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package require psfgen

set nCARBON [lindex $argv 0]
set nQUARTERS [lindex $argv 1]
set GUEST [lindex $argv 2]
set GUESTSEGNAME [lindex $argv 3]

set QUARTERS 0${nQUARTERS}-quarter
set TSBDIR ../../02_cpp-writer/${QUARTERS}/tsb35-c${nCARBON}_${QUARTERS}_TSB
set GUESTDIR ../../02_cpp-writer/${QUARTERS}/tsb35-c${nCARBON}_${QUARTERS}_${GUESTSEGNAME}
set GRAPDIR ../../02_cpp-writer/${QUARTERS}/tsb35-c${nCARBON}_${QUARTERS}_LAY

topology ../../02_cpp-writer/${QUARTERS}/tsb35-c${nCARBON}_${QUARTERS}_with-${GUEST}_TOP.top

pdb ${TSBDIR}A-PDB.pdb
segment TSBA {pdb ${TSBDIR}A-PDB.pdb}
coordpdb ${TSBDIR}A-PDB.pdb TSBA

pdb ${TSBDIR}B-PDB.pdb
segment TSBB {pdb ${TSBDIR}B-PDB.pdb}
coordpdb ${TSBDIR}B-PDB.pdb TSBB

pdb ${GUESTDIR}-PDB.pdb
segment ${GUESTSEGNAME} {pdb ${GUESTDIR}-PDB.pdb}
coordpdb ${GUESTDIR}-PDB.pdb ${GUESTSEGNAME}

pdb ${GRAPDIR}1-PDB.pdb
segment LAY1 {pdb ${GRAPDIR}1-PDB.pdb}
coordpdb ${GRAPDIR}1-PDB.pdb LAY1

pdb ${GRAPDIR}2-PDB.pdb
segment LAY2 {pdb ${GRAPDIR}2-PDB.pdb}
coordpdb ${GRAPDIR}2-PDB.pdb LAY2

pdb ${GRAPDIR}3-PDB.pdb
segment LAY3 {pdb ${GRAPDIR}3-PDB.pdb}
coordpdb ${GRAPDIR}3-PDB.pdb LAY3

pdb ${GRAPDIR}4-PDB.pdb
segment LAY4 {pdb ${GRAPDIR}4-PDB.pdb}
coordpdb ${GRAPDIR}4-PDB.pdb LAY4

pdb ${GRAPDIR}5-PDB.pdb
segment LAY5 {pdb ${GRAPDIR}5-PDB.pdb}
coordpdb ${GRAPDIR}5-PDB.pdb LAY5

pdb ${GRAPDIR}6-PDB.pdb
segment LAY6 {pdb ${GRAPDIR}6-PDB.pdb}
coordpdb ${GRAPDIR}6-PDB.pdb LAY6

writepdb ../../04_NAMD/${QUARTERS}/tsb35-c${nCARBON}_${QUARTERS}_with-${GUEST}_simPDB.pdb
writepsf ../../04_NAMD/${QUARTERS}/tsb35-c${nCARBON}_${QUARTERS}_with-${GUEST}_simPSF.psf

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writpdb tsb35-c${nCARBON}_${QUARTERS}_with-${GUEST}_simPDB.pdb
writepsf tsb35-c${nCARBON}_${QUARTERS}_with-${GUEST}_simPSF.psf

#####
# Generate fixedAtoms file
#####

mol load pdb tsb35-c${nCARBON}_${QUARTERS}_with-${GUEST}_simPDB.pdb
mol addfile tsb35-c${nCARBON}_${QUARTERS}_with-${GUEST}_simPSF.psf

set all [atomselect top all]

set overlayer [atomselect top "segname TSBA TSBB ${GUESTSEGNAME}"]
set graphite [atomselect top "segname LAY1 LAY2 LAY3 LAY4 LAY5 LAY6"]

$all set beta 0
$graphite set beta 1

$all writpdb tsb35-c${nCARBON}_${QUARTERS}_with-${GUEST}_fixedPDB.pdb
$all writpdb ../../04_NAMD/${QUARTERS}/tsb35-c${nCARBON}_${QUARTERS}_with-${GUEST}_fixedPDB.pdb

#mol delete all
#exit
```