**Supplementary Data**

**Coordinates for the ARCase [Co(Biot-en-tBu2-Salphen)] 4 ‧ Sav\*\_α16 S122V-K131H**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| N 22.022 16.408 -0.327  C 23.489 16.604 -0.460  C 24.261 15.397 -1.078  O 24.129 14.259 -0.616  C 24.084 16.923 0.915  C 25.564 17.274 0.853  O 25.873 18.422 0.644  O 26.371 16.390 1.015  H 21.611 17.226 0.075  H 21.625 16.245 -1.229  H 21.844 15.621 0.263  H 23.666 17.449 -1.127  H 23.544 17.760 1.359  H 23.955 16.063 1.575  N 25.074 15.632 -2.118  C 25.704 14.507 -2.809  C 26.562 13.671 -1.842  O 26.429 12.445 -1.780  C 26.563 15.009 -3.974  C 27.167 13.904 -4.823  C 28.084 14.442 -5.904  N 28.583 13.552 -6.755  O 28.345 15.647 -5.975  H 25.262 16.571 -2.435  H 24.920 13.865 -3.212  H 25.958 15.641 -4.625  H 27.377 15.620 -3.587  H 27.748 13.242 -4.180  H 26.362 13.347 -5.305  H 29.194 13.848 -7.490  H 28.345 12.583 -6.662  N 27.421 14.322 -1.045  C 28.253 13.581 -0.088  C 27.420 12.961 1.027  O 27.703 11.837 1.471  C 29.322 14.491 0.501  H 27.505 15.328 -1.096  H 28.740 12.765 -0.622  H 29.929 13.927 1.209  H 29.956 14.873 -0.299  H 28.847 15.324 1.016  N 26.386 13.671 1.482  C 25.552 13.147 2.548  C 24.871 11.848 2.170  O 24.905 10.882 2.934  H 26.172 14.578 1.093  H 26.162 12.981 3.438  H 24.793 13.881 2.811  N 24.243 11.799 0.982  C 23.551 10.583 0.573  C 24.526 9.439 0.340  O 24.255 8.289 0.703  C 22.729 10.823 -0.706  C 21.565 11.773 -0.423  C 22.220 9.503 -1.266  C 20.874 12.282 -1.668  H 24.240 12.597 0.363  H 22.868 10.288 1.370  H 23.356 11.306 -1.456  H 20.825 11.268 0.195  H 21.927 12.635 0.139  H 21.641 9.692 -2.171  H 23.065 8.858 -1.504  H 21.587 9.015 -0.526  H 20.061 12.950 -1.386  H 21.591 12.823 -2.286  H 20.472 11.440 -2.231  N 25.635 9.712 -0.337  C 26.604 8.670 -0.656  C 27.073 7.955 0.604  O 27.507 8.593 1.577  C 27.818 9.253 -1.405  C 28.819 8.155 -1.733  O 27.381 9.874 -2.620  H 25.814 10.660 -0.638  H 26.124 7.939 -1.308  H 28.304 10.004 -0.782  H 27.035 10.748 -2.426  H 29.670 8.585 -2.261  H 29.162 7.687 -0.810  H 28.342 7.405 -2.363  N 27.039 6.618 0.570  C 27.498 5.821 1.684  C 26.597 4.626 1.886  O 25.843 4.231 0.984  H 26.684 6.154 -0.255  H 28.521 5.490 1.498  H 27.516 6.431 2.586  N 26.670 4.073 3.097  C 25.932 2.871 3.459  C 24.882 3.209 4.505  O 25.191 3.871 5.507  C 26.870 1.773 3.991  C 26.087 0.507 4.303  O 27.873 1.480 3.010  H 27.263 4.512 3.787  H 25.436 2.488 2.567  H 27.363 2.122 4.900  H 27.731 0.596 2.661  H 26.766 -0.258 4.678  H 25.331 0.724 5.059  H 25.601 0.148 3.397  N 23.662 2.721 4.281  C 22.492 3.022 5.087  C 21.932 1.709 5.598  O 22.063 0.683 4.931  C 21.434 3.773 4.277  C 21.838 5.172 3.918  C 22.505 5.566 2.798  C 21.597 6.376 4.687  C 22.149 7.437 3.964  C 20.969 6.633 5.912  N 22.699 6.925 2.817  C 22.095 8.744 4.424  C 20.914 7.944 6.372  C 21.461 8.971 5.646  H 23.567 2.100 3.489  H 22.801 3.638 5.930  H 21.227 3.230 3.354  H 20.505 3.820 4.844  H 22.837 4.900 2.004  H 23.170 7.462 2.102  H 20.530 5.822 6.491  H 22.524 9.574 3.862  H 20.423 8.136 7.326  H 21.400 9.988 6.035  N 21.340 1.747 6.792  C 20.752 0.572 7.414  C 19.347 0.909 7.876  O 19.069 2.054 8.275  C 21.609 0.083 8.583  C 23.078 -0.047 8.253  C 23.909 1.061 8.337  C 23.596 -1.274 7.865  C 25.252 0.942 8.034  C 24.938 -1.392 7.563  C 25.765 -0.290 7.646  O 27.102 -0.408 7.345  H 21.304 2.630 7.281  H 20.699 -0.222 6.669  H 21.507 0.772 9.422  H 21.247 -0.890 8.915  H 23.501 2.026 8.641  H 22.944 -2.145 7.798  H 25.904 1.813 8.100  H 25.346 -2.357 7.257  H 27.518 0.457 7.396  N 18.453 -0.066 7.863  C 17.141 0.291 8.394  C 16.781 -0.607 9.579  O 17.598 -1.405 10.072  C 16.082 0.206 7.312  C 15.843 -1.203 6.845  N 15.140 -1.345 5.751  O 16.296 -2.165 7.478  H 18.608 -1.006 7.525  H 17.184 1.318 8.763  H 15.143 0.616 7.687  H 16.385 0.812 6.458  H 14.949 -2.260 5.394  H 14.793 -0.540 5.273  N 15.544 -0.422 10.057  C 15.069 -1.063 11.280  C 14.778 -2.554 11.098  O 14.612 -3.270 12.088  C 13.811 -0.353 11.790  C 12.550 -0.686 11.009  C 12.438 0.111 9.723  N 11.762 -0.459 8.732  O 12.955 1.228 9.622  H 14.919 0.187 9.547  H 15.845 -0.975 12.040  H 13.641 -0.618 12.832  H 13.960 0.724 11.744  H 12.562 -1.746 10.754  H 11.682 -0.461 11.628  H 11.655 0.020 7.860  H 11.361 -1.365 8.857  N 14.702 -3.034 9.857  C 14.505 -4.452 9.575  C 15.817 -5.252 9.498  O 15.765 -6.476 9.320  C 13.737 -4.604 8.256  C 12.304 -4.055 8.253  C 11.713 -4.185 6.856  C 11.467 -4.814 9.273  H 14.783 -2.386 9.086  H 13.922 -4.888 10.386  H 14.289 -4.090 7.471  H 13.687 -5.663 8.004  H 12.318 -2.996 8.512  H 10.695 -3.795 6.854  H 12.320 -3.618 6.150  H 11.700 -5.235 6.562  H 10.449 -4.424 9.271  H 11.450 -5.874 9.015  H 11.902 -4.690 10.264  N 16.989 -4.616 9.605  C 18.255 -5.288 9.311  C 18.763 -5.149 7.875  O 19.887 -5.616 7.579  H 17.004 -3.649 9.895  H 19.034 -4.902 9.968  H 18.158 -6.353 9.518  N 17.990 -4.515 6.981  C 18.436 -4.313 5.602  C 19.406 -3.140 5.520  O 19.420 -2.249 6.371  C 17.249 -4.065 4.691  O 16.341 -5.131 4.748  H 17.082 -4.168 7.260  H 18.962 -5.211 5.273  H 16.749 -3.143 4.987  H 17.597 -3.934 3.668  H 15.601 -4.880 4.190  N 20.182 -3.122 4.435  C 21.207 -2.116 4.201  C 21.275 -1.771 2.731  O 21.033 -2.626 1.879  C 22.588 -2.592 4.687  C 23.051 -3.797 3.882  O 23.540 -1.530 4.545  H 20.042 -3.851 3.751  H 20.944 -1.217 4.758  H 22.527 -2.868 5.740  H 23.081 -0.687 4.554  H 24.028 -4.119 4.240  H 22.335 -4.609 3.998  H 23.123 -3.524 2.830  N 21.677 -0.550 2.418  C 22.047 -0.385 1.033  C 23.178 0.603 0.889  O 23.475 1.402 1.792  C 20.844 0.081 0.210  C 20.423 1.494 0.501  C 20.973 2.555 -0.201  C 19.476 1.762 1.477  C 20.586 3.855 0.066  C 19.086 3.060 1.744  C 19.642 4.107 1.038  H 21.743 0.242 3.043  H 22.390 -1.349 0.649  H 21.079 0.008 -0.852  H 19.996 -0.574 0.402  H 21.719 2.355 -0.972  H 19.037 0.936 2.035  H 21.027 4.680 -0.494  H 18.339 3.259 2.515  H 19.337 5.131 1.250  N 23.849 0.453 -0.246  C 25.055 1.171 -0.581  C 24.714 1.993 -1.812  O 24.318 1.437 -2.833  C 26.239 0.226 -0.858  C 26.520 -0.650 0.365  C 27.476 1.023 -1.242  C 27.523 -1.752 0.110  H 23.474 -0.213 -0.907  H 25.317 1.814 0.257  H 25.983 -0.447 -1.676  H 26.896 -0.029 1.179  H 25.591 -1.108 0.707  H 28.303 0.341 -1.433  H 27.270 1.604 -2.140  H 27.743 1.696 -0.427  H 27.670 -2.330 1.023  H 27.151 -2.407 -0.678  H 28.472 -1.316 -0.199  N 24.851 3.308 -1.725  C 24.455 4.152 -2.831  C 25.551 5.176 -3.109  O 26.168 5.719 -2.187  C 23.130 4.872 -2.515  C 23.307 5.821 -1.340  C 22.643 5.621 -3.746  H 25.230 3.735 -0.890  H 24.319 3.525 -3.713  H 22.386 4.131 -2.222  H 22.361 6.321 -1.131  H 23.621 5.258 -0.461  H 24.063 6.566 -1.584  H 21.706 6.127 -3.516  H 23.390 6.357 -4.043  H 22.484 4.916 -4.562  N 25.755 5.460 -4.402  C 26.605 6.549 -4.857  C 25.681 7.601 -5.435  O 24.833 7.277 -6.265  C 27.637 6.093 -5.906  C 28.478 7.271 -6.374  O 28.495 5.097 -5.334  H 25.290 4.880 -5.087  H 27.148 6.945 -3.999  H 27.120 5.659 -6.761  H 28.871 4.558 -6.034  H 29.200 6.930 -7.116  H 27.829 8.026 -6.821  H 29.005 7.703 -5.525  N 25.824 8.834 -4.978  C 25.052 9.960 -5.480  C 25.879 10.651 -6.553  O 27.055 10.968 -6.309  C 24.683 10.901 -4.341  H 26.503 8.990 -4.247  H 24.137 9.572 -5.927  H 24.106 11.738 -4.733  H 24.088 10.362 -3.603  H 25.591 11.275 -3.871  N 25.267 10.851 -7.745  C 25.930 11.526 -8.856  C 25.664 13.020 -8.834  O 24.661 13.502 -8.289  H 24.322 10.518 -7.865  H 27.003 11.345 -8.805  H 25.577 11.107 -9.798  N 26.600 13.797 -9.394  C 26.355 15.232 -9.408  C 25.087 15.564 -10.206  O 24.412 16.550 -9.907  C 27.556 15.970 -9.980  H 27.453 13.440 -9.798  H 26.195 15.559 -8.381  H 27.358 17.041 -9.984  H 28.435 15.766 -9.367  H 27.740 15.632 -10.998  N 24.732 14.703 -11.152  C 23.598 14.800 -12.051  C 22.285 14.346 -11.422  O 21.284 14.217 -12.135  C 23.866 13.976 -13.312  C 24.048 12.491 -13.022  O 23.919 12.109 -11.884  O 24.315 11.756 -13.942  H 25.348 13.906 -11.222  H 23.467 15.846 -12.330  H 23.037 14.096 -14.009  H 24.764 14.348 -13.807  N 22.280 14.006 -10.146  C 21.059 13.584 -9.493  C 20.817 12.090 -9.507  O 19.825 11.637 -8.931  H 23.138 14.039 -9.612  H 21.071 13.911 -8.453  H 20.207 14.065 -9.971  N 21.677 11.312 -10.149  C 21.505 9.863 -10.213  C 21.846 9.198 -8.873  O 22.737 9.644 -8.157  C 22.358 9.275 -11.328  H 22.472 11.732 -10.609  H 20.455 9.655 -10.425  H 22.218 8.195 -11.361  H 22.059 9.709 -12.282  H 23.406 9.500 -11.140  N 21.126 8.120 -8.535  C 21.527 7.197 -7.477  C 21.834 5.870 -8.149  O 21.099 5.457 -9.049  C 20.422 7.032 -6.426  C 19.976 8.320 -5.722  C 18.817 8.011 -4.784  C 21.151 8.917 -4.961  H 20.269 7.944 -9.040  H 22.425 7.588 -7.001  H 19.547 6.597 -6.906  H 20.772 6.341 -5.660  H 19.623 9.037 -6.464  H 18.500 8.927 -4.285  H 17.984 7.604 -5.358  H 19.136 7.283 -4.040  H 20.833 9.833 -4.462  H 21.504 8.201 -4.218  H 21.958 9.145 -5.658  N 22.911 5.215 -7.725  C 23.268 3.904 -8.256  C 23.833 3.097 -7.106  O 24.513 3.659 -6.234  C 24.289 3.995 -9.406  C 25.590 4.611 -8.916  O 24.551 2.682 -9.920  H 23.496 5.635 -7.017  H 22.366 3.429 -8.644  H 23.881 4.609 -10.207  H 24.604 2.058 -9.193  H 26.301 4.668 -9.741  H 25.396 5.614 -8.534  H 26.008 3.996 -8.120  N 23.602 1.786 -7.114  C 24.265 0.986 -6.096  C 23.637 -0.381 -5.959  O 23.167 -0.966 -6.931  H 22.999 1.329 -7.782  H 25.319 0.874 -6.350  H 24.218 1.503 -5.138  N 23.652 -0.874 -4.722  C 23.090 -2.176 -4.383  C 22.230 -2.024 -3.129  O 22.411 -1.105 -2.330  C 24.188 -3.231 -4.154  C 25.066 -3.364 -5.389  O 24.999 -2.845 -3.037  H 24.072 -0.316 -3.994  H 22.469 -2.511 -5.214  H 23.728 -4.194 -3.936  H 25.131 -1.894 -3.051  H 25.836 -4.114 -5.209  H 24.454 -3.669 -6.238  H 25.536 -2.407 -5.606  N 21.288 -2.929 -2.973  C 20.372 -2.954 -1.859  C 20.382 -4.374 -1.337  O 20.183 -5.307 -2.118  C 18.964 -2.516 -2.269  C 18.028 -2.295 -1.102  C 17.695 -1.006 -0.715  C 17.504 -3.381 -0.418  C 16.840 -0.802 0.352  C 16.649 -3.179 0.647  C 16.317 -1.896 1.032  O 15.466 -1.695 2.095  H 21.218 -3.641 -3.686  H 20.736 -2.268 -1.094  H 19.024 -1.587 -2.839  H 18.523 -3.270 -2.921  H 18.107 -0.151 -1.252  H 17.766 -4.394 -0.722  H 16.578 0.210 0.657  H 16.236 -4.034 1.185  H 15.047 -2.527 2.329  N 20.617 -4.564 -0.040  C 20.639 -5.918 0.509  C 19.531 -6.020 1.547  O 19.532 -5.269 2.530  C 21.996 -6.243 1.138  C 22.128 -7.672 1.644  C 23.495 -7.974 2.192  O 24.364 -7.144 2.063  O 23.672 -9.036 2.742  H 20.781 -3.780 0.575  H 20.444 -6.623 -0.299  H 22.786 -6.071 0.407  H 22.178 -5.573 1.978  H 21.391 -7.840 2.427  H 21.912 -8.357 0.825  N 18.551 -6.893 1.302  C 17.408 -7.033 2.185  C 17.623 -8.147 3.180  O 18.168 -9.189 2.799  C 16.164 -7.297 1.340  O 15.024 -7.327 2.138  H 18.674 -7.626 0.589  H 17.287 -6.084 2.753  H 16.056 -6.514 0.555  H 16.270 -8.277 0.831  H 14.895 -6.419 2.507  N 17.179 -7.935 4.436  C 17.183 -8.957 5.482  C 15.929 -9.838 5.476  O 15.873 -10.827 6.222  C 17.338 -8.313 6.853  H 16.828 -7.013 4.651  H 18.029 -9.620 5.306  H 17.339 -9.086 7.621  H 18.278 -7.762 6.892  H 16.510 -7.627 7.029  N 14.939 -9.596 4.551  C 13.612 -10.210 4.580  C 13.235 -10.878 3.279  O 13.092 -10.193 2.237  C 12.521 -9.255 5.140  C 12.840 -8.819 6.582  C 12.316 -8.005 4.300  H 15.065 -8.853 3.845  H 13.674 -11.015 5.255  H 11.554 -9.806 5.163  H 12.060 -8.151 6.945  H 12.863 -9.718 7.197  H 13.804 -8.314 6.640  H 11.525 -7.390 4.774  H 13.245 -7.405 4.245  H 11.975 -8.270 3.280  N 13.105 -12.243 3.215  C 12.097 -12.890 2.351  C 10.719 -12.798 2.985  O 10.597 -12.296 4.136  C 12.468 -14.362 2.104  O 12.396 -15.107 3.293  H 13.374 -12.790 4.063  H 12.076 -12.390 1.363  H 11.825 -14.808 1.309  H 13.511 -14.409 1.727  H 11.469 -15.477 3.351  N 9.629 -13.344 2.373  C 8.313 -13.462 3.021  C 8.014 -14.908 3.386  O 8.853 -15.813 3.112  C 7.263 -12.869 2.080  H 9.737 -13.757 1.421  H 8.282 -12.886 3.971  H 6.253 -12.876 2.541  H 7.519 -11.820 1.834  H 7.238 -13.427 1.122  N 6.874 -15.237 4.188  C 6.507 -16.628 4.510  C 5.525 -17.146 3.469  O 4.293 -17.167 3.718  C 5.951 -16.695 5.951  C 7.029 -16.591 6.979  N 7.696 -15.444 7.186  O 7.275 -17.557 7.735  H 6.158 -14.487 4.332  H 7.399 -17.295 4.458  H 5.202 -15.894 6.122  H 5.435 -17.668 6.098  H 8.444 -15.438 7.905  H 7.493 -14.598 6.618  N 5.957 -17.375 2.192  C 5.124 -17.035 1.020  C 5.468 -17.953 -0.151  O 6.065 -17.489 -1.154  C 5.351 -15.535 0.711  C 4.241 -14.870 -0.106  C 4.516 -13.390 -0.204  O 4.173 -12.624 0.741  O 5.428 -12.991 -0.975  H 6.991 -17.371 2.043  H 4.045 -17.178 1.249  H 5.400 -14.998 1.683  H 6.334 -15.395 0.210  H 4.196 -15.321 -1.123  H 3.257 -15.040 0.387  N 5.265 -19.380 -0.065  C 6.240 -20.404 -0.480  C 6.717 -20.277 -1.906  O 7.949 -20.375 -2.129  C 5.557 -21.754 -0.194  C 4.692 -21.400 0.990  C 4.244 -19.968 0.783  H 7.129 -20.325 0.184  H 4.963 -22.070 -1.063  H 6.258 -22.571 0.032  H 3.861 -22.061 1.068  H 5.295 -21.464 1.907  H 3.263 -19.934 0.261  H 4.169 -19.457 1.767  N 5.836 -19.978 -2.988  C 6.326 -19.845 -4.380  C 7.101 -18.558 -4.597  O 8.193 -18.590 -5.228  C 5.159 -19.929 -5.377  C 4.681 -21.345 -5.504  O 4.394 -22.004 -4.471  O 4.702 -21.921 -6.624  H 4.817 -20.127 -2.809  H 7.026 -20.685 -4.601  H 4.320 -19.279 -5.042  H 5.486 -19.565 -6.377  N 6.638 -17.359 -4.131  C 7.427 -16.117 -4.238  C 8.646 -16.094 -3.320  O 9.582 -15.290 -3.582  C 6.528 -14.909 -3.968  H 5.751 -17.365 -3.578  H 7.803 -16.026 -5.281  H 7.087 -13.972 -4.174  H 5.636 -14.940 -4.630  H 6.188 -14.904 -2.909  N 8.843 -17.070 -2.291  C 9.942 -17.022 -1.315  C 11.054 -18.010 -1.645  O 12.230 -17.720 -1.303  C 9.385 -17.267 0.088  H 8.127 -17.817 -2.188  H 10.395 -16.005 -1.317  H 10.193 -17.185 0.846  H 8.610 -16.505 0.316  H 8.926 -18.277 0.152  N 10.841 -19.089 -2.462  C 11.908 -19.768 -3.231  C 12.390 -18.867 -4.342  O 13.619 -18.750 -4.555  C 11.358 -21.071 -3.814  C 12.387 -21.911 -4.559  C 13.513 -22.373 -3.677  O 13.400 -22.241 -2.482  O 14.489 -22.858 -4.201  H 9.860 -19.284 -2.745  H 12.734 -20.007 -2.560  H 10.945 -21.683 -3.012  H 10.546 -20.846 -4.505  H 11.891 -22.783 -4.982  H 12.793 -21.323 -5.382  N 11.491 -17.955 -4.976  C 11.938 -16.896 -5.886  C 12.819 -15.864 -5.220  O 13.633 -15.225 -5.931  H 10.470 -18.124 -4.858  H 12.497 -17.353 -6.729  H 11.055 -16.384 -6.309  N 12.660 -15.496 -3.917  C 13.589 -14.561 -3.246  C 14.847 -15.259 -2.764  O 15.870 -14.576 -2.476  C 12.877 -13.880 -2.064  C 13.529 -12.568 -1.718  C 13.234 -11.423 -2.475  C 14.407 -12.449 -0.627  C 13.740 -10.230 -2.120  C 14.915 -11.245 -0.309  C 14.564 -10.115 -1.065  H 11.924 -15.981 -3.359  H 13.906 -13.778 -3.972  H 11.812 -13.685 -2.322  H 12.862 -14.558 -1.181  H 12.552 -11.490 -3.314  H 14.670 -13.318 -0.041  H 13.443 -9.348 -2.658  H 15.563 -11.138 0.552  H 14.926 -9.138 -0.783  N 14.832 -16.592 -2.460  C 15.911 -17.269 -1.727  C 17.161 -17.427 -2.584  O 17.077 -17.743 -3.770  C 15.449 -18.638 -1.253  C 16.434 -19.371 -0.355  C 15.927 -20.711 0.038  N 15.925 -21.639 -1.080  C 16.990 -22.361 -1.479  N 18.135 -22.250 -0.841  N 16.885 -23.180 -2.510  H 14.022 -17.159 -2.785  H 16.212 -16.633 -0.894  H 14.515 -18.537 -0.703  H 15.253 -19.275 -2.116  H 17.379 -19.503 -0.883  H 16.603 -18.788 0.550  H 16.562 -21.124 0.821  H 14.908 -20.619 0.408  H 15.062 -21.752 -1.596  H 18.215 -21.624 -0.052  H 18.933 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-3.153  H 20.388 1.536 -3.079  H 19.737 3.765 -5.122  H 21.234 2.801 -5.121  H 20.216 2.865 -6.581  N 18.810 1.589 -8.390  C 18.912 2.787 -9.202  C 17.869 3.783 -8.709  O 16.806 3.381 -8.219  C 18.707 2.486 -10.698  C 19.728 1.467 -11.182  O 17.386 1.969 -10.907  H 17.896 1.216 -8.177  H 19.911 3.206 -9.076  H 18.817 3.404 -11.273  H 17.135 1.420 -10.160  H 19.567 1.267 -12.241  H 20.733 1.863 -11.034  H 19.615 0.543 -10.617  N 18.144 5.069 -8.889  C 17.168 6.062 -8.505  C 17.657 7.443 -8.803  O 18.589 7.617 -9.585  H 19.020 5.371 -9.288  H 16.234 5.879 -9.037  H 16.955 5.969 -7.440  N 17.022 8.428 -8.173  C 17.325 9.849 -8.393  C 17.282 10.568 -7.057  O 16.647 10.107 -6.094  C 16.332 10.489 -9.353 | C 16.366 9.936 -10.770  C 17.597 10.353 -11.492  N 17.575 9.936 -12.885  C 18.004 8.740 -13.332  N 18.487 7.857 -12.487  N 17.943 8.456 -14.622  H 16.298 8.176 -7.515  H 18.349 9.931 -8.757  H 15.322 10.356 -8.972  H 16.523 11.560 -9.412  H 16.340 8.847 -10.737  H 15.502 10.305 -11.324  H 17.686 11.439 -11.462  H 18.467 9.903 -11.015  H 17.211 10.590 -13.565  H 18.533 8.074 -11.501  H 18.809 6.961 -12.822  H 17.573 9.137 -15.272  H 18.266 7.562 -14.956  N 17.876 11.755 -7.030  C 17.668 12.646 -5.893  C 17.727 14.076 -6.403  O 18.250 14.337 -7.486  C 18.709 12.410 -4.797  C 20.080 12.954 -5.131  C 20.480 14.183 -4.626  C 20.937 12.225 -5.941  C 21.732 14.681 -4.930  C 22.190 12.723 -6.245  C 22.587 13.946 -5.743  O 23.835 14.441 -6.047  H 18.474 12.055 -7.787  H 16.679 12.450 -5.477  H 18.374 12.874 -3.870  H 18.804 11.341 -4.610  H 19.806 14.756 -3.988  H 20.623 11.260 -6.339  H 22.047 15.645 -4.533  H 22.864 12.151 -6.883  H 24.201 13.952 -6.788  N 17.202 14.995 -5.587  C 17.171 16.430 -5.899  C 18.589 16.994 -5.833  O 19.197 17.019 -4.757  C 16.259 17.186 -4.929  C 16.084 18.653 -5.301  O 16.760 19.103 -6.196  O 15.276 19.307 -4.687  H 16.809 14.673 -4.714  H 16.791 16.556 -6.913  H 15.278 16.712 -4.907  H 16.673 17.129 -3.921  N 19.131 17.437 -6.963  C 20.510 17.919 -6.975  C 20.660 19.327 -6.412  O 21.792 19.783 -6.245  C 21.048 17.886 -8.393  O 20.385 18.818 -9.203  H 18.599 17.447 -7.821  H 21.112 17.262 -6.344  H 22.116 18.103 -8.382  H 20.922 16.887 -8.807  H 20.178 19.562 -8.633  N 19.568 20.032 -6.115  C 19.619 21.406 -5.612  C 18.616 21.543 -4.476  O 17.545 22.152 -4.633  C 19.343 22.393 -6.737  H 18.670 19.589 -6.247  H 20.621 21.587 -5.222  H 19.385 23.410 -6.348  H 20.094 22.273 -7.518  H 18.354 22.204 -7.151  N 18.920 20.980 -3.307  C 17.978 21.042 -2.181  C 17.712 22.486 -1.777  O 18.510 23.389 -2.015  C 18.702 20.272 -1.073  C 19.629 19.363 -1.805  C 20.103 20.178 -2.979  H 17.034 20.557 -2.472  H 19.227 20.974 -0.408  H 17.972 19.729 -0.455  H 20.452 19.050 -1.147  H 19.101 18.447 -2.112  H 20.953 20.807 -2.670  H 20.397 19.506 -3.798  N 16.540 22.693 -1.187  C 16.205 23.974 -0.601  C 17.180 24.296 0.524  O 17.725 23.414 1.197  C 14.767 23.969 -0.102  H 15.866 21.942 -1.146  H 16.308 24.737 -1.373  H 14.531 24.938 0.336  H 14.093 23.774 -0.936  H 14.647 23.191 0.651  N 17.423 25.585 0.706  C 18.315 26.049 1.755  C 17.574 26.434 3.025  O 18.204 26.927 3.966  C 19.148 27.250 1.270  C 19.996 26.859 0.069  O 18.274 28.325 0.904  H 16.979 26.263 0.103  H 19.002 25.241 2.007  H 19.802 27.588 2.074  H 17.953 28.760 1.698  H 20.578 27.720 -0.260  H 20.670 26.049 0.346  H 19.348 26.529 -0.742  N 16.267 26.216 3.084  C 15.524 26.625 4.270  C 15.483 25.556 5.322  O 14.673 25.745 6.237  C 14.092 27.012 3.896  C 13.278 25.837 3.370  O 13.811 24.756 3.298  O 12.130 26.033 3.049  H 15.773 25.771 2.323  H 16.023 27.488 4.709  H 13.585 27.423 4.771  H 14.112 27.791 3.134  N 16.288 24.495 5.214  C 16.225 23.380 6.138  C 15.390 22.191 5.689  O 15.441 21.140 6.338  H 16.962 24.473 4.462  H 17.233 23.011 6.333  H 15.818 23.718 7.090  N 14.608 22.312 4.624  C 13.879 21.130 4.197  C 14.854 20.030 3.802  O 16.021 20.281 3.482  C 12.967 21.464 3.033  O 12.060 22.474 3.379  H 14.497 23.173 4.106  H 13.280 20.771 5.035  H 13.566 21.786 2.181  H 12.422 20.571 2.729  H 12.548 23.299 3.323  N 14.359 18.791 3.834  C 15.162 17.666 3.403  C 15.287 17.587 1.886  O 14.710 18.362 1.127  H 13.417 18.627 4.159  H 16.158 17.741 3.840  H 14.720 16.741 3.772  N 16.074 16.607 1.448  C 16.405 16.377 0.046  C 15.521 15.257 -0.503  O 15.714 14.080 -0.137  C 17.891 16.016 -0.135  C 18.191 15.702 -1.592  O 18.707 17.115 0.291  H 16.458 15.993 2.152  H 16.210 17.294 -0.511  H 18.131 15.145 0.476  H 18.147 17.806 0.655  H 19.245 15.449 -1.700  H 17.580 14.859 -1.915  H 17.961 16.572 -2.206  N 14.585 15.619 -1.407  C 13.715 14.620 -2.036  C 14.533 13.594 -2.811  O 15.458 13.945 -3.552  C 12.702 15.298 -2.948  H 14.479 16.591 -1.658  H 13.181 14.091 -1.247  H 12.064 14.543 -3.407  H 12.090 15.984 -2.363  H 13.226 15.851 -3.725  N 14.163 12.317 -2.669  C 14.907 11.255 -3.333  C 14.005 10.046 -3.458  O 12.912 10.000 -2.882  C 16.175 10.893 -2.547  C 15.963 10.538 -1.070  C 15.205 9.220 -0.969  C 17.312 10.448 -0.372  H 13.364 12.076 -2.100  H 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-15.447  H 13.345 -7.641 -14.713  N 17.998 -11.448 -9.590  C 19.462 -11.425 -9.724  C 19.878 -12.810 -10.221  O 19.039 -13.643 -10.587  C 20.148 -11.070 -8.418  C 21.466 -10.379 -8.626  N 21.747 -9.396 -7.809  O 22.232 -10.738 -9.528  H 17.517 -12.336 -9.586  H 19.730 -10.678 -10.474  H 19.498 -10.417 -7.831  H 20.312 -11.976 -7.834  H 22.611 -8.901 -7.901  H 21.098 -9.140 -7.094  N 21.186 -13.074 -10.265  C 21.716 -14.314 -10.842  C 21.090 -15.572 -10.256  O 20.927 -16.555 -10.984  C 23.223 -14.362 -10.675  C 23.937 -13.405 -11.590  N 25.162 -13.086 -11.260  O 23.379 -12.956 -12.597  H 21.829 -12.393 -9.886  H 21.481 -14.328 -11.907  H 23.485 -14.124 -9.644  H 23.580 -15.373 -10.877  H 25.686 -12.454 -11.831  H 25.576 -13.474 -10.436  N 20.732 -15.564 -8.974  C 20.178 -16.730 -8.305  C 18.815 -16.499 -7.676  O 18.487 -17.153 -6.675  C 21.157 -17.223 -7.238  C 22.536 -17.537 -7.771  C 23.542 -16.585 -7.700  C 22.795 -18.780 -8.335  C 24.801 -16.873 -8.189  C 24.055 -19.067 -8.823  C 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-5.060 -9.553  H 9.302 -3.589 -9.109  N 10.399 -3.102 -5.550  C 9.988 -2.028 -4.629  C 10.489 -0.652 -5.065  O 11.654 -0.540 -5.481  C 10.422 -2.366 -3.192  C 9.998 -1.335 -2.176  O 9.887 -3.592 -2.809  H 11.302 -3.585 -5.370  H 8.892 -1.998 -4.613  H 11.525 -2.454 -3.181  H 8.931 -3.444 -2.600  H 10.396 -1.581 -1.172  H 10.430 -0.416 -2.516  H 8.898 -1.232 -2.123  N 9.676 0.396 -4.862  C 10.145 1.770 -5.025  C 10.017 2.487 -3.697  O 8.975 2.374 -3.026  C 9.355 2.524 -6.112  C 9.834 3.963 -6.219  O 9.533 1.869 -7.375  H 8.718 0.232 -4.589  H 11.193 1.746 -5.327  H 8.295 2.518 -5.861  H 10.379 2.124 -7.751  H 9.264 4.480 -6.992  H 9.690 4.466 -5.263  H 10.892 3.976 -6.479  N 11.084 3.207 -3.320  C 11.095 4.027 -2.117  C 10.945 5.463 -2.566  O 11.502 5.855 -3.596  C 12.388 3.845 -1.320  C 12.474 2.527 -0.611  C 12.234 2.294 0.710  C 12.828 1.246 -1.189  C 12.775 0.307 -0.155  C 13.177 0.829 -2.478  N 12.413 0.963 0.994  C 13.063 -1.033 -0.367  C 13.463 -0.515 -2.690  C 13.439 -1.422 -1.608  H 11.910 3.174 -3.901  H 10.248 3.740 -1.495  H 13.243 3.932 -1.988  H 12.471 4.639 -0.577  H 11.943 3.052 1.433  H 12.299 0.535 1.902  H 13.220 1.544 -3.298  H 13.023 -1.768 0.438  H 13.735 -0.832 -3.699  H 13.720 -2.446 -1.783  N 10.252 6.261 -1.778  C 10.137 7.671 -2.108  C 10.239 8.451 -0.800  O 9.567 8.090 0.168  C 8.827 7.963 -2.813  O 8.696 9.331 -3.083  H 9.797 5.911 -0.947  H 10.968 7.942 -2.761  H 8.781 7.398 -3.744  H 7.997 7.631 -2.189  H 9.316 9.777 -2.502  N 11.092 9.468 -0.719  C 11.137 10.188 0.546  C 12.185 11.260 0.553  O 12.492 11.851 -0.480  H 11.696 9.760 -1.473  H 10.164 10.637 0.743  H 11.338 9.488 1.355  N 12.721 11.529 1.753  C 13.704 12.592 1.877  C 14.913 12.149 2.691  O 14.807 11.304 3.599  C 13.069 13.829 2.518  C 11.985 14.479 1.676  C 11.514 15.800 2.257  N 10.597 16.459 1.558  O 11.968 16.221 3.323  H 12.455 11.006 2.575  H 14.051 12.862 0.880  H 12.630 13.557 3.479  H 13.840 14.575 2.709  H 12.379 14.667 0.677  H 11.130 13.806 1.619  H 10.249 17.336 1.891  H 10.257 16.081 0.697  N 16.052 12.752 2.349  C 17.293 12.681 3.121  C 17.363 13.902 4.028  O 17.055 15.019 3.587  C 18.517 12.610 2.205  C 19.816 12.968 2.893  C 20.449 12.038 3.704  C 20.374 14.224 2.712  C 21.635 12.364 4.332  C 21.560 14.550 3.340  C 22.190 13.625 4.147  O 23.372 13.950 4.772  H 16.034 13.289 1.493  H 17.270 11.779 3.732  H 18.612 11.602 1.800  H 18.380 13.289 1.363  H 20.011 11.050 3.846  H 19.876 14.955 2.075  H 22.133 11.633 4.970  H 21.998 15.538 3.198  H 23.604 14.858 4.565  N 17.764 13.692 5.286  C 17.984 14.771 6.247  C 19.426 14.640 6.762  O 19.866 13.541 7.136  C 16.986 14.690 7.417  C 17.249 15.802 8.421  C 15.562 14.765 6.888  H 17.919 12.737 5.576  H 17.855 15.724 5.732  H 17.131 13.744 7.939  H 16.535 15.728 9.240  H 18.261 15.706 8.812  H 17.139 16.769 7.929  H 14.861 14.705 7.720  H 15.419 15.709 6.359  H 15.382 13.937 6.203  N 20.159 15.752 6.764  C 21.544 15.781 7.184  C 21.696 15.950 8.690  O 20.775 15.723 9.477  H 19.720 16.609 6.456  H 22.036 14.857 6.879  H 22.059 16.599 6.682  N 22.915 16.324 9.088  C 23.311 16.444 10.478  C 23.992 15.185 10.983  O 24.106 14.168 10.282  H 23.588 16.532 8.364  H 23.988 17.291 10.591  H 22.433 16.651 11.090  N 24.440 15.265 12.246  C 25.153 14.154 12.868  C 24.298 12.901 12.884  O 24.797 11.795 12.627  C 25.587 14.526 14.280  H 24.282 16.108 12.779  H 26.040 13.944 12.270  H 26.117 13.686 14.730  H 26.246 15.393 14.241  H 24.710 14.763 14.878  N 23.007 13.058 13.189  C 22.046 11.958 13.170  C 21.264 11.995 11.853  O 20.039 12.168 11.817  C 21.090 12.050 14.362  C 21.750 11.830 15.716  C 22.256 10.426 15.898  O 21.746 9.542 15.253  O 23.155 10.238 16.685  H 22.692 13.983 13.443  H 22.595 11.017 13.227  H 20.618 13.032 14.375  H 20.298 11.308 14.251  H 22.585 12.522 15.818  H 21.029 12.057 16.501  N 22.018 11.820 10.761  C 21.475 11.821 9.403  C 20.451 10.701 9.210  O 20.619 9.582 9.716  C 22.597 11.695 8.383  H 23.009 11.682 10.894  H 20.959 12.768 9.245  H 22.176 11.697 7.377  H 23.283 12.535 8.490  H 23.136 10.763 8.549  N 19.390 10.990 8.458  C 18.307 10.025 8.267  C 17.867 10.023 6.807  O 17.990 11.036 6.104  C 17.119 10.355 9.159  C 17.393 10.262 10.651  C 17.573 8.855 11.090  N 17.706 8.750 12.535  C 18.873 8.829 13.204  N 19.996 9.014 12.546  N 18.888 8.722 14.520  H 19.329 11.893 8.010  H 18.695 9.026 8.466  H 16.776 11.366 8.948  H 16.295 9.676 8.932  H 18.303 10.814 10.889  H 16.555 10.689 11.204  H 16.710 8.265 10.783  H 18.473 8.444 10.635  H 16.863 8.606 13.075  H 19.984 9.097 11.539  H 20.870 9.075 13.047  H 18.024 8.579 15.026  H 19.762 8.781 15.022  N 17.297 8.900 6.371  C 16.445 8.899 5.177  C 15.104 8.302 5.575  O 15.056 7.223 6.182  C 17.066 8.093 4.022  C 18.356 8.761 3.538  C 16.074 7.951 2.878  C 19.102 7.962 2.495  H 17.450 8.033 6.866  H 16.312 9.928 4.847  H 17.340 7.100 4.378  H 18.123 9.739 3.118  H 19.023 8.921 4.385  H 16.530 7.380 2.070  H 15.183 7.434 3.231  H 15.798 8.941 2.512  H 20.005 8.500 2.201  H 19.377 6.991 2.907  H 18.467 7.820 1.622  N 14.018 9.018 5.285  C 12.684 8.584 5.683  C 11.911 8.336 4.405  O 11.688 9.274 3.647  C 11.993 9.606 6.567  C 12.619 9.708 7.931  N 13.191 10.848 8.225  O 12.585 8.756 8.716  H 14.122 9.883 4.775  H 12.775 7.648 6.236  H 12.030 10.585 6.088  H 10.943 9.338 6.682  H 13.625 10.974 9.118  H 13.195 11.594 7.559  N 11.523 7.095 4.150  C 10.827 6.799 2.897  C 9.529 6.040 3.132  O 9.388 5.268 4.095  C 11.727 5.989 1.945  C 12.880 6.845 1.443  O 12.250 4.846 2.635  H 11.698 6.345 4.804  H 10.581 7.742 2.407  H 11.140 5.645 1.095  H 12.392 5.067 3.558  H 13.504 6.257 0.772  H 12.485 7.709 0.909  H 13.476 7.183 2.288  N 8.623 6.227 2.171  C 7.458 5.385 1.955  C 7.716 4.494 0.747  O 8.324 4.932 -0.236  C 6.198 6.229 1.744  C 4.925 5.416 1.581  C 3.683 6.287 1.552  N 2.992 6.293 0.419  O 3.347 6.946 2.540  H 8.778 7.017 1.561  H 7.312 4.764 2.839  H 6.063 6.899 2.594  H 6.319 6.847 0.855  H 4.977 4.863 0.643  H 4.839 4.724 2.419  H 2.164 6.848 0.340  H 3.299 5.743 -0.358  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-4.024 -4.246  O 4.004 -4.523 -3.787  C 6.273 -4.302 -2.060  C 6.507 -5.808 -2.320  C 7.721 -6.065 -3.198  C 6.711 -6.511 -0.984  H 4.735 -2.074 -2.273  H 7.018 -3.289 -3.843  H 7.094 -3.888 -1.440  H 5.355 -4.247 -1.450  H 5.617 -6.255 -2.809  H 7.811 -7.154 -3.374  H 7.627 -5.562 -4.180  H 8.627 -5.731 -2.671  H 6.872 -7.598 -1.135  H 7.584 -6.077 -0.458  H 5.810 -6.388 -0.350  N 5.293 -4.050 -5.584  C 4.284 -4.554 -6.528  C 4.698 -5.896 -7.076  O 5.757 -5.989 -7.750  C 4.041 -3.535 -7.646  C 3.034 -4.084 -8.646  O 3.539 -2.316 -7.085  H 6.157 -3.599 -5.957  H 3.309 -4.683 -6.020  H 4.977 -3.323 -8.162  H 2.549 -2.377 -7.027  H 2.868 -3.349 -9.434  H 3.419 -5.005 -9.082  H 2.060 -4.300 -8.171  N 3.905 -6.995 -6.900  C 4.165 -8.309 -7.534  C 3.553 -8.395 -8.915  O 2.479 -7.793 -9.167  C 3.753 -9.493 -6.607  C 2.394 -9.302 -5.918  C 3.823 -10.850 -7.322  H 2.975 -6.835 -6.455  H 5.246 -8.411 -7.698  H 4.507 -9.540 -5.791  H 1.675 -8.765 -6.565  H 1.945 -10.271 -5.612  H 2.523 -8.700 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4.867  H 2.528 4.638 5.347  H 3.796 6.639 4.405  N 9.993 2.796 5.621  C 11.308 2.423 6.184  C 12.046 3.684 6.596  O 12.049 4.667 5.852  C 12.146 1.635 5.175  C 11.679 0.194 5.012  O 11.316 -0.406 5.995  O 11.688 -0.289 3.906  H 9.950 3.484 4.883  H 11.143 1.807 7.069  H 12.103 2.127 4.203  H 13.188 1.629 5.493  N 12.767 3.634 7.715  C 13.678 4.712 8.096  C 15.114 4.196 8.144  O 15.381 3.167 8.777  C 13.293 5.318 9.459  C 14.320 6.353 9.891  O 12.005 5.941 9.362  H 12.679 2.828 8.317  H 13.613 5.501 7.346  H 13.244 4.528 10.207  H 12.113 6.860 9.110  H 14.032 6.770 10.856  H 15.298 5.880 9.978  H 14.368 7.150 9.152  N 16.027 4.898 7.467  C 17.418 4.466 7.323  C 18.319 5.360 8.159  O 18.066 6.569 8.285  C 17.857 4.506 5.858  C 17.085 3.576 4.968  C 15.889 3.977 4.391  C 17.550 2.295 4.707  C 15.177 3.121 3.572  C 16.842 1.438 3.887  C 15.653 1.852 3.319  H 15.735 5.765 7.039  H 17.503 3.443 7.694  H 17.743 5.519 5.473  H 18.913 4.246 5.788  H 15.514 4.981 4.589  H 18.490 1.969 5.156  H 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8.225  H -20.025 3.299 9.104  H -18.932 3.519 11.299  H -17.250 1.523 10.205  H -19.682 1.392 12.288  H -20.847 1.975 11.075  H -19.729 0.651 10.671  N -18.258 5.159 8.897  C -17.282 6.148 8.503  C -17.772 7.532 8.788  O -18.703 7.714 9.568  H -19.134 5.465 9.294  H -16.348 5.971 9.037  H -17.069 6.044 7.440  N -17.135 8.512 8.148  C -17.439 9.933 8.354  C -17.396 10.639 7.010  O -16.761 10.169 6.051  C -16.447 10.583 9.307  C -16.480 10.046 10.729  C -17.711 10.470 11.446  N -17.689 10.067 12.844  C -18.119 8.875 13.304  N -18.601 7.984 12.467  N -18.058 8.604 14.596  H -16.412 8.252 7.492  H -18.463 10.020 8.717  H -15.436 10.447 8.928  H -16.637 11.656 9.355  H -16.455 8.957 10.708  H -15.617 10.420 11.280  H -17.800 11.555 11.406  H -18.582 10.016 10.975  H -17.325 10.727 13.518  H -18.648 8.191 11.479  H -18.923 7.090 12.811  H -17.688 9.292 15.239  H -18.379 7.713 14.940  N -17.991 11.826 6.971  C -17.782 12.705 5.825  C -17.841 14.141 6.320  O -18.364 14.413 7.401  C -18.823 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-19.915 27.567 -2.292  H -18.066 28.741 -1.928  H -20.692 27.722 0.041  H -20.783 26.046 -0.549  H -19.461 26.536 0.534  N -16.380 26.185 -3.287  C -15.638 26.581 -4.477  C -15.596 25.502 -5.519  O -14.787 25.681 -6.436  C -14.205 26.972 -4.108  C -13.391 25.802 -3.571  O -13.925 24.722 -3.487  O -12.243 26.001 -3.252  H -15.886 25.748 -2.522  H -16.136 27.441 -4.926  H -13.699 27.374 -4.987  H -14.226 27.759 -3.354  N -16.402 24.441 -5.401  C -16.339 23.318 -6.314  C -15.504 22.134 -5.852  O -15.555 21.076 -6.490  H -17.076 24.427 -4.649  H -17.347 22.946 -6.505  H -15.932 23.647 -7.268  N -14.722 22.265 -4.789  C -13.993 21.087 -4.349  C -14.967 19.991 -3.943  O -16.134 20.246 -3.626  C -13.080 21.432 -3.189  O -12.173 22.439 -3.545  H -14.610 23.130 -4.279  H -13.394 20.720 -5.184  H -13.680 21.764 -2.341  H -12.536 20.543 -2.876  H -12.662 23.265 -3.498  N -14.473 18.752 -3.963  C -15.276 17.632 -3.521  C -15.401 17.568 -2.002  O -14.824 18.351 -1.253  H -13.531 18.585 -4.286  H 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6.527  H -13.965 1.618 9.414  H -11.373 2.124 8.516  H -12.040 0.180 9.962  H -13.237 -0.704 8.986  H -11.746 -0.095 8.230  N -14.457 -0.923 6.679  C -15.210 -2.167 6.656  C -14.326 -3.224 7.295  O -13.171 -3.399 6.877  C -15.583 -2.576 5.219  C -16.318 -3.909 5.218  C -16.434 -1.491 4.576  H -13.543 -0.892 6.250  H -16.122 -2.032 7.238  H -14.670 -2.713 4.641  H -16.574 -4.183 4.194  H -15.676 -4.678 5.649  H -17.229 -3.822 5.808  H -16.694 -1.787 3.560  H -17.345 -1.352 5.158  H -15.873 -0.557 4.550  N -14.858 -3.925 8.301  C -14.142 -5.059 8.892  C -14.629 -6.349 8.234  O -15.840 -6.588 8.158  C -14.344 -5.085 10.400  H -15.767 -3.674 8.661  H -13.080 -4.936 8.681  H -13.806 -5.932 10.826  H -13.964 -4.159 10.834  H -15.406 -5.180 10.623  N -13.693 -7.170 7.741  C -14.045 -8.333 6.922  C -14.388 -9.538 7.798  O -13.746 -10.594 7.749  C -12.926 -8.673 5.925  C -12.642 -7.559 4.960  C -11.440 -7.033 4.734  C -13.492 -6.983 4.035  C -12.749 -6.110 3.305  C -14.821 -7.197 3.719  N 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 H -23.453 -15.535 7.477  H -22.119 -19.440 8.649  H -25.707 -16.041 8.356  H -24.373 -19.946 9.527  H -26.438 -19.204 9.835  N -18.166 -15.457 8.404  C -16.843 -15.191 7.844  C -15.988 -14.437 8.845  O -16.506 -13.754 9.727  C -16.966 -14.417 6.539  H -18.493 -14.899 9.180  H -16.362 -16.148 7.643  H -15.972 -14.227 6.134  H -17.544 -15.002 5.823  H -17.470 -13.470 6.725  N -14.685 -14.583 8.678  C -13.747 -13.791 9.453  C -12.423 -13.856 8.717  O -11.691 -14.846 8.839  C -13.625 -14.290 10.881  C -12.797 -13.379 11.744  N -12.991 -13.461 13.036  O -11.981 -12.598 11.239  H -14.330 -15.249 8.006  H -14.099 -12.759 9.473  H -14.618 -14.385 11.320  H -13.171 -15.281 10.883  H -12.468 -12.879 13.657  H -13.661 -14.107 13.399  N -12.125 -12.841 7.926  C -10.888 -12.862 7.114  C -9.729 -12.261 7.883  O -8.603 -12.129 7.337  C -11.128 -12.147 5.784  H -12.744 -12.050 7.824  H -10.598 -13.909 6.863  H -10.252 -12.284 5.111  H -12.019 -12.582 5.284  H -11.287 -11.064 5.943  N -9.922 -11.792 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-10.263 7.795  H 3.605 -11.523 8.845  H 3.955 -11.114 7.141  H 5.424 -14.551 8.667  H 4.571 -13.461 9.707  N 4.928 -8.201 9.669  C 4.269 -6.894 9.743  C 4.753 -5.980 8.668  O 4.018 -5.026 8.295  C 4.550 -6.241 11.075  H 5.505 -8.501 10.443  H 3.171 -7.022 9.626  H 4.062 -5.268 11.106  H 4.156 -6.870 11.874  H 5.623 -6.113 11.212  N 5.999 -6.134 8.131  C 6.457 -5.229 7.081  C 5.559 -5.358 5.839  O 5.307 -4.334 5.154  C 7.906 -5.539 6.700  C 8.100 -6.923 6.160  C 8.366 -8.049 6.879  C 8.048 -7.323 4.839  C 8.254 -8.677 4.836  C 7.722 -6.638 3.667  N 8.464 -9.134 6.077  C 8.103 -9.427 3.676  C 7.551 -7.371 2.543  C 7.719 -8.782 2.552  H 6.632 -6.838 8.484  H 6.396 -4.206 7.454  H 8.245 -4.826 5.948  H 8.546 -5.420 7.575  H 8.474 -8.085 7.962  H 8.621 -10.130 6.361  H 7.540 -5.571 3.671  H 8.231 -10.499 3.696  H 7.222 -6.884 1.641  H 7.512 -9.351 1.654  N 5.042 -6.578 5.460  C 4.200 -6.803 4.259  C 2.713 -6.621 4.508  O 1.928 -6.672 3.527  C 4.530 -8.184 3.607  H 5.328 -7.413 6.012  H 4.466 -6.029 3.507  H 4.560 -8.049 2.504  H 5.541 -8.485 3.915  C 3.662 -9.393 3.883  N 3.671 -10.491 3.099  C 2.876 -9.638 4.925  C 2.853 -11.365 3.709  N 2.372 -10.880 4.804  H 4.195 -10.673 2.211  H 2.666 -8.990 5.753  H 2.626 -12.358 3.330  N 2.204 -6.429 5.767  C 0.775 -6.620 6.113  C -0.195 -5.915 5.192  O -1.366 -6.367 5.100  C 0.492 -6.161 7.551  O 0.718 -4.781 7.680  H 2.885 -6.454 6.553  H 0.544 -7.706 6.058  H -0.567 -6.377 7.814  H 1.122 -6.736 8.268  H 1.656 -4.670 7.997  N 0.097 -4.699 4.642  C -0.949 -3.786 4.139  C -0.933 -3.720 2.637  O -0.029 -3.071 2.061  C -0.761 -2.385 4.752  C -1.817 -1.407 4.285  O -0.876 -2.457 6.145  H 1.088 -4.373 4.663  H -1.950 -4.136 4.451  H 0.240 -1.977 4.473  H -0.016 -2.830 6.475  H -1.639 -0.458 4.814  H -1.721 -1.210 3.205  H -2.835 -1.786 4.514  N -1.979 -4.187 1.898  C -2.194 -3.779 0.495  C -2.439 -2.277 0.398  O -3.131 -1.707 1.277  C -3.375 -4.558 -0.120  C -3.024 -5.972 -0.621  C -2.455 -6.874 0.470  C -4.275 -6.625 -1.201  H -2.681 -4.782 2.383  H -1.299 -4.031 -0.092  H -4.187 -4.626 0.620  H -3.760 -3.990 -0.996  H -2.273 -5.878 -1.429  H -2.265 -7.887 0.057  H -1.482 -6.492 0.836  H -3.159 -6.963 1.323  H -4.041 -7.651 -1.551  H -5.067 -6.696 -0.428  H -4.656 -6.039 -2.063  N -2.052 -1.566 -0.701  C -2.666 -0.271 -1.087  C -3.308 -0.389 -2.452  O -2.721 -0.998 -3.385  C -1.647 0.908 -1.039  C -0.537 0.662 -2.054  C -2.291 2.257 -1.316  H -1.478 -2.068 -1.408  H -3.474 -0.023 -0.371  H -1.205 0.913 -0.043  H 0.221 1.431 -1.961  H -0.047 -0.308 -1.850  H -0.908 0.684 -3.099  H -1.535 3.040 -1.263  H -2.737 2.251 -2.311  H -3.066 2.450 -0.573  N -4.403 0.355 -2.731  C -4.970 0.523 -4.061  C -5.997 1.638 -4.073  O -6.126 2.412 -3.117  H -4.873 0.827 -1.950  H -4.175 0.729 -4.776  H -5.457 -0.428 -4.361  N -6.722 1.727 -5.200  C -7.673 2.800 -5.413  C -8.953 2.204 -6.004  O -8.907 1.218 -6.758  C -7.099 3.874 -6.343  C -5.862 4.529 -5.812  C -5.687 5.697 -5.150  N -4.609 3.969 -5.943  C -3.715 4.767 -5.383  N -4.343 5.820 -4.896  H -6.601 1.027 -5.918  H -7.914 3.267 -4.458  H -6.861 3.428 -7.310  H -7.849 4.645 -6.514  H -6.466 6.408 -4.871  H -2.641 4.585 -5.334  H -3.910 6.595 -4.411  N -10.107 2.740 -5.589  C -11.422 2.362 -6.148  C -12.161 3.618 -6.572  O -12.164 4.609 -5.839  C -12.260 1.583 -5.130  C -11.794 0.145 -4.953  O -11.431 -0.466 -5.931  O -11.803 -0.328 -3.842  H -10.064 3.435 -4.858  H -11.257 1.737 -7.026  H -12.217 2.086 -4.165  H -13.303 1.574 -5.449  N -12.881 3.557 -7.692  C -13.793 4.631 -8.082  C -15.229 4.114 -8.125  O -15.495 3.080 -8.749  C -13.408 5.223 -9.451  C -14.434 6.253 -9.895  O -12.119 5.846 -9.361  H -12.794 2.745 -8.285  H -13.728 5.428 -7.341  H -13.359 4.425 -10.192  H -12.227 6.768 -9.118  H -14.147 6.660 -10.864  H -15.413 5.780 -9.976  H -14.482 7.059 -9.163  N -16.141 4.823 -7.456  C -17.533 4.392 -7.308  C -18.433 5.279 -8.152  O -18.180 6.486 -8.291  C -17.972 4.448 -5.843  C -17.199 3.525 -4.944  C -16.003 3.933 -4.370  C -17.665 2.249 -4.669  C -15.292 3.085 -3.543  C -16.957 1.400 -3.841  C -15.768 1.820 -3.277  H -15.849 5.694 -7.036  H -17.617 3.366 -7.667  H -17.857 5.464 -5.467  H -19.027 4.189 -5.770  H -15.628 4.935 -4.579  H -18.603 1.917 -5.115  H -14.354 3.419 -3.099  H -17.335 0.399 -3.634  H -15.207 1.150 -2.627  N -19.502 4.680 -8.694  C -20.485 5.410 -9.479  C -21.870 5.159 -8.886  O -22.064 4.231 -8.096  C -20.454 4.995 -10.962  C -19.056 5.170 -11.536  O -20.848 3.623 -11.084  H -19.625 3.687 -8.551  H -20.253 6.474 -9.422  H -21.153 5.611 -11.528  H -21.413 3.520 -11.854  H -19.054 4.872 -12.584  H -18.758 6.215 -11.454  H -18.355 4.548 -10.980  N -22.836 5.975 -9.301  C -24.243 5.688 -8.996  C -24.878 4.762 -10.026  O -25.967 4.232 -9.786  C -25.044 6.987 -8.907  C -24.682 7.869 -7.719  C -25.553 9.114 -7.670  C -25.253 9.953 -6.436  N -25.910 9.406 -5.217  H -22.607 6.804 -9.831  H -24.291 5.181 -8.031  H -24.894 7.571 -9.815  H -26.108 6.755 -8.840  H -24.812 7.307 -6.794  H -23.637 8.171 -7.796  H -25.378 9.719 -8.560  H -26.604 8.823 -7.651  H -24.176 9.984 -6.271  H -25.603 10.973 -6.595  H -25.687 9.991 -4.424  H -26.911 9.391 -5.352  H -25.579 8.468 -5.049  N -24.201 4.505 -11.135  C -24.721 3.637 -12.182  C -23.884 2.373 -12.210  O -22.659 2.440 -12.370  C -24.674 4.330 -13.558  C -25.187 3.396 -14.644  C -25.490 5.614 -13.519  H -23.291 4.929 -11.255  H -25.757 3.389 -11.943  H -23.638 4.566 -13.799  H -25.146 3.903 -15.608  H -24.566 2.502 -14.677  H -26.217 3.117 -14.425  H -25.452 6.099 -14.493  H -26.526 5.379 -13.272  H -25.081 6.283 -12.763  N -24.544 1.227 -12.020  C -23.865 -0.069 -11.892  C -23.257 -0.467 -13.234  O -23.956 -0.417 -14.258  C -24.833 -1.149 -11.404  C -24.222 -2.541 -11.302  C -25.289 -3.593 -11.036  C -24.739 -4.998 -11.228  N -24.316 -5.244 -12.633  H -25.552 1.261 -11.965  H -23.061 0.033 -11.162  H -25.213 -0.878 -10.419  H -25.686 -1.206 -12.080  H -23.710 -2.782 -12.234  H -23.495 -2.560 -10.492  H -25.655 -3.491 -10.014  H -26.125 -3.444 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