Total non-bonded energies (Elec+VdW) av01 -4200 **-**-4400 **-**-4400 --4600 -5000 **-**-5000 **-**500 1500 1000 2000 1000 1500 2000 sw06 -4250 **-**Energy (kcal/mol) -4500 · -5000 -5000 **-**-5250 · 1000 500 1000 500 1500 1500 2000 sw22 sw25 -4250 **-**-4500 **-**-4750 · -5000 --5000 –5250 **-**-5250 · 1000 500 1500 2000 500 1000 1500 2000

TIME (x5000fs)