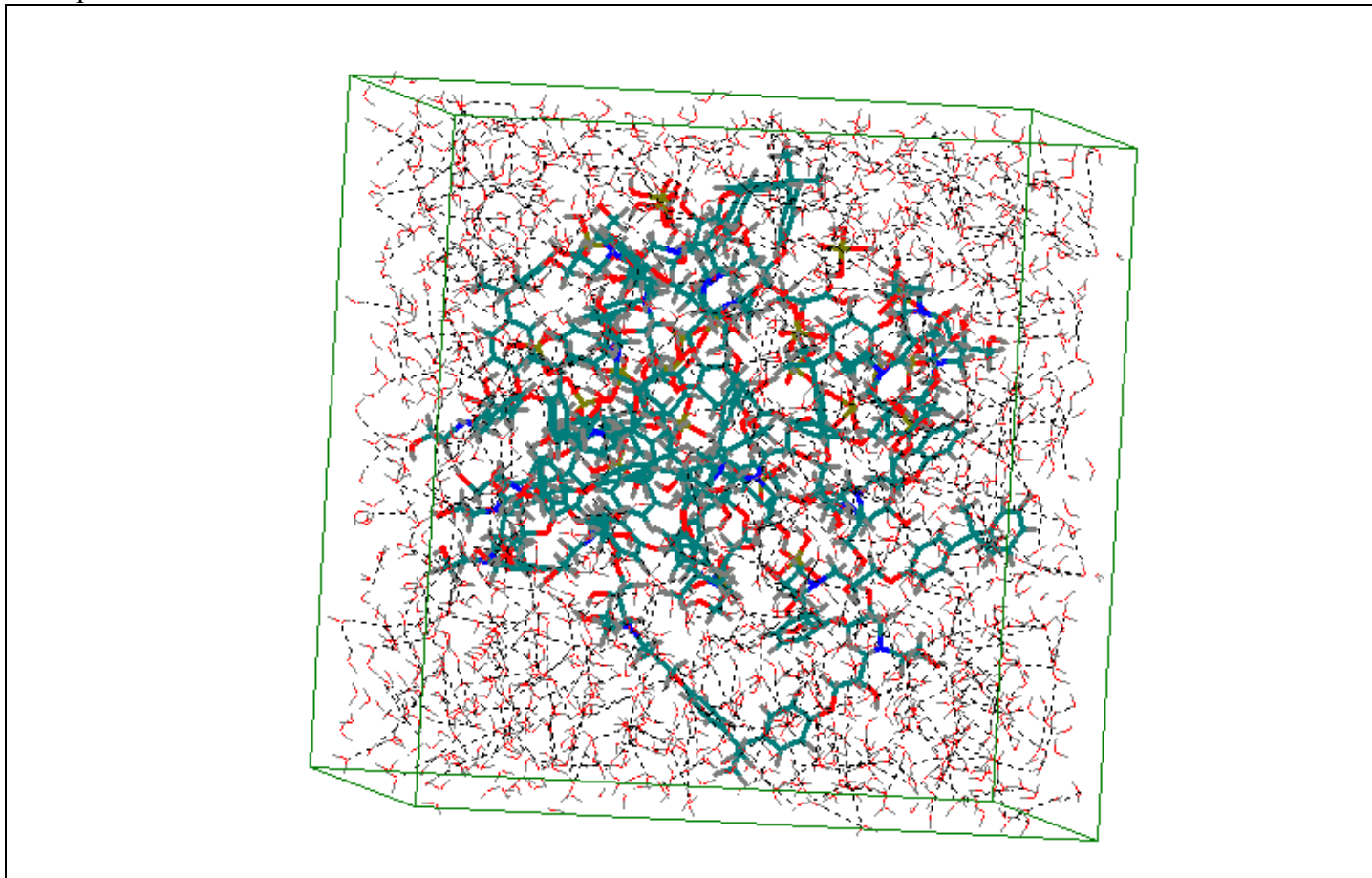


Hdispersion01.hin



Dispersion with population:

1 neutral PHAE 3-11 copolymer, n=4; 1 neutral PHAE 3-11 copolymer, n=20; 22 phosphoric acid, undissociated
2 lactic acid, undissociated; 26 molecules (1416 atoms)

Translated all to near origin, Minimized system with MM+; E=798 kcal

Imposed periodic box 50x50x50; Removed boundary conditions, recommenced MM+ minimization; E=871 kcal

Imposed periodic box 40x40x40; 1541 water added to solvate