

```

forcefield amber
sys 0 0 1
view 40 0.15058 57.4 17.4 0.04949906 0.5118667 0.8576376 -0.8401311 -0.4430261
0.3129017 0.5401198 -0.7360165 0.4081058 -0.86644 -1.8893 -55.21
seed 0
mol 1
atom 1 - C CA - 0 0.6174496 4.348619 0.06800047 3 2 s 9 s 14 s
atom 2 - C CA - 0 -0.1405912 4.102345 -1.063262 3 1 s 3 s 15 s
atom 3 - C CA - 0 0.2373727 3.110379 -1.952814 3 2 s 4 s 16 s
atom 4 - C CB - 0 1.394996 2.318304 -1.721511 4 3 s 5 s 8 s 10 s
atom 5 - C CB - 0 2.161185 2.560286 -0.5617862 4 4 s 6 s 9 s 10 s
atom 6 - C C5 - 0 3.251375 1.682818 -0.5793154 4 5 s 7 s 10 s 12 s
atom 7 - C C5 - 0 3.189911 0.9300277 -1.75558 4 6 s 8 s 10 s 37 s
atom 8 - C C5 - 0 2.036932 1.31033 -2.451727 4 7 s 4 s 10 s 11 s
atom 9 - C CA - 0 1.753806 3.598433 0.3221232 3 1 s 5 s 13 s
atom 10 - C DC - 0 2.378515 1.738006 -1.411306 6 8 s 4 s 5 s 6 s 7 s 17 s
atom 11 - H HA - 0 1.783098 1.004809 -3.30351 1 8 s
atom 12 - H HA - 0 3.950156 1.662434 0.0495031 1 6 s
atom 13 - H HA - 0 2.327688 3.790913 1.216767 1 9 s
atom 14 - H HA - 0 0.3194271 5.125622 0.7566214 1 1 s
atom 15 - H HA - 0 -1.024879 4.69101 -1.258351 1 2 s
atom 16 - H HA - 0 -0.3317083 2.966048 -2.859186 1 3 s
atom 17 - Zr ZR - 0 1.219782 0.1957982 -0.33981 4 10 s 27 s 34 s 35 s
atom 18 - C CA - 0 -2.893651 0.6068944 0.5645774 3 19 s 26 s 31 s
atom 19 - C CA - 0 -2.854589 1.248055 -0.6611595 3 18 s 20 s 32 s
atom 20 - C CA - 0 -1.958729 0.8370547 -1.634218 3 19 s 21 s 33 s
atom 21 - C CB - 0 -1.057725 -0.2372359 -1.398197 4 20 s 22 s 25 s 27 s
atom 22 - C CB - 0 -1.090144 -0.8833699 -0.1444735 4 21 s 23 s 26 s 27 s
atom 23 - C C5 - 0 -0.1420205 -1.911656 -0.1708695 4 22 s 24 s 27 s 29 s
atom 24 - C C5 - 0 0.4466392 -1.933925 -1.439777 4 23 s 25 s 27 s 36 s
atom 25 - C C5 - 0 -0.105981 -0.8916892 -2.190435 4 24 s 21 s 27 s 28 s
atom 26 - C CA - 0 -2.030627 -0.4438077 0.8287479 3 18 s 22 s 30 s
atom 27 - C DC - 0 -0.3692833 -1.149608 -1.063196 6 25 s 21 s 22 s 23 s 24 s 17
s
atom 28 - H HA - 0 0.07104779 -0.7127501 -3.095933 1 25 s
atom 29 - H HA - 0 0.0152839 -2.529735 0.5198386 1 23 s
atom 30 - H HA - 0 -2.059545 -0.9253348 1.79527 1 26 s
atom 31 - H HA - 0 -3.595623 0.9295157 1.319371 1 18 s
atom 32 - H HA - 0 -3.53075 2.066049 -0.8624855 1 19 s
atom 33 - H HA - 0 -1.977224 1.31144 -2.603854 1 20 s
atom 34 - Cl CI - 0 0.3430986 1.268747 1.674567 1 17 s
atom 35 - Cl CI - 0 2.888252 -1.287398 0.6536561 1 17 s
atom 36 - Si SI - 0 1.628333 -3.246437 -2.061002 4 24 s 41 s 42 s 43 s
atom 37 - Si SI - 0 4.513425 -0.2327637 -2.393242 4 7 s 38 s 39 s 40 s
atom 38 - C CT - 0 4.03711 -0.8845111 -4.100317 4 37 s 44 s 45 s 46 s
atom 39 - C CT - 0 6.134755 0.7223555 -2.537874 4 37 s 47 s 48 s 49 s
atom 40 - H HC - 0 4.694602 -1.323634 -1.488297 1 37 s
atom 41 - C CT - 0 1.536822 -4.760827 -0.9378029 4 36 s 50 s 51 s 55 s
atom 42 - H HC - 0 2.965086 -2.747837 -2.06148 1 36 s
atom 43 - C CT - 0 1.138625 -3.747701 -3.813772 4 36 s 52 s 53 s 54 s
atom 44 - H HC - 0 3.01992 -1.27209 -4.073139 1 38 s
atom 45 - H HC - 0 4.095048 -0.07368945 -4.826334 1 38 s
atom 46 - H HC - 0 4.722353 -1.680801 -4.390316 1 38 s
atom 47 - H HC - 0 6.424268 1.096829 -1.556077 1 39 s
atom 48 - H HC - 0 6.913415 0.06134164 -2.918464 1 39 s
atom 49 - H HC - 0 6.002428 1.560305 -3.222524 1 39 s
atom 50 - H HC - 0 1.862527 -4.488575 0.06626731 1 41 s

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atom 51 - H HC - 0 2.18576 -5.543562 -1.330771 1 41 s
atom 52 - H HC - 0 1.854473 -4.474685 -4.196881 1 43 s
atom 53 - H HC - 0 1.132028 -2.868423 -4.457372 1 43 s
atom 54 - H HC - 0 0.1435885 -4.191985 -3.797555 1 43 s
atom 55 - H HC - 0 0.5097418 -5.124316 -0.9016936 1 41 s
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selectatom 7 molecule 1
selectatom 24 molecule 1
selectatom 36 molecule 1
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selection Theta 4
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selectatom 7 molecule 1
selectatom 17 molecule 1
selectatom 34 molecule 1
endselection Theta
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