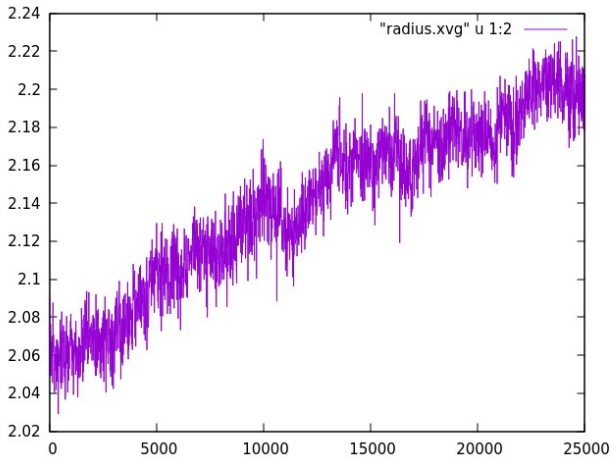
# Weekly Report: June 17 -June 21

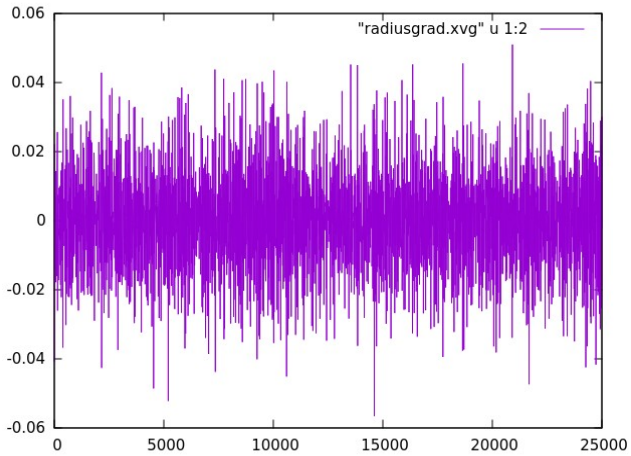
-Vatsa Shah

**1) For 1.8 nm *hexagonal ice* seed in 10x10x10 nm^3 box of water at 230K.**

Radius(nm) Vs Time(ps)

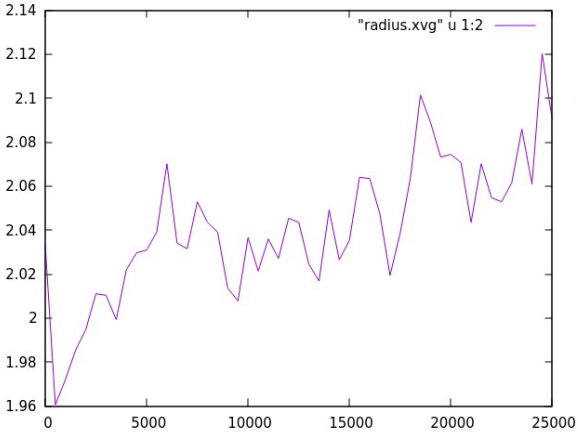



Radius Change(nm) Vs Time (ps)

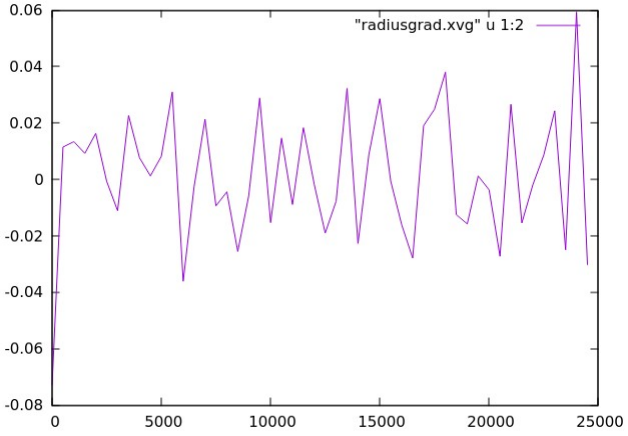



**2) For 1.8 nm *hexagonal ice* seed in 10x10x10 nm^3 box of water at 240K.**

Radius(nm) Vs Time(ps)

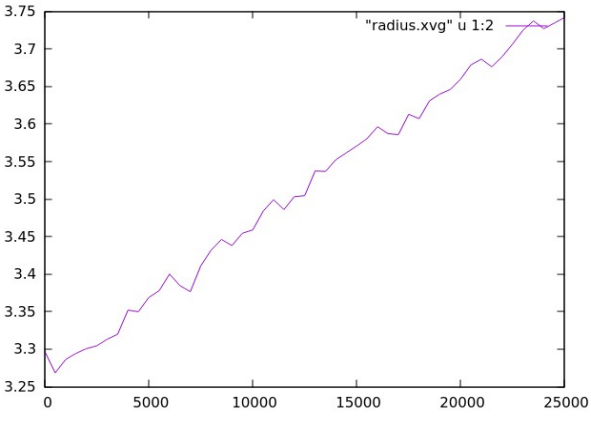



Radius Change(nm) Vs Time(ps)

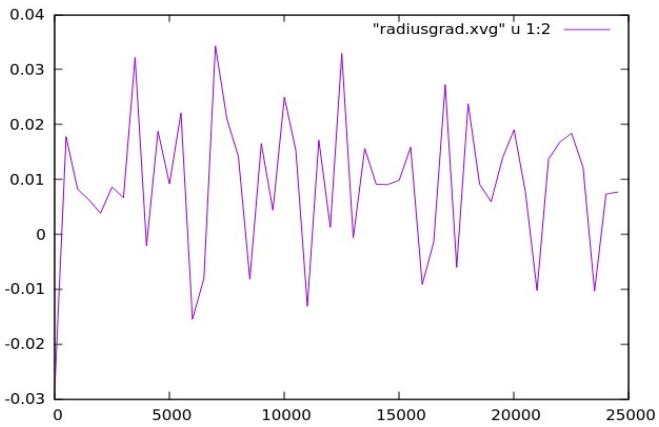



**3) For 3 nm *hexagonal ice* seed in 12x12x12 nm^3 box of water at 240K.**

Radius(nm) Vs Time(ps)

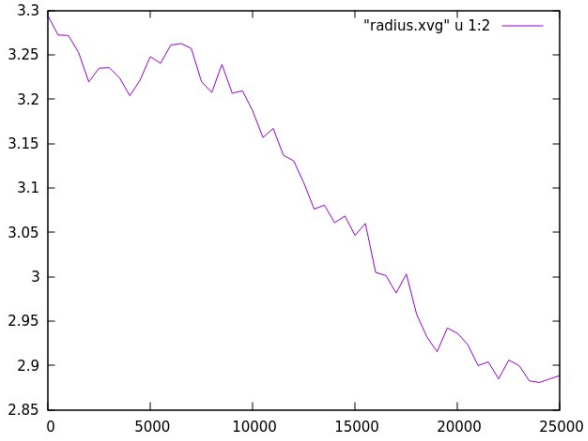



Radius Change(nm) Vs Time(ps)

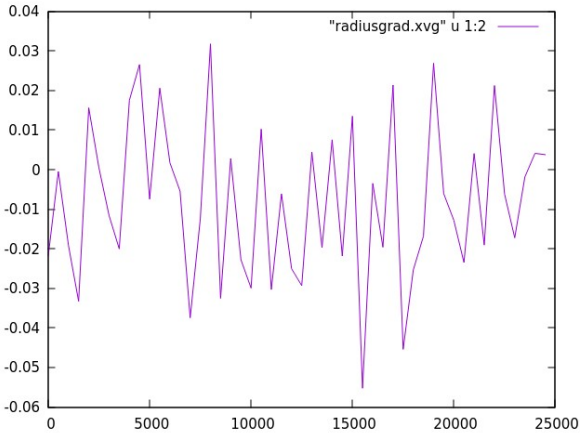


**4) For 3 nm *hexagonal ice* seed in 12x12x12 nm^3 box of water at 255K.**

Radius(nm) Vs Time(ps)

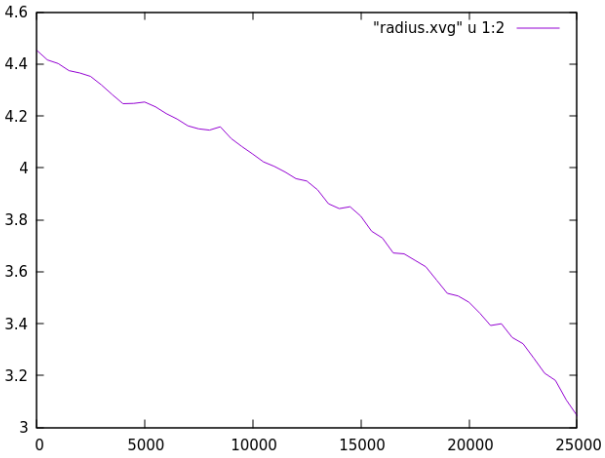



Radius Change(nm) Vs Time(ps)

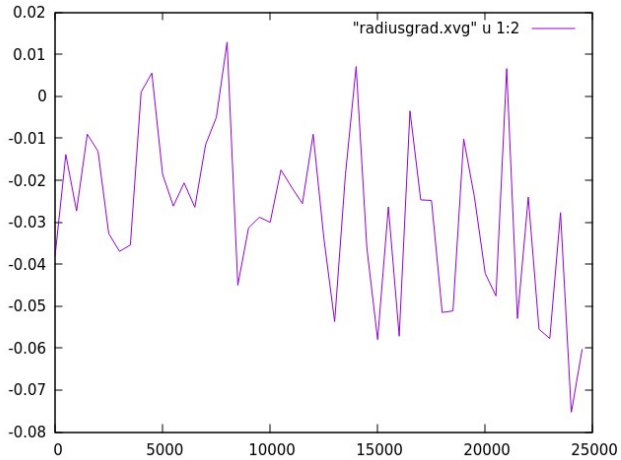



**5) For 4 nm *hexagonal ice* seed in 14x14x14 nm^3 box of water at 260K.**

Radius(nm) Vs Time(ps)

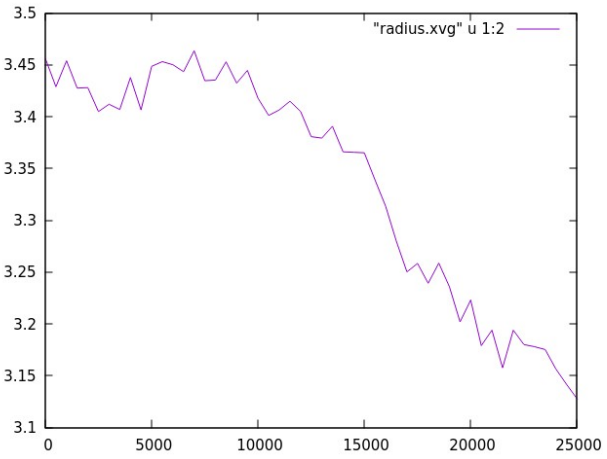



Radius Change(nm) Vs Time(ps)

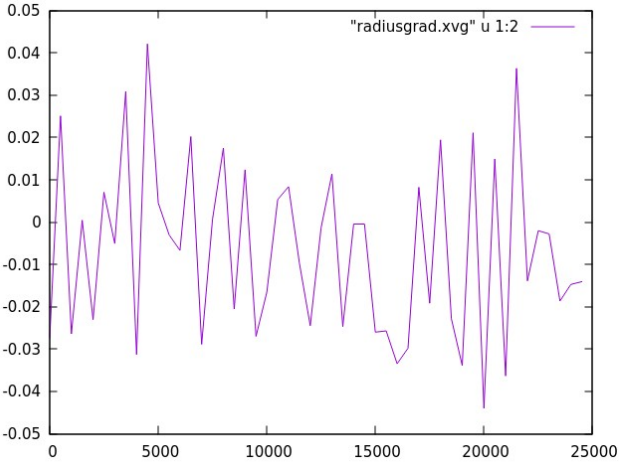



**6) For 3 nm *cubic ice* seed in 12x12x12 nm^3 box of water at 255K.**

Radius(nm) Vs Time(ps)

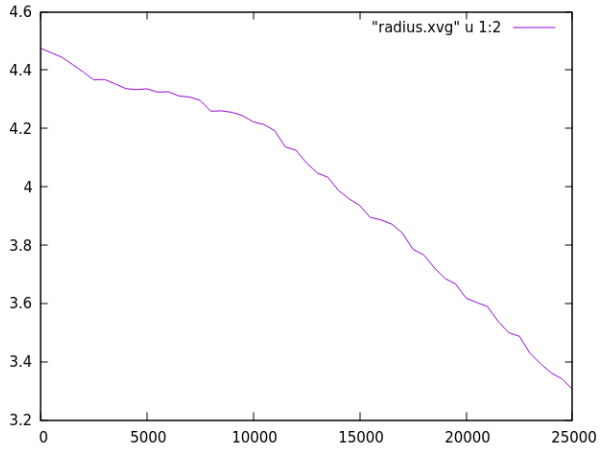



Radius Change(nm) Vs Time(ps)

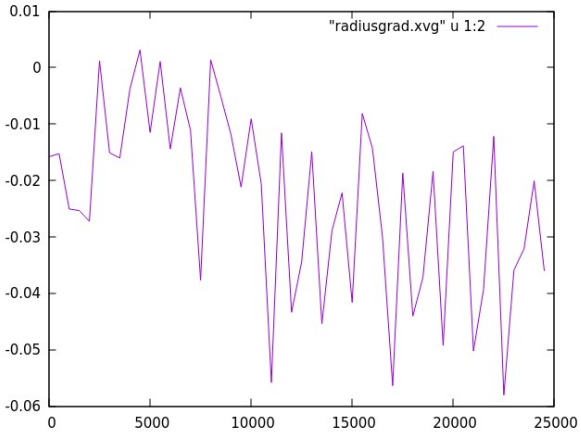


**7) For 4 nm *Cubic ice* seed in 14x14x14 nm^3 box of water at 260K.**

Radius(nm) Vs Time(ps)




Radius Change(nm) Vs Time(ps)




**Performed simulation to get stable Single Stranded TmAFP (Pdb Id code - 1EZG) Protein by energy minimization follwed by npt production run (Performing on chain A of 1EZG)->**

*1) gmx pdb2gmx -f 1ezg.pdb* ( used tip4p water model and amber 99sb-ildn)

*2)* Removed all atoms from B strand of protein and did the changes in topology file by subtracting nos. of B atoms from overall atoms in protein. Also box size can be fixed by changing the x,y and z coordinates of conf.gro file (last line).

*3) gmx solvate -cp conf.gro -cs tip4p -o tmafp_chain_A_solvated.gro -p topol_chain_A.top*
(Added water molecule to the surroundings of protein to fill the box)

*4) gmx grompp -f em.mdp -c tmafp_chain_A_solvated.gro -p topol_chain_A.top -o addion.tpr -maxwarn 2* (adding ions)

*5) gmx genion -s addion.tpr -o tmafp_chain_A_solvated_ionadded.gro -p topol_chain_A.top -pname NA -nname CL -np 2*
(Replacing 2 SOL molecule with 2 NA atoms in order to neutralize the system)

*6)* Performing Energy minimization->

*gmx grompp -f em.mdp -c tmafp_chain_A_solvated_ionadded.gro -p topol_chain_A.top -o em.tpr*
*gmx mdrun -s em.tpr -v -deffnm em -ntmpi 4*

*7)* Performing NPT Equlillibrium step->

*gmx grompp -f npteq-t300.mdp -c em.gro -p topol_chain_A.top -o npt_300_1bar_tmafp_chainA_2na_eq.tpr*

*gmx mdrun -s npt_300_1bar_tmafp_chainA_2na_eq.tpr -v -deffnm npt_300_1bar_tmafp_chainA_2na_eq -ntmpi 4*

*8)* Performing NPT Production run step->

*gmx grompp -f nptprod-t300.mdp -c npt_300_1bar_tmafp_chainA_2na_eq.gro -p topol_chain_A.top -o npt_300_tmafp_chainA_2na_prod.tpr*

*gmx mdrun -s npt_300_tmafp_chainA_2na_prod.tpr -v -deffnm npt_300_tmafp_chainA_2na_prod -ntmpi 4*

**Performed same above simulations on B chain of protein TmAFP.**

**Performed addition of previously prepared box of protein to the slab of ice->**

*1) D*isplaced ice slab by 4nm in downwards direction.

*gmx editconf -f ice.gro -translate 0 0 -4 -o ice.gro*

*2) D*isplaced protein chain by 4.3 nm in upward direction.

*gmx editconf -translate 0 0 4.3 -f npt_300K_1bar_tmafp_eq.gro -o protein.gro*

*3)* Combined the above two files in order to perform further simulations ->

*python ../../hom-seeding/script/combin_grofile.py -i1 protein.gro -i2 ice.gro -d 2 -o protein_on_ice.gro*