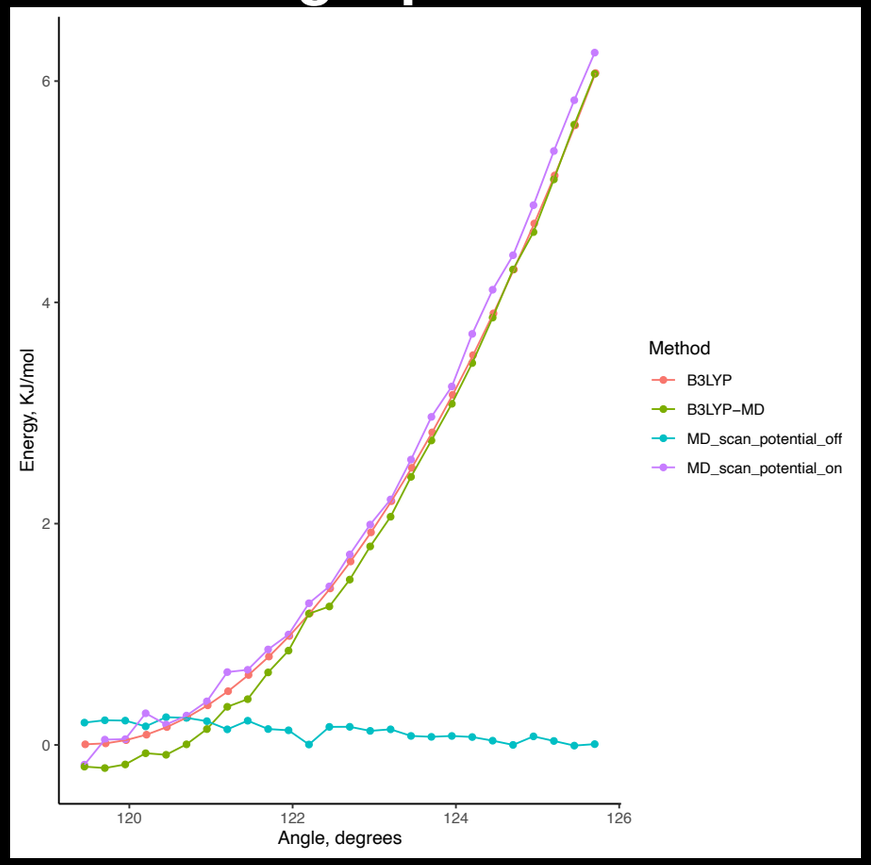
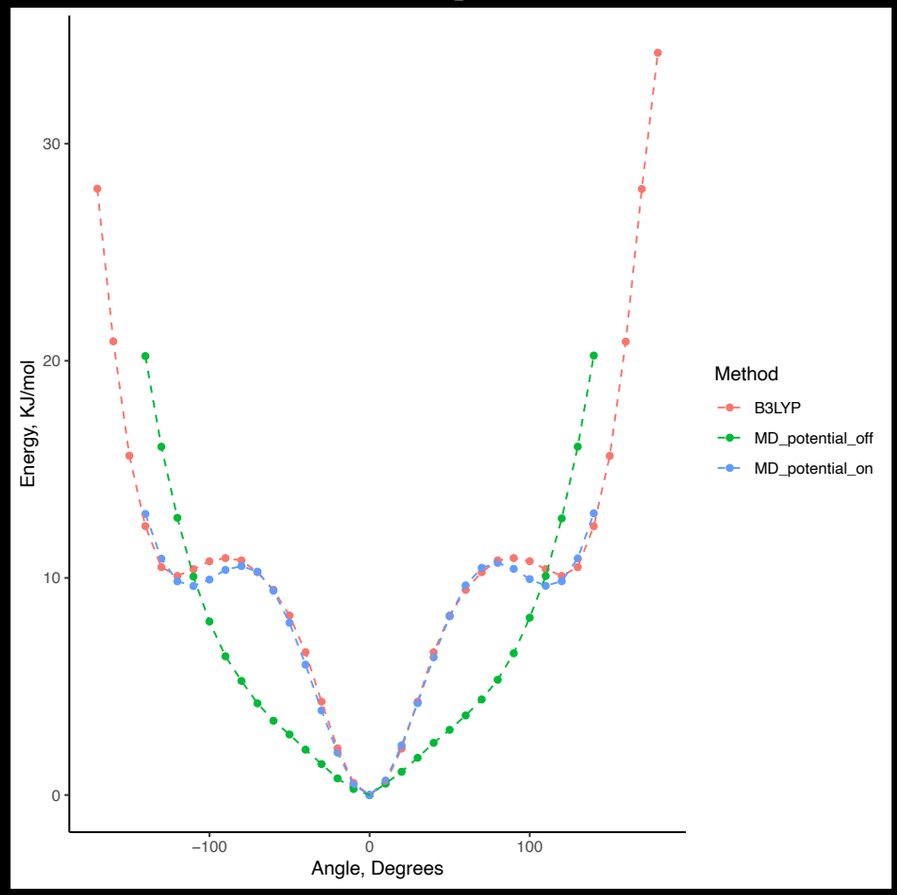
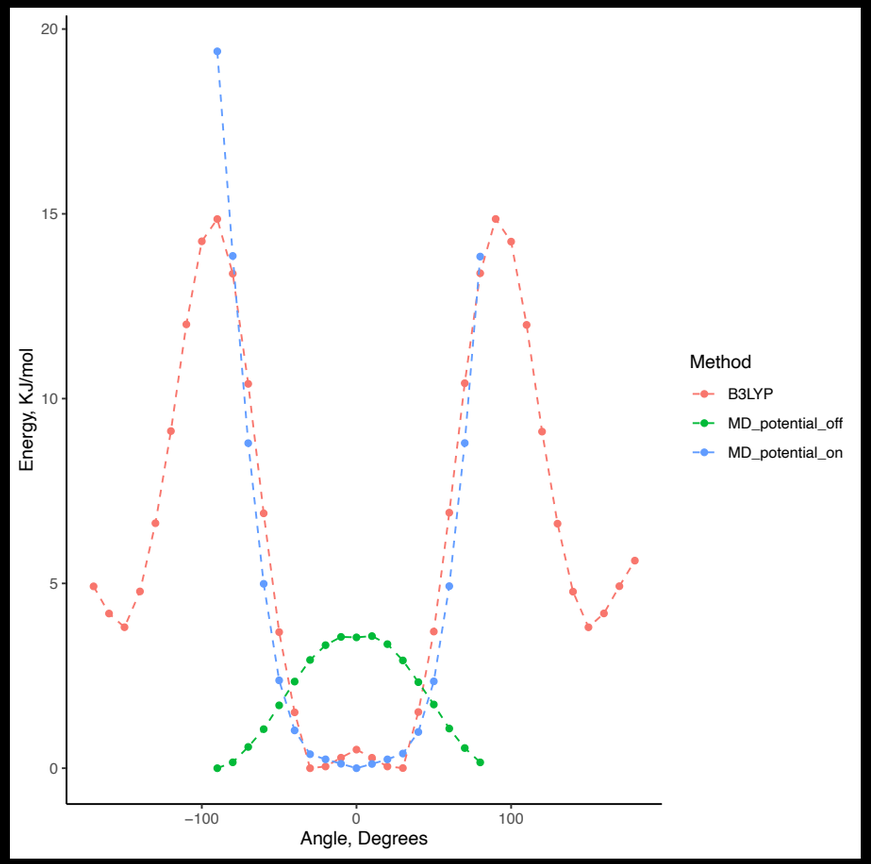
C-C-O Angle potential



Inner dihedral potential

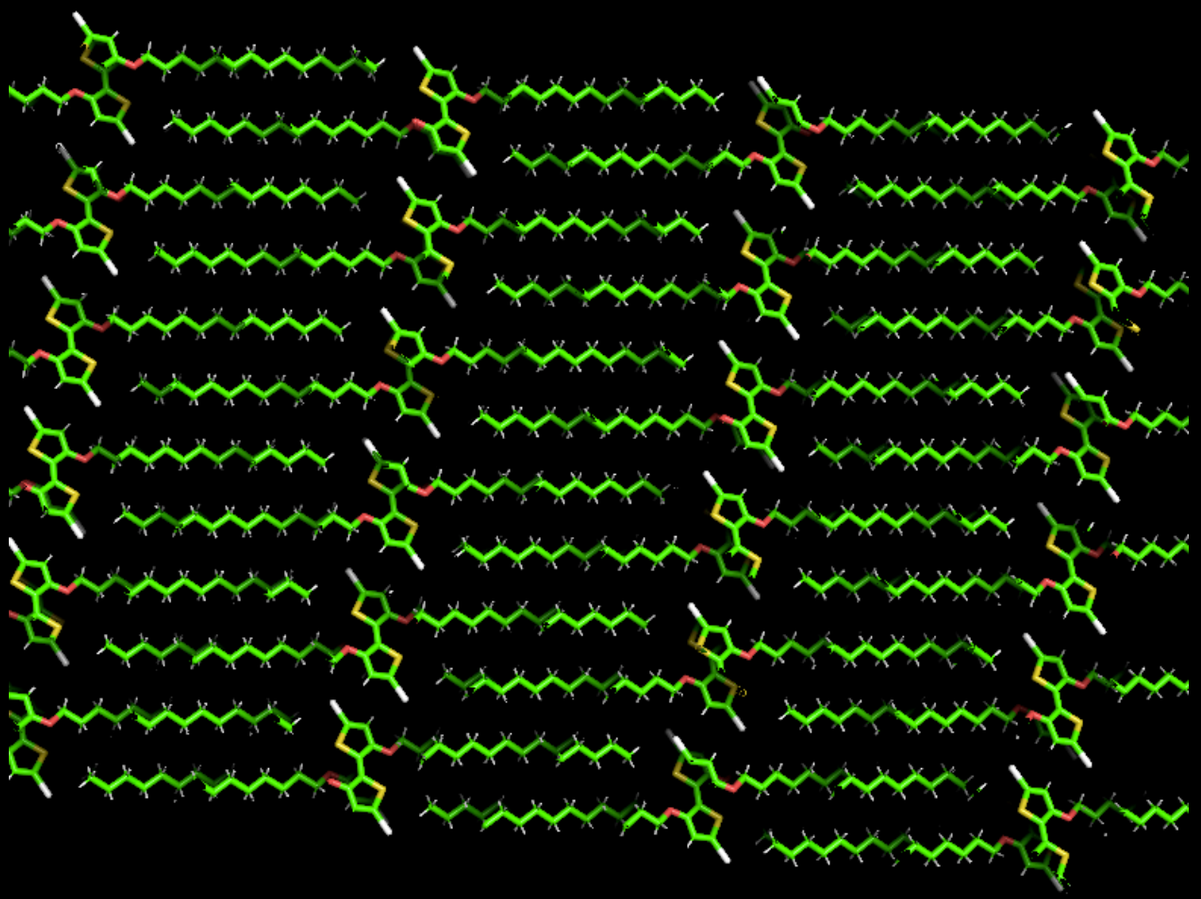


Outer dihedral potential

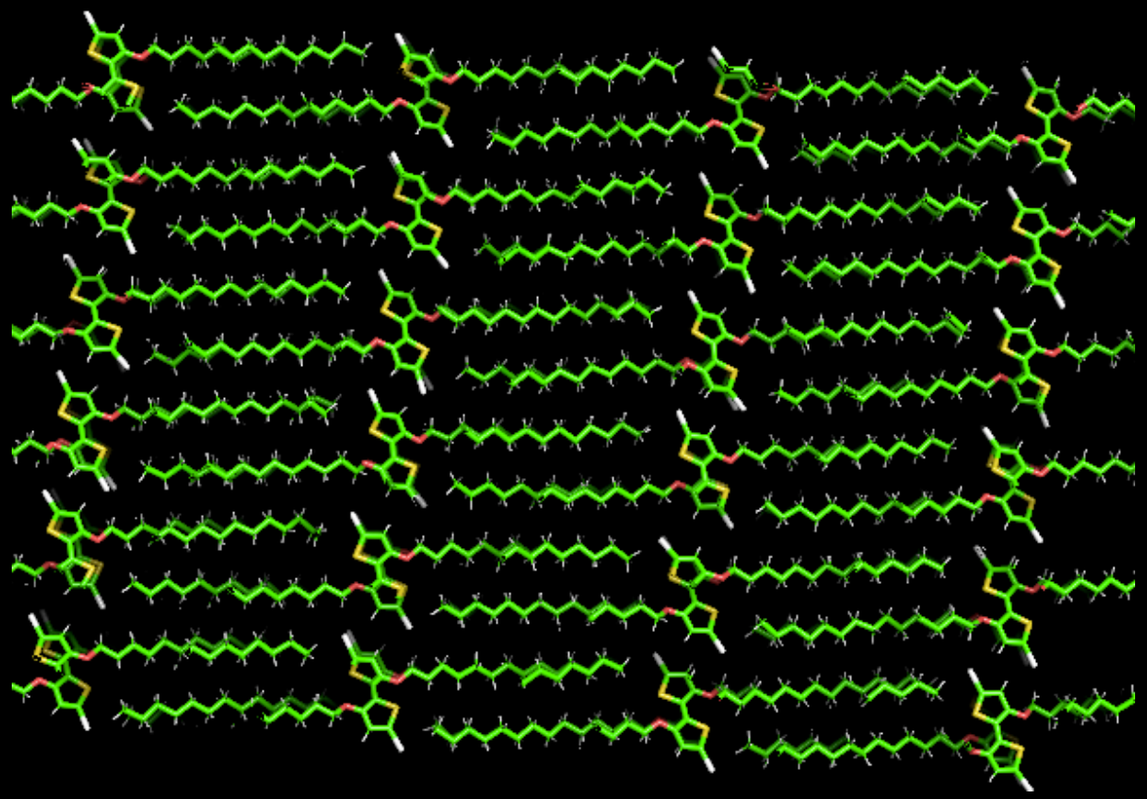


Alkylated side-chains, Bromine terminals

Before MD



After 500ps



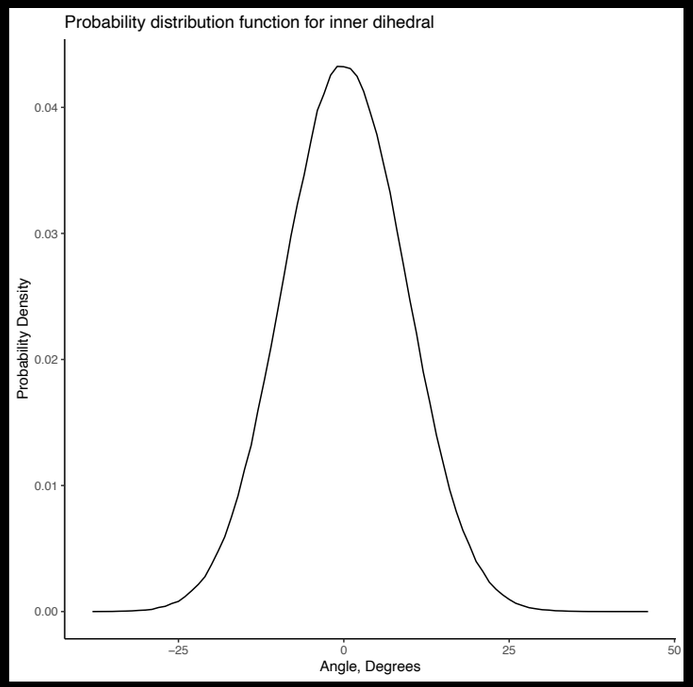
- crystal structure maintained on the nanosecond time scale

Lattice parameters before -
a = 4.165
b = 9.298
c = 23.806
alpha = 91.86
beta = 91.48
zeta = 96.45

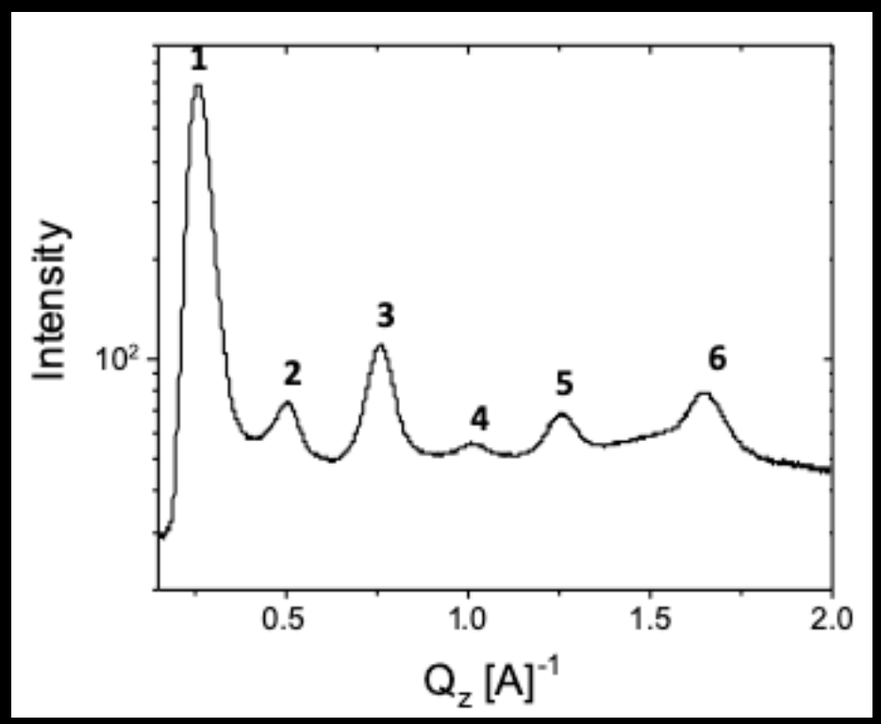
Lattice parameters after -
a = 4.157
b = 9.281
c = 23.763

Lattice parameters accurate to within 0.2%

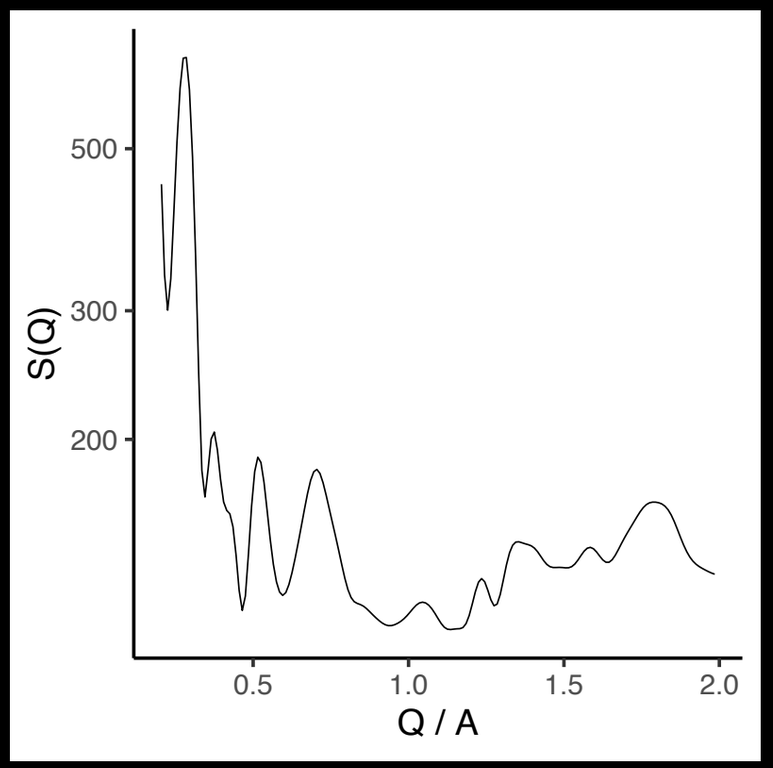
Prob. Distribution fn. for inner dihedral



Alex' x-ray pattern (experiment)



My x-ray pattern (MD)



Fairly good agreement (peak intensity agreement could be improved with bigger simulation box)