Commands for DNA-Protein MD Simulations

Step One: Prepare the Protein Topology

gmx pdb2gmx -f mol10.pdb -o mol10_processed.gro -water spce -ignh
Select AMBER forcefield
Mol10: Name of the complex

Step Two: Prepare the Ligand Topology

gmx editconf -f mol10_processed.gro -o mol10_newbox.gro -c -d 1.0 -bt cubic

Step Three: Defining the Unit Cell & Adding Solvent

gmx solvate -cp mol10_newbox.gro -cs spc216.gro -o mol10_solv.gro -p topol.top

Step Four: Adding Ions

gmx grompp -f ions.mdp -c mol10_solv.gro -p topol.top -o ions.tpr
gmx genion -s ions.tpr -o mol10_solv_ions.gro -p topol.top -pname NA -nname CL -neutral
select 17 for 'sol'

Step Five: Energy Minimization

gmx grompp -f minim.mdp -c mol10_solv_ions.gro -p topol.top -o em.tpr

Step Six: Equilibration

gmx mdrun -v -deffnm em
gmx energy -f em.edr -o potential.xvg
selected 10
gmx grompp -f nvt.mdp -c em.gro -r em.gro -p topol.top -o nvt.tpr
gmx mdrun -v -deffnm nvt
gmx energy -f nvt.edr -o temperature.xvg

Step Seven: Equilibration, Part 2

gmx grompp -f npt.mdp -c nvt.gro -r nvt.gro -t nvt.cpt -p topol.top -o npt.tpr
gmx energy -f npt.edr -o pressure.xvg
gmx energy -f npt.edr -o density.xvg

Step 8: <u>Production MD</u>

gmx grompp -f md.mdp -c npt.gro -r npt.gro -t npt.cpt -p topol.top -o md_0_1.tpr
gmx mdrun -v -deffnm md_0_1

Step 9: <u>Analysis</u>

gmx mdrun -v -deffnm md_0_1
gmx trjconv -s md_0_1.tpr -f md_0_1.xtc -o md_0_1_noPBC.xtc -pbc mol -ur compact
select 0
*we can use nojump after "-pbc"
OR
gmx trjconv -s md_0_1.tpr -f md_0_1.xtc -o md_0_1_noPBC.xtc -pbc mol -center
select 1 (protein) and 0

A. <u>RMSD calculations</u>

gmx rms -s md_0_1.tpr -f md_0_1_noPBC.xtc -o rmsd.xvg -tu ns
Select Protein and DNA

B. <u>RMSF calculations</u>

gmx rmsf -f md_0_1.trr -s md_0_1.tpr -o rmsf.xvg -res
type 4 (backbone)

C. <u>radius of gyration</u>

gmx gyrate -s md_0_1.tpr -f md_0_1_noPBC.xtc -o gyrate.xvg
type 4 for both

D. <u>Compute and analyze hydrogen bonds</u> (H-bonds)

gmx hbond -f md_0_1.trr -s md_0_1.tpr -num
type 5 (mainchain) 8(sidechain)

E. <u>Compute solvent accessible surface area</u> (SASA)

gmx sasa -f md_0_1.trr -s md_0_1.tpr -o sasa.xvg
Select Protein and DNA

Reference:

J.A. Lemkul (2018) "From Proteins to Perturbed Hamiltonians: A Suite of Tutorials for the GROMACS-2018 Molecular Simulation Package, v1.0" *Living J. Comp. Mol. Sci.* 1 (1): 5068.