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TINKER .key file to run dileucine
or met enk simulations
with the oplsmixed.prm force field.
E. Lyman 2006

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Force Field Selection

PARAMETERS /home/zuckerman/elyman/bin/TINKER/params/oplsmixed10.prm

extra params for mixed force filed

Bond 1 217 268.0 1.5290
Bond 23 217 337.0 1.4490
Bond 1 218 268.0 1.5290
Bond 23 218 337.0 1.4490
Bond 218 21 317.0 1.5220
Bond 23 249 337.0 1.4490

Angle 21 23 217 50.00 121.90
Angle 217 23 24 38.00 118.40
Angle 1 1 217 58.35 112.70
Angle 217 1 217 58.35 112.70
Angle 217 1 2 37.50 110.70
Angle 23 216 219 80.000 109.700
Angle 1 1 218 58.35 112.70
Angle 218 1 2 37.50 110.70
Angle 1 218 217 58.35 112.70
Angle 21 23 218 50.00 121.90
Angle 218 23 24 38.00 118.40
Angle 23 218 21 63.00 110.10
Angle 23 218 219 80.000 109.700
Angle 21 218 219 63.00 111.10
Angle 218 21 22 80.00 120.40
Angle 218 21 23 70.00 116.60
Angle 218 219 218 58.35 112.70
Angle 21 23 249 50.00 121.90
Angle 249 23 24 38.00 118.40

Torsion 1 21 23 217 2.300 0.0 1 6.089 180.0 2
 Torsion 22 21 23 217 6.089 180.0 2
 Torsion 1 1 1 217 1.300 0.0 1 -0.050 180.0 2 0.200 0.0 3
 Torsion 2 1 1 217 0.300 0.0 3
 Torsion 21 23 216 219 0.462 180.0 2
 Torsion 214 23 216 219
 Torsion 23 216 219 218 0.845 0.0 1 -0.962 180.0 2 0.713 0.0 3
 Torsion 23 1 1 218 0.845 0.0 1 -0.962 180.0 2 0.713 0.0 3
 Torsion 21 1 1 218 -1.697 0.0 1 -0.456 180.0 2 0.585 0.0
 Torsion 2 1 1 218 0.300 0.0 3
 Torsion 1 21 23 218 6.089 180.0 2
 Torsion 22 21 23 218 6.089 180.0 2
 Torsion 1 1 218 217 1.300 0.0 1 -0.050 180.0 2 0.200 0.0 3
 Torsion 2 1 218 217 0.300 0.0 3
 Torsion 21 23 218 21 -2.365 0.0 1 0.912 180.0 2 -0.850 0.0 3
 Torsion 21 23 218 219 0.462 180.0 2
 Torsion 24 23 218 21
 Torsion 24 23 218 219
 Torsion 23 218 21 22
 Torsion 23 218 21 23 1.816 0.0 1 1.222 180.0 2 1.581 0.0 3
 Torsion 219 218 21 22
 Torsion 219 218 21 23 1.173 0.0 1 0.189 180.0 2 -1.200 0.0 3
 Torsion 23 218 219 218 0.845 0.0 1 -0.962 180.0 2 0.713 0.0 3
 Torsion 21 218 219 218 -1.697 0.0 1 -0.456 180.0 2 0.585 0.0 3
 Torsion 218 21 23 249 2.300 0.0 1 6.089 180.0 2
 Torsion 218 21 23 24 4.900 180.0 2
 Torsion 22 21 23 249 4.900 180.0 2
 Torsion 218 219 218 217 1.300 0.0 1 -0.050 180.0 2 0.200 0.0 3
 Torsion 1 21 23 249 2.300 0.0 1 6.089 180.0 2

INTEGRATE stochastic
 SOLVATE gbsa
 FRICTION 5.0
 ARCHIVE

