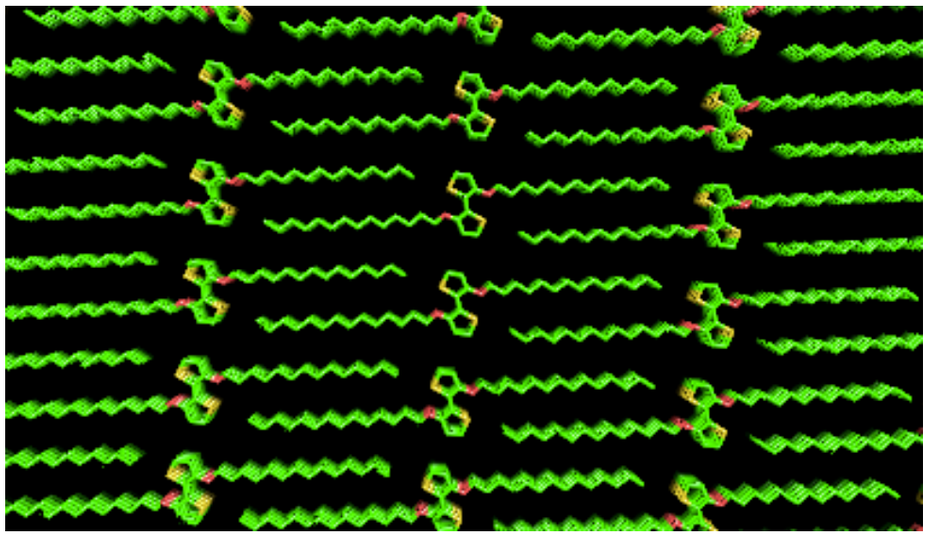
Annealing protocol -

1) Heat from 300K to annealing temperature over 1ns
2) Cool from annealing temperature to 300K at a rate of 10K/1ns

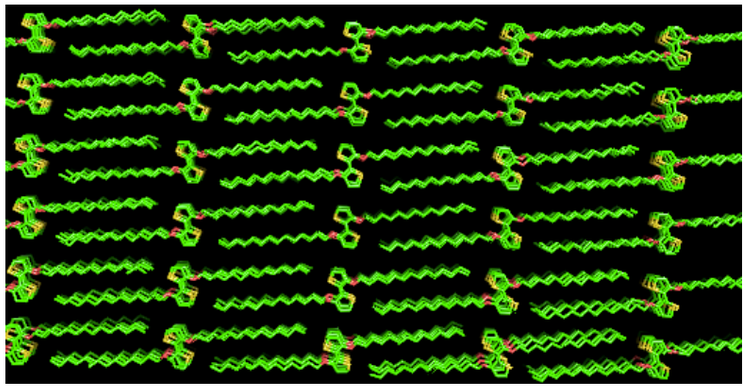
Before MD



a = 4.17
b = 9.30
c = 23.80
alpha = 91.86
beta = 91.48
gamma = 96.45

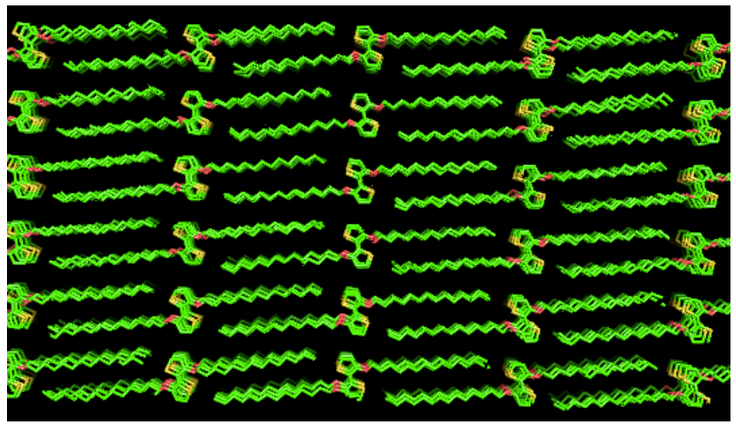
After MD

Without annealing



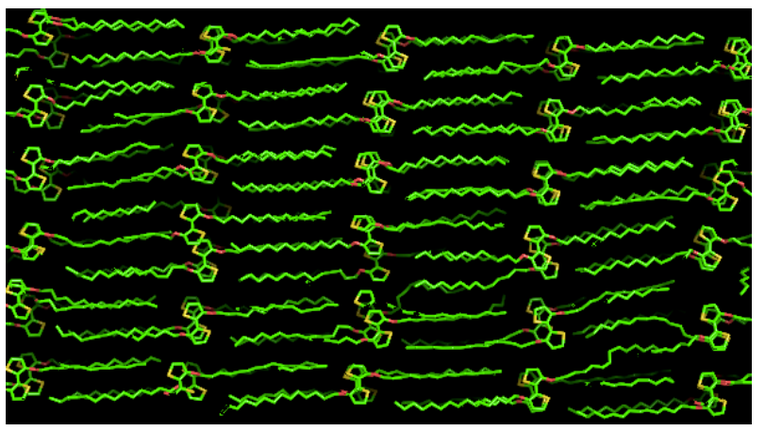
a = 4.16
b = 9.28
c = 23.78
alpha = 91.97
beta = 91.28
gamma = 96.10

Annealed at 350K



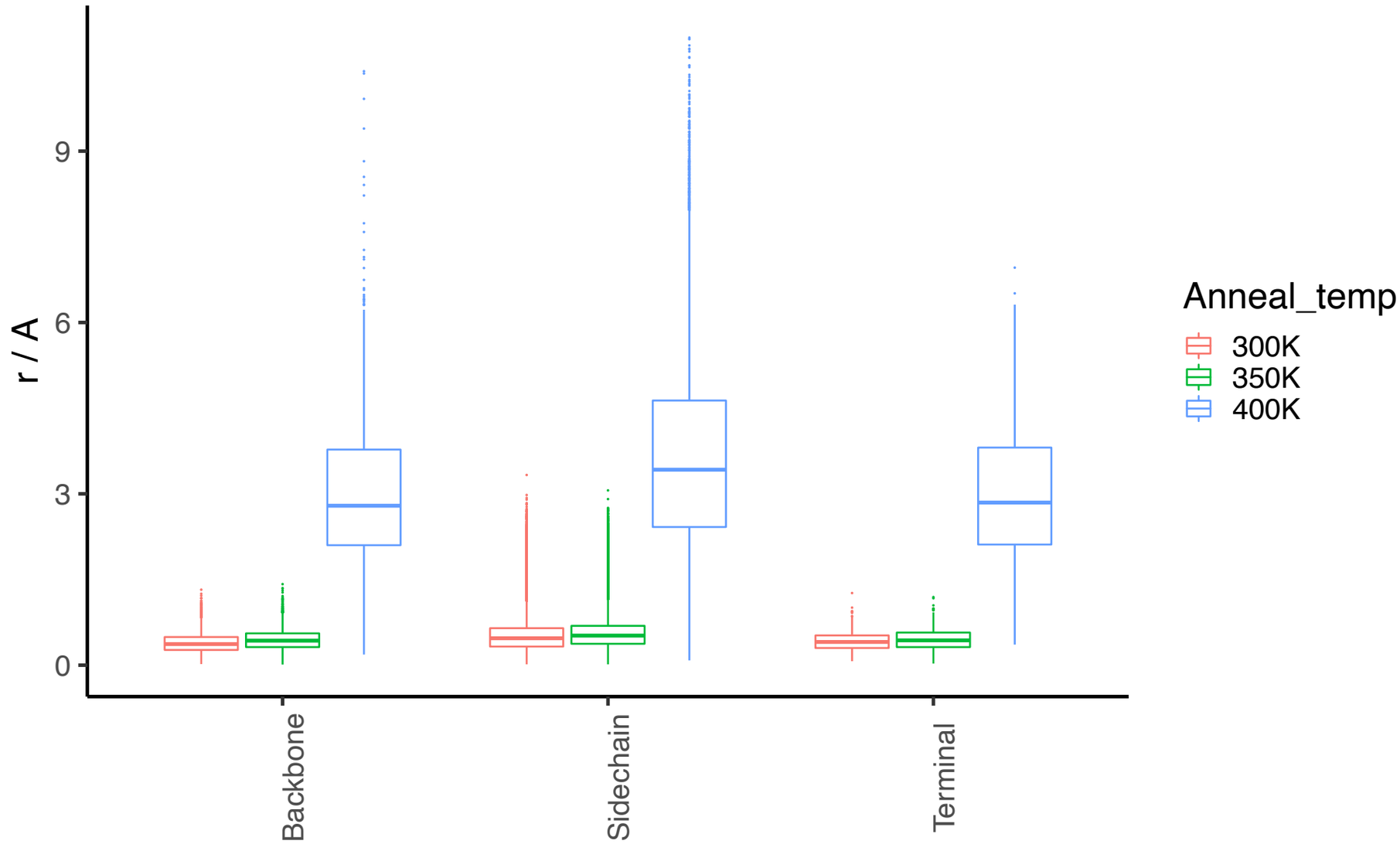
a = 4.16
b = 9.28
c = 23.76
alpha = 92.21
beta = 91.70
gamma = 97.13

Annealed at 400K

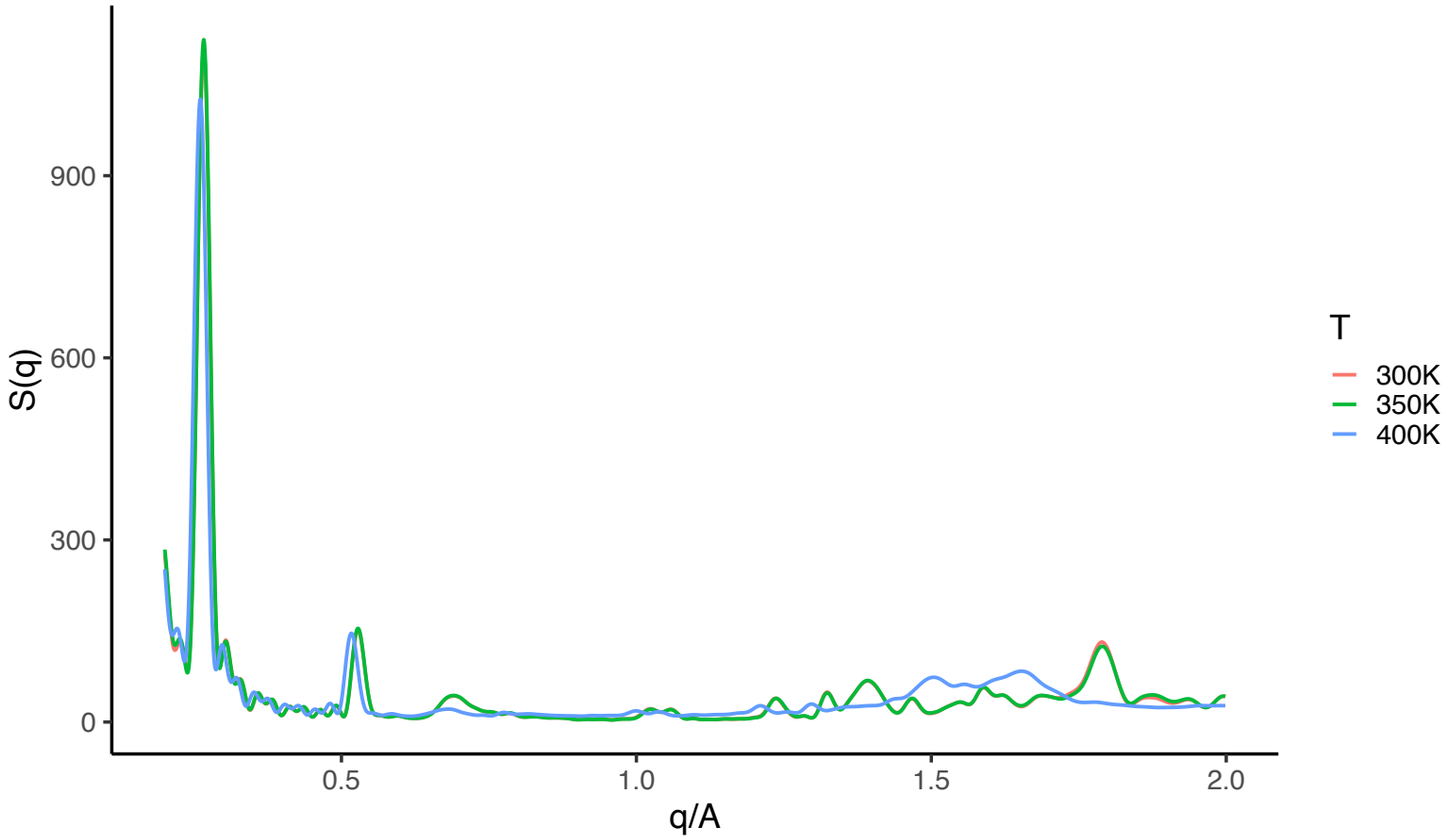


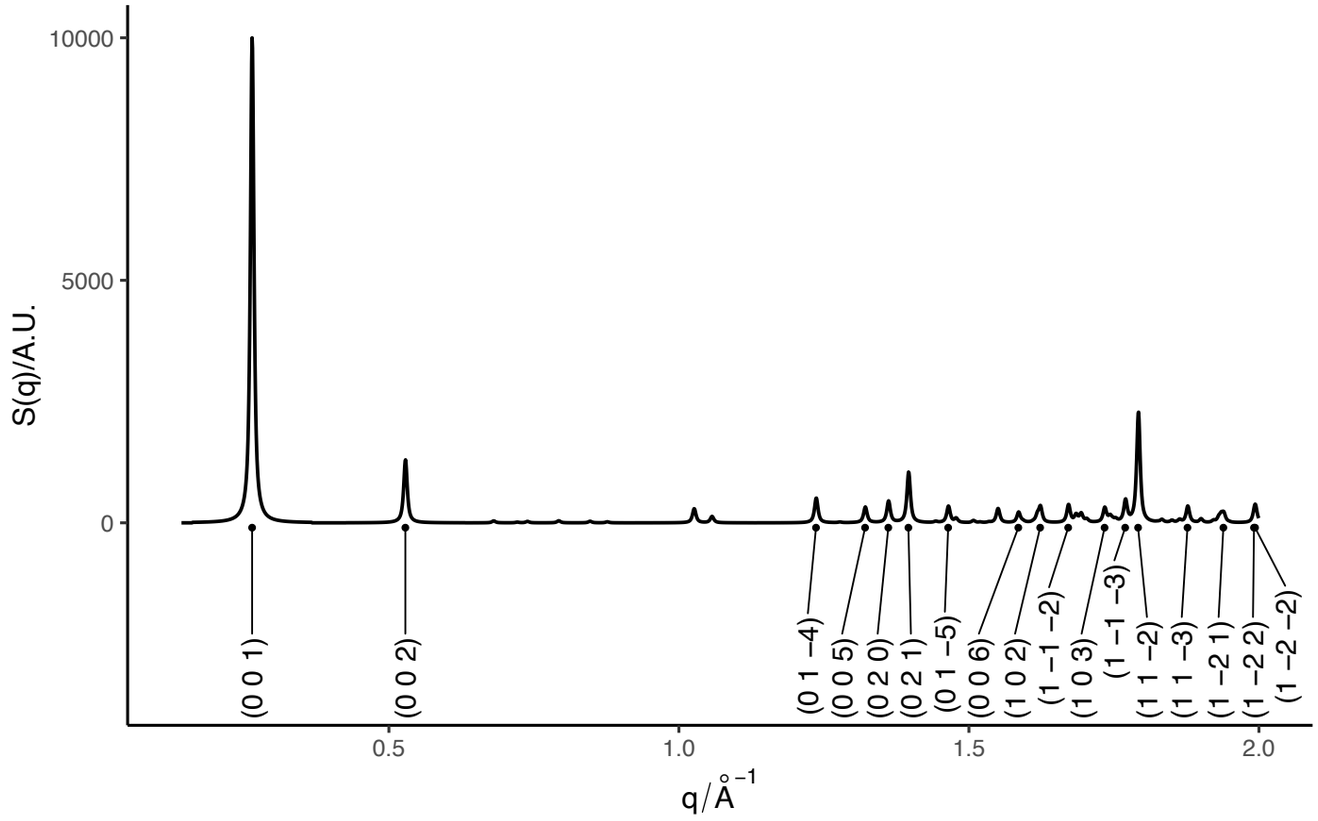
a = 4.25
b = 9.48
c = 24.29
alpha = 90.71
beta = 88.89
gamma = 96.21

r = the displacement of an atom at time t, from its initial position at t=0 (where it is perfectly crystalline)



Crystal structure resistant to annealing at 350K, however crystallinity is slightly broken when annealed at 400K. Average atomic displacements for the non-annealed simulation and the annealed simulation at 350K are around 1+/-1A, which is very small.





The same is seen in the simulated spectra from MD (top). When compared to the spectra from Mercury (bottom) peaks are preserved. Many of the peaks match up, so the crystal structure hasn't changed. When annealed at 400K, the higher q-peaks change as expected. Low-q peaks are still preserved, so long range order is preserved even when annealed at 400K.