

An Alternating Sheared AA Pair and Elements of Stability for a Single Sheared Purine-Purine Pair Flanked by Sheared GA Pairs

Supporting Information

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Table S1. List of Distance Restraints (in Å) Used for the Structural Modeling of $\begin{smallmatrix} \text{GGU} & \text{GGA} & \text{GGCU} \\ \text{PCCA} & \text{AAG} & \text{CCG} \end{smallmatrix}$. See text for Dihedral Angle Restraints. Values in fifth column are measured distances of corresponding internal loop in the crystal structure in H68 of *D. radiodurans* LSU rRNA (PDB: 1NKW) (*I*).

Hydrogen bond restraints				
1:G5'_1:H1	1:C_19:N3	1.800	2.500	
1:G5'_1:O6	1:C_19:H42	1.800	2.500	
1:G5'_1:H22	1:C_19:O2	1.800	2.500	
1:G_2:H1	1:C_18:N3	1.800	2.500	
1:G_2:O6	1:C_18:H42	1.800	2.500	
1:G_2:H22	1:C_18:O2	1.800	2.500	
1:G_7:H1	1:C_13:N3	1.800	2.500	
1:G_7:O6	1:C_13:H42	1.800	2.500	
1:G_7:H22	1:C_13:O2	1.800	2.500	
1:G_8:H1	1:C_12:N3	1.800	2.500	
1:G_8:O6	1:C_12:H42	1.800	2.500	
1:G_8:H22	1:C_12:O2	1.800	2.500	
1:C_9:N3	1:G5'_11:H1	1.800	2.500	
1:C_9:H42	1:G5'_11:O6	1.800	2.500	
1:C_9:O2	1:G5'_11:H22	1.800	2.500	
Distance restraints from SNOESY				
1:G_8:H1	1:G_7:H1	2.768	6.459	
1:G_4:H1	1:U_3:H3	3.002	7.000	5.50
1:G_4:H1	1:G_5:H1	2.423	5.654	6.04
1:G_5:H1	1:G_14:H1	2.500	7.000	7.82

1:G_2:H1	1:U_3:H3	2.228	5.200	
1:G_2:H1	1:G5'_1:H1	3.079	7.000	
1:U_3:H3	1:A_17:H2	1.800	4.022	3.28
1:U_3:H3	1:A_17:H61	1.964	4.582	3.84
1:U_3:H3	1:A_17:H62	1.800	4.102	2.46
1:G_4:H1	1:A_17:H61	3.275	7.000	3.99
1:G_4:H1	1:A_17:H62	2.467	5.757	3.46
1:G5'_1:H1	1:P3'_20:H6	3.102	7.000	
1:C_19:H41	1:P3'_20:H6	2.081	4.857	
1:C_19:H42	1:P3'_20:H6	1.846	4.308	
1:G5'_11:H1	1:U3'_10:H1'	2.428	5.664	
1:G5'_1:H1	1:P3'_20:H1'	2.062	4.811	
1:G_2:H1	1:U_3:H1'	2.204	5.144	
1:U_3:H3	1:G_4:H1'	2.369	5.528	3.57
1:G_2:H1	1:C_19:H1'	2.107	5.917	
1:G5'_1:H1	1:G_2:H1'	2.368	5.526	
1:G_7:H1	1:G_14:H1'	2.040	4.761	3.58
1:G_5:H1	1:G_14:H2'	2.413	5.631	7.07
1:G_14:H1	1:G_5:H1'	1.800	7.000	10.76
Distance restraints from D ₂ O NOESY				
1:G5'_1:H8	1:G5'_1:H1'	2.446	4.543	
1:G5'_1:H8	1:G_2:H8	3.312	6.000	
1:G5'_1:H1'	1:G5'_1:H3'	2.528	4.696	
1:G5'_1:H1'	1:G5'_1:H4'	2.315	4.299	
1:G5'_1:H1'	1:G_2:H8	3.145	5.841	
1:G5'_1:H2'	1:G5'_1:H8	3.123	5.800	
1:G5'_1:H2'	1:G5'_1:H1'	1.928	3.581	
1:G5'_1:H2'	1:G_2:H8	1.800	3.188	
1:G5'_1:H2'	1:G_2:H1'	2.950	5.479	
1:G5'_1:H3'	1:G5'_1:H8	2.256	4.190	
1:G5'_1:H3'	1:G_2:H8	2.078	3.860	
1:G_2:H8	1:G_2:H1'	2.689	4.994	
1:G_2:H8	1:G_2:H3'	2.238	4.157	
1:G_2:H1'	1:G_2:H3'	2.530	4.699	
1:G_2:H1'	1:G_2:H4'	2.567	4.768	
1:G_2:H2'	1:G_2:H8	2.864	5.318	
1:G_2:H2'	1:G_2:H1'	2.128	3.952	
1:G_2:H3'	1:U_3:H6	2.125	3.947	
1:G_2:H4'	1:G_2:H8	2.614	4.854	
1:U_3:H6	1:G_2:H2'	1.806	3.354	
1:U_3:H6	1:U_3:H5	1.800	3.162	
1:U_3:H6	1:U_3:H3'	2.064	3.833	2.89
1:U_3:H1'	1:G_2:H2'	2.837	5.269	
1:U_3:H1'	1:U_3:H6	2.896	5.379	3.55
1:U_3:H1'	1:U_3:H3'	3.102	5.761	3.86
1:U_3:H2'	1:U_3:H1'	1.985	3.686	2.80
1:U_3:H3'	1:G_4:H8	1.938	3.599	2.23
1:G_4:H8	1:U_3:H6	3.334	6.000	4.44
1:G_4:H8	1:U_3:H1'	3.432	6.000	4.76
1:G_4:H8	1:U_3:H2'	1.800	3.342	2.15
1:G_4:H8	1:G_4:H1'	2.936	5.453	3.73
1:G_4:H8	1:G_4:H2'	2.631	4.886	4.09
1:G_4:H8	1:G_4:H3'	2.022	3.755	2.69
1:G_4:H1'	1:U_3:H2'	2.884	5.355	3.41
1:G_4:H1'	1:G_4:H2'	1.969	3.656	2.78
1:G_4:H1'	1:G_4:H3'	3.085	5.730	3.80
1:G_4:H1'	1:G_4:H4'	2.741	5.091	3.53

1:G_4:H1'	1:A_17:H2	2.181	4.051	3.05
1:G_4:H2'	1:G_5:H8	2.446	4.543	2.06
1:G_4:H3'	1:G_4:H2'	1.927	3.578	2.44
1:G_4:H3'	1:G_5:H8	2.170	4.029	3.69
1:G_4:H4'	1:G_4:H2'	2.672	4.962	3.86
1:G_5:H8	1:G_5:H1'	3.002	5.574	3.77
1:G_5:H8	1:G_5:H2'	1.800	2.778	4.04
1:G_5:H1'	1:G_5:H4'	2.809	5.216	3.40
1:G_5:H2'	1:G_5:H1'	2.288	4.250	2.78
1:G_5:H3'	1:G_5:H8	2.331	4.329	2.66
1:A_6:H2	1:G_7:H1'	2.690	4.996	4.80
1:A_6:H8	1:G_5:H1'	2.329	4.325	5.30
1:A_6:H8	1:A_6:H2'	2.934	5.449	3.88
1:A_6:H8	1:G_7:H8	2.630	4.884	3.61
1:A_6:H3'	1:A_6:H8	2.116	3.929	2.67
1:G_7:H8	1:A_6:H2'	2.375	4.411	2.32
1:G_7:H8	1:A_6:H3'	1.800	5.000	2.59
1:G_7:H8	1:G_7:H1'	1.954	5.500	3.49
1:G_7:H8	1:G_7:H3'	1.800	3.310	3.75
1:G_8:H8	1:G_7:H1'	3.095	5.748	
1:G_8:H8	1:G_8:H1'	2.767	5.138	
1:G_8:H8	1:G_8:H2'	2.916	5.415	
1:G_8:H1'	1:G_8:H3'	2.291	4.255	
1:G_8:H1'	1:G_8:H4'	2.367	4.395	
1:G_8:H2'	1:G_8:H1'	1.907	3.541	
1:G_8:H3'	1:G_8:H8	1.800	5.000	
1:C_9:H5	1:G_8:H2'	2.761	5.127	
1:C_9:H6	1:G_8:H1'	3.251	6.000	
1:C_9:H6	1:G_8:H2'	1.800	3.016	
1:C_9:H6	1:G_8:H3'	1.811	5.000	
1:C_9:H6	1:C_9:H5	1.800	3.111	
1:C_9:H6	1:C_9:H1'	2.537	4.711	
1:C_9:H6	1:C_9:H3'	1.800	3.312	
1:C_9:H1'	1:U3'_10:H6	2.843	5.279	
1:C_9:H1'	1:G_8:H2'	2.542	4.720	
1:C_9:H1'	1:C_9:H3'	2.678	4.973	
1:C_9:H1'	1:U3'_10:H6	3.172	5.892	
1:C_9:H2'	1:C_9:H1'	1.935	3.594	
1:C_9:H2'	1:U3'_10:H5	2.690	4.996	
1:C_9:H2'	1:U3'_10:H6	1.800	3.136	
1:C_9:H2'	1:U3'_10:H1'	2.401	4.459	
1:C_9:H3'	1:U3'_10:H6	2.372	4.405	
1:C_9:H4'	1:C_9:H1'	2.749	5.105	
1:U3'_10:H5	1:U3'_10:H6	1.800	3.194	
1:U3'_10:H6	1:U3'_10:H1'	2.792	5.185	
1:U3'_10:H2'	1:U3'_10:H6	2.290	4.252	
1:U3'_10:H2'	1:U3'_10:H1'	2.074	3.852	
1:U3'_10:H3'	1:U3'_10:H6	1.873	3.478	
1:U3'_10:H3'	1:U3'_10:H1'	2.560	4.754	
1:G5'_11:H8	1:G5'_11:H1'	2.511	4.663	
1:G5'_11:H8	1:G5'_11:H4'	2.890	5.367	
1:G5'_11:H1'	1:G5'_11:H3'	2.480	4.605	
1:G5'_11:H1'	1:G5'_11:H4'	2.342	4.349	
1:G5'_11:H1'	1:C_12:H6	3.153	5.855	
1:G5'_11:H2'	1:G5'_11:H8	2.596	4.820	
1:G5'_11:H2'	1:G5'_11:H1'	1.898	3.525	
1:G5'_11:H3'	1:G5'_11:H8	2.404	4.465	

1:G5'_11:H3'	1:C_12:H6	1.860	3.454	
1:C_12:H5	1:G5'_11:H2'	2.729	5.068	
1:C_12:H5	1:G5'_11:H3'	2.520	4.679	
1:C_12:H6	1:G5'_11:H2'	1.800	3.133	
1:C_12:H6	1:C_12:H5	1.800	3.226	
1:C_12:H6	1:C_12:H1'	2.736	5.081	
1:C_12:H1'	1:G5'_11:H2'	3.024	5.616	
1:C_12:H1'	1:C_13:H6	3.219	5.978	
1:C_12:H2'	1:C_12:H1'	2.047	3.801	
1:C_12:H2'	1:C_13:H6	1.800	3.052	
1:C_12:H3'	1:C_12:H6	1.829	3.397	
1:C_12:H3'	1:C_12:H1'	2.409	4.473	
1:C_13:H6	1:C_12:H3'	2.448	4.545	
1:C_13:H6	1:C_13:H5	1.822	3.383	
1:C_13:H6	1:C_13:H3'	2.279	4.233	3.07
1:C_13:H1'	1:C_12:H2'	2.718	5.047	
1:C_13:H1'	1:C_13:H6	2.662	4.944	3.52
1:C_13:H1'	1:C_13:H3'	2.755	5.116	3.89
1:C_13:H1'	1:G_14:H8	3.394	6.000	5.24
1:C_13:H2'	1:C_13:H1'	1.986	3.689	2.80
1:C_13:H2'	1:G_14:H8	2.130	3.956	2.87
1:C_13:H2'	1:G_14:H1'	2.577	4.787	3.27
1:C_13:H3'	1:G_14:H8	2.121	3.938	2.21
1:C_13:H4'	1:C_13:H1'	2.741	5.091	3.29
1:G_14:H8	1:G_14:H3'	2.242	4.163	2.86
1:G_14:H1'	1:G_14:H3'	3.099	5.755	3.87
1:G_14:H2'	1:G_14:H8	2.060	3.826	3.99
1:G_14:H2'	1:G_14:H1'	2.118	3.934	2.79
1:G_14:H2'	1:A_15:H8	2.098	3.895	4.79
1:A_15:H2	1:A_6:H1'	2.496	4.636	10.23
1:A_15:H1'	1:A_6:H2	2.635	4.894	5.63
1:A_15:H1'	1:A_15:H2'	2.357	4.377	2.79
1:A_15:H1'	1:A_15:H3'	2.666	4.951	3.81
1:A_15:H3'	1:A_15:H8	2.505	4.652	1.91
1:A_16:H2	1:A_17:H1'	2.350	4.364	4.37
1:A_16:H8	1:A_15:H2'	2.082	3.867	2.83
1:A_16:H8	1:A_15:H3'	2.534	4.706	3.86
1:A_16:H8	1:A_16:H3'	2.280	4.234	2.85
1:A_16:H8	1:A_16:H4'	3.047	5.660	4.39
1:A_16:H8	1:A_17:H8	3.366	6.000	3.93
1:A_16:H1'	1:A_15:H2	2.172	4.035	10.78
1:A_16:H1'	1:A_15:H2'	3.050	5.665	5.83
1:A_16:H1'	1:A_16:H8	2.868	5.326	3.81
1:A_16:H1'	1:A_16:H2'	1.912	3.552	2.81
1:A_16:H1'	1:A_16:H3'	2.870	5.329	3.87
1:A_16:H1'	1:A_16:H4'	2.475	4.596	3.25
1:A_16:H1'	1:A_17:H8	3.410	6.000	5.15
1:A_16:H2'	1:A_16:H8	3.069	5.700	3.88
1:A_16:H2'	1:A_17:H8	1.845	3.427	2.72
1:A_17:H2	1:C_18:H1'	2.440	4.532	
1:A_17:H8	1:A_17:H3'	1.889	3.508	2.72
1:A_17:H8	1:A_16:H3'	1.800	5.000	2.62
1:A_17:H8	1:A_17:H1'	2.886	5.359	3.80
1:A_17:H8	1:C_18:H5	3.041	5.648	
1:A_17:H1'	1:A_16:H2'	2.720	5.052	3.74
1:A_17:H1'	1:A_17:H3'	2.776	5.156	3.85
1:A_17:H1'	1:A_17:H4'	2.571	4.775	3.26

1:A_17:H1'	1:C_18:H6	2.816	5.229	
1:A_17:H2'	1:A_17:H1'	1.967	3.654	2.80
1:A_17:H3'	1:C_18:H6	2.353	4.371	
1:C_18:H6	1:A_17:H2'	1.800	3.283	
1:C_18:H6	1:C_18:H5	1.800	3.188	
1:C_18:H6	1:C_18:H2'	2.932	5.444	
1:C_18:H6	1:C_18:H3'	1.822	3.383	
1:C_18:H1'	1:A_17:H2'	2.909	5.403	
1:C_18:H1'	1:C_18:H3'	2.102	3.904	
1:C_18:H1'	1:C_18:H4'	2.537	4.711	
1:C_18:H1'	1:C_18:H1'	1.921	3.567	
1:C_18:H3'	1:C_19:H6	2.100	3.900	
1:C_19:H5	1:C_18:H2'	2.716	5.045	
1:C_19:H5	1:C_18:H3'	2.566	4.766	
1:C_19:H6	1:C_18:H2'	1.800	3.117	
1:C_19:H6	1:C_19:H5	1.800	3.252	
1:C_19:H6	1:C_19:H1'	2.675	4.968	
1:C_19:H1'	1:C_18:H2'	3.024	5.616	
1:C_19:H1'	1:C_19:H3'	2.762	5.130	
1:C_19:H1'	1:P3'_20:H8	3.380	6.000	
1:C_19:H2'	1:C_19:H6	2.436	5.500	
1:C_19:H2'	1:C_19:H1'	1.841	3.418	
1:C_19:H2'	1:P3'_20:H8	1.804	3.351	
1:C_19:H3'	1:C_19:H6	1.800	3.328	
1:C_19:H3'	1:P3'_20:H8	2.190	4.067	
1:C_19:H4'	1:C_19:H1'	2.731	5.073	
1:P3'_20:H8	1:P3'_20:H1'	2.699	5.013	
1:P3'_20:H1'	1:P3'_20:H3'	2.703	5.020	
1:P3'_20:H1'	1:P3'_20:H4'	2.633	4.890	
1:P3'_20:H2'	1:P3'_20:H8	2.770	5.144	
1:P3'_20:H2'	1:P3'_20:H1'	2.109	3.916	
1:P3'_20:H3'	1:P3'_20:H8	1.929	3.583	
1:P3'_20:H4'	1:P3'_20:H8	2.963	5.502	

Table S2. List of Distance Restraints (in Å) Used for the Structural Modeling ofGGU GAA GGCU
PCCG AAG CCG . See text for Dihedral Angle Restraints.

Hydrogen bond restraints

1:G5'_1:H1	1:C_19:N3	1.800	2.500
1:G5'_1:O6	1:C_19:H42	1.800	2.500
1:G5'_1:H22	1:C_19:O2	1.800	2.500
1:G_2:H1	1:C_18:N3	1.800	2.500
1:G_2:O6	1:C_18:H42	1.800	2.500
1:G_2:H22	1:C_18:O2	1.800	2.500
1:G_7:H1	1:C_13:N3	1.800	2.500
1:G_7:O6	1:C_13:H42	1.800	2.500
1:G_7:H22	1:C_13:O2	1.800	2.500
1:G_8:H1	1:C_12:N3	1.800	2.500
1:G_8:O6	1:C_12:H42	1.800	2.500
1:G_8:H22	1:C_12:O2	1.800	2.500
1:C_9:N3	1:G5'_11:H1	1.800	2.500
1:C_9:H42	1:G5'_11:O6	1.800	2.500
1:C_9:O2	1:G5'_11:H22	1.800	2.500

Distance restraints from SNOESY

1:G_7:H1	1:G_14:H1'	2.153	4.000
1:G_17:H1	1:G_4:H1'	1.800	5.000
1:G_2:H1	1:U_3:H3	1.888	4.406
1:G_2:H1	1:G_17:H1	2.081	4.855
1:P3'_20:H6	1:G5'_1:H1	2.184	5.097
1:U_3:H3	1:C_18:H42	2.291	5.347
1:U_3:H3	1:C_18:H41	2.638	6.156
1:C_19:H42	1:P3'_20:H6	2.363	5.514
1:P3'_20:H6	1:C_19:H41	1.900	4.433
1:G5'_1:H1	1:P3'_20:H1'	2.120	4.946

Distance restraints from D₂O NOESY

1:A_6:H1'	1:A_15:H2	1.800	4.857 ^a
1:A_16:H1'	1:A_15:H2	1.800	4.299 ^a
1:A_15:H1'	1:A_6:H2	1.800	4.140 ^a
1:A_15:H8	1:A_5:H2	2.000	5.000 ^a
1:G_14:H1'	1:A_5:H2	1.800	5.000 ^a
1:G_14:H2'	1:A_5:H2	2.000	5.000 ^a
1:G_14:H1'	1:A_15:H8	2.000	5.495 ^a
1:A_16:H8	1:A_15:H2'	1.800	3.990 ^a
1:A_6:H8	1:A_5:H1'	1.800	4.119 ^a
1:G_4:H3'	1:A_5:H8	1.800	5.000 ^a
1:A_16:H8	1:A_15:H3'	1.800	5.000 ^a
1:G_4:H8	1:A_5:H8	3.401	6.000 ^a
1:A_15:H8	1:A_16:H8	3.084	5.727 ^a
1:A_16:H2	1:A_5:H4'	2.834	5.262 ^a
1:A_6:H1'	1:A_5:H2	1.800	5.000 ^b
1:A_16:H1'	1:A_5:H2	1.800	5.000 ^b
1:A_5:H1'	1:A_16:H2	1.800	5.000 ^b
1:A_5:H8	1:A_15:H2	1.800	5.000 ^b
1:G_4:H1'	1:A_15:H2	1.800	5.000 ^b
1:G_4:H2'	1:A_15:H2	1.800	5.000 ^b
1:A_5:H8	1:G_4:H1'	1.800	5.516 ^b
1:A_6:H8	1:A_5:H2'	1.800	4.658 ^b
1:A_15:H1'	1:A_16:H8	1.800	4.340 ^b

1:A_15:H8	1:G_14:H3'	1.800	5.000 ^b
1:A_5:H3'	1:A_6:H8	1.800	4.907 ^b
1:A_6:H8	1:A_5:H8	3.270	6.000 ^b
1:A_6:H2	1:A_15:H4'	3.000	6.000 ^b
1:A_5:H8	1:G_4:H2'	1.800	5.000
1:A_5:H8	1:A_5:H1'	1.800	4.965
1:A_5:H8	1:A_5:H2'	1.800	3.191 ^c
1:A_5:H2'	1:A_5:H1'	1.800	3.938
1:A_5:H3'	1:A_5:H1'	1.800	4.810
1:A_5:H3'	1:A_5:H8	1.800	5.000
1:A_5:H4'	1:A_5:H1'	1.800	4.411
1:A_15:H8	1:A_15:H1'	1.800	5.043
1:A_15:H8	1:A_15:H2'	1.800	5.000
1:A_15:H8	1:A_15:H3'	1.800	4.265
1:A_15:H1'	1:A_15:H3'	1.800	5.000
1:A_15:H1'	1:A_15:H4'	1.800	4.420
1:A_15:H2'	1:A_15:H1'	1.800	3.646
1:G_14:H2'	1:A_15:H8	1.800	4.762
1:G5'_1:H8	1:G5'_1:H1'	2.637	4.897
1:G5'_1:H8	1:G5'_1:H2'	2.645	4.911
1:G5'_1:H8	1:G5'_1:H4'	2.863	5.318
1:G5'_1:H1'	1:G5'_1:H3'	2.531	4.700
1:G5'_1:H1'	1:G5'_1:H4'	2.506	4.654
1:G5'_1:H1'	1:G_2:H8	2.872	5.334
1:G5'_1:H2'	1:G5'_1:H1'	1.936	3.596
1:G5'_1:H2'	1:G_2:H8	1.800	3.191
1:G5'_1:H3'	1:G5'_1:H8	2.352	4.367
1:G_2:H8	1:G5'_1:H3'	1.988	3.692
1:G_2:H8	1:G5'_1:H8	3.259	6.000
1:G_2:H8	1:G_2:H1'	2.625	4.875
1:G_2:H8	1:G_2:H2'	2.983	5.540
1:G_2:H8	1:G_2:H3'	2.303	4.278
1:G_2:H8	1:U_3:H5	2.759	5.124
1:G_2:H1'	1:G5'_1:H2'	3.001	5.573
1:G_2:H1'	1:G_2:H2'	1.889	3.508
1:G_2:H1'	1:G_2:H3'	2.891	5.369
1:G_2:H2'	1:U_3:H1'	2.486	4.617
1:G_2:H3'	1:U_3:H6	2.140	3.974
1:G_2:H4'	1:G_2:H8	2.594	4.817
1:G_2:H4'	1:G_2:H1'	2.769	5.143
1:U_3:H5	1:G_2:H2'	2.574	4.780
1:U_3:H6	1:G_2:H1'	2.962	5.501
1:U_3:H6	1:G_2:H2'	1.847	3.430
1:U_3:H6	1:U_3:H5	1.800	3.329
1:U_3:H6	1:U_3:H1'	2.401	4.458
1:U_3:H6	1:U_3:H3'	2.161	4.013
1:U_3:H1'	1:U_3:H3'	2.903	5.391
1:U_3:H1'	1:U_3:H4'	2.604	4.836
1:U_3:H2'	1:U_3:H6	2.325	5.000
1:U_3:H2'	1:U_3:H1'	1.954	3.629
1:U_3:H2'	1:G_4:H1'	2.373	4.408
1:U_3:H4'	1:U_3:H6	2.590	4.811
1:G_4:H8	1:U_3:H6	3.032	5.632
1:G_4:H8	1:U_3:H1'	3.252	6.000
1:G_4:H8	1:U_3:H2'	1.883	3.497
1:G_4:H8	1:U_3:H3'	1.942	3.606
1:G_4:H1'	1:G_4:H8	2.747	5.102

1:G_4:H1'	1:G_4:H2'	2.149	3.990
1:G_4:H1'	1:G_4:H4'	2.626	4.877
1:G_4:H2'	1:G_4:H8	2.482	4.610
1:G_4:H3'	1:G_4:H8	1.988	3.692
1:G_4:H3'	1:G_4:H1'	2.586	4.803
1:A_6:H8	1:A_6:H1'	2.569	5.500
1:A_6:H8	1:A_6:H3'	2.146	3.985
1:A_6:H1'	1:A_6:H2'	2.665	4.950
1:A_6:H1'	1:A_6:H3'	3.017	5.602
1:A_6:H2'	1:A_6:H8	2.691	4.998
1:A_6:H3'	1:G_7:H8	1.800	3.321
1:G_7:H8	1:A_6:H8	2.477	4.600
1:G_7:H8	1:A_6:H1'	3.796	6.000
1:G_7:H8	1:A_6:H2'	2.983	5.540
1:G_7:H8	1:G_7:H1'	2.374	4.409
1:G_7:H8	1:G_7:H2'	1.938	5.000
1:G_7:H1'	1:A_6:H2	2.462	4.572
1:G_7:H2'	1:G_8:H8	1.800	3.028
1:G_7:H2'	1:G_8:H1'	2.995	5.562
1:G_7:H3'	1:G_7:H8	1.800	5.000
1:G_7:H3'	1:G_8:H8	1.931	5.000
1:G_8:H8	1:G_7:H1'	2.675	4.968
1:G_8:H8	1:G_8:H1'	2.818	5.233
1:G_8:H8	1:G_8:H2'	3.057	5.676
1:G_8:H8	1:G_7:H8	3.200	5.943
1:G_8:H8	1:C_9:H5	3.137	5.826
1:G_8:H1'	1:C_9:H6	3.149	5.849
1:G_8:H2'	1:G_8:H1'	1.874	3.480
1:G_8:H2'	1:C_9:H5	2.654	4.928
1:G_8:H2'	1:C_9:H6	1.800	3.104
1:G_8:H3'	1:G_8:H8	1.973	3.664
1:G_8:H3'	1:G_8:H1'	2.515	4.672
1:G_8:H3'	1:C_9:H5	2.525	4.689
1:G_8:H3'	1:C_9:H6	2.149	3.990
1:G_8:H4'	1:G_8:H8	2.583	5.000
1:G_8:H4'	1:G_8:H1'	2.645	4.911
1:C_9:H5	1:U3'_10:H5	2.520	4.680
1:C_9:H6	1:G_8:H8	2.835	5.265
1:C_9:H6	1:C_9:H5	1.800	3.160
1:C_9:H6	1:U3'_10:H6	2.910	5.404
1:C_9:H1'	1:G_8:H2'	2.875	5.339
1:C_9:H1'	1:C_9:H6	2.545	4.727
1:C_9:H1'	1:C_9:H3'	2.478	4.602
1:C_9:H2'	1:C_9:H6	2.394	5.000
1:C_9:H2'	1:C_9:H1'	1.869	3.472
1:C_9:H3'	1:C_9:H6	1.928	3.580
1:C_9:H5	1:C_9:H3'	2.682	4.981
1:C_9:H4'	1:C_9:H1'	2.490	4.624
1:U3'_10:H5	1:C_9:H6	3.010	5.590
1:U3'_10:H5	1:C_9:H2'	2.450	4.551
1:U3'_10:H5	1:C_9:H3'	2.452	5.000
1:U3'_10:H6	1:C_9:H1'	2.773	5.149
1:U3'_10:H6	1:C_9:H2'	1.800	3.327
1:U3'_10:H6	1:C_9:H3'	2.085	3.872
1:U3'_10:H6	1:U3'_10:H5	1.800	3.267
1:U3'_10:H1'	1:U3'_10:H6	2.557	4.749
1:U3'_10:H1'	1:C_9:H2'	2.642	4.907

1:U3'_10:H2'	1:U3'_10:H6	2.288	4.249
1:U3'_10:H2'	1:U3'_10:H1'	2.024	3.760
1:U3'_10:H3'	1:U3'_10:H6	1.926	3.578
1:U3'_10:H3'	1:U3'_10:H1'	2.279	4.233
1:U3'_10:H4'	1:U3'_10:H1'	2.477	4.601
1:U3'_10:H4'	1:U3'_10:H6	2.466	5.000
1:G5'_11:H8	1:C_12:H6	2.682	4.981
1:G5'_11:H8	1:G5'_11:H1'	2.596	4.821
1:G5'_11:H8	1:G5'_11:H2'	2.498	4.639
1:G5'_11:H8	1:G5'_11:H3'	2.225	4.132
1:G5'_11:H1'	1:G5'_11:H3'	2.559	4.752
1:G5'_11:H1'	1:G5'_11:H4'	2.415	4.485
1:G5'_11:H1'	1:C_12:H6	2.863	5.318
1:G5'_11:H2'	1:G5'_11:H1'	1.896	3.522
1:G5'_11:H2'	1:C_12:H5	2.480	4.605
1:G5'_11:H2'	1:C_12:H6	1.800	3.220
1:G5'_11:H3'	1:C_12:H6	2.057	3.821
1:G5'_11:H8	1:G5'_11:H4'	3.017	5.602
1:G5'_11:H8	1:C_12:H5	3.603	6.000
1:C_12:H5	1:G5'_11:H3'	2.775	5.153
1:C_12:H6	1:C_12:H5	1.800	3.118
1:C_12:H6	1:C_12:H2'	2.173	5.000
1:C_12:H1'	1:G5'_11:H2'	2.908	5.401
1:C_12:H1'	1:C_12:H6	2.482	4.610
1:C_12:H1'	1:C_12:H2'	1.850	3.436
1:C_12:H1'	1:C_13:H6	2.957	5.492
1:C_12:H2'	1:C_13:H5	2.857	5.306
1:C_12:H2'	1:C_13:H6	1.800	3.296
1:C_12:H3'	1:C_12:H6	1.935	3.593
1:C_12:H3'	1:C_12:H1'	2.134	3.963
1:C_12:H4'	1:C_12:H1'	2.477	4.599
1:C_13:H6	1:C_13:H5	1.800	3.323
1:C_13:H6	1:C_13:H3'	2.011	3.735
1:C_13:H1'	1:C_12:H2'	2.775	5.153
1:C_13:H1'	1:C_13:H6	2.588	4.807
1:C_13:H1'	1:C_13:H3'	2.321	4.310
1:C_13:H1'	1:C_13:H4'	2.231	4.143
1:C_13:H1'	1:G_14:H8	3.288	6.000
1:C_13:H2'	1:C_13:H1'	1.861	3.455
1:G_14:H8	1:C_13:H6	2.968	5.512
1:G_14:H8	1:C_13:H2'	1.983	3.682
1:G_14:H8	1:C_13:H3'	1.800	3.251
1:G_14:H8	1:G_14:H2'	2.022	5.000
1:G_14:H1'	1:G_14:H8	2.785	5.173
1:G_14:H1'	1:G_14:H2'	1.993	3.701
1:G_14:H1'	1:G_14:H3'	2.818	5.233
1:G_14:H3'	1:G_14:H8	2.190	4.067
1:G_14:H4'	1:G_14:H1'	2.486	4.617
1:A_16:H2	1:G_17:H1'	2.400	4.457
1:A_16:H8	1:A_16:H2'	2.246	5.000
1:A_16:H8	1:G_17:H8	2.766	5.136
1:A_16:H1'	1:A_16:H8	2.755	5.117
1:A_16:H1'	1:A_16:H2'	1.945	3.612
1:A_16:H1'	1:A_16:H3'	2.612	4.851
1:A_16:H1'	1:A_16:H4'	2.464	4.576
1:A_16:H2'	1:G_17:H8	1.989	3.695
1:A_16:H3'	1:A_16:H8	2.129	3.953

1:A_16:H3'	1:G_17:H8	1.800	5.000
1:G_17:H3'	1:G_17:H8	1.800	5.000
1:G_17:H8	1:A_16:H1'	3.552	6.000
1:G_17:H8	1:C_18:H5	2.955	5.487
1:G_17:H1'	1:G_17:H8	2.529	4.697
1:G_17:H2'	1:G_17:H8	2.120	5.000
1:G_17:H2'	1:C_18:H6	1.800	3.194
1:G_17:H3'	1:C_18:H6	1.945	3.612
1:G_17:H3'	1:C_18:H5	2.560	4.754
1:C_18:H5	1:C_18:H6	1.800	3.299
1:C_18:H5	1:C_18:H3'	2.281	5.000
1:C_18:H6	1:G_17:H8	2.835	5.265
1:C_18:H6	1:G_17:H1'	2.857	5.305
1:C_18:H6	1:C_18:H1'	2.522	4.683
1:C_18:H6	1:C_18:H2'	2.720	5.051
1:C_18:H6	1:C_18:H3'	1.800	3.305
1:C_18:H1'	1:C_18:H2'	1.885	3.502
1:C_18:H1'	1:C_18:H3'	2.543	4.723
1:C_18:H1'	1:C_18:H4'	2.240	4.160
1:C_18:H1'	1:C_19:H6	2.506	6.000
1:C_18:H3'	1:C_19:H6	2.324	4.317
1:G_17:H2'	1:C_18:H5	2.396	4.449
1:C_19:H6	1:C_18:H2'	1.800	3.142
1:C_19:H6	1:C_19:H5	1.800	3.177
1:C_19:H6	1:C_19:H2'	2.304	5.000
1:C_19:H6	1:C_19:H3'	1.800	3.309
1:C_19:H1'	1:C_18:H2'	2.875	5.339
1:C_19:H1'	1:C_19:H6	2.598	4.825
1:C_19:H1'	1:C_19:H2'	1.815	3.371
1:C_19:H1'	1:C_19:H3'	2.586	4.803
1:C_19:H1'	1:P3'_20:H8	3.338	6.000
1:C_19:H2'	1:P3'_20:H8	1.800	3.198
1:C_19:H2'	1:P3'_20:H1'	2.533	4.704
1:C_19:H3'	1:P3'_20:H8	2.049	3.805
1:C_19:H4'	1:C_19:H1'	2.490	4.625
1:P3'_20:H2	1:G5'_1:H1'	3.149	5.849
1:P3'_20:H8	1:C_19:H6	3.270	6.000
1:P3'_20:H8	1:P3'_20:H1'	2.832	5.259
1:P3'_20:H8	1:P3'_20:H2'	2.408	4.472
1:P3'_20:H1'	1:P3'_20:H2'	2.015	3.742
1:P3'_20:H1'	1:P3'_20:H3'	2.612	4.851
1:P3'_20:H3'	1:P3'_20:H8	1.976	3.670
1:P3'_20:H4'	1:P3'_20:H8	2.560	4.754
1:P3'_20:H4'	1:P3'_20:H1'	2.396	4.450

^a For the structure modeling of A6/A15/A16 only; ^b For the structure modeling of A6/A5/A16 only; ^c Loosened upper bound to 4.50 Å for the structural modeling of A6/A5/A16.

Table S3a. List of the chemical shift assignments for $\frac{\text{GGU GGA GGCU}}{\text{PCCA AAG CCG}}$ at 30 °C referenced to TSP.

	H6/H8	H2/H5	H1'	H2'	H3'	H4'	H5/H5" ^{na}	Imino/amino ^b
G1	8.14	- ^c	5.95	4.89	4.55	4.47	4.14/3.99	11.88
G2	7.28	-	5.78	4.67	4.43	4.49	4.55/4.12	13.17 (8.40/6.16)
U3	7.32	5.02	5.14	4.42	4.22			12.53
G4	7.79	-	5.43	3.62	4.62	4.35	4.53/4.11	10.48
G5	8.11	-	5.65	5.01	4.95	4.72		9.77
A6	7.72	8.11	5.11	4.70	4.48			
G7	7.43	-	4.22					12.78
G8	7.18	-	5.74	4.50	4.37	4.44	4.03	13.29
C9	7.43	5.14	5.60	4.35	4.26	4.40	4.16/4.03	8.48/7.05
U10	7.74	5.56	5.73	3.97	4.16	4.14	4.02	10.95
G11	8.10	-	5.85	4.83	4.53	4.45	4.11/3.94	13.34
C12	7.83	5.23	5.64	4.53	4.48	4.59	4.44/4.16	8.73/6.83
C13	7.50	5.26	5.53	4.65	4.31	4.46	4.26/4.14	7.98/6.52
G14	7.99	-	5.72	4.53	4.93	4.65	4.46/4.27	9.33
A15	8.18	7.16	5.51	4.80	4.64	4.56		
A16	7.06	8.17	5.81	4.91	4.37	4.57	4.12	
A17	7.77	7.91	5.06	4.30	4.52	4.42		(7.82/6.64)
C18	7.36	5.24	5.26	4.15	4.35	4.52	4.01	8.36/7.09
C19	7.62	5.39	5.47	4.36	4.48	4.35	4.07	8.06/7.05
P20	8.84/8.43	8.13	6.15	4.17	4.34	4.31		-

^aThe H5' and H5'' assignments are not stereospecific.

^b Imino and amino proton were assigned at 5 °C.

^c Not applicable and labeled with -.

^d Assignments in parentheses are tentative.

Table S3b. List of the chemical shift assignments for $\frac{\text{GGU GAA GGCU}}{\text{PCCG AAG CCG}}$ at 30 °C referenced to TSP unless otherwise noted.

	H6/H8	H2/H5	H1'	H2'	H3'	H4'	H5'/H5" ^{na}	Imino/amino ^b	³¹ P ^c
G1	8.14	- ^d	5.94	4.87	4.55	4.47	4.13/4.00	11.93	-
G2	7.32	-	5.77	4.65	4.42	4.47	4.55/4.14	13.34	0.44
U3	7.23	5.26	5.20	4.44	4.21	4.38	4.06	11.49	0.09
G4	7.90	-	5.35	3.67	4.82	4.40	4.48/4.15		-0.56
A5	8.24	8.28	5.68	4.95	4.82	4.65	4.45/4.16		-0.05
A6	7.62	7.94	5.44	4.74	4.40		4.47/4.25		2.20
G7	7.47	-	4.27	4.33	4.37	4.40	4.47/4.10	12.61	(0.18) ^e
G8	7.13	-	5.71	4.49	4.39	4.43	4.27/4.01	13.22	-0.11
C9	7.42	5.12	5.59	4.37	4.26	4.39	4.16/4.03	8.47/7.08	-0.39
U10	7.74	5.55	5.73	3.96	4.16	4.14	4.31/4.03	10.95	0.25
G11	8.11	-	5.86	4.83	4.54	4.44	4.13/3.96	13.35	-
C12	7.83	5.25	5.65	4.57	4.49	4.50	4.43/4.16	8.72/6.89	-0.09
C13	7.41	5.32	5.45	4.48	4.24	4.43	4.45/4.13	8.10/6.59	0.62
G14	7.92	-	5.55	4.24	4.92	4.50	4.41/4.13		-0.21
A15	8.16	7.83	5.72	4.92	4.80	4.59	4.52/4.22		0.28
A16	7.52	8.06	5.42	4.80	4.36	4.52	4.47/4.21		1.41
G17	7.32	-	4.70	4.33	4.37			11.46 (6.36/5.40)	(0.17)
C18	7.59	5.37	5.41	4.19	4.43	4.36	4.09/4.04	8.29/7.06	0.23
C19	7.65	5.44	5.48	4.36	4.48	4.37	4.29/4.08	8.06/7.07	0.34
P20	8.84/8.44	8.13	6.15	4.17	4.33	4.31	4.44/4.10	-	0.38

^a The H5' and H5'' assignments are not stereospecific.

^b Imino and amino proton were assigned at 5 °C.

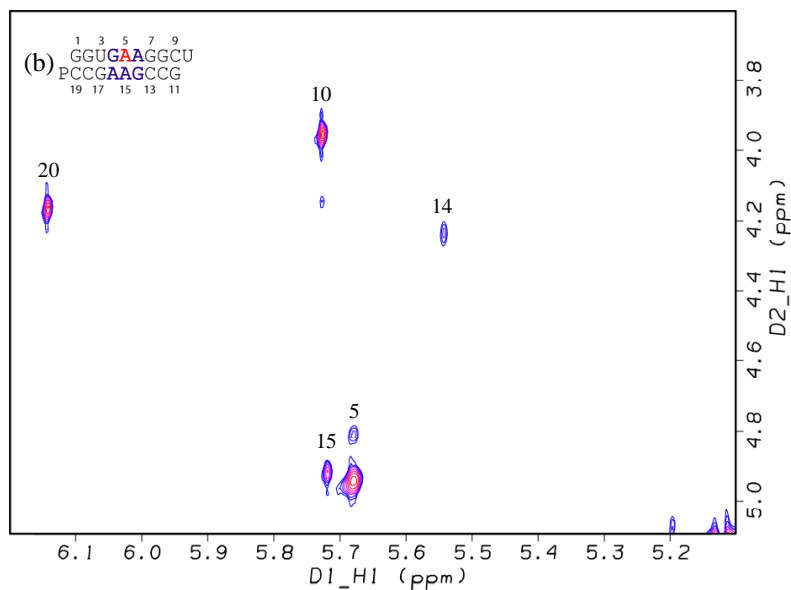
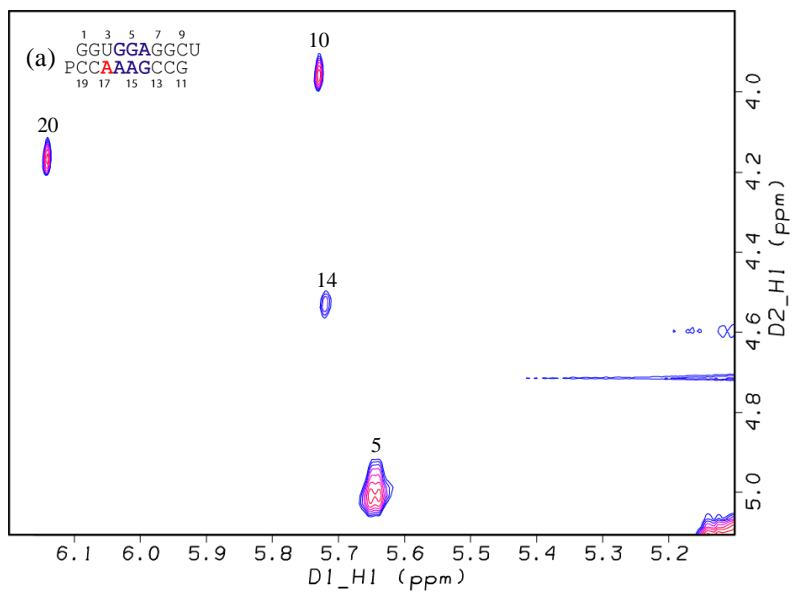
^c Referenced to external standard of 85% H₃PO₄ at 0 ppm.

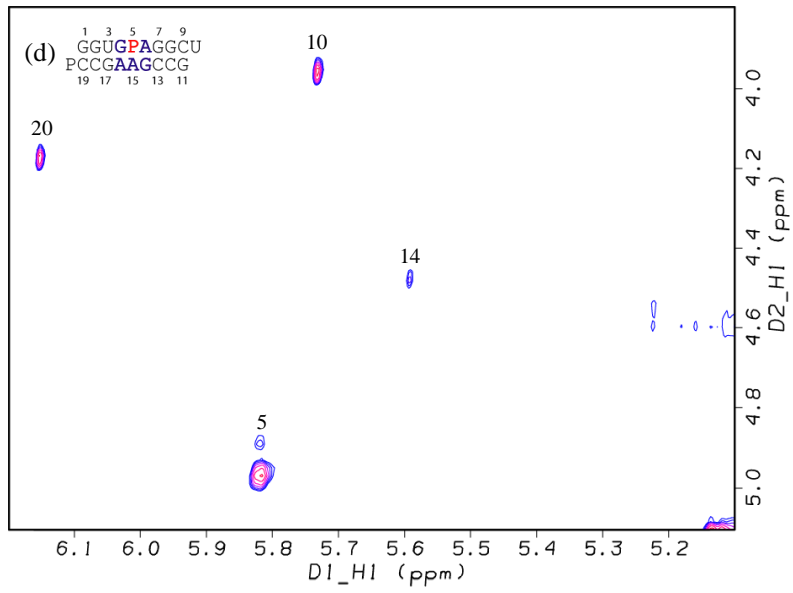
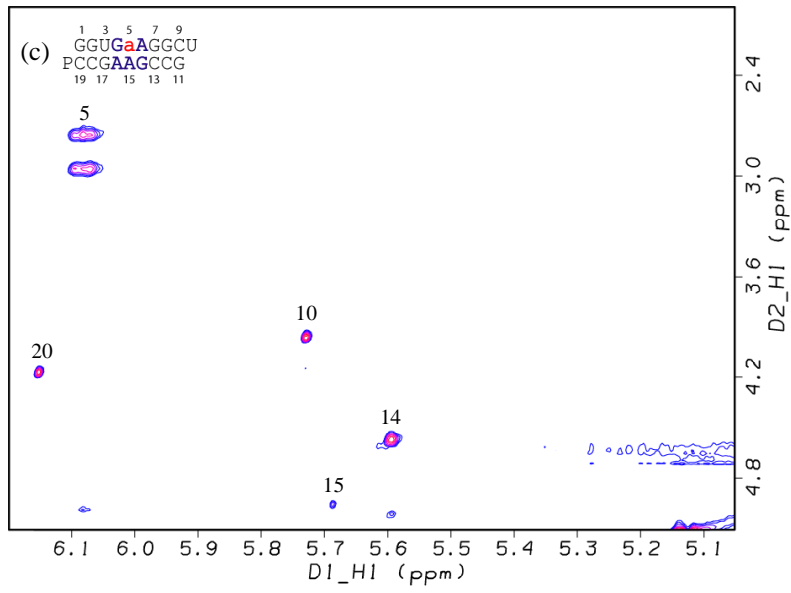
^d Not applicable and labeled with -.

^e Assignments in parentheses are tentative.

Figure S1. The 40 ms mixing time TOCSY spectra (H1'-sugar region) of $\begin{matrix} \text{GGU} & \text{GGA} & \text{GGCU} \\ \text{PCCA} & \text{AAG} & \text{CCG} \end{matrix}$,

$\begin{matrix} \text{GGU} & \text{GAA} & \text{GGCU} \\ \text{PCCG} & \text{AAG} & \text{CCG} \end{matrix}$, $\begin{matrix} \text{GGU} & \text{GaA} & \text{GGCU} \\ \text{PCCG} & \text{AAG} & \text{CCG} \end{matrix}$, $\begin{matrix} \text{GGU} & \text{GPA} & \text{GGCU} \\ \text{PCCG} & \text{AAG} & \text{CCG} \end{matrix}$, $\begin{matrix} \text{GGU} & \text{GIA} & \text{GGCU} \\ \text{PCCG} & \text{AAG} & \text{CCG} \end{matrix}$, and $\begin{matrix} \text{GGU} & \text{GAA} & \text{GGCU} \\ \text{PCCG} & \text{AIG} & \text{CCG} \end{matrix}$ at 30 °C.





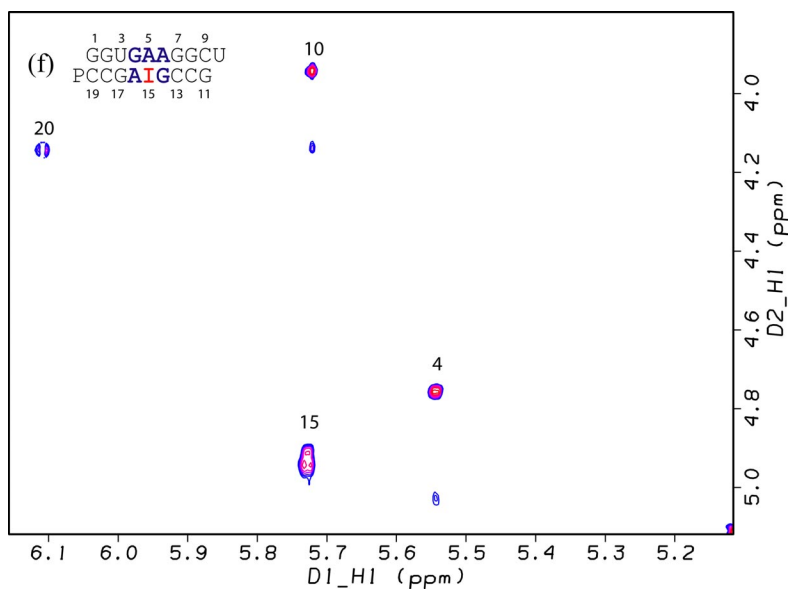
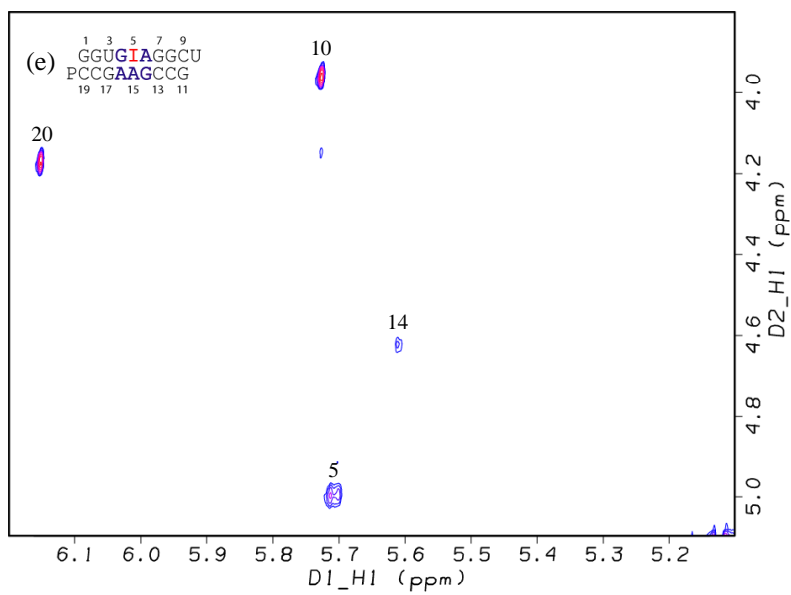


Figure S2. One-dimensional proton spectra (9–14.5 ppm) in 90:10 (v:v) H₂O:D₂O at 5 °C. (a) $\frac{\text{GGU GDA GGCUCU}}{\text{PCCG AAG CCG}}$, 0.9 mM, pH 7.0; (b) $\frac{\text{GGU GIA GGCUCU}}{\text{PCCG AAG CCG}}$, 2.4 mM, pH 5.7; (c) $\frac{\text{GGU GAA GGCUCU}}{\text{PCCG AIG CCG}}$, 0.8 mM, pH 6.5; (d) $\frac{\text{GGU GPA GGCUCU}}{\text{PCCG AAG CCG}}$, 0.9 mM, pH 6.9; and (e) $\frac{\text{GGU GaA GGCUCU}}{\text{PCCG AAG CCG}}$, 1.6 mM, pH 6.9. Numbers on spectra correspond to assignments with numbering starting at left most (5') nucleotide of top strand and ending at left most (3') nucleotide of bottom strand. The value to the right of each duplex is the free energy increment in kcal/mol for formation of the internal loop at 37 °C, at pH7 in 1 M NaCl. Spectra for $\frac{\text{GGU GGA GGCUCU}}{\text{PCCA AAG CCG}}$ and $\frac{\text{GGU GAA GGCUCU}}{\text{PCCG AAG CCG}}$ were published in ref (2).

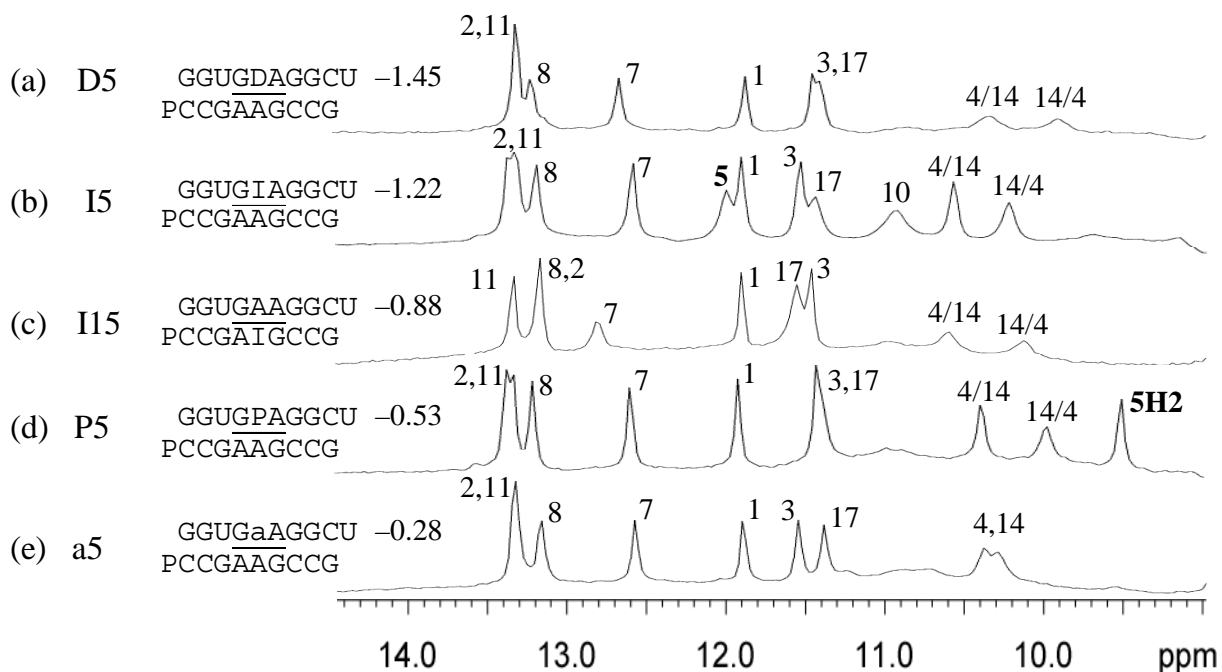
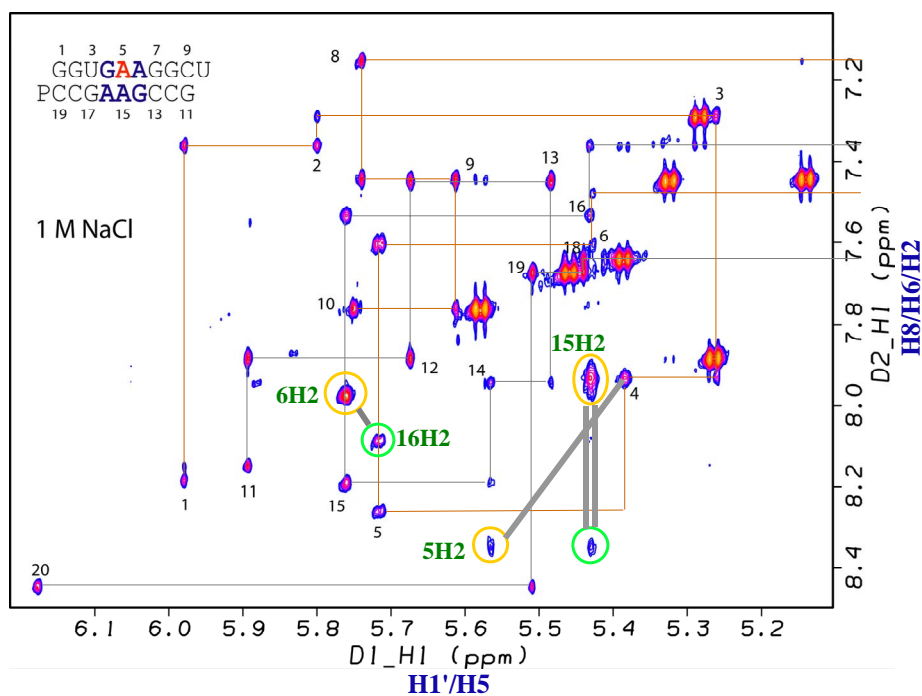


Figure S3:(H8/H6/H2)-(H1'/H5) region of the 400 ms mixing time NOESY spectrum of A5 duplex (Figure 2) at 30 °C in 1 M NaCl, 10 mM sodium phosphate, 0.5 mM disodium EDTA, pH7. As in Figure 3b for the A5 sequence at 80 mM NaCl, yellow and green circles connected by gray lines identify related cross peaks of major and minor conformations, respectively. Note that chemical shifts are only mildly salt dependent, although A6H1' and A16H1' overlap at 1 M NaCl so their cross peaks to A15H2 (major conformation) and A5H2 (minor conformation) are not resolved. A15H2 and G4H8 are also overlapped and the cross peak A15H2-G4H1' is overlapped with G4H8-G4H1'.



References:

1. Harms, J., Schluenzen, F., Zarivach, R., Bashan, A., Gat, S., Agmon, I., Bartels, H., Franceschi, F., and Yonath, A. (2001) High resolution structure of the large ribosomal subunit from a mesophilic Eubacterium. *Cell* 107, 679-688.
2. Chen, G., and Turner, D. H. (2006) Consecutive GA pairs stabilize medium size RNA internal loops. *Biochemistry In press*.