

E_{angle} (kJ/mol/K)

1 ps

10 ps

100 ps

0.36

0.29

0

1000

2000

3000

4000

5000

simulation time (ps)

0

1000

2000

3000

4000

5000

simulation time (ps)

0

1000

2000

3000

4000

5000

simulation time (ps)