1. UCSF Chimera, which allows the phi and psi of each residue to be specified.
   Tools -> Structure Editing -> Build -> Peptide
   - paste the sequence in the box
   - assign fully extended phi, psi values to all non-P residues (-179,179)
   - give all Pro residues PPII dihedral angles (-80, 160)
   - save as CTD_chimera.pdb

1. Check the sequence is correct in the PDB file. Check all dihedrals are trans (they are)
   a. g_chi -s CTD_chimera.pdb -f CTD_chimera.pdb -omega

2. pdb2gmx -f CTD_chimera.pdb -o init.gro -p init.top -ignh -ter -vsite hydrogens -v # CHARMM22STAR

3. editconf -f init.gro -o editconf.gro -bt dodecahedron -d 1.5 -center 0 0 0

4. genbox -cp editconf.gro -cs spc216 -o genbox.gro -p init.top

5. /usr/local/gromacs/4.6/465-impi403-fftw332-gcc447-2/bin/grompp -f em.mdp -c genbox.gro -p init.top -o genbox.tpr [make the tpr for genion]

6. echo 13 | genion -s genbox.tpr -conc 0.15 -o genbox_genion.pdb -neutral -p init.top

Energy Minimization

7. /usr/local/gromacs/4.6/465-impi403-fftw332-gcc447-2/bin/grompp -f em.mdp -c genbox_genion.pdb -p init.top -o em.tpr

8. mdrun -s em.tpr