

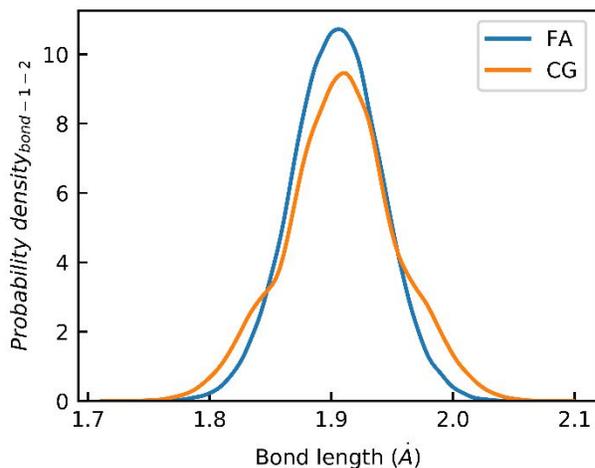
## Supporting Information

# Molecular Dynamics Simulation of Photo-induced Free Radical Polymerization

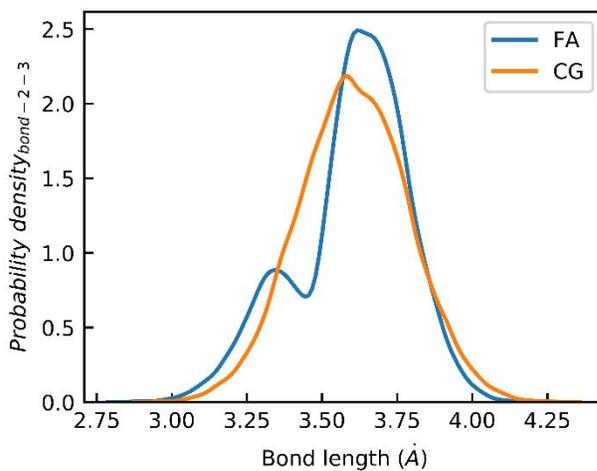
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University, University Park, PA 16801, United States

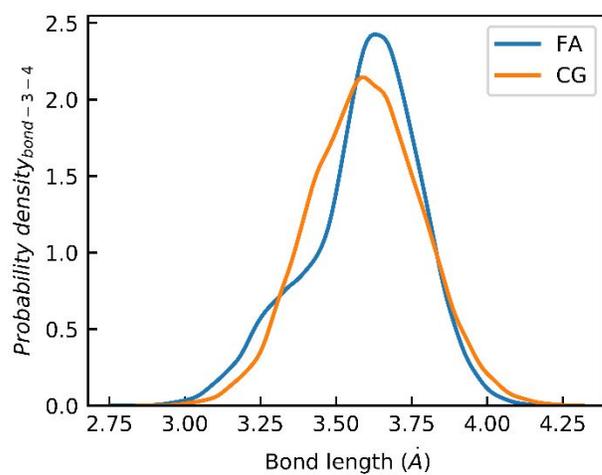
## 1. Probability density function for bonding lengths



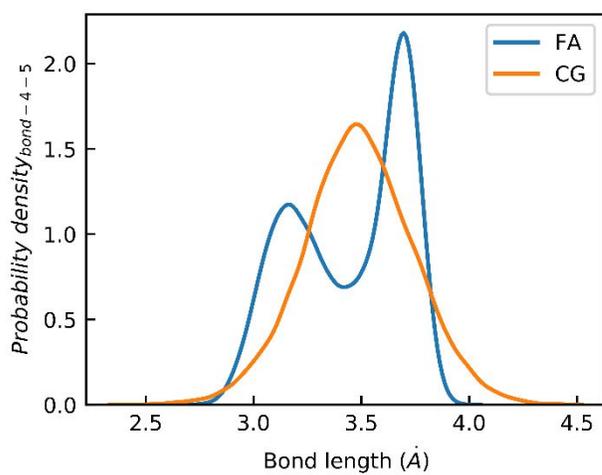
**Figure S1.** The probability density function of the bond lengths between bead 1 and 2 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



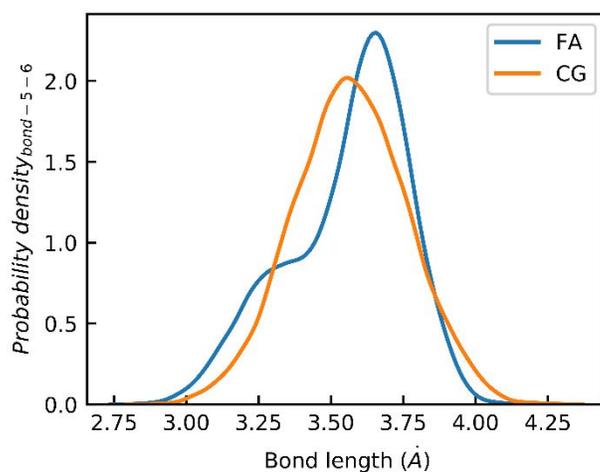
**Figure S2.** The probability density function of the bond lengths between bead 2 and 3 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



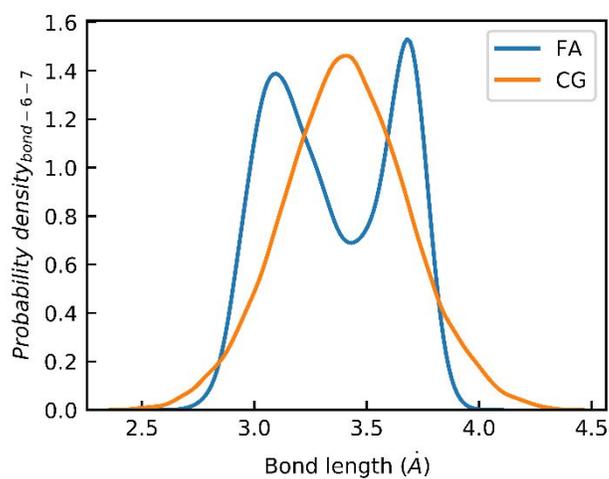
**Figure S3.** The probability density function of the bond lengths between bead 3 and 4 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



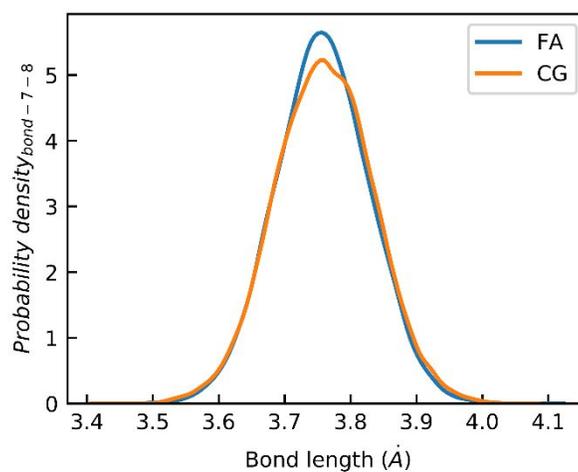
**Figure S4.** The probability density function of the bond lengths between bead 4 and 5 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



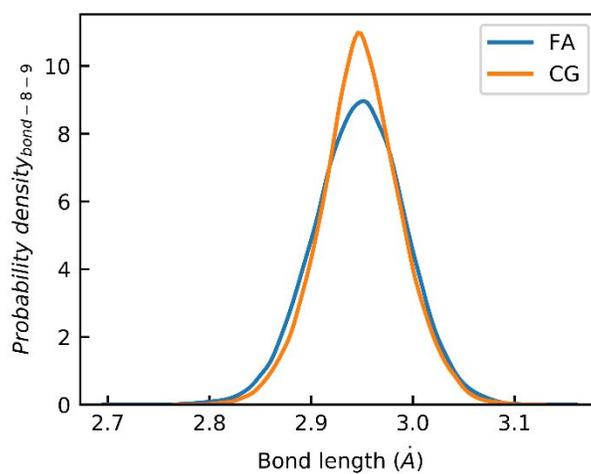
**Figure S5.** The probability density function of the bond lengths between bead 5 and 6 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



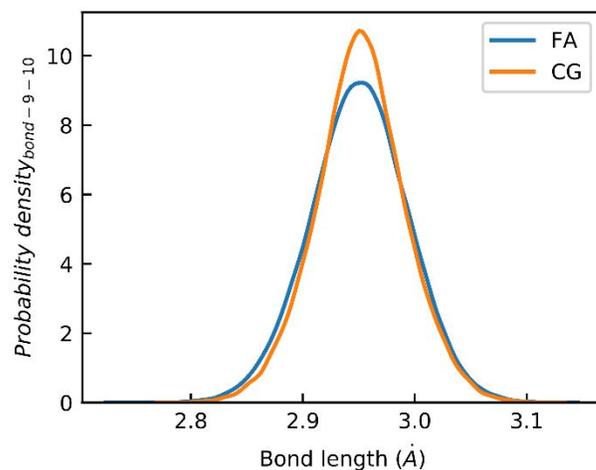
**Figure S6.** The probability density function of the bond lengths between bead 6 and 7 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



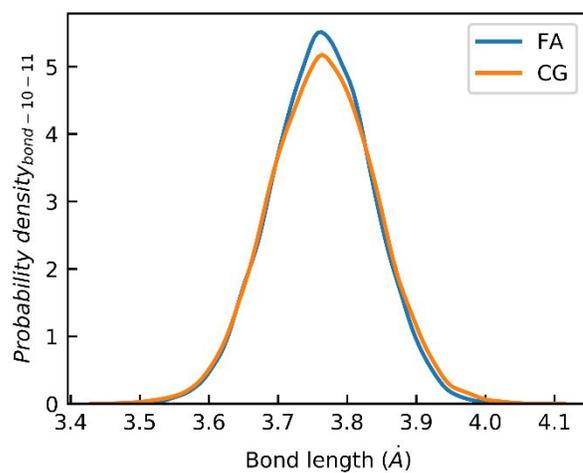
**Figure S7.** The probability density function of the bond lengths between bead 7 and 8 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



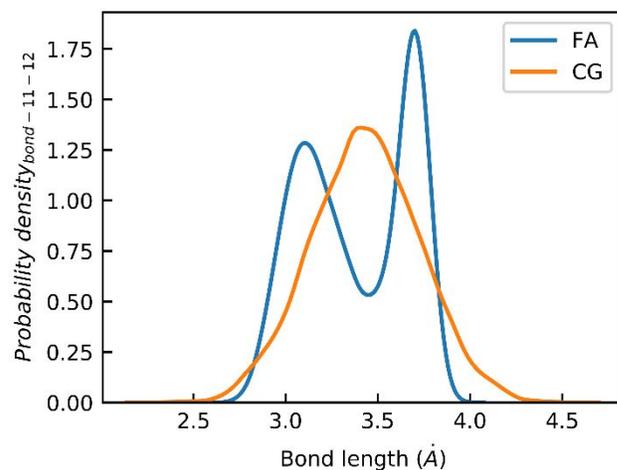
**Figure S8.** The probability density function of the bond lengths between bead 8 and 9 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



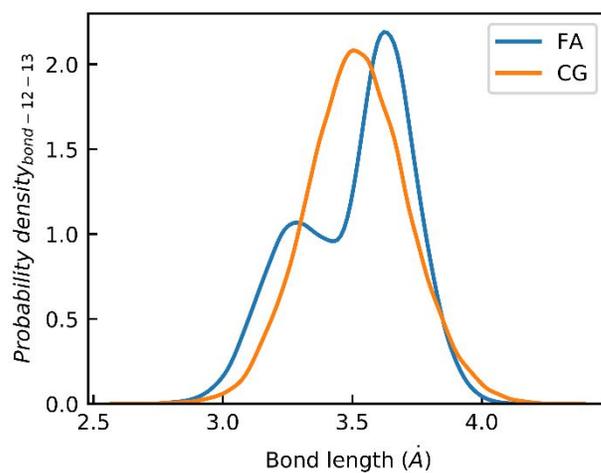
**Figure S9.** The probability density function of the bond lengths between bead 9 and 10 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



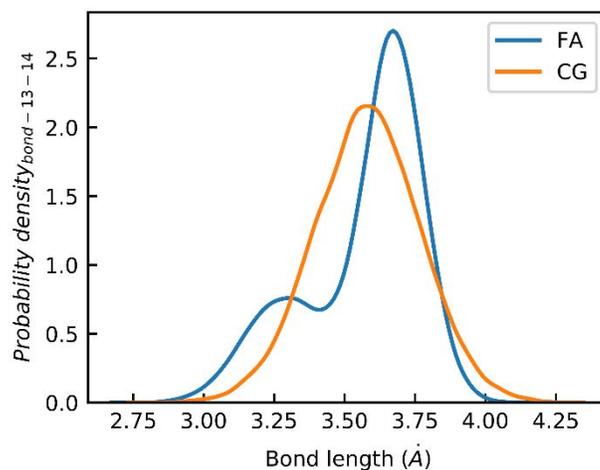
**Figure S10.** The probability density function of the bond lengths between bead 10 and 11 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



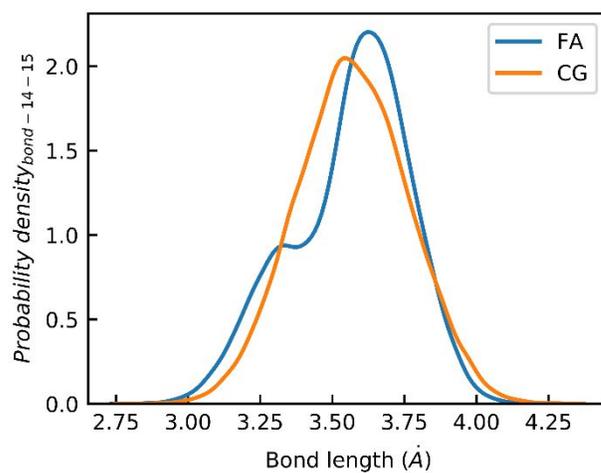
**Figure S11.** The probability density function of the bond lengths between bead 11 and 12 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



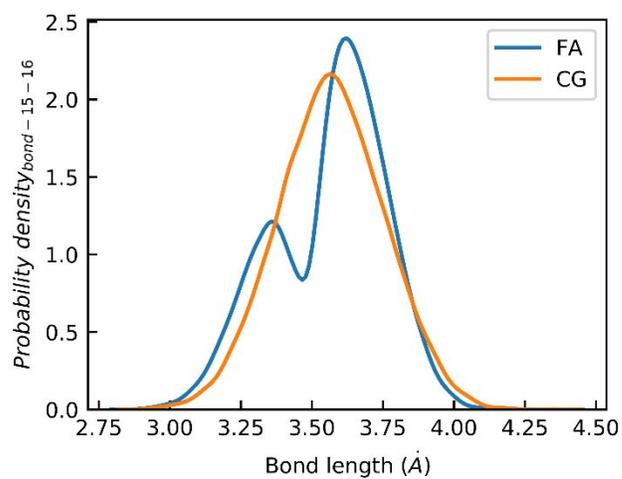
**Figure S12.** The probability density function of the bond lengths between bead 12 and 13 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



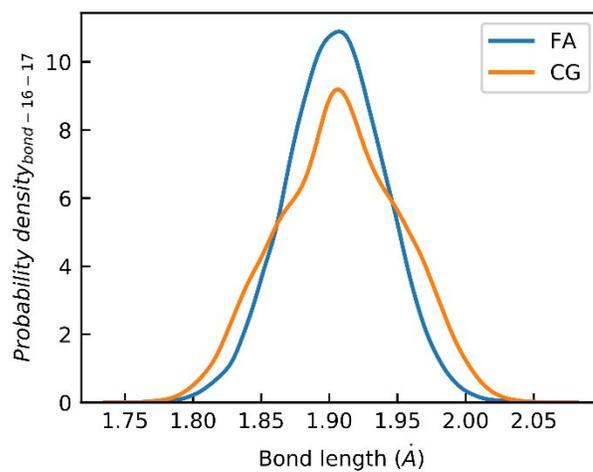
**Figure S13.** The probability density function of the bond lengths between bead 13 and 14 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



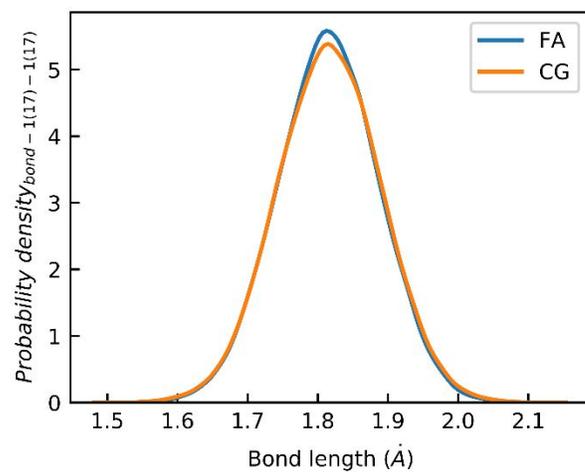
**Figure S14.** The probability density function of the bond lengths between bead 14 and 15 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



**Figure S15.** The probability density function of the bond lengths between bead 15 and 16 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

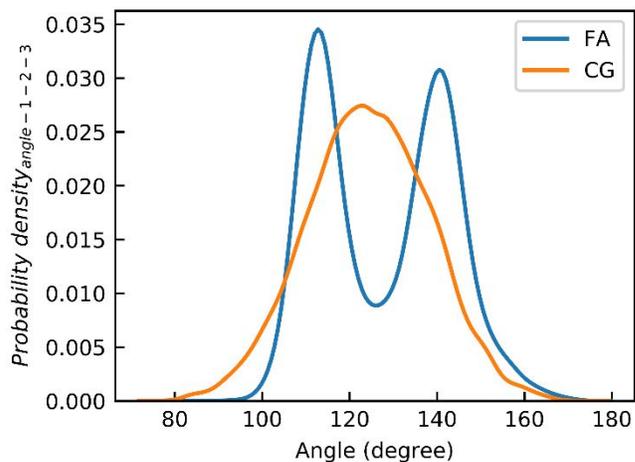


**Figure S16.** The probability density function of the bond lengths between bead 16 and 17 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

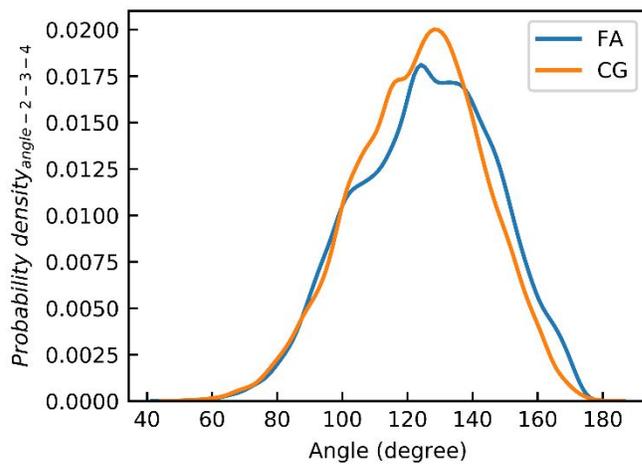


**Figure S17.** The probability density function of the bond lengths between bead 1(or 17) and 1(or 17) obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

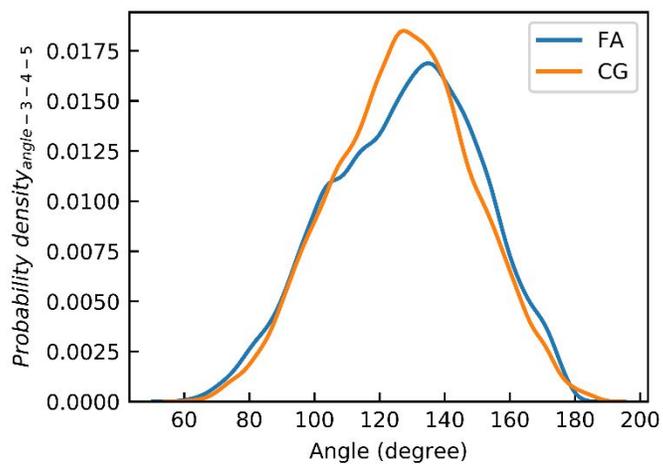
## 2. Probability density function for angles



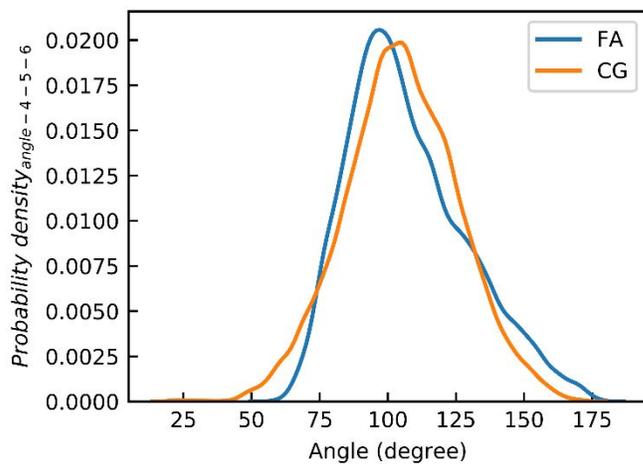
**Figure S18.** The probability density function of the angle between bead 1, 2 and 3 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



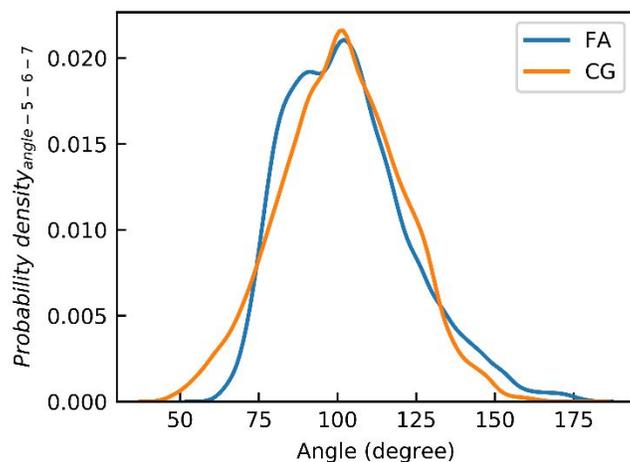
**Figure S19.** The probability density function of the angle between bead 2, 3 and 4 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



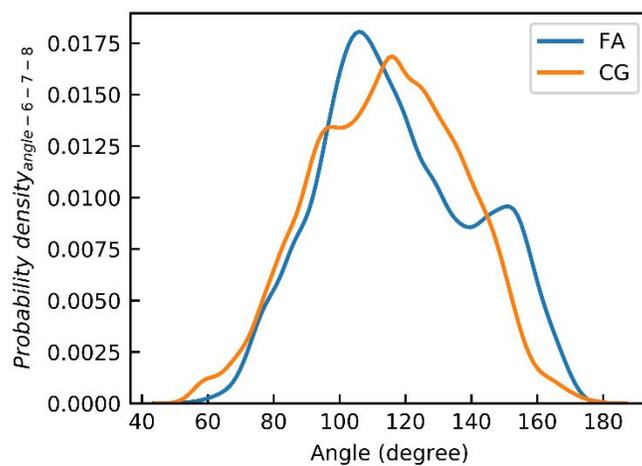
**Figure S20.** The probability density function of the angle between bead 3, 4 and 5 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



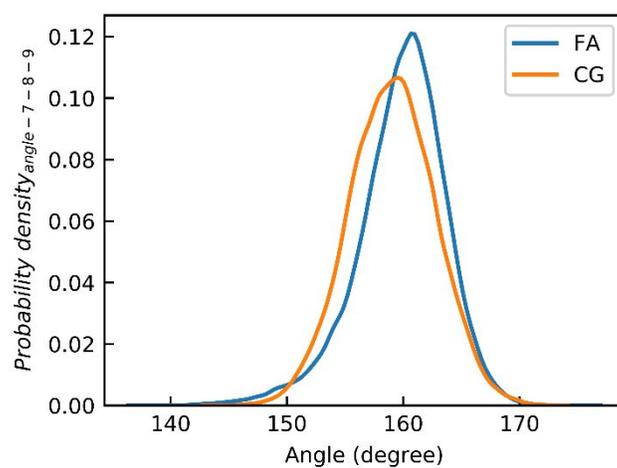
**Figure S21.** The probability density function of the angle between bead 4, 5 and 6 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



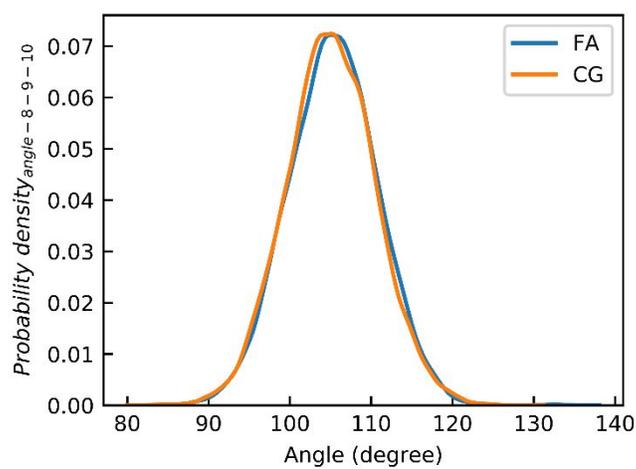
**Figure S22.** The probability density function of the angle between bead 5, 6 and 7 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



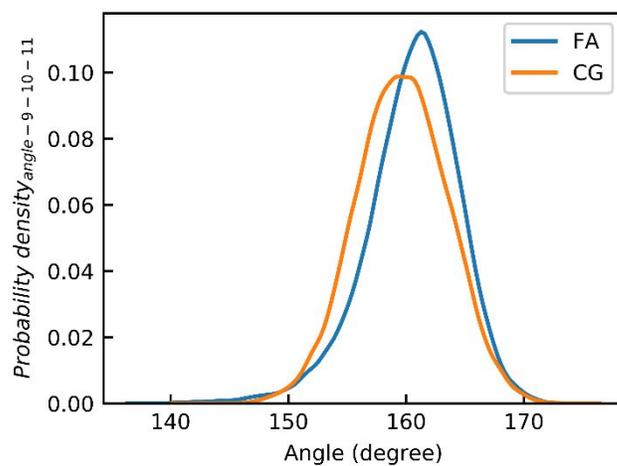
**Figure S23.** The probability density function of the angle between bead 6, 7 and 8 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



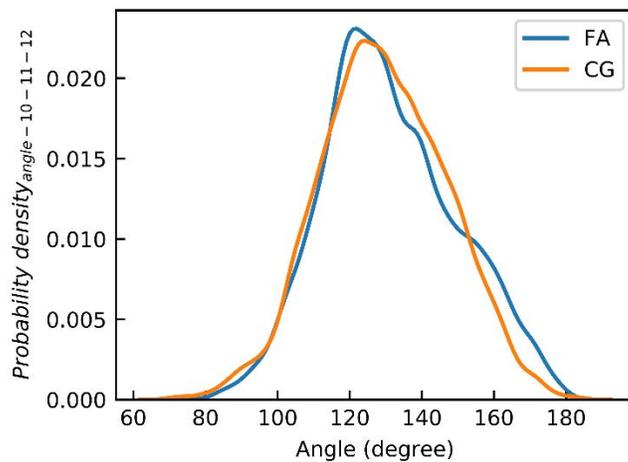
**Figure S24.** The probability density function of the angle between bead 7, 8 and 9 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



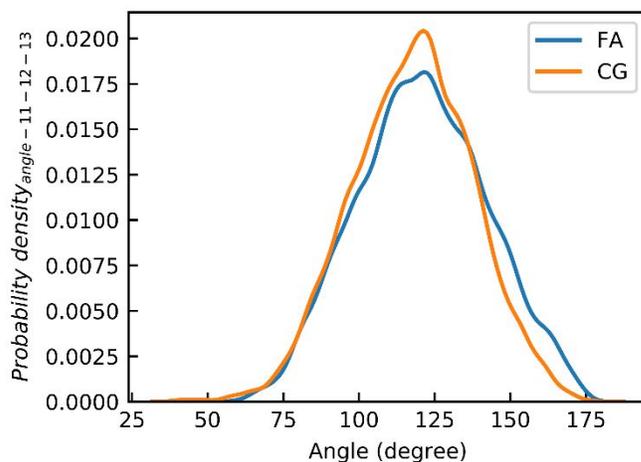
**Figure S25.** The probability density function of the angle between bead 8, 9 and 10 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



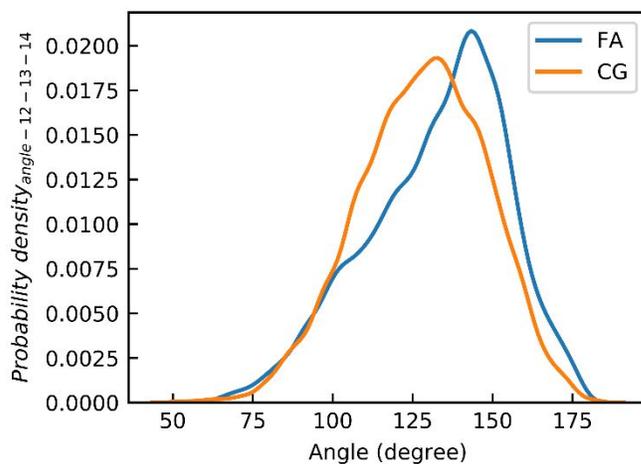
**Figure S26.** The probability density function of the angle between bead 9, 10 and 11 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



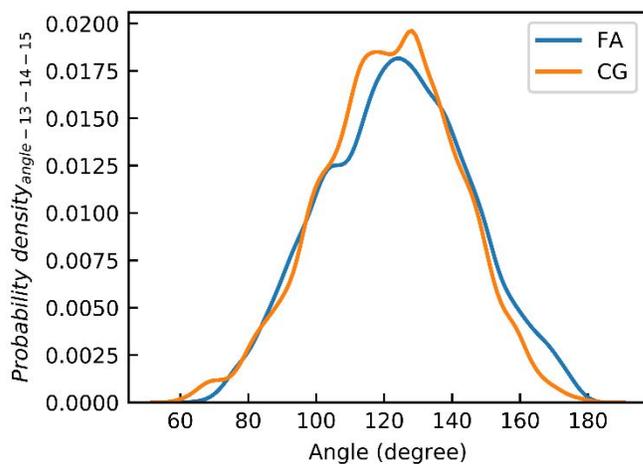
**Figure S27.** The probability density function of the angle between bead 10, 11 and 12 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



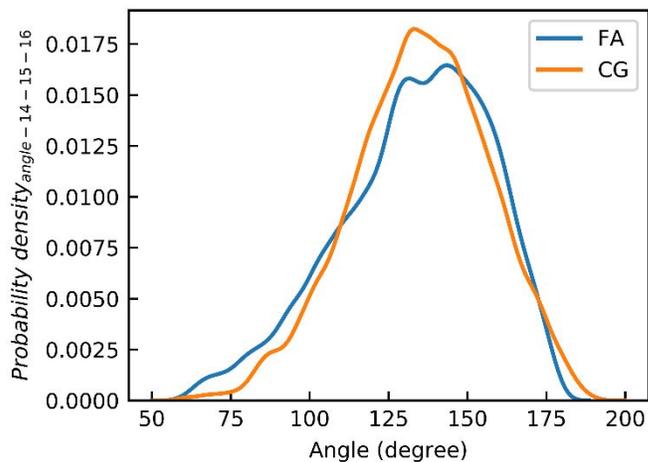
**Figure S28.** The probability density function of the angle between bead 11, 12 and 13 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



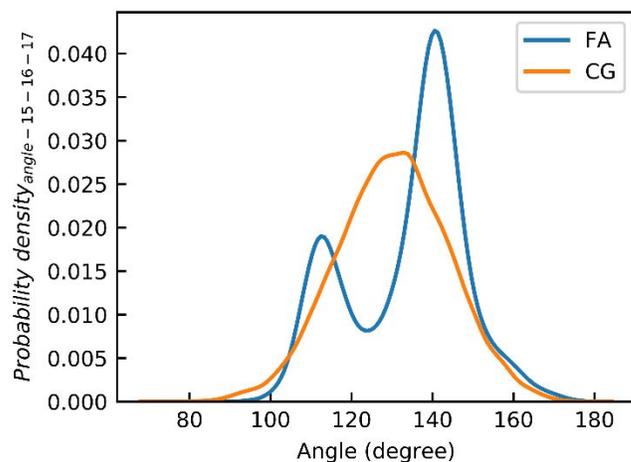
**Figure S29.** The probability density function of the angle between bead 12, 13 and 14 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



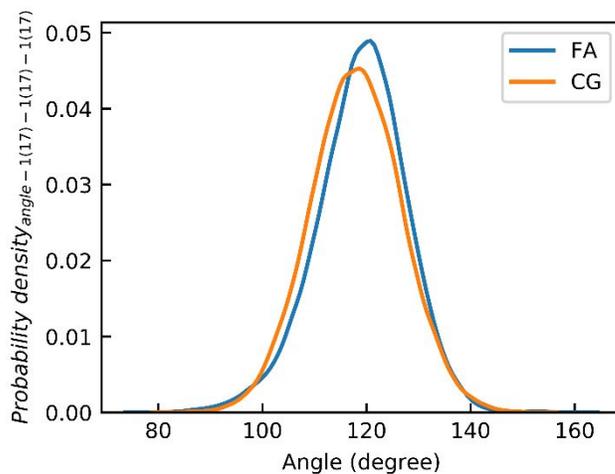
**Figure S30.** The probability density function of the angle between bead 13, 14 and 15 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



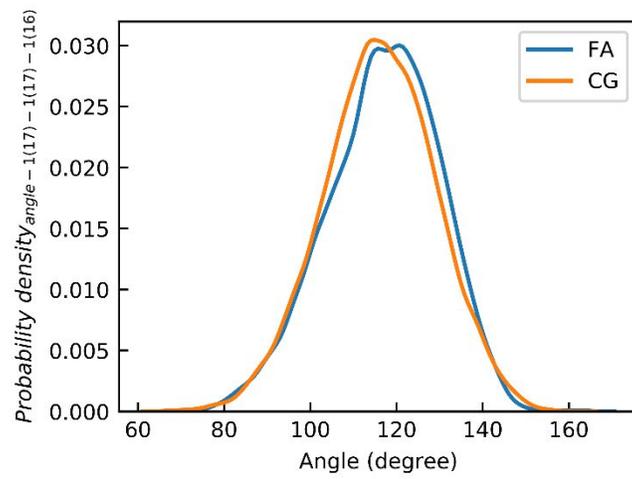
**Figure S31.** The probability density function of the angle between bead 14, 15 and 16 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



**Figure S32.** The probability density function of the angle between bead 15, 16 and 17 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



**Figure S33.** The probability density function of the angle between bead 1(or 17), 1(or 17) and 1(or 17) obtained from the coarse-grained (CG) model and the full-atomic (FA) model.



**Figure S34.** The probability density function of the angle between bead 1(or 17), 1(or 17) and 2(or 16) obtained from the coarse-grained (CG) model and the full-atomic (FA) model.