Supporting Information

NMR study of RNA structures in the 3⁻end of the Hepatitis C Virus genome

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Figure S1: The 3' $X^{2SL-IrAID}$ RNA adopts a similar structure as 3'X. Overlay of the aromatic region of the 2D 1H-1H NOESY spectra collected for 3'X (black) and 3' $X^{2SL-IrAID}$ (red) is shown. The modest spectral changes were caused by the mutations in 3' $X^{2SL-IrAID}$, and the assignment of the mutant sequences in the upper stem of SL2/3 are marked. Adenosine C2-H proton NOE connectivities are marked in purple.



Figure S2: (A) Secondary structure of the SL2/3 control oligonucleotides. (B) Portion of the 2D 1H-1H NOESY spectrum collected for the SL2/3 control RNA in ²H₂O. Inter- and intra- residue ribose-to-aromatic proton NOE connectivities are labeled. Adenosine C2-H proton NOE connectivities are marked in purple.



Figure S3: (A) Secondary structure of the kissing-interaction control oligonucleotides. (B) Portion of the 2D 1H-1H NOESY spectrum collected for the Kissing-loop control RNA in 2 H₂O. Inter- and intra- residue ribose-to-aromatic proton NOE connectivities are labeled. Adenosine C2-H proton NOE connectivities are marked in purple.



Figure. S4: The ion-induced free energy for each predicted 3D structure of the 3'X 2SL conformation. The bulk concentrations [Mg²⁺] correspond to 0 mM (black), 0.2 mM (red), 2 mM (blue), and 6 mM (pink).



Figure. S5: 5BSL3.2 bulge residues are not affected upon formation of the kissing-loop interaction. The C2-H of A_{9298} gave characteristic NOEs to U_{9299} -H1' and G_{9274} -H1' in the 2D NOESY spectra of 3'END in both PI buffer (A) and PI buffer containing 6 mM MgCl₂ (B). The assignments were made by referencing with the assigned NOESY spectrum of 5BSL3.2 collected in PI buffer (C).