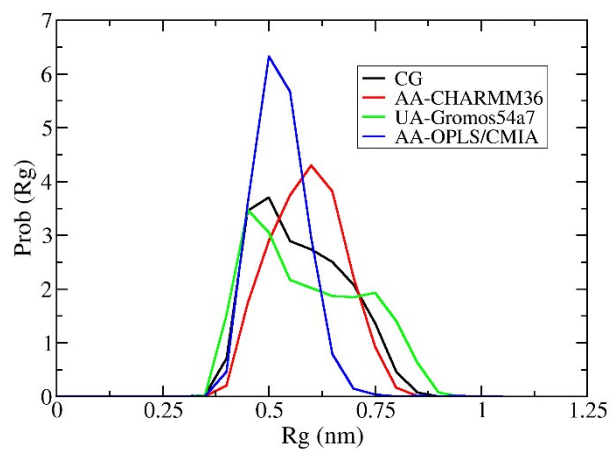
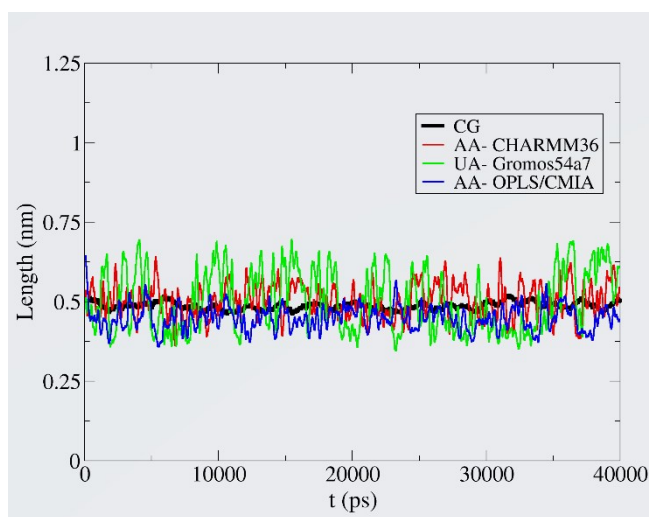


Figure SI-1. Probability distribution of end to end distances of CG PEG₉ (black) with the AA-CHARMM36 (red), UA-GROMACS541a7 (green) and AA-OPLS/CM1A (blue) FFs.



(a)



(b)

Figure SI-2. (a) Probability distribution and (b) average radius of gyration of CG-PEG₉ (black) compared to the AA-CHARMM36 (red), UA-GROMACS541a7 (green) and AA-OPLS/CM1A (blue) FFs.

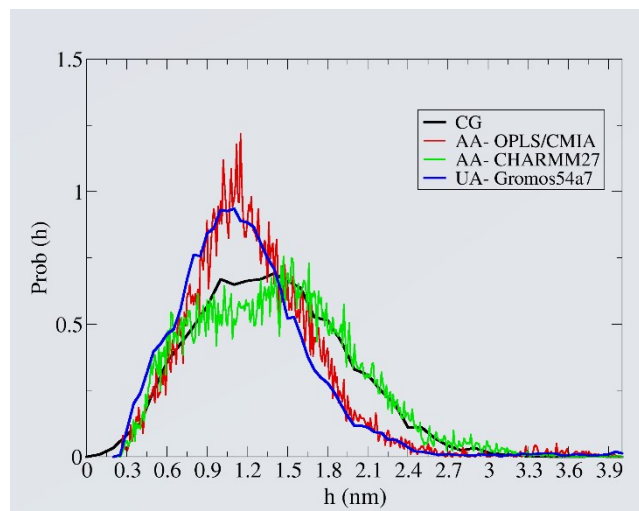


Figure SI-3. Probability distribution of end-to-end distances of CG PCL₁₀ and 3 tested AA/UA FFs

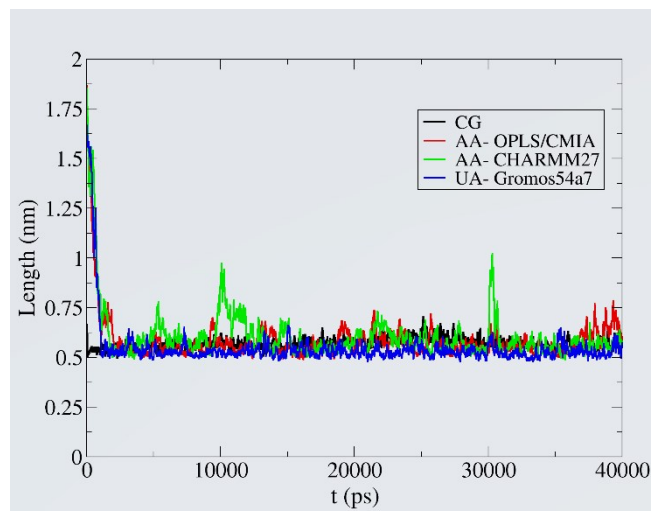
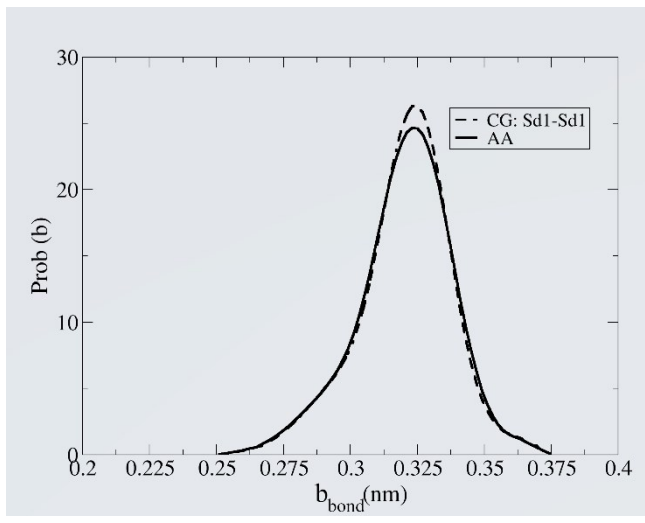
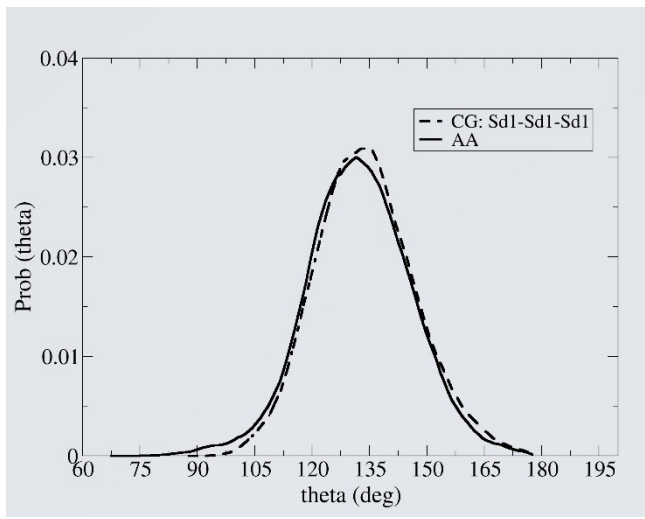


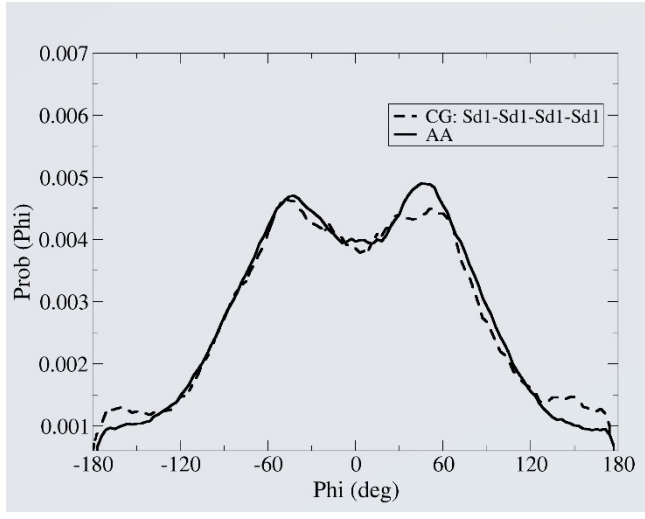
Figure SI-4. Average radius of gyration of CG PCL₁₀ and 3 tested AA/UA FFs.



(a)

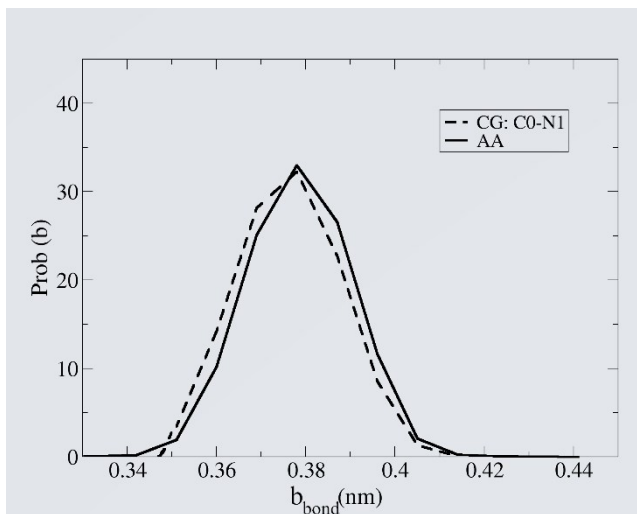


(b)

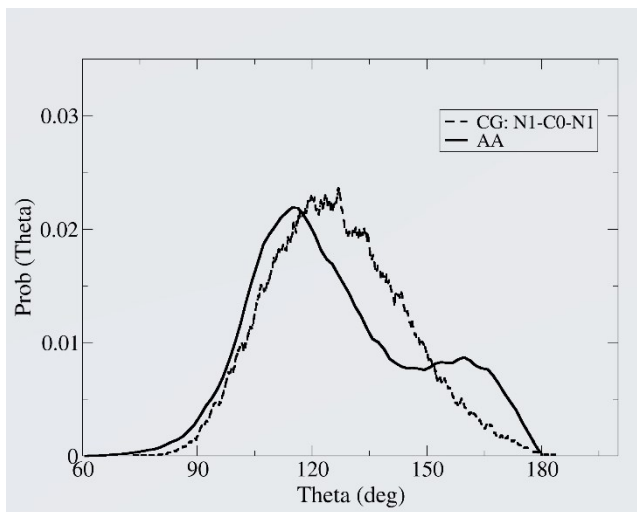


(c)

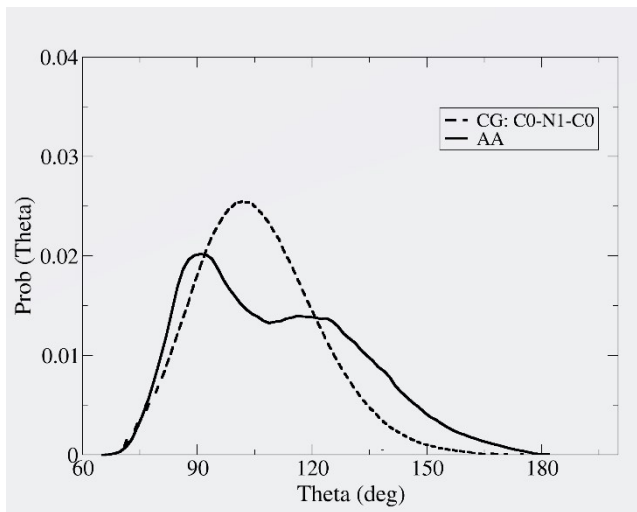
Figure SI-5. Probability distributions of (a) core bonds Sd1-Sd1, (b) core angles Sd1-Sd1-Sd1, and (c) core dihedrals Sd1-Sd1-Sd1 of PEG₉ from all-atom (solid line) and CG (dashed line).



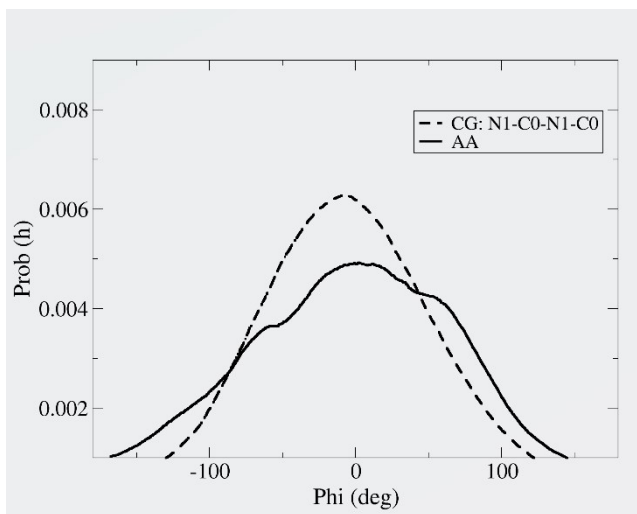
(a)



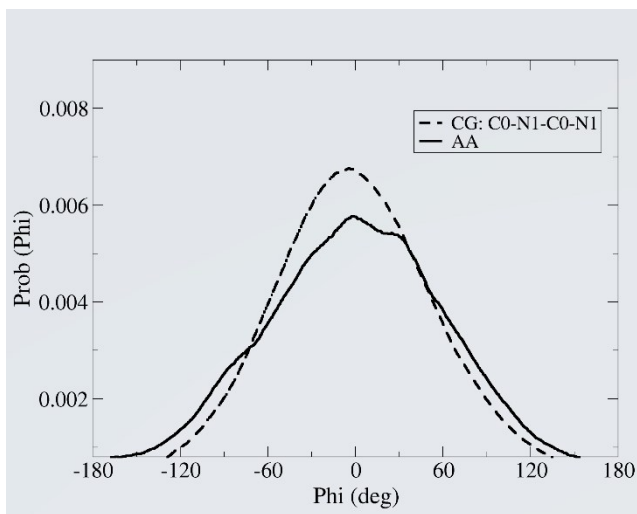
(b)



(c)



(d)



(e)

Figure SI-6. Probability distributions of **(a)** core bonds C0-N1, **(b)** core angles N1-C0-N1, **(c)** core angles C0-N1-C0, **(d)** core dihedrals N1-C0-N1-C0 and **(e)** core dihedrals C0-N1-C0-N1 of PCL₁₀ from all-atom (solid line) and CG (dashed line).