**Input Data for**: **fdMD\_OneTraj.cmd**

The User MUST modify the **fdMD\_OneTraj.cmd file :**

@ num\_res\_prot = 387 # Number of the protein

@ num\_lig = 26 # Number of Ligands in the simulation

# The program will superpose ALL the snapshots of the MD to the FIRST snapshot using the Alpha

# Carbons ( CA ) of the Protein and the residues [ini\_res\_sup , ifi\_res\_sup ]

@ ini\_res\_sup = 51 # Initial protein residue to superpose

@ ifi\_res\_sup = 82 # Final protein residue to superpose

# The USER can use a X-Ray structure as reference to superpose the full trajectory.

# However, this X-Ray file MUST contain ONLY the protein and the ligand

# ( No wat,Na+,Cl- …) and MUST be well prepared (like the MD system).

set xray = 'no'

if ( $xray == 'yes' ) then

set ref\_pdb = "Name\_Of\_XRay\_PDB.pdb"

endif

set dir\_traj = .

set top\_name = 2ohk\_Sol\_vdw2301\_ZeroB.top

set top\_file = $dir\_traj/$top\_name

set prefix\_traj = 2ohk

@ ini\_traj = 1