

The following input files were used for 2L7X and are reported here as an example of the protocol used to run the MD simulations for all systems.

NONBONDED SIMULATIONS input files

min.in

Minimization with Cartesian restraints for the solute

```
&cntrl  
imin=1, maxcyc=200,  
ntpr=5,  
ntr=1,restraint_wt=10,restraintmask='1-77'  
/  

```

min2.in

Minimization with Cartesian

```
&cntrl  
imin=1, maxcyc=500,  
ntpr=5,  
ntr=0  
/  

```

heat1.in

Heating up the system equilibration stage 1

```
&cntrl  
nstlim=50000, dt=0.002, ntx=1, irest=0, ntpr=500, ntwr=5000, ntwx=50,  
temp1=100.0, temp0=300.0, ntt=1, tautp=2.0, ig=-1,  
  
ntb=1, ntp=0,  
  
ntc=2, ntf=2,  
  
nrespa=2,  
&end
```

heat2.in

Constant pressure constant temperature equilibration stage 2

```
&cntrl  
nstlim=5000, dt=0.002, ntx=5, irest=1, ntpr=500, ntwr=5000, ntwx=5000,  
temp0=300.0, ntt=1, tautp=2.0,  
  
ntb=2, ntp=1,  
  
ntc=2, ntf=2,
```

```
nrespa=1,  
&end
```

dina.in

Constant pressure constant temperature production run

```
&cntrl
```

```
nstlim=50000000, dt=0.002, ntx=5, irest=1, ntp=500, ntwr=5000, ntwx=5000,  
temp0=300.0, ntt=1, tautp=2.0,
```

```
ntb=2, ntp=1,
```

```
ntc=2, ntf=2,
```

```
nrespa=1,  
&end
```

dina2.in

Constant pressure constant temperature production run

```
&cntrl
```

```
nstlim=50000000, dt=0.002, ntx=5, irest=1, ntp=5000, ntwr=5000, ntwx=5000,  
temp0=300.0, ntt=1, tautp=2.0,
```

```
ntb=2, ntp=1,
```

```
ntc=2, ntf=2,
```

```
nrespa=1,  
&end
```

dina3.in

Constant pressure constant temperature production run

```
&cntrl
```

```
nstlim=50000000, dt=0.002, ntx=5, irest=1, ntp=5000, ntwr=5000, ntwx=5000,  
temp0=300.0, ntt=1, tautp=2.0,
```

```
ntb=2, ntp=1,
```

```
ntc=2, ntf=2,
```

```
nrespa=1,  
&end
```

dina4.in

Constant pressure constant temperature production run

```
&cntrl  
nstim=50000000, dt=0.002, ntx=5, irest=1, ntp=5000, ntwr=5000, ntwx=5000,  
temp0=300.0, ntt=1, tautp=2.0,
```

```
ntb=2, ntp=1,
```

```
ntc=2, ntf=2,
```

```
nrespa=1,  
&end
```

dina5.in

Constant pressure constant temperature production run

```
&cntrl  
nstim=50000000, dt=0.002, ntx=5, irest=1, ntp=5000, ntwr=5000, ntwx=5000,  
temp0=300.0, ntt=1, tautp=2.0,
```

```
ntb=2, ntp=1,
```

```
ntc=2, ntf=2,
```

```
nrespa=1,  
&end
```

BONDED SIMULATIONS input files

min.in

```
&cntrl  
imin=1, maxcyc=200,  
ntpr=5,  
ntr=1, restraint_wt=10, restraintmask=':1-77'  
/
```

min2.in

Minimization with Cartesian

```
&cntrl  
imin=1, maxcyc=500,  
ntpr=5,  
ntr=0  
/
```

heat1.in

Heating up the system equilibration stage 1

```
&cntrl  
nstlim=50000, dt=0.002, ntx=1, irest=0, ntpr=500, ntwr=5000, ntwx=50,  
temp0=100.0, temp0=300.0, ntt=1, tautp=2.0, ig=-1,  
  
ntb=1, ntp=0,  
  
ntc=2, ntf=2,  
  
nrespa=2,  
&end
```

heat2.in

Constant pressure constant temperature equilibration stage 2

```
&cntrl  
nstlim=5000, dt=0.002, ntx=5, irest=1, ntpr=500, ntwr=5000, ntwx=5000,  
temp0=300.0, ntt=1, tautp=2.0,  
  
ntb=2, ntp=1,  
  
ntc=2, ntf=2,  
  
nrespa=1,  
&end
```

dina.in

Constant pressure constant temperature production run

```
&cntrl  
nstlim=50000000, dt=0.002, ntx=5, irest=1, ntpr=500, ntwr=50000, ntwx=5000,  
temp0=300.0, ntt=1, tautp=2.0,  
  
ntb=2, ntp=1,  
  
ntc=2, ntf=2,
```

```
nrespa=1,  
&end
```

dina2.in

Constant pressure constant temperature production run

```
&cntrl
```

```
nstlim=50000000, dt=0.002, ntx=5, irest=1, ntp=500, ntwr=50000, ntwx=5000,  
temp0=300.0, ntt=1, tautp=2.0,
```

```
ntb=2, ntp=1,
```

```
ntc=2, ntf=2,
```

```
nrespa=1,  
&end
```

dina3.in

Constant pressure constant temperature production run

```
&cntrl
```

```
nstlim=50000000, dt=0.002, ntx=5, irest=1, ntp=500, ntwr=50000, ntwx=5000,  
temp0=300.0, ntt=1, tautp=2.0,
```

```
ntb=2, ntp=1,
```

```
ntc=2, ntf=2,
```

```
nrespa=1,  
&end
```

dina4.in

Constant pressure constant temperature production run

```
&cntrl
```

```
nstlim=50000000, dt=0.002, ntx=5, irest=1, ntp=500, ntwr=50000, ntwx=5000,  
temp0=300.0, ntt=1, tautp=2.0,
```

```
ntb=2, ntp=1,
```

```
ntc=2, ntf=2,
```

```
nrespa=1,  
&end
```

dina5.in

Constant pressure constant temperature production run

&cntrl

nstlim=50000000, dt=0.002, ntx=5, irest=1, ntpr=500, ntwr=50000, ntwx=5000,
temp0=300.0, ntt=1, tautp=2.0,

ntb=2, ntp=1,

ntc=2, ntf=2,

nrespa=1,

&end