Table 4: Supplementary Material: Calculated and experimental[35] mean values of the backbone dihedral angles (in degrees) for residues A4 - U11 of the UUCG hairpin, including their standard deviations. For the loop residues U6 - G9, the calculated distribution functions showed two peaks. This confirms the presence of at least two conformational states as shown in Figure 1. The NMR study also reported two values for some angles of C8 and C9, which, however, do not directly correspond to the two conformational states observed in the MD simulation.

		α	β	γ	δ	ϵ	ζ
A4	MD	-72.±9.	178.±10.	60.±8.	78.±6.	-152.±11.	-70.± 9.
	NMR	-79.±7.	173.±5.	63.±6.	91.±2.	-157.±3.	-73.± 3.
C5	MD	-72.±9.	171.±10.	59.±8.	78.±6.	-162.±15.	-67.± 13.
	NMR	-72.±4.	163.±3.	62.±5.	92.±1.	-147.±9.	-68.± 10.
U6	MD	-71.±9.	173.±9.	61.±7.	72.±6.	-168.±10.	-88.± 18.
		158.±11.	-158.±9.	-172.±10.	153.±6.	-94.±10.	-125.± 10.
	NMR	-80.±11.	180.±15.	50.±3.	92.±1.	-166.±3.	-98.± 4.
U7	MD	-63.±10.	177.±17.	-171.±12.	147.±9.	-83.±10.	-70.± 15.
		-161.±10.		56.±9.		-164.±10.	61.± 16.
		68.±15.					
	NMR	-143.±5.	113.±3.	63.±5.	134.±1.	-102.±5.	-57.± 4.
C8	MD	-62.±15.	177.±10.	57.±8.	144.±9.	-91.±11.	72.± 11.
		-93.±15.					
	NMR	-57.±4.	174.±4.	45.±2.	136.±3.	-114.±9.	106.± 6.
		30.±8.	-143.±6.	-170.±5.			
G9	MD	67.±12.	-172.±11.	-178.±7.	86.±8.	-84.±10.	-59.± 9.
					108.±8.	-175.±10.	56.± 11.
	NMR	-58.±12.	135.±6.	-28.±8.	91.±1.	-147.±10.	-43.± 44.
		110.±8.	-130.±12.				
G10	MD	-69.±9.	79.±11.	176.±15.	82.±7.	-155.±8.	-62.± 8.
		-132.±10.					
	NMR	-125.±15.	90.±15.	-171.±28.	96.±2.	-151.±2.	-68.± 3.
U11	MD	-74.±9.	175.±8.	60.±8.	78.±6.	-155.±9.	-70.± 13.
	NMR	-66.±3.	173.±4.	53.±4.	89.±1.	-156.±7.	-91.± 5.

Table 5: Supplementary Material: Calculated and experimental[35;37] dihedral angles χ ($O_{4'}$-$C_{1'}$-N_1-C_2 for pyrimidine and $O_{4'}$-$C_{1'}$-N_9-C_4 for purine) including their standard deviation, obtained for the fourteen residues of the UUCG hairpin. The base of residue U7 adopts both anti (77 %) and syn (23 %) conformations during the simulation.

	χ_{MD} (degree)	χ_{exp} [35] (degree)	χ_{exp} [37] (degree)
G1	-171.±9.		
G2	-163.±8.		-168.±2.
C3	-163.±9.		
A4	-156.±9.	-149.±3.	-162.±1.
C5	-153.±11.	-141.±3.	-169.±8.
U6	-147.±17.	-142.±3.	-164.±4.
U7	-131.±19.; 48.±12.	-147±6.	-143.±9.
C8	-137.±12.	-126.±1.	-150.±6.
G9	61.±20.	61.±14.	44.±4.
G10	-161.±9.	-166.±2.	-145.±13.
U11	-153.±8.	-153.±2.	
G12	-171.±8.		-168.±4.
C13	-159.±7.		-171.±3.
C14	-148.±12.		-162.±5.

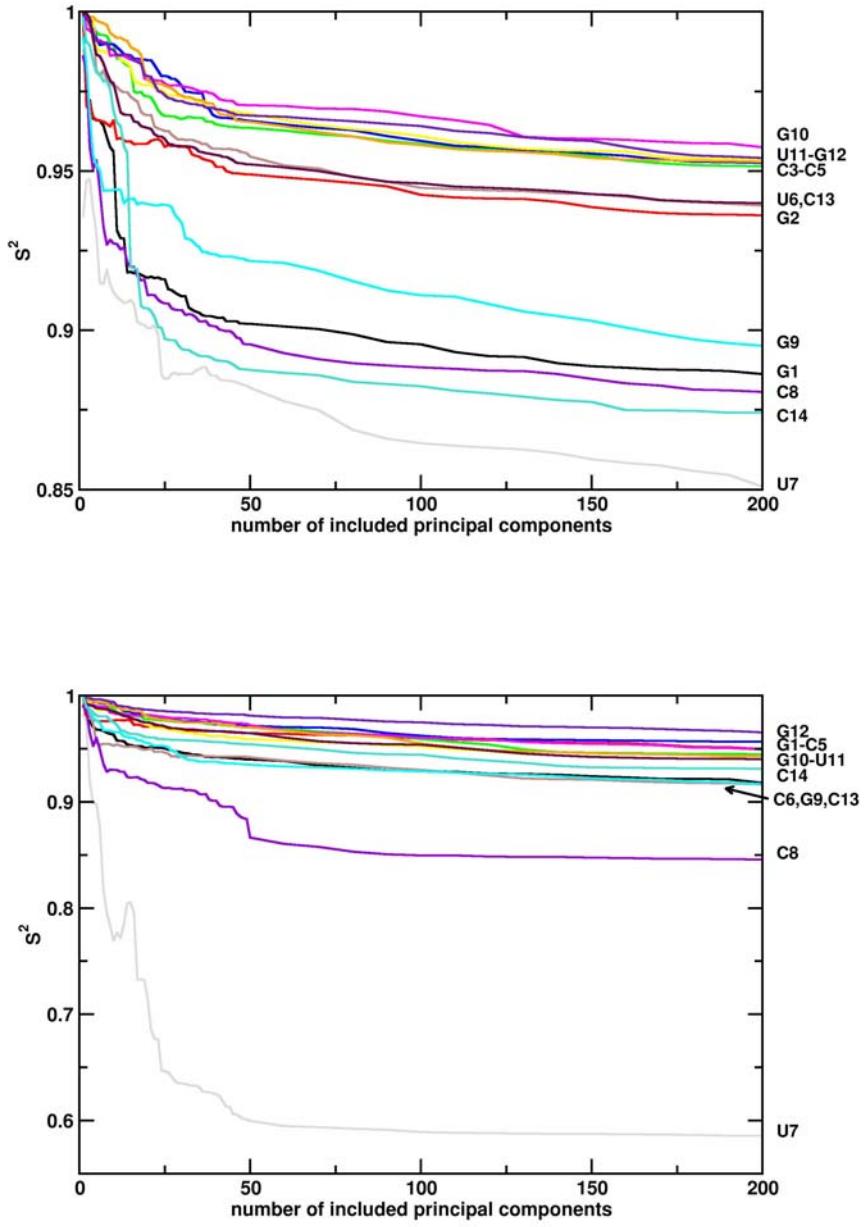

Figure 6: Supplementary Material: Order parameter S^2 (100 ps Lipari-Szabo fit) for $C_{1'}$ (top) and C_6/C_8 (bottom) obtained for the fourteen residues of the UUCG hairpin, plotted as a function of the number of included principal components.