```
# NAMD configuration file

##############################################

set nCARBONS         ;# 6,8,10,12,14
set nQUARTERS        ;# 0,1,2,3,4
set TIME         ;# total time at end of this simulation (ie: 12)

set MOLECULE        tsb35-c${nCARBONS}
set GUEST
set LATTICE         ${MOLECULE}_0${nQUARTERS}-quarter_with-${GUEST}

set temperature      ;# in Kelvin

set minSteps         ;# minimize of previous simulation (ie: 20000)
set previousRunSteps     ;# numsteps of previous simulation (ie: 6000000)

set RESTARTTIME      ;# total time of previous simulation (ie: 06)
set RESTARTTEMP     $temperature

set runSteps         ;# numsteps for this simulation (ie: 6000000)

##############################################

timestep        1.0
firsttimestep       [expr $previousRunSteps+$minSteps]
stepspercycle       4

cutoff          10.0
switching       on
switchdist      8.0
pairlistdist        12.0
margin          1.0

coordinates         ../../${LATTICE}_simPDB.pdb
structure       ../../${LATTICE}_simPSF.psf
parameters      ../../../CHARMM-parameters/${MOLECULE}_charmm.params
paraTypeCharmm      on

wrapAll         on
wrapNearest     on

exclude         scaled1-4
1-4scaling      0.4

#temperature        $temperature
rescaleFreq     10
rescaleTemp         $temperature

CoMmotion       yes
rigidBonds      all

fixedAtoms      on
```

```
fixedAtomsFile      ../../${LATTICE}_fixedPDB.pdb
fixedAtomsCol       B

outputname      ${LATTICE}_${temperature}K_${TIME}ns_OUTPUT
binaryoutput        no
outputEnergies      1000

restartname         ${LATTICE}_${temperature}K_${TIME}ns_RESTART
restartfreq     5000

DCDfile         ${LATTICE}_${temperature}K_${TIME}ns_DCD.dcd
DCDfreq         1000

if {1} {
set inputname       ../${RESTARTTIME}ns/${LATTICE}_${RESTARTTEMP}K_${RESTARTTIME}ns_RESTART
binCoordinates      ${inputname}.coor
extendedSystem      ${inputname}.xsc
binVelocities       ${inputname}.vel    ;# DO NOT USE temperature OR reinitvels WITH THIS
}

run         $runSteps
```