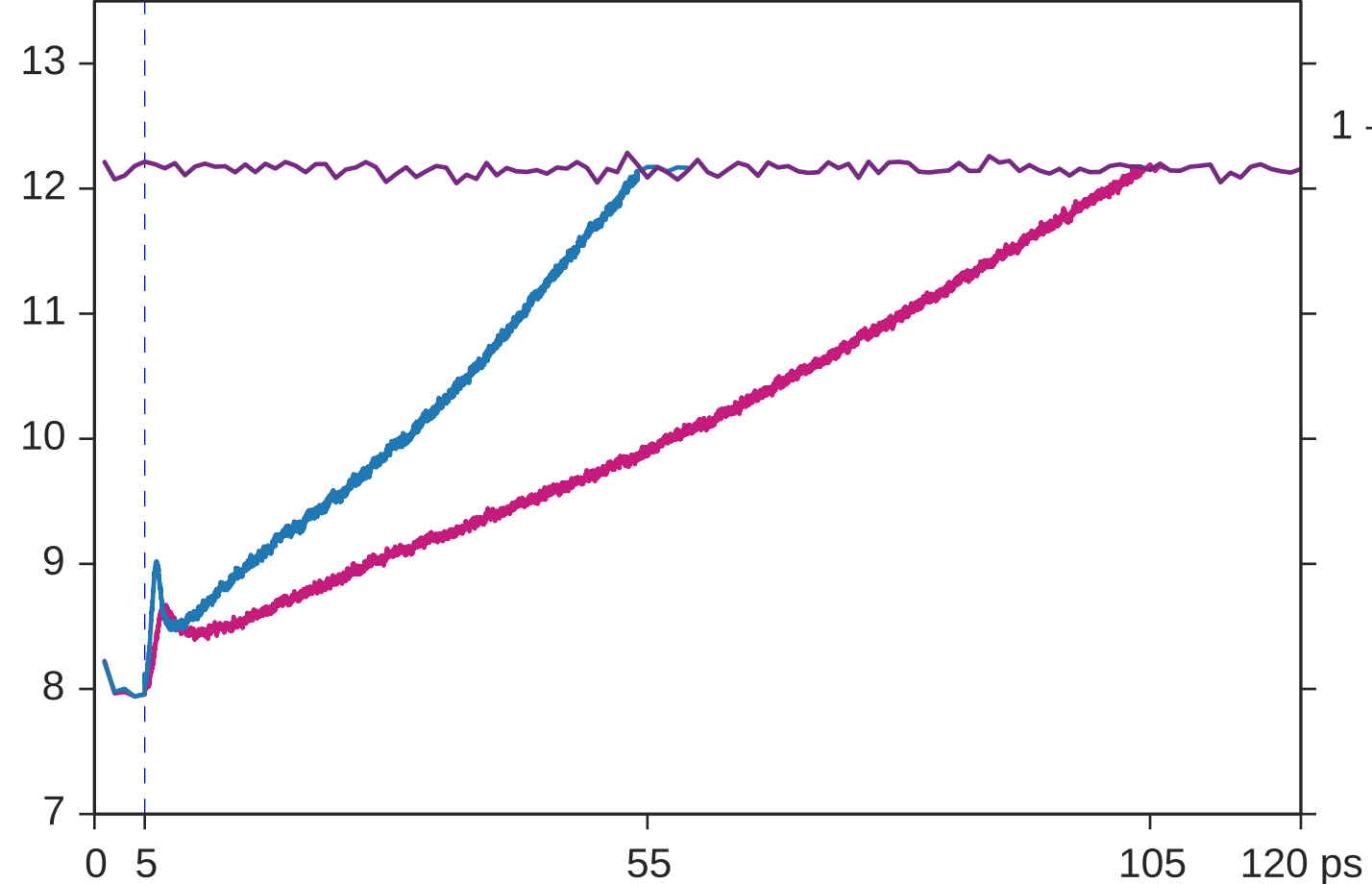
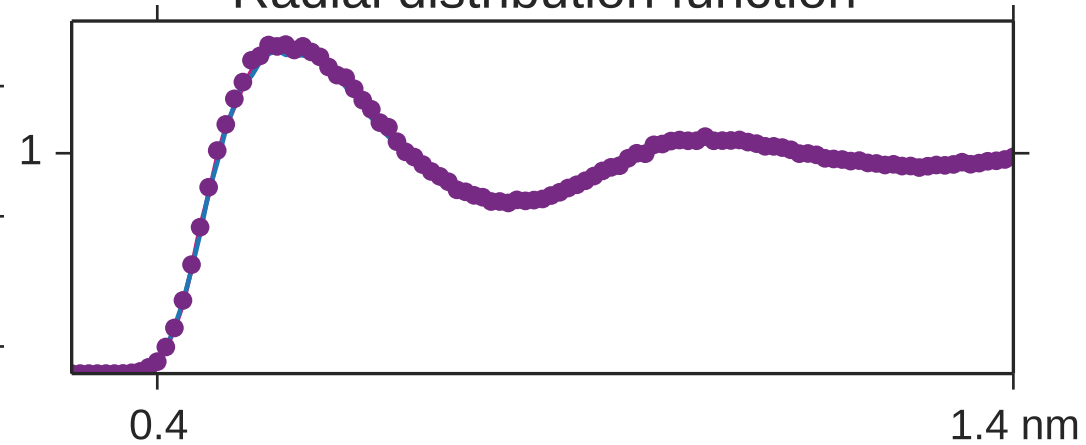


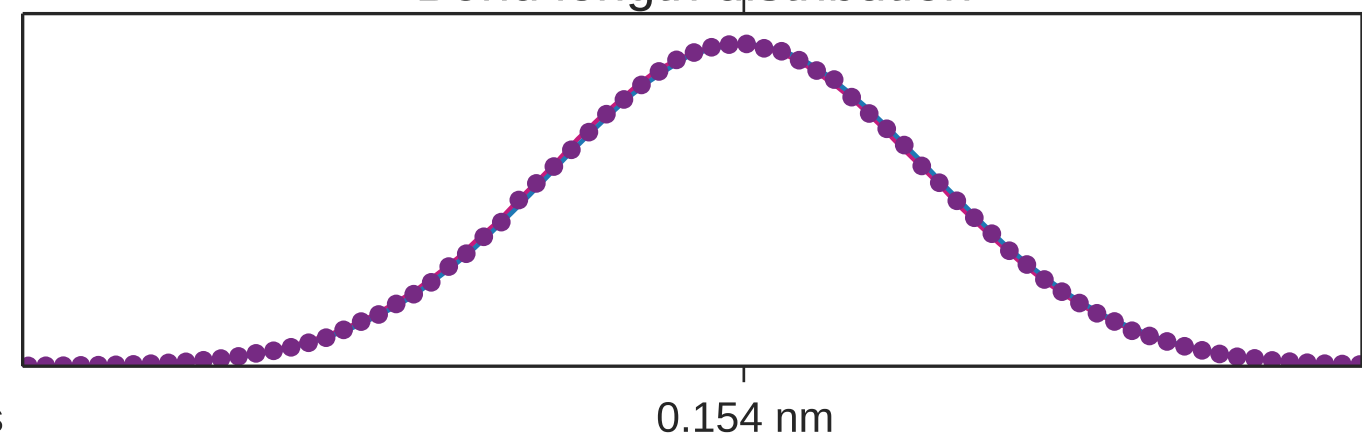
kJ/mol/N Change in total potential energy during backmapping



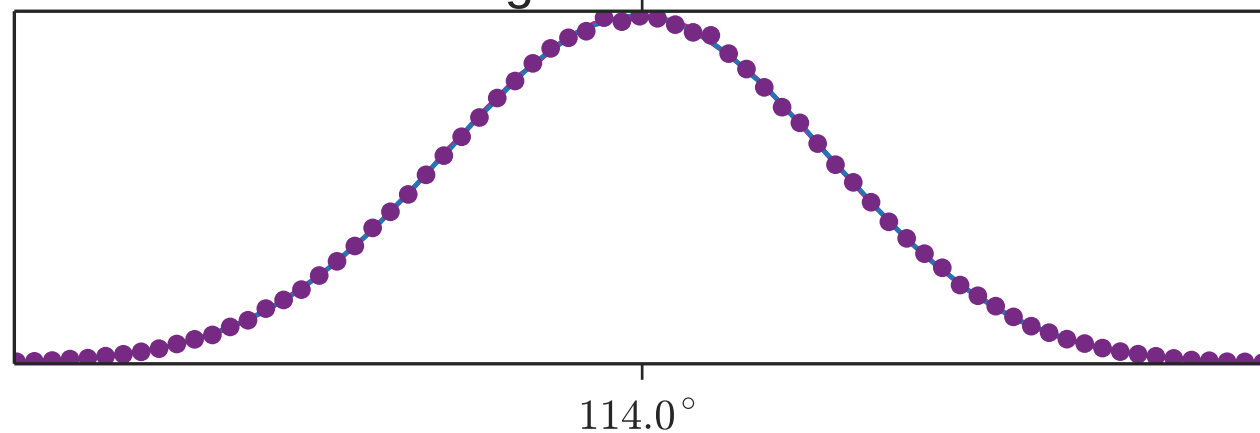
Radial distribution function



Bond length distribution



Angle distribution



Dihedral distribution

