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#!/bin/bash
mpirun -np 12 $AMBERHOME/bin/sander.MPI -O -i min.in -o min.out -p
complex_sol.prmtop -c complex_sol.inpcrd -r min.rst -ref
complex_sol.inpcrd
mpirun -np 12 $AMBERHOME/bin/sander.MPI -O -i min2.in -o min2.out -p
complex_sol.prmtop -c min.rst -r min2.rst -ref min.rst

/usr/local/amber16/bin/pmemd.cuda -O -i heat.in -o heat.out -p
complex_sol.prmtop -c min2.rst -r heat.rst -x heat.mdcrd -ref min2.rst
/usr/local/amber16/bin/pmemd.cuda -O -i density.in -o density.out -p
complex_sol.prmtop -c heat.rst -r density.rst -x density.mdcrd -ref
heat.rst
/usr/local/amber16/bin/pmemd.cuda -O -i equil.in -o equil.out -p
complex_sol.prmtop -c density.rst -r equil.rst -x equil.mdcrd

/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod1.out -p
complex_sol.prmtop -c equil.rst -r prod1.rst -x prod1.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod2.out -p
complex_sol.prmtop -c prod1.rst -r prod2.rst -x prod2.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod3.out -p
complex_sol.prmtop -c prod2.rst -r prod3.rst -x prod3.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod4.out -p
complex_sol.prmtop -c prod3.rst -r prod4.rst -x prod4.mdcrd

/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod5.out -p
complex_sol.prmtop -c prod4.rst -r prod5.rst -x prod5.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod6.out -p
complex_sol.prmtop -c prod5.rst -r prod6.rst -x prod6.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod7.out -p
complex_sol.prmtop -c prod6.rst -r prod7.rst -x prod7.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod8.out -p
complex_sol.prmtop -c prod7.rst -r prod8.rst -x prod8.mdcrd

/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod9.out -p
complex_sol.prmtop -c prod8.rst -r prod9.rst -x prod9.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod10.out -p
complex_sol.prmtop -c prod9.rst -r prod10.rst -x prod10.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod11.out -p
complex_sol.prmtop -c prod10.rst -r prod11.rst -x prod11.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod12.out -p
complex_sol.prmtop -c prod11.rst -r prod12.rst -x prod12.mdcrd

/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod13.out -p
complex_sol.prmtop -c prod12.rst -r prod13.rst -x prod13.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod14.out -p
complex_sol.prmtop -c prod13.rst -r prod14.rst -x prod14.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod15.out -p
complex_sol.prmtop -c prod14.rst -r prod15.rst -x prod15.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod16.out -p
complex_sol.prmtop -c prod15.rst -r prod16.rst -x prod16.mdcrd

/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod17.out -p
complex_sol.prmtop -c prod16.rst -r prod17.rst -x prod17.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod18.out -p
complex_sol.prmtop -c prod17.rst -r prod18.rst -x prod18.mdcrd
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod19.out -p

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complex_sol.prmtop -c prod18.rst -r prod19.rst -x prod19.mdcrd  
/usr/local/amber16/bin/pmemd.cuda -O -i prod.in -o prod20.out -p  
complex_sol.prmtop -c prod19.rst -r prod20.rst -x prod20.mdcrd
```