

##GROMACS MD TRAJECTORY ANALYSIS

###source /usr/local/gromacs/bin/GMXRC

####check for jump and trim trajectory

```
gmx trjconv -s 8ID2_md.tpr -f 8ID2_md.xtc -o traj_nojump.xtc -pbc nojump -b 0 -e 1 -tu ns
```

```
gmx trjconv -s 8ID2_md.tpr -f 8ID2_md.trr -o traj_nojump.trr -pbc nojump -b 0 -e 1 -tu ns
```

```
`select group 'system':1`
```

##First frame for the analysis

```
1. gmx trjconv -s 8ID2_md.tpr -f 8ID2_md.trr -o firstframe.gro -b 0 -e 2
```

```
`select group 'system':1`
```

##RMSD CALCULATION

```
1. gmx rms -s firstframe.gro -f traj_nojump.xtc -o rmsd_backbone.svg -tu ns
```

```
`select group 'Backbone' :4`
```

```
again
```

```
`select group 'Backbone' :4`
```

##RMSF CALCULATION

```
1. gmx rmsf -f traj_nojump.xtc -s 8ID2_md.tpr -o rmsf_per_residue.svg -ox average.pdb -oq  
bfactors_residue.pdb -res
```

```
`select group 'protein' :1`
```

##RADIUS OF GYRATION

```
1. gmx gyrate -s 8ID2_md.tpr -f traj_nojump.xtc -o pro_radius_of_gyration.svg
```

```
`select group 'protein':1`
```

NOTE: gyrate doesnt have time unit option.

##RAMACHANDRAN PLOT

```
1. gmx rama -f traj_nojump.xtc -s 8ID2_md.tpr -o ramachandran.svg
```