A

RMSD
C-alpha after lsq fit to Protein

RMSD (nm)

0.0
0.1
0.2

0
2
4
6
8
10

Time (ns)

B

GROMACS Energies

(K), (bar)

400
200
0
−200
−400

Temperature
Pressure

0
2000
4000
6000
8000
10000

Time (ps)