH B 609 38.256 38.707 63.838 1.00 33.32 O

HETATM 6561 O HOH B 610 29.327 11.713 54.856 1.00 18.17 O

HETATM 6562 O HOH B 611 79.117 -1.814 63.269 1.00 20.83 O

HETATM 6563 O HOH B 612 64.846 -3.428 55.648 1.00 13.46 O

HETATM 6564 O HOH B 613 36.401 38.678 70.003 1.00 41.36 O

HETATM 6565 O HOH B 614 59.262 0.842 73.782 1.00 15.22 O

HETATM 6566 O HOH B 615 54.925 26.139 91.400 1.00 20.46 O

HETATM 6567 O HOH B 616 63.093 -10.060 53.014 1.00 15.58 O

HETATM 6568 O HOH B 617 49.053 45.202 69.217 1.00 26.51 O

HETATM 6569 O HOH B 618 56.280 7.605 81.440 1.00 18.51 O

HETATM 6570 O HOH B 619 41.293 2.116 83.380 1.00 25.39 O

HETATM 6571 O HOH B 620 37.913 -1.854 80.273 1.00 21.84 O

HETATM 6572 O HOH B 621 47.807 1.947 84.591 1.00 25.74 O

HETATM 6573 O HOH B 622 37.598 38.854 66.311 1.00 25.73 O

HETATM 6574 O HOH B 623 46.250 29.095 92.292 1.00 23.19 O

HETATM 6575 O HOH B 624 66.452 -12.058 47.243 1.00 29.25 O

HETATM 6576 O HOH B 625 65.796 -5.967 58.107 1.00 17.43 O

HETATM 6577 O HOH B 626 62.573 0.503 71.335 1.00 17.81 O

HETATM 6578 O HOH B 627 75.712 10.317 77.562 1.00 27.87 O

HETATM 6579 O HOH B 628 56.403 4.854 82.705 1.00 27.37 O

HETATM 6580 O HOH B 629 55.694 1.468 67.930 1.00 17.84 O

HETATM 6581 O HOH B 630 49.159 22.539 91.533 1.00 31.52 O

HETATM 6582 O HOH B 631 59.233 3.596 85.613 1.00 30.66 O

HETATM 6583 O HOH B 632 65.394 11.165 85.606 1.00 41.95 O

HETATM 6584 O HOH B 633 44.278 45.030 74.312 1.00 43.13 O

HETATM 6585 O HOH B 634 63.630 7.555 72.245 1.00 23.23 O

HETATM 6586 O HOH B 635 58.158 27.678 91.127 1.00 44.34 O

HETATM 6587 O HOH B 636 57.939 -6.432 46.227 1.00 21.96 O

HETATM 6588 O HOH B 637 41.083 0.528 65.376 1.00 19.70 O

HETATM 6589 O HOH B 638 73.278 -12.694 49.972 1.00 39.31 O

HETATM 6590 O HOH B 639 63.685 -2.823 58.862 1.00 21.54 O

HETATM 6591 O HOH B 640 27.807 5.312 61.108 1.00 26.57 O

HETATM 6592 O HOH B 641 34.769 40.294 60.073 1.00 31.61 O

HETATM 6593 O HOH B 642 65.526 -2.490 62.550 1.00 24.70 O

HETATM 6594 O HOH B 643 79.826 1.547 73.369 1.00 44.74 O

HETATM 6595 O HOH B 644 58.329 1.266 84.310 1.00 26.87 O

HETATM 6596 O HOH B 645 38.879 41.134 68.493 1.00 20.74 O

HETATM 6597 O HOH B 646 62.698 0.063 65.736 1.00 40.53 O

HETATM 6598 O HOH B 647 54.246 -1.205 85.443 1.00 40.82 O

HETATM 6599 O HOH B 648 68.619 11.173 79.567 1.00 43.15 O

HETATM 6600 O HOH B 649 77.030 11.278 79.701 1.00 35.22 O

HETATM 6601 O HOH B 650 38.565 2.234 63.704 1.00 33.96 O

HETATM 6602 O HOH B 651 55.374 4.308 80.188 1.00 20.02 O

HETATM 6603 O HOH B 652 40.884 20.698 92.029 1.00 36.78 O

HETATM 6604 O HOH B 653 80.046 -1.431 68.232 1.00 32.84 O

HETATM 6605 O HOH B 654 57.922 -3.662 46.357 1.00 21.19 O

HETATM 6606 O HOH B 655 66.453 -12.845 44.575 1.00 33.09 O

HETATM 6607 O HOH B 656 56.499 -7.561 48.112 1.00 19.00 O

HETATM 6608 O HOH B 657 23.384 31.659 54.106 1.00 48.12 O

HETATM 6609 O HOH B 658 53.415 1.954 66.166 1.00 19.92 O

HETATM 6610 O HOH B 659 33.918 0.850 71.670 1.00 14.83 O

HETATM 6611 O HOH B 660 40.441 25.068 93.614 1.00 35.43 O

HETATM 6612 O HOH B 661 80.967 -2.924 61.520 1.00 32.45 O

HETATM 6613 O HOH B 662 61.944 -1.170 60.386 1.00 20.61 O

HETATM 6614 O HOH B 663 13.886 37.680 65.528 1.00 46.35 O

HETATM 6615 O HOH B 664 59.508 -1.957 68.908 1.00 15.98 O

HETATM 6616 O HOH B 665 59.411 -2.121 64.867 1.00 25.36 O

HETATM 6617 O HOH B 666 56.242 24.063 90.414 1.00 38.24 O

HETATM 6618 O HOH B 667 43.820 20.153 91.774 1.00 46.30 O

HETATM 6619 O HOH B 668 32.228 19.566 95.332 1.00 51.91 O

HETATM 6620 O HOH B 669 35.347 21.116 95.818 1.00 48.80 O

HETATM 6621 O HOH B 670 45.576 39.475 69.490 1.00 15.73 O

HETATM 6622 O HOH B 671 40.028 26.086 75.565 1.00 13.96 O

HETATM 6623 O HOH B 672 45.740 14.371 59.688 1.00 17.51 O

HETATM 6624 O HOH B 673 48.952 38.428 68.066 1.00 17.13 O

HETATM 6625 O HOH B 674 46.984 7.433 74.217 1.00 22.51 O

HETATM 6626 O HOH B 675 30.719 9.404 75.388 1.00 16.29 O

HETATM 6627 O HOH B 676 67.012 17.815 78.594 1.00 20.12 O

HETATM 6628 O HOH B 677 47.585 10.719 67.083 1.00 13.57 O

HETATM 6629 O HOH B 678 33.598 20.032 90.878 1.00 21.75 O

HETATM 6630 O HOH B 679 68.231 10.451 73.728 1.00 16.46 O

HETATM 6631 O HOH B 680 43.634 9.841 78.303 1.00 16.24 O

HETATM 6632 O HOH B 681 40.760 21.706 88.894 1.00 16.47 O

HETATM 6633 O HOH B 682 38.158 30.228 59.352 1.00 16.66 O

HETATM 6634 O HOH B 683 58.860 18.306 69.627 1.00 17.81 O

HETATM 6635 O HOH B 684 22.149 14.997 68.684 1.00 20.63 O

HETATM 6636 O HOH B 685 35.272 4.628 68.108 1.00 17.09 O

HETATM 6637 O HOH B 686 65.985 19.519 80.870 1.00 21.66 O

HETATM 6638 O HOH B 687 40.367 25.132 90.977 1.00 20.81 O

HETATM 6639 O HOH B 688 21.851 18.021 69.333 1.00 16.18 O

HETATM 6640 O HOH B 689 31.369 11.858 74.543 1.00 18.49 O

HETATM 6641 O HOH B 690 17.808 24.910 78.704 1.00 23.04 O

HETATM 6642 O HOH B 691 28.559 8.610 76.946 1.00 20.96 O

HETATM 6643 O HOH B 692 60.792 -5.035 47.769 1.00 17.78 O

HETATM 6644 O HOH B 693 33.652 22.604 75.238 1.00 22.38 O

HETATM 6645 O HOH B 694 35.359 4.861 80.797 1.00 23.40 O

HETATM 6646 O HOH B 695 46.594 14.080 68.733 1.00 21.55 O

HETATM 6647 O HOH B 696 63.590 20.763 84.982 1.00 19.64 O

HETATM 6648 O HOH B 697 74.342 -1.233 54.475 1.00 21.73 O

HETATM 6649 O HOH B 698 37.365 10.658 59.322 1.00 14.32 O

HETATM 6650 O HOH B 699 15.418 15.312 72.203 1.00 26.22 O

HETATM 6651 O HOH B 700 71.524 -1.524 54.644 1.00 17.91 O

HETATM 6652 O HOH B 701 49.299 27.037 66.582 1.00 21.72 O

HETATM 6653 O HOH B 702 46.413 14.947 66.224 1.00 22.90 O

HETATM 6654 O HOH B 703 47.232 20.905 88.864 1.00 18.96 O

HETATM 6655 O HOH B 704 66.468 21.995 79.451 1.00 22.09 O

HETATM 6656 O HOH B 705 44.015 30.768 65.921 1.00 19.06 O

HETATM 6657 O HOH B 706 80.390 10.180 68.199 1.00 25.18 O

HETATM 6658 O HOH B 707 37.250 6.559 81.638 1.00 34.82 O

HETATM 6659 O HOH B 708 71.286 -4.128 54.158 1.00 20.97 O

HETATM 6660 O HOH B 709 56.212 37.804 76.549 1.00 28.96 O

HETATM 6661 O HOH B 710 62.738 31.410 79.943 1.00 23.44 O

HETATM 6662 O HOH B 711 55.812 26.646 85.106 1.00 18.33 O

HETATM 6663 O HOH B 712 40.446 9.995 63.359 1.00 19.18 O

HETATM 6664 O HOH B 713 40.736 22.945 60.167 1.00 20.80 O

HETATM 6665 O HOH B 714 37.814 29.760 63.398 1.00 19.88 O

HETATM 6666 O HOH B 715 44.706 6.939 74.554 1.00 29.39 O

HETATM 6667 O HOH B 716 17.881 23.772 87.804 1.00 29.70 O

HETATM 6668 O HOH B 717 32.224 4.076 66.085 1.00 22.48 O

HETATM 6669 O HOH B 718 30.888 -0.396 79.058 1.00 19.40 O

HETATM 6670 O HOH B 719 60.683 21.162 84.985 1.00 24.22 O

HETATM 6671 O HOH B 720 18.674 4.394 80.227 1.00 23.38 O

HETATM 6672 O HOH B 721 37.446 4.288 66.254 1.00 19.10 O

HETATM 6673 O HOH B 722 24.528 -1.283 83.336 1.00 28.51 O

HETATM 6674 O HOH B 723 80.063 2.471 62.079 1.00 23.50 O

HETATM 6675 O HOH B 724 70.211 18.086 69.866 1.00 18.55 O

HETATM 6676 O HOH B 725 56.178 10.780 71.036 1.00 25.89 O

HETATM 6677 O HOH B 726 18.496 5.354 71.356 1.00 23.33 O

HETATM 6678 O HOH B 727 45.313 11.437 65.148 1.00 28.79 O

HETATM 6679 O HOH B 728 42.809 12.334 69.095 1.00 21.16 O

HETATM 6680 O HOH B 729 44.174 22.401 64.807 1.00 25.62 O

HETATM 6681 O HOH B 730 57.347 21.425 67.816 1.00 20.74 O

HETATM 6682 O HOH B 731 66.260 26.020 83.221 1.00 29.83 O

HETATM 6683 O HOH B 732 28.898 21.658 78.433 1.00 23.95 O

HETATM 6684 O HOH B 733 48.366 36.721 76.127 1.00 20.40 O

HETATM 6685 O HOH B 734 19.564 5.120 75.929 1.00 24.11 O

HETATM 6686 O HOH B 735 33.142 34.652 52.905 1.00 25.14 O

HETATM 6687 O HOH B 736 34.051 0.728 80.792 1.00 21.40 O

HETATM 6688 O HOH B 737 38.019 10.239 84.353 1.00 25.34 O

HETATM 6689 O HOH B 738 74.443 14.488 78.708 1.00 33.09 O

HETATM 6690 O HOH B 739 24.053 26.009 61.353 1.00 28.35 O

HETATM 6691 O HOH B 740 55.027 41.926 67.520 1.00 32.79 O

HETATM 6692 O HOH B 741 29.686 5.693 76.483 1.00 18.02 O

HETATM 6693 O HOH B 742 41.264 11.826 64.833 1.00 22.51 O

HETATM 6694 O HOH B 743 40.927 11.327 67.486 1.00 18.72 O

HETATM 6695 O HOH B 744 56.193 22.886 87.417 1.00 27.98 O

HETATM 6696 O HOH B 745 19.443 17.928 77.301 1.00 30.68 O

HETATM 6697 O HOH B 746 63.111 33.117 75.004 1.00 35.86 O

HETATM 6698 O HOH B 747 32.430 36.114 55.115 1.00 31.33 O

HETATM 6699 O HOH B 748 43.522 30.810 86.463 1.00 22.34 O

HETATM 6700 O HOH B 749 53.081 35.130 84.311 1.00 26.42 O

HETATM 6701 O HOH B 750 66.355 15.427 83.285 1.00 28.92 O

HETATM 6702 O HOH B 751 49.370 23.987 68.149 1.00 30.04 O

HETATM 6703 O HOH B 752 47.407 19.013 58.399 1.00 27.92 O

HETATM 6704 O HOH B 753 50.436 8.197 85.788 1.00 29.70 O

HETATM 6705 O HOH B 754 57.180 32.897 80.665 1.00 24.58 O

HETATM 6706 O HOH B 755 54.793 34.095 87.292 1.00 32.39 O

HETATM 6707 O HOH B 756 18.862 3.382 77.790 1.00 25.63 O

HETATM 6708 O HOH B 757 46.148 28.299 67.542 1.00 24.22 O

HETATM 6709 O HOH B 758 29.021 22.218 75.811 1.00 31.13 O

HETATM 6710 O HOH B 759 44.457 7.296 82.590 1.00 27.19 O

HETATM 6711 O HOH B 760 63.012 33.322 77.521 1.00 45.11 O

HETATM 6712 O HOH B 761 66.598 12.361 82.873 1.00 39.32 O

HETATM 6713 O HOH B 762 53.530 32.414 68.056 1.00 20.44 O

HETATM 6714 O HOH B 763 39.652 32.668 81.405 1.00 34.21 O

HETATM 6715 O HOH B 764 24.403 15.122 91.107 1.00 37.80 O

HETATM 6716 O HOH B 765 14.222 28.955 71.133 1.00 47.13 O

HETATM 6717 O HOH B 766 46.166 34.020 62.402 1.00 29.04 O

HETATM 6718 O HOH B 767 59.181 19.610 86.510 1.00 23.85 O

HETATM 6719 O HOH B 768 52.992 12.901 69.450 1.00 26.92 O

HETATM 6720 O HOH B 769 41.398 4.248 64.046 1.00 37.52 O

HETATM 6721 O HOH B 770 47.284 18.703 90.343 1.00 32.40 O

HETATM 6722 O HOH B 771 32.907 12.150 87.240 1.00 28.05 O

HETATM 6723 O HOH B 772 50.139 15.011 88.970 1.00 29.38 O

HETATM 6724 O HOH B 773 27.035 17.070 66.295 1.00 34.39 O

HETATM 6725 O HOH B 774 38.880 29.257 89.170 1.00 39.28 O

HETATM 6726 O HOH B 775 76.919 22.512 71.902 1.00 30.98 O

HETATM 6727 O HOH B 776 31.088 21.636 93.737 1.00 43.86 O

HETATM 6728 O HOH B 777 33.844 22.810 91.061 1.00 22.07 O

HETATM 6729 O HOH B 778 55.474 41.111 74.636 1.00 30.92 O

HETATM 6730 O HOH B 779 73.860 14.414 63.485 1.00 33.29 O

HETATM 6731 O HOH B 780 56.503 20.229 86.653 1.00 26.47 O

HETATM 6732 O HOH B 781 15.243 8.042 73.548 1.00 32.43 O

HETATM 6733 O HOH B 782 39.792 29.853 61.686 1.00 28.35 O

HETATM 6734 O HOH B 783 47.017 25.803 67.435 1.00 30.30 O

HETATM 6735 O HOH B 784 41.112 25.206 61.744 1.00 27.80 O

HETATM 6736 O HOH B 785 48.937 10.923 85.960 1.00 26.41 O

HETATM 6737 O HOH B 786 82.343 14.151 68.462 1.00 34.71 O

HETATM 6738 O HOH B 787 67.088 23.682 81.657 1.00 31.91 O

HETATM 6739 O HOH B 788 41.317 32.151 62.084 1.00 36.41 O

HETATM 6740 O HOH B 789 72.634 -5.502 52.365 1.00 38.19 O

HETATM 6741 O HOH B 790 25.025 17.233 68.713 1.00 32.34 O

HETATM 6742 O HOH B 791 27.061 24.855 68.866 1.00 27.50 O

HETATM 6743 O HOH B 792 14.149 4.383 76.650 1.00 35.66 O

HETATM 6744 O HOH B 793 23.656 32.701 59.481 1.00 28.83 O

HETATM 6745 O HOH B 794 60.896 32.503 70.408 1.00 35.43 O

HETATM 6746 O HOH B 795 51.512 24.390 64.450 1.00 33.77 O

HETATM 6747 O HOH B 796 33.825 9.107 83.949 1.00 27.54 O

HETATM 6748 O HOH B 797 30.285 33.995 74.833 1.00 43.08 O

HETATM 6749 O HOH B 798 27.708 18.437 69.974 1.00 32.37 O

HETATM 6750 O HOH B 799 29.714 27.321 49.560 1.00 26.37 O

HETATM 6751 O HOH B 800 19.116 0.802 77.911 1.00 38.17 O

HETATM 6752 O HOH B 801 43.658 1.609 65.666 1.00 30.72 O

HETATM 6753 O HOH B 802 46.103 31.476 87.257 1.00 36.73 O

HETATM 6754 O HOH B 803 48.646 35.349 84.391 1.00 36.58 O

HETATM 6755 O HOH B 804 11.782 18.844 66.862 1.00 31.21 O

HETATM 6756 O HOH B 805 26.333 30.552 78.568 1.00 37.91 O

HETATM 6757 O HOH B 806 81.306 13.101 78.185 1.00 36.03 O

HETATM 6758 O HOH B 807 44.070 27.359 65.537 1.00 40.94 O

HETATM 6759 O HOH B 808 57.433 41.854 68.783 1.00 35.68 O

HETATM 6760 O HOH B 809 20.422 25.194 59.637 1.00 28.08 O

HETATM 6761 O HOH B 810 14.705 21.954 94.581 1.00 38.00 O

HETATM 6762 O HOH B 811 23.151 4.476 89.628 1.00 41.65 O

HETATM 6763 O HOH B 812 9.819 14.267 66.155 1.00 32.14 O

HETATM 6764 O HOH B 813 41.798 12.287 85.607 1.00 35.32 O

HETATM 6765 O HOH B 814 20.827 23.221 94.362 1.00 36.65 O

HETATM 6766 O HOH B 815 39.078 32.976 76.496 1.00 27.67 O

HETATM 6767 O HOH B 816 29.919 17.244 68.458 1.00 35.48 O

HETATM 6768 O HOH B 817 57.239 12.211 87.145 1.00 24.83 O

HETATM 6769 O HOH B 818 43.603 11.193 84.660 1.00 41.50 O

HETATM 6770 O HOH B 819 33.074 16.953 69.462 1.00 28.93 O

HETATM 6771 O HOH B 820 39.565 27.787 90.814 1.00 30.22 O

HETATM 6772 O HOH B 821 71.647 15.714 78.842 1.00 30.16 O

HETATM 6773 O HOH B 822 43.747 10.073 81.631 1.00 34.65 O

HETATM 6774 O HOH B 823 24.222 7.095 90.410 1.00 39.40 O

HETATM 6775 O HOH B 824 19.009 16.409 79.804 1.00 31.36 O

HETATM 6776 O HOH B 825 21.837 29.133 53.668 1.00 42.78 O

HETATM 6777 O HOH B 826 68.903 16.169 79.480 1.00 33.81 O

HETATM 6778 O HOH B 827 33.321 29.833 85.968 1.00 33.59 O

HETATM 6779 O HOH B 828 55.683 19.411 89.512 1.00 33.93 O

HETATM 6780 O HOH B 829 33.354 33.809 49.989 1.00 43.54 O

HETATM 6781 O HOH B 830 17.537 19.349 78.836 1.00 31.56 O

HETATM 6782 O HOH B 831 44.790 12.317 67.278 1.00 26.01 O

HETATM 6783 O HOH B 832 48.798 44.458 73.151 1.00 31.70 O

HETATM 6784 O HOH B 833 41.235 31.397 87.055 1.00 40.67 O

HETATM 6785 O HOH B 834 32.111 30.636 79.243 1.00 31.74 O

HETATM 6786 O HOH B 835 51.518 39.672 76.164 1.00 34.74 O

HETATM 6787 O HOH B 836 35.204 18.552 92.609 1.00 35.38 O

HETATM 6788 O HOH B 837 59.519 32.828 79.809 1.00 36.12 O

HETATM 6789 O HOH B 838 48.850 38.823 75.490 1.00 36.71 O

HETATM 6790 O HOH B 839 27.318 22.954 62.026 1.00 42.48 O

HETATM 6791 O HOH B 840 29.970 34.641 60.021 1.00 39.04 O

HETATM 6792 O HOH B 841 26.331 27.328 76.104 1.00 37.35 O

HETATM 6793 O HOH B 842 16.238 6.006 89.975 1.00 36.87 O

HETATM 6794 O HOH B 843 69.934 -6.862 42.548 1.00 36.34 O

HETATM 6795 O HOH B 844 28.818 21.409 69.294 1.00 37.50 O

HETATM 6796 O HOH B 845 44.725 12.931 87.311 1.00 43.00 O

HETATM 6797 O HOH B 846 26.897 22.797 79.568 1.00 40.26 O

HETATM 6798 O HOH B 847 25.830 8.563 88.575 1.00 30.98 O

HETATM 6799 O HOH B 848 28.570 33.456 73.211 1.00 32.81 O

HETATM 6800 O HOH B 849 61.243 24.208 87.500 1.00 39.11 O

HETATM 6801 O HOH B 850 23.497 22.470 60.559 1.00 43.97 O

HETATM 6802 O HOH B 851 43.482 24.551 62.561 1.00 35.58 O

HETATM 6803 O HOH B 852 22.044 27.736 55.890 1.00 34.74 O

HETATM 6804 O HOH B 853 21.760 30.601 61.734 1.00 39.61 O

HETATM 6805 O HOH B 854 33.817 4.363 82.930 1.00 33.40 O

HETATM 6806 O HOH B 855 31.853 33.068 79.572 1.00 37.11 O

HETATM 6807 O HOH B 856 26.806 6.354 87.523 1.00 37.66 O

HETATM 6808 O HOH B 857 29.361 18.014 65.034 1.00 31.67 O

HETATM 6809 O HOH B 858 30.115 24.192 65.532 1.00 38.89 O

HETATM 6810 O HOH B 859 24.319 21.433 62.804 1.00 35.77 O

HETATM 6811 O HOH B 860 26.072 22.080 60.140 1.00 37.67 O

HETATM 6812 O HOH B 861 46.142 11.798 85.826 1.00 38.21 O

HETATM 6813 O HOH B 862 55.012 22.157 90.267 1.00 32.75 O

HETATM 6814 O HOH B 863 47.309 41.444 75.927 1.00 39.52 O

HETATM 6815 O HOH B 864 39.062 33.974 79.087 1.00 39.00 O

HETATM 6816 O HOH B 865 25.232 3.843 87.596 1.00 36.35 O

HETATM 6817 O HOH B 866 14.332 33.182 87.991 1.00 36.99 O

HETATM 6818 O HOH B 867 45.428 2.557 85.987 1.00 40.82 O

HETATM 6819 O HOH B 868 23.985 30.011 83.129 1.00 38.83 O

HETATM 6820 O HOH B 869 19.975 30.679 80.538 1.00 42.00 O

HETATM 6821 O HOH B 870 35.223 28.398 84.786 1.00 32.50 O

HETATM 6822 O HOH B 871 6.833 18.946 87.751 1.00 36.99 O

HETATM 6823 O HOH B 872 83.035 9.586 67.390 1.00 45.93 O

HETATM 6824 O HOH B 873 30.072 30.022 87.641 1.00 45.23 O

HETATM 6825 O HOH B 874 13.110 14.655 95.855 1.00 43.57 O

HETATM 6826 O HOH B 875 77.913 -1.673 55.275 1.00 41.83 O

HETATM 6827 O HOH B 876 29.206 35.039 68.626 1.00 36.04 O

HETATM 6828 O HOH B 877 23.153 23.235 82.841 1.00 45.17 O

HETATM 6829 O HOH B 878 22.786 1.707 87.622 1.00 39.52 O

HETATM 6830 O HOH B 879 22.628 31.669 80.534 1.00 43.35 O

HETATM 6831 O HOH B 880 41.034 34.700 62.914 1.00 29.89 O

HETATM 6832 O HOH B 881 41.787 39.411 78.456 1.00 38.09 O

HETATM 6833 O HOH B 882 15.988 2.980 77.951 1.00 44.70 O

HETATM 6834 O HOH B 883 23.980 28.793 79.732 1.00 42.89 O

HETATM 6835 O HOH B 884 81.515 12.568 63.489 1.00 37.00 O

HETATM 6836 O HOH B 885 82.553 7.017 67.952 1.00 30.60 O

HETATM 6837 O HOH B 886 34.741 26.412 54.891 1.00 19.10 O

HETATM 6838 O HOH B 887 58.668 10.508 71.751 1.00 18.61 O

HETATM 6839 O HOH B 888 63.922 23.555 72.844 1.00 18.30 O

HETATM 6840 O HOH B 889 37.463 12.421 56.158 1.00 19.94 O

HETATM 6841 O HOH B 890 56.189 30.544 64.553 1.00 22.50 O

HETATM 6842 O HOH B 891 59.491 18.675 72.521 1.00 13.65 O

HETATM 6843 O HOH B 892 57.542 26.421 66.997 1.00 22.82 O

HETATM 6844 O HOH B 893 28.267 27.669 90.440 1.00 40.96 O

HETATM 6845 O HOH B 894 27.721 21.429 93.851 1.00 35.99 O

HETATM 6846 O HOH B 895 83.863 5.220 65.696 1.00 48.23 O

HETATM 6847 O HOH B 896 60.704 1.897 44.690 1.00 34.32 O

HETATM 6848 O HOH B 897 83.705 21.004 72.889 1.00 47.66 O

HETATM 6849 O HOH B 898 36.374 33.180 45.125 1.00 41.93 O

HETATM 6850 O HOH B 899 38.813 33.533 61.699 1.00 38.68 O

HETATM 6851 O HOH B 900 15.988 25.235 76.006 1.00 41.55 O

HETATM 6852 O HOH B 901 14.917 22.139 73.686 1.00 37.34 O

HETATM 6853 O HOH B 902 10.509 18.913 64.547 1.00 39.11 O

HETATM 6854 O HOH B 903 48.687 12.306 69.065 1.00 14.50 O

HETATM 6855 O HOH B 904 23.818 -1.551 80.653 1.00 21.32 O

HETATM 6856 O HOH B 905 29.351 29.390 84.615 1.00 33.53 O

HETATM 6857 O HOH B 906 22.814 15.142 92.914 1.00 46.47 O

HETATM 6858 O HOH B 907 11.985 9.642 73.117 1.00 38.55 O

HETATM 6859 O HOH B 908 79.206 17.696 77.930 1.00 40.11 O

HETATM 6860 O HOH B 909 56.782 12.875 89.629 1.00 44.37 O

HETATM 6861 O HOH B 910 53.184 24.050 62.466 1.00 32.23 O

HETATM 6862 O HOH B 911 53.479 34.659 65.317 1.00 35.15 O

HETATM 6863 O HOH B 912 43.593 4.236 66.137 1.00 32.13 O

HETATM 6864 O HOH B 913 52.448 24.642 67.125 1.00 43.66 O

HETATM 6865 O HOH B 914 22.421 27.163 62.913 1.00 43.96 O

HETATM 6866 O HOH B 915 5.651 11.919 89.619 1.00 46.39 O

HETATM 6867 O HOH B 916 48.259 12.788 62.649 1.00 33.38 O

HETATM 6868 O HOH B 917 46.517 9.016 83.569 1.00 34.33 O

HETATM 6869 O HOH B 918 12.185 11.224 64.168 1.00 42.60 O

HETATM 6870 O HOH B 919 24.827 24.218 69.970 1.00 34.79 O

HETATM 6871 O HOH B 920 58.700 16.451 89.867 1.00 44.03 O

HETATM 6872 O HOH B 921 59.816 14.198 89.064 1.00 46.56 O

HETATM 6873 O HOH B 922 48.649 16.843 62.618 1.00 37.96 O

HETATM 6874 O HOH B 923 21.893 28.237 93.493 1.00 49.40 O

HETATM 6875 O HOH B 924 63.294 19.986 88.001 1.00 48.21 O

HETATM 6876 O HOH B 925 57.661 24.693 88.467 1.00 52.54 O

HETATM 6877 O HOH B 926 62.666 30.084 84.775 1.00 46.03 O

HETATM 6878 O HOH B 927 31.125 23.110 74.348 1.00 27.57 O

HETATM 6879 O HOH B 928 25.493 22.019 81.839 1.00 41.19 O

HETATM 6880 O HOH B 929 56.891 32.076 89.736 1.00 46.27 O

HETATM 6881 O HOH B 930 26.284 32.223 74.449 1.00 42.29 O

HETATM 6882 O HOH B 931 31.345 18.238 90.873 1.00 24.49 O

HETATM 6883 O HOH B 932 48.329 31.813 89.675 1.00 44.98 O

HETATM 6884 O HOH B 933 48.698 16.567 90.239 1.00 41.91 O

HETATM 6885 O HOH B 934 30.497 17.712 92.741 1.00 48.59 O

HETATM 6886 O HOH B 935 28.573 10.441 68.180 1.00 35.30 O

HETATM 6887 O HOH B 936 13.461 24.867 67.668 1.00 43.57 O

HETATM 6888 O HOH B 937 31.332 19.525 68.336 1.00 39.19 O

HETATM 6889 O HOH B 938 43.801 34.532 84.075 1.00 41.10 O

HETATM 6890 O HOH B 939 38.756 8.525 82.783 1.00 42.91 O

HETATM 6891 O HOH B 940 29.745 31.301 49.047 1.00 46.37 O

HETATM 6892 O HOH B 941 14.024 22.257 68.155 1.00 47.10 O

HETATM 6893 O HOH B 942 61.404 30.788 68.695 1.00 34.34 O

HETATM 6894 O HOH B 943 48.909 20.362 68.916 1.00 43.33 O

HETATM 6895 O HOH B 944 36.497 29.754 88.109 1.00 46.58 O

HETATM 6896 O HOH B 945 49.567 16.510 68.947 1.00 47.42 O

HETATM 6897 O HOH B 946 36.819 26.332 91.673 1.00 43.68 O

HETATM 6898 O HOH B 947 46.321 20.822 64.922 1.00 49.56 O

HETATM 6899 O HOH B 948 35.250 22.667 93.420 1.00 43.60 O

HETATM 6900 O HOH B 949 23.038 27.741 82.399 1.00 48.13 O

HETATM 6901 O HOH B 950 26.203 31.644 88.950 1.00 40.36 O

HETATM 6902 O HOH B 951 43.392 15.267 87.041 1.00 33.12 O

HETATM 6903 O HOH B 952 24.144 21.787 70.807 1.00 47.31 O

HETATM 6904 O HOH B 953 22.756 29.610 71.426 1.00 34.65 O

HETATM 6905 O HOH B 954 52.876 10.910 71.476 1.00 54.63 O

HETATM 6906 O HOH B 955 46.911 16.899 60.207 1.00 30.89 O