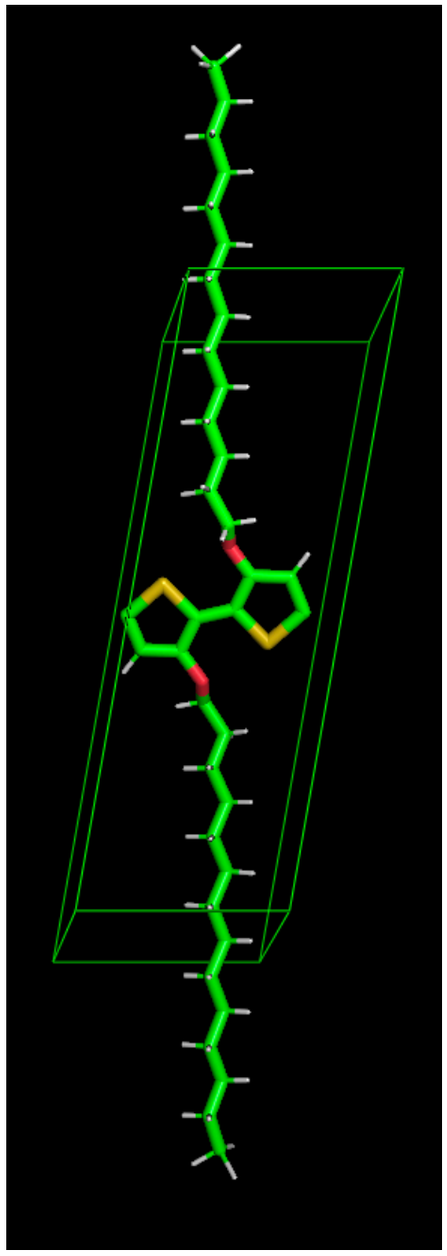
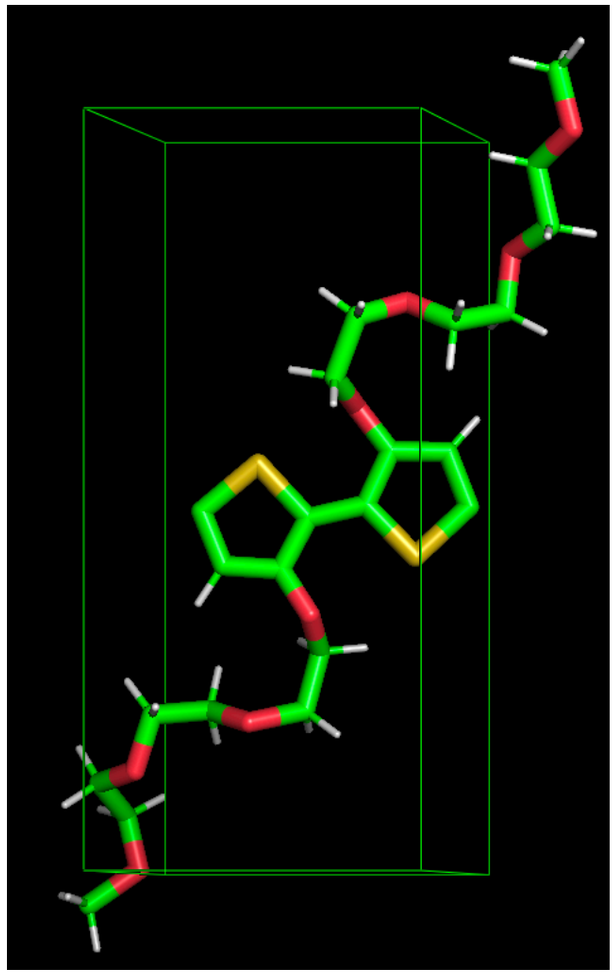
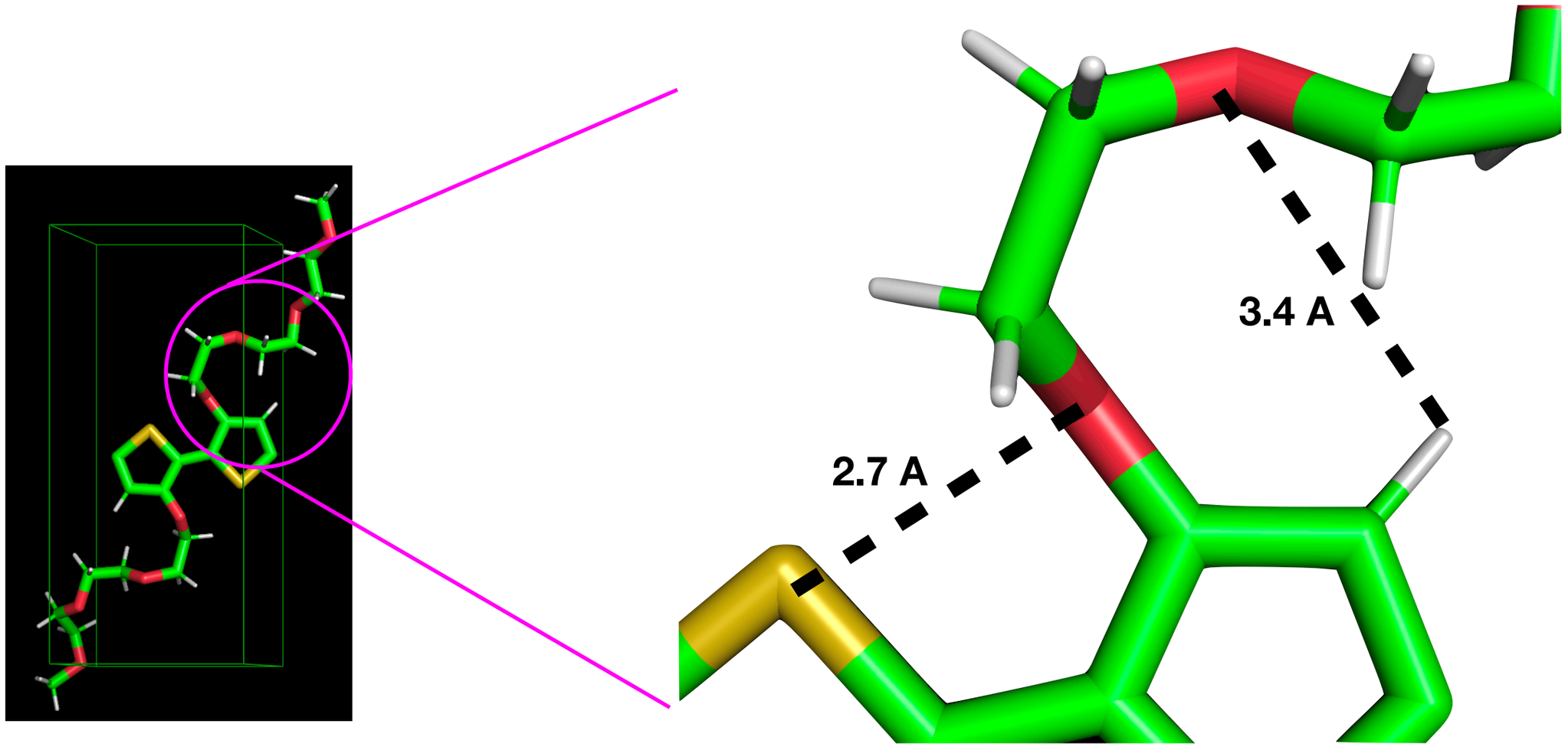
Monomer conformations seen in MD





Where we are at with the crystal structures - A completely resolved crystal structure is seen for the alkylated polymer (cell axis and angles all knows and agrees well with experimental X-ray spectra). Glycolated polymers equilibrate and maintain a crystal structure when run in NVT and the structure agrees with X-ray spectra. A monomer conformer in the structure is shown here. It isn't fully relaxed as I am having issues with the NPT stage of the equilibration, but I am quite confident it is a `good` structure.

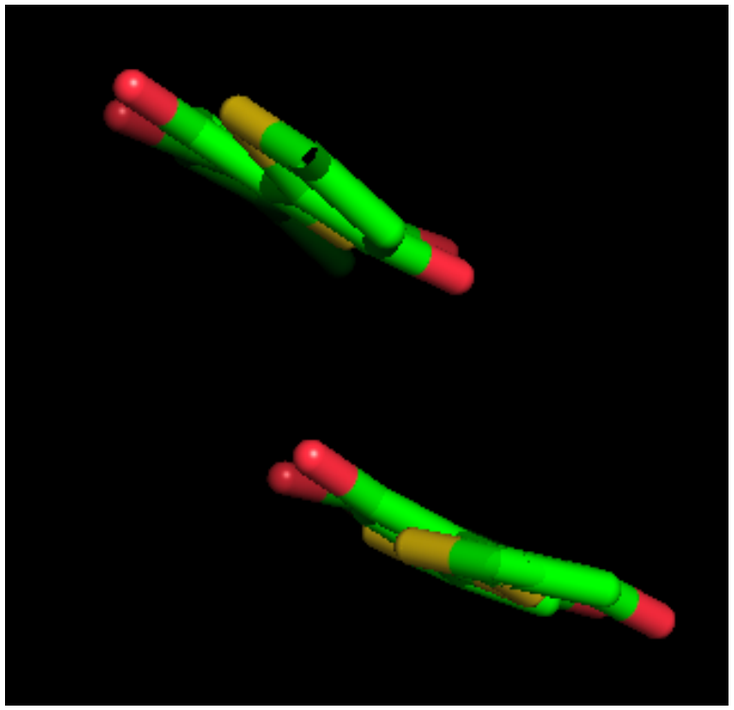
Implications of this side chain conformation and potential reason for it



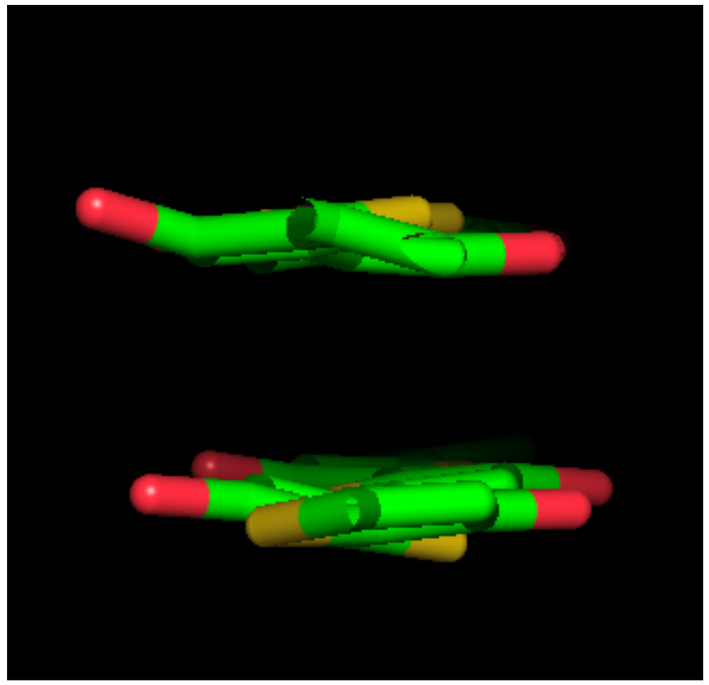
I am have been wondering about the O-H interaction shown here. Whether this has a ‘pinning’ effect of the side chain to the backbone. 3.4A seems a bit long for an O-H interaction, but if I take the structure show here and do an energy minimisation in Gaussian, this length goes down to 2.6A (sort of hydrogen bond length?). together with the first oxygen being ‘pinned’ to the sulphur atom, this might allow for a cavity to form when alkyl spacers are put in the sidechain

What about the pi stack?

Alkylated polymer pi stack



Glycolated polymer pi stack



Cannot confirm pi-stack distance in the glycolated polymer as it hasn’t equilibrated in NPT yet (just NVT). But in the glycolated polymer case there is significant more overlap of the backbones.