Alkoxylated Bithiophene Polymer Crystal

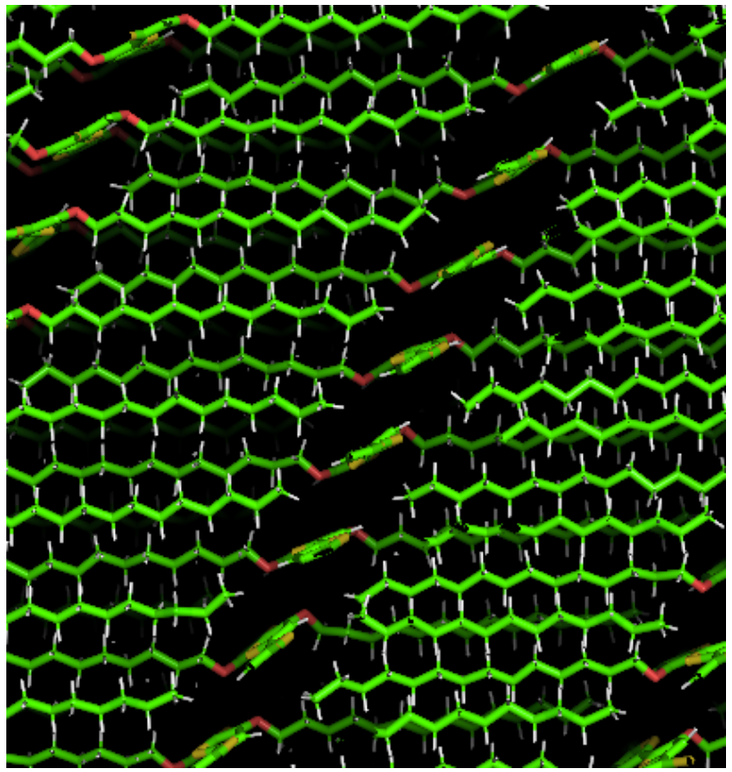
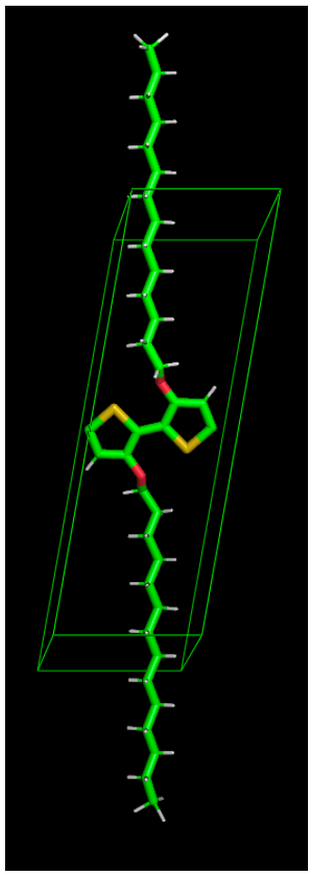
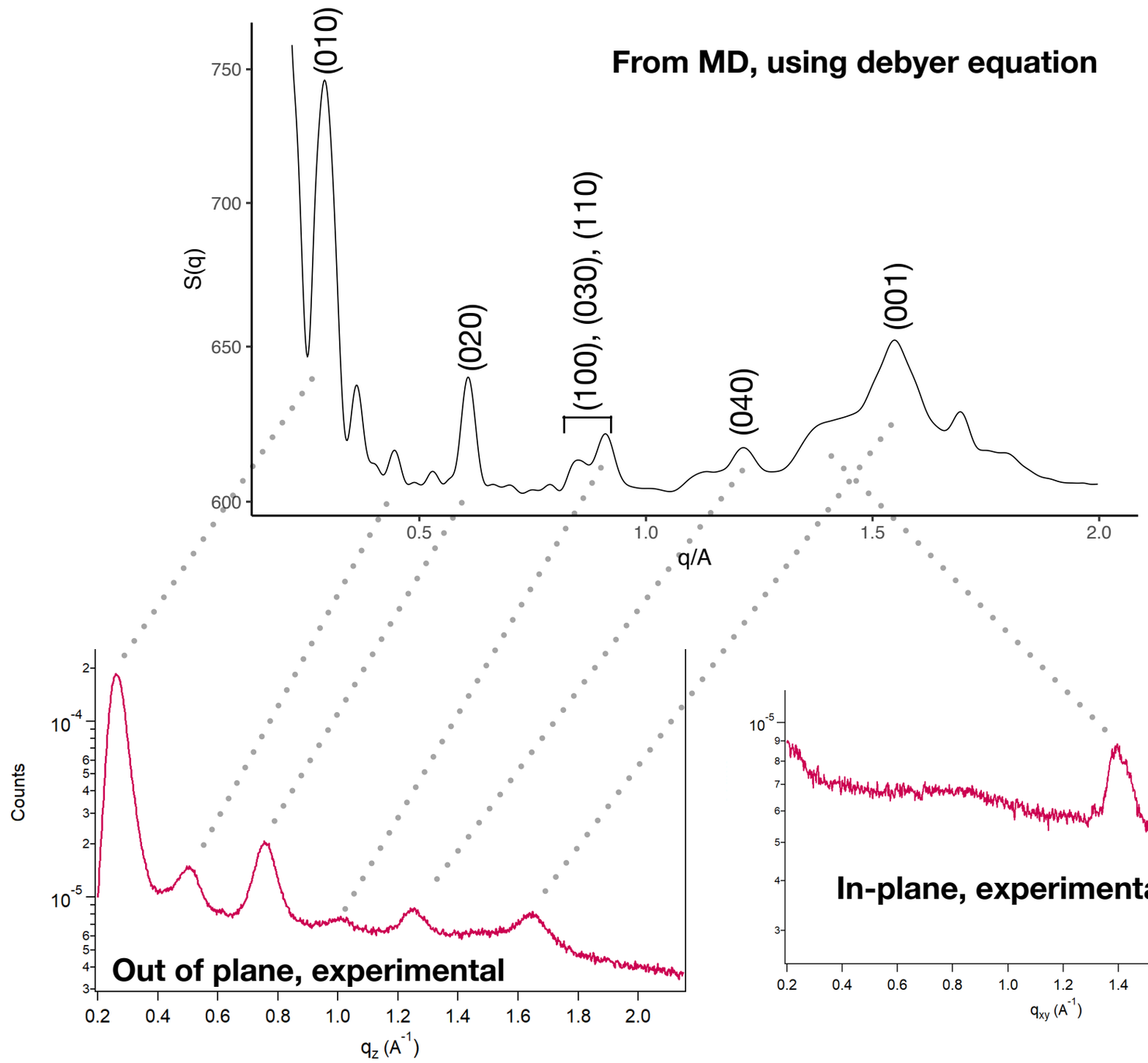


Image of crystal looking along backbones



a = 7.67
b = 21.85
c = 5.84
alpha = 65.27
beta = 79.60
gamma = 92.02
Symmetry = P1



In general the lamellar peaks, (0n0), seem to be at lower q's than in the data, suggesting the model over-predicts the lamellar stack distance. The pi-stack peak, (001), is also at lower q value than the data, showing that it over-predicts the pi-stack distance. Peaks that I haven't labelled are because in the structure factor calculations there are many peaks in that area, so it is unclear which are showing peaks.

Glycoxylated Bithiophene Polymer Crystal

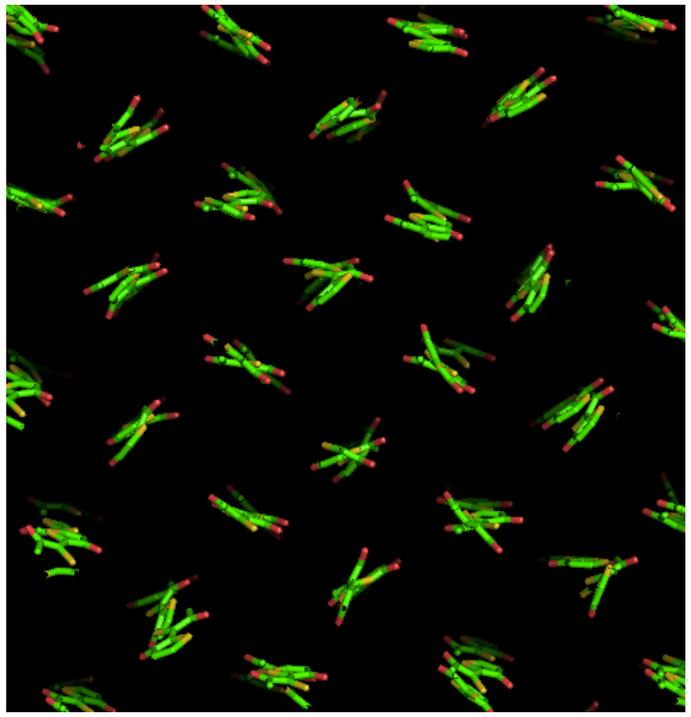
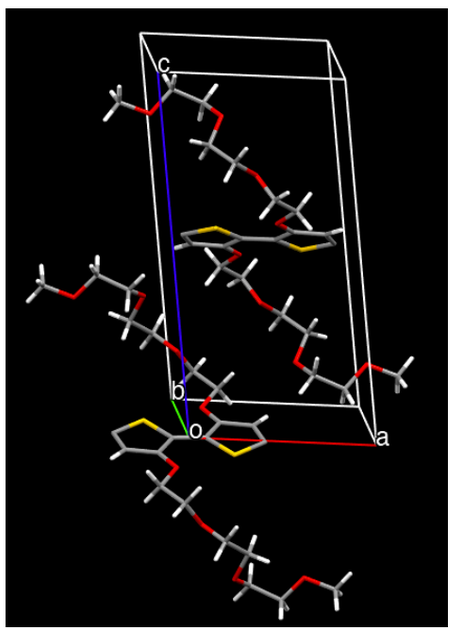
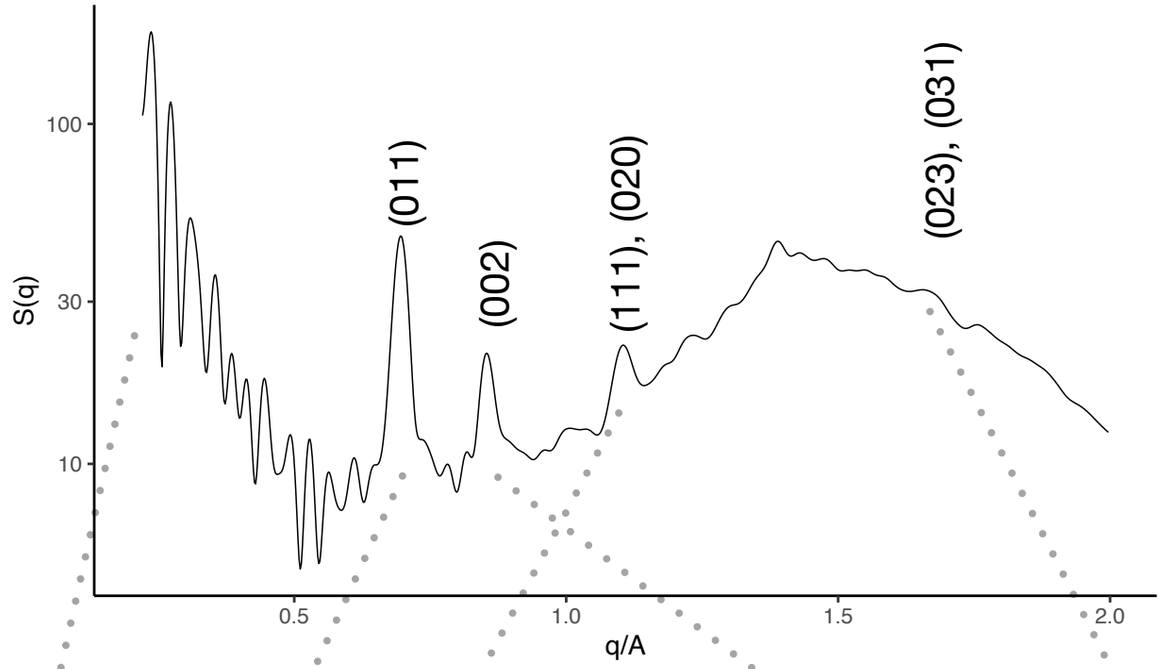
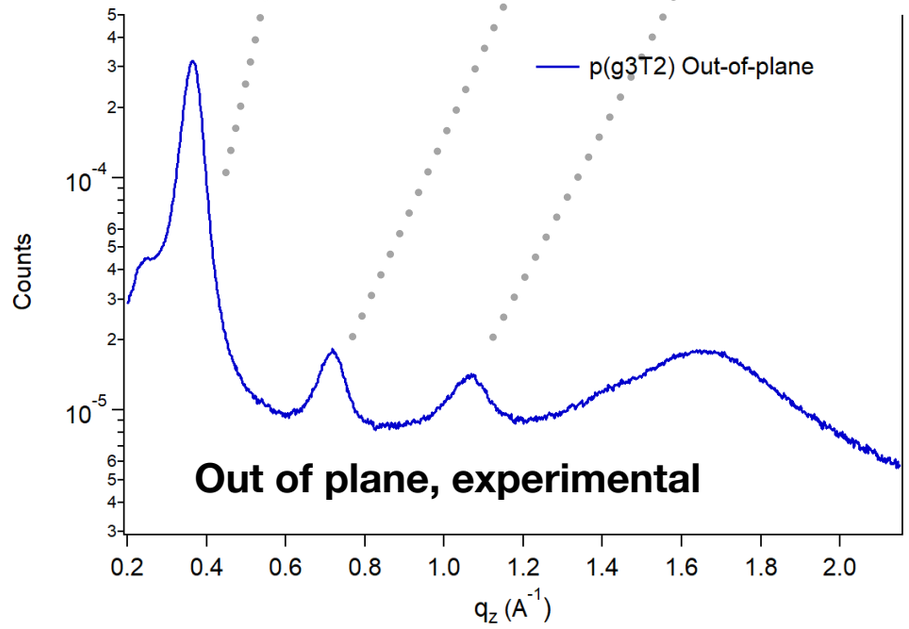


Image of crystal looking along backbones. Only backbone structure shown for clarity

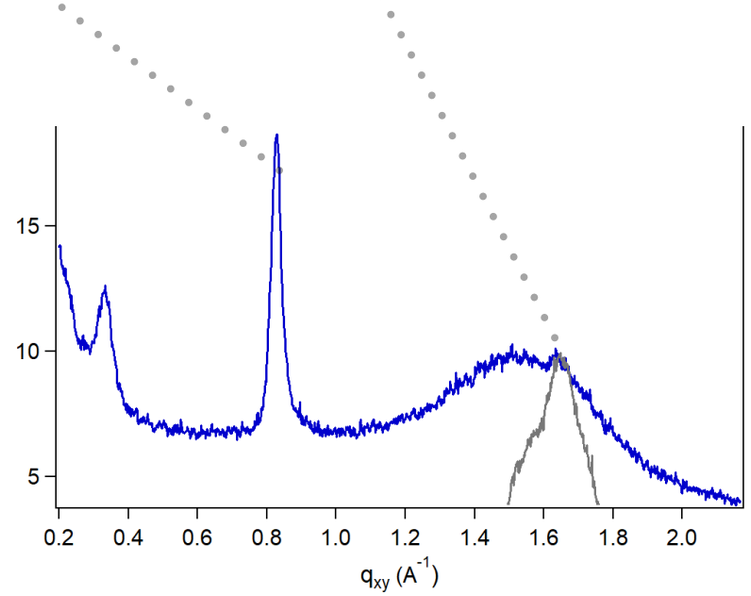


a = 7.96
b = 12.2
c = 15.7
alpha = 90.00
beta = 97.71
gamma = 90.00
Symmetry = P21/n





Out of plane, experimental



In-plane, experimental

Oscillations at low-q in the simulated pattern may be occurring due to artefacts from the limited size of the box that is simulated. The lattice parameters are only approximate, as further analysis of the MD structure files are needed to extract the exact ones. The polymer crystal adopts a herringbone structure, as opposed to a pi stack. Worthwhile to keep testing other structures with pic stacks to see if good agreement is reached with other structures. So far these haven't been stable in MD however.

General formal followed for crystal design

1) Lattice parameters taken from experimental XRD

↓

2) Unit cell angles (alpha, beta and gamma) taken so as to reproduce elements of monomer crystals (eg to maintain nature of pi-stack)

↓

3) Atomic structure inside unit cell is initially the same as for the monomer crystal, with additional rotation so the backbone lies along a unit cell axis (and they link up to form a polymer)

↓

4) Run in MD and observe structural rearrangements (particularly in energy minimisation step and NVT)

↓

Is it stable in NPT? → No → Redesign Crystal, taking into account The structural rearrangements seen in step 4

↓ Yes

Structure obtained, extract cell parameters and see if xrd patterns agree with experiments