

Alkyl Monomer Crystal

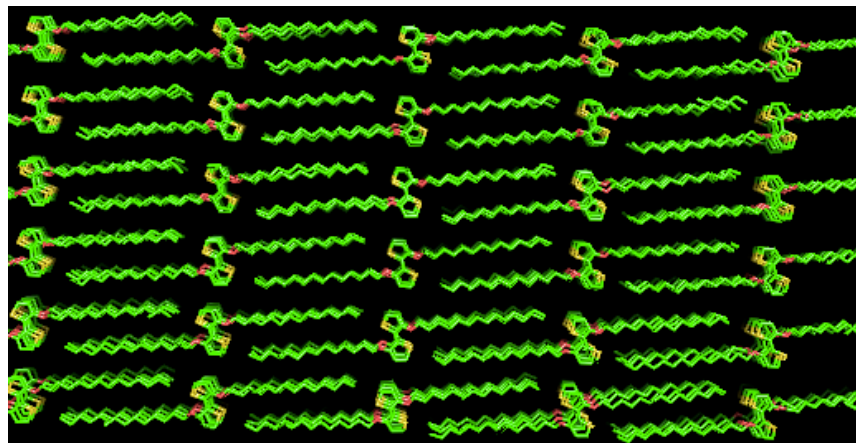
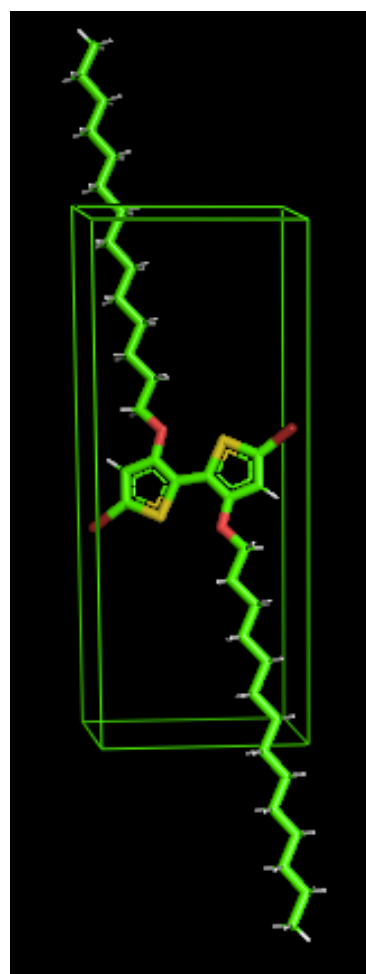


Image of super cell stabilised in MD



Parameters after MD

$$a = 4.16$$

$$b = 9.28$$

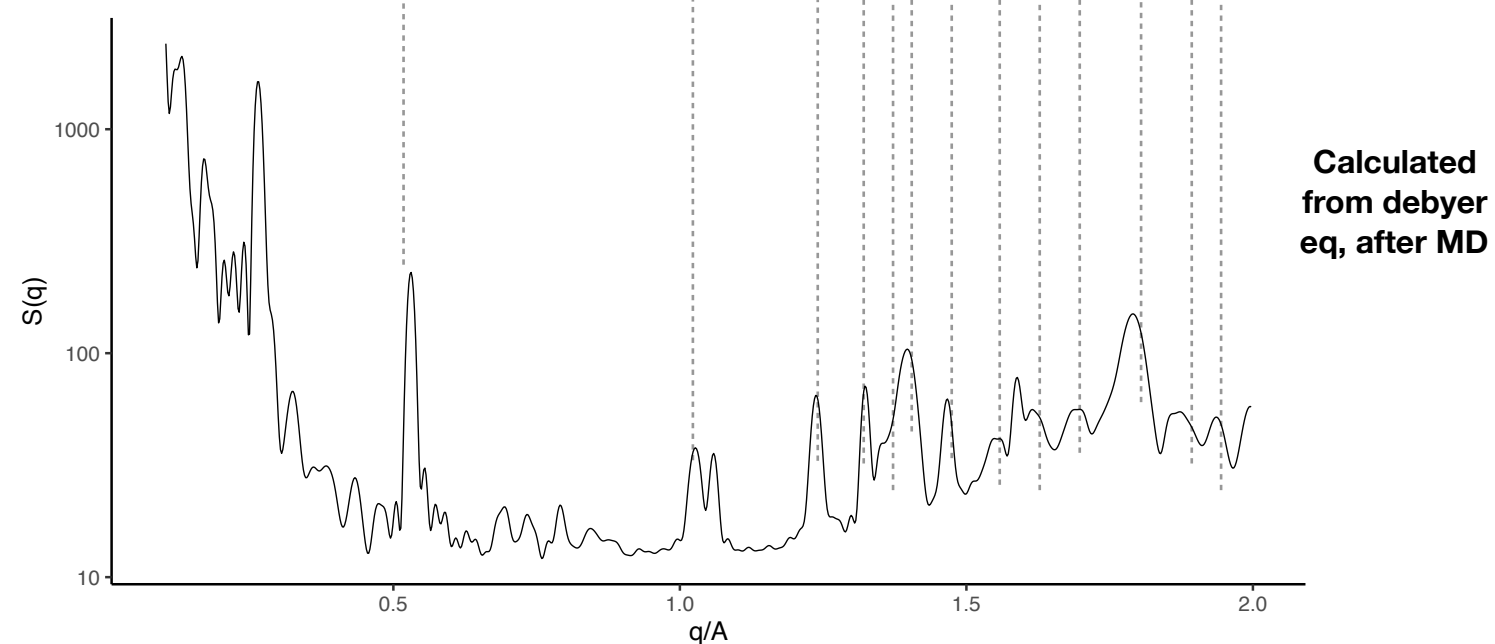
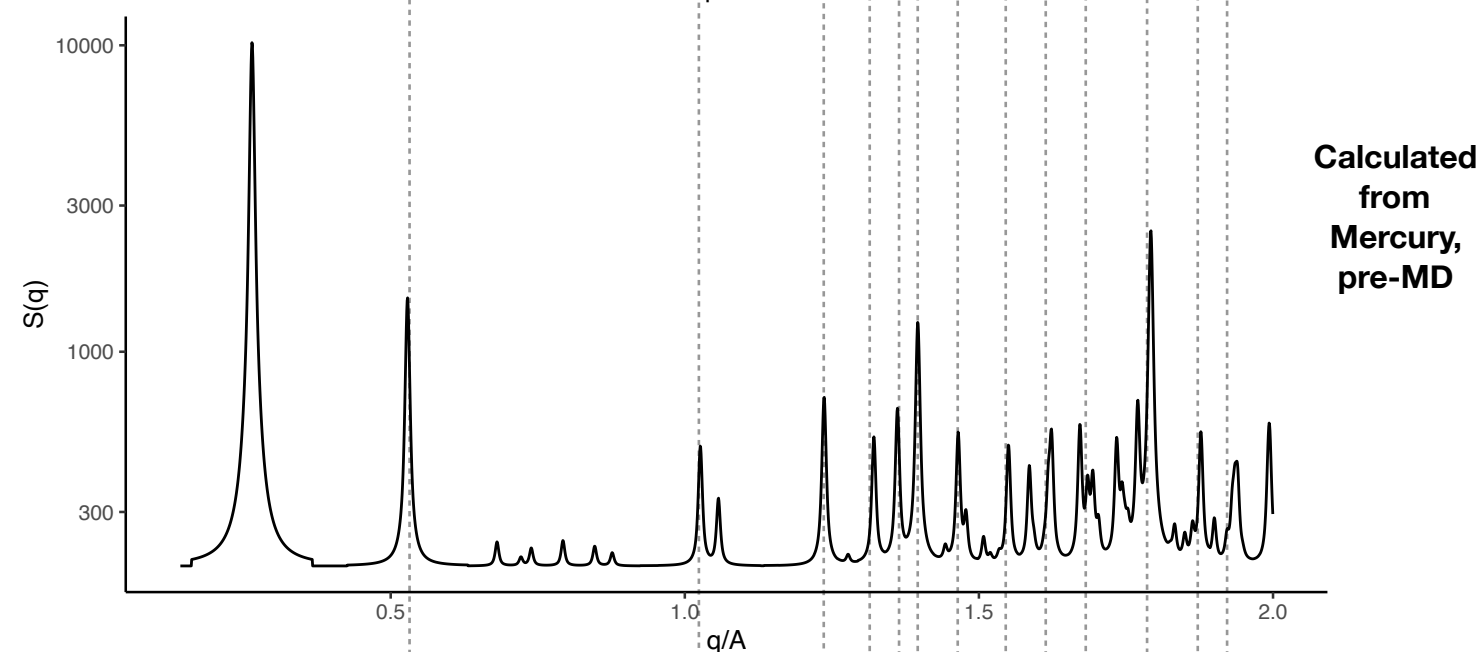
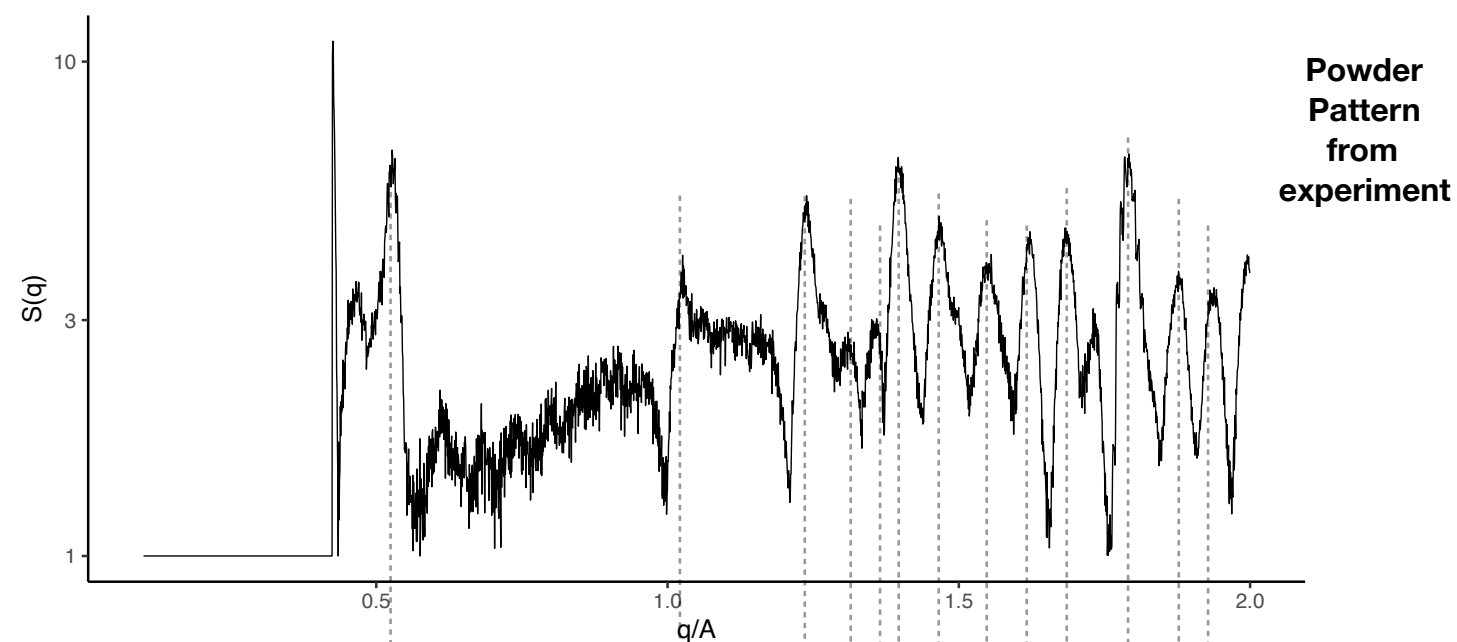
$$c = 23.78$$

$$\alpha = 91.97$$

$$\beta = 91.28$$

$$\gamma = 96.10$$

Strong agreement seen between the experiment, the theoretical structure factor and the calculated structure factor after equilibration in MD.



Glycol Monomer Crystal

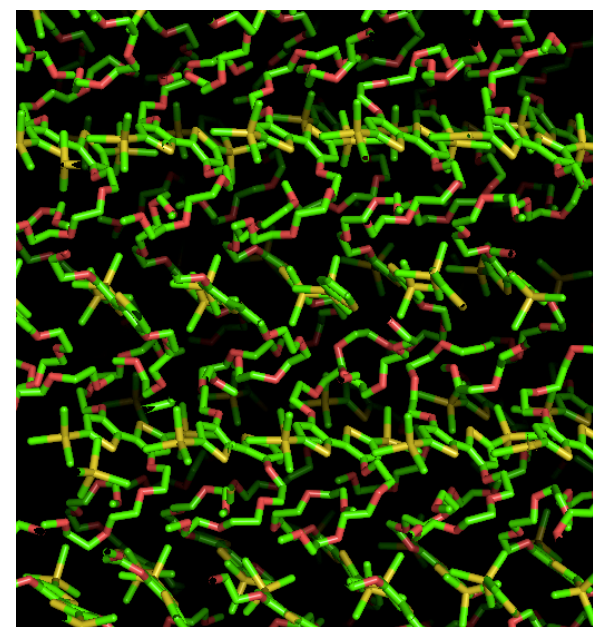
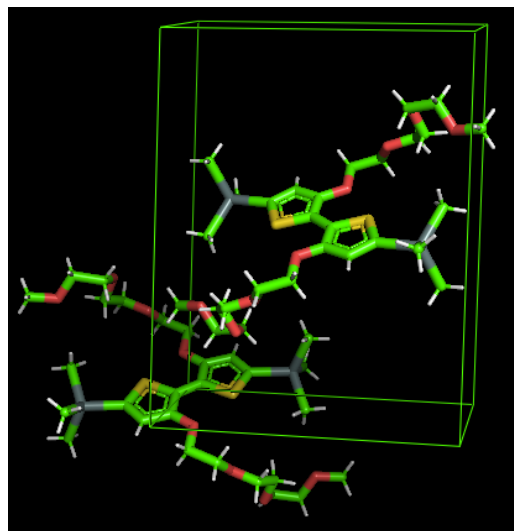


Image of super cell
stabilised in MD



Parameters
after MD

$a = 7.17$
 $b = 14.36$
 $c = 18.45$
 $\alpha = 89.25$
 $\beta = 96.78$
 $\gamma = 91.19$

Strong agreement seen between the
experiment, the theoretical structure
factor and the calculated structure factor
after equilibration in MD.

