```
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
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atom 1 - C CA - 0 1.274967 -2.038414 -5.733374 3 2 s 9 s 14 s
atom 2 - C CA - 0 1.843825 -2.946391 -4.857368 3 1 s 3 s 15 s
atom 3 - C CA - 0 2.39226 -2.514242 -3.660622 3 2 s 4 s 16 s
atom 4 - C CB - 0 2.409225 -1.134387 -3.313098 4 3 s 5 s 8 s 10 s
atom 5 - C CB - 0 1.833463 -0.2111112 -4.211584 4 4 s 6 s 9 s 10 s
atom 6 - C C5 - 0 2.028316 1.06892 -3.688954 4 5 s 7 s 10 s 12 s
atom 7 - C C5 - 0 2.705609 0.9531227 -2.472944 4 6 s 8 s 10 s 37 s
atom 8 - C C5 - 0 2.932376 -0.4083313 -2.232714 4 7 s 4 s 10 s 11 s
atom 9 - C CA - 0 1.254348 -0.6898966 -5.419279 3 1 s 5 s 13 s
atom 10 - C DC - 0 2.361151 0.05027741 -3.162889 6 8 s 4 s 5 s 6 s 7 s 17 s
atom 11 - H HA - 0 3.402933 -0.7683938 -1.502872 1 8 s
atom 12 - H HA - 0 1.801366 1.874361 -4.116897 1 6 s
atom 13 - H HA - 0 0.8031718 0.009974757 -6.107508 1 9 s
atom 14 - H HA - 0 0.8371698 -2.383471 -6.658674 1 1 s
atom 15 - H HA - 0 1.860798 -3.996697 -5.108019 1 2 s
atom 16 - H HA - 0 2.907826 -3.227883 -3.036901 1 3 s
atom 17 - Zr ZR - 0 0.4364929 -0.01842479 -2.103837 4 10 s 27 s 34 s 35 s
atom 18 - C CA - 0 -1.050952 3.092877 0.3765516 3 19 s 26 s 31 s
atom 19 - C CA - 0 -2.244581 2.467238 0.05963274 3 18 s 20 s 32 s
atom 20 - C CA - 0 -2.269855 1.105842 -0.1959607 3 19 s 21 s 33 s
atom 21 - C CB - 0 -1.088048 0.3206305 -0.09538133 4 20 s 22 s 25 s 27 s
atom 22 - C CB - 0 0.1291096 0.9556252 0.2311897 4 21 s 23 s 26 s 27 s
atom 23 - C C5 - 0 1.115955 -0.03588626 0.316354 4 22 s 24 s 27 s 29 s
atom 24 - C C5 - 0 0.5150901 -1.27323 0.05564106 4 23 s 25 s 27 s 36 s
atom 25 - C C5 - 0 -0.8381897 -1.049471 -0.2072552 4 24 s 21 s 27 s 28 s
atom 26 - C CA - 0 0.1244565 2.362391 0.4449977 3 18 s 22 s 30 s
atom 27 - C DC - 0 -0.01452158 -0.2125875 0.03757031 6 25 s 21 s 22 s 23 s 24 s
17 s
atom 28 - H HA - 0 -1.485522 -1.712849 -0.3635709 1 25 s
atom 29 - H HA - 0 2.010844 0.09720377 0.5706561 1 23 s
atom 30 - H HA - 0 1.038324 2.864998 0.7219022 1 26 s
atom 31 - H HA - 0 -1.033454 4.157304 0.5591469 1 18 s
atom 32 - H HA - 0 -3.154217 3.04539 -0.01054093 1 19 s
atom 33 - H HA - 0 -3.203223 0.6308268 -0.4601786 1 20 s
atom 34 - Cl CI - 0 -0.8888313 -1.768763 -3.177673 1 17 s
atom 35 - Cl CI - 0 -0.7032822 2.010451 -2.854258 1 17 s
atom 36 - Si SI - 0 1.322069 -2.956019 0.1708445 4 24 s 41 s 42 s 43 s
atom 37 - Si SI - 0 3.283312 2.418054 -1.461649 4 7 s 38 s 39 s 40 s
atom 38 - C CT - 0 5.124543 2.673048 -1.785929 4 37 s 44 s 45 s 46 s
atom 39 - C CT - 0 2.353526 3.985262 -1.958813 4 37 s 47 s 48 s 49 s
atom 40 - H HC - 0 3.094374 2.159495 -0.06935631 1 37 s
atom 41 - C CT - 0 2.63703 -2.920422 1.524525 4 36 s 50 s 51 s 55 s
atom 42 - H HC - 0 1.932104 -3.300664 -1.069993 1 36 s
atom 43 - C CT - 0 0.01645835 -4.251327 0.5971384 4 36 s 52 s 53 s 54 s
atom 44 - H HC - 0 5.671252 1.776842 -1.492843 1 38 s
atom 45 - H HC - 0 5.282987 2.865287 -2.84707 1 38 s
atom 46 - H HC - 0 5.48147 3.523369 -1.204854 1 38 s
atom 47 - H HC - 0 1.290174 3.864814 -1.757566 1 39 s
atom 48 - H HC - 0 2.736552 4.830086 -1.386771 1 39 s
atom 49 - H HC - 0 2.501702 4.172587 -3.022188 1 39 s
atom 50 - H HC - 0 3.398675 -2.182765 1.271792 1 41 s
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atom 51 - H HC - 0 3.098567 -3.904212 1.609485 1 41 s
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atom 53 - H HC - 0 0.4935466 -5.224504 0.7118264 1 43 s
atom 54 - H HC - 0 -0.7205292 -4.301185 -0.2044304 1 43 s
atom 55 - H HC - 0 2.173021 -2.65249 2.473735 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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