Supporting Information:

Coarse-Grained Model for Simulation of RNA Three-Dimensional Structures

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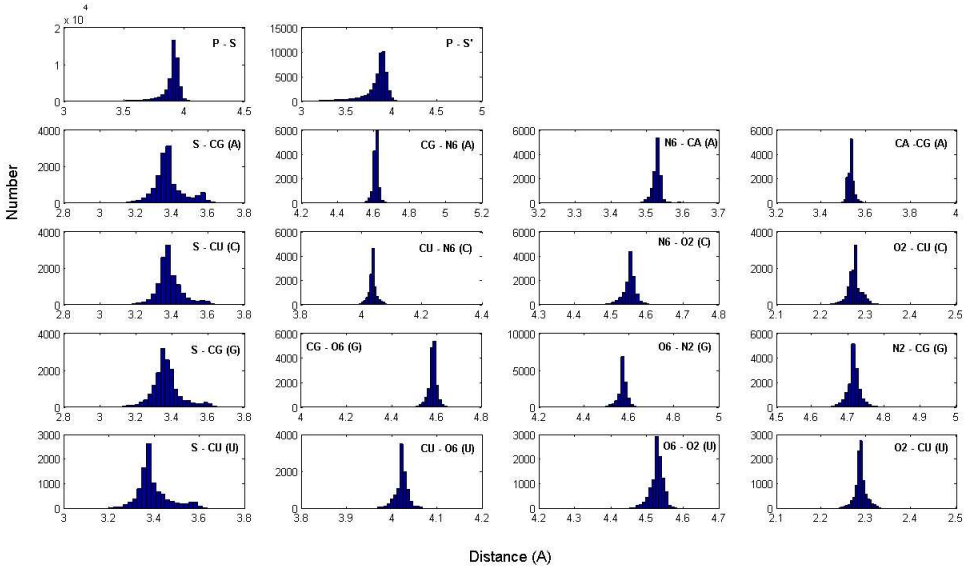

Figure S1: Histogram of the bond length distributions between CG atoms obtained from statistical structures. The bond types are defined in Table 2.

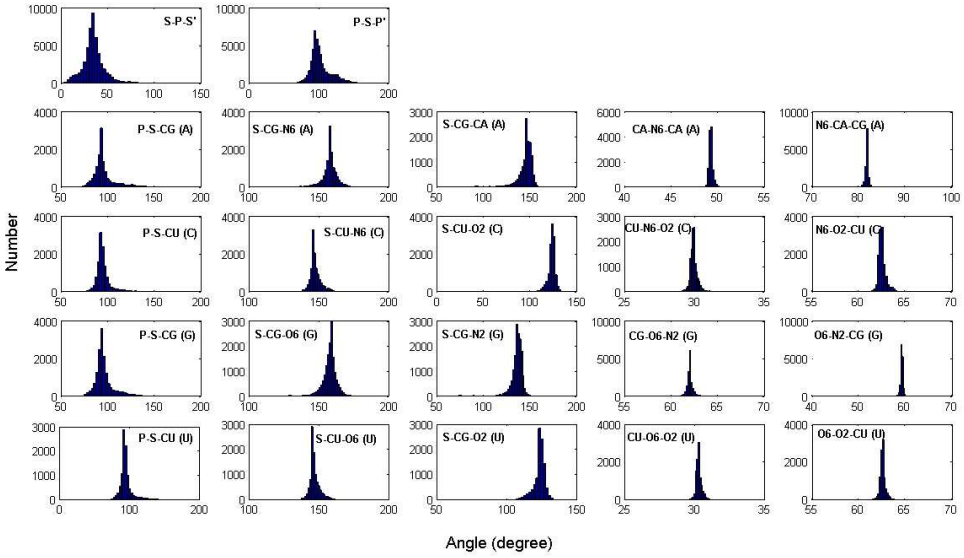

Figure S2: Histogram of the bond angle distributions between CG atoms obtained from statistical structures. The angle types are defined in Table 3. The primes at atoms S and P indicate the atoms come from their neighbor residues.

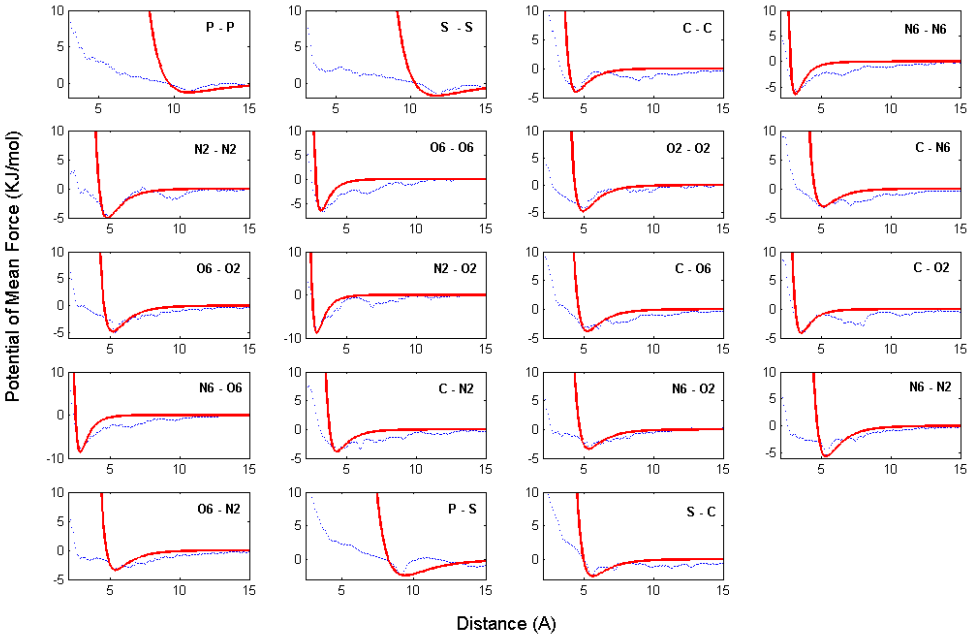

Figure S3: Potential of mean force for similar and unlike pairs of CG atoms. The blue dotted lines are the statistical results and the red solid lines are the fitted Buckingham potential curves. The potential of mean force were obtained from the intermolecular RDF for the 9 CG atoms, whose values are used as the initial values of the non-bonded parameters.

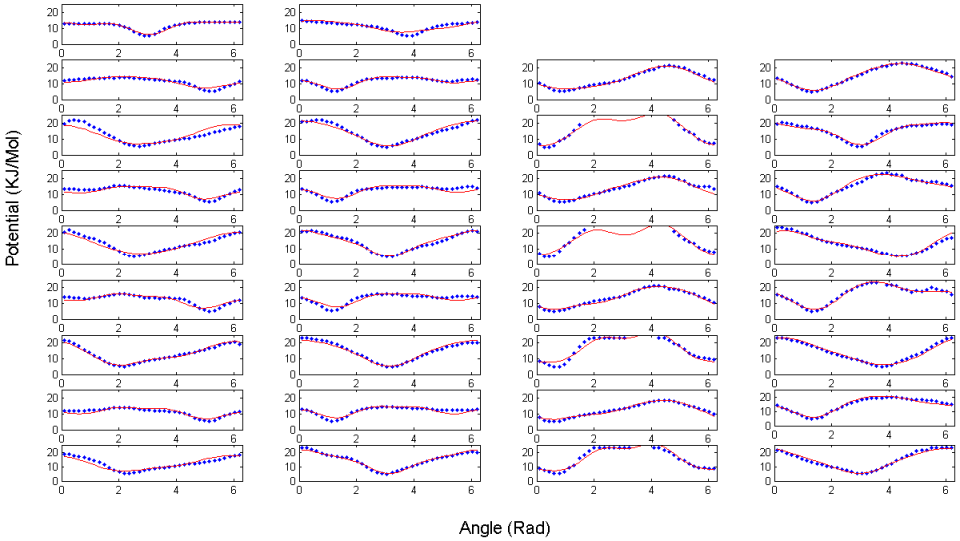

Figure S4: Torsion potential between CG atoms obtained from statistical structures. The blue dot is the statistical results and the red line is the fitting curve. The torsion types are defined in Table 5. The primes at atoms S and P indicate the atoms come from their neighbor residues.

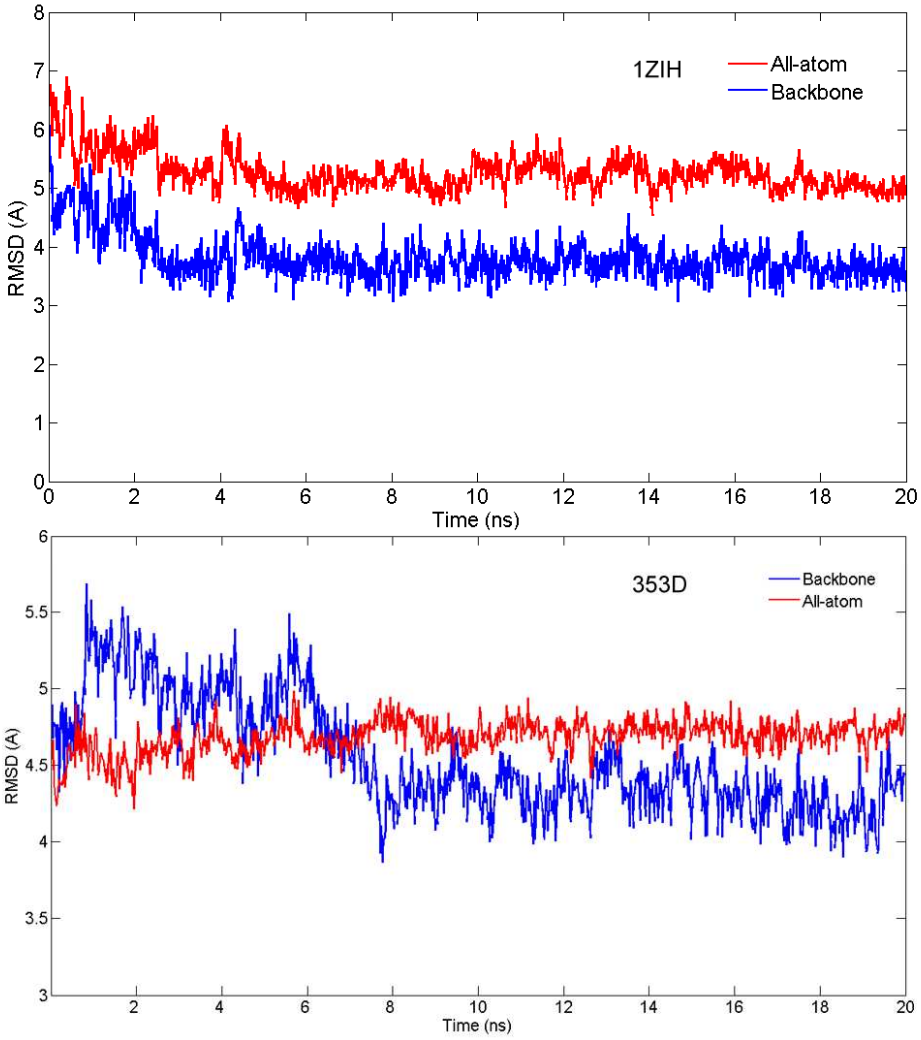

Figure S5: The all-atom (blue line) and backbone (red line) RMSDs of the RNA 1ZIH and 353D compared to their native structures. The simulation started from the last snapshot of simulated annealing simulation in Figure 3a. Simulation was performed for 20 ns with GB/SA solvation model.