Weekly Report: June 2 -June 7

-Vatsa Shah

Visualized *prod_xx_dxdxd_2X0-dt500.gro* in vmd ->

1) *vmd prod_1.8_10x10x10_220.gro prod_1.8_10x10x10_220-dt500.xtc*
2) open *TkConsole* and give following command ->

source q6ave_prod.tcl

3) In representation select “selected atoms” as “user 1” and you will observe cluster of hexagonal ice for different time frames.

Done above visualization ->

For 1.8 nm ice seed (Ih) in 10x10x10 nm^3 box of water, for temperatures 300K to 220K,230K, and 240K,
For 3 nm ice seed (Ih) in 12x12x12 nm^3 box of water, for temperatures 300K to 240K,245K,250K and 255K,
For 4 nm ice seed (Ih) in 14x14x14 nm^3 box of water, for temperatures 300K to 255K and 260K.

Observation ->

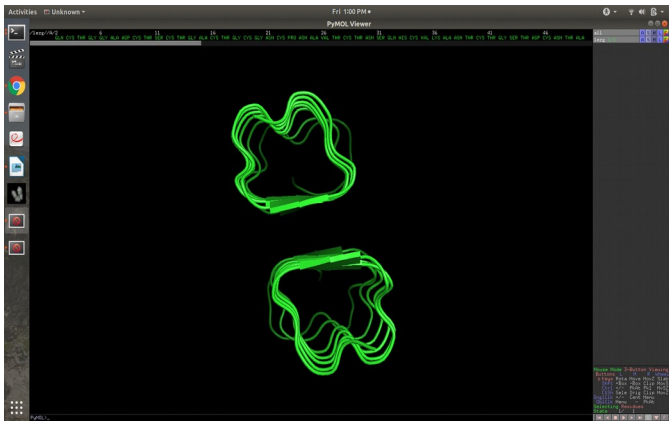
For 1.8 nm ice seed (Ih) in 10x10x10 nm^3 box of water and for temperatures 300K to 220K,230K, and 240K, The ice seed is growing in size.
For 3 nm ice seed (Ih) in 12x12x12 nm^3 box of water, for temperatures 300K to 240K,245K and 250K, the ice seed grows in size.
For 3 nm ice seed (Ih) in 12x12x12 nm^3 box of water, for temperature at 255K, the ice seed dissociates.
For 4 nm ice seed (Ih) in 14x14x14 nm^3 box of water, for temperatures 300K and 255K, the ice seed grows in size.
For 4 nm ice seed (Ih) in 14x14x14 nm^3 box of water, for temperature at 260K, the ice seed dissociates.

Ran simmulations for Cubic ice (Ic) seed for ->

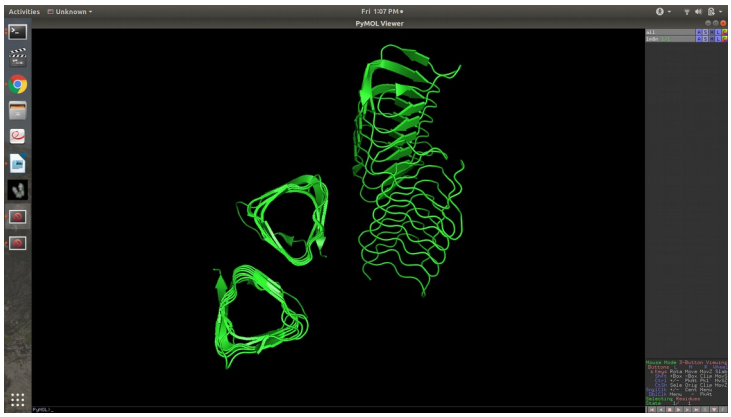
For 3 nm ice seed (Ic) in 12x12x12 nm^3 box of water, for temperature at 255K.
For 4 nm ice seed (Ic) in 14x14x14 nm^3 box of water, for temperature at 260K.

Visualized following Anti-freezing protein’s ice binding sites in PyMol ->

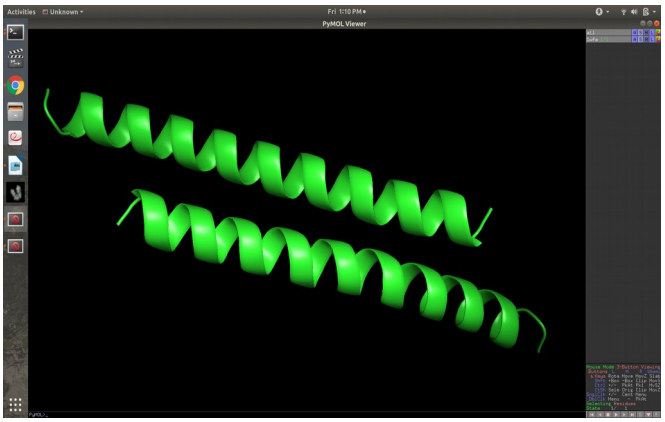
1) 1ezg.pdb
2) 1m8n.pdb
3) 1wfa.pdb
4) 3p4g.pdb



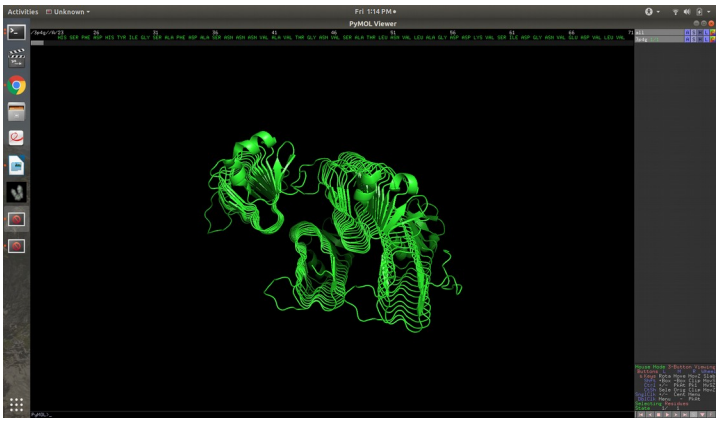
1ezg.pdb



1m8n.pdb



1wfa.pdb



3p4g.pdb