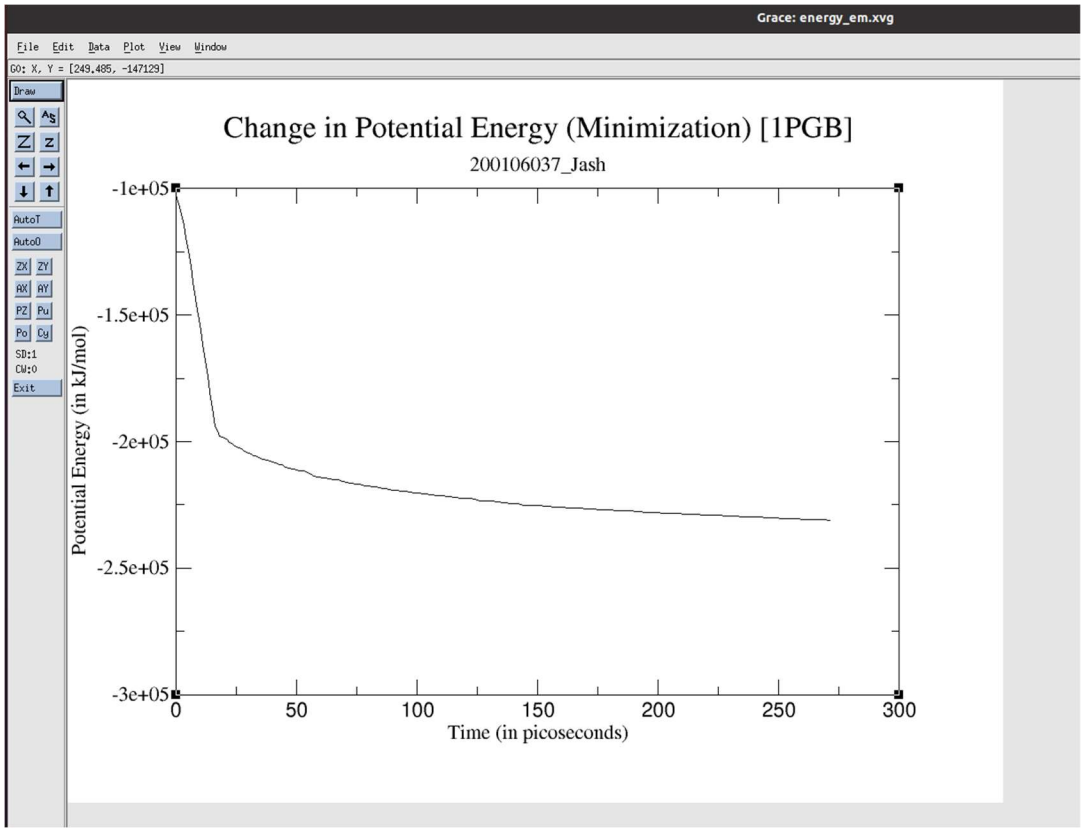
XVG file (Grace Output Image Screenshots)

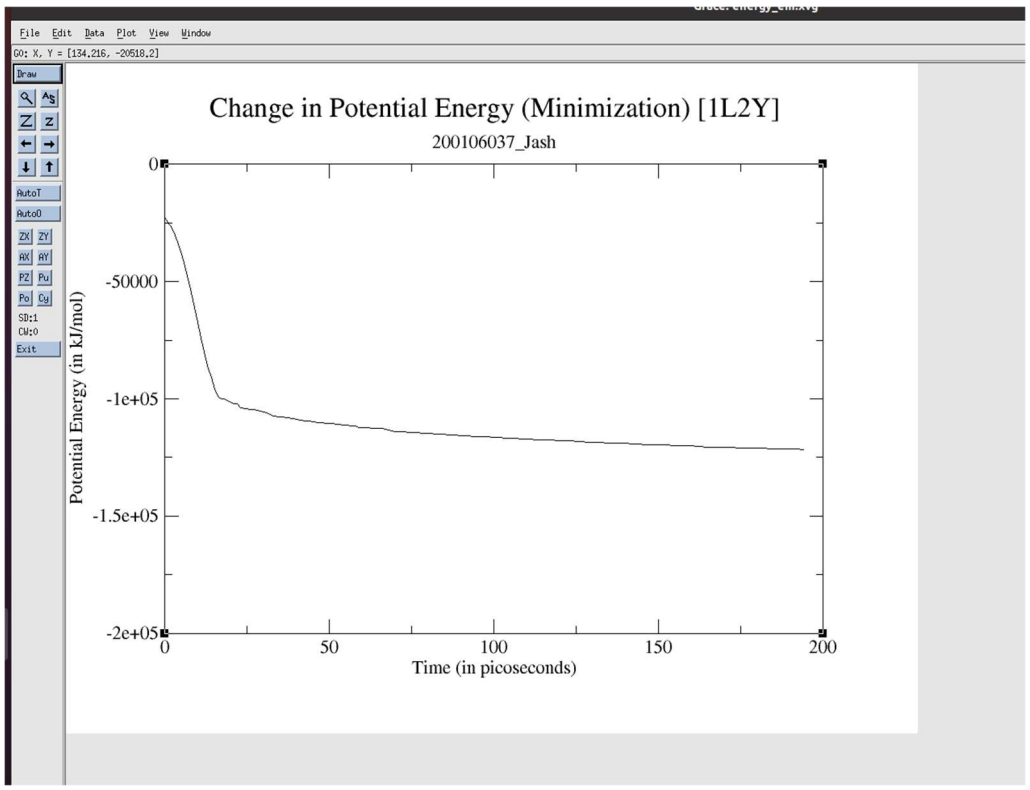
Q2. Energy Minimization –

The information we can infer from this plot is that after our process of energy minimzation the overall potential energy of the Protein is reduced. We observe that after a steep decline, the plot stabalizes after a given point of time. Thus, indicating that the lowest possible energy conformation is obtained. As we know, low potential energy means more stability. Thus, we are making our protein molecule more stable for our MD simulation.

Protein G [1PGB.pdb]



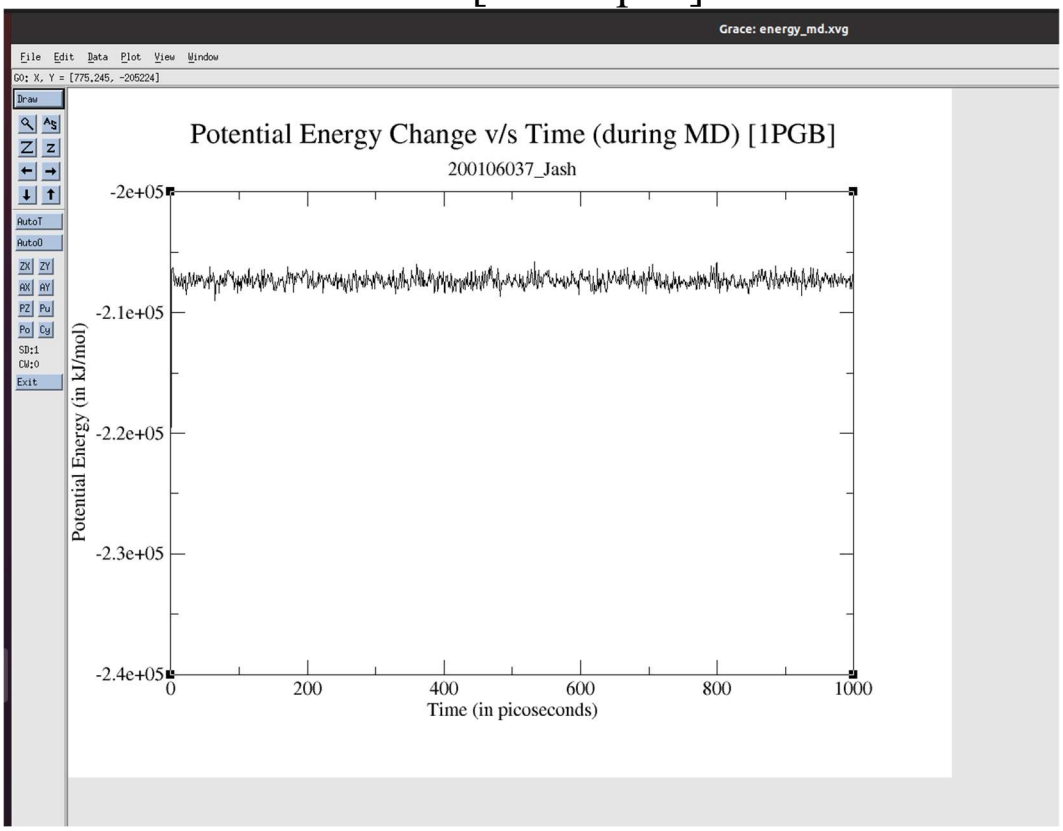
Trp Cage [1L2Y.pdb]



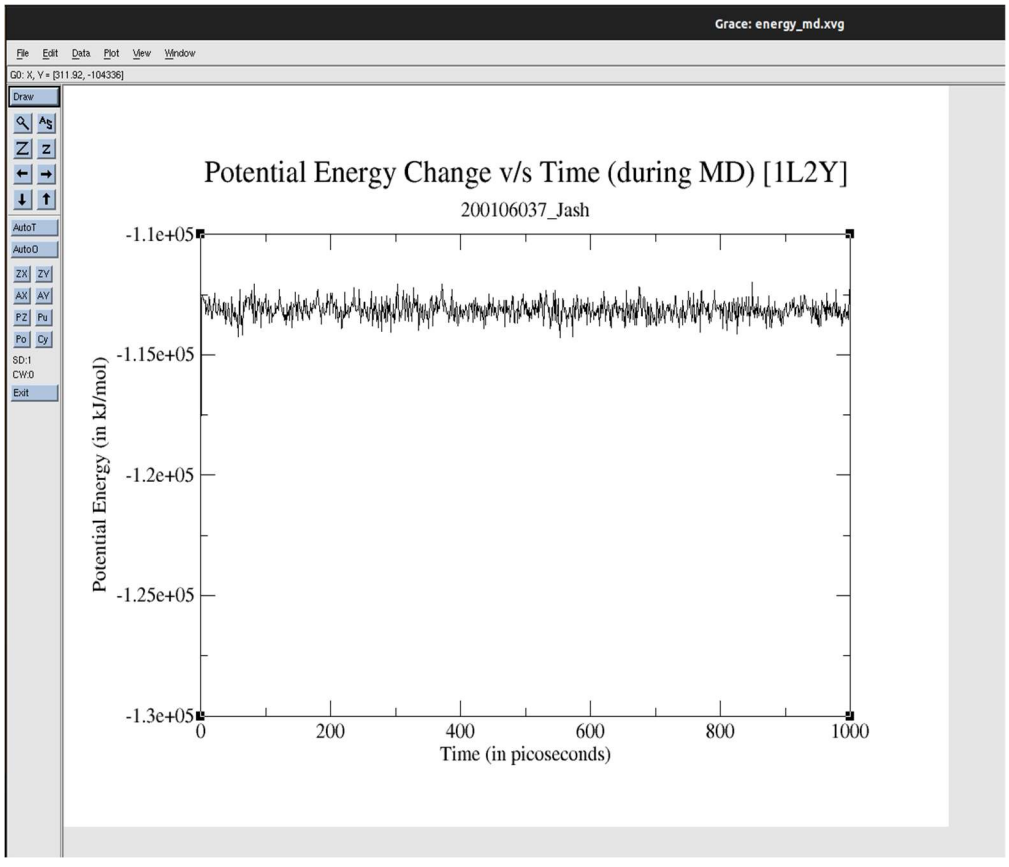
Q4. Potential Energy during MD Simulation –

MD Simulation considers all the conformations of protein structure. So, some conformations may have more potential energy and some may have less potential energy depending upon the stability of the structure. Thus, we get a plot with varying potential energy some peaks are up whereas some are down. We can notice that the range of the energy fluctuations is very limited and the energies are not changing dramatically like we saw in PE change during energy minimization step. The peaks signify the potential energy of that structural conformation of the protein molecule.

Protein G [1PGB.pdb]



Trp Cage [1L2Y.pdb]

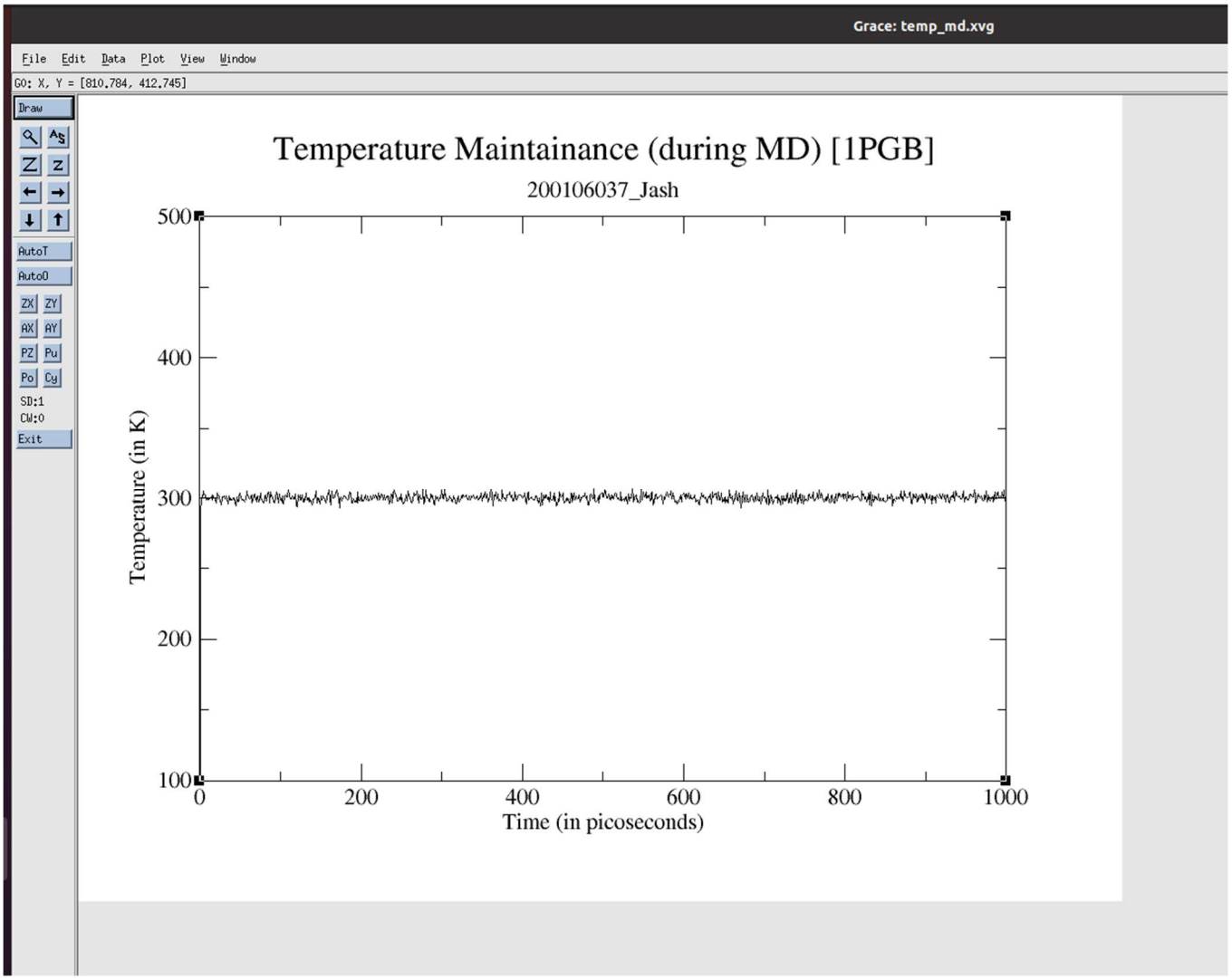


Q6. Temperature and Pressure Maintainance during MD Simulation -

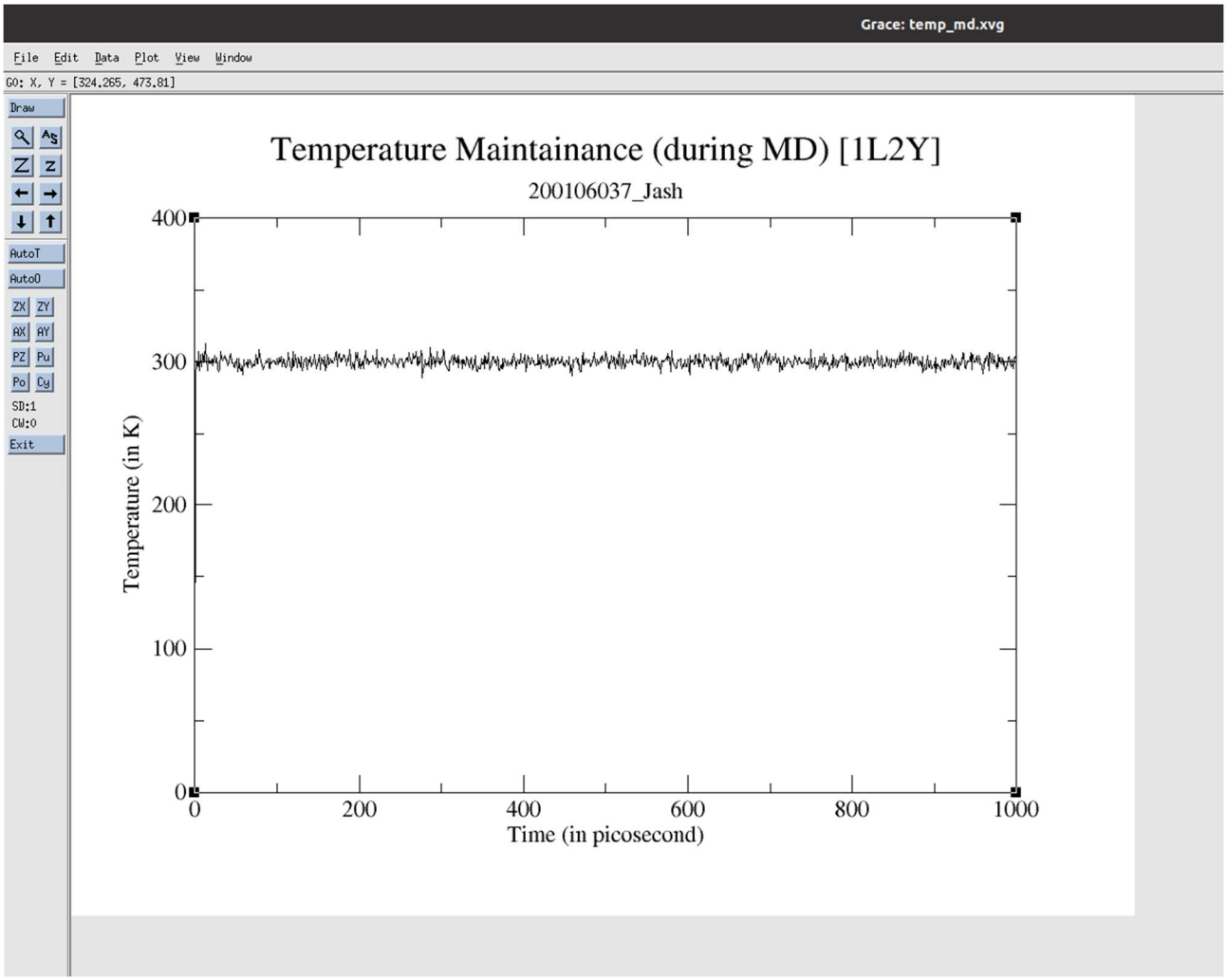
Temperature -
Initial temperature was set to 300K. So, during MD the temperature may have varied but as we can see from the plot that the variation in the temperature is very small. Thus, our temperature is maintained at 300K throughout the whole MD simulation.

The temperature is controlled using techniques like Berendsen thermostats. There are many other methods similar to Berendsen thermostat. A Thermostats acts like a heat bath which virtually exchanges energy with out simulated system and thus maintains a desired temperture of the system.
These methods allow for the system to equilibrate to a desired temperature by coupling it to a heat or by simulating collisions with an external gas.

Protein G [1PGB.pdb]



Trp Cage [1L2Y.pdb]

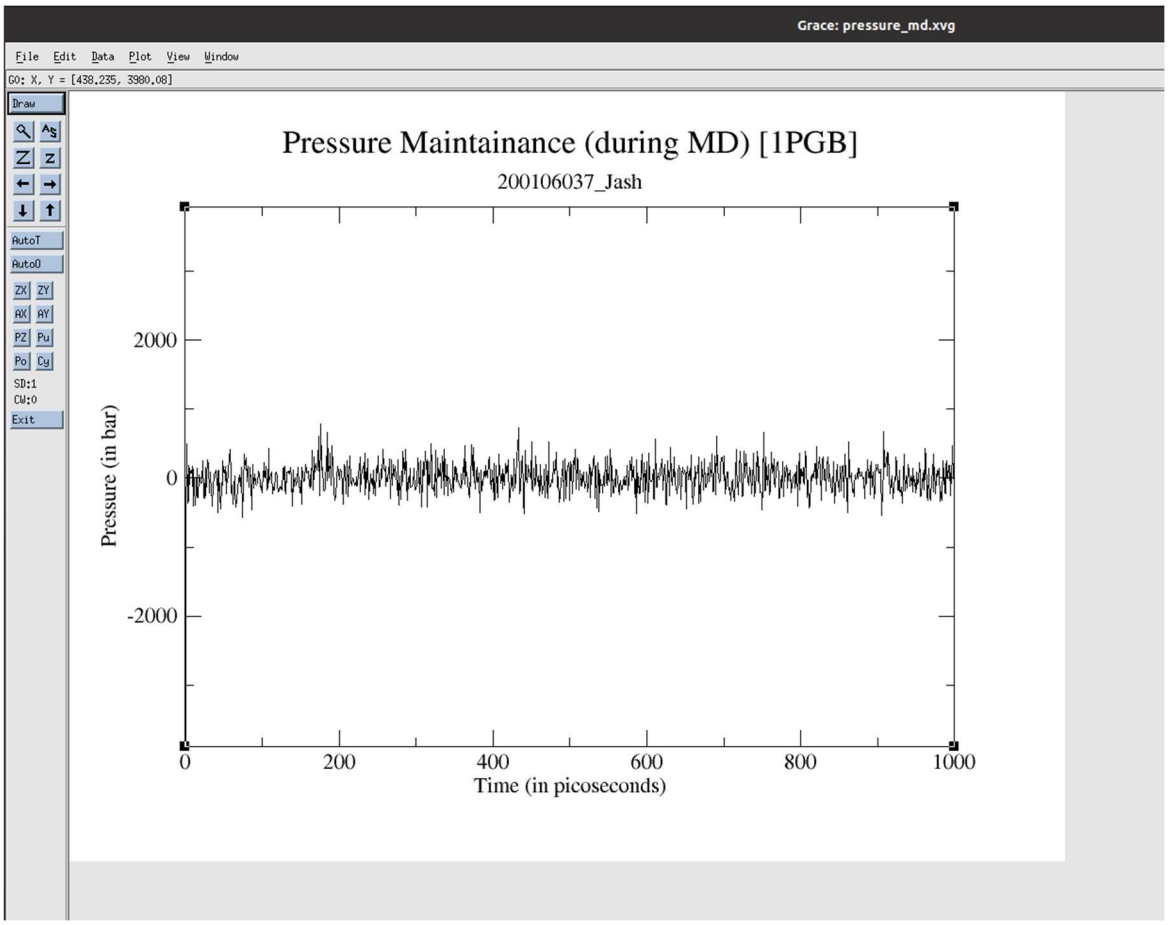


Pressure -

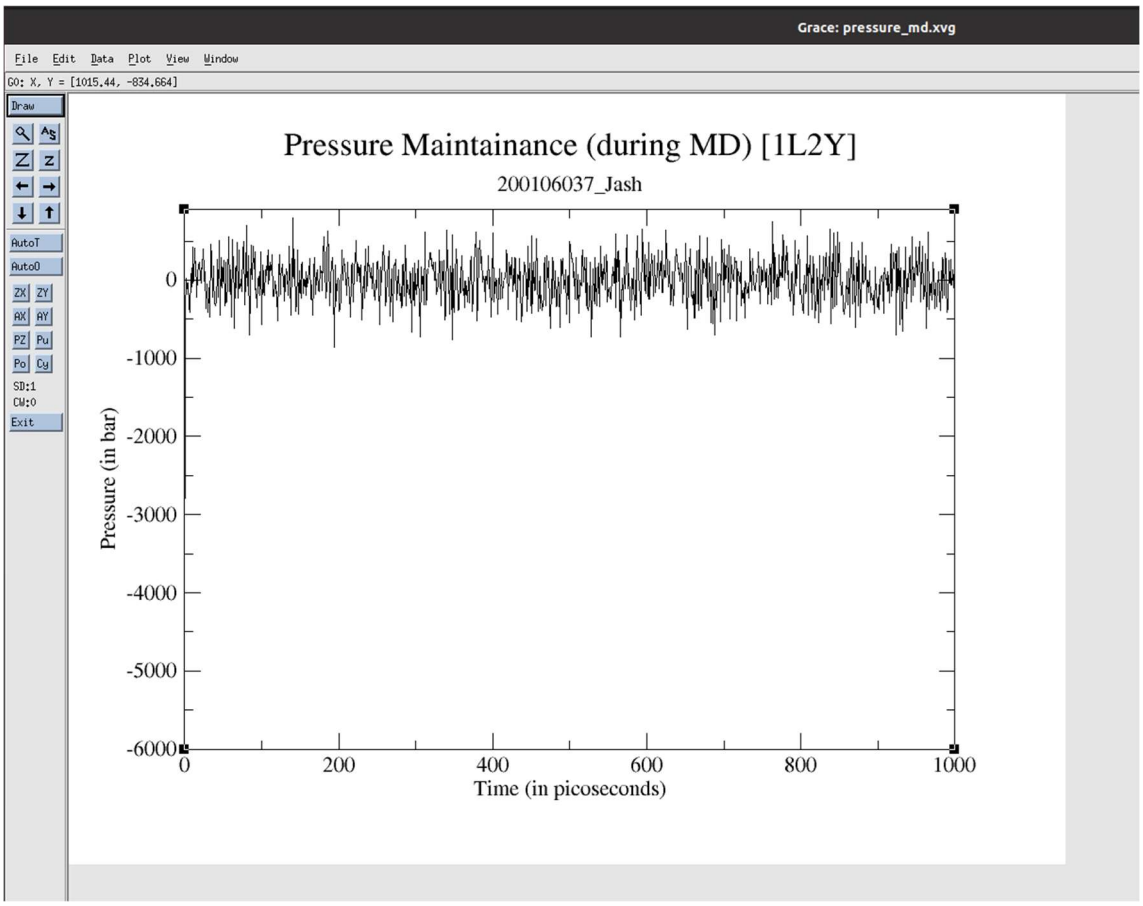
Initial pressure was set to 0 bar. So, during MD simulation the pressure might have varied but as we can see from the plot that the pressure variation during the process is very small. Thus, our pressure is maintained at 0 bar throughout the whole MD simulation.

Similar to the thermostats, the simulations use a barostat to controll and maintain the given pressure durnig the MD simulation.
For e.g. --
Parrinello-Rahman barostat: This technique allows for the simulation of systems with variable volume by coupling the system to a pressure bath. The pressure bath exerts a pressure on the system, which causes the system to equilibrate to a desired pressure while allowing for fluctuations in volume.

Protein G [1PGB.pdb]



Trp Cage [1L2Y.pdb]



Theoretical answers to the Questions in Assignment :

Q5. Time taken for whole MD Simulation can be found out from the md.log file which gives the log output of the whole operation.

Protein G [1PGB.pdb]

Total Time taken = 1hour 2min 17 seconds (3737seconds)

```
               Core t (s)   Wall t (s)        (%)
       Time:    14951.450     3737.862      400.0
                         1h02:17
                 (ns/day)    (hour/ns)
Performance:       23.115        1.038
```

Trp Cage [1L2Y.pdb]

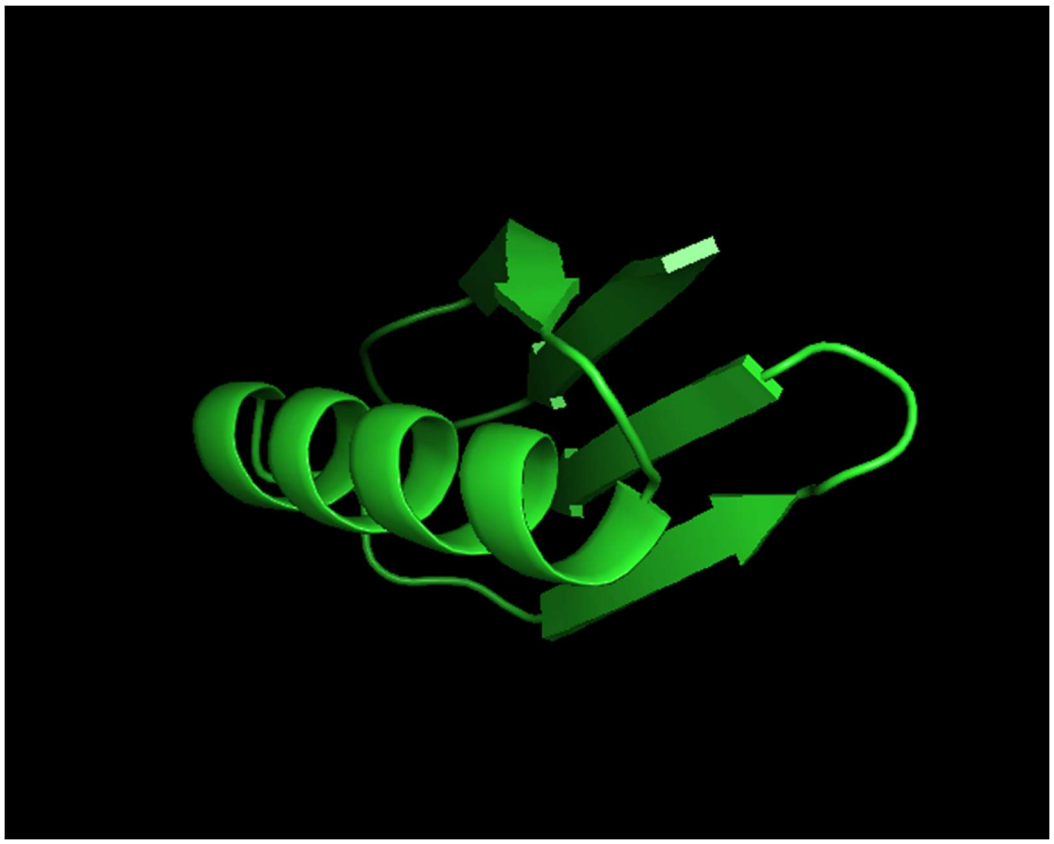
Total Time taken = 1022.282 Seconds

```
               Core t (s)   Wall t (s)        (%)
       Time:    12267.381     1022.282     1200.0
                 (ns/day)    (hour/ns)
Performance:       84.517        0.284
```

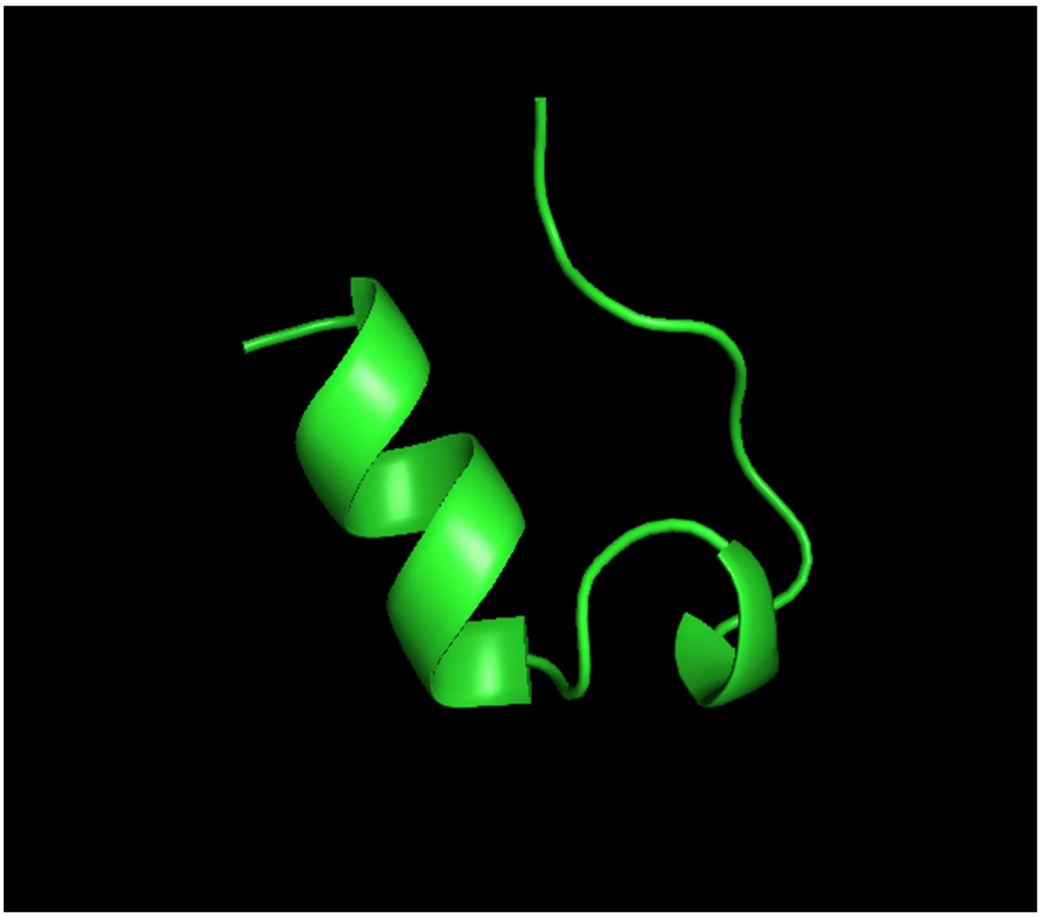
GRO file (PyMol Image Screenshots)

1. Vaccum

Protein G [1PGB.pdb]

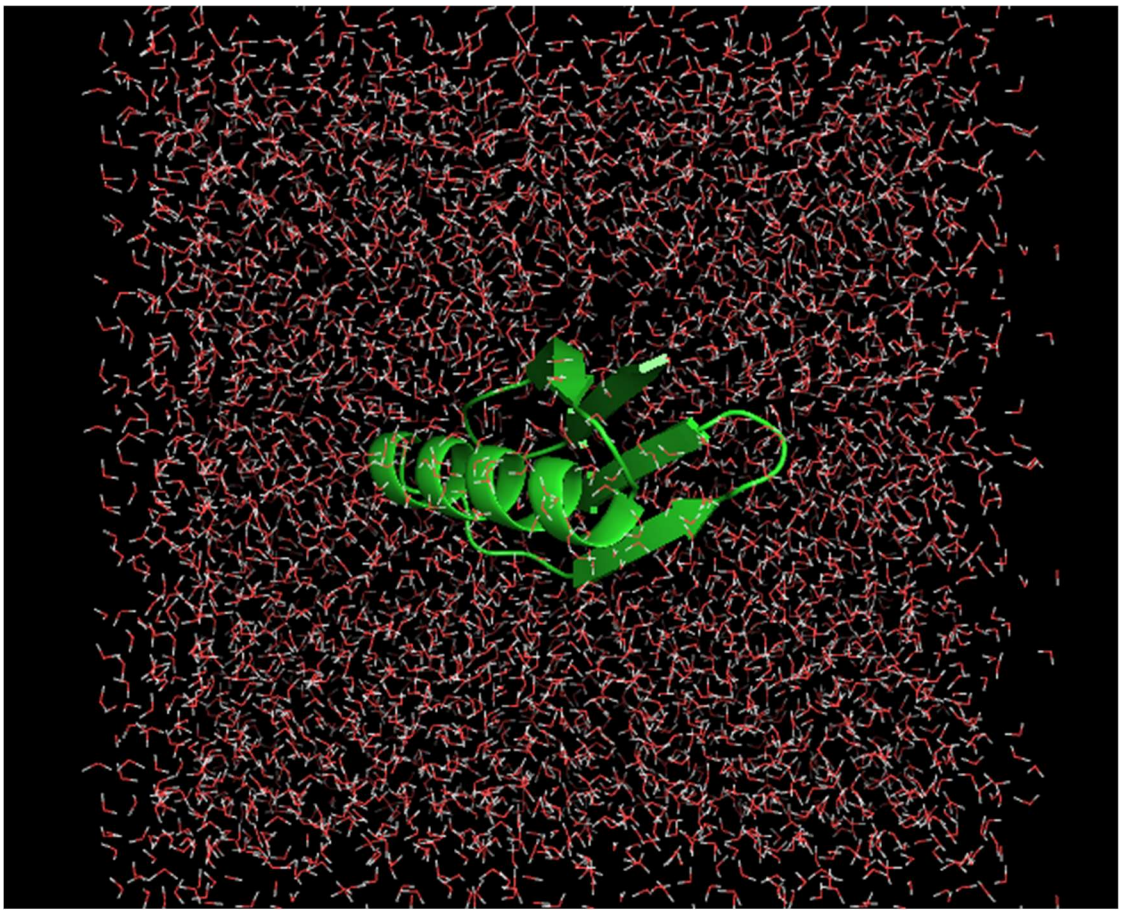


Trp Cage [1L2Y.pdb]

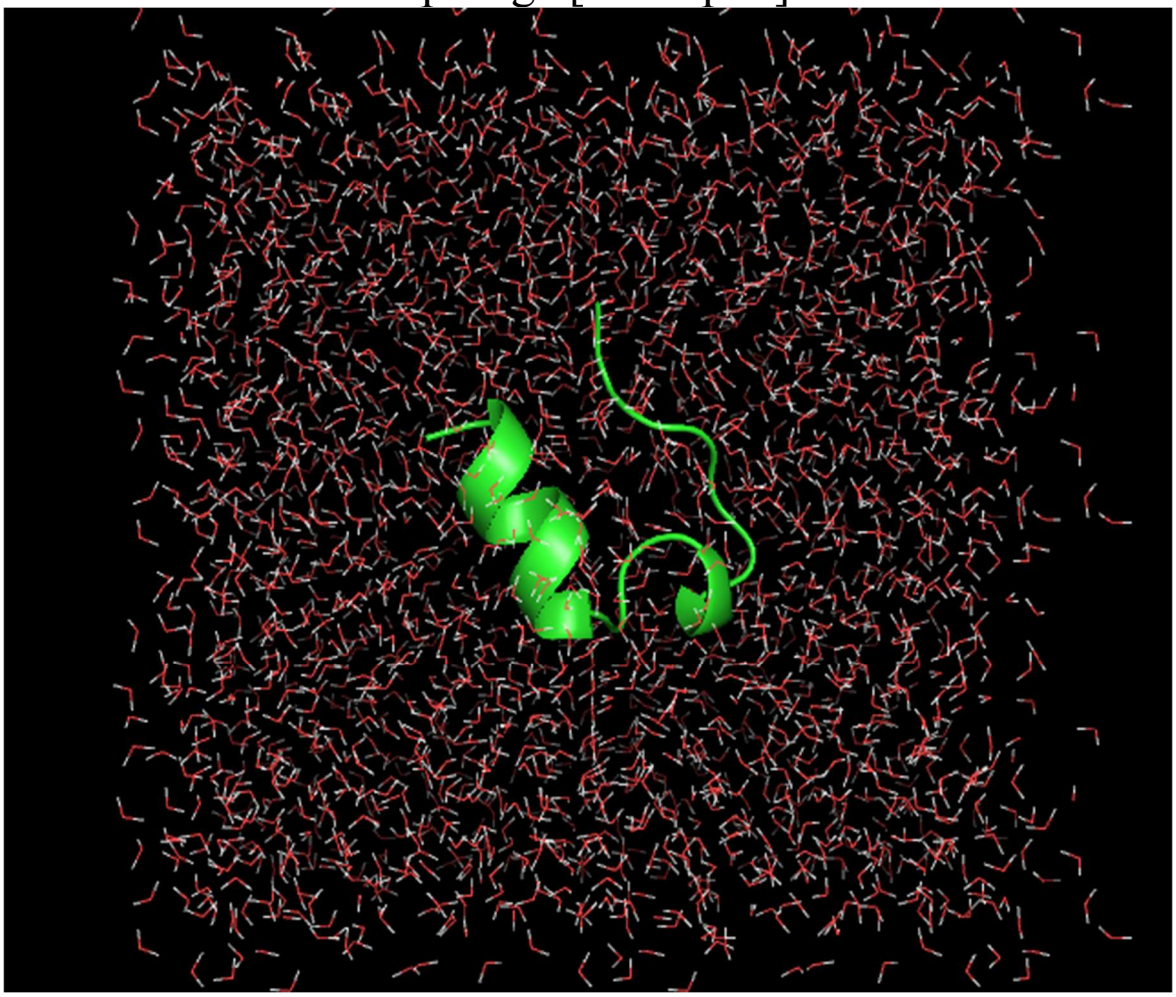


2. Solvation

Protein G [1PGB.pdb]

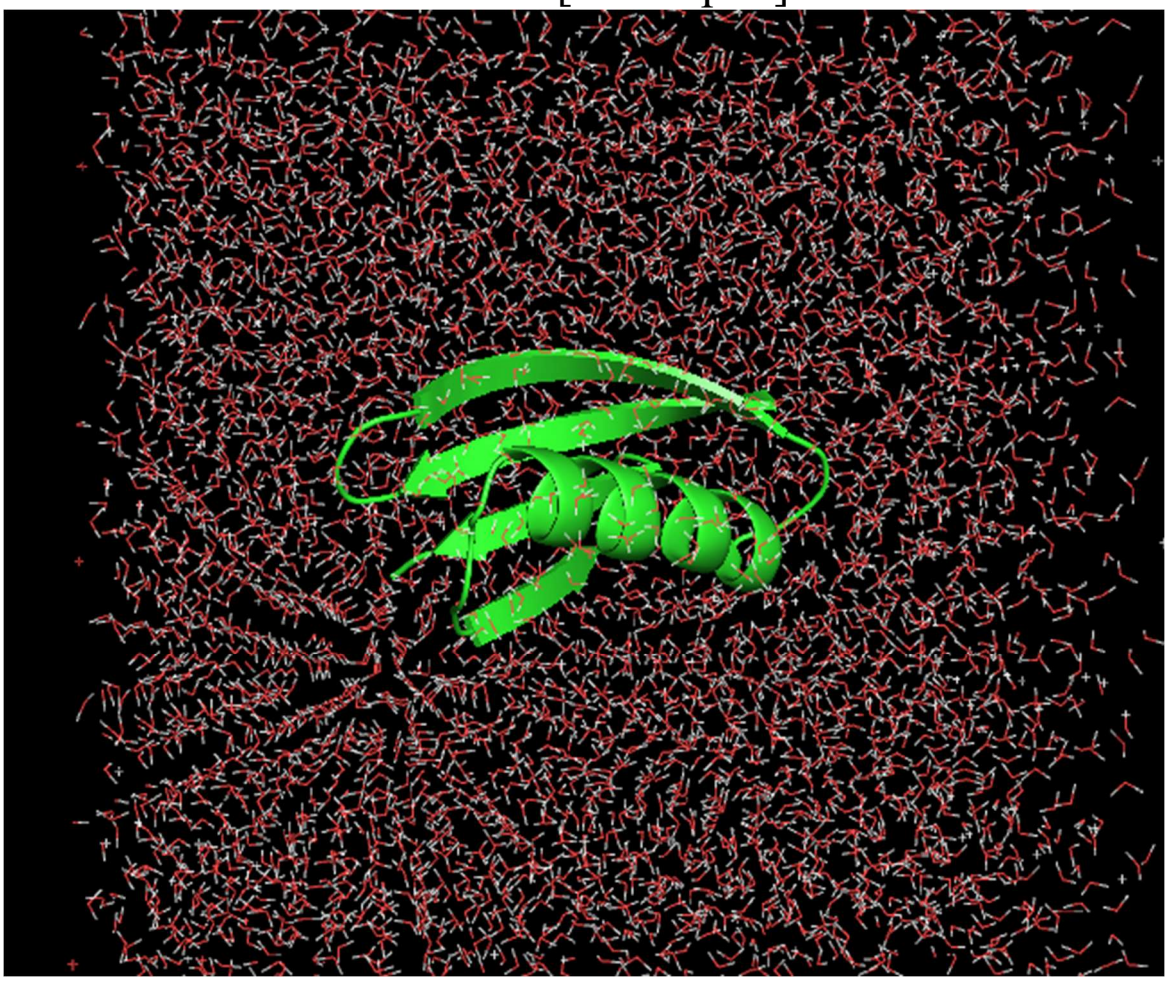


Trp Cage [1L2Y.pdb]



3. Energy Minimization

Protein G [1PGB.pdb]



Trp Cage [1L2Y.pdb]