Supporting Information for:

The Mechanisms of RNA SHAPE Chemistry

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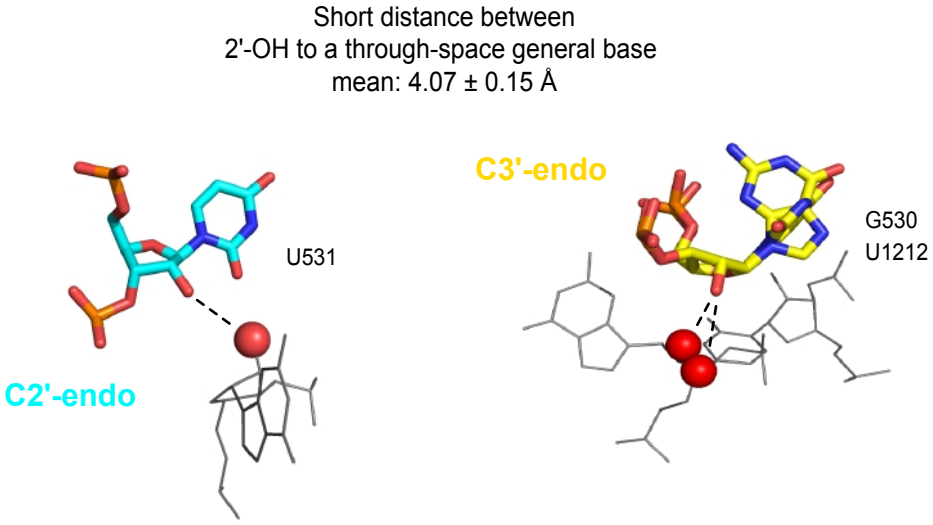
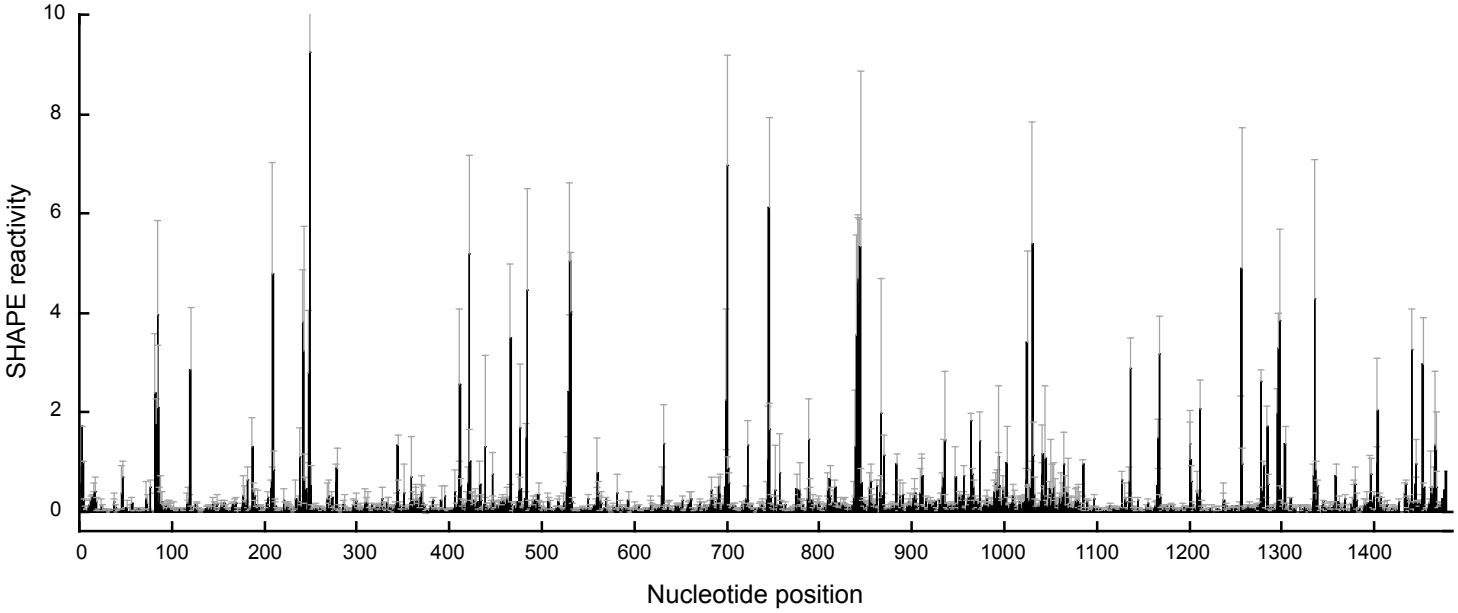


Supporting Figure 1: Nucleotides in which the 2'-OH group is close to a through-space group capable of hydrogen bond formation and general base catalysis. Nucleotides in the C2'- or C3'-endo ribose conformations are illustrated in cyan and yellow, respectively. Through-space neighbors are shown in gray with the hydrogen-bonding functional group illustrated with a red sphere.



Supporting Figure 2: SHAPE reactivity histogram reporting the mean of three independent experiments. Standard deviations at each nucleotide are indicated with gray error bars. These data have been deposited in the SNRNASM database.

Table S1: Conformations of nucleotides with high SHAPE reactivities (0.7 – 2.0), B-factor less than 60, and well-defined position in the ribosome crystal.

Position	Facilitating interaction(s)	Conforms to model	Non-adjacent interaction
235	5.1 Å PO-to-2'-OH distance 3.4 Å distance to O4	[a]	
244	5.1 Å PO-to-2'-OH distance	[a]	
251	3.3 Å distance to OP2(268)	✔	✔
352	2.8 Å distance to O1P	✔	
561	2.5 Å distance to O1P	✔	
758	3.0 Å distance to N6(583)	✔	✔
789	2.6 Å distance to N7(791)	✔	✔
812	2.8 Å distance to N1(765)	✔	✔
867	2.6 Å distance to N1(873)	✔	✔
871	5.3 Å PO-to-2'-OH distance		
911	3.4 Å distance to O4(912) 5.3 Å PO-to-2'-OH distance	✔	✔
912	5.2 Å PO-to-2'-OH Å distance	✔	
1201	2.0 Å distance to O1P(1200) 2.5 Å distance to OP	✔	✔
1396	2.7 Å distance to O1P(15)	✔	✔
1403	3.2 Å distance to N1(1499)	✔	✔
1404	2.8 Å distance to O2'(1519)	✔	✔
1467	5.1 Å PO-to-2'-OH distance	[a]	
1468	2.6 Å distance to O2'(318)	✔	✔

[a] Does not fully conform. PO vector is oriented away from the 2'-OH but is not as long as for the hyper-reactive nucleotides. Numbers in parentheses indicate interactions with non-adjacent nucleotides.