Commands to Run Molecular Dynamics Simulations of Protein in Water

Step-1: Clean your structure from water

```
grep -v HOH your_structure.pdb > str_clean.pdb
```

Note: You need to perform this step if your structure is downloaded from protein databank

Step-2: Creation of topology file

```
gmx pdb2gmx -f str_clean.pdb -o str_processed.gro -water spce
```

Step-3: Solvation

```
gmx editconf -f str_processed.gro -o str_newbox.gro -c -d 1.0 -bt cubic
```

Once the above command is successfully executed then type the following command in terminal

```
gmx solvate -cp str_newbox.gro -cs spc216.gro -o str_solv.gro -p topol.top
```

Step-4: Ionization

```
gmx grompp -f ions.mdp -c str_solv.gro -p topol.top -o ions.tpr
```

Once the above command is successfully executed then type the following command in terminal

```
gmx genion -s ions.tpr -o str_solv_ions.gro -p topol.top -pname NA -nname CL -neutral
```

Step-5: Energy Minimization

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

Once the above command is successfully executed then type the following command in terminal

```
gmx mdrun -v -deffnm em
```

Step-6: Equilibration
For temperature equilibration

```
gmx grompp -f nvt.mdp -c em.gro -r em.gro -p topol.top -o nvt.tpr
```

Once the above command is successfully executed then type the following command in terminal

```
gmx mdrun -deffnm nvt -v
```

If you want to plot the energy then use the following command

```
gmx energy -f nvt.edr -o temperature.xvg
```

For Pressure equilibration

```
gmx grompp -f npt.mdp -c nvt.gro -r nvt.gro -t nvt.cpt -p topol.top -o
npt.tpr
```

Once the above command is successfully executed then type the following command in terminal

```
gmx mdrun -deffnm npt -v
```

If you want to plot the energy then use the following command

```
gmx energy -f npt.edr -o pressure.xvg
```

Step-6: Production

```
gmx grompp -f md.mdp -c npt.gro -t npt.cpt -p topol.top -o md_0_1.tpr
```

Once the above command is successfully executed then type the following command in terminal

```
gmx mdrun -deffnm md_0_1 -v
```

If you have gpu installed in your system the use the following command instead of above-mentione

```
gmx mdrun -deffnm md_0_1 -v -nb gpu
```