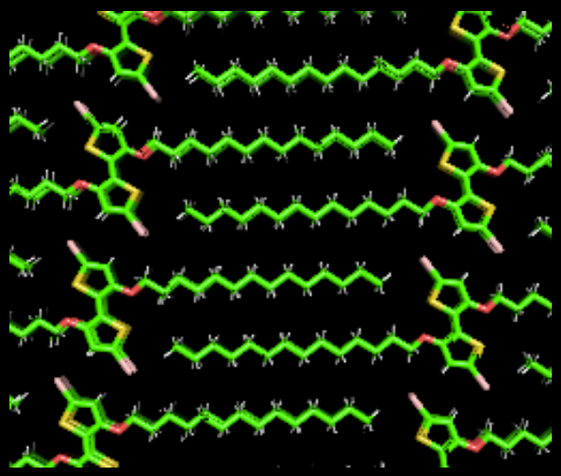
Alkylated Crystal Structure (units in angstrom)

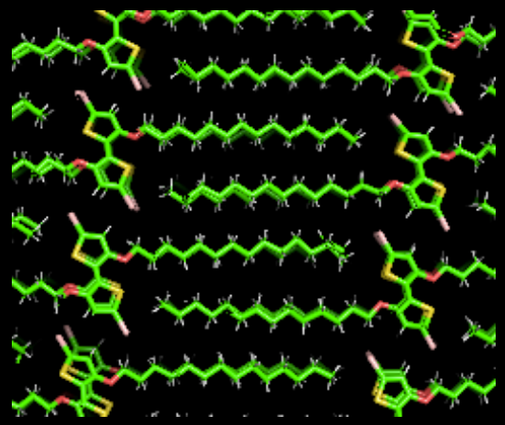
Run times up to 60ns

Before



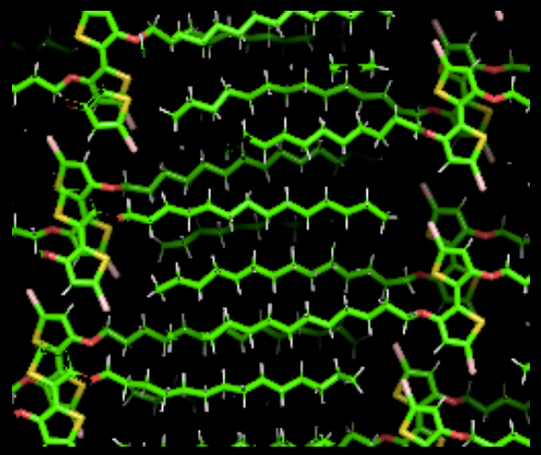
a = 4.165
b = 9.298
c = 23.806
Alpha = 91.86
Beta = 91.48
Gamma = 96.45

No annealing



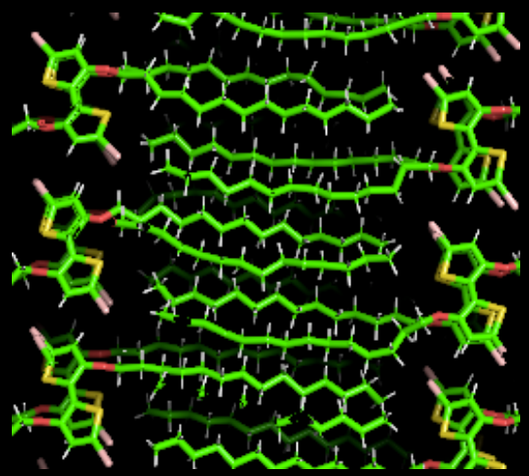
a = 4.16
b = 9.28
c = 23.76
Alpha = 91.61
Beta = 91.44
Gamma = 96.39

Annealed at 350K



a = 4.23
b = 9.46
c = 24.23
Alpha = 92.90
Beta = 89.80
Gamma = 96.24

Annealed at 400K

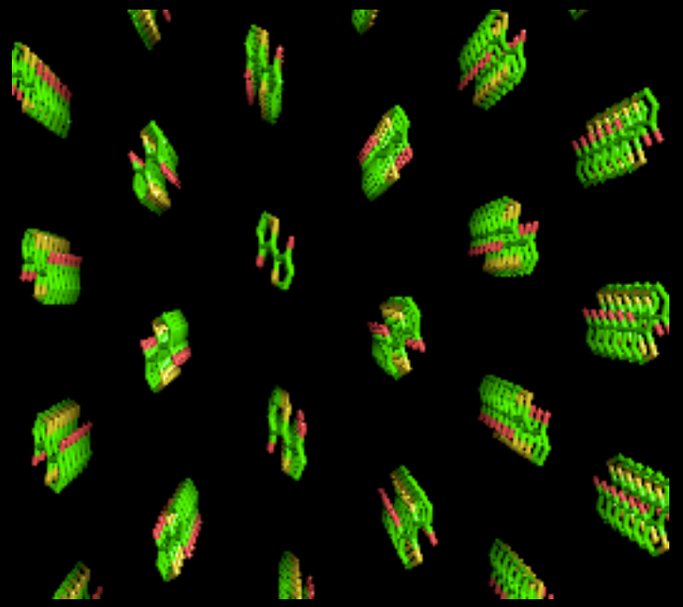


a = 4.21
b = 9.39
c = 24.05
Alpha = 93.55
Beta = 89.69
Gamma = 94.87

Resilient to Annealing

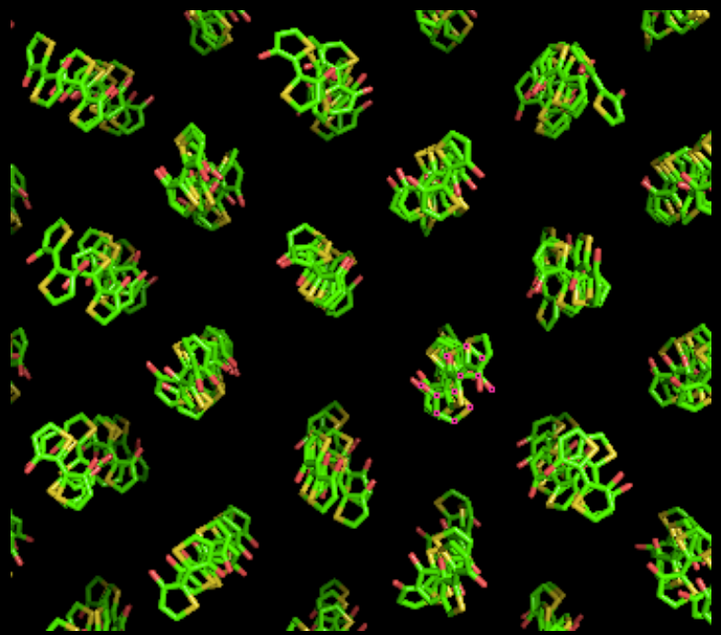
Glycolated Crystal Structure - re-run with better optimised C-C-O Angle parameters

Before (only backbones shown)



20ns

After (only backbones shown)



a = 7.01
b = 14.02
c = 18.01
Alpha = 90.00
Beta = 97.71
Gamma = 90.00

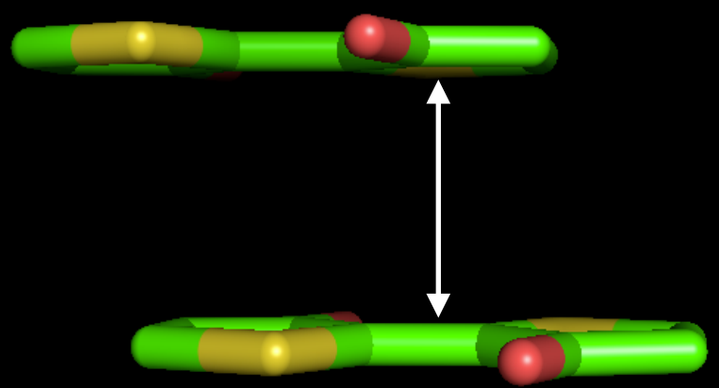
a = 7.21
b = 14.44
c = 18.55
Alpha = 90.00
Beta = 97.71
Gamma = 90.00

Atomic Displacements
dx = 0.461 +/- 2.30
dy = 0.501 +/- 1.90
Dz = 0.871 +/- 1.91

Much more stable than last week

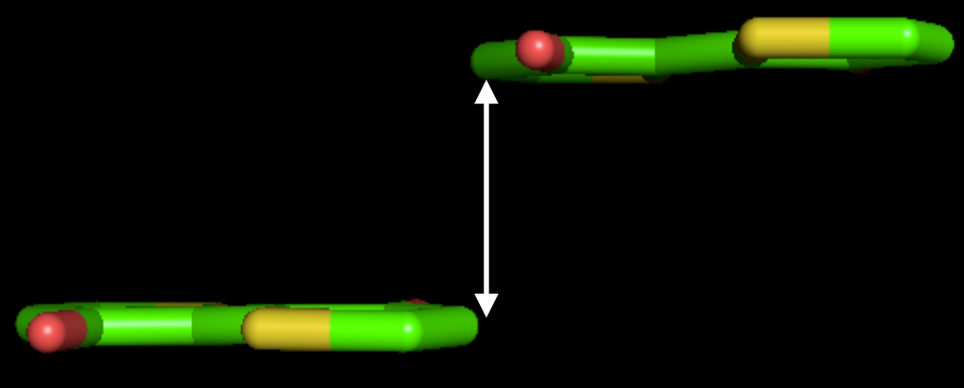
Pi-pi spacing

Alkylated structure



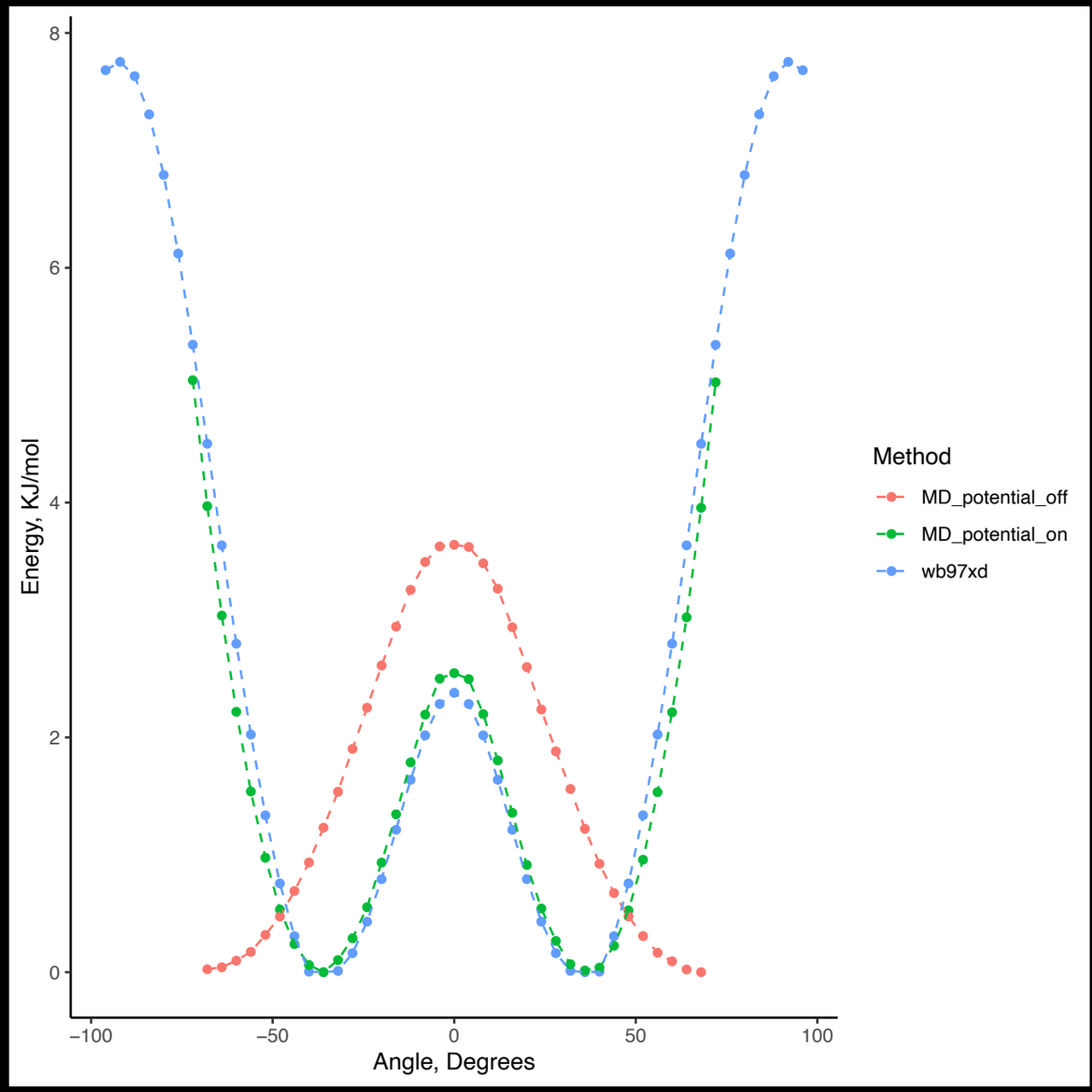
Pi-pi distance before - 3.58
Pi-pi distance after MD - 3.67

Glycolated structure



Pi-pi distance before - 3.64
Pi-pi distance after MD - 3.66
Does this even count as a pi-stack?

Outer dihedral scan now fitted also. Doing CCSD and MP2/4 to check the barrier height.



Let’s do some polymer simulations!