

Supporting Information

Molecular Dynamics Simulation of Photo-induced Free Radical Polymerization

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1. Probability density function for bonding lengths

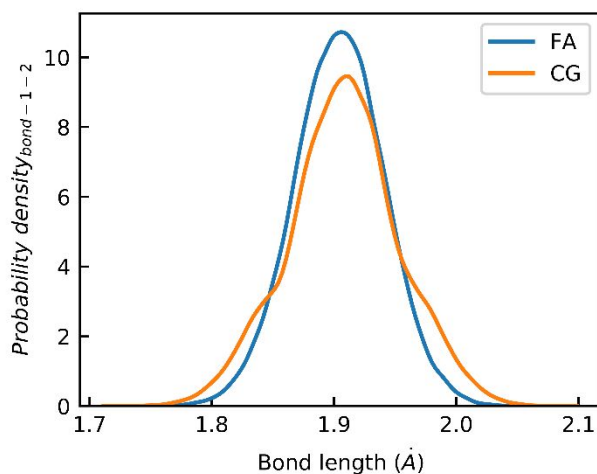


Figure S1. The probability density function of the bond lengths between bead 1 and 2 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

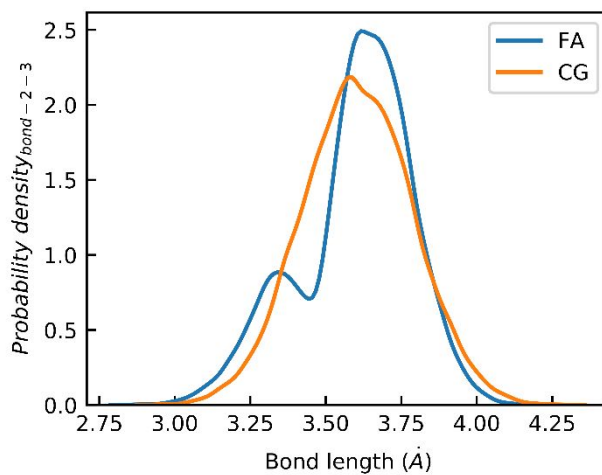


Figure S2. The probability density function of the bond lengths between bead 2 and 3 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

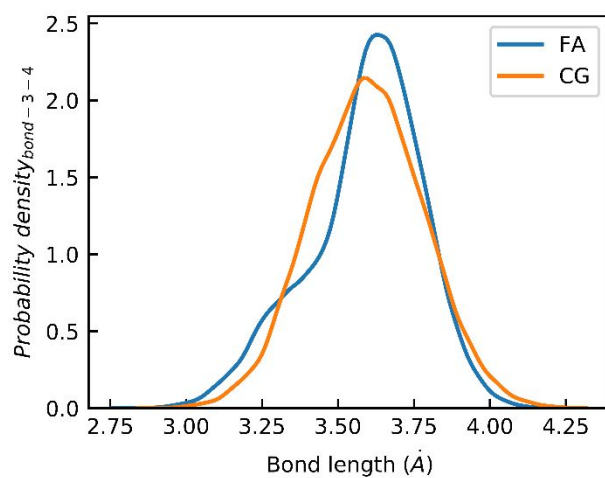


Figure S3. The probability density function of the bond lengths between bead 3 and 4 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

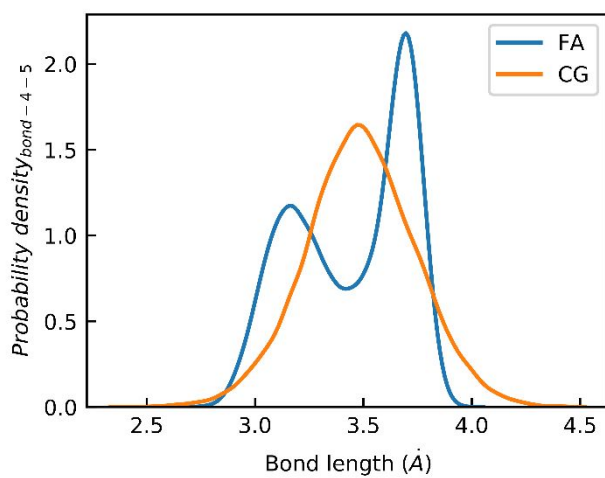


Figure S4. The probability density function of the bond lengths between bead 4 and 5 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

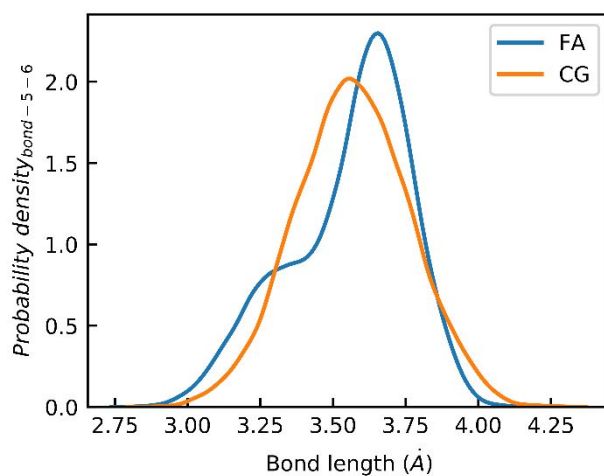


Figure S5. The probability density function of the bond lengths between bead 5 and 6 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

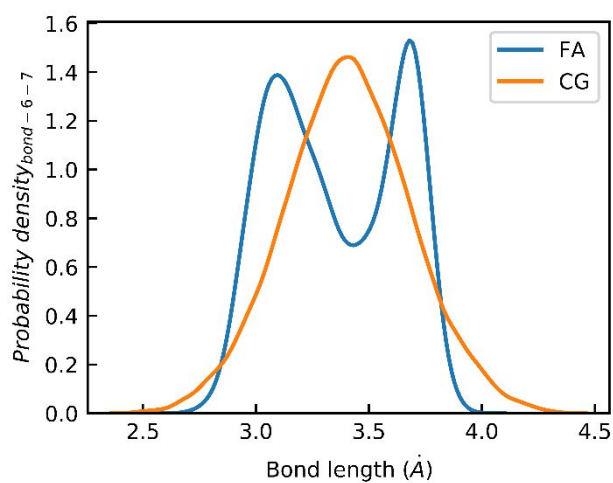


Figure S6. The probability density function of the bond lengths between bead 6 and 7 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

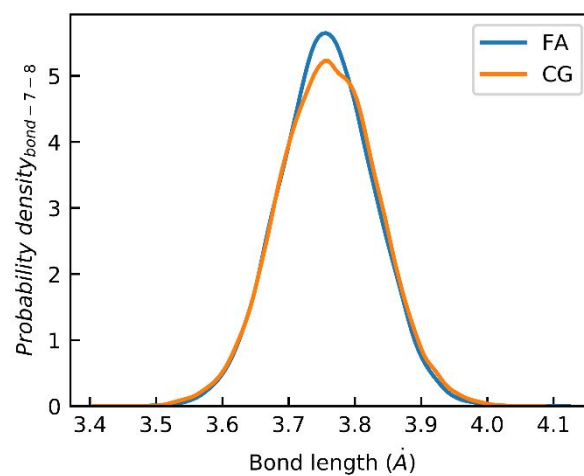


Figure S7. The probability density function of the bond lengths between bead 7 and 8 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

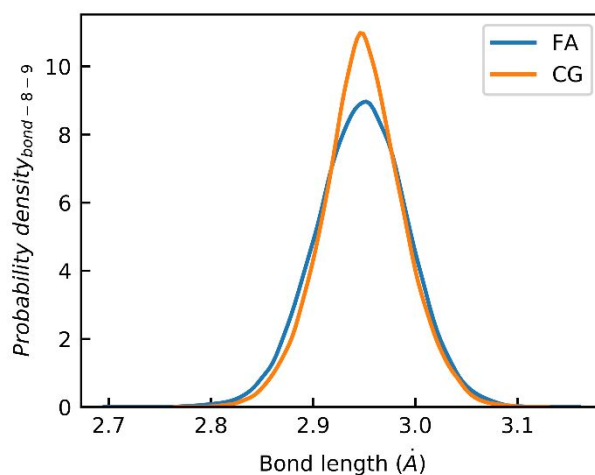


Figure S8. The probability density function of the bond lengths between bead 8 and 9 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

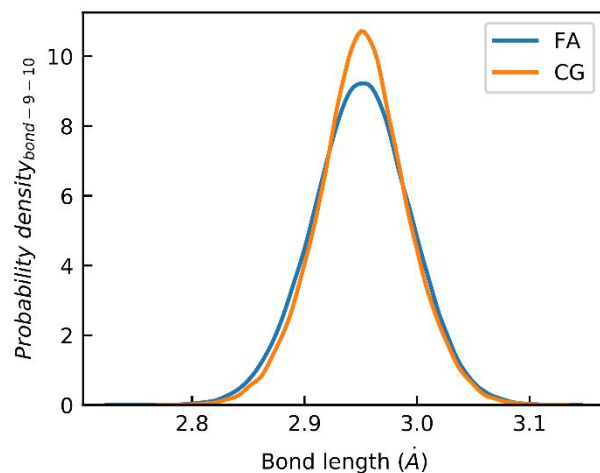


Figure S9. The probability density function of the bond lengths between bead 9 and 10 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

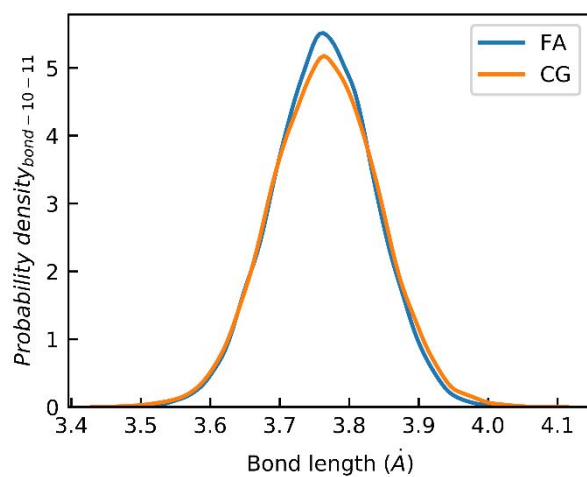


Figure S10. The probability density function of the bond lengths between bead 10 and 11 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

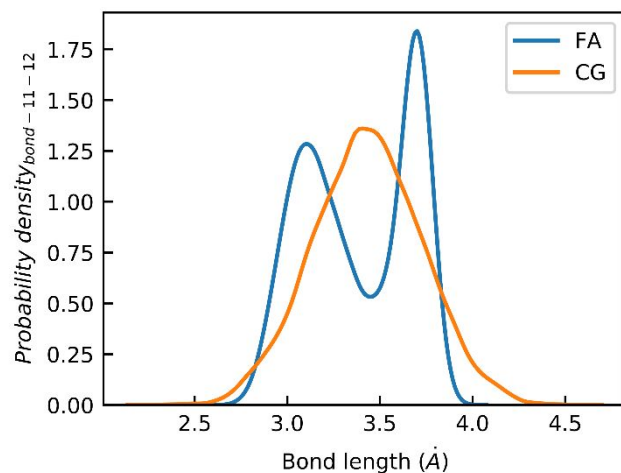


Figure S11. The probability density function of the bond lengths between bead 11 and 12 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

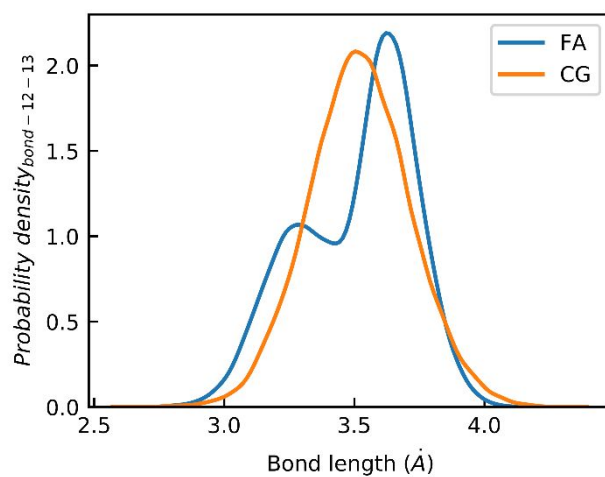


Figure S12. The probability density function of the bond lengths between bead 12 and 13 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

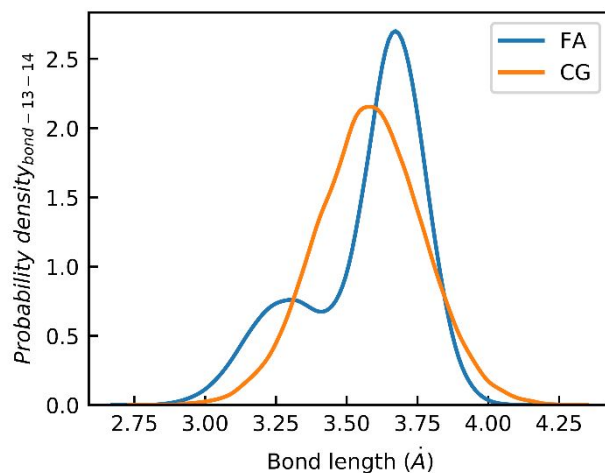


Figure S13. The probability density function of the bond lengths between bead 13 and 14 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

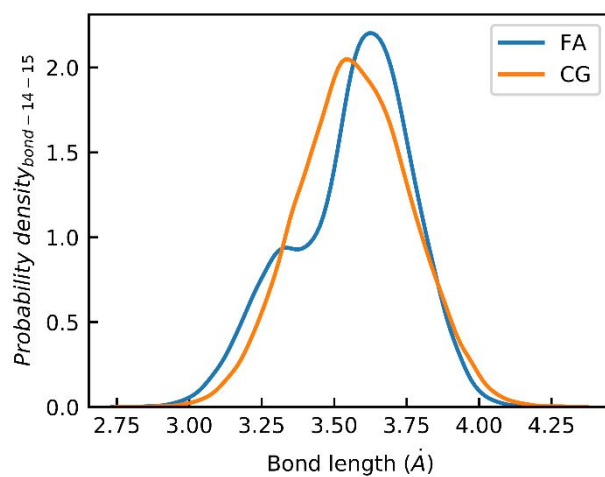


Figure S14. The probability density function of the bond lengths between bead 14 and 15 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

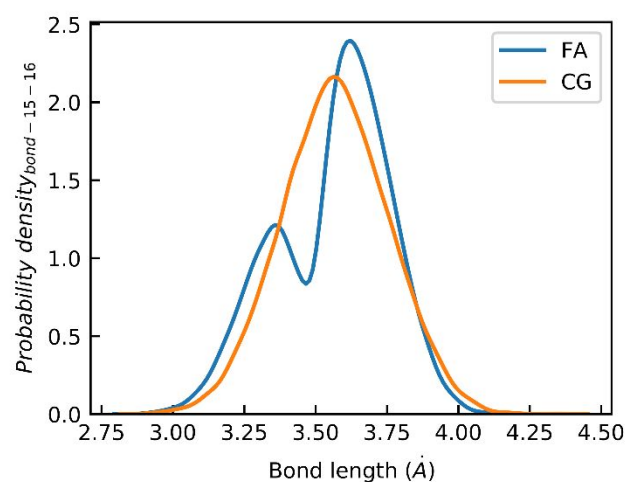


Figure S15. The probability density function of the bond lengths between bead 15 and 16 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

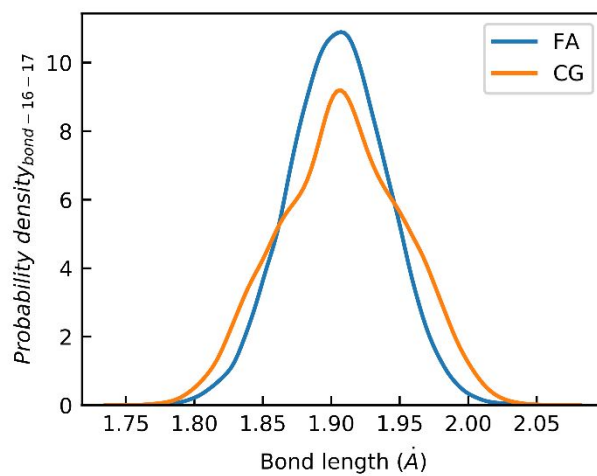


Figure S16. The probability density function of the bond lengths between bead 16 and 17 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

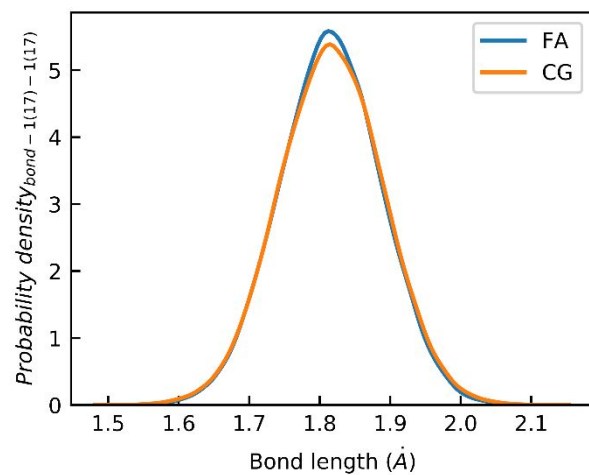


Figure S17. The probability density function of the bond lengths between bead 1(or 17) and 1(or 17) obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

2. Probability density function for angles

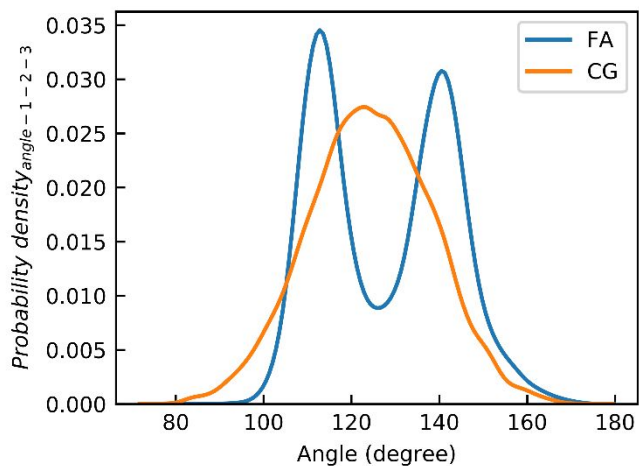


Figure S18. The probability density function of the angle between bead 1, 2 and 3 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

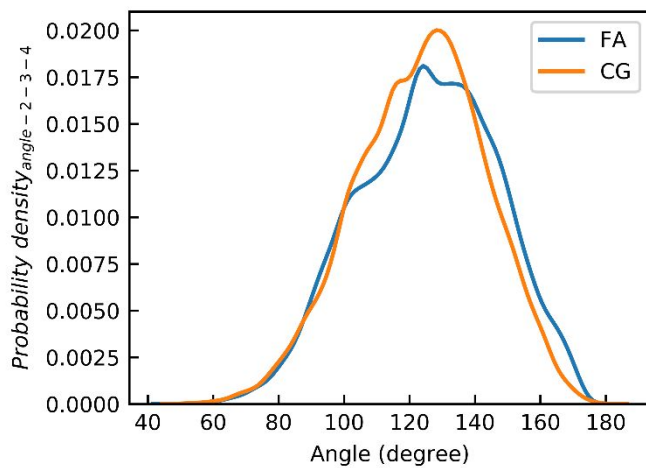


Figure S19. The probability density function of the angle between bead 2, 3 and 4 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

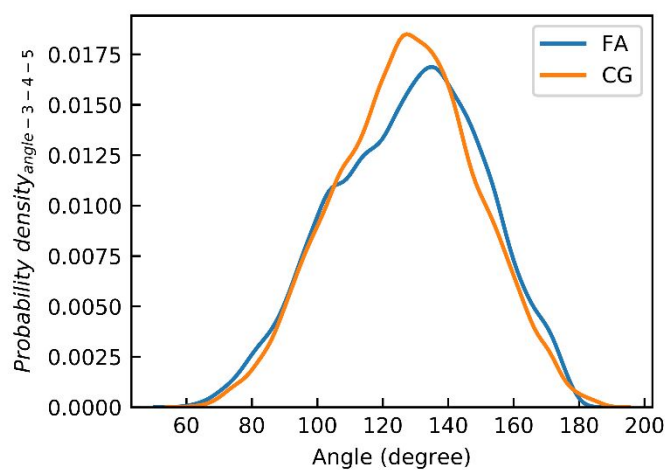


Figure S20. The probability density function of the angle between bead 3, 4 and 5 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

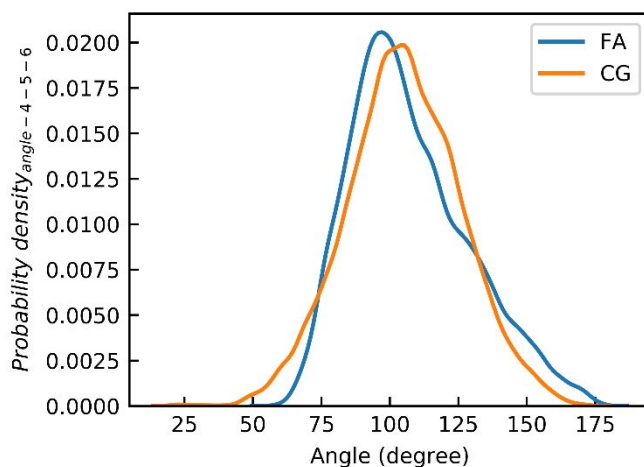


Figure S21. The probability density function of the angle between bead 4, 5 and 6 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

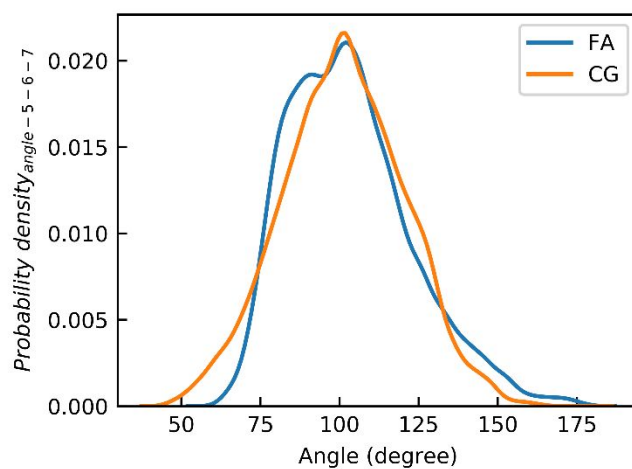


Figure S22. The probability density function of the angle between bead 5, 6 and 7 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

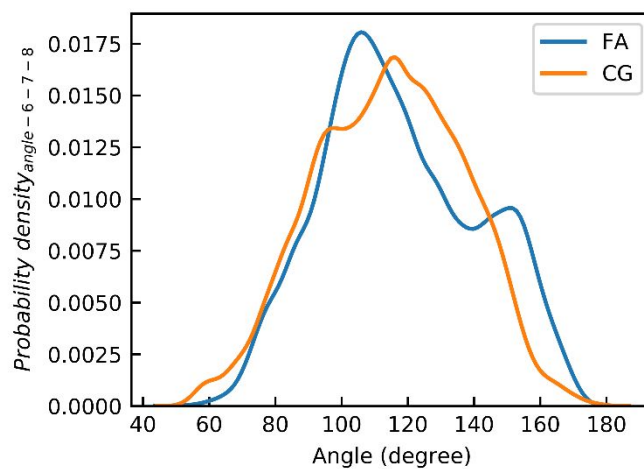


Figure S23. The probability density function of the angle between bead 6, 7 and 8 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

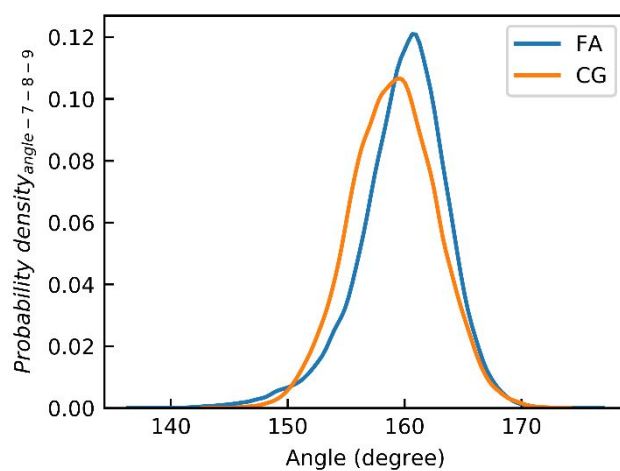


Figure S24. The probability density function of the angle between bead 7, 8 and 9 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

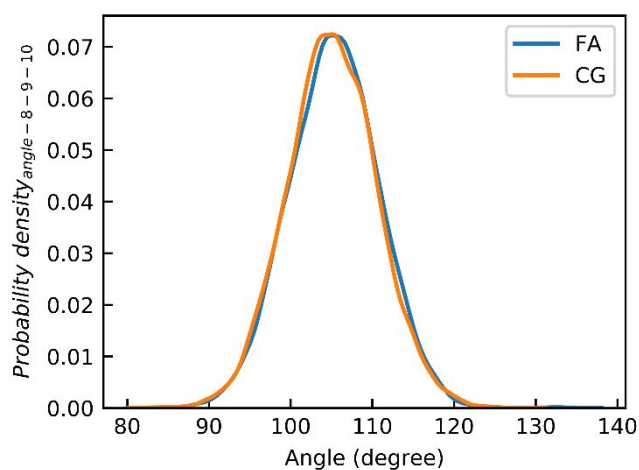


Figure S25. The probability density function of the angle between bead 8, 9 and 10 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

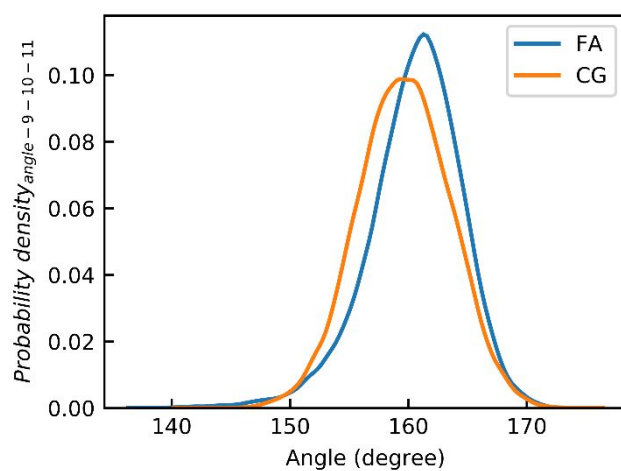


Figure S26. The probability density function of the angle between bead 9, 10 and 11 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

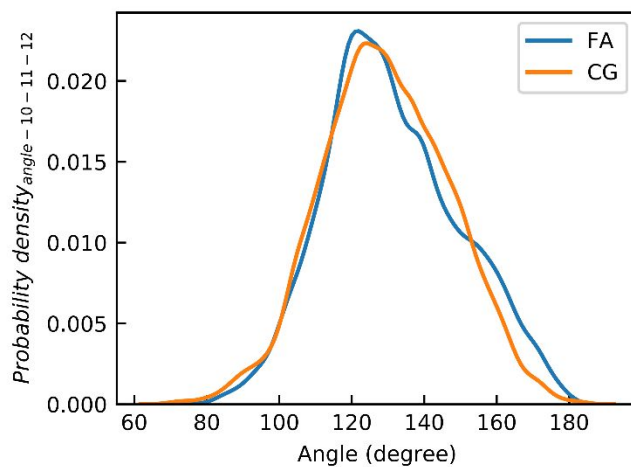


Figure S27. The probability density function of the angle between bead 10, 11 and 12 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

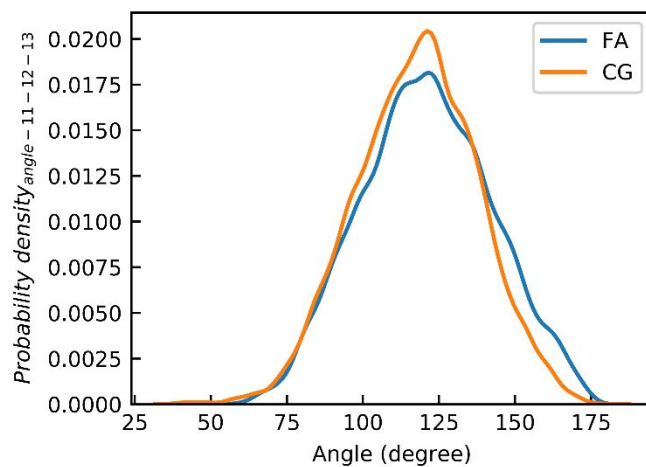


Figure S28. The probability density function of the angle between bead 11, 12 and 13 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

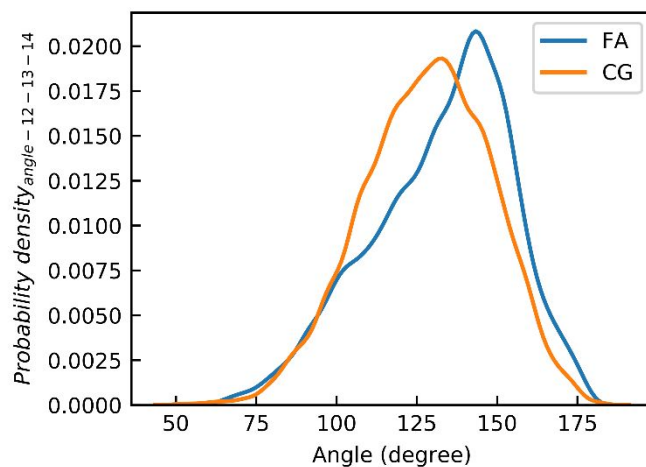


Figure S29. The probability density function of the angle between bead 12, 13 and 14 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

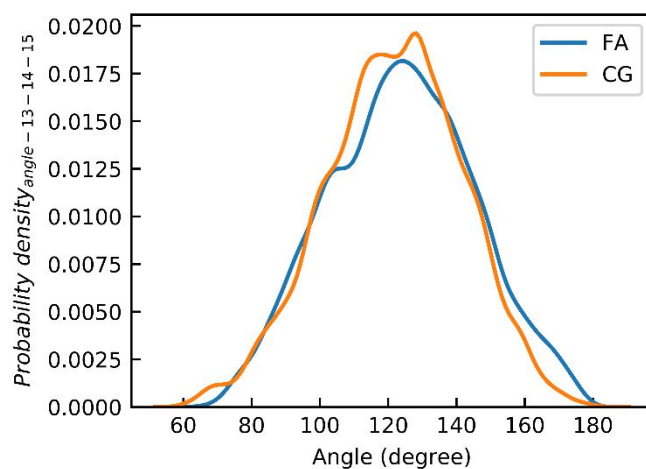


Figure S30. The probability density function of the angle between bead 13, 14 and 15 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

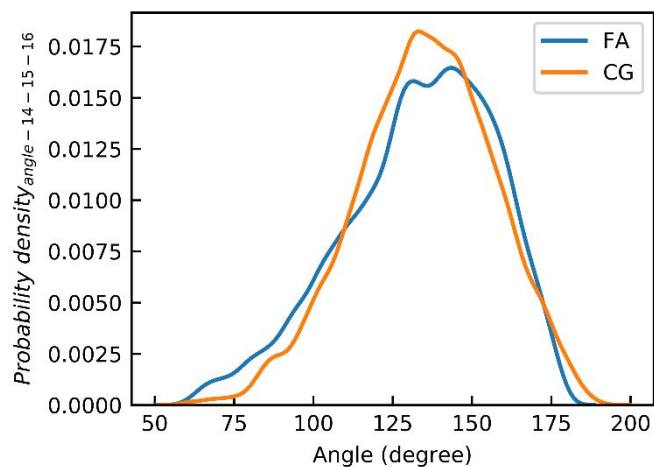


Figure S31. The probability density function of the angle between bead 14, 15 and 16 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

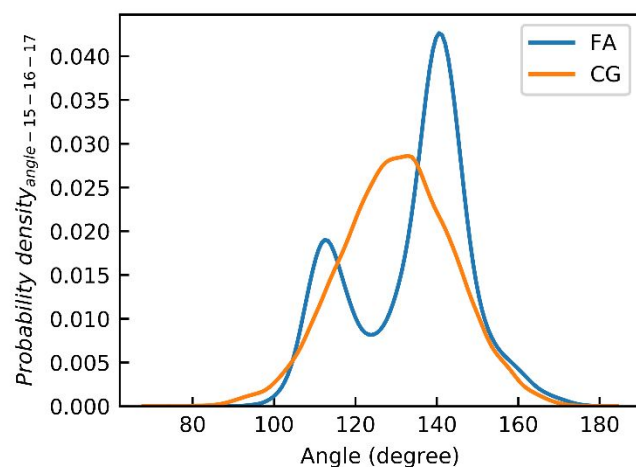


Figure S32. The probability density function of the angle between bead 15, 16 and 17 obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

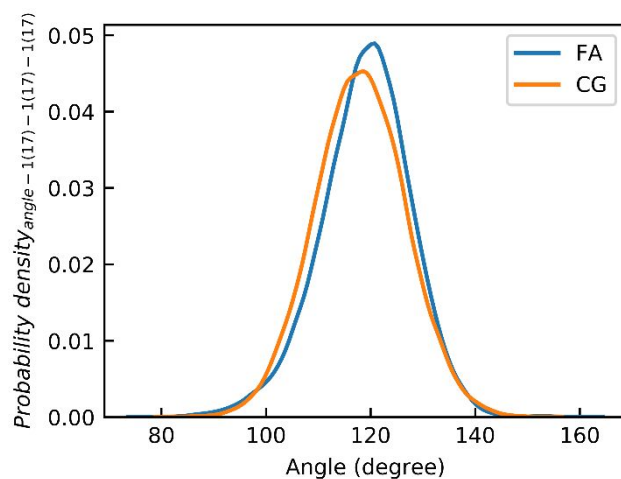


Figure S33. The probability density function of the angle between bead 1(or 17), 1(or 17) and 1(or 17) obtained from the coarse-grained (CG) model and the full-atomic (FA) model.

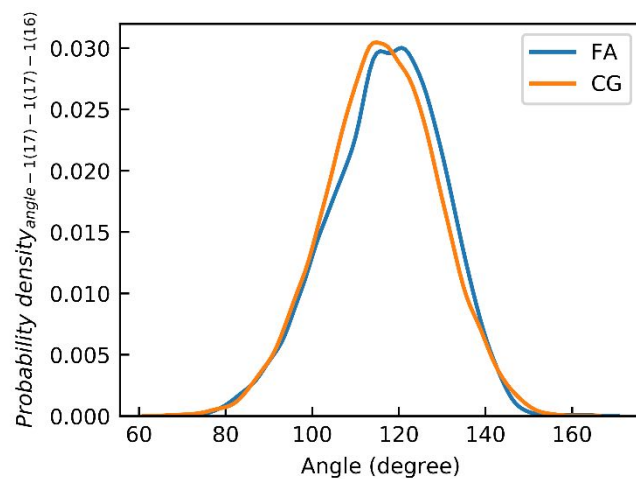


Figure S34. The probability density function of the angle between bead 1(or 17), 1(or 17) and 2(or 16) obtained from the coarse-grained (CG) model and the full-atomic (FA) model.