# GROMACS
# Lysozyme in Water

| Command | Purpose | Flags/Parameters Explained | Notes / Mnemonics |
|---|---|---|---|
| **grep -v HOH 1aki.pdb > 1AKI_clean.pdb** | Remove water molecules from PDB file | -v: inverse match (exclude lines with "HOH") | Clean PDB from water |
| **gmx pdb2gmx -f 1AKI_clean.pdb -o 1AKI_processed.gro -water spce** | Generate topology and processed structure file | -f: input file, -o: output file, -water spce: use SPC/E water model | "pdb2gmx" = PDB to GROMACS format |
| **gmx editconf -f 1AKI_processed.gro -o 1AKI_newbox.gro -c -d 1.0 -bt cubic** | Define box for solvation | -c: center, -d 1.0: 1 nm distance, -bt cubic: box type | "editconf" = edit configuration |
| **gmx solvate -cp 1AKI_newbox.gro -cs spc216.gro -o 1AKI_solv.gro -p topol.top** | Add water molecules | -cp: protein config, -cs: solvent config, -p: update topology | "solvate" = add solvent |
| **gmx grompp -f ions.mdp -c 1AKI_solv.gro -p topol.top -o ions.tpr** | Prepare for ion addition | grompp: preprocessor, -f: parameter file, -c: structure, -p: topology | "grompp" = GROMACS preprocessor |
| **gmx genion -s ions.tpr -o 1AKI_solv_ions.gro -p topol.top -pname NA -nname CL -neutral** | Add ions to neutralize system | -pname, -nname: names of ions, -neutral: neutralize charge | "genion" = generate ions |
| **gmx grompp -f minim.mdp -c 1AKI_solv_ions.gro -p topol.top -o em.tpr** | Prepare energy minimization | em.tpr: energy minimization input | "minim" = minimization |
| **gmx mdrun -v -deffnm em** | Run energy minimization | -v: verbose, -deffnm: default filenames prefix | "mdrun" = run MD simulation |
| **gmx energy -f em.edr -o potential.xvg** | Extract potential energy | -f: energy file, -o: output xvg plot | Potential energy check |
| **gmx grompp -f nvt.mdp -c em.gro -r em.gro -p topol.top -o nvt.tpr** | Prep for NVT equilibration | -r: reference structure | "NVT" = constant Number, Volume, Temperature |
| **gmx mdrun -deffnm nvt** | Run NVT equilibration | Output: nvt.gro, nvt.edr etc. | |
| **gmx energy -f nvt.edr -o temperature.xvg** | Check temperature stability | Temperature plot | |

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|---|---|---|---|
| **gmx grompp -f npt.mdp -c nvt.gro -r nvt.gro -t nvt.cpt -p topol.top -o npt.tpr** | Prep for NPT equilibration | -t: checkpoint (continuation) | "NPT" = constant Number, Pressure, Temperature |
| **gmx mdrun -deffnm npt** | Run NPT equilibration | Output: npt.gro, npt.edr | |
| **gmx energy -f npt.edr -o pressure.xvg** | Extract pressure profile | | |
| **gmx energy -f npt.edr -o density.xvg** | Extract density profile | | |
| **gmx grompp -f md.mdp -c npt.gro -t npt.cpt -p topol.top -o md_0_1.tpr** | Prep final production MD run | md.mdp: production parameters | |
| **gmx mdrun -deffnm md_0_1** | Run final MD simulation | Produces .xtc, .gro, .edr, .log | |
| **gmx trjconv -s md_0_1.tpr -f md_0_1.xtc -o md_0_1_noPBC.xtc -pbc mol -center** | Remove PBC and center molecule | -pbc mol: remove jumps, -center: center molecule | "trjconv" = trajectory conversion |
| **gmx rms -s md_0_1.tpr -f md_0_1_noPBC.xtc -o rmsd.xvg -tu ns** | Compute RMSD of MD run | -tu ns: time unit in nanoseconds | |
| **gmx rms -s em.tpr -f md_0_1_noPBC.xtc -o rmsd_xtal.xvg -tu ns** | RMSD vs. crystal structure | Compares simulation to starting (minimized) state | |
| **gmx gyrate -s md_0_1.tpr -f md_0_1_noPBC.xtc -o gyrate.xvg** | Radius of gyration plot | Measures compactness | |

- **pdb2gmx**: Convert PDB to GROMACS
- **editconf**: Edit box (Confine molecule)
- **solvate**: Solvent addition
- **grompp**: Pre-process input
- **genion**: Add IONs

- **mdrun**: Run simulation
- **energy**: Extract energy terms
- **trjconv**: Trajectory conversion (post-processing)
- **rms / gyrate**: Analysis (structure deviation and compactness)

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START

**1. Remove water from PDB**

grep -v HOH 1aki.pdb > 1AKI_clean.pdb

**2. Generate topology and coordinate file**

gmx pdb2gmx -f 1AKI_clean.pdb -o 1AKI_processed.gro -water spce

**3. Define simulation box**

gmx editconf -f 1AKI_processed.gro -o 1AKI_newbox.gro -c -d 1.0 -bt cubic

**4. Solvate the protein**

gmx solvate -cp 1AKI_newbox.gro -cs spc216.gro -o 1AKI_solv.gro -p topol.top

**5. Add ions to neutralize**

gmx grompp -f ions.mdp -c 1AKI_solv.gro -p topol.top -o ions.tpr

gmx genion -s ions.tpr -o 1AKI_solv_ions.gro -p topol.top -pname NA -nname CL -neutral

**6. Energy minimization**

gmx grompp -f minim.mdp -c 1AKI_solv_ions.gro -p topol.top -o em.tpr

gmx mdrun -v -deffnm em

gmx energy -f em.edr -o potential.xvg

**7. NVT equilibration (constant volume)**

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

gmx mdrun -deffnm nvt

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

**8. NPT equilibration (constant pressure)**

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

gmx mdrun -deffnm npt

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

gmx energy -f npt.edr -o density.xvg

**9. Production MD run**

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

gmx mdrun -deffnm md_0_1

**10. Post-MD analysis**

- Remove PBC and center: gmx trjconv -s md_0_1.tpr -f md_0_1.xtc -o md_0_1_noPBC.xtc -pbc mol -center
- RMSD analysis: gmx rms -s md_0_1.tpr -f md_0_1_noPBC.xtc -o rmsd.xvg -tu ns
- RMSD vs. crystal: gmx rms -s em.tpr -f md_0_1_noPBC.xtc -o rmsd_xtal.xvg -tu ns
- Radius of gyration: gmx gyrate -s md_0_1.tpr -f md_0_1_noPBC.xtc -o gyrate.xvg

END