Note: Steps 1 to 5 were executed exclusively on CPU processors, while Step 6 (production MD) was conducted on a hybrid GPU/CPU system to enhance computational efficiency.

GROMACS Commands (CPU):

Step 1 - Generate Topology

echo 15 | gmx_mpi pdb2gmx -f 6bfa_noWater_noLigand_fullSideChains_Chimera.pdb -o test_str_processed.gro -water spce

Step 2 - Solvation

Step 2.1: Creating simulation box.
gmx_mpi editconf -f test_str_processed.gro -o str_newbox.gro -c -d 1.0 -bt cubic

Step 2.2: Adding water molecules.
gmx_mpi solvate -cp str_newbox.gro -cs spc216.gro -o str_solv.gro -p topol.top

Step 3 - Ionization

Step 3.1: Preparing system for ion addition.
gmx_mpi grompp -f ions.mdp -c str_solv.gro -p topol.top -o ions.tpr

Step 3.2: Adding ions to neutralize the system. (Selection 13 = SOL)
gmx_mpi genion -s ions.tpr -o str_solv_ions.gro -p topol.top -pname NA -nname CL -neutral

Step 4 - Energy Minimization

Step 4.1: Preparing input for energy minimization.
gmx_mpi grompp -f minim.mdp -c str_solv_ions.gro -p topol.top -o em.tpr

Step 4.2: Running energy minimization.
srun gmx_mpi mdrun -v -deffnm em

Step 5 - Equilibration (NVT & NPT)

Step 5.1: Running NVT equilibration.
gmx_mpi grompp -f nvt.mdp -c em.gro -r em.gro -p topol.top -po mdout.mdp -o nvt.tpr
srun gmx_mpi mdrun -deffnm nvt -v

Step 5.2: Extracting total energy from NVT.
cho -e "16\n0" | gmx_mpi energy -f nvt.edr -o temperature.xvg

Step 5.3: Running NPT equilibration.
gmx_mpi grompp -f npt.mdp -c nvt.gro -r nvt.gro -t nvt.cpt -p topol.top -o npt.tpr

srun gmx_mpi mdrun -deffnm npt -v
Step 5.4: Extracting density from NPT.
echo -e "24\n0" | gmx_mpi energy -f npt.edr -o pressure.xvg

Step 6 - Final MD (100 ns)

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

GROMACS Command (GPU/CPU)

srun gmx_mpi mdrun -nb gpu -pme cpu -bonded cpu -deffnm md_0_1 -v