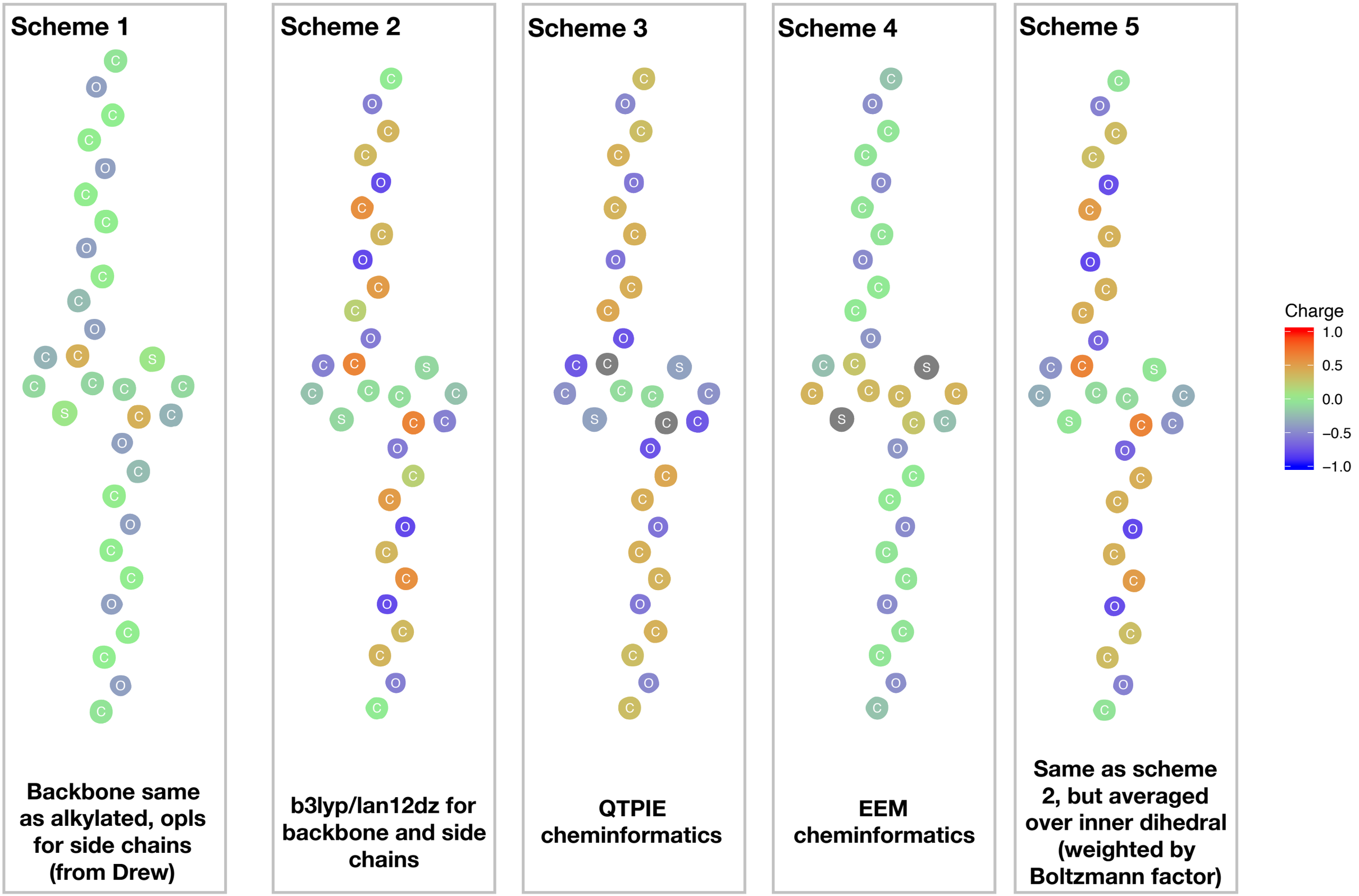
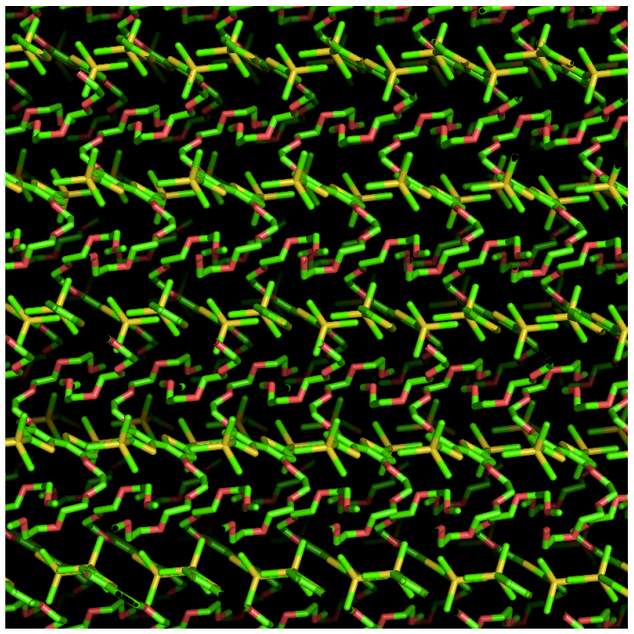
Glycolated Monomer Crystal Structure
Different Charge Schemes



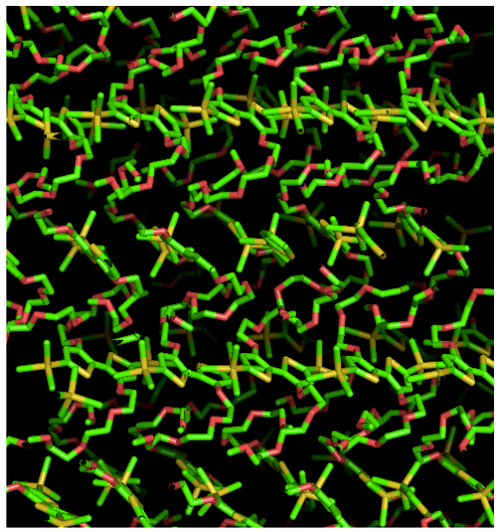
MD stability results

Before MD



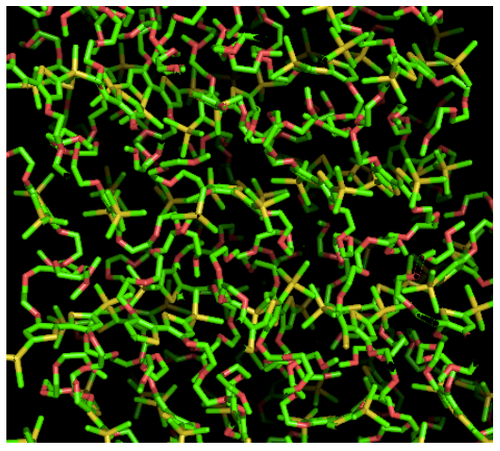
a = 7.01
b = 14.03
c = 18.02
α = 90.00
β = 97.71
γ = 90.00

CP scheme 1



a = 7.17
b = 14.36
c = 18.45
α = 89.25
β = 96.78
γ = 91.19

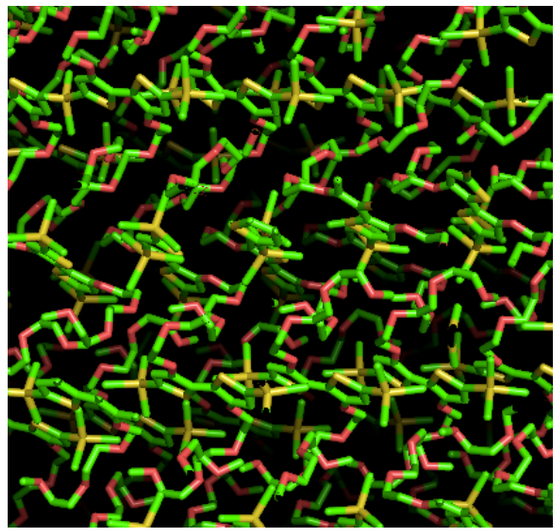
CP scheme 2



a = 7.21
b = 14.43
c = 18.54
α = 90.52
β = 101.49
γ = 93.20

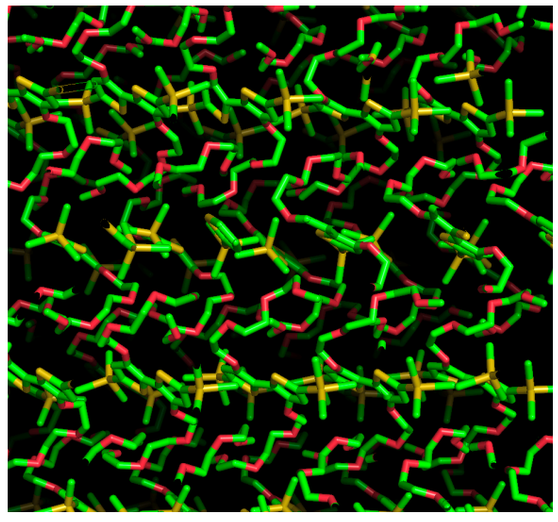
CP scheme 3 crashes!

CP scheme 4



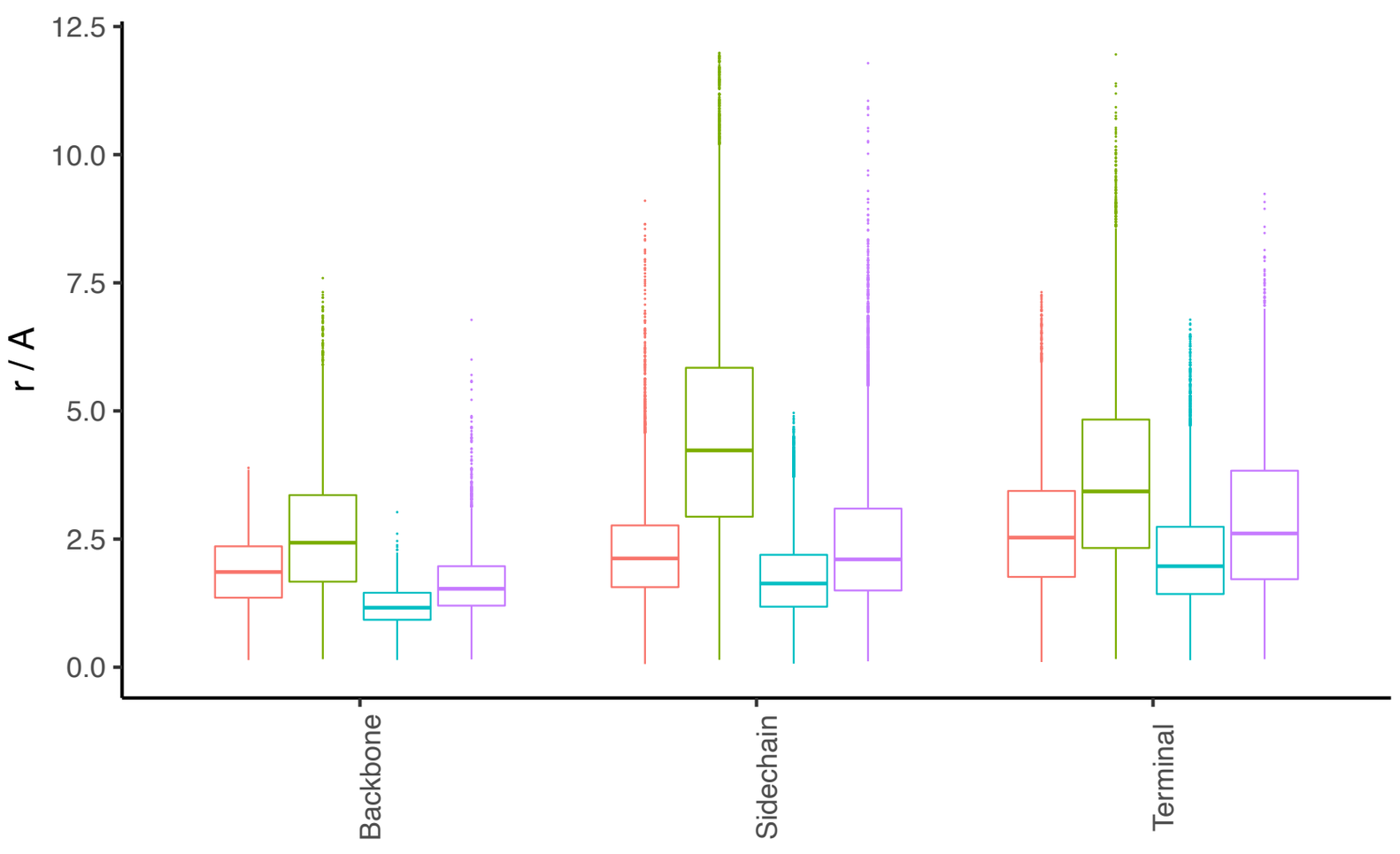
a = 6.99
b = 14.00
c = 17.97
α = 90.06
β = 98.61
γ = 90.14

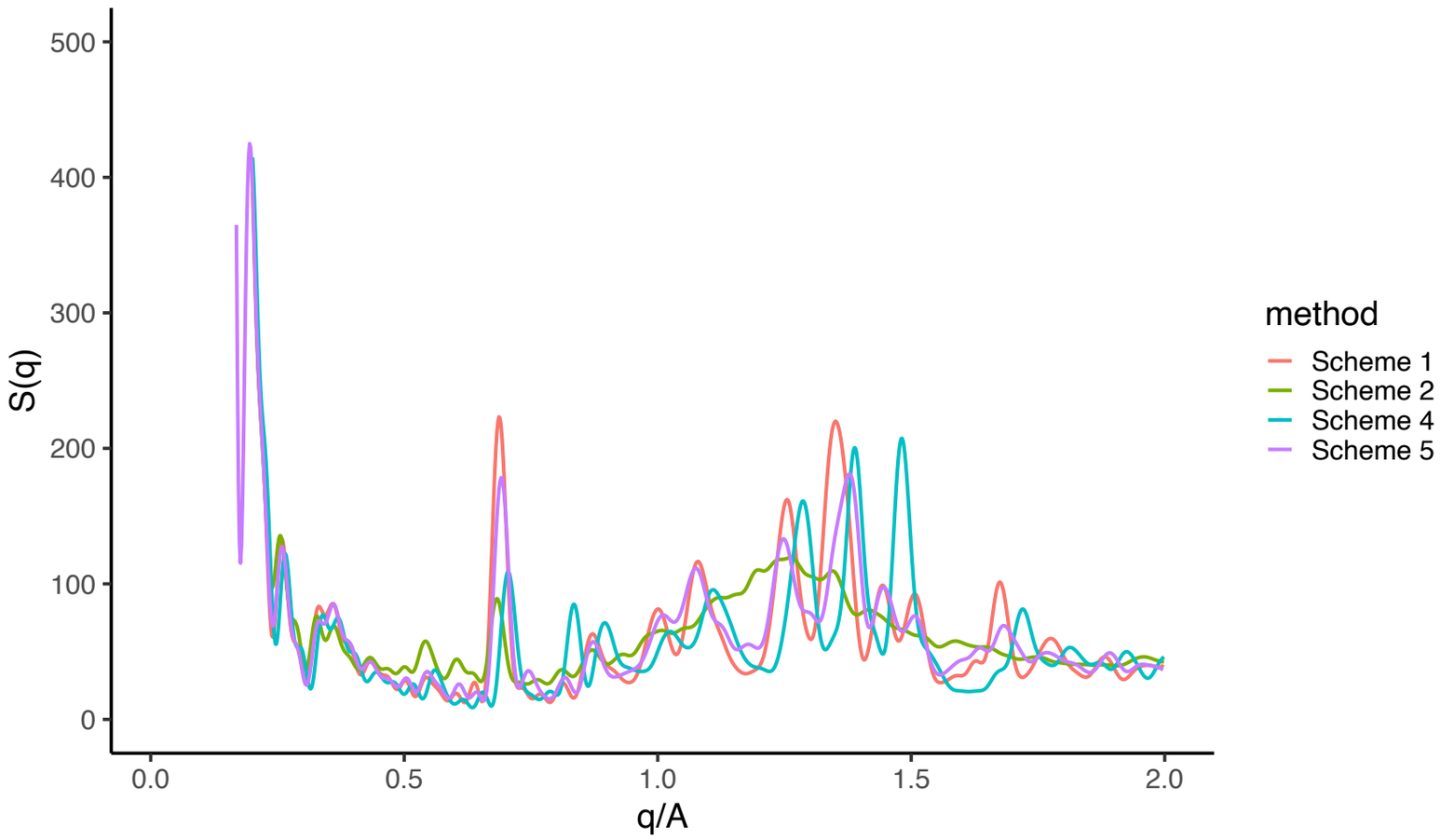
CP scheme 5



a = 7.15
b = 14.32
c = 18.38
α = 90.63
β = 95.90
γ = 90.94

Simulations using parameters from b3lyp/lan12dz perform badly (scheme 1). Significantly improved if averaged over the dihedral (scheme 5). Both simulations using opls and EEM do well (scheme 2 and 4). The EEM method actually slightly outperforms opls (more easily seen on the next slide)

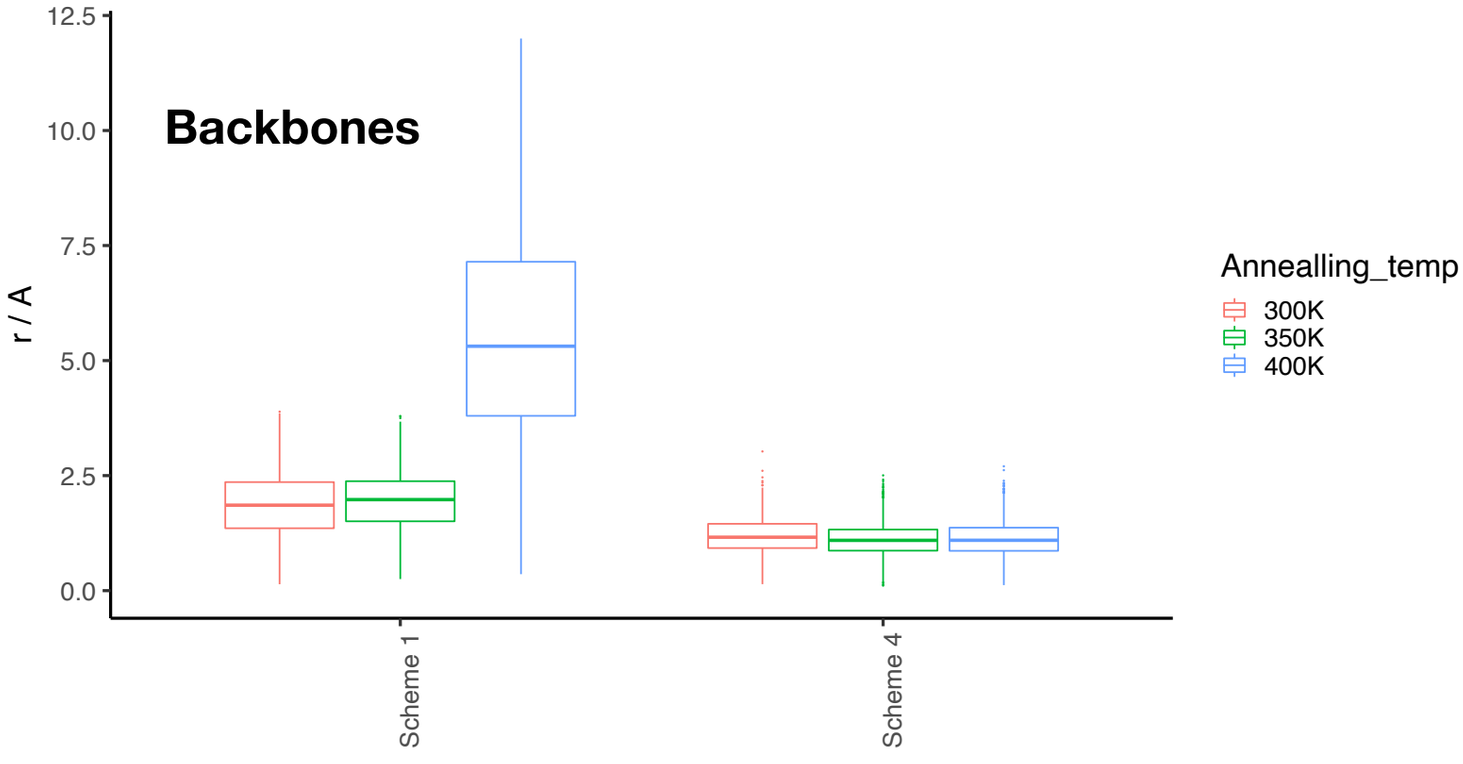


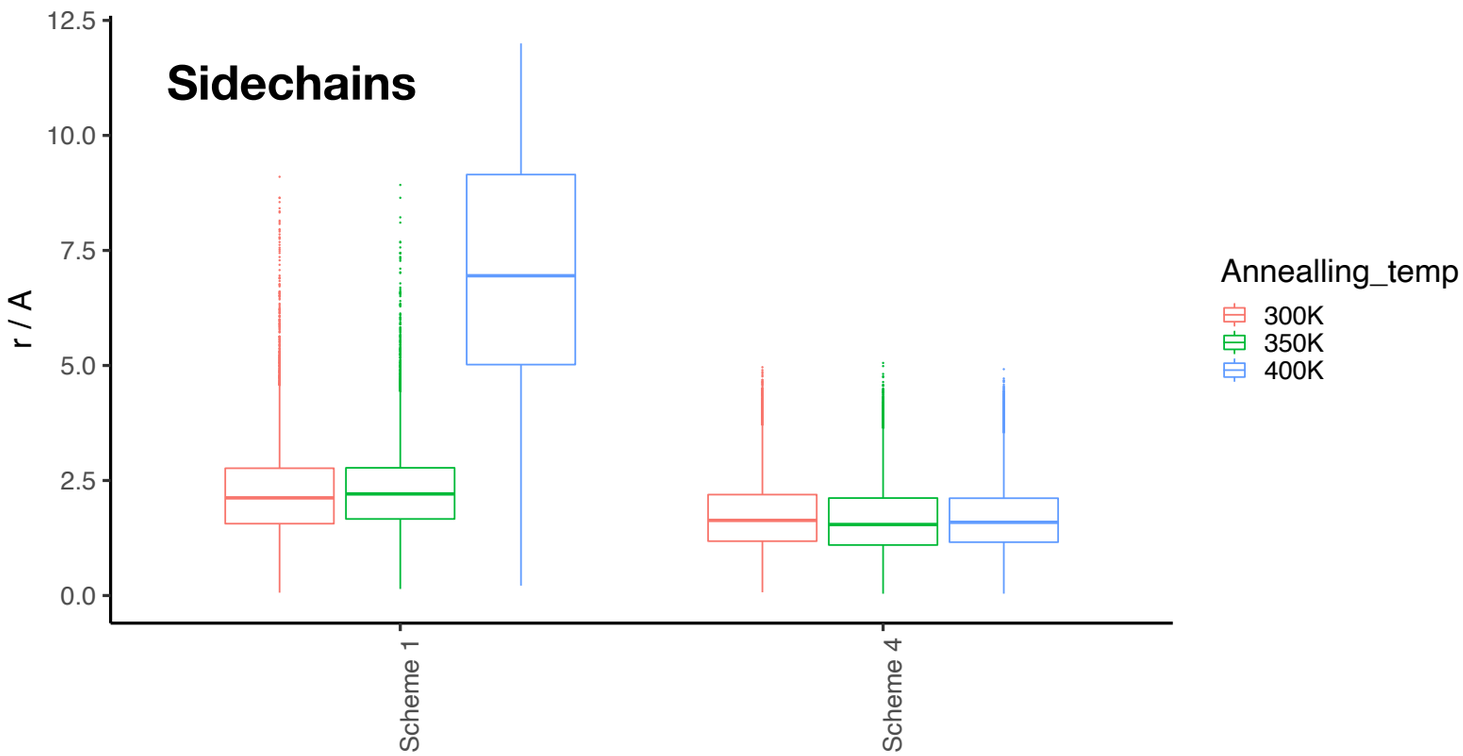


Top - boxplot of atomic displacement vectors. Scheme 4 wins in modelling the crystal structure the best, with atomic displacement vectors all close to 1.5 A (quite small).

Bottom - X-ray diffraction patterns of simulations. Scheme 2 convincingly fails to model the structure, whilst all other schemes show strong peaks, therefore maintaining their crystallinity.

Annealing Scheme 1 and Scheme 4





Scheme 4 recovers the crystal structure after annealing much more readily than scheme 1 does!

Conclusion - EEM cheminformatics parameters for electrostatic potentials are the best!