Useful commands VMD (TkConsole)

1) Make a selection of atoms: it can be done with any selection criteria of VMD such as atom type, name, residue, distances,... For example:

set seleccio [atomselect top "protein"]
set seleccio [atomselect top "all and not x*x+y*y<36"]

2) Obtain **information** from atom selection

Number of atoms in a selection:
$seleccio num

Maximum and minimum values of coordinates from a selection
measure minmax $seleccio

Calculate charge from a selection
eval vecadd [$seleccio get charge]

Center of coordinates from a selection
measure center $sel weight mass

Save coordinates of a selection in a pdb
$seleccio writepdb myselection.pdb

Save structure/topology of a selection in psf format
$seleccio writepsf lamevaseleccio.psf

3) **Modify** a selection of atoms

Change atom properties (such as charge, mass,...)
$seleccio set charge 0.060 #changes the charge of seleccio

Move selected atoms (for example move -6.0 in z coordinate)
$seleccio moveby {0 0 -6.0}

Move selected atoms in a way that the geometric center will be in 0,0,0
set com [measure center $seleccio]
$seleccio moveby [vecscale -1.0 $com]

rotate respect to axis not passing from the CM of the molecule (for example a protein)
set com [measure center $seleccio weight mass]
set matrix [transaxis z 45]
$seleccio moveby [vecscale -1.0 $com]
$seleccio move $matrix
$seleccio moveby $com

Define periodic boundary conditions: one component of (a b c) or the full vector:
molinfo top set a 17.194
pbc set {17.194 17.018 40} -all -molid top

-NOTE: To save memory, when finishing with a selection use: $seleccio delete