

Correction to NMR of CCCC RNA Reveals a Right-Handed Helix and Revised Parameters for AMBER Force Field Torsions Improve Structural Predictions from Molecular Dynamics

Jason D. Tubbs, David E. Condon, Scott D. Kennedy, Melanie Hauser, Philip C. Bevilacqua, and Douglas H. Turner*

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The labeling of Figure 5A has been corrected.

The trajectory for $\delta 4$ has been replaced with the correct trajectory (the corrected Figure S5 in the original Supporting Information appears below).

The trajectory for $\delta 1$ has been replaced with the correct trajectory (the corrected Figure S10 in the original Supporting Information appears below).

Funding for the research was missing and should have been listed as, "Funding from NIH Grant GM22939 (D.H.T.) and NSF Grant CHE-1213667s".

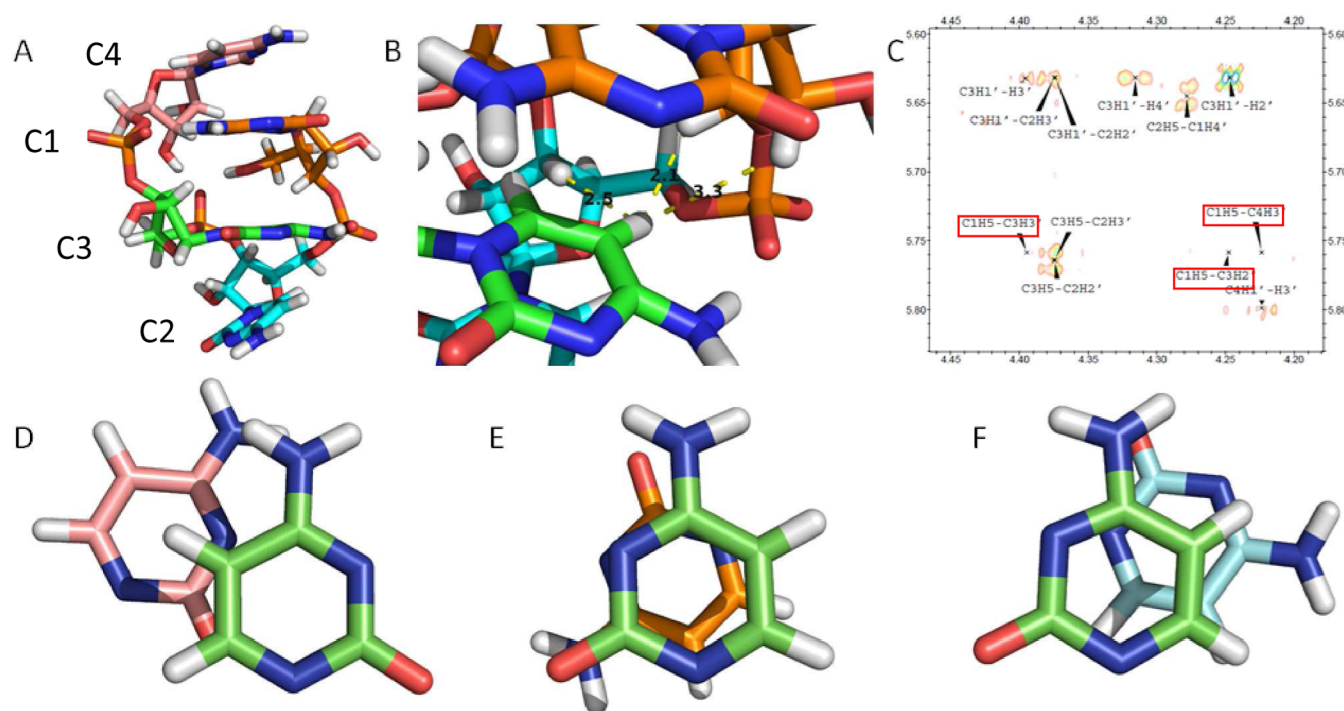


Figure 5. (A) 3D representation of r(CCCC) when C1 intercalates between C3 and C4 after 770 ns in the MD simulation with A-form (C3'-endo/anti) starting structure with the parm99TOR force field; (B) C1 intercalated between C3 and C4. The distances shown correspond to C1H5–C4H3' (2.5 Å), C1H5–C3H3' (2.1 Å), and C1H5–C3H2' (3.3 Å); (C) 200 ms NOESY of r(CCCC) showing the absence of the hypothetical H–H cross-peaks, red boxed labels, predicted by the parm99TOR simulation after 770 ns; (D) typical A-form base stacking between C1 and C2 (from nugen structure); (E) the base stacking between C1 and C3 after C1 intercalates between C3 and C4 observed after 770 ns; (F) the base stacking between C1 and C4 after C1 intercalates between C3 and C4 observed after 770 ns. The residues C1, C2, C3, and C4 are green, pink, orange, and cyan, respectively.

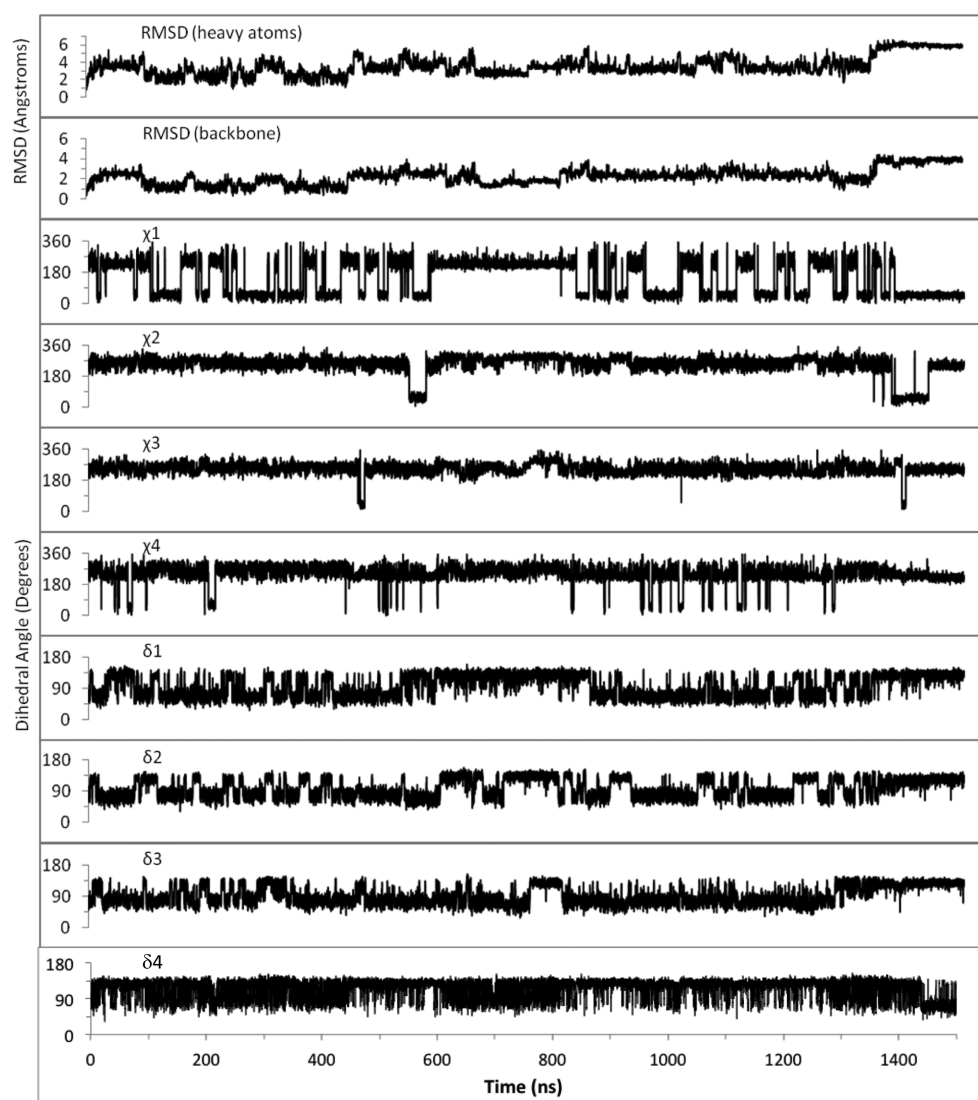


Figure S5. Time evolution (in ns) of r(CCCC) with parm99 force field. The starting structure is A-form r(CCCC) after minimization. Top two plots show the heavy atom RMS deviations (in Å) of the whole structure and of the backbone, respectively, relative to A-form r(CCCC). The remaining plots correspond to the χ and δ dihedral angles for each residue. A delta dihedral angle, δ , of 78° to 90° and 140° to 152° correspond to sugar puckers of C3'-endo and C2'-endo, respectively. Anti, high anti, and syn conformations were defined by a chi dihedral angle, χ , 180° to 239°, 240° to 300°, and 0° to 120°, respectively.

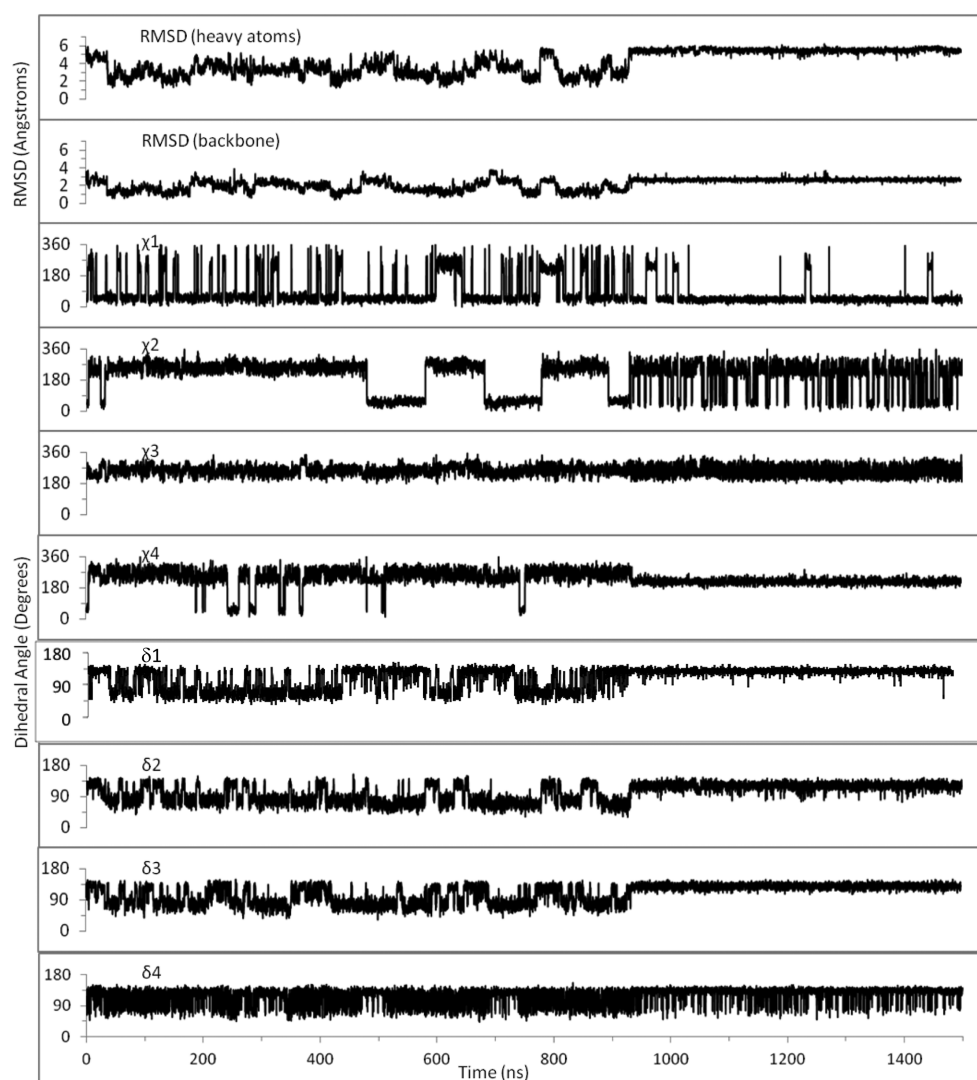


Figure S10. Time evolution (in ns) of $r(\text{CCCC})$ with parm99 force field. The starting structure is C2'-endo/syn $r(\text{CCCC})$ after minimization. Top two plots show the heavy atom RMS deviations (in Å) of the whole structure and of the backbone, respectively, relative to A-form $r(\text{CCCC})$. The remaining plots correspond to the χ and δ dihedral angles for each residue. Delta dihedral angles, δ , of 78° to 90° and 140° to 152° correspond to sugar pucker of C3'-endo and C2'-endo, respectively. Anti, high anti, and syn conformations were defined by a chi dihedral angle, χ , of 180° to 239° , 240° to 300° , and 0° to 120° , respectively. After 931 ns, C₄ forms a looplike structure with C₁ stacking on C₄ with overlapping carbonyls and aminos.