

Solution Structure of an RNA Internal Loop with Three Consecutive Sheared GA Pairs

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Supporting Information

Table S1. List of Distance and Dihedral Angle Restraints Used for Modeling.

Hydrogen bond restraints					
<i>Atom 1</i>	<i>Atom 2</i>	<i>Lower limit</i>	<i>Upper limit</i>		
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, upper limits loosened with the note *					
<i>Hydrogen 1</i>	<i>Hydrogen 2</i>	<i>lower limit</i>	<i>upper limit</i>	<i>NMR distance</i>	<i>note</i>
from SNOESY spectrum with 150 ms mixing time					
1:U_3:H3	1:G_2:H1	1.750	4.082	2.916	
1:G_17:H1	1:G_2:H1	1.940	4.527	3.234	
1:U_3:H3	1:G_4:H1	2.828	6.599	4.713	
1:G_4:H1	1:G_5:H1	2.340	5.459	3.899	
1:G_14:H1	1:G_5:H1	2.500	7.000	-	*
1:U_3:H3	1:C_18:H42	2.252	5.255	3.754	*
1:U_3:H3	1:C_18:H41	2.166	7.000	3.609	
1:P3'_20:H6	1:C_19:H41	1.942	4.531	3.237	
1:P3'_20:H6	1:C_19:H42	1.780	4.153	2.966	
1:G5'_11:H1	1:U3'_10:H1'	2.404	5.610	4.007	
1:G_7:H1	1:G_14:H1'	1.864	4.305	3.107	
1:G_17:H1	1:G_4:H1'	1.442	3.364	2.403	
1:P3'_20:H1'	1:G5'_1:H1	2.125	4.958	3.542	
1:G_2:H1	1:U_3:H1'	2.068	4.825	3.446	
1:U_3:H2'	1:G_17:H1	2.410	5.624	4.017	
1:G_5:H1	1:G_14:H2'	2.502	5.838	4.170	
1:P3'_20:H6	1:G5'_1:H1	2.217	5.172	3.695	
from D₂O NOESY spectrum with 100 ms mixing time unless otherwise noted					
1:G_2:H1'	1:G5'_1:H2'	2.798	5.196	3.997	200ms
1:G_2:H3'	1:U_3:H5	2.188	4.064	3.126	200ms

1:G_5:H8	1:G_4:H8	2.360	6.000	3.371	*200ms
1:G_17:H8	1:C_18:H5	3.294	6.000	4.706	200ms
1:G_17:H8	1:C_18:H6	3.268	6.000	4.668	200ms
1:A_15:H2	1:A_16:H2	3.493	6.000	4.99	200ms
1:A_15:H2	1:A_6:H8	3.839	6.000	5.484	200ms
1:G_7:H8	1:A_6:H8	2.557	4.749	3.653	200ms
1:G_7:H2'	1:G_8:H1'	2.614	4.855	3.735	200ms
1:G_8:H2'	1:C_9:H5	2.988	5.549	4.268	200ms
1:G5'_11:H8	1:C_12:H5	3.481	6.000	4.973	200ms
1:C_12:H1'	1:G5'_11:H2'	3.281	6.000	4.687	200ms
1:A_16:H1'	1:A_15:H2'	3.057	5.677	4.367	200ms
1:G5'_1:H8	1:G5'_1:H1'	2.819	5.235	4.027	
1:G5'_1:H8	1:G5'_1:H2'	2.680	4.977	3.829	
1:G5'_1:H8	1:G5'_1:H3'	2.309	4.288	3.298	
1:G5'_1:H1'	1:G5'_1:H3'	2.703	5.020	3.862	
1:G5'_1:H1'	1:G5'_1:H4'	2.318	4.305	3.312	
1:G5'_1:H2'	1:G5'_1:H1'	1.922	3.570	2.746	
1:G5'_1:H3'	1:G_2:H8	2.040	3.788	2.914	
1:G_2:H8	1:G5'_1:H1'	2.966	5.508	4.237	200ms
1:G_2:H8	1:G5'_1:H2'	1.683	3.125	2.404	
1:G_2:H8	1:G_2:H1'	2.978	5.530	4.254	
1:G_2:H8	1:G_2:H2'	2.831	5.257	4.044	200ms
1:G_2:H1'	1:G_2:H2'	1.975	3.668	2.821	
1:G_2:H1'	1:G_2:H3'	2.798	5.196	3.997	
1:G_2:H1'	1:G_2:H4'	2.320	4.309	3.314	
1:G_2:H3'	1:G_2:H8	2.247	4.172	3.209	
1:G_2:H3'	1:U_3:H6	1.991	3.697	2.844	
1:U_3:H5	1:G_2:H8	2.493	4.629	3.561	
1:U_3:H6	1:G_2:H1'	3.087	5.733	4.410	200ms
1:U_3:H6	1:G_2:H2'	1.745	3.241	2.493	
1:U_3:H6	1:U_3:H2'	2.728	5.066	3.897	200ms
1:U_3:H6	1:U_3:H5	1.826	3.391	2.608	
1:U_3:H1'	1:G_2:H2'	2.431	4.516	3.474	
1:U_3:H1'	1:U_3:H6	2.365	4.392	3.378	
1:U_3:H1'	1:U_3:H3'	2.350	4.363	3.357	
1:U_3:H1'	1:G_4:H8	2.563	6.000	3.661	*
1:U_3:H2'	1:U_3:H1'	1.919	3.563	2.741	
1:U_3:H3'	1:U_3:H6	2.210	4.104	3.157	
1:G_4:H8	1:U_3:H2'	1.717	3.188	2.453	
1:G_4:H8	1:U_3:H3'	1.958	3.636	2.797	
1:G_4:H8	1:G_4:H2'	2.844	5.282	4.063	
1:G_4:H8	1:G_4:H3'	2.188	4.063	3.125	
1:G_4:H1'	1:U_3:H2'	2.192	4.071	3.131	
1:G_4:H1'	1:G_4:H8	2.796	5.192	3.994	
1:G_4:H1'	1:G_4:H2'	1.857	3.449	2.653	
1:G_4:H1'	1:G_4:H4'	2.238	4.156	3.197	
1:G_5:H8	1:G_4:H2'	2.730	5.071	3.900	
1:G_5:H8	1:G_4:H3'	2.408	4.473	3.441	

1:G_5:H8	1:G_5:H2'	1.432	2.659	2.045	
1:G_5:H1'	1:G_5:H8	3.290	6.000	4.699	
1:G_5:H2'	1:G_5:H1'	2.232	4.144	3.188	
1:G_5:H3'	1:G_5:H8	2.462	4.573	3.518	
1:A_6:H2	1:G_7:H1'	2.380	4.420	3.400	
1:A_6:H2	1:A_15:H1'	2.125	3.946	3.035	
1:A_6:H8	1:G_5:H1'	2.301	4.274	3.288	
1:A_6:H8	1:A_6:H1'	3.059	5.682	4.371	200ms
1:A_6:H8	1:A_6:H2'	3.633	6.000	5.190	200ms
1:A_6:H8	1:A_6:H3'	1.971	3.660	2.815	
1:G_7:H8	1:A_6:H2'	2.883	5.354	4.118	
1:G_7:H8	1:A_6:H3'	1.561	2.899	2.230	
1:G_7:H8	1:G_7:H1'	2.463	4.575	3.519	
1:G_7:H2'	1:G_8:H8	1.659	3.081	2.370	
1:G_7:H3'	1:G_7:H8	1.739	5.000	2.484	
1:G_7:H3'	1:G_8:H8	1.711	5.000	2.444	*
1:G_8:H8	1:G_7:H1'	2.743	5.095	3.919	
1:G_8:H8	1:G_8:H1'	2.716	5.043	3.879	
1:G_8:H1'	1:G_8:H4'	2.230	4.142	3.186	
1:G_8:H1'	1:C_9:H6	2.701	5.017	3.859	200ms
1:G_8:H2'	1:G_8:H8	3.177	5.900	4.539	
1:G_8:H2'	1:G_8:H1'	1.807	3.356	2.582	
1:G_8:H3'	1:G_8:H8	1.805	3.352	2.578	
1:G_8:H3'	1:C_9:H6	2.366	4.393	3.380	
1:C_9:H6	1:G_8:H2'	1.617	3.002	2.309	
1:C_9:H6	1:C_9:H5	1.691	3.140	2.415	
1:C_9:H1'	1:G_8:H2'	2.464	4.577	3.521	
1:C_9:H1'	1:C_9:H6	2.432	4.517	3.475	
1:C_9:H1'	1:C_9:H3'	2.440	4.532	3.486	
1:C_9:H1'	1:U3'_10:H6	2.798	5.196	3.997	
1:C_9:H2'	1:C_9:H1'	1.793	3.330	2.562	
1:C_9:H3'	1:C_9:H6	1.772	3.290	2.531	
1:C_9:H3'	1:U3'_10:H6	2.322	4.313	3.317	
1:C_9:H4'	1:C_9:H1'	2.346	4.357	3.351	
1:U3'_10:H5	1:C_9:H2'	2.333	4.332	3.332	
1:U3'_10:H6	1:C_9:H2'	1.688	3.134	2.411	
1:U3'_10:H6	1:U3'_10:H5	1.721	3.196	2.459	
1:U3'_10:H1'	1:U3'_10:H6	3.162	5.873	4.518	
1:U3'_10:H1'	1:U3'_10:H2'	2.021	3.753	2.887	
1:U3'_10:H2'	1:U3'_10:H6	2.183	4.055	3.119	
1:U3'_10:H3'	1:U3'_10:H6	1.709	3.175	2.442	
1:U3'_10:H3'	1:U3'_10:H1'	2.296	4.265	3.280	
1:U3'_10:H5	1:C_9:H5	2.574	4.780	3.677	200ms
1:U3'_10:H5	1:C_9:H6	3.162	5.872	4.517	200ms
1:U3'_10:H5	1:C_9:H3'	3.135	5.823	4.479	200ms
1:U3'_10:H1'	1:C_9:H2'	2.729	5.069	3.899	200ms
1:G5'_11:H8	1:G5'_11:H1'	2.454	4.558	3.506	
1:G5'_11:H8	1:G5'_11:H2'	2.705	5.024	3.865	

1:G5'_11:H8	1:G5'_11:H3'	2.274	4.223	3.249	
1:G5'_11:H1'	1:G5'_11:H2'	1.868	3.468	2.668	
1:G5'_11:H1'	1:G5'_11:H3'	2.905	5.396	4.151	
1:G5'_11:H1'	1:G5'_11:H4'	2.611	4.849	3.730	
1:G5'_11:H1'	1:C_12:H6	3.226	5.991	4.609	
1:C_12:H6	1:G5'_11:H2'	1.652	3.068	2.360	
1:C_12:H6	1:C_12:H5	1.754	3.257	2.505	
1:C_12:H1'	1:C_12:H6	2.507	4.655	3.581	
1:C_12:H1'	1:C_13:H6	3.102	5.760	4.431	200ms
1:C_12:H2'	1:C_12:H1'	1.835	3.408	2.621	
1:C_12:H2'	1:C_13:H5	2.632	4.888	3.76	
1:C_12:H3'	1:C_12:H6	1.732	3.217	2.475	
1:C_12:H3'	1:C_12:H1'	2.367	4.396	3.382	
1:C_13:H6	1:C_12:H2'	1.532	2.845	2.188	
1:C_13:H6	1:C_13:H5	1.790	3.324	2.557	
1:C_13:H6	1:C_13:H1'	2.733	5.075	3.904	200ms
1:C_13:H1'	1:C_12:H2'	2.484	4.613	3.548	
1:C_13:H1'	1:C_13:H2'	1.894	3.518	2.706	
1:C_13:H1'	1:C_13:H3'	2.766	5.137	3.952	
1:C_13:H1'	1:C_13:H4'	2.216	4.116	3.166	
1:C_13:H1'	1:G_14:H8	3.666	6.000	5.237	200ms
1:C_13:H3'	1:C_13:H6	1.960	3.640	2.800	
1:C_13:H3'	1:G_14:H8	1.924	3.574	2.749	
1:G_14:H8	1:C_13:H2'	1.973	3.664	2.818	
1:G_14:H8	1:G_14:H3'	1.949	3.620	2.785	
1:G_14:H1'	1:G_14:H8	2.703	5.020	3.862	
1:G_14:H1'	1:G_14:H3'	2.974	5.523	4.248	
1:G_14:H1'	1:G_14:H4'	2.511	4.664	3.588	
1:G_14:H1'	1:A_15:H8	3.266	6.000	4.666	
1:G_14:H8	1:G_14:H2'	1.894	3.818	2.706	*
1:G_14:H2'	1:G_14:H1'	1.872	3.477	2.674	
1:G_14:H2'	1:G_14:H3'	1.653	3.069	2.361	
1:A_15:H2	1:A_6:H1'	2.149	3.991	3.070	
1:A_15:H2	1:A_16:H1'	2.060	3.825	2.942	
1:A_15:H8	1:G_14:H2'	2.016	3.743	2.879	
1:A_15:H8	1:A_15:H3'	2.091	3.884	2.987	
1:A_15:H1'	1:A_15:H8	3.152	5.853	4.502	200ms
1:A_15:H1'	1:A_15:H2'	2.296	4.263	3.279	
1:A_16:H2	1:G_17:H1'	2.537	4.712	3.625	
1:A_16:H8	1:A_15:H1'	3.281	6.000	4.687	200ms
1:A_16:H8	1:A_15:H2'	1.939	3.602	2.771	
1:A_16:H8	1:A_15:H3'	2.392	4.442	3.417	
1:A_16:H8	1:A_16:H1'	2.624	4.873	3.749	
1:A_16:H1'	1:A_16:H4'	2.545	4.727	3.636	
1:A_16:H1'	1:G_17:H8	2.988	5.549	4.268	200ms
1:A_16:H2'	1:A_16:H8	2.970	5.515	4.243	
1:A_16:H2'	1:A_16:H1'	1.863	3.460	2.662	
1:A_16:H2'	1:G_17:H8	1.847	3.431	2.639	

1:A_16:H3'	1:A_16:H8	2.286	4.245	3.265	
1:A_16:H3'	1:A_16:H2'	1.717	3.188	2.453	
1:A_16:H3'	1:G_17:H8	1.661	3.085	2.373	
1:G_17:H2'	1:G_17:H8	2.034	5.000	2.906	
1:G_17:H2'	1:C_18:H6	1.602	2.975	2.288	
1:G_17:H2'	1:C_18:H1'	2.748	5.103	3.925	
1:G_17:H3'	1:C_18:H6	1.820	3.379	2.599	
1:C_18:H5	1:C_18:H6	1.697	3.151	2.424	
1:C_18:H1'	1:C_18:H3'	2.338	4.343	3.341	
1:C_18:H1'	1:C_19:H6	2.892	5.371	4.132	
1:C_18:H2'	1:C_18:H6	2.570	4.772	3.671	
1:C_18:H2'	1:C_18:H1'	1.889	3.509	2.699	
1:C_18:H2'	1:C_19:H6	1.686	3.132	2.409	
1:C_18:H3'	1:C_18:H6	1.672	3.105	2.389	
1:C_18:H3'	1:C_19:H6	1.868	5.000	2.668	
1:C_18:H4'	1:C_18:H1'	2.141	3.976	3.058	
1:C_19:H6	1:C_19:H5	1.720	3.195	2.457	
1:C_19:H1'	1:C_18:H2'	2.798	5.196	3.997	
1:C_19:H1'	1:C_19:H6	2.728	5.067	3.897	
1:C_19:H1'	1:C_19:H3'	2.404	4.465	3.434	
1:C_19:H1'	1:P3'_20:H8	3.145	5.841	4.493	200ms
1:C_19:H2'	1:C_19:H1'	1.903	3.534	2.718	
1:C_19:H3'	1:C_19:H6	1.669	3.099	2.384	
1:C_19:H4'	1:C_19:H1'	2.023	3.758	2.890	
1:P3'_20:H8	1:C_19:H3'	2.162	4.014	3.088	
1:P3'_20:H8	1:P3'_20:H1'	2.936	5.453	4.195	
1:P3'_20:H1'	1:P3'_20:H3'	2.735	5.079	3.907	
1:P3'_20:H1'	1:P3'_20:H4'	2.365	4.392	3.378	
1:P3'_20:H2'	1:P3'_20:H8	2.494	4.632	3.563	
1:P3'_20:H2'	1:P3'_20:H1'	2.057	3.820	2.938	
1:P3'_20:H3'	1:P3'_20:H8	1.701	3.160	2.431	
1:P3'_20:H2	1:G5'_1:H1'	2.941	5.461	4.021	200ms
1:C_19:H2'	1:P3'_20:H8	1.902	3.533	2.717	200ms
1:P3'_20:H8	1:C_19:H6	3.322	6.000	4.745	200ms

Dihedral angle restraints

<i>Atom 1</i>	<i>Atom 2</i>	<i>Atom 3</i>	<i>Atom 4</i>	<i>Lower limit</i>	<i>Upper limit</i>
alpha O3'-P-O5'-C5'; A-form -68					
1:G5'_1:O3'	1:G_2:P	1:G_2:O5'	1:G_2:C5'	-120	120
1:G_2:O3'	1:U_3:P	1:U_3:O5'	1:U_3:C5'	-120	120
1:A_6:O3'	1:G_7:P	1:G_7:O5'	1:G_7:C5'	-120	120
1:G_7:O3'	1:G_8:P	1:G_8:O5'	1:G_8:C5'	-120	120
1:G_8:O3'	1:C_9:P	1:C_9:O5'	1:C_9:C5'	-120	120
1:C_9:O3'	1:U3'_10:P	1:U3'_10:O5'	1:U3'_10:C5'	-120	120

1:G5'_11:O3'	1:C_12:P	1:C_12:O5'	1:C_12:C5'	-120	120
1:C_12:O3'	1:C_13:P	1:C_13:O5'	1:C_13:C5'	-120	120
1:A_16:O3'	1:G_17:P	1:G_17:O5'	1:G_17:C5'	-120	120
1:G_17:O3'	1:C_18:P	1:C_18:O5'	1:C_18:C5'	-120	120
1:C_18:O3'	1:C_19:P	1:C_19:O5'	1:C_19:C5'	-120	120
1:C_19:O3'	1:P3'_20:P	1:P3'_20:O5'	1:P3'_20:C5'	-120	120

beta P-O5'-C5'-C4'; A-form 178

1:G_2:P	1:G_2:O5'	1:G_2:C5'	1:G_2:C4'	150	-150
1:U_3:P	1:U_3:O5'	1:U_3:C5'	1:U_3:C4'	150	-150
1:G_7:P	1:G_7:O5'	1:G_7:C5'	1:G_7:C4'	150	-150
1:G_8:P	1:G_8:O5'	1:G_8:C5'	1:G_8:C4'	150	-150
1:C_9:P	1:C_9:O5'	1:C_9:C5'	1:C_9:C4'	150	-150
1:C_12:P	1:C_12:O5'	1:C_12:C5'	1:C_12:C4'	150	-150
1:C_13:P	1:C_13:O5'	1:C_13:C5'	1:C_13:C4'	150	-150
1:G_17:P	1:G_17:O5'	1:G_17:C5'	1:G_17:C4'	150	-150
1:C_18:P	1:C_18:O5'	1:C_18:C5'	1:C_18:C4'	150	-150
1:C_19:P	1:C_19:O5'	1:C_19:C5'	1:C_19:C4'	150	-150

gamma O5'-C5'-C4'-C3'; A-form 54

1:G5'_1:O5'	1:G5'_1:C5'	1:G5'_1:C4'	1:G5'_1:C3'	30	90
1:G_2:O5'	1:G_2:C5'	1:G_2:C4'	1:G_2:C3'	30	90
1:U_3:O5'	1:U_3:C5'	1:U_3:C4'	1:U_3:C3'	30	90
1:G_7:O5'	1:G_7:C5'	1:G_7:C4'	1:G_7:C3'	30	90
1:G_8:O5'	1:G_8:C5'	1:G_8:C4'	1:G_8:C3'	30	90
1:C_9:O5'	1:C_9:C5'	1:C_9:C4'	1:C_9:C3'	30	90
1:G5'_11:O5'	1:G5'_11:C5'	1:G5'_11:C4'	1:G5'_11:C3'	30	90
1:C_12:O5'	1:C_12:C5'	1:C_12:C4'	1:C_12:C3'	30	90
1:C_13:O5'	1:C_13:C5'	1:C_13:C4'	1:C_13:C3'	30	90
1:G_17:O5'	1:G_17:C5'	1:G_17:C4'	1:G_17:C3'	30	90
1:C_18:O5'	1:C_18:C5'	1:C_18:C4'	1:C_18:C3'	30	90
1:C_19:O5'	1:C_19:C5'	1:C_19:C4'	1:C_19:C3'	30	90

delta C5'-C4'-C3'-O3'; A-form 82

1:G5'_1:C5'	1:G5'_1:C4'	1:G5'_1:C3'	1:G5'_1:O3'	55	115
1:G_2:C5'	1:G_2:C4'	1:G_2:C3'	1:G_2:O3'	55	115
1:U_3:C5'	1:U_3:C4'	1:U_3:C3'	1:U_3:O3'	55	115
1:G_4:C5'	1:G_4:C4'	1:G_4:C3'	1:G_4:O3'	55	115
1:G_5:C5'	1:G_5:C4'	1:G_5:C3'	1:G_5:O3'	130	-170
1:A_6:C5'	1:A_6:C4'	1:A_6:C3'	1:A_6:O3'	55	-170
1:G_7:C5'	1:G_7:C4'	1:G_7:C3'	1:G_7:O3'	55	115
1:G_8:C5'	1:G_8:C4'	1:G_8:C3'	1:G_8:O3'	55	115
1:C_9:C5'	1:C_9:C4'	1:C_9:C3'	1:C_9:O3'	55	115
1:U3'_10:C5'	1:U3'_10:C4'	1:U3'_10:C3'	1:U3'_10:O3'	55	-170
1:G5'_11:C5'	1:G5'_11:C4'	1:G5'_11:C3'	1:G5'_11:O3'	55	115
1:C_12:C5'	1:C_12:C4'	1:C_12:C3'	1:C_12:O3'	55	115
1:C_13:C5'	1:C_13:C4'	1:C_13:C3'	1:C_13:O3'	55	115
1:G_14:C5'	1:G_14:C4'	1:G_14:C3'	1:G_14:O3'	55	-170
1:A_15:C5'	1:A_15:C4'	1:A_15:C3'	1:A_15:O3'	55	115
1:A_16:C5'	1:A_16:C4'	1:A_16:C3'	1:A_16:O3'	55	115
1:G_17:C5'	1:G_17:C4'	1:G_17:C3'	1:G_17:O3'	55	115

1:C_18:C5'	1:C_18:C4'	1:C_18:C3'	1:C_18:O3'	55	115
1:C_19:C5'	1:C_19:C4'	1:C_19:C3'	1:C_19:O3'	55	115
1:P3'_20:C5'	1:P3'_20:C4'	1:P3'_20:C3'	1:P3'_20:O3'	55	-170
epsilon C4'-C3'-O3'-P; A-form -153					
1:G5'_1:C4'	1:G5'_1:C3'	1:G5'_1:O3'	1:G_2:P	-180	-100
1:G_2:C4'	1:G_2:C3'	1:G_2:O3'	1:U_3:P	-180	-100
1:U_3:C4'	1:U_3:C3'	1:U_3:O3'	1:G_4:P	-180	-100
1:G_7:C4'	1:G_7:C3'	1:G_7:O3'	1:G_8:P	-180	-100
1:G_8:C4'	1:G_8:C3'	1:G_8:O3'	1:C_9:P	-180	-100
1:C_9:C4'	1:C_9:C3'	1:C_9:O3'	1:U3'_10:P	-180	-100
1:G5'_11:C4'	1:G5'_11:C3'	1:G5'_11:O3'	1:C_12:P	-180	-100
1:C_12:C4'	1:C_12:C3'	1:C_12:O3'	1:C_13:P	-180	-100
1:C_13:C4'	1:C_13:C3'	1:C_13:O3'	1:G_14:P	-180	-100
1:G_17:C4'	1:G_17:C3'	1:G_17:O3'	1:C_18:P	-180	-100
1:C_18:C4'	1:C_18:C3'	1:C_18:O3'	1:C_19:P	-180	-100
1:C_19:C4'	1:C_19:C3'	1:C_19:O3'	1:P3'_20:P	-180	-100
zeta C3'-O3'-P-O5'; A-form -71					
1:G5'_1:C3'	1:G5'_1:O3'	1:G_2:P	1:G_2:O5'	-120	120
1:G_2:C3'	1:G_2:O3'	1:U_3:P	1:U_3:O5'	-120	120
1:U_3:C3'	1:U_3:O3'	1:G_4:P	1:G_4:O5'	-120	120
1:G_7:C3'	1:G_7:O3'	1:G_8:P	1:G_8:O5'	-120	120
1:G_8:C3'	1:G_8:O3'	1:C_9:P	1:C_9:O5'	-120	120
1:C_9:C3'	1:C_9:O3'	1:U3'_10:P	1:U3'_10:O5'	-120	120
1:G5'_11:C3'	1:G5'_11:O3'	1:C_12:P	1:C_12:O5'	-120	120
1:C_12:C3'	1:C_12:O3'	1:C_13:P	1:C_13:O5'	-120	120
1:C_13:C3'	1:C_13:O3'	1:G_14:P	1:G_14:O5'	-120	120
1:G_17:C3'	1:G_17:O3'	1:C_18:P	1:C_18:O5'	-120	120
1:C_18:C3'	1:C_18:O3'	1:C_19:P	1:C_19:O5'	-120	120
1:C_19:C3'	1:C_19:O3'	1:P3'_20:P	1:P3'_20:O5'	-120	120
chi Glycosidic torsions; A-form -158					
1:G5'_1:O4'	1:G5'_1:C1'	1:G5'_1:N9	1:G5'_1:C4	150	-130
1:G_2:O4'	1:G_2:C1'	1:G_2:N9	1:G_2:C4	150	-130
1:U_3:O4'	1:U_3:C1'	1:U_3:N1	1:U_3:C2	150	-130
1:G_7:O4'	1:G_7:C1'	1:G_7:N9	1:G_7:C4	150	-130
1:G_8:O4'	1:G_8:C1'	1:G_8:N9	1:G_8:C4	150	-130
1:C_9:O4'	1:C_9:C1'	1:C_9:N1	1:C_9:C2	150	-130
1:U3'_10:O4'	1:U3'_10:C1'	1:U3'_10:N1	1:U3'_10:C2	150	-130
1:G5'_11:O4'	1:G5'_11:C1'	1:G5'_11:N9	1:G5'_11:C4	150	-130
1:C_12:O4'	1:C_12:C1'	1:C_12:N1	1:C_12:C2	150	-130
1:C_13:O4'	1:C_13:C1'	1:C_13:N1	1:C_13:C2	150	-130
1:G_17:O4'	1:G_17:C1'	1:G_17:N9	1:G_17:C4	150	-130
1:C_18:O4'	1:C_18:C1'	1:C_18:N1	1:C_18:C2	150	-130
1:C_19:O4'	1:C_19:C1'	1:C_19:N1	1:C_19:C2	150	-130
1:P3'_20:O4'	1:P3'_20:C1'	1:P3'_20:N9	1:P3'_20:C4	150	-130

Table S2. Summary of NOE distance restraints.

Nucleotide	Total	Intra-nucleotide	Inter-nucleotide
G1	13	6	7
G2	19	6	13
U3	22	6	16
G4	15	5	10
G5	11	4	7
A6	11	3	8
G7	11	2	9
G8	14	5	9
C9	19	6	13
U10	15	6	9
G11	11	6	5
C12	13	5	8
C13	13	6	7
G14	15	7	8
A15	14	3	11
A16	16	6	10
G17	13	1	12
C18	17	6	11
C19	16	6	10
P20	15	6	9

Table S3. List of the chemical shift assignments at 30 °C.

	H6/H8	H2/H5	H1'	H2'	H3'	H4'	H5'/H5'' ^a	Imino/amino ^b	³¹ P
G1	8.15	- ^c	5.95	4.86	4.55	4.47	4.13/3.99	11.91	-
G2	7.38	-	5.78	4.68	4.42	4.48	4.55/4.14	13.37	-1.75
U3	7.31	5.30	5.23	4.59	4.27	4.07	4.41/4.10	11.50	-2.18
G4	7.86	-	5.30	3.61	4.70	4.35	4.47/4.11	10.33	-2.59
G5	8.14	-	5.67	5.06	4.98	4.76	4.69/4.47	9.74	-2.85
A6	7.77	8.14	5.21	4.71	4.50	4.42	4.20		
G7	7.50	-	4.21	(4.33) ^d	(4.35)	4.42	4.28/4.07	12.82	-1.66
G8	7.17	-	5.73	4.49	4.38	4.42	4.35/4.02	13.30	-2.22
C9	7.42	5.15	5.58	4.35	4.25	4.38	4.15/4.02	8.47/7.02	-2.48
U10	7.73	5.54	5.73	3.99	4.15	4.13	4.31/4.02	10.95	-1.84
G11	8.10	-	5.85	4.82	4.53	4.44	4.15/3.98	13.34	-
C12	7.84	5.21	5.64	4.52	4.49	4.57	4.44/4.15	8.73/6.82	-2.28
C13	7.51	5.24	5.52	4.67	4.30	4.45	4.26/4.14	8.04/6.49	-1.84
G14	7.99	-	5.68	4.45	4.93	4.62	4.51/4.26	9.40	-1.98
A15	8.25	7.13	5.50	4.78	4.64	4.56	(4.56/4.23)		-2.65
A16	7.10	8.22	5.86	4.89	4.28	4.55	4.38/4.10		-1.36
G17	7.19	-	4.75	4.30	4.37		4.55/4.09	11.48 (6.37/5.42)	-1.89
C18	7.58	5.39	5.41	4.17	4.44	4.37	4.07/4.04	8.29/7.06	-1.98
C19	7.64	5.43	5.48	4.37	4.48	4.35	4.32/4.08	8.09/7.06	-1.98
P20	8.85/8.45	8.16	6.15	4.16	4.33	4.31	4.44/4.10	-	-1.70

^aThe H5' and H5'' assignments are not stereospecific.^bImino and amino proton were assigned at 5 °C.^cNot applicable.^dAssignments in parentheses are tentative.

Figure S1. 1D ^{31}P spectrum at 30 °C.

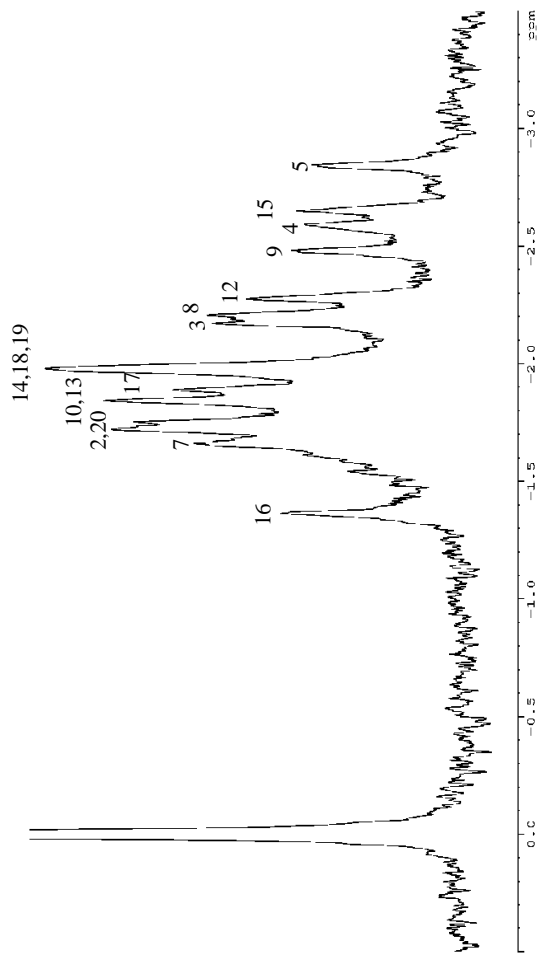


Figure S2. SNOESY spectrum at 5 °C. Assignments on the diagonal are imino protons, the cross peaks are labeled by corresponding amino protons unless otherwise noted. Tentative assignments are in parentheses. Weak cross-peaks of U3H3-G4H1 and G5H1-G14H2' are seen at lower contour level.

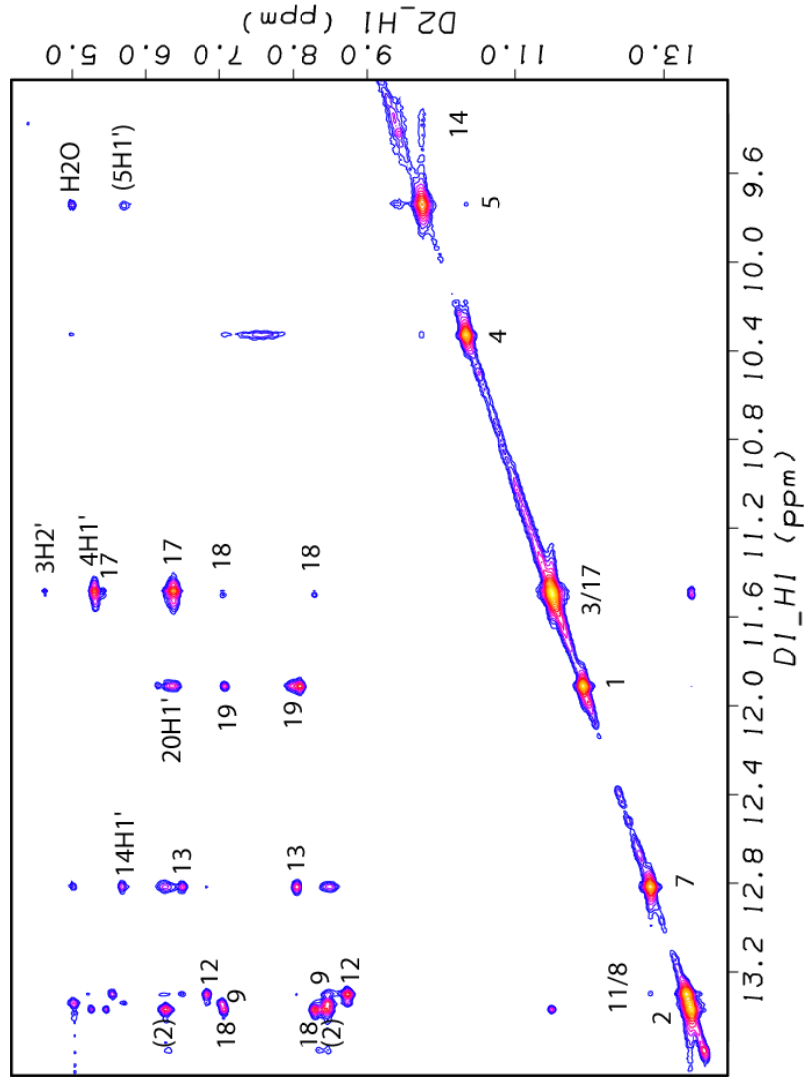


Figure S3. The H1'-C1' and H5-C5 region of an HSQC spectrum at 30 °C.

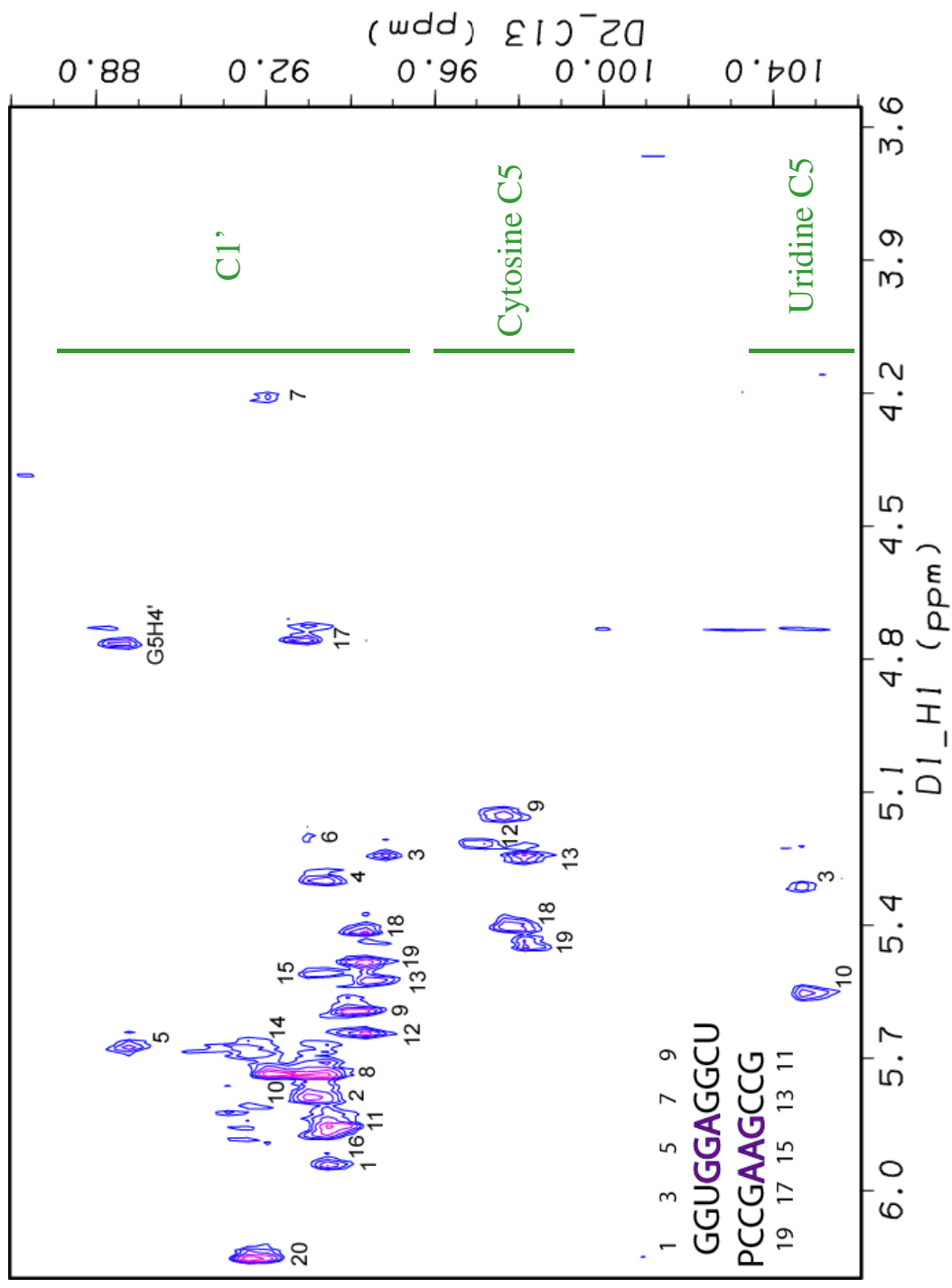


Figure S4. The H1'-H2' region (top) and H5-H6 region (bottom) of a TOCSY spectrum at 30 °C

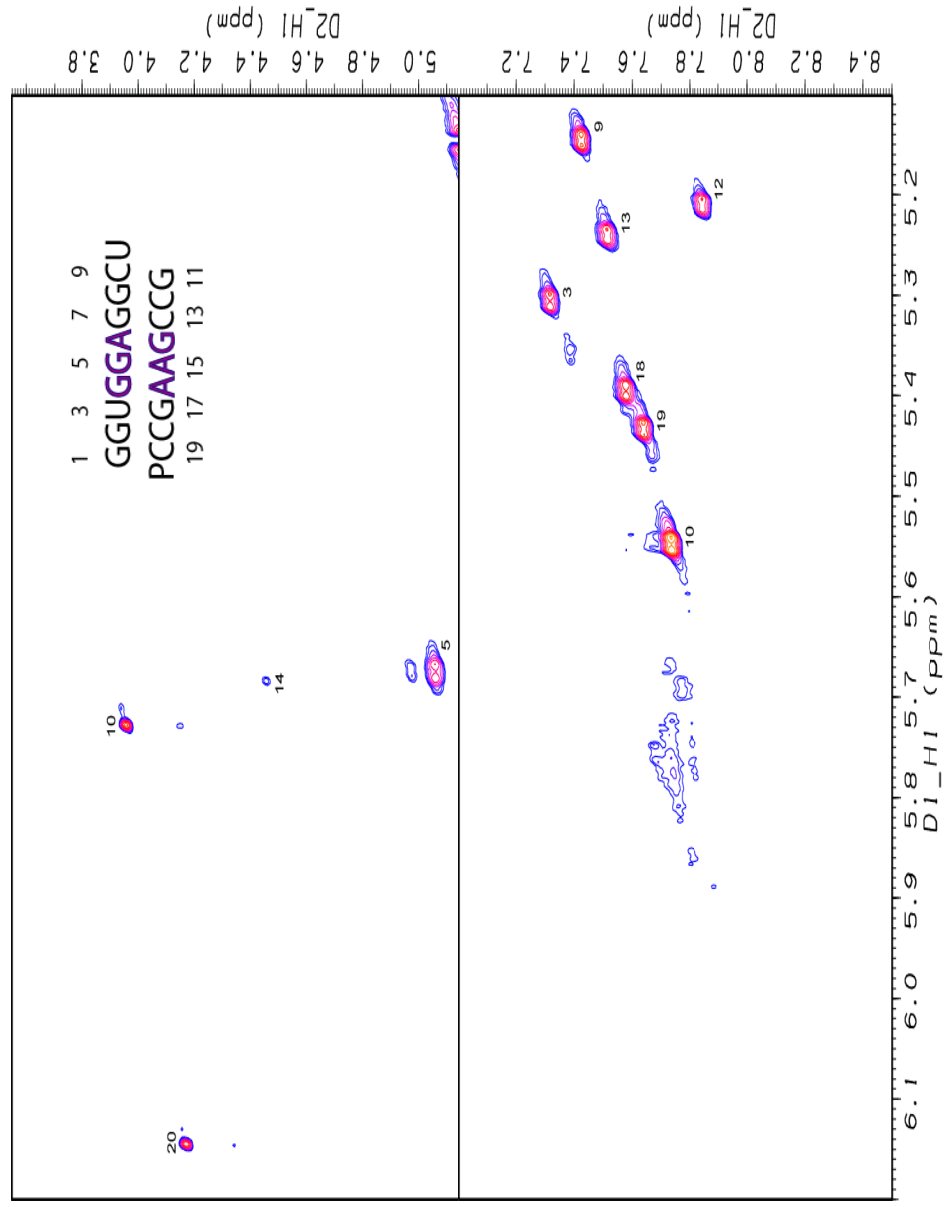


Figure S5. HMQC (aromatic) at 30 °C.

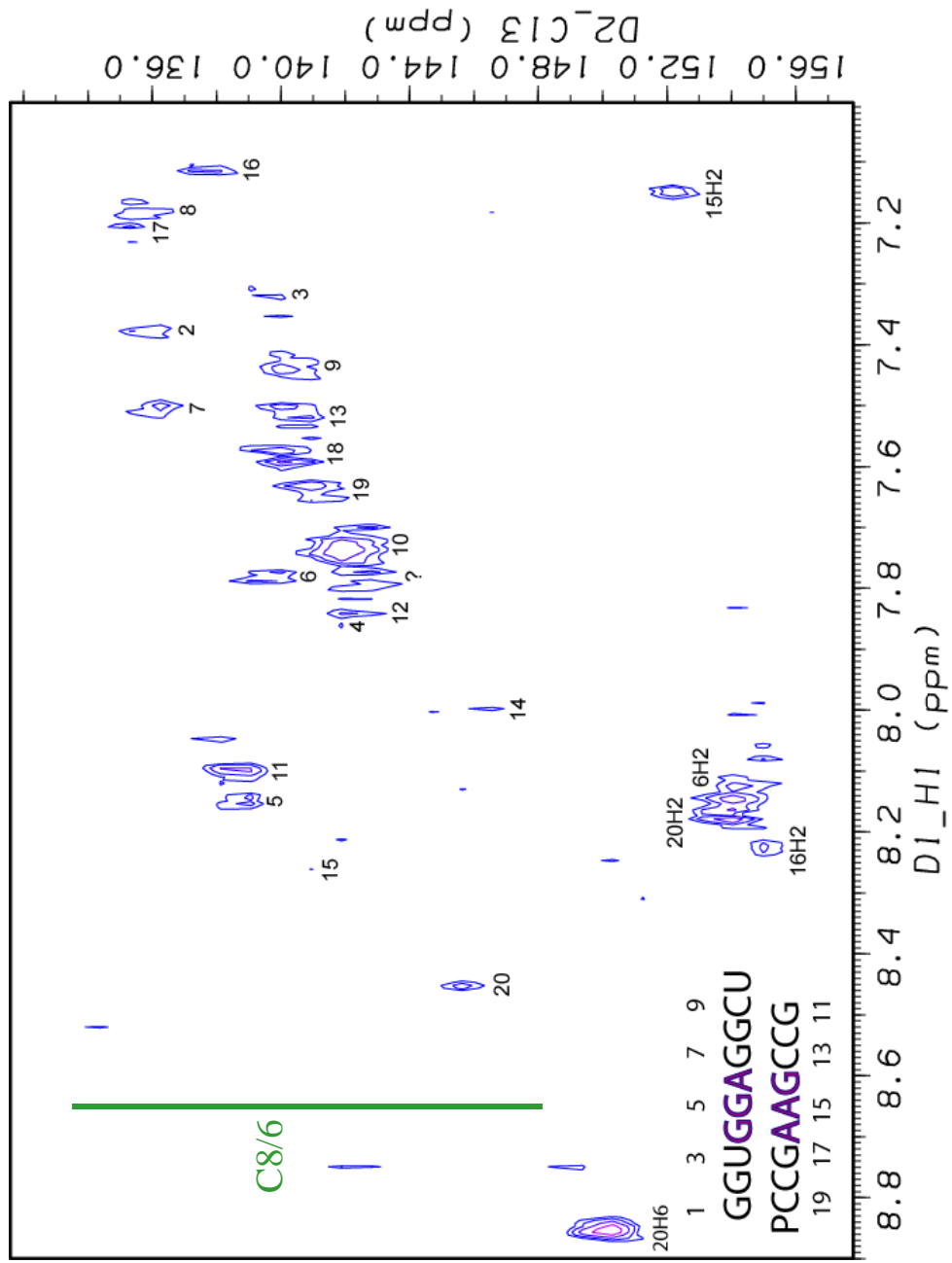


Figure S6. SNOESY spectrum at 40 °C. Only imino protons from G2, G8, U3 and G17 are observable. Note the cross-peaks between U3 and G17 imino protons.

