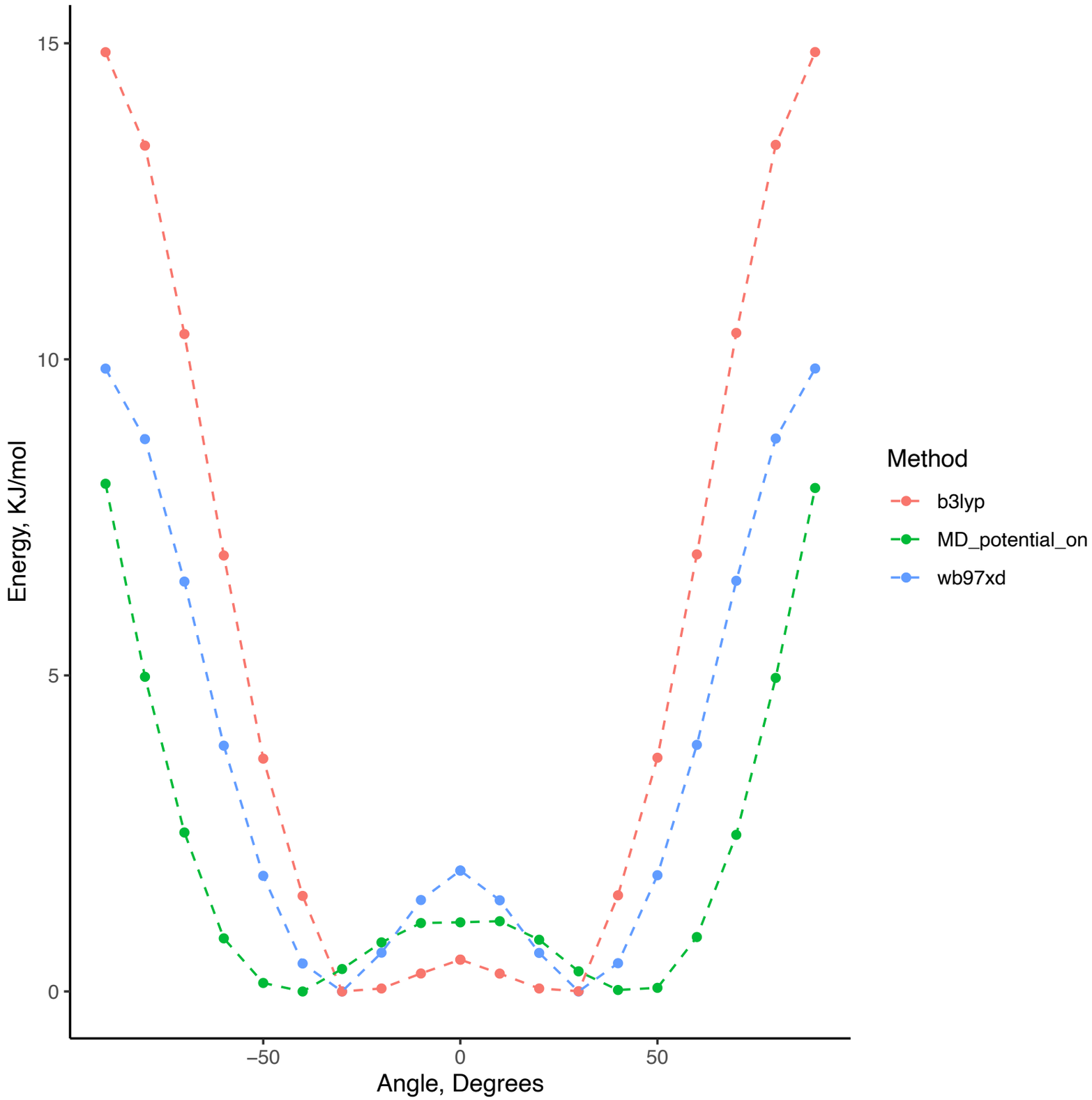
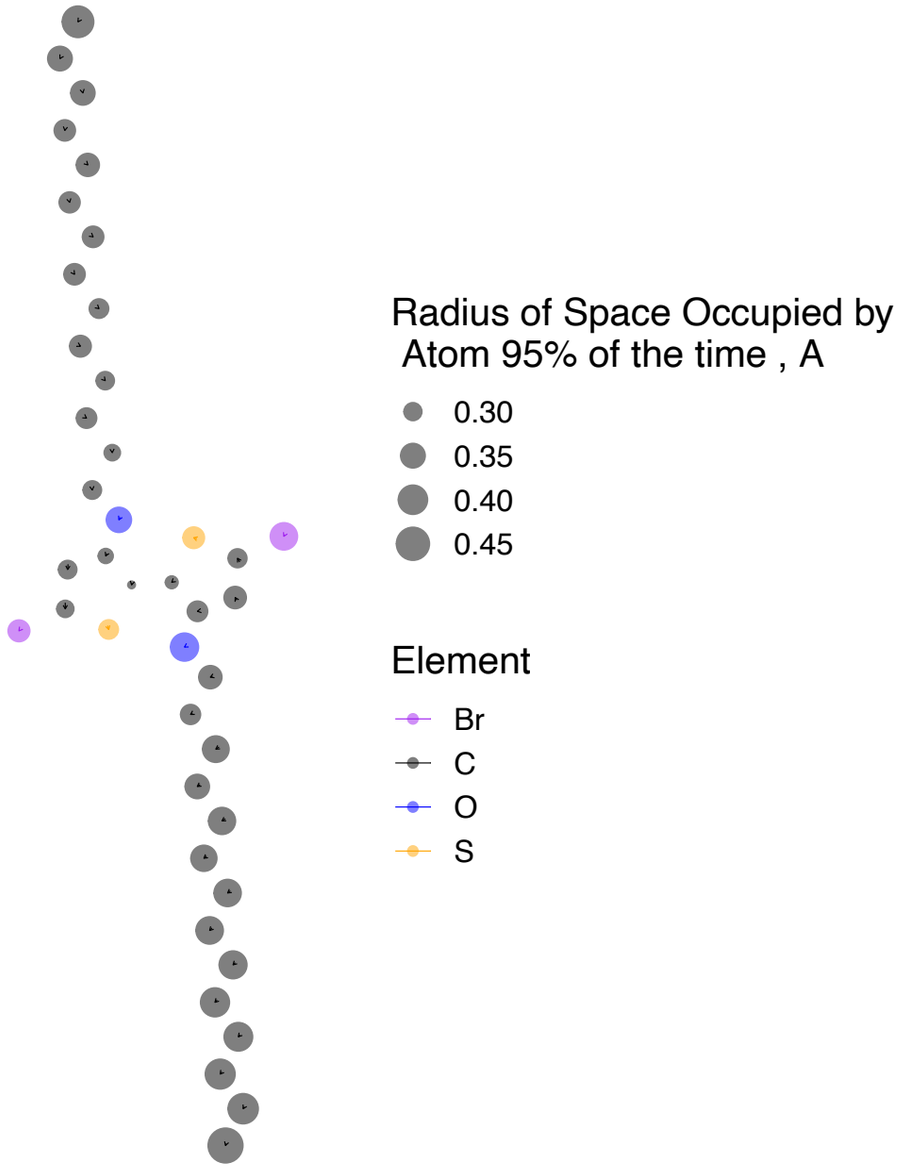
Outer dihedral scan

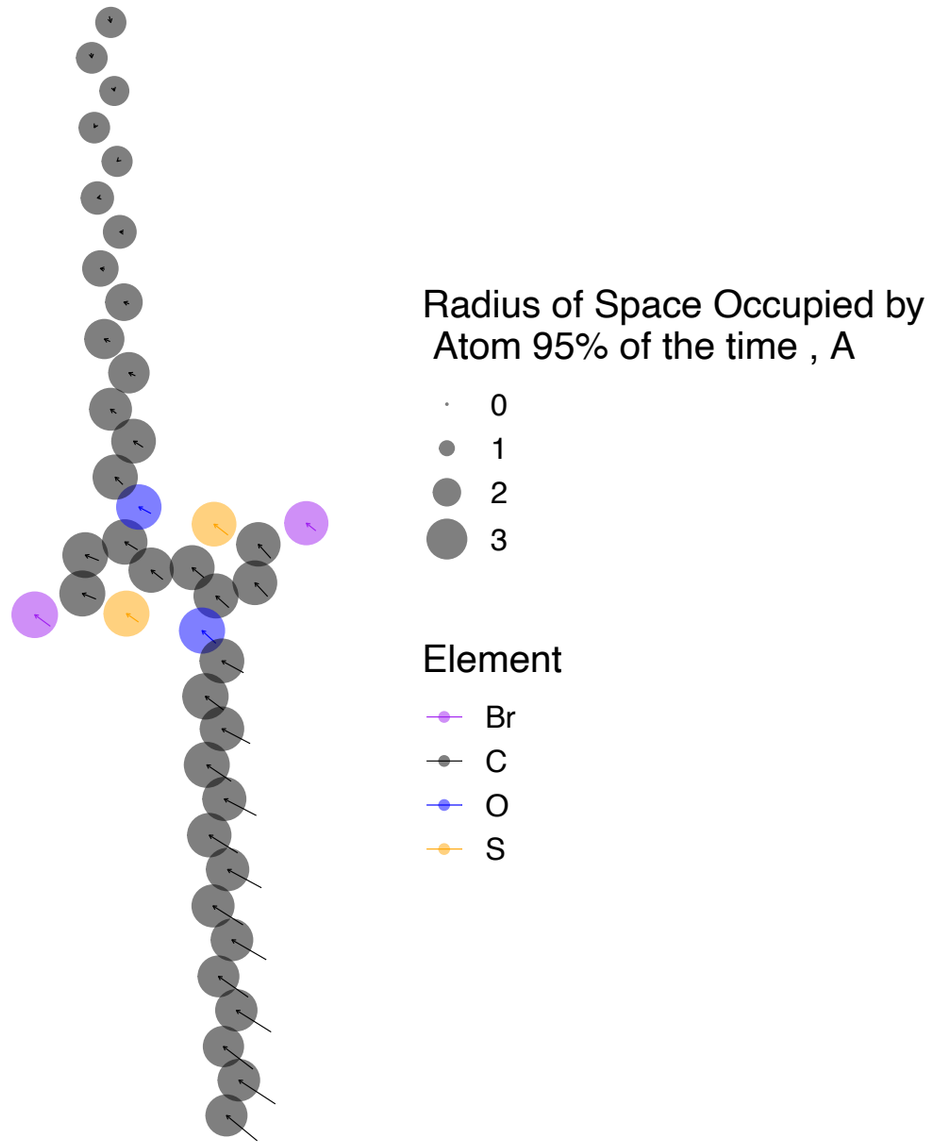


Alkylated Crystal Structure

Without Annealing



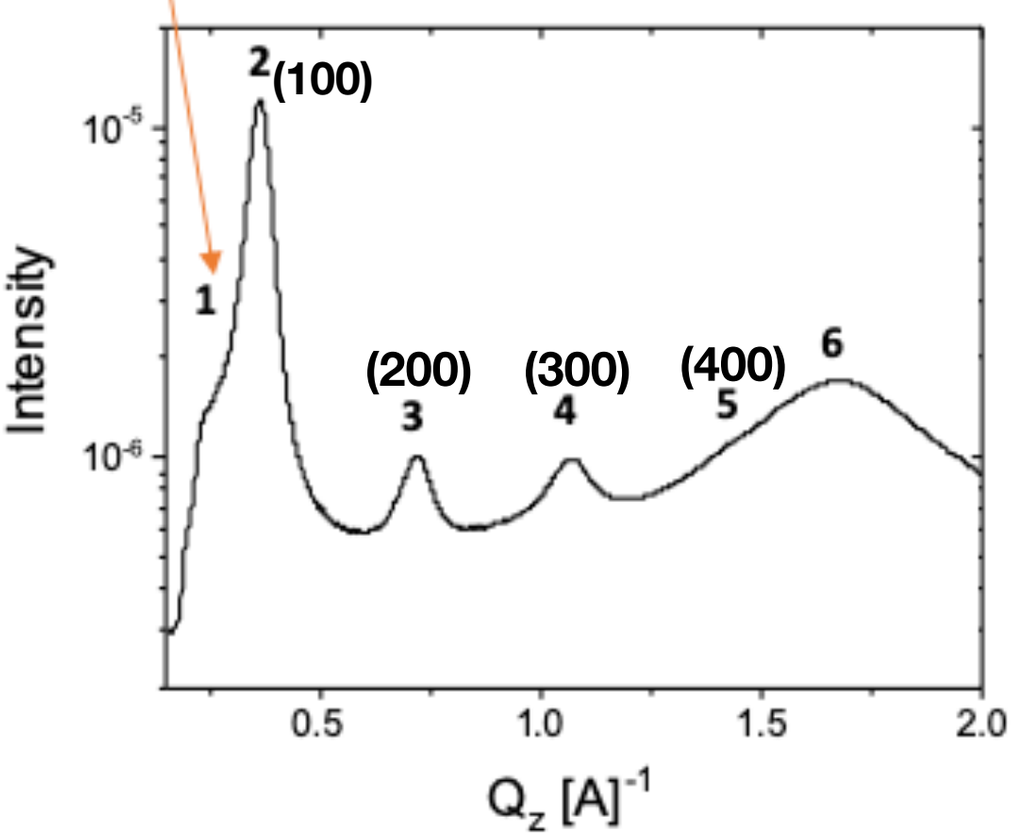
Annealed at 400K



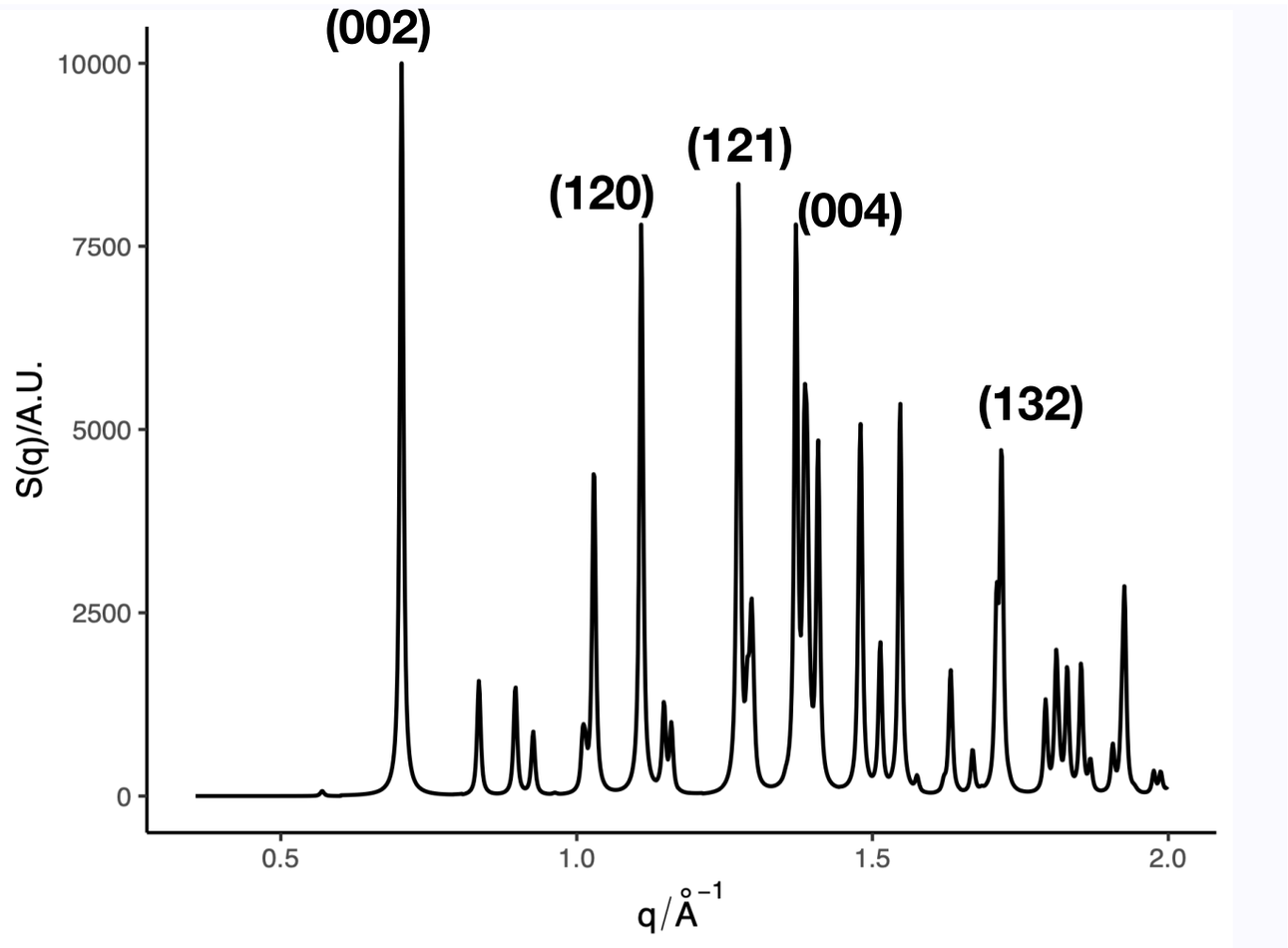
Plots showing the average position (position of dots) and average displacement of each atom (arrows), and twice the standard deviation of the displacement vectors (size of dots). Statistics are averaged over both space and time (hoping the system is ergodic)

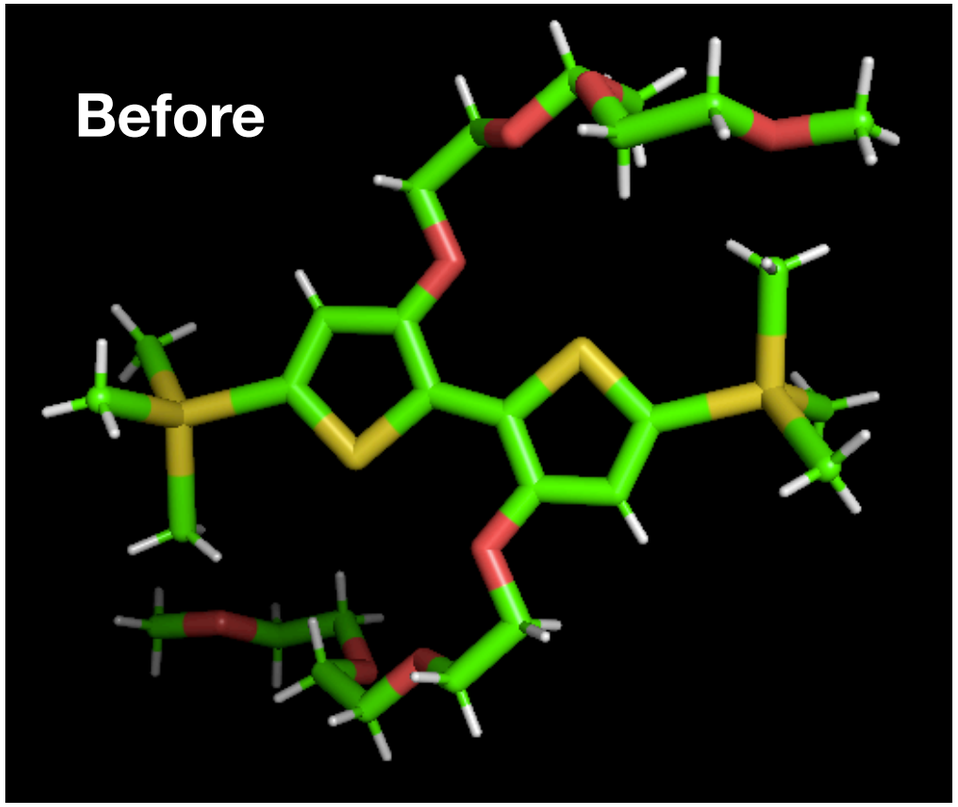
Glycolated Crystal Structure

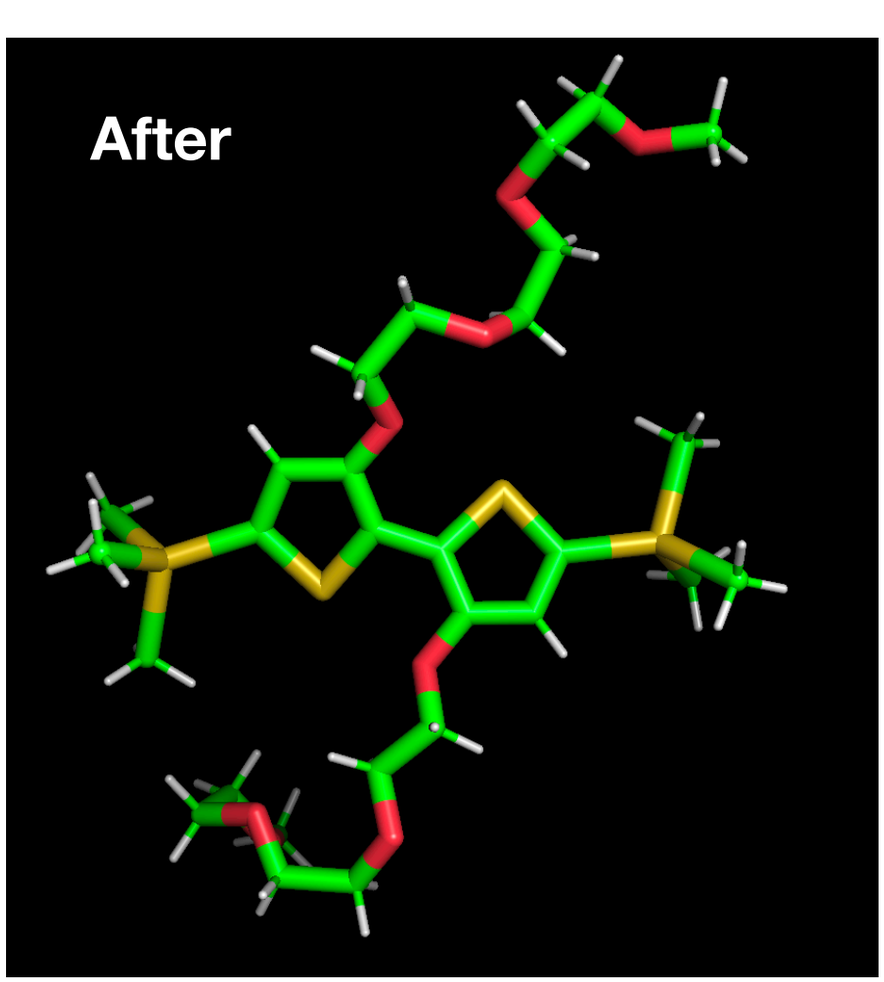
Peak 1 here is most possibly the Yoneda peak, which is due to total reflection of the incident beam on the surface of the polymer and is not a polymer feature. The q value of this peaks matches very closely the expected peak position of the Yoneda peak (q ~0.22)



Structure Factor obtained from Mercury using their .cif file







After equilibrating for 20 ns (!)