

Supplementary Table 1

Torsion Angles of RNA Duplexes (GA8)

Non-standard torsions in bold, Comparison to NMR structure 1YFV

Torsions/ Residue	Alpha P-O5'	Beta O5'-C5'	Gamma C5'-C4'	Delta C4'-C3'	Epsilon C3'-O3'	Zeta O3'-P	Chi C1'-N
Gua 101	85.59	-156.82	-62.33	-171.44
Gua 201				81.39	-145.43	-72.36	-176.29
Gua 301				86.12	-155.56	-62.65	-171.99
1YFV-1				93.57	-141.54	-78.58	173.30
Gua 102	-63.20	-169.64	46.20	81.93	-147.84	-74.78	-158.98
Gua 202	-68.38	175.12	65.88	78.11	-142.17	-75.05	-175.19
Gua 302	-62.87	-169.64	45.66	81.36	-147.24	-75.25	-158.48
1YFV-2	-76.37	177.39	57.43	90.31	-152.52	-65.29	-172.45
Cyt 103	-51.82	159.78	55.18	78.30	-149.32	-72.41	-172.14
Cyt 203	-55.53	171.98	54.05	78.92	-132.15	-62.15	-160.58
Cyt 303	-51.25	160.54	54.58	78.81	-148.89	-73.19	-171.26
1YFV-3	-79.53	176.43	58.65	90.14	-158.83	-49.53	-158.28
Gua 104	156.72	-149.13	171.42	89.06	-139.20	-136.13	-165.14
Gua 204	-72.46	165.70	62.36	83.00	-145.59	-147.86	-164.93
Gua 304	156.39	-148.91	172.57	89.30	-138.73	-135.25	-166.15
1YFV-4	-83.56	-176.97	54.37	89.29	179.95	-108.26	-158.89
Ade 105	-53.35	157.42	44.66	84.16	-130.12	-59.30	-172.28
Ade 205	-42.29	128.49	52.16	76.82	-152.61	-45.03	-171.23
Ade 305	-54.04	158.20	44.70	84.82	-129.95	-60.07	-170.93
1YFV-5	-72.45	-169.61	55.75	93.03	-140.94	-51.82	-167.35
Gua 106	-57.60	168.13	51.10	82.74	-134.29	-96.80	-166.43
Gua 206	-74.85	177.84	55.83	84.58	-154.61	-65.93	-176.29
Gua 306	-55.77	167.72	49.53	82.51	-134.77	-98.25	-167.15
1YFV-6	-68.92	165.47	60.58	88.60	-156.31	-65.64	-166.98
Cyt 107	-48.97	142.22	56.23	80.47	-133.47	-79.86	-179.00
Cyt 207	-66.06	178.60	53.56	79.30	-144.87	-81.21	-171.01
Cyt 307	-48.07	140.86	55.43	80.16	-133.06	-80.80	-179.77
1YFV-7	-77.72	179.57	56.25	89.59	-153.81	-64.62	-159.92
Cyt 108	-65.23	159.21	71.02	72.90	-164.98
Cyt 208	-67.63	172.41	54.18	73.44			-156.23
Cyt 308	-65.83	157.30	72.82	72.29			-163.61
1YFV-8	-70.43	171.35	55.71	80.75			-158.97
Gua 109	82.18	-150.35	-69.23	-176.40
Gua 209				84.22	-154.28	-68.71	-178.19
Gua 110	-65.13	-174.85	50.04	84.30	-139.50	-79.14	-162.43
Gua 210	-76.39	-172.92	54.95	82.42	-144.65	-75.98	-170.90
Cyt 111	-74.43	153.36	70.53	81.84	-128.16	-72.73	-173.53
Cyt 211	-51.83	166.94	56.42	79.31	-147.62	-52.96	-159.95
Gua 112	-70.01	148.60	70.47	91.38	-120.89	-149.80	-172.44
Gua 212	-62.98	-177.48	50.51	82.27	-174.61	-115.05	-150.40
Ade 113	-52.84	128.69	55.72	80.65	-135.58	-57.80	-177.75
Ade 213	-45.09	167.32	45.35	84.51	-140.30	-56.35	-158.40
Gua 114	-71.95	171.33	53.61	78.67	-144.22	-78.99	-163.27
Gua 214	-58.88	166.64	47.79	83.06	-156.06	-63.86	-168.51
Cyt 115	-29.32	149.59	51.04	79.47	-149.41	-124.58	-168.47
Cyt 215	-65.80	-173.99	45.53	77.75	-155.48	-55.75	-162.88
Cyt 116	143.81	-119.12	166.85	74.66	-177.15
Cyt 216	-125.23	142.90	135.95	88.53			-164.65

Supplementary Table 2

Torsion Angles of RNA Duplexes (IGA8)

Non-standard torsions in bold

Torsions/ Residue	Alpha P-O5'	Beta O5'-C5'	Gamma C5'-C4'	Delta C4'-C3'	Epsilon C3'-O3'	Zeta O3'-P	Chi C1'-N
Gua 101	83.80	-151.88	-77.66	-175.43
Gua 201				87.61	-142.36	-77.32	-166.84
Gua 301				86.99	-142.11	-76.05	-166.81
Ino 102	-68.05	-173.54	54.05	85.75	-153.54	-65.29	-153.38
Ino 202	-45.55	161.94	45.47	74.00	-145.51	-73.98	-164.84
Ino 302	-46.97	163.81	45.62	74.51	-145.39	-73.62	-164.66
Cyt 103	-66.00	168.03	56.25	76.39	-136.26	-58.78	-169.05
Cyt 203	-61.84	165.27	57.10	79.71	-150.20	-59.65	-163.31
Cyt 303	-61.81	165.18	56.81	79.25	-151.06	-59.31	-163.40
Gua 104	-59.07	165.45	62.50	84.60	-159.59	-139.64	-155.38
Gua 204	-58.40	171.33	55.59	84.68	-153.81	-128.17	-147.28
Gua 304	-58.45	171.96	54.93	85.19	-153.98	-128.62	-146.92
Ade 105	-43.93	150.95	49.30	82.58	-136.26	-53.54	-167.25
Ade 205	-58.40	163.51	45.57	80.23	-135.88	-57.42	-165.64
Ade 305	-56.81	163.08	46.10	79.40	-136.23	-56.15	-165.44
Gua 106	-67.03	176.29	56.40	84.17	-153.54	-63.27	-159.63
Gua 206	-48.36	162.27	54.82	78.98	-146.76	-72.48	-172.05
Gua 306	-47.86	161.85	53.96	79.20	-148.01	-72.12	-171.81
Cyt 107	-65.57	-175.36	46.54	82.59	-151.88	-94.01	-159.33
Cyt 207	-66.91	172.77	54.34	77.42	-147.84	-70.50	-161.23
Cyt 307	-68.45	173.73	54.66	78.09	-148.47	-69.86	-162.02
Cyt 108	153.30	-134.89	173.54	77.79	-171.05
Cyt 208	-53.34	164.84	59.90	69.17			-160.96
Cyt 308	-54.34	165.45	60.23	68.60			-160.60
Gua 109	87.89	-149.94	-66.17	-173.87
Gua 209				83.75	-161.97	-66.20	-171.60
Ino 110	-67.96	-174.69	50.18	81.19	-153.35	-85.04	-159.83
Ino 210	-66.56	-166.76	52.03	82.73	-148.57	-71.09	-164.86
Cyt 111	-63.65	169.33	49.96	85.53	-136.90	-47.86	-157.10
Cyt 211	-61.25	178.73	52.64	85.64	-144.94	-81.41	-158.45
Gua 112	-78.02	179.79	64.06	92.34	-152.54	-130.69	-158.68
Gua 212	135.54	-134.34	177.32	85.60	-98.37	-165.25	169.97
Ade 113	-55.85	150.51	54.19	83.94	-136.90	-57.12	-171.78
Ade 213	-60.23	127.84	46.95	74.29	-149.15	-42.57	-174.12
Gua 114	-71.84	179.79	62.19	83.31	-153.35	-67.90	-164.16
Gua 214	-74.11	-179.96	60.95	85.20	-147.96	-71.80	-171.47
Cyt 115	-73.82	169.33	59.82	83.44	-149.94	-69.75	-163.43
Cyt 215	-75.32	-179.99	54.25	80.32	-155.85	-69.32	-168.01
Cyt 116	-70.60	-174.69	54.53	75.05	-160.30
Cyt 216	-60.96	173.27	60.39	-51.10			-158.86

Supplementary Table 3

Data and Refinement Statistics for IGA8 and GA8

Resolution (Å) (per IGA8 asymmetric unit)	30.0 - 2.7
Total number of measurements	24938
Total number of unique reflections	5239
Number of non-hydrogen RNA atoms	855
Number of solvent molecules	20
$R_{\text{merge}}(\%)^a$	12.2
Completeness(%)	70.7
Space Group	P6(4)
Cell Dimensions	
GA8 (Å)	a=b= 69.65, c= 68.36, $\gamma= 120^\circ$
IGA8 (Å)	a=b= 69.65, c=67.81, $\gamma= 120^\circ$
$R_{\text{cryst}}(\%)^b$	GA8 24.1 IGA8 23.8
$R_{\text{free}}(\%)^c$	GA8 25.5 IGA8 29.7
Average B-factor (Å ²)	
RNA GA8/IGA8	65.2/54.7
Solvent GA8/IGA8	52.3/36.7
RMS Deviations from ideality	
Bond length (Å) GA8/IGA8	0.006/0.005
Bond angle (°) GA8/IGA8	1.074/0.973

^a $R_{\text{merge}} = \frac{\sum_h \sum_i |I(h,i) - \langle I(h) \rangle|}{\sum_h \sum_i I(h,i)}$, where $I(h,i)$ is the intensity for the i th measurement of reflection h and $\langle I(h) \rangle$ is the mean value of $I(h,i)$ for all I measurements.

^b $R_{\text{cryst}} = \frac{\sum_{hkl} ||F_{\text{obs}}| - |F_{\text{calc}}||}{\sum_{hkl} |F_{\text{obs}}|}$, where F_{obs} denotes the observed structure factor amplitude, and F_{calc} denotes the structure factor amplitude calculated from the model; 10% of reflections were used to calculate ^c R_{free} .