

E_{rb_dih} (kJ/mol/K)

1 ps

1.66

1.00

0 1000 2000 3000 4000 5000

simulation time (ps)

10 ps

0 1000 2000 3000 4000 5000

simulation time (ps)

100 ps

0 1000 2000 3000 4000 5000

simulation time (ps)

