Trajectory Visualization with VMD

/home/nct00/nct00002/GromacsUbiquitin/* (or your traj.!)

Trajectory (Dry, 1000 snapshots):

→*.**imaged.rot.10.xtc**

Topology needed!! → **1_*.dry.pdb**

cp 1_*.pdb 1_*.dry.pdb
vim/edit 1_*.dry.pdb
→ Remove everything after the protein (SOL, Cl-, Na+)

VMD: 1_*.pdb (VM)

VMD: dry.pdb + xtc (Load Data into Molecule)

Trajectory Analysis with Gromacs

http://manual.gromacs.org/programs/byname.html

g_*NAME*_mpi

- Convert trajectory from xtc to trr:

*/apps/GROMACS/4.6.4/bin/**trjconv_mpi** –f *.rot.10.xtc –o *.rot.10.trr*

- Compute RMSd (*out rmsd.xvg*):

*/apps/GROMACS/4.6.4/bin/**g_rms_mpi** –f *.rot.10.xtc –s *.tpr*

- Compute RMSf (*out rmsf.xvg*):

*/apps/GROMACS/4.6.4/bin/**g_rmsf_mpi** –f *.rot.10.xtc –s *.tpr*

- Compute Clusters of structures (*out rmsd-clust.xpm / cluster.log*):

*/apps/GROMACS/4.6.4/bin/**g_cluster_mpi** –f *.rot.10.xtc –s *.tpr*

Trajectory Analysis with AmberTools

http://ambermd.org/tutorials/analysis/ *(Virtual Machine)*

- Load trajectory with cpptraj:

*cpptraj *.dry.pdb*

*trajin *.trr*

***rmsd** @N,C,CA,CO out ubiq.rmsd.dat*

go

atomicfluct !@H* out ubiq.rmsf.dat

distance :74@CZ :40@CD out ubiq.loop.dist.dat (ARG_CZ – GLN_CD)
analyze statistics all

Type *help*!!