

Supporting Information

A Computational Model for Predicting Experimental RNA and DNA Nearest-Neighbor Free Energy Rankings

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All calculations performed at the MP2(full)/6-311G** level of theory.

Table S1. RNA monomer total energies in Hartrees with methyl groups or H atoms replacing sugar. PCM values in parenthesis.

Name	Energy Methyl	Energy Hydrogen
A	-505.5475 (-505.5592341)	-466.3364801 (-466.3499013)
C	-433.3125 (-433.3327027)	-394.1020954 (-394.1242706)
G	-580.6518 (-580.6762143)	-541.4409947 (-541.4666228)
U	-453.1882 (-453.2010314)	-413.9818761 (-413.9950282)

Table S2. RNA H-bonding total energies, BSSE corrected, in Hartrees with methyl groups of H atoms replacing sugar. PCM values in parenthesis and not BSSE corrected.

Name	Energy Methyl	Energy Hydrogen
AU	-958.753955432667 (-958.7798559)	-880.333941825190 (-880.3630386)
GC	-1014.005513675605 (-1014.0417625)	-935.584481328308 (-935.6217226)

Table S3. RNA intra-strand dimer total energies, BSSE corrected, in Hartrees with methyl groups of H atoms replacing sugar. PCM values in parenthesis and not BSSE corrected.

Name	Energy Methyl	Energy Hydrogen
5'AA3'	-1011.10087708361 (-1011.132611)	-932.673191165635 (-932.708138)
5'AC3'	-938.864073427099 (-938.9054593)	-860.44168109387 (-860.4866108)
5'AG3'	-1086.2068134335 (-1086.248233)	-1007.78620197666 (-1007.832343)
5'AU3'	-958.741768680442 (-958.7723064)	-880.321643779543 (-880.3556082)
5'CA3'	-938.863797042051 (-938.9000833)	-860.441484683877 (-860.4812826)
5'CC3'	-866.626698043469 (-866.6753431)	-788.204929672991 (-788.2575625)
5'CG3'	-1013.97019365581 (-1014.015916)	-935.548146121855 (-935.5967764)
5'CU3'	-886.507903993872 (-886.542489)	-808.088516474724 (-808.1266389)
5'GA3'	-1086.20942350544 (-1086.250727)	-1007.78684951668 (-1007.830527)
5'GC3'	-1013.97901959855 (-1014.024989)	-935.557107818996 (-935.6055383)
5'GG3'	-1161.30449729058 (-1161.366013)	-1082.88218350098 (-1082.945538)
5'GU3'	-1033.84323452231 (-1033.890567)	-955.423438476563 (-955.4733128)
5'UA3'	-958.74125501757 (-958.7676762)	-880.317757765525 (-880.3478481)
5'UC3'	-886.505843835831 (-886.5432242)	-808.081563674384 (-808.1225769)
5'UG3'	-1033.84303371525 (-1033.884715)	-955.422808087448 (-955.4666413)
5'UU3'	-906.377438918791 (-906.408667)	-827.960244074473 (-827.9949716)

Table S4. RNA inter-strand dimer total energies, BSSE corrected, in Hartrees with methyl groups of H atoms replacing sugar. PCM values in parenthesis and not BSSE corrected.

Name	Energy Methyl	Energy Hydrogen
5'_A3' 3'_A_5'	-1011.09328143182 (-1011.12413)	-932.671140521484 (-932.6711405)
5'_A3' 3'_C_5'	-938.860218554063 (-938.8970634)	-860.438575013156 (-860.4792379)
5'_A3' 3'_G_5'	-1086.20417139122 (-1086.242546)	-1007.78217497475 (-1007.823428)
5'_A3' 3'_U_5'	-958.739995667483 (-958.765096)	-880.319972494016 (-880.3482914)
5'_C3' 3'_C_5'	-866.62351198996 (-866.6655722)	-788.191765623309 (-788.2417044)
5'_C3' 3'_G_5'	-1013.96992837519 (-1014.014412)	-935.548456965801 (-935.5960913)
5'_C3' 3'_U_5'	-886.504315294478 (-886.5359224)	-808.084753334739 (-808.1200325)
5'_G3' 3'_G_5'	-1161.30462562111 (-1161.359148)	-1082.88275246767 (-1082.939548)
5'_G3' 3'_U_5'	-1033.838231652 (-1033.880986)	-955.418603859058 (-955.4638349)
5'_U3' 3'_U_5'	-906.375217977412 (-906.4023451)	-827.958079797836 (-827.9886102)
5'_A_3' 3'_A5'	-1011.0954346442 (-1011.120089)	-932.673344770499 (-932.7015913)
5'_A_3' 3'_C5'	-938.859336208788 (-938.8923247)	-860.437898272345 (-860.4747833)
5'_A_3' 3'_G5'	-1086.20311666235 (-1086.242546)	-1007.78137018682 (-1007.818419)
5'_A_3' 3'_U5'	-958.736567880997 (-958.7606758)	-880.316666962476 (-880.3440581)
5'_C_3' 3'_C5'	-866.623509278486 (-866.6655791)	-788.202370362433 (-788.2487205)
5'_C_3' 3'_G5'	-1013.96907787355 (-1014.009617)	-935.54673782373 (-935.5908336)
5'_C_3' 3'_U5'	-886.501605289368 (-886.533948)	-808.082232940612 (-808.1181524)
5'_G_3' 3'_G5'	-1161.27925196128 (-1161.35414)	-1082.87753922336 (-1082.934935)
5'_G_3' 3'_U5'	-1033.83916438441 (-1033.877545)	-955.4195976 (-955.4605689)
5'_U_3' 3'_U5'	-906.375209187984 (-906.4009909)	-827.95879979263 (-827.9939355)

Table S5. DNA monomer total energies in Hartrees with methyl groups or H atoms replacing sugar. PCM values in parenthesis.

Name	Energy Methyl	Energy Hydrogen
A	-505.5470926 (-505.5587826)	-466.3361022 (-466.3495757)
C	-433.3130117 (-433.3330602)	-394.102419 (-394.1245858)
G	-580.6517317 (-580.6765157)	-541.44136 (-541.4671002)
T	-492.4060958 (-492.4177803)	-453.1976146 (-453.2108213)

Table S6. DNA H-bonding total energies, BSSE corrected, in Hartrees with methyl groups of H atoms replacing sugar. PCM values in parenthesis and not BSSE corrected.

Name	Energy Methyl	Energy Hydrogen
AT	-997.9753639 (-998.0005419)	-919.5552777 (-919.5835695)
GC	-1014.008336 (-1014.042085)	-935.5872965 (-935.6241115)

Table S7. DNA intra-strand dimer total energies, BSSE corrected, in Hartrees with methyl groups of H atoms replacing sugar. PCM values in parenthesis and not BSSE corrected.

Name	Energy Methyl	Energy Hydrogen
5'AA3'	-1011.101851 (-1011.135926)	-932.6747553 (-932.7107958)
5'AC3'	-938.8660637 (-938.9057521)	-860.4433509 (-860.4876392)
5'AG3'	-1086.209383 (-1086.253389)	-1007.786197 (-1007.832365)
5'AT3'	-997.9585773 (-997.9933122)	-919.539795 (-919.5747433)
5'CA3'	-938.8654398 (-938.9036428)	-860.4414147 (-860.4834004)
5'CC3'	-866.6271133 (-866.6772506)	-788.204357 (-788.2585035)
5'CG3'	-1013.973169 (-1014.020637)	-935.5505374 (-935.6008546)
5'CT3'	-925.7270765 (-925.7642996)	-847.3057851 (-847.3464205)
5'GA3'	-1086.211169 (-1086.254725)	-1007.788071 (-1007.8338)
5'GC3'	-1013.978037 (-1014.025777)	-935.5565931 (-935.6060391)
5'GG3'	-1161.30728 (-1161.371929)	-1082.884388 (-1082.950566)
5'GT3'	-1073.063987 (-1073.110868)	-994.6431738 (-994.6925395)
5'TA3'	-997.9606155 (-997.9884672)	-919.5378961 (-919.5692481)
5'TC3'	-925.7245146 (-925.7626217)	-847.3039047 (-847.3455576)
5'TG3'	-1073.063358 (-1073.109243)	-994.6440148 (-994.6875331)
5'TT3'	-984.816878 (-984.8553329)	-906.405192 (-906.4393285)

Table S8. DNA inter-strand dimer total energies, BSSE corrected, in Hartrees with methyl groups of H atoms replacing sugar. PCM values in parenthesis and not BSSE corrected.

Name	Energy Methyl	Energy Hydrogen
5'_A3'	-1011.096584	-932.6745715
3'_A_5'	(-1011.124569)	(-932.7059697)
5'_A3'	-938.8589627	-860.4372615
3'_C_5'	(-938.894928)	(-860.4770832)
5'_A3'	-1086.204219	-1007.782888
3'_G_5'	(-1086.2434)	(-1007.824883)
5'_A3'	-997.9577576	-919.53391
3'_T_5'	(-997.9818636)	(-919.5622585)
5'_C3'	-866.6215669	-788.1999819
3'_C_5'	(-866.666432)	(-788.249419)
5'_C3'	-1013.969617	-935.5482372
3'_G_5'	(-1014.013806)	(-935.5955964)
5'_C3'	-925.7221946	-847.3030499
3'_T_5'	(-925.7542063)	(-847.3390018)
5'_G3'	-1161.309278	-1082.887515
3'_G_5'	(-1161.362804)	(-1082.943425)
5'_G3'	-1073.060696	-994.6415426
3'_T_5'	(-1073.100361)	(-994.6842852)
5'_T3'	-984.8142657	-906.397052
3'_T_5'	(-984.8389258)	(-906.4250272)
5'_A_3'	-1011.09485	-932.6662757
3'_A5'	(-1011.121345)	(-932.702827)
5'_A_3'	-938.8596748	-860.4321686
3'_C5'	(-938.8935426)	(-860.4705511)
5'_A_3'	-1086.203963	-1007.782235
3'_G5'	(-1086.239779)	(-1007.82098)
5'_A_3'	-997.9565883	-919.5373663
3'_T5'	(-997.980473)	(-919.5648659)
5'_C_3'	-866.624198	-788.2027494
3'_C5'	(-866.666799)	(-788.249755)
5'_C_3'	-1013.971494	-935.5502696
3'_G5'	(-1014.011384)	(-935.5932798)
5'_C_3'	-925.722491	-847.3035256
3'_T5'	(-925.7539225)	(-847.338854)
5'_G_3'	-1161.301292	-1082.887515
3'_G5'	(-1161.358098)	(-1082.943425)
5'_G_3'	-1073.060468	-994.6415687
3'_T5'	(-1073.097909)	(-994.6819965)
5'_T_3'	-984.8144478	-906.3973664
3'_T5'	(-984.8387663)	(-906.4248778)

Table S9. RNA monomer dipole moments in Debye with methyl groups or H atoms replacing sugar. PCM values in parenthesis.

Name	Dipole Moment Methyl	Dipole Moment Hydrogens
A	2.4518 (3.3037)	2.42 (3.176)
C	7.4992 (9.7311)	7.9238 (10.0489)
G	8.1679 (10.2939)	7.7732 (9.8142)
U	5.4682 (6.9076)	4.9181 (6.1882)

Table S10. RNA intra-strand dimer dipole moments in Debye with methyl groups or H atoms replacing sugar. PCM values in parenthesis.

Name	Dipole Moments Methyl	Dipole Moments Hydrogen
5'AA3'	2.4565 (6.341)	2.4399 (6.1402)
5'AC3'	7.5036 (12.9185)	7.9242 (13.1649)
5'AG3'	8.1601 (8.1038)	7.7984 (7.0915)
5'AU3'	5.3788 (9.032)	5.1354 (8.3538)
5'CA3'	2.4629 (11.3473)	2.4256 (11.6797)
5'CC3'	7.5032 (19.5963)	7.9242 (19.3048)
5'CG3'	8.1467 (1.4681)	7.775 (1.7187)
5'CU3'	5.3769 (10.9782)	5.4458 (11.2093)
5'GA3'	2.4629 (11.5633)	2.4256 (10.5321)
5'GC3'	7.5032 (10.7982)	7.9242 (10.0592)
5'GG3'	8.1467 (19.5444)	7.775 (18.6819)
5'GU3'	5.3769 (15.4611)	5.1355 (14.4348)
5'UA3'	2.4608 (10.1256)	2.4256 (9.7986)
5'UC3'	7.5031 (15.7853)	7.9242 (15.8495)
5'UG3'	8.1564 (10.2213)	7.775 (9.1642)
5'UU3'	5.3831 (13.0541)	5.1355 (12.409)

Table S11. RNA inter-strand dimer dipole moments in Debye with methyl groups or H atoms replacing sugar. PCM values in parenthesis.

Name	Dipole Moments Methyl	Dipole Moments Hydrogen
5'_A3'	2.4462	2.4256
3'_A_5'	(0.2191)	(0.8218)
5'_A3'	2.4508	7.9238
3'_C_5'	(7.2912)	(8.2144)
5'_A3'	2.4492	7.7732
3'_G_5'	(11.5559)	(10.7458)
5'_A3'	5.4658	5.1449
3'_U_5'	(4.4167)	(3.6179)
5'_C3'	7.4981	7.8788
3'_C_5'	(18.3506)	(12.7565)
5'_C3'	8.1655	7.7732
3'_G_5'	(11.5586)	(11.4201)
5'_C3'	5.463	5.1449
3'_U_5'	(3.5811)	(4.5567)
5'_G3'	8.1637	7.7732
3'_G_5'	(18.8066)	(17.7676)
5'_G3'	5.4633	5.1449
3'_U_5'	(15.7209)	(14.8279)
5'_U3'	5.4639	5.1449
3'_U_5'	(6.4778)	(5.3338)
5'_A_3'	2.4446	2.421
3'_A5'	(3.1095)	(3.8886)
5'_A_3'	2.4431	7.9293
3'_C5'	(11.58)	(11.58)
5'_A_3'	8.1643	7.7689
3'_G5'	(11.5559)	(7.6355)
5'_A_3'	5.4692	5.1471
3'_U5'	(4.4431)	(4.8109)
5'_C_3'	7.4988	7.9293
3'_C5'	(18.3526)	(19.2505)
5'_C_3'	8.1648	7.7689
3'_G5'	(1.2924)	(1.1315)
5'_C_3'	5.4691	5.1471
3'_U5'	(10.2122)	(11.0116)
5'_G_3'	7.7661	7.7732
3'_G5'	(19.2879)	(19.109)
5'_G_3'	5.4695	5.1471
3'_U5'	(10.5889)	(9.8271)
5'_U_3'	5.3783	5.1449
3'_U5'	(0.7269)	(12.5111)

Table S12. DNA monomer dipole moments in Debye with methyl groups or H atoms replacing sugar. PCM values in parenthesis.

Name	Dipole Moments Methyl	Dipole Moments Hydrogen
A	2.4955 (3.3551)	2.4799 (3.2469)
C	7.452 (9.6661)	7.882 (9.9908)
G	8.1638 (10.2821)	7.7887 (9.8342)
T	5.1734 (6.668)	5.1734 (6.668)

Table S13. DNA intra-strand dimer dipole moments in Debye with methyl groups or H atoms replacing sugar. PCM values in parenthesis.

Name	Dipole Moments Methyl	Dipole Moments Hydrogen
5'AA3'	2.5713 (6.3417)	2.4972 (6.1737)
5'AC3'	2.4955 (12.9122)	7.882 (13.1081)
5'AG3'	2.5034 (7.8624)	7.7953 (7.087)
5'AT3'	2.5326 (8.6347)	7.4272 (8.1174)
5'CA3'	7.4478 (11.0902)	2.4851 (11.6529)
5'CC3'	7.452 (18.356)	7.882 (18.9205)
5'CG3'	8.1488 (1.3168)	7.7969 (1.1802)
5'CT3'	5.1655 (10.6886)	4.923 (10.9244)
5'GA3'	2.4969 (11.94)	2.4851 (10.956)
5'GC3'	7.452 (11.3918)	7.882 (10.7111)
5'GG3'	8.1573 (19.59)	7.7953 (18.7526)
5'GT3'	5.1734 (15.4722)	4.9229 (14.52)
5'TA3'	2.5094 (9.9426)	2.4851 (9.6872)
5'TC3'	7.4517 (15.7007)	7.882 (15.8063)
5'TG3'	8.1638 (9.4625)	7.7954 (8.444)
5'TT3'	5.1639 (12.4936)	4.9207 (11.9623)

Table S14. DNA inter-strand dimer dipole moments in Debye with methyl groups or H atoms replacing sugar. PCM values in parenthesis.

Name	Dipole Moments Methyl	Dipole Moments Hydrogen
5'_A3'	2.4914	2.4851
3'_A_5'	(0.3771)	(0.6921)
5'_A3'	7.4497	7.8778
3'_C_5'	(7.0771)	(8.0174)
5'_A3'	8.1809	2.4851
3'_G_5'	(12.0407)	(11.1677)
5'_A3'	5.079	5.2959
3'_T_5'	(4.0888)	(3.8873)
5'_C3'	7.4466	7.882
3'_C_5'	(11.3604)	(12.5221)
5'_C3'	8.1812	7.7888
3'_G_5'	(12.003)	(11.7662)
5'_C3'	5.107	7.882
3'_T_5'	(3.2819)	(4.2485)
5'_G3'	8.1786	7.7888
3'_G_5'	(19.4987)	(18.3859)
5'_G3'	5.0827	4.9015
3'_T_5'	(15.7846)	(14.9729)
5'_T3'	5.1934	4.9229
3'_T_5'	(6.2159)	(5.1096)
5'_A_3'	2.4931	2.4384
3'_A_5'	(3.5472)	(4.289)
5'_A_3'	7.4488	7.8766
3'_C_5'	(10.9311)	(11.7556)
5'_A_3'	8.1829	7.7907
3'_G_5'	(8.0760)	(7.3429)
5'_A_3'	5.0796	4.9034
3'_T_5'	(4.5386)	(5.0577)
5'_C_3'	7.448	7.8766
3'_C_5'	(18.3005)	(19.2063)
5'_C_3'	8.1801	7.7907
3'_G_5'	1.473)	(1.3364)
5'_C_3'	5.0973	4.9034
3'_T_5'	(10.6883)	(11.4753)
5'_G_3'	8.1796	7.7888
3'_G_5'	(19.6082)	(18.3859)
5'_G_3'	5.0795	4.9034
3'_T_5'	(9.6376)	(8.9953)
5'_T_3'	5.1842	4.9133
3'_T_5'	(1.823)	(2.5954)

Table S15. RNA monomer geometries with methyls.

A				C			
6	1.724991000	-0.265570000	0.001146000	7	1.111448000	0.435521000	-0.000886000
6	0.363927000	-0.619158000	0.000581000	6	0.632260000	-0.868679000	-0.003563000
7	-0.292773000	-1.837004000	0.002882000	7	-0.712864000	-1.080299000	-0.000994000
6	-1.551578000	-1.516032000	-0.001488000	6	-1.562757000	-0.046691000	-0.003090000
7	-1.774130000	-0.169457000	-0.000715000	6	-1.091657000	1.314015000	-0.002051000
6	-0.530030000	0.415557000	0.004073000	6	0.247655000	1.498100000	-0.000871000
7	-0.269974000	1.732678000	0.000127000	7	-2.859363000	-0.298208000	0.003867000
6	1.037527000	1.937715000	-0.002757000	1	-3.195011000	-1.271864000	0.010192000
7	2.029070000	1.041529000	0.004382000	1	-3.534172000	0.479606000	0.002417000
1	1.349193000	2.982271000	-0.012217000	1	-1.782954000	2.156605000	-0.002491000
1	-2.353983000	-2.253032000	-0.005960000	1	0.648112000	2.511763000	-0.000184000
7	2.719294000	-1.172790000	-0.003014000	8	1.448714000	-1.798093000	-0.000241000
1	2.497959000	-2.178787000	-0.006385000	6	2.561882000	0.622943000	0.003574000
1	3.700521000	-0.860541000	-0.002432000	1	2.780861000	1.690922000	0.005423000
6	-3.045054000	0.539317000	-0.000674000	1	2.999981000	0.151283000	-0.876280000
1	-2.822451000	1.607019000	-0.027912000	1	2.994629000	0.149194000	0.884952000
1	-3.635749000	0.272743000	-0.878341000				
1	-3.614603000	0.314657000	0.902334000				
G				U			
6	0.229790000	0.990730000	0.002189000	7	1.072951000	0.451611000	-0.003368000
7	1.377313000	1.783995000	-0.000038000	6	0.631959000	-0.848149000	0.001207000
6	2.357605000	0.915092000	-0.001362000	7	-0.734645000	-1.013628000	0.000774000
7	1.945675000	-0.400894000	-0.002627000	6	-1.687182000	-0.004247000	-0.003815000
6	0.562268000	-0.339128000	0.000943000	6	-1.129270000	1.326323000	-0.005155000
7	-0.259771000	-1.425703000	-0.000599000	6	0.201462000	1.515930000	0.001686000
6	-1.535946000	-1.077007000	0.002590000	1	-1.794620000	2.188439000	-0.011137000
7	-1.974214000	0.239696000	-0.002842000	1	-1.085016000	-1.982645000	0.004198000
6	-1.135705000	1.366328000	-0.002398000	8	-2.885160000	-0.278064000	0.005407000
1	3.407593000	1.206785000	-0.001443000	1	0.596781000	2.531786000	0.011098000
8	-1.630306000	2.495616000	0.003085000	8	1.382651000	-1.810843000	-0.003095000
1	-2.991175000	0.402497000	-0.007826000	6	2.527121000	0.646597000	0.003415000
7	-2.501033000	-1.997483000	0.000424000	1	2.732430000	1.714950000	-0.059167000
1	-3.488872000	-1.707616000	-0.005060000	1	2.976739000	0.133368000	-0.846224000
1	-2.257830000	-2.998909000	0.004108000	1	2.961080000	0.240759000	0.916881000
6	2.756319000	-1.606734000	0.001352000				
1	2.079225000	-2.462069000	-0.019745000				
1	3.369362000	-1.658547000	0.902459000				
1	3.402376000	-1.640043000	-0.877283000				

Table S16. RNA monomer geometries with hydrogens.

A				C			
6	0.702603000	0.740855000	-0.003792000	6	1.177799000	-0.494676000	-0.002501000
6	0.171408000	-0.518497000	-0.000615000	7	-0.068493000	-1.043222000	-0.001160000
6	-1.232535000	-0.601048000	-0.001291000	6	-1.154432000	-0.261302000	-0.003455000
7	-1.924140000	0.548478000	-0.004596000	6	-1.046940000	1.174629000	-0.001347000
6	-1.257778000	1.706439000	0.002935000	6	0.200771000	1.695067000	0.001043000
7	0.049803000	1.913678000	0.000067000	7	1.307557000	0.888695000	0.001222000
1	-1.876046000	2.604112000	0.012391000	1	0.328710000	2.777430000	0.002566000
7	1.171013000	-1.474916000	-0.002777000	1	-1.930712000	1.812436000	-0.001948000
6	2.269679000	-0.782024000	0.001761000	7	-2.343619000	-0.836015000	0.002294000
7	2.066691000	0.567712000	0.001004000	1	-2.419139000	-1.863134000	0.007857000
7	-1.899231000	-1.770710000	0.002839000	1	-3.194887000	-0.256615000	0.000667000
1	-2.929574000	-1.776418000	0.002410000	8	2.204767000	-1.184417000	0.001043000
1	-1.378945000	-2.659978000	0.006299000	1	2.246595000	1.256699000	0.003578000
1	3.260763000	-1.235611000	0.006058000				
1	2.754591000	1.303846000	0.003091000				
G				U			
6	1.666934000	-0.591002000	-0.002804000	7	-0.047982000	-0.980709000	0.002898000
7	0.670419000	-1.461159000	-0.000064000	6	1.212902000	-0.413453000	0.000465000
6	-0.543079000	-0.841629000	-0.001544000	7	1.207016000	0.986229000	0.003534000
6	-0.823597000	0.500151000	-0.002339000	6	0.029485000	1.695159000	-0.001088000
6	0.241574000	1.433455000	0.002730000	6	-1.187578000	1.114284000	-0.002000000
7	1.487357000	0.785054000	0.003106000	6	-1.303393000	-0.335539000	0.000123000
7	-2.202156000	0.713817000	-0.000220000	1	0.145431000	2.771867000	-0.002456000
6	-2.705604000	-0.495526000	0.000597000	1	-2.094209000	1.699660000	-0.003194000
7	-1.761184000	-1.500302000	0.001624000	8	-2.330485000	-0.982252000	-0.000221000
1	-3.777727000	-0.690742000	0.000464000	1	-0.065259000	-1.992591000	0.002005000
1	-1.898724000	-2.498031000	0.002383000	8	2.240836000	-1.057060000	-0.003569000
8	0.194400000	2.665405000	-0.002312000	1	2.109501000	1.434216000	0.003938000
1	2.331623000	1.374906000	0.008417000				
7	2.936761000	-0.998685000	-0.000616000				
1	3.699425000	-0.307174000	0.005222000				
1	3.154450000	-2.005965000	-0.004637000				

Table S17. RNA intra-strand dimer geometries with methyls. The stacks are written 5' TO 3'.

AA				AC			
7	-3.212158000	0.840746000	-0.182680000	6	-3.178933000	0.875660000	-0.966814000
6	-3.712601000	-0.141120000	-0.987968000	7	-3.043959000	-0.406734000	-0.810499000
7	-3.112457000	-1.284881000	-0.850773000	6	-2.066475000	-0.525010000	0.161350000
6	-2.144093000	-1.042656000	0.107116000	6	-1.640252000	0.705847000	0.575440000
6	-2.194093000	0.255292000	0.532530000	7	-2.362145000	1.615191000	-0.161243000
7	-1.415610000	0.856757000	1.445699000	7	-0.706429000	0.990840000	1.496541000
6	-0.533256000	-0.003857000	1.928936000	6	-0.209140000	-0.127507000	2.001248000
7	-0.366797000	-1.294442000	1.626194000	7	-0.525918000	-1.392724000	1.711683000
6	-1.162255000	-1.854654000	0.702534000	6	-1.460198000	-1.633259000	0.779480000
1	0.151631000	0.395218000	2.677154000	7	-1.774862000	-2.906557000	0.475659000
7	-0.991092000	-3.151859000	0.385403000	1	-2.490146000	-3.103702000	-0.239190000
1	-1.595330000	-3.592827000	-0.323081000	1	-1.300469000	-3.683634000	0.958097000
1	-0.256020000	-3.703455000	0.851293000	1	0.565194000	0.001543000	2.757499000
1	-4.538154000	0.019790000	-1.681206000	1	-3.878487000	1.319745000	-1.674924000
6	-3.664273000	2.216620000	-0.051302000	6	-2.285935000	3.062971000	-0.034089000
1	-4.697218000	2.254604000	0.298413000	1	-3.232271000	3.471723000	0.323439000
1	-3.587490000	2.743193000	-1.003953000	1	-2.032858000	3.523398000	-0.990339000
1	-3.021825000	2.703336000	0.684283000	1	-1.504465000	3.285035000	0.694229000
6	0.480094000	1.655250000	-1.169763000	6	1.387702000	1.162845000	-1.098383000
7	0.518885000	0.383009000	-1.429628000	7	2.496210000	1.031526000	-0.305029000
6	1.663256000	-0.055762000	-0.787519000	6	2.955618000	-0.225143000	0.070307000
6	2.285422000	0.976995000	-0.142441000	7	2.285072000	-1.330173000	-0.357152000
7	1.516789000	2.088523000	-0.394951000	6	1.202079000	-1.209803000	-1.134691000
7	3.416206000	0.938850000	0.580279000	6	0.707097000	0.081266000	-1.538524000
6	3.896442000	-0.294119000	0.607978000	7	0.580128000	-2.308509000	-1.522610000
7	3.404082000	-1.401006000	0.043407000	1	-0.255711000	-2.242047000	-2.121034000
6	2.274735000	-1.317242000	-0.676689000	1	0.930851000	-3.230334000	-1.227241000
7	1.780157000	-2.426466000	-1.256965000	1	-0.175603000	0.181196000	-2.170520000
1	0.914472000	-2.374132000	-1.812738000	8	3.958656000	-0.296263000	0.790385000
1	2.267321000	-3.326657000	-1.144577000	1	1.047968000	2.159095000	-1.380440000
1	4.821826000	-0.425315000	1.169027000	6	3.222023000	2.196183000	0.197572000
1	-0.306147000	2.314230000	-1.536661000	1	2.767312000	3.098898000	-0.211123000
6	1.747877000	3.420950000	0.140023000	1	3.181328000	2.219863000	1.286824000
1	0.985308000	3.676970000	0.877133000	1	4.269908000	2.135008000	-0.097188000
1	1.746227000	4.161391000	-0.661310000				
1	2.725827000	3.414858000	0.623724000				
AG				AU			
6	-2.450236000	0.169023000	0.607870000	7	-2.386558000	1.576337000	-0.136361000
6	-2.383000000	-1.115307000	0.145138000	6	-1.653100000	0.661249000	0.581546000
6	-1.336688000	-1.905431000	0.653866000	7	-0.722911000	0.939040000	1.508507000
7	-0.502550000	-1.339604000	1.539187000	6	-0.211397000	-0.183063000	1.990135000
6	-0.693684000	-0.063842000	1.886850000	7	-0.512073000	-1.445965000	1.674475000
7	-1.635148000	0.775703000	1.484935000	6	-1.443283000	-1.679088000	0.737331000
7	-3.532620000	0.734466000	-0.024156000	6	-2.063657000	-0.566129000	0.142076000
6	-4.050142000	-0.244770000	-0.821815000	7	-3.042637000	-0.440276000	-0.827312000
7	-3.402874000	-1.368918000	-0.754581000	6	-3.193929000	0.843248000	-0.957170000
7	-1.141572000	-3.187279000	0.291367000	1	-3.899128000	1.292908000	-1.656103000
1	-1.775104000	-3.632327000	-0.388395000	1	0.561287000	-0.059798000	2.749033000
1	-0.358876000	-3.723051000	0.693830000	7	-1.741742000	-2.949749000	0.407253000
1	0.024329000	0.341313000	2.599919000	1	-2.454511000	-3.141191000	-0.311647000
1	-4.924332000	-0.096978000	-1.455817000	1	-1.257466000	-3.730512000	0.873649000
6	-4.015532000	2.091865000	0.164958000	6	-2.335477000	3.021509000	0.021821000
1	-5.033252000	2.091892000	0.559166000	1	-1.581767000	3.241416000	0.779634000

1	-3.994484000	2.647357000	-0.774265000	1	-2.059613000	3.506889000	-0.915741000
1	-3.354717000	2.576489000	0.885804000	1	-3.298955000	3.409520000	0.356297000
6	1.957664000	1.065201000	-0.333038000	6	0.695642000	0.137690000	-1.551972000
7	3.144569000	1.096416000	0.335859000	6	1.362129000	1.204397000	-1.081932000
6	3.732510000	-0.088943000	0.348517000	7	2.478821000	1.057621000	-0.291232000
7	3.201576000	-1.218575000	-0.258063000	6	2.955629000	-0.178406000	0.067703000
6	1.980230000	-1.260427000	-0.950038000	7	2.250137000	-1.254902000	-0.422901000
6	1.349292000	0.006774000	-0.955840000	6	1.123404000	-1.202646000	-1.230866000
7	0.138757000	0.402911000	-1.526993000	8	3.943150000	-0.338378000	0.767137000
6	0.056892000	1.676411000	-1.231646000	1	2.593086000	-2.191221000	-0.163901000
7	1.126051000	2.158827000	-0.506786000	8	0.572853000	-2.237604000	-1.599603000
1	-0.784364000	2.300825000	-1.532979000	1	-0.180129000	0.285523000	-2.184489000
8	1.594674000	-2.322053000	-1.444326000	1	1.011336000	2.206510000	-1.331211000
1	3.744519000	-2.092133000	-0.196316000	6	3.139167000	2.245001000	0.261025000
7	4.907626000	-0.267669000	0.953429000	1	4.066151000	1.921394000	0.734394000
1	5.354818000	-1.195687000	0.946505000	1	2.498400000	2.718974000	1.004576000
1	5.369004000	0.522508000	1.427623000	1	3.361256000	2.950142000	-0.539944000
6	1.309815000	3.483819000	0.058210000				
1	0.587198000	3.665175000	0.855351000				
1	1.199925000	4.246325000	-0.714453000				
1	2.318514000	3.534532000	0.471071000				
CA				CC			
7	3.068366000	-0.877541000	0.044337000	7	-2.578837000	-0.781205000	-0.343786000
6	2.002225000	-0.541239000	0.869449000	6	-3.053791000	0.369818000	0.273234000
7	1.636676000	0.765774000	0.980073000	7	-2.356694000	1.531017000	0.134965000
6	2.290283000	1.713614000	0.298118000	6	-1.232816000	1.566903000	-0.591356000
6	3.397082000	1.391044000	-0.564670000	6	-0.720891000	0.388002000	-1.241797000
6	3.743187000	0.087311000	-0.654869000	6	-1.428648000	-0.752936000	-1.086560000
1	4.575242000	-0.201911000	-1.296675000	1	-1.077409000	-1.668444000	-1.561919000
1	3.930935000	2.162351000	-1.119592000	1	0.195029000	0.415093000	-1.832491000
7	1.904637000	2.969008000	0.438684000	8	-4.094836000	0.297215000	0.937019000
1	2.391164000	3.717115000	-0.075115000	7	-0.586449000	2.714034000	-0.695076000
1	1.117353000	3.199197000	1.061503000	1	-0.949662000	3.554188000	-0.223667000
8	1.423428000	-1.444975000	1.484814000	1	0.280947000	2.767158000	-1.248211000
6	3.455909000	-2.285085000	-0.027740000	6	-3.304419000	-2.026865000	-0.105110000
1	4.346785000	-2.375963000	-0.649700000	1	-4.356657000	-1.892759000	-0.356801000
1	3.656521000	-2.663938000	0.974747000	1	-3.238431000	-2.298649000	0.948605000
1	2.646357000	-2.880222000	-0.451050000	1	-2.864730000	-2.814279000	-0.717637000
6	-2.427772000	-0.754389000	-0.100097000	7	2.262025000	-1.457980000	-0.073620000
7	-3.581661000	-0.773840000	0.585915000	6	3.185240000	-0.697147000	-0.739968000
6	-4.009362000	0.461745000	0.790880000	6	3.289853000	0.632537000	-0.519416000
7	-3.449664000	1.617486000	0.420262000	6	2.388005000	1.206350000	0.445398000
6	-2.299258000	1.591581000	-0.270300000	7	1.489649000	0.456422000	1.094422000
6	-1.738692000	0.334371000	-0.557890000	6	1.401436000	-0.880566000	0.851877000
7	-0.591349000	-0.054626000	-1.226244000	1	3.848194000	-1.173185000	-1.462297000
6	-0.616633000	-1.352093000	-1.166470000	1	4.022760000	1.242151000	-1.047685000
7	-1.698679000	-1.849324000	-0.499588000	7	2.441612000	2.498223000	0.715000000
1	-4.948258000	0.549180000	1.337828000	1	1.800745000	2.906168000	1.410397000
7	-1.736668000	2.751942000	-0.655994000	1	3.124012000	3.097129000	0.229196000
1	-0.854194000	2.744387000	-1.187232000	8	0.585288000	-1.606411000	1.432800000
1	-2.188643000	3.646394000	-0.419396000	6	2.169932000	-2.903662000	-0.277581000
1	0.153616000	-1.983631000	-1.607968000	1	1.186205000	-3.168400000	-0.665540000
6	-1.958528000	-3.228266000	-0.117509000	1	2.299271000	-3.418355000	0.674617000
1	-1.891983000	-3.883294000	-0.987446000	1	2.943568000	-3.212440000	-0.980761000
1	-1.246091000	-3.550450000	0.643354000				

1	-2.968479000	-3.273133000	0.292694000				
CG				CU			
6	-2.279193000	0.451407000	0.928447000	7	-2.281931000	1.420318000	-0.061872000
7	-3.409382000	0.763191000	0.182775000	6	-1.413461000	0.843616000	0.856681000
6	-4.090012000	-0.211683000	-0.496619000	7	-1.487097000	-0.496382000	1.087182000
6	-3.687768000	-1.501924000	-0.463119000	6	-2.378796000	-1.249808000	0.433048000
6	-2.515117000	-1.799218000	0.317882000	6	-3.288563000	-0.676784000	-0.524774000
7	-1.856097000	-0.841797000	0.980987000	6	-3.198406000	0.655883000	-0.733380000
7	-2.072054000	-3.040745000	0.400351000	1	-3.867779000	1.131455000	-1.450074000
1	-1.237304000	-3.253169000	0.964952000	1	-4.016059000	-1.289264000	-1.057191000
1	-2.561341000	-3.795789000	-0.100518000	7	-2.418250000	-2.544577000	0.690951000
1	-4.226019000	-2.281107000	-1.002573000	1	-3.095269000	-3.146203000	0.200998000
1	-4.972965000	0.058325000	-1.075731000	1	-1.771734000	-2.952049000	1.381378000
8	-1.697385000	1.363284000	1.528780000	8	-0.603849000	1.572715000	1.442653000
6	-3.854367000	2.154399000	0.169546000	6	-2.212366000	2.868677000	-0.250146000
1	-3.089224000	2.793136000	-0.272902000	1	-3.011601000	3.177176000	-0.924700000
1	-4.024038000	2.499889000	1.189859000	1	-2.318040000	3.370458000	0.712154000
1	-4.776038000	2.226267000	-0.408855000	1	-1.246334000	3.154391000	-0.667426000
6	0.166257000	1.385021000	-1.251807000	7	2.565243000	0.797160000	-0.347398000
7	1.270022000	1.941857000	-0.641165000	6	3.055567000	-0.330618000	0.262226000
6	2.075949000	0.863554000	-0.316309000	7	2.319424000	-1.479104000	0.071635000
7	3.283152000	0.962476000	0.308202000	6	1.150247000	-1.595530000	-0.666291000
6	3.838151000	-0.224108000	0.495033000	6	0.711434000	-0.358379000	-1.265868000
7	3.257843000	-1.418119000	0.090707000	6	1.407459000	0.776502000	-1.090943000
6	2.015225000	-1.530097000	-0.553990000	1	1.047945000	1.699872000	-1.546537000
6	1.419744000	-0.260279000	-0.746031000	1	-0.197101000	-0.345608000	-1.868619000
7	0.203753000	0.078794000	-1.341792000	8	0.575689000	-2.678122000	-0.756225000
7	5.025806000	-0.342141000	1.090267000	1	2.671931000	-2.336088000	0.521862000
1	5.523169000	0.498102000	1.420008000	8	4.079306000	-0.341659000	0.926936000
1	5.446703000	-1.273373000	1.220262000	6	3.223549000	2.078488000	-0.070051000
1	3.778017000	-2.287778000	0.277296000	1	3.383760000	2.618928000	-1.002980000
8	1.585487000	-2.643830000	-0.862122000	1	4.182193000	1.866335000	0.403334000
1	-0.666199000	1.980352000	-1.627311000	1	2.607224000	2.672929000	0.604399000
6	1.461593000	3.319939000	-0.224443000				
1	2.491808000	3.428883000	0.118032000				
1	0.781590000	3.565185000	0.592838000				
1	1.202950000	3.478757000	-1.272479000				
GA				GC			
7	-1.449943000	0.893387000	1.275252000	7	-3.126947000	-0.532389000	-0.855777000
6	-2.219469000	0.199665000	0.390391000	6	-2.099806000	-0.616035000	0.084474000
6	-2.142896000	-1.122329000	0.036086000	6	-1.461059000	-1.753788000	0.635097000
6	-1.151082000	-1.943974000	0.625045000	7	-0.465219000	-1.384453000	1.553951000
7	-0.364442000	-1.220060000	1.535838000	6	-0.139543000	-0.078101000	1.890395000
6	-0.527450000	0.125844000	1.832124000	7	-0.732506000	0.983527000	1.369276000
7	-3.261133000	0.745381000	-0.340891000	6	-1.701537000	0.635532000	0.476935000
6	-3.748867000	-0.300955000	-1.095081000	7	-2.485254000	1.537526000	-0.222951000
7	-3.118853000	-1.434534000	-0.910551000	6	-3.315183000	0.756047000	-0.998848000
1	-4.585825000	-0.193961000	-1.784728000	1	-4.062754000	1.174179000	-1.672540000
7	0.329343000	0.618750000	2.727457000	1	0.063688000	-2.139764000	2.012754000
1	0.274191000	1.610637000	3.001563000	8	-1.677399000	-2.947605000	0.416121000
1	1.045833000	0.008424000	3.144616000	7	0.839982000	0.050964000	2.786244000
1	0.390644000	-1.725738000	2.020473000	1	1.140986000	0.988934000	3.088938000
8	-0.927442000	-3.142646000	0.443055000	1	1.295440000	-0.786363000	3.175242000
6	-3.748846000	2.111099000	-0.266430000	6	-2.452901000	2.985267000	-0.102538000
1	-4.778663000	2.136746000	0.094087000	1	-1.715051000	3.238244000	0.660546000

1	-3.699932000	2.594412000	-1.243758000	1	-2.166557000	3.449869000	-1.047456000
1	-3.114033000	2.653861000	0.436120000	1	-3.427922000	3.368044000	0.203293000
6	2.235026000	0.931418000	-0.375401000	6	0.558224000	0.094614000	-1.747851000
7	3.374857000	0.932720000	0.333988000	6	1.230861000	1.187614000	-1.323975000
6	3.866823000	-0.293829000	0.405787000	7	2.375121000	1.074736000	-0.580083000
7	3.377903000	-1.427108000	-0.107041000	6	2.880208000	-0.174371000	-0.239834000
6	2.239116000	-1.382712000	-0.815683000	7	2.218723000	-1.290707000	-0.651752000
6	1.614643000	-0.132222000	-0.970045000	6	1.100887000	-1.188323000	-1.381061000
7	0.458490000	0.269922000	-1.615026000	7	0.489480000	-2.297584000	-1.755463000
6	0.411066000	1.551317000	-1.406673000	1	-0.372544000	-2.245012000	-2.316986000
7	1.453079000	2.024926000	-0.663236000	1	0.874551000	-3.213747000	-1.486435000
7	1.747807000	-2.518987000	-1.344077000	8	3.914544000	-0.228846000	0.436063000
1	0.874951000	-2.496974000	-1.890583000	1	-0.352843000	0.179864000	-2.340516000
1	2.244645000	-3.409531000	-1.201294000	1	0.855547000	2.178297000	-1.579271000
1	4.800168000	-0.393896000	0.960022000	6	3.112144000	2.250933000	-0.125270000
1	-0.385682000	2.187851000	-1.790159000	1	3.175603000	2.255179000	0.963283000
6	1.703200000	3.388880000	-0.226987000	1	4.130096000	2.228875000	-0.515501000
1	0.884934000	3.748008000	0.399260000	1	2.597170000	3.147330000	-0.472070000
1	1.823008000	4.054766000	-1.083116000				
1	2.627948000	3.382565000	0.352253000				
GG				GU			
6	-2.470139000	0.117972000	0.469126000	6	-1.714405000	0.584627000	0.487104000
7	-1.670587000	0.807681000	1.330181000	7	-0.752086000	0.913370000	1.393894000
6	-0.692706000	0.053440000	1.804618000	6	-0.146268000	-0.158233000	1.878535000
7	-0.506039000	-1.275973000	1.453007000	7	-0.453829000	-1.455956000	1.494954000
6	-1.323290000	-1.995567000	0.566054000	6	-1.442610000	-1.805434000	0.560837000
6	-2.373954000	-1.188536000	0.065579000	6	-2.095152000	-0.657314000	0.049293000
7	-3.395071000	-1.501975000	-0.831728000	7	-3.121192000	-0.553788000	-0.890179000
6	-4.070075000	-0.384505000	-0.939429000	6	-3.326179000	0.736333000	-0.987844000
7	-3.570535000	0.652346000	-0.179887000	7	-2.508440000	1.500561000	-0.182387000
1	-4.950059000	-0.282946000	-1.574151000	8	-1.642602000	-2.993445000	0.298949000
8	-1.073818000	-3.179614000	0.329947000	1	0.084016000	-2.220088000	1.928039000
1	0.292305000	-1.771834000	1.874321000	1	-4.077713000	1.168297000	-1.648270000
7	0.200798000	0.545103000	2.664031000	7	0.829439000	-0.048247000	2.781071000
1	0.959822000	-0.054379000	3.016711000	1	1.117293000	0.882236000	3.117754000
1	0.131425000	1.525177000	2.974927000	1	1.295087000	-0.892818000	3.141279000
6	-4.086652000	2.001596000	-0.041578000	6	-2.517633000	2.940763000	0.006770000
1	-5.103517000	1.990443000	0.355223000	1	-3.465001000	3.270953000	0.436192000
1	-4.084130000	2.519915000	-1.002269000	1	-2.356594000	3.456660000	-0.941308000
1	-3.439817000	2.536130000	0.656612000	1	-1.710745000	3.192409000	0.697090000
6	1.915009000	1.016668000	-0.532160000	7	2.358437000	1.114863000	-0.542521000
7	3.105400000	1.079421000	0.128271000	6	1.207584000	1.252118000	-1.284444000
6	3.703103000	-0.100130000	0.176446000	6	0.550132000	0.180461000	-1.755942000
7	3.178009000	-1.253361000	-0.389445000	6	1.024359000	-1.155827000	-1.487547000
6	1.953133000	-1.327783000	-1.072386000	7	2.183530000	-1.198800000	-0.726272000
6	1.311804000	-0.066554000	-1.116147000	6	2.880518000	-0.116850000	-0.235511000
7	0.094834000	0.300832000	-1.692817000	8	3.899025000	-0.268388000	0.419989000
6	0.004212000	1.582681000	-1.439074000	1	2.560278000	-2.132006000	-0.505873000
7	1.073482000	2.097279000	-0.736865000	1	0.821717000	2.250620000	-1.493082000
8	1.573491000	-2.408180000	-1.529153000	1	-0.353759000	0.321120000	-2.349325000
1	3.728439000	-2.120033000	-0.302206000	8	0.485967000	-2.195269000	-1.861584000
7	4.883065000	-0.249401000	0.779910000	6	3.038821000	2.309480000	-0.034921000
1	5.340636000	0.559649000	1.225078000	1	3.340147000	2.951407000	-0.862972000
1	5.337804000	-1.173532000	0.800879000	1	2.376448000	2.861206000	0.632460000
1	-0.843834000	2.190065000	-1.755788000	1	3.923679000	1.982055000	0.511297000

6	1.274429000	3.454625000	-0.263184000				
1	0.490510000	3.734693000	0.442485000				
1	1.277662000	4.158891000	-1.096811000				
1	2.242642000	3.493007000	0.238839000				
UA				UC			
6	-3.755924000	-0.105223000	-0.653076000	7	2.285649000	-1.412385000	-0.078209000
6	-3.413286000	-1.402095000	-0.578430000	6	1.425581000	-0.874351000	0.846394000
6	-2.318985000	-1.831666000	0.257686000	7	1.544054000	0.481975000	1.052865000
7	-1.691251000	-0.797905000	0.938025000	6	2.437581000	1.336162000	0.422353000
6	-2.017207000	0.538544000	0.875231000	6	3.301498000	0.680540000	-0.528922000
7	-3.069214000	0.855950000	0.052660000	6	3.210883000	-0.642336000	-0.744881000
8	-1.390383000	1.370407000	1.512666000	1	3.882631000	-1.114115000	-1.461449000
1	-0.904057000	-1.055485000	1.550644000	1	4.037284000	1.266192000	-1.079107000
8	-1.941580000	-2.992125000	0.402558000	8	2.454972000	2.533469000	0.698475000
1	-4.593225000	0.190850000	-1.284388000	1	0.906734000	0.903836000	1.743648000
1	-3.969223000	-2.139443000	-1.156639000	8	0.595190000	-1.533572000	1.452287000
6	-3.472266000	2.262769000	-0.043920000	6	2.199621000	-2.862053000	-0.288047000
1	-2.853645000	2.833334000	0.649116000	1	3.016063000	-3.166186000	-0.942549000
1	-3.320130000	2.632138000	-1.058295000	1	2.277134000	-3.380866000	0.667081000
1	-4.522105000	2.371419000	0.229153000	1	1.246004000	-3.127989000	-0.743392000
7	0.591269000	0.043983000	-1.222743000	6	-3.054082000	0.343147000	0.274505000
6	1.740113000	-0.343607000	-0.556153000	7	-2.372125000	1.514300000	0.144967000
6	2.303864000	-1.600050000	-0.271453000	6	-1.247989000	1.569856000	-0.579713000
7	3.454945000	-1.624585000	0.418033000	6	-0.719899000	0.402217000	-1.237503000
6	4.012281000	-0.468248000	0.790348000	6	-1.412800000	-0.748933000	-1.090874000
7	3.581520000	0.766723000	0.588114000	7	-2.563364000	-0.797329000	-0.349721000
6	2.427066000	0.745885000	-0.096905000	7	-0.616612000	2.726043000	-0.674861000
7	1.695067000	1.839874000	-0.493663000	1	0.250641000	2.794294000	-1.226558000
6	0.613584000	1.341390000	-1.160525000	1	-0.991355000	3.558139000	-0.198213000
7	1.743632000	-2.760985000	-0.658850000	8	-4.094840000	0.252388000	0.936504000
1	0.860668000	-2.754479000	-1.189287000	1	-1.049037000	-1.656505000	-1.571998000
1	2.197901000	-3.654829000	-0.424356000	1	0.196259000	0.445330000	-1.826876000
1	4.951867000	-0.554533000	1.336292000	6	-3.294118000	-2.047215000	-0.147398000
1	-0.158527000	1.971970000	-1.600135000	1	-2.799049000	-2.840120000	-0.708418000
6	1.983776000	3.224126000	-0.152556000	1	-3.312167000	-2.297477000	0.913535000
1	2.995821000	3.259253000	0.253148000	1	-4.324578000	-1.933262000	-0.484598000
1	1.927394000	3.855080000	-1.040689000				
1	1.283096000	3.586137000	0.601140000				
UG				UU			
6	-4.104860000	-0.224428000	-0.498975000	7	-2.304813000	1.371658000	-0.057774000
7	-3.409944000	0.745365000	0.186648000	6	-3.222569000	0.599069000	-0.731803000
6	-2.295905000	0.449201000	0.931828000	6	-3.296744000	-0.727433000	-0.532450000
7	-1.917371000	-0.874790000	0.938455000	6	-2.422450000	-1.384644000	0.408187000
6	-2.549148000	-1.915428000	0.272495000	7	-1.537504000	-0.527853000	1.047211000
6	-3.710387000	-1.508524000	-0.480544000	6	-1.435847000	0.832308000	0.857699000
1	-1.083205000	-1.116385000	1.492642000	8	-0.611764000	1.493717000	1.469789000
8	-1.660345000	1.289142000	1.549720000	1	-0.893298000	-0.950756000	1.730933000
1	-4.991627000	0.054133000	-1.067602000	8	-2.424746000	-2.585479000	0.669106000
1	-4.274921000	-2.252729000	-1.041378000	1	-4.026958000	-1.314854000	-1.088144000
8	-2.120505000	-3.063591000	0.362366000	1	-3.901868000	1.071796000	-1.440584000
6	-3.836240000	2.146520000	0.167118000	6	-2.281710000	2.822136000	-0.274078000
1	-4.822672000	2.202546000	-0.293457000	1	-3.226798000	3.267104000	0.037929000
1	-3.880137000	2.535217000	1.184618000	1	-1.472264000	3.235095000	0.328250000
1	-3.135570000	2.758208000	-0.401404000	1	-2.107954000	3.042151000	-1.327614000
6	2.075250000	0.846137000	-0.313861000	7	2.550462000	0.818381000	-0.349550000

7	3.282652000	0.943556000	0.310501000	6	3.058202000	-0.300166000	0.262819000
6	3.837560000	-0.243499000	0.494594000	7	2.338587000	-1.459876000	0.077126000
7	3.256984000	-1.436558000	0.087855000	6	1.170016000	-1.595709000	-0.658440000
6	2.014161000	-1.546986000	-0.556712000	6	0.712203000	-0.367017000	-1.261196000
6	1.418778000	-0.276682000	-0.745820000	6	1.391877000	0.778452000	-1.091059000
7	0.202650000	0.063830000	-1.340481000	8	4.083089000	-0.294143000	0.925821000
6	0.165342000	1.369865000	-1.247654000	1	2.704308000	-2.310180000	0.529473000
7	1.269357000	1.925242000	-0.636137000	1	1.018171000	1.695016000	-1.548971000
1	-0.667154000	1.966110000	-1.621616000	1	-0.197415000	-0.369433000	-1.862441000
8	1.584193000	-2.659997000	-0.867128000	8	0.611174000	-2.686852000	-0.743961000
1	3.777107000	-2.306684000	0.272402000	6	3.218210000	2.103381000	-0.111973000
7	5.025379000	-0.362967000	1.089214000	1	3.360349000	2.623877000	-1.058833000
1	5.446201000	-1.294530000	1.217065000	1	2.621661000	2.716309000	0.563388000
1	5.522944000	0.476499000	1.420627000	1	4.185802000	1.897494000	0.345236000
6	1.491550000	3.312348000	-0.266130000				
1	0.822176000	3.603153000	0.544827000				
1	1.330448000	3.963832000	-1.126302000				
1	2.525106000	3.409306000	0.069492000				

Table S18. RNA intra-strand dimer geometries with hydrogens. The stacks are written 5' TO 3'.

AA				AC			
6	2.271700000	-0.710649000	0.550087000	7	0.687761000	-1.242516000	1.575158000
6	2.292522000	0.574056000	0.083991000	6	1.601293000	-0.997231000	0.622806000
6	1.362406000	1.458900000	0.658277000	6	2.001100000	0.213928000	0.131490000
7	0.542751000	0.974123000	1.603207000	6	1.388060000	1.346837000	0.695911000
6	0.637780000	-0.313711000	1.945879000	7	0.473563000	1.146563000	1.656810000
7	1.466580000	-1.237887000	1.485756000	6	0.181604000	-0.104443000	2.023844000
7	3.250021000	-1.375248000	-0.151293000	7	2.324794000	-1.936698000	-0.073387000
6	3.799871000	-0.449204000	-0.989804000	6	3.116147000	-1.232757000	-0.934326000
7	3.266529000	0.730602000	-0.885935000	7	2.963745000	0.054379000	-0.849231000
7	1.262958000	2.753157000	0.301038000	1	3.810504000	-1.706471000	-1.628208000
1	1.886405000	3.136575000	-0.424089000	7	1.677538000	2.605060000	0.314222000
1	0.563551000	3.360040000	0.752882000	1	2.377452000	2.771292000	-0.423336000
1	4.610229000	-0.678510000	-1.681718000	1	1.199245000	3.401521000	0.759790000
1	-0.063538000	-0.649488000	2.709795000	1	-0.577712000	-0.201188000	2.799886000
1	3.491689000	-2.347956000	-0.048663000	1	2.264648000	-2.935218000	0.046771000
6	-2.246033000	-1.197032000	-0.079211000	6	-0.790972000	-0.529671000	-1.481343000
7	-3.367888000	-1.071934000	0.647592000	6	-1.299238000	0.775059000	-1.143269000
6	-3.777203000	0.186632000	0.638591000	7	-2.370682000	0.923985000	-0.354753000
7	-3.226693000	1.245444000	0.036750000	6	-3.016495000	-0.164388000	0.147057000
6	-2.108843000	1.074988000	-0.685978000	7	-2.543852000	-1.433664000	-0.163906000
6	-1.570682000	-0.222107000	-0.759818000	6	-1.446995000	-1.594054000	-0.968036000
7	-0.457442000	-0.745229000	-1.393418000	8	-4.008205000	-0.066753000	0.879611000
6	-0.489123000	-2.008837000	-1.093544000	1	-1.096500000	-2.599766000	-1.198655000
7	-1.543435000	-2.357880000	-0.300200000	1	0.082372000	-0.652772000	-2.122185000
7	-1.556092000	2.135513000	-1.303601000	7	-0.701240000	1.858677000	-1.604383000
1	-1.990626000	3.065055000	-1.217371000	1	0.125300000	1.770225000	-2.212794000
1	-0.698572000	2.016582000	-1.861765000	1	-1.061329000	2.790699000	-1.356026000
1	-4.689814000	0.387822000	1.199827000	1	-3.046760000	-2.214473000	0.229353000
1	-1.760124000	-3.269769000	0.048375000				
1	0.155417000	-2.733187000	-1.367370000				
AG				AU			
6	1.968703000	0.441255000	-0.871460000	6	1.618875000	-0.933180000	0.671913000
7	0.963875000	0.563371000	-1.758463000	6	2.008084000	0.248742000	0.106473000
6	0.295204000	-0.566579000	-1.846122000	6	1.386334000	1.409126000	0.601252000
7	0.492880000	-1.717078000	-1.209666000	7	0.474625000	1.260780000	1.574143000
6	1.501669000	-1.807108000	-0.330398000	6	0.193448000	0.032337000	2.017806000
6	2.297723000	-0.659503000	-0.134763000	7	0.708494000	-1.126967000	1.639036000
7	3.396819000	-0.412511000	0.668524000	7	2.349332000	-1.907685000	0.033547000
6	3.694998000	0.826641000	0.414092000	6	3.133848000	-1.251506000	-0.870309000
7	2.874299000	1.408790000	-0.513526000	7	2.970896000	0.037133000	-0.864182000
7	1.710626000	-2.964086000	0.319868000	1	3.831309000	-1.761251000	-1.534927000
1	4.520907000	1.352607000	0.894121000	7	1.664952000	2.643854000	0.142522000
1	2.482151000	-3.041269000	0.997997000	1	2.362625000	2.770187000	-0.605006000
1	1.099355000	-3.772927000	0.140456000	1	1.180594000	3.462238000	0.539115000
1	-0.543322000	-0.557946000	-2.542078000	1	-0.564155000	-0.022765000	2.799575000
1	2.904448000	2.349591000	-0.872804000	1	2.297589000	-2.897396000	0.214909000
6	-0.993361000	0.838839000	0.949739000	6	-3.007194000	-0.190125000	0.165184000
6	-1.805048000	1.334246000	-0.054602000	7	-2.322381000	0.839312000	-0.441894000
7	-2.830356000	0.706768000	-0.687846000	6	-1.209768000	0.718154000	-1.261940000
6	-3.022542000	-0.530449000	-0.238443000	6	-0.773203000	-0.643303000	-1.458000000
7	-2.254859000	-1.109817000	0.752033000	6	-1.419495000	-1.664665000	-0.873079000
6	-1.192192000	-0.478473000	1.421737000	7	-2.523410000	-1.451053000	-0.079674000

7	-0.060550000	1.804128000	1.336087000	1	-1.062293000	-2.683192000	-1.029404000
6	-0.330448000	2.829155000	0.569437000	8	-3.983743000	0.028823000	0.864049000
7	-1.379740000	2.620628000	-0.300368000	1	0.092683000	-0.844611000	-2.089364000
1	0.225304000	3.765916000	0.614837000	1	-2.670848000	1.793393000	-0.269589000
8	-0.579084000	-1.089925000	2.296658000	8	-0.677231000	1.716825000	-1.740762000
1	-2.477330000	-2.078191000	1.020813000	1	-3.022837000	-2.202873000	0.368117000
7	-3.993148000	-1.292444000	-0.752263000				
1	-4.132859000	-2.251987000	-0.405754000				
1	-4.601384000	-0.919236000	-1.495294000				
1	-1.771766000	3.250463000	-0.981540000				
CA				CC			
6	2.062208000	-0.996661000	0.850949000	6	-1.348703000	-1.266361000	-0.737296000
7	1.745155000	0.321408000	0.978697000	7	-1.408381000	0.053610000	-1.066331000
6	2.433296000	1.253250000	0.308772000	6	-2.285819000	0.864536000	-0.463697000
6	3.527421000	0.901275000	-0.558673000	6	-3.194524000	0.375574000	0.540608000
6	3.825164000	-0.413065000	-0.665946000	6	-3.118417000	-0.938917000	0.847147000
7	3.115197000	-1.361346000	0.021018000	7	-2.216475000	-1.762418000	0.227827000
1	4.645967000	-0.724446000	-1.311860000	8	-0.552506000	-2.046946000	-1.273181000
8	1.450454000	-1.886329000	1.454826000	1	-3.787550000	-1.351596000	1.602023000
7	2.094254000	2.520092000	0.465800000	1	-3.910422000	1.034879000	1.031178000
1	2.608059000	3.256338000	-0.038493000	7	-2.312072000	2.136947000	-0.816938000
1	1.316012000	2.771079000	1.091941000	1	-2.977969000	2.781648000	-0.368268000
1	4.089372000	1.659490000	-1.103806000	1	-1.666387000	2.483954000	-1.540389000
1	3.321467000	-2.346421000	-0.044653000	1	-2.144013000	-2.745445000	0.441466000
6	-2.372652000	-1.033551000	-0.119095000	6	1.495049000	-1.076917000	1.175921000
7	-3.526463000	-1.019301000	0.567176000	7	2.639861000	-1.179757000	0.431427000
6	-3.908259000	0.228464000	0.788361000	6	3.136796000	-0.082557000	-0.261651000
7	-3.306285000	1.367473000	0.432489000	7	2.466731000	1.100746000	-0.196464000
6	-2.157630000	1.308089000	-0.258917000	6	1.348294000	1.209513000	0.530996000
6	-1.643858000	0.034883000	-0.563067000	6	0.813973000	0.087524000	1.259412000
7	-0.511665000	-0.387489000	-1.236976000	1	1.126226000	-1.951225000	1.711689000
6	-0.584825000	-1.683805000	-1.194024000	8	4.171973000	-0.221988000	-0.923938000
7	-1.684479000	-2.149372000	-0.533113000	1	-0.097568000	0.173935000	1.851179000
1	0.161581000	-2.337559000	-1.644056000	7	0.728424000	2.375374000	0.562401000
1	-4.843280000	0.343387000	1.336860000	1	-0.134247000	2.484200000	1.114770000
7	-1.552597000	2.451802000	-0.629806000	1	1.107552000	3.174493000	0.035447000
1	-1.971243000	3.359181000	-0.381403000	1	3.162130000	-2.039260000	0.355771000
1	-0.671009000	2.418576000	-1.161533000				
1	-1.957564000	-3.105148000	-0.368760000				
CG				CU			
6	2.372234000	-0.920678000	0.939089000	6	-1.367050000	-1.229542000	-0.756565000
7	2.015245000	0.392009000	0.998736000	7	-1.416445000	0.096114000	-1.063720000
6	2.727299000	1.319482000	0.348013000	6	-2.288687000	0.903450000	-0.448845000
6	3.889221000	0.968575000	-0.426750000	6	-3.202430000	0.404681000	0.546021000
6	4.225391000	-0.340232000	-0.467489000	6	-3.136534000	-0.915245000	0.830795000
7	3.490740000	-1.284154000	0.199228000	7	-2.239859000	-1.735060000	0.199061000
1	5.097843000	-0.650614000	-1.042269000	1	-3.809788000	-1.335391000	1.577846000
8	1.740093000	-1.806139000	1.527966000	8	-0.575916000	-2.007046000	-1.304301000
1	4.470628000	1.723286000	-0.956115000	1	-3.914104000	1.061076000	1.046539000
7	2.347506000	2.581357000	0.437037000	7	-2.304979000	2.181705000	-0.780947000
1	2.878487000	3.314172000	-0.054291000	1	-2.966702000	2.823821000	-0.322502000
1	1.520367000	2.831879000	0.997204000	1	-1.655702000	2.535845000	-1.497699000
1	3.724798000	-2.265052000	0.182173000	1	-2.175010000	-2.722009000	0.396445000
6	-1.988581000	-1.100601000	-0.340546000	6	1.468599000	-1.105753000	1.166743000
7	-3.204013000	-1.142442000	0.274363000	7	2.620380000	-1.192085000	0.418615000

6	-3.699196000	0.069495000	0.466495000	6	3.127995000	-0.111240000	-0.258176000
7	-3.055670000	1.235319000	0.075827000	7	2.415567000	1.060610000	-0.129850000
6	-1.804051000	1.288544000	-0.558906000	6	1.254204000	1.242432000	0.607198000
6	-1.272643000	-0.008543000	-0.756608000	6	0.795904000	0.050824000	1.279970000
7	-1.236223000	-2.216175000	-0.668014000	1	1.094605000	-1.994034000	1.677148000
6	-0.100846000	-1.711853000	-1.266199000	8	4.146941000	-0.158743000	-0.928619000
7	-0.070991000	-0.404775000	-1.346157000	1	-0.108341000	0.090754000	1.887960000
1	0.703026000	-2.346073000	-1.640313000	8	0.701330000	2.339519000	0.637866000
8	-1.315726000	2.381166000	-0.855114000	1	2.781311000	1.883077000	-0.631017000
1	-3.532236000	2.128978000	0.265472000	1	3.140245000	-2.049607000	0.320766000
7	-4.883819000	0.243539000	1.053980000				
1	-5.257665000	1.194043000	1.188244000				
1	-5.425898000	-0.572667000	1.373459000				
1	-1.486657000	-3.176049000	-0.493957000				
GA				GC			
6	2.302220000	-0.686351000	0.258981000	6	1.658555000	-0.977863000	-0.431895000
7	1.503289000	-1.446602000	1.059059000	7	0.689374000	-1.885441000	-0.126305000
6	0.630649000	-0.709146000	1.726052000	6	0.093190000	-1.601239000	1.020001000
7	0.540732000	0.670770000	1.609600000	7	0.416010000	-0.502590000	1.803947000
6	1.358201000	1.463360000	0.787443000	6	1.411977000	0.439034000	1.497693000
6	2.296709000	0.672755000	0.080468000	6	2.054168000	0.128439000	0.274259000
7	3.279722000	1.052131000	-0.833779000	7	3.082582000	0.794857000	-0.392326000
6	3.843295000	-0.080319000	-1.174240000	6	3.274174000	0.075059000	-1.469895000
7	3.304661000	-1.187950000	-0.554134000	7	2.445301000	-1.022362000	-1.570619000
1	4.666400000	-0.141880000	-1.885765000	1	4.023547000	0.321970000	-2.221583000
8	1.200554000	2.685918000	0.766216000	8	1.625607000	1.375269000	2.270853000
1	-0.180163000	1.149293000	2.168226000	1	-0.115289000	-0.367845000	2.675900000
7	-0.244026000	-1.267210000	2.564015000	7	-0.887032000	-2.370576000	1.495354000
1	-0.921144000	-0.678390000	3.068675000	1	-1.186056000	-3.206238000	0.971647000
1	-0.242110000	-2.287893000	2.706191000	1	-1.345006000	-2.129563000	2.385326000
1	3.564334000	-2.156232000	-0.650938000	1	2.401921000	-1.718008000	-2.297645000
6	-2.193352000	-1.068202000	-0.521054000	6	-1.270412000	0.042749000	-2.021397000
7	-3.324737000	-1.099924000	0.201035000	7	-2.415794000	-0.454674000	-1.459155000
6	-3.746322000	0.131745000	0.439496000	6	-2.924363000	0.088687000	-0.285585000
7	-3.199350000	1.293901000	0.069937000	7	-2.265179000	1.123015000	0.305252000
6	-2.071567000	1.280343000	-0.657321000	6	-1.146264000	1.616016000	-0.239642000
6	-1.519812000	0.028524000	-0.982946000	6	-0.600005000	1.071214000	-1.456088000
7	-0.394192000	-0.348440000	-1.693782000	1	-0.892353000	-0.399358000	-2.942865000
6	-0.416873000	-1.646728000	-1.654217000	8	-3.959600000	-0.394221000	0.188483000
7	-1.476813000	-2.155784000	-0.961263000	1	0.311944000	1.470528000	-1.900449000
1	0.339216000	-2.270255000	-2.130228000	7	-0.537182000	2.617044000	0.369799000
7	-1.522189000	2.447364000	-1.041964000	1	0.325608000	3.013527000	-0.029639000
1	-0.657124000	2.449304000	-1.601151000	1	-0.924829000	3.000664000	1.243054000
1	-1.966848000	3.337410000	-0.776630000	1	-2.930217000	-1.221540000	-1.864764000
1	-4.667319000	0.209362000	1.017476000				
1	-1.708245000	-3.121752000	-0.792618000				
GG				GU			
7	1.742936000	-1.333538000	1.203371000	6	-1.677098000	0.302735000	-0.995460000
6	2.585027000	-0.616246000	0.407901000	7	-0.713603000	1.126708000	-1.494604000
6	2.569724000	0.725759000	0.128874000	6	-0.108936000	1.812315000	-0.538286000
6	1.569221000	1.544936000	0.706463000	7	-0.418645000	1.691560000	0.809049000
7	0.707581000	0.796600000	1.524979000	6	-1.408652000	0.844884000	1.333857000
6	0.811911000	-0.568820000	1.749834000	6	-2.059956000	0.117875000	0.307734000
7	3.652153000	-1.153589000	-0.292204000	7	-3.086580000	-0.823115000	0.389376000
6	4.215774000	-0.082539000	-0.953025000	6	-3.289805000	-1.172465000	-0.856666000

7	3.610059000	1.059018000	-0.738723000	7	-2.470349000	-0.533410000	-1.763090000
1	5.089310000	-0.177671000	-1.597576000	1	-4.041239000	-1.904575000	-1.151493000
8	1.393066000	2.758908000	0.583206000	8	-1.610541000	0.821819000	2.549859000
1	-0.059909000	1.298580000	1.993712000	1	0.118449000	2.266189000	1.473932000
7	-0.111853000	-1.083421000	2.562556000	7	0.867631000	2.675128000	-0.822087000
1	-0.833616000	-0.474436000	2.972527000	1	1.332356000	3.194157000	-0.064117000
1	-0.103168000	-2.090719000	2.780018000	1	1.157074000	2.822126000	-1.800162000
1	3.934363000	-2.120385000	-0.297995000	1	-2.436516000	-0.632179000	-2.764824000
6	-1.175073000	-0.053498000	-1.139744000	6	1.244456000	-1.566898000	-1.297027000
6	-1.844610000	-1.147848000	-0.657682000	7	2.395691000	-0.813029000	-1.306559000
7	-3.038067000	-1.199463000	-0.001834000	6	2.916256000	-0.270059000	-0.158459000
6	-3.562701000	0.004648000	0.158748000	7	2.217344000	-0.538143000	0.997789000
7	-2.966892000	1.171638000	-0.298463000	6	1.057641000	-1.292443000	1.103556000
6	-1.738252000	1.234853000	-0.975751000	6	0.585110000	-1.818138000	-0.154597000
7	0.018451000	-0.438796000	-1.752592000	1	0.859849000	-1.967624000	-2.235603000
6	0.030038000	-1.741916000	-1.620378000	1	-0.319043000	-2.427155000	-0.177228000
7	-1.070217000	-2.253847000	-0.965696000	8	3.935057000	0.401948000	-0.137199000
1	0.840093000	-2.367558000	-1.995595000	8	0.517477000	-1.454517000	2.195419000
8	-1.292313000	2.328117000	-1.330628000	1	2.592934000	-0.138722000	1.870017000
1	-3.463541000	2.058287000	-0.128468000	1	2.905669000	-0.612938000	-2.152173000
7	-4.732670000	0.168429000	0.777706000				
1	-5.130151000	1.112547000	0.886768000				
1	-5.239792000	-0.649346000	1.146732000				
1	-1.286328000	-3.212673000	-0.745876000				
UA				UC			
7	3.120689000	-1.326644000	0.014253000	6	-1.377560000	-1.270450000	-0.715797000
6	3.839202000	-0.373509000	-0.670407000	7	-2.249106000	-1.708270000	0.250025000
6	3.539974000	0.932094000	-0.566894000	6	-3.146125000	-0.860303000	0.858133000
6	2.460432000	1.379289000	0.279110000	6	-3.196346000	0.444259000	0.541198000
7	1.798447000	0.352220000	0.936740000	6	-2.317409000	0.997087000	-0.460283000
6	2.079681000	-0.992633000	0.844211000	7	-1.454526000	0.069058000	-1.025764000
8	1.425344000	-1.817048000	1.463415000	8	-0.571532000	-2.000294000	-1.271561000
1	4.666296000	-0.683280000	-1.308566000	1	-3.828483000	-1.254061000	1.610881000
1	4.120301000	1.663119000	-1.128940000	1	-3.910426000	1.093506000	1.046809000
1	1.020153000	0.622273000	1.555332000	8	-2.298706000	2.169567000	-0.827746000
8	2.121894000	2.548191000	0.449832000	1	-0.808004000	0.416145000	-1.748860000
1	3.341606000	-2.377146000	-0.053240000	1	-2.202757000	-2.760923000	0.500048000
6	-2.368835000	-1.030145000	-0.129895000	6	3.130439000	-0.116097000	-0.244468000
7	-3.523482000	-1.027648000	0.555114000	7	2.476666000	1.077687000	-0.214388000
6	-3.912874000	0.216217000	0.784860000	6	1.355008000	1.220670000	0.502110000
7	-3.317223000	1.361291000	0.437929000	6	0.800071000	0.125332000	1.255257000
6	-2.167459000	1.313668000	-0.252548000	6	1.465241000	-1.050223000	1.206474000
6	-1.645851000	0.045741000	-0.565288000	7	2.613469000	-1.188084000	0.472983000
7	-0.510433000	-0.365078000	-1.240907000	1	1.080562000	-1.905241000	1.761862000
6	-0.575999000	-1.662079000	-1.207406000	8	4.167979000	-0.286898000	-0.895618000
7	-1.673634000	-2.138875000	-0.551159000	1	-0.114119000	0.239602000	1.838146000
1	0.174751000	-2.308158000	-1.661277000	7	0.751406000	2.395452000	0.499222000
7	-1.568759000	2.463574000	-0.614458000	1	-0.113340000	2.530435000	1.042498000
1	-0.686395000	2.439383000	-1.145381000	1	1.145271000	3.175400000	-0.045354000
1	-1.993025000	3.366654000	-0.359996000	1	3.124089000	-2.056422000	0.423089000
1	-4.849172000	0.321666000	1.333084000				
1	-1.941267000	-3.097406000	-0.394033000				
UG				UU			
7	3.493391000	-1.256036000	0.192526000	6	-3.164050000	-0.847399000	0.843620000
6	2.388475000	-0.919637000	0.934203000	7	-2.263938000	-1.684997000	0.225793000

7	2.072203000	0.420376000	0.959184000	6	-1.391287000	-1.232049000	-0.732020000
6	2.757253000	1.440513000	0.314515000	7	-1.470456000	0.111447000	-1.023634000
6	3.904204000	0.991419000	-0.436442000	6	-2.336514000	1.029759000	-0.447251000
6	4.238355000	-0.309309000	-0.472472000	6	-3.216388000	0.461305000	0.544616000
1	5.115663000	-0.620227000	-1.038997000	1	-3.847159000	-1.252950000	1.589394000
8	1.709413000	-1.738397000	1.533983000	8	-0.582526000	-1.952450000	-1.296075000
1	1.245825000	0.692132000	1.511065000	1	-0.823149000	0.469845000	-1.740479000
8	2.382044000	2.605962000	0.419558000	8	-2.319539000	2.207237000	-0.798454000
1	4.507387000	1.717000000	-0.981215000	1	-3.932922000	1.102004000	1.057606000
1	3.725645000	-2.236366000	0.178799000	1	-2.207374000	-2.669005000	0.434852000
6	-1.986328000	-1.091818000	-0.349443000	7	2.601886000	-1.197581000	0.451907000
7	-3.201932000	-1.142263000	0.264480000	6	3.125260000	-0.137818000	-0.245893000
6	-3.702202000	0.066480000	0.463430000	7	2.427025000	1.045226000	-0.145276000
7	-3.063249000	1.237214000	0.080002000	6	1.265454000	1.257116000	0.583370000
6	-1.811494000	1.299306000	-0.553658000	6	0.790028000	0.085926000	1.279701000
6	-1.274645000	0.005597000	-0.758655000	6	1.448671000	-1.081035000	1.193703000
7	-0.071035000	-0.382226000	-1.349802000	1	1.061882000	-1.953504000	1.721547000
6	-0.095564000	-1.689863000	-1.277539000	8	4.145862000	-0.212242000	-0.911349000
7	-1.229201000	-2.202352000	-0.683007000	1	2.804713000	1.852202000	-0.662509000
1	0.711122000	-2.318568000	-1.654890000	8	0.726169000	2.361360000	0.588544000
8	-1.327494000	2.395646000	-0.843151000	1	-0.115761000	0.150028000	1.883309000
1	-3.543592000	2.127777000	0.274607000	1	3.111381000	-2.063361000	0.374330000
7	-4.887868000	0.232203000	1.051217000				
1	-5.265694000	1.180359000	1.190837000				
1	-5.426771000	-0.588084000	1.365573000				
1	-1.475787000	-3.164253000	-0.514742000				

Table S19. RNA inter-strand dimer geometries with methyls.

3'AA				5'AA			
6	2.493804000	0.695551000	-0.305072000	7	-5.715379000	0.078213000	-0.369845000
6	2.677685000	-0.646462000	-0.492135000	6	-5.702933000	-1.285284000	-0.308900000
7	1.968383000	-1.477121000	-1.272741000	7	-4.590464000	-1.777092000	0.146864000
6	0.999718000	-0.812060000	-1.881829000	6	-3.810139000	-0.663079000	0.399889000
7	0.686825000	0.484464000	-1.795327000	6	-4.486313000	0.484631000	0.093791000
6	1.426317000	1.281360000	-1.008506000	7	-4.056715000	1.751599000	0.202929000
7	3.762451000	-0.983445000	0.282316000	6	-2.820810000	1.773588000	0.677040000
6	4.159176000	0.172774000	0.889410000	7	-2.038964000	0.749449000	1.030347000
7	3.432880000	1.203038000	0.575271000	6	-2.505157000	-0.501579000	0.898700000
1	5.005838000	0.227246000	1.572958000	1	-6.547265000	-1.903201000	-0.614333000
1	0.369544000	-1.403537000	-2.546177000	7	-1.717073000	-1.537629000	1.242404000
7	1.122948000	2.590128000	-0.926049000	1	-2.063819000	-2.502905000	1.144866000
1	1.684018000	3.211579000	-0.326023000	1	-0.767427000	-1.365101000	1.603028000
1	0.329960000	2.969131000	-1.462549000	1	-2.380405000	2.763573000	0.795920000
6	4.331015000	-2.316252000	0.411947000	6	-6.783992000	0.956167000	-0.822150000
1	5.383916000	-2.314989000	0.129994000	1	-7.672466000	0.839818000	-0.197668000
1	4.229913000	-2.683818000	1.433110000	1	-7.041762000	0.747423000	-1.862661000
1	3.779025000	-2.972788000	-0.260636000	1	-6.420304000	1.979431000	-0.741024000
7	-0.687108000	0.484204000	1.795003000	7	2.038550000	0.749823000	-1.030347000
6	-1.426362000	1.280870000	1.008514000	6	2.505137000	-0.501231000	-0.898728000
6	-2.493983000	0.695236000	0.304888000	6	3.810068000	-0.662812000	-0.399928000
6	-2.677579000	-0.646153000	0.492273000	6	4.486216000	0.484281000	-0.093782000
7	-1.968473000	-1.476777000	1.272599000	7	4.057092000	1.751957000	-0.202833000
6	-0.999436000	-0.811876000	1.882187000	6	2.820879000	1.773648000	-0.676963000
1	-0.369263000	-1.403239000	2.546515000	7	4.590634000	-1.776841000	-0.146935000
7	-3.432919000	1.202871000	-0.575259000	6	5.703148000	-1.284848000	0.308854000
6	-4.159194000	0.172812000	-0.889405000	7	5.715127000	0.077778000	0.369826000
7	-1.122993000	2.589986000	0.926101000	7	1.717566000	-1.537863000	-1.242443000
1	-0.329762000	2.969785000	1.462924000	1	2.380065000	2.763624000	-0.795828000
1	-1.684072000	3.211817000	0.326082000	1	0.767817000	-1.365471000	-1.603066000
1	-5.006159000	0.226579000	-1.573341000	1	2.063685000	-2.502831000	-1.144988000
7	-3.762449000	-0.983491000	-0.282323000	1	6.547433000	-1.902931000	0.614257000
6	-4.330784000	-2.316291000	-0.411900000	6	6.783640000	0.955978000	0.822211000
1	-3.779742000	-2.972376000	0.261899000	1	7.672394000	0.839152000	0.198217000
1	-4.228225000	-2.684604000	-1.432648000	1	7.040863000	0.747756000	1.862962000
1	-5.384088000	-2.314849000	-0.131457000	1	6.420106000	1.979133000	0.740348000
3'AC				5'AC			
6	2.541610000	-0.970105000	-0.800490000	6	-2.465609000	-0.196205000	0.710294000
7	3.659108000	-1.067267000	0.019465000	7	-2.055048000	1.080884000	0.725137000
6	4.222216000	0.052982000	0.570069000	6	-2.868735000	2.029373000	0.252637000
6	3.711462000	1.282681000	0.336369000	7	-4.089594000	1.906061000	-0.244373000
6	2.552528000	1.356302000	-0.515047000	6	-4.463547000	0.616978000	-0.234397000
7	2.006205000	0.257168000	-1.048059000	6	-3.749054000	-0.463683000	0.201280000
7	1.997849000	2.525715000	-0.778296000	7	-5.662014000	0.112886000	-0.681952000
1	1.164784000	2.576336000	-1.381742000	6	-5.595015000	-1.235810000	-0.483147000
1	2.399097000	3.386525000	-0.380341000	7	-4.475777000	-1.630451000	0.044820000
1	4.156495000	2.177105000	0.772034000	1	-6.404715000	-1.917493000	-0.743344000
1	5.099383000	-0.049192000	1.208832000	1	-2.472832000	3.044577000	0.280608000
8	2.064028000	-2.008521000	-1.273803000	7	-1.644946000	-1.157220000	1.174587000
6	4.200432000	-2.402173000	0.270505000	1	-0.713176000	-0.908138000	1.537086000
1	5.072684000	-2.313794000	0.918167000	1	-1.948890000	-2.141636000	1.167441000
1	4.501124000	-2.865340000	-0.669262000	1	-6.419099000	0.650880000	-1.072441000
1	3.434772000	-3.033115000	0.721921000	7	3.567324000	0.306197000	-0.574700000

7	-0.704498000	0.671974000	1.493944000	6	3.750901000	-1.013102000	-0.438389000
6	-1.447136000	1.404452000	0.649584000	6	4.542872000	1.180950000	-0.204669000
6	-2.549629000	0.779774000	0.039826000	7	5.734996000	0.685885000	0.309738000
7	-3.501757000	1.220486000	-0.862192000	6	4.976620000	-1.549825000	0.093363000
6	-4.262740000	0.184200000	-1.048333000	6	5.930365000	-0.661886000	0.449951000
7	-3.877009000	-0.914387000	-0.336213000	8	4.410788000	2.405969000	-0.316796000
6	-2.761344000	-0.530334000	0.369369000	1	5.127385000	-2.624002000	0.203605000
7	-2.049904000	-1.296176000	1.211860000	1	6.874266000	-1.025409000	0.857368000
6	-1.047011000	-0.599592000	1.722334000	7	2.779447000	-1.825478000	-0.814135000
1	-0.412148000	-1.137301000	2.426706000	1	1.906986000	-1.439228000	-1.200870000
1	-5.127948000	0.192035000	-1.710448000	1	2.895950000	-2.844177000	-0.719624000
7	-1.113712000	2.688875000	0.424214000	1	6.434309000	1.364790000	0.569132000
1	-1.676839000	3.261043000	-0.221188000				
1	-0.295706000	3.098499000	0.896844000				
6	-4.476051000	-2.240349000	-0.319273000				
1	-3.914636000	-2.842383000	0.396723000				
1	-4.413310000	-2.706421000	-1.303713000				
1	-5.519965000	-2.187568000	-0.006640000				
3'AG				5'AG			
7	-0.708801000	0.017742000	1.744283000	6	2.684153000	-0.577740000	-0.760110000
6	-1.405559000	1.133385000	1.252077000	7	2.181029000	0.636151000	-1.030430000
6	-1.008819000	-1.303108000	1.442354000	6	2.907113000	1.718992000	-0.738490000
7	-2.005616000	-1.667146000	0.652357000	7	4.117474000	1.790321000	-0.206826000
6	-2.687435000	-0.591290000	0.168566000	6	4.585777000	0.557030000	0.040885000
6	-2.467125000	0.741665000	0.400432000	6	3.967169000	-0.640174000	-0.187534000
7	-0.219935000	-2.211274000	2.018175000	7	1.951780000	-1.671797000	-1.041675000
1	-0.377347000	-3.214777000	1.844337000	7	4.772818000	-1.693971000	0.205396000
1	0.546122000	-1.909837000	2.636374000	6	5.842640000	-1.118081000	0.664761000
1	0.084585000	0.192579000	2.377298000	7	5.803508000	0.244634000	0.597911000
8	-1.048431000	2.268039000	1.576069000	1	6.691887000	-1.670901000	1.066232000
7	-3.398451000	1.520341000	-0.286867000	1	2.327250000	-2.609311000	-0.837725000
6	-4.144218000	0.640138000	-0.907386000	1	1.016045000	-1.571421000	-1.461156000
7	-3.778174000	-0.669924000	-0.680989000	1	2.438363000	2.675369000	-0.970387000
1	-4.981292000	0.918874000	-1.547051000	1	6.506088000	0.905715000	0.888511000
6	-4.373153000	-1.884361000	-1.210988000	7	-2.018650000	0.723322000	0.798368000
1	-5.414216000	-1.976908000	-0.893246000	6	-2.361283000	-0.638969000	0.809718000
1	-3.805085000	-2.728260000	-0.822891000	6	-3.649162000	-0.849767000	0.261200000
1	-4.326688000	-1.893382000	-2.302262000	6	-4.371810000	0.222637000	-0.194321000
6	0.992981000	-0.081038000	-2.149094000	7	-4.029856000	1.541925000	-0.201876000
7	0.691076000	1.135277000	-1.684565000	6	-2.829744000	1.742185000	0.316947000
6	1.433732000	1.657302000	-0.696167000	7	-4.363180000	-2.035386000	0.081066000
6	2.492624000	0.879603000	-0.194717000	6	-5.483966000	-1.642935000	-0.471661000
6	2.665610000	-0.349244000	-0.769012000	7	-5.567752000	-0.282270000	-0.675069000
7	1.952815000	-0.905658000	-1.761372000	1	-6.282524000	-2.333358000	-0.746928000
1	0.360851000	-0.443998000	-2.959646000	7	-2.311283000	2.968406000	0.399415000
7	1.141477000	2.886417000	-0.231871000	8	-1.569288000	-1.463009000	1.271306000
1	1.705081000	3.297667000	0.525925000	1	-1.097170000	0.985686000	1.175363000
1	0.354449000	3.414584000	-0.634276000	1	-2.850100000	3.778174000	0.063218000
7	3.431860000	1.095564000	0.798059000	1	-1.372178000	3.103661000	0.799063000
6	4.147553000	0.011400000	0.795727000	1	-6.319903000	0.252053000	-1.078974000
1	4.991351000	-0.146511000	1.466631000				
7	3.743622000	-0.910324000	-0.126261000				
6	4.333977000	-2.203399000	-0.434965000				
1	4.386020000	-2.828772000	0.458959000				
1	5.337134000	-2.085454000	-0.850497000				

1	3.696348000	-2.683522000	-1.175797000				
3'AU				5'AU			
6	-1.450859000	1.423243000	0.632960000	6	-2.450995000	-0.339826000	0.825474000
6	-2.552840000	0.790784000	0.030338000	7	-2.020505000	0.930567000	0.848279000
6	-2.762640000	-0.516097000	0.373631000	6	-2.836401000	1.899665000	0.423859000
7	-2.049742000	-1.272174000	1.223675000	7	-4.076592000	1.803735000	-0.029407000
6	-1.047508000	-0.568981000	1.726322000	6	-4.469768000	0.520345000	-0.028999000
7	-0.706805000	0.700588000	1.484508000	6	-3.756389000	-0.578734000	0.359921000
7	-3.878163000	-0.908959000	-0.327309000	7	-4.506327000	-1.731513000	0.209433000
6	-4.265728000	0.181634000	-1.050632000	6	-5.638131000	-1.310555000	-0.269106000
7	-3.506026000	1.220811000	-0.875711000	7	-5.691627000	0.042482000	-0.440636000
1	-0.411562000	-1.098478000	2.435917000	1	-2.424114000	2.908217000	0.455550000
7	-1.119260000	2.705687000	0.394035000	7	-1.628624000	-1.321398000	1.241206000
1	-0.301552000	3.121296000	0.861931000	1	-0.680333000	-1.092939000	1.573159000
1	-1.683485000	3.270350000	-0.256990000	1	-1.947781000	-2.300916000	1.227451000
1	-5.131293000	0.181423000	-1.712327000	1	-6.467337000	-1.975214000	-0.511295000
6	-4.485298000	-2.230549000	-0.284739000	6	-6.789855000	0.849211000	-0.950359000
1	-3.914110000	-2.828426000	0.423773000	1	-7.669861000	0.756018000	-0.310199000
1	-4.448428000	-2.706572000	-1.266944000	1	-7.048812000	0.551280000	-1.968623000
1	-5.522843000	-2.168412000	0.050078000	1	-6.457207000	1.886156000	-0.953680000
6	2.570888000	1.474483000	-0.505105000	7	3.588093000	0.044109000	-0.657243000
6	3.732183000	1.300411000	0.332872000	6	3.690323000	-1.337316000	-0.571154000
6	4.229529000	0.076346000	0.576102000	6	4.966139000	-1.799900000	-0.081261000
7	3.658335000	-1.048148000	0.025886000	6	5.936512000	-0.928713000	0.244703000
6	2.549761000	-0.977873000	-0.780471000	7	5.741780000	0.428639000	0.135292000
7	2.057051000	0.287698000	-1.008184000	6	4.561987000	0.958324000	-0.324479000
1	4.211825000	2.173361000	0.774432000	8	4.362329000	2.157908000	-0.431588000
1	5.101571000	-0.027733000	1.221082000	1	2.694952000	0.422830000	-1.004566000
8	2.022616000	-1.958687000	-1.281822000	8	2.750358000	-2.053797000	-0.907803000
8	2.035722000	2.547814000	-0.772780000	1	5.145856000	-2.868690000	0.025324000
1	1.224903000	0.360386000	-1.611152000	1	6.894951000	-1.305136000	0.602513000
6	4.190547000	-2.389445000	0.288337000	6	6.794020000	1.388475000	0.488103000
1	5.077543000	-2.292109000	0.911712000	1	7.094213000	1.962729000	-0.389372000
1	4.449814000	-2.880369000	-0.649796000	1	6.428091000	2.084186000	1.243207000
1	3.444956000	-2.999986000	0.799093000	1	7.647847000	0.836395000	0.876995000
3'CC				5'CC			
7	-3.501888000	0.269948000	0.567883000	7	3.501569000	0.269995000	-0.570583000
6	-3.630619000	-1.062808000	0.572250000	6	3.630294000	-1.062762000	-0.574873000
6	-4.852870000	-1.700634000	0.156919000	6	4.852841000	-1.700539000	-0.160337000
6	-5.861278000	-0.893399000	-0.238940000	6	5.861533000	-0.893256000	0.234698000
7	-5.721910000	0.468540000	-0.242831000	7	5.722171000	0.468684000	0.238516000
6	-4.532048000	1.061818000	0.161037000	6	4.532021000	1.061913000	-0.164575000
8	-4.451455000	2.296290000	0.144503000	8	4.451443000	2.296388000	-0.148140000
7	-2.607154000	-1.792266000	0.978788000	7	2.606536000	-1.792269000	-0.980586000
1	-1.736989000	-1.333242000	1.282188000	1	1.736155000	-1.333282000	-1.283420000
1	-2.680882000	-2.819229000	0.991603000	1	2.680252000	-2.819234000	-0.993323000
1	-4.958944000	-2.785746000	0.161276000	1	4.958908000	-2.785651000	-0.164633000
1	-6.804700000	-1.334867000	-0.561657000	1	6.805185000	-1.334685000	0.556795000
6	-6.813839000	1.352858000	-0.648155000	6	6.808536000	1.352220000	0.661207000
1	-7.670742000	0.745447000	-0.940600000	1	6.481013000	1.967882000	1.499326000
1	-6.493726000	1.978653000	-1.481619000	1	7.665284000	0.744662000	0.952680000
1	-7.083288000	2.010599000	0.178602000	1	7.082233000	2.021062000	-0.155318000
6	3.630628000	-1.062658000	-0.572250000	6	-3.630132000	-1.062451000	0.574827000
7	3.502118000	0.269309000	-0.568181000	7	-3.501622000	0.269515000	0.570497000
6	4.532250000	1.061522000	-0.161519000	6	-4.532044000	1.061679000	0.164473000

7	5.722217000	0.468798000	0.242491000	7	-5.722300000	0.468906000	-0.238610000
6	5.861627000	-0.893467000	0.238916000	6	-5.861711000	-0.893357000	-0.234762000
6	4.852478000	-1.701353000	-0.156789000	6	-4.852281000	-1.701195000	0.160322000
1	4.958682000	-2.786044000	-0.160890000	1	-4.958484000	-2.785886000	0.164637000
7	2.607389000	-1.792281000	-0.978609000	7	-2.606604000	-1.792025000	0.980546000
1	1.736452000	-1.333983000	-1.282150000	1	-1.735448000	-1.333690000	1.283405000
1	2.680833000	-2.819321000	-0.991199000	1	-2.680041000	-2.819063000	0.993319000
8	4.451725000	2.295892000	-0.145267000	8	-4.451527000	2.296047000	0.148007000
1	6.804559000	-1.334559000	0.561713000	1	-6.804874000	-1.334489000	-0.556828000
6	6.813082000	1.353619000	0.649216000	6	-6.808786000	1.352529000	-0.660809000
1	7.670386000	0.746721000	0.941547000	1	-6.482201000	1.967101000	-1.500092000
1	7.082317000	2.012459000	-0.176735000	1	-7.080930000	2.022386000	0.155403000
1	6.492007000	1.978323000	1.483129000	1	-7.666253000	0.745079000	-0.950384000
3'CG				5'CG			
6	2.560164000	1.514009000	-0.461880000	7	3.666486000	-0.060355000	-0.683325000
7	2.006546000	0.503596000	-1.143425000	6	3.867508000	-1.369000000	-0.489147000
6	2.529874000	-0.750873000	-1.066751000	6	5.116046000	-1.869767000	0.024508000
7	3.643117000	-0.970941000	-0.264622000	6	6.073610000	-0.956956000	0.302880000
6	4.213699000	0.057183000	0.437406000	7	5.860060000	0.380922000	0.103651000
6	3.715056000	1.311860000	0.374966000	6	4.645692000	0.839775000	-0.391655000
8	2.045498000	-1.709310000	-1.680295000	7	2.891766000	-2.206894000	-0.789744000
7	2.016930000	2.713697000	-0.562383000	8	4.497720000	2.056540000	-0.559005000
1	1.187152000	2.855198000	-1.155221000	1	5.281308000	-2.935495000	0.181868000
1	2.424466000	3.507331000	-0.047393000	1	3.021303000	-3.218786000	-0.649539000
1	4.166329000	2.133309000	0.931865000	1	2.001750000	-1.848040000	-1.163645000
1	5.087112000	-0.140364000	1.058385000	1	7.034279000	-1.291935000	0.693756000
6	4.180694000	-2.319015000	-0.216651000	6	6.889927000	1.375202000	0.401663000
1	5.054464000	-2.329513000	0.435064000	1	7.132775000	1.940374000	-0.498658000
1	4.457517000	-2.644486000	-1.219742000	1	7.777504000	0.864045000	0.774230000
1	3.423883000	-3.009677000	0.157314000	1	6.507167000	2.071268000	1.148776000
7	-0.721100000	0.519408000	1.443237000	6	-2.265078000	-0.571446000	0.854999000
6	-1.418993000	1.485577000	0.700362000	7	-1.942199000	0.791304000	0.745362000
6	-2.517705000	0.912116000	0.015057000	6	-2.794140000	1.772390000	0.256089000
6	-2.766701000	-0.429532000	0.145616000	7	-4.020090000	1.530360000	-0.177521000
7	-2.083452000	-1.359112000	0.870495000	6	-4.343099000	0.210325000	-0.074163000
6	-1.052197000	-0.826807000	1.505624000	6	-3.580250000	-0.826600000	0.397662000
7	-0.255970000	-1.573212000	2.272158000	7	-2.288352000	3.006506000	0.237168000
1	-0.434958000	-2.583279000	2.370869000	1	-2.857075000	3.790003000	-0.111777000
1	0.537313000	-1.140334000	2.765308000	1	-1.329114000	3.174117000	0.571383000
1	0.098136000	0.833252000	1.982766000	1	-1.003619000	1.084319000	1.050802000
8	-1.032812000	2.656382000	0.705901000	8	-1.436014000	-1.359384000	1.314530000
7	-3.462415000	1.508035000	-0.820698000	7	-5.558503000	-0.333585000	-0.452688000
6	-4.244251000	0.515333000	-1.166016000	6	-5.444384000	-1.679304000	-0.177328000
7	-3.889756000	-0.699493000	-0.618261000	7	-4.287577000	-2.027806000	0.328667000
1	-5.100542000	0.638696000	-1.828668000	1	-6.248441000	-2.392519000	-0.364327000
6	-4.503589000	-2.000732000	-0.819073000	6	-6.690734000	0.388172000	-1.007700000
1	-5.573729000	-1.953859000	-0.607814000	1	-7.560427000	0.308285000	-0.352172000
1	-4.031255000	-2.701074000	-0.132118000	1	-6.947381000	0.002028000	-1.996380000
1	-4.350972000	-2.350325000	-1.842923000	1	-6.405399000	1.435172000	-1.096353000
3'CU				5'CU			
6	4.330479000	0.122985000	0.710545000	7	-3.511864000	0.251029000	0.569861000
6	3.787355000	1.357616000	0.624163000	6	-3.640498000	-1.080876000	0.557631000
6	2.601063000	1.493575000	-0.181551000	6	-4.862699000	-1.714305000	0.135198000
7	2.061820000	0.443443000	-0.812716000	6	-5.872047000	-0.901524000	-0.249831000
6	2.630032000	-0.789691000	-0.712904000	7	-5.732510000	0.460670000	-0.236741000

7	3.774269000	-0.946077000	0.060021000	6	-4.542205000	1.048275000	0.173698000
1	5.228808000	-0.024846000	1.309412000	7	-2.617044000	-1.815533000	0.954265000
8	2.160259000	-1.783363000	-1.279988000	8	-4.461573000	2.282745000	0.172579000
1	4.227028000	2.211489000	1.140063000	1	-1.745852000	-1.361079000	1.262812000
7	2.014116000	2.670541000	-0.302794000	1	-2.690577000	-2.842643000	0.954269000
1	1.162164000	2.764766000	-0.873154000	1	-4.969002000	-2.798955000	0.126027000
1	2.409766000	3.493796000	0.173513000	1	-6.815246000	-1.338530000	-0.577370000
6	4.350501000	-2.286921000	0.151758000	6	-6.818599000	1.348695000	-0.649224000
1	4.605970000	-2.649876000	-0.844111000	1	-7.094474000	2.006923000	0.175287000
1	3.622416000	-2.976259000	0.580588000	1	-6.491027000	1.975274000	-1.479194000
1	5.242392000	-2.246310000	0.777043000	1	-7.674657000	0.744492000	-0.949562000
7	-2.110224000	0.464690000	0.770524000	7	3.540700000	0.208649000	-0.559514000
6	-2.636644000	-0.805786000	0.699401000	6	3.601535000	-1.177177000	-0.604055000
7	-3.770785000	-0.937657000	-0.062454000	6	4.866897000	-1.721104000	-0.174306000
6	-4.334502000	0.132653000	-0.718310000	6	5.866182000	-0.913335000	0.220387000
6	-3.803858000	1.363498000	-0.627273000	7	5.711954000	0.453451000	0.240530000
6	-2.613841000	1.600699000	0.152926000	6	4.544873000	1.058497000	-0.154071000
8	-2.115381000	-1.737676000	1.291933000	8	4.380935000	2.268208000	-0.146319000
1	-1.258531000	0.583230000	1.337878000	1	2.656510000	0.644459000	-0.859585000
8	-2.047872000	2.683561000	0.283990000	8	2.637264000	-1.830885000	-0.995283000
1	-4.278115000	2.193679000	-1.149723000	1	5.014887000	-2.800017000	-0.170129000
1	-5.228027000	-0.020748000	-1.322769000	1	6.815798000	-1.349769000	0.530359000
6	-4.326744000	-2.290550000	-0.175055000	6	6.792441000	1.344674000	0.677839000
1	-3.630173000	-2.945354000	-0.700698000	1	6.479205000	1.918281000	1.550917000
1	-4.501789000	-2.703332000	0.817911000	1	7.660480000	0.737079000	0.927610000
1	-5.265369000	-2.233465000	-0.723683000	1	7.047021000	2.045154000	-0.117670000
3'GG				5'GG			
6	-2.466276000	0.903903000	0.303516000	6	-2.889309000	1.520894000	0.659158000
7	-3.397693000	1.436937000	-0.587788000	7	-4.114861000	1.405351000	0.174499000
6	-4.132736000	0.406342000	-0.924767000	6	-4.492443000	0.101469000	0.057357000
7	-3.759471000	-0.775338000	-0.319943000	7	-5.721285000	-0.320323000	-0.421895000
6	-2.675725000	-0.439994000	0.474212000	6	-5.667569000	-1.697147000	-0.367340000
7	-1.990239000	-1.319195000	1.257484000	7	-4.536351000	-2.172039000	0.091780000
6	-1.001932000	-0.729560000	1.910019000	6	-3.782880000	-1.030273000	0.365162000
7	-0.713224000	0.624141000	1.810251000	6	-2.467828000	-0.909157000	0.876668000
6	-1.413856000	1.538742000	1.007121000	7	-2.088858000	0.438021000	0.994532000
7	-0.211226000	-1.420453000	2.732287000	1	-6.494520000	-2.334713000	-0.679142000
1	-0.360467000	-2.431907000	2.861525000	8	-1.681140000	-1.796519000	1.213804000
1	0.548076000	-0.943339000	3.237957000	1	-1.145734000	0.637835000	1.356926000
8	-1.066935000	2.721556000	0.983678000	7	-2.333968000	2.718601000	0.848283000
1	0.074158000	0.984907000	2.367579000	1	-1.376107000	2.789155000	1.218962000
1	-4.966851000	0.476594000	-1.622532000	1	-2.863719000	3.573424000	0.623214000
6	-4.385163000	-2.082671000	-0.415578000	6	-6.811343000	0.527948000	-0.872271000
1	-5.342195000	-2.100652000	0.112280000	1	-7.044705000	0.333677000	-1.919124000
1	-4.548211000	-2.350964000	-1.461369000	1	-7.702949000	0.363483000	-0.267217000
1	-3.715458000	-2.808433000	0.043427000	1	-6.492471000	1.564626000	-0.764019000
6	1.001970000	-0.729565000	-1.909818000	7	2.052956000	0.512287000	-0.990574000
7	0.713227000	0.624177000	-1.810281000	6	2.463704000	-0.828590000	-0.908741000
6	1.413983000	1.538579000	-1.007112000	6	3.780742000	-0.932727000	-0.400305000
6	2.465978000	0.903896000	-0.303978000	7	4.560493000	-2.064528000	-0.157444000
6	2.675710000	-0.439730000	-0.474119000	6	5.680274000	-1.575695000	0.314592000
7	1.990304000	-1.319612000	-1.257168000	7	5.702535000	-0.200583000	0.406115000
8	1.067150000	2.721449000	-0.983716000	6	4.464900000	0.206227000	-0.061955000
7	0.211235000	-1.420554000	-2.732030000	7	4.056870000	1.504016000	-0.144201000
1	-0.074315000	0.985532000	-2.367868000	6	2.829097000	1.604244000	-0.625942000

1	-0.548466000	-0.943268000	-3.238288000	8	1.697482000	-1.724071000	-1.269821000
1	0.360095000	-2.432064000	-2.861630000	1	1.105538000	0.699095000	-1.347765000
7	3.397934000	1.437225000	0.587961000	1	6.522874000	-2.202760000	0.609494000
6	4.132510000	0.406256000	0.924469000	7	2.246192000	2.793686000	-0.783020000
7	3.759399000	-0.775547000	0.320007000	1	1.286776000	2.851271000	-1.151983000
1	4.966859000	0.476806000	1.622530000	1	2.755661000	3.652751000	-0.534978000
6	4.385127000	-2.082770000	0.415393000	6	6.993078000	0.186567000	0.949745000
1	5.340996000	-2.101367000	-0.114547000	1	7.801691000	-0.144491000	0.298097000
1	3.714344000	-2.808897000	-0.041454000	1	7.135850000	-0.236841000	1.943950000
1	4.550435000	-2.350025000	1.461095000	1	7.012470000	1.274228000	1.018422000
3'GU				5'GU			
7	-3.467469000	1.510576000	-0.831173000	6	-2.802237000	1.759217000	0.272386000
6	-2.521078000	0.921344000	0.008878000	7	-4.028451000	1.521651000	-0.163713000
6	-1.423888000	1.501018000	0.690102000	6	-4.351279000	0.201040000	-0.073335000
7	-0.724038000	0.541024000	1.439029000	7	-5.567543000	-0.338230000	-0.457436000
6	-1.052645000	-0.805428000	1.509610000	6	-5.453942000	-1.687238000	-0.195182000
7	-2.082945000	-1.344043000	0.877719000	7	-4.296955000	-2.040389000	0.307445000
6	-2.767841000	-0.419632000	0.147295000	6	-3.589438000	-0.840825000	0.388377000
7	-3.890351000	-0.696954000	-0.614844000	6	-2.273674000	-0.590045000	0.848314000
6	-4.246967000	0.513862000	-1.169817000	7	-1.951309000	0.773484000	0.752035000
1	-5.103729000	0.631780000	-1.833489000	1	-1.012591000	1.064189000	1.060315000
8	-1.039995000	2.672618000	0.688362000	7	-2.296249000	2.993156000	0.265629000
1	0.094799000	0.860354000	1.976837000	1	-1.337136000	3.158088000	0.601455000
7	-0.254982000	-1.545620000	2.280721000	1	-2.865388000	3.781476000	-0.075905000
1	-0.431675000	-2.555463000	2.386095000	8	-1.444871000	-1.383011000	1.300246000
1	0.537915000	-1.108030000	2.771714000	1	-6.257077000	-2.397777000	-0.389267000
6	-4.517595000	-1.995866000	-0.788105000	6	-6.697096000	0.387392000	-1.012341000
1	-4.428309000	-2.336906000	-1.822269000	1	-6.414193000	1.438737000	-1.082485000
1	-5.573341000	-1.951767000	-0.512173000	1	-7.571807000	0.294933000	-0.366885000
1	-4.005761000	-2.701664000	-0.135908000	1	-6.942781000	0.016367000	-2.008463000
7	2.057604000	0.532206000	-1.097909000	7	3.709751000	-0.116375000	-0.664052000
6	2.578890000	1.630492000	-0.428879000	6	3.846232000	-1.487564000	-0.498490000
6	3.734840000	1.328404000	0.379599000	6	5.131978000	-1.889072000	0.018552000
6	4.220947000	0.077819000	0.447330000	6	6.079479000	-0.976523000	0.294851000
7	3.643037000	-0.951584000	-0.259660000	7	5.851184000	0.366980000	0.107295000
6	2.538804000	-0.757203000	-1.051477000	6	4.659679000	0.839596000	-0.383436000
8	2.005901000	-1.651763000	-1.689448000	1	7.046126000	-1.307595000	0.674738000
1	1.228869000	0.697518000	-1.687141000	1	5.338064000	-2.945121000	0.186662000
8	2.053835000	2.735711000	-0.542443000	8	2.925293000	-2.245563000	-0.794329000
1	4.219628000	2.125157000	0.942839000	1	2.808297000	0.219230000	-1.033532000
1	5.089123000	-0.124908000	1.073798000	8	4.430394000	2.025651000	-0.559618000
6	4.176178000	-2.316870000	-0.207978000	6	6.878686000	1.370474000	0.405187000
1	4.410204000	-2.665461000	-1.213761000	1	7.747568000	0.861265000	0.819522000
1	3.441316000	-2.997316000	0.225000000	1	6.498612000	2.094597000	1.124291000
1	5.079171000	-2.312702000	0.400179000	1	7.162446000	1.904338000	-0.500567000
3'UU				5'UU			
6	4.336444000	0.138831000	0.710652000	6	-4.557166000	1.044473000	0.161376000
6	3.807509000	1.370233000	0.627696000	7	-3.552400000	0.190473000	0.556495000
6	2.616170000	1.613115000	-0.149680000	6	-3.612282000	-1.195831000	0.584269000
7	2.110542000	0.481001000	-0.772354000	6	-4.877280000	-1.735390000	0.147988000
6	2.635551000	-0.790855000	-0.709098000	6	-5.877128000	-0.923591000	-0.236890000
7	3.770751000	-0.927725000	0.050199000	7	-5.723840000	0.443443000	-0.240499000
1	4.283866000	2.197704000	1.154272000	8	-2.647554000	-1.853562000	0.967546000
1	5.231405000	-0.019199000	1.313561000	8	-4.394059000	2.254302000	0.168257000
8	2.051062000	2.697264000	-0.274110000	1	-2.668503000	0.623229000	0.861804000

1	1.258035000	0.603336000	-1.337734000	1	-5.024528000	-2.814275000	0.130762000
8	2.112542000	-1.718585000	-1.305570000	1	-6.826451000	-1.356897000	-0.552106000
6	4.361908000	-2.264467000	0.179124000	6	-6.810192000	1.338116000	-0.654611000
1	4.189089000	-2.664476000	1.178237000	1	-7.150597000	1.940667000	0.187504000
1	5.433328000	-2.212338000	-0.014373000	1	-7.633845000	0.730544000	-1.029512000
1	3.883496000	-2.913427000	-0.554411000	1	-6.460256000	2.011188000	-1.437311000
7	-2.114049000	0.476995000	0.770093000	7	3.548851000	0.195284000	-0.560196000
6	-2.639274000	-0.794023000	0.699828000	6	4.552733000	1.051326000	-0.165608000
7	-3.774496000	-0.927073000	-0.060211000	7	5.720627000	0.452755000	0.236666000
6	-4.340362000	0.142647000	-0.715178000	6	5.875203000	-0.914573000	0.233900000
6	-3.810840000	1.374038000	-0.625005000	6	4.877187000	-1.727656000	-0.150431000
6	-2.619822000	1.612476000	0.153287000	6	3.611428000	-1.190694000	-0.587054000
1	-1.261572000	0.596419000	1.336083000	8	2.647864000	-1.850285000	-0.969902000
8	-2.054758000	2.695922000	0.283432000	1	6.824700000	-1.346108000	0.549372000
1	-4.286786000	2.203723000	-1.146706000	8	4.388002000	2.261299000	-0.173256000
1	-5.234694000	-0.011683000	-1.318205000	1	2.664499000	0.626409000	-0.865774000
8	-2.116105000	-1.725368000	1.291537000	1	5.025514000	-2.806893000	-0.132536000
6	-4.338228000	-2.277610000	-0.160459000	6	6.827537000	1.309912000	0.675986000
1	-3.642843000	-2.944038000	-0.670768000	1	7.710955000	1.122958000	0.065477000
1	-4.526482000	-2.677310000	0.835985000	1	7.059645000	1.118514000	1.723646000
1	-5.272343000	-2.221259000	-0.719344000	1	6.511936000	2.346380000	0.556695000

Table S20. RNA inter-strand dimer geometries with hydrogens.

5'A_3' 3'_A5'				5'_A3' 3'_A_5'			
6	-1.072461000	-1.097051000	1.841578000	6	2.848036000	1.896744000	-0.551425000
7	-2.016854000	-1.761959000	1.194474000	7	2.082612000	0.872603000	-0.939024000
6	-2.694811000	-0.931348000	0.386926000	6	2.542527000	-0.378423000	-0.786867000
7	-3.748477000	-1.268697000	-0.429605000	6	3.824136000	-0.539918000	-0.230748000
6	-4.121106000	-0.112405000	-1.051802000	6	4.486082000	0.607793000	0.105008000
7	-3.407702000	0.917657000	-0.709440000	7	4.061729000	1.874759000	-0.023041000
6	-2.504003000	0.410037000	0.206858000	7	1.770446000	-1.414476000	-1.165149000
6	-1.464789000	0.995680000	0.951793000	1	0.837704000	-1.241951000	-1.567478000
7	-0.756947000	0.199026000	1.766679000	1	2.112539000	-2.379751000	-1.052355000
1	-4.940601000	-0.058648000	-1.768423000	7	4.592496000	-1.653928000	0.056581000
7	-1.158415000	2.304792000	0.881311000	6	5.683684000	-1.162116000	0.561175000
1	-0.386840000	2.684599000	1.448817000	1	2.413321000	2.886729000	-0.689687000
1	-1.695532000	2.926614000	0.259740000	7	5.693409000	0.201380000	0.622622000
1	-0.468825000	-1.688403000	2.530117000	1	6.513664000	-1.780031000	0.903699000
1	-4.145396000	-2.189258000	-0.530199000	1	6.420167000	0.806855000	0.969494000
7	0.756710000	0.199204000	-1.767015000	7	-2.082170000	0.872933000	0.939050000
6	1.072747000	-1.097323000	-1.841155000	6	-2.848087000	1.896755000	0.551370000
7	2.016780000	-1.762376000	-1.194539000	7	-4.062087000	1.875060000	0.022952000
6	2.694933000	-0.931704000	-0.386737000	6	-4.485952000	0.607382000	-0.105009000
7	3.748496000	-1.268676000	0.429661000	6	-2.542461000	-0.378125000	0.786884000
6	4.121118000	-0.112446000	1.051820000	6	-3.824018000	-0.539709000	0.230774000
7	3.407705000	0.917815000	0.709422000	7	-5.693120000	0.200874000	-0.622595000
6	2.503867000	0.410315000	-0.207056000	6	-5.683843000	-1.161752000	-0.561163000
6	1.464787000	0.996113000	-0.951818000	7	-4.592605000	-1.653741000	-0.056551000
7	1.158426000	2.304884000	-0.881348000	1	-6.513768000	-1.779838000	-0.903665000
1	0.387086000	2.683880000	-1.448536000	7	-1.770880000	-1.414754000	1.165136000
1	1.695539000	2.926346000	-0.259794000	1	-2.412977000	2.886733000	0.689651000
1	0.469105000	-1.688810000	-2.529689000	1	-2.112336000	-2.379723000	1.052439000
1	4.940327000	-0.057963000	1.768040000	1	-0.838037000	-1.242360000	1.567472000
1	4.145385000	-2.189247000	0.530282000	1	-6.419700000	0.806580000	-0.969435000
5'_A3' 3'_C_5'				5'A_3' 3'_C5'			
6	-1.104578000	-0.915637000	1.693998000	6	-2.465609000	-0.196205000	0.710294000
7	-2.094431000	-1.612058000	1.158465000	7	-2.055048000	1.080884000	0.725137000
6	-2.786049000	-0.845286000	0.300458000	6	-2.868735000	2.029373000	0.252637000
7	-3.884200000	-1.228924000	-0.432303000	7	-4.089594000	1.906061000	-0.244373000
6	-4.253574000	-0.129401000	-1.151612000	6	-4.463547000	0.616978000	-0.234397000
7	-3.498043000	0.907103000	-0.945544000	6	-3.749054000	-0.463683000	0.201280000
6	-2.567475000	0.465530000	-0.021712000	7	-5.662014000	0.112886000	-0.681952000
6	-1.480377000	1.089947000	0.615342000	6	-5.595015000	-1.235810000	-0.483147000
7	-0.757639000	0.356557000	1.476021000	7	-4.475777000	-1.630451000	0.044820000
7	-1.142605000	2.374985000	0.400187000	1	-6.404715000	-1.917493000	-0.743344000
1	-0.336465000	2.784381000	0.892974000	1	-2.472832000	3.044577000	0.280608000
1	-1.690531000	2.947853000	-0.257560000	7	-1.644946000	-1.157220000	1.174587000
1	-5.102674000	-0.121049000	-1.834257000	1	-0.713176000	-0.908138000	1.537086000
1	-0.486375000	-1.454094000	2.412476000	1	-1.948890000	-2.141636000	1.167441000
1	-4.309744000	-2.142113000	-0.422554000	1	-6.419099000	0.650880000	-1.072441000
7	2.013508000	-0.052015000	-1.000987000	7	3.567324000	0.306197000	-0.574700000
6	2.543742000	-1.279330000	-0.742724000	6	3.750901000	-1.013102000	-0.438389000
7	3.641342000	-1.377098000	0.103609000	6	4.542872000	1.180950000	-0.204669000
6	4.190260000	-0.257391000	0.669434000	7	5.734996000	0.685885000	0.309738000

6	3.684337000	0.972343000	0.425632000	6	4.976620000	-1.549825000	0.093363000
6	2.546084000	1.046595000	-0.453187000	6	5.930365000	-0.661886000	0.449951000
7	1.997001000	2.216063000	-0.727685000	8	4.410788000	2.405969000	-0.316796000
1	1.178597000	2.267124000	-1.350834000	1	5.127385000	-2.624002000	0.203605000
1	2.387955000	3.076478000	-0.318780000	1	6.874266000	-1.025409000	0.857368000
1	4.118136000	1.866338000	0.873341000	7	2.779447000	-1.825478000	-0.814135000
1	5.051944000	-0.360033000	1.328862000	1	1.906986000	-1.439228000	-1.200870000
8	2.078412000	-2.317276000	-1.229094000	1	2.895950000	-2.844177000	-0.719624000
1	4.003108000	-2.303207000	0.272965000	1	6.434309000	1.364790000	0.569132000
5' _A3' 3'G_5'				5' A_3' 3' _G5'			
6	1.075345000	-0.517049000	2.167490000	6	2.684153000	-0.577740000	-0.760110000
7	0.777513000	-1.477802000	1.287371000	7	2.181029000	0.636151000	-1.030430000
6	1.488915000	-1.564336000	0.152735000	6	2.907113000	1.718992000	-0.738490000
6	2.511820000	-0.620888000	-0.049964000	7	4.117474000	1.790321000	-0.206826000
7	3.413719000	-0.416031000	-1.079054000	6	4.585777000	0.557030000	0.040885000
6	4.108567000	0.610066000	-0.689260000	6	3.967169000	-0.640174000	-0.187534000
7	3.725394000	1.102687000	0.524536000	7	1.951780000	-1.671797000	-1.041675000
6	2.685098000	0.305893000	0.940417000	7	4.772818000	-1.693971000	0.205396000
7	2.003049000	0.423744000	2.090795000	6	5.842640000	-1.118081000	0.664761000
7	1.200971000	-2.536709000	-0.732298000	7	5.803508000	0.244634000	0.597911000
1	0.440969000	-3.202967000	-0.535320000	1	6.691887000	-1.670901000	1.066232000
1	1.740823000	-2.613443000	-1.606200000	1	2.327250000	-2.609311000	-0.837725000
1	0.470084000	-0.507134000	3.074068000	1	1.016045000	-1.571421000	-1.461156000
1	4.921255000	1.036609000	-1.276322000	1	2.438363000	2.675369000	-0.970387000
1	4.107793000	1.885086000	1.031210000	1	6.506088000	0.905715000	0.888511000
7	-0.781420000	0.803125000	-1.420514000	7	-2.018650000	0.723322000	0.798368000
6	-1.093477000	1.902271000	-0.632914000	6	-2.361283000	-0.638969000	0.809718000
7	-2.063896000	1.909026000	0.266233000	6	-3.649162000	-0.849767000	0.261200000
6	-2.705266000	0.708536000	0.328390000	6	-4.371810000	0.222637000	-0.194321000
7	-3.761785000	0.425581000	1.177711000	7	-4.029856000	1.541925000	-0.201876000
6	-4.093809000	-0.884412000	0.903515000	6	-2.829744000	1.742185000	0.316947000
7	-3.357641000	-1.441043000	-0.026102000	7	-4.363180000	-2.035386000	0.081066000
6	-2.469759000	-0.430820000	-0.396503000	6	-5.483966000	-1.642935000	-0.471661000
6	-1.436630000	-0.437855000	-1.365143000	7	-5.567752000	-0.282270000	-0.675069000
1	-4.898799000	-1.410812000	1.415818000	1	-6.282524000	-2.333358000	-0.746928000
1	-0.011345000	0.905718000	-2.096677000	7	-2.311283000	2.968406000	0.399415000
8	-1.071890000	-1.354461000	-2.104569000	8	-1.569288000	-1.463009000	1.271306000
7	-0.345769000	2.985705000	-0.846867000	1	-1.097170000	0.985686000	1.175363000
1	-0.514660000	3.844005000	-0.302065000	1	-2.850100000	3.778174000	0.063218000
1	0.399969000	2.964628000	-1.556311000	1	-1.372178000	3.103661000	0.799063000
1	-4.176738000	1.057591000	1.843104000	1	-6.319903000	0.252053000	-1.078974000
5' _A3' 3'U_5'				5' A_3' 3' _U5'			
7	-3.886614000	-1.228707000	-0.404943000	7	-4.099738000	1.897760000	-0.218655000
6	-2.788203000	-0.828596000	0.318562000	6	-4.473776000	0.608698000	-0.228179000
7	-2.094116000	-1.576880000	1.190781000	6	-2.878867000	2.013458000	0.280159000
6	-1.104815000	-0.868175000	1.711000000	6	-3.759351000	-0.478478000	0.191095000
7	-0.760423000	0.400022000	1.467225000	6	-2.475886000	-0.218814000	0.704090000
6	-1.485574000	1.114822000	0.593041000	7	-2.065242000	1.057878000	0.738251000
6	-2.572380000	0.475911000	-0.029987000	7	-4.486149000	-1.642699000	0.017005000
7	-3.504923000	0.897329000	-0.961213000	6	-5.605364000	-1.240043000	-0.504925000
6	-4.258872000	-0.144405000	-1.145558000	7	-5.672276000	0.111510000	-0.683305000
1	-0.484730000	-1.391103000	2.439258000	1	-2.482899000	3.028098000	0.323483000
1	-5.108864000	-0.151167000	-1.827108000	7	-1.655283000	-1.186797000	1.153786000

7	-1.150368000	2.395902000	0.351842000	1	-0.723496000	-0.943288000	1.520007000
1	-0.344324000	2.816463000	0.835294000	1	-1.959292000	-2.170972000	1.131750000
1	-1.700161000	2.954568000	-0.316477000	1	-6.415109000	-1.917659000	-0.775402000
1	-4.310518000	-2.142264000	-0.376412000	1	-6.429328000	0.655399000	-1.065606000
7	2.061066000	-0.027788000	-0.957455000	7	3.608039000	0.249850000	-0.553943000
6	2.550181000	-1.290750000	-0.708499000	6	3.727252000	-1.129632000	-0.459024000
7	3.639865000	-1.352953000	0.123852000	6	4.990549000	-1.571743000	0.079772000
6	4.196534000	-0.223288000	0.678344000	6	5.935191000	-0.685269000	0.438466000
6	3.703203000	0.998041000	0.414092000	7	5.724774000	0.668702000	0.316883000
6	2.561396000	1.163706000	-0.451902000	6	4.555311000	1.179421000	-0.188480000
1	5.053540000	-0.320933000	1.344151000	1	6.885032000	-1.046340000	0.833127000
1	4.171225000	1.875177000	0.859806000	1	5.181833000	-2.637416000	0.196910000
8	2.031039000	2.234054000	-0.740290000	1	2.723018000	0.614218000	-0.935699000
1	1.243015000	0.038858000	-1.580092000	8	4.342203000	2.375577000	-0.307366000
8	2.036210000	-2.276289000	-1.214243000	8	2.811122000	-1.861001000	-0.827831000
1	4.002590000	-2.273799000	0.312663000	1	6.424412000	1.342345000	0.585004000
5' _C3' 3'C_5'				5'C_3' 3'_C5'			
6	-2.599179000	1.139283000	0.152654000	6	4.535019000	1.264473000	-0.012762000
6	-3.774614000	1.007229000	-0.668546000	7	3.518771000	0.472292000	-0.453030000
6	-4.318004000	-0.226846000	-0.765660000	6	3.647367000	-0.859672000	-0.453033000
7	-3.771363000	-1.298035000	-0.110718000	6	4.854964000	-1.498398000	0.002153000
6	-2.637362000	-1.144782000	0.677394000	6	5.850599000	-0.690542000	0.430785000
7	-2.069137000	0.087695000	0.788174000	7	5.711125000	0.671719000	0.429940000
1	-5.208642000	-0.372400000	-1.376772000	7	2.637996000	-1.589265000	-0.892766000
1	-4.206431000	1.862777000	-1.187607000	1	1.777461000	-1.130943000	-1.224618000
7	-2.012757000	2.315363000	0.284724000	1	2.711829000	-2.616302000	-0.903055000
1	-1.168038000	2.407117000	0.866735000	1	4.961262000	-2.583088000	0.001414000
1	-2.400914000	3.140282000	-0.194029000	1	6.782460000	-1.131660000	0.784244000
8	-2.175690000	-2.140437000	1.248313000	8	4.453986000	2.498840000	0.000978000
1	-4.191659000	-2.300134000	-0.175185000	1	6.441578000	1.291798000	0.744860000
6	2.637280000	-1.144945000	-0.677554000	6	-3.647470000	-0.860037000	0.453036000
7	3.771441000	-1.298012000	0.110736000	7	-3.518685000	0.472722000	0.453032000
6	4.317956000	-0.226598000	0.765593000	6	-4.534980000	1.264623000	0.012750000
6	3.774729000	1.007211000	0.668740000	7	-5.710967000	0.671375000	-0.429935000
6	2.598969000	1.139715000	-0.152831000	6	-5.850366000	-0.690566000	-0.430758000
7	2.069145000	0.087302000	-0.788158000	6	-4.855452000	-1.497832000	-0.002173000
1	5.208504000	-0.371843000	1.376591000	1	-6.782705000	-1.132010000	-0.784249000
1	4.206706000	1.862946000	1.188041000	1	-4.961594000	-2.582946000	-0.001410000
7	2.012439000	2.315718000	-0.284959000	7	-2.637857000	-1.589527000	0.892796000
1	1.167945000	2.407485000	-0.866698000	1	-2.711949000	-2.616493000	0.903078000
1	2.400950000	3.140682000	0.194259000	1	-1.778103000	-1.130526000	1.224582000
8	2.176021000	-2.140651000	-1.248050000	8	-4.453908000	2.499097000	-0.001000000
1	4.191921000	-2.300032000	0.175220000	1	-6.441628000	1.291171000	-0.744930000
5' _C3' 3'G_5'				5'C_3' 3'_G5'			
6	2.563283000	1.281696000	-0.229453000	6	4.639060000	1.093716000	-0.253167000
6	3.692525000	0.921724000	0.589192000	7	5.847658000	0.664576000	0.281336000
6	4.180427000	-0.330186000	0.442793000	6	6.092312000	-0.668633000	0.476050000
7	3.622833000	-1.211857000	-0.444444000	6	5.171916000	-1.605422000	0.155204000
6	2.534362000	-0.840852000	-1.224658000	6	3.928635000	-1.135172000	-0.398487000
7	2.022188000	0.413651000	-1.092961000	7	3.697155000	0.169121000	-0.587966000
1	5.034468000	-0.644293000	1.042326000	1	7.047645000	-0.980109000	0.898189000
1	4.133538000	1.626921000	1.294011000	1	5.362009000	-2.667553000	0.308796000
7	2.031504000	2.486707000	-0.131391000	7	2.988721000	-1.997371000	-0.741520000

1	1.219890000	2.740177000	-0.711946000	1	3.142193000	-3.006534000	-0.605873000
1	2.429792000	3.172420000	0.526119000	1	2.102675000	-1.660195000	-1.143939000
8	2.060913000	-1.670525000	-2.010244000	8	4.462258000	2.307408000	-0.414758000
1	3.971442000	-2.150154000	-0.568150000	1	6.580348000	1.304382000	0.547882000
7	-0.777579000	0.006334000	1.382221000	6	-2.842874000	1.808185000	0.134966000
6	-1.447352000	1.096380000	0.802910000	7	-1.981102000	0.846821000	0.645700000
6	-2.530152000	0.665566000	-0.001832000	6	-2.268400000	-0.525578000	0.731368000
7	-3.446586000	1.410446000	-0.744386000	6	-3.558537000	-0.813365000	0.224747000
6	-4.225218000	0.503368000	-1.280025000	6	-4.333537000	0.206167000	-0.264843000
7	-3.894895000	-0.793021000	-0.945708000	7	-4.045104000	1.535811000	-0.344617000
6	-2.792109000	-0.675065000	-0.116496000	7	-4.228146000	-2.033415000	0.119535000
7	-2.136207000	-1.725756000	0.451164000	6	-5.375690000	-1.712836000	-0.424576000
6	-1.119699000	-1.325821000	1.197480000	7	-5.518525000	-0.368202000	-0.691721000
1	-5.061478000	0.751587000	-1.933181000	1	-6.151736000	-2.446677000	-0.646791000
1	0.028190000	0.210574000	1.990300000	8	-1.433970000	-1.294233000	1.213299000
7	-0.350770000	-2.204883000	1.841432000	1	-1.062827000	1.163284000	0.987328000
1	-0.539532000	-3.214359000	1.755745000	7	-2.372400000	3.056291000	0.145372000
1	0.431202000	-1.875001000	2.424164000	1	-1.430914000	3.247704000	0.515367000
8	-1.053321000	2.243266000	1.025042000	1	-2.950583000	3.826788000	-0.216726000
1	-4.338053000	-1.652024000	-1.228719000	1	-6.300233000	0.115717000	-1.102970000
5'_C3' 3'_U_5'				5'_C_3' 3'_U5'			
7	3.774506000	-1.288565000	0.099794000	6	-4.547019000	1.251500000	0.025952000
6	4.323301000	-0.221862000	0.760409000	7	-3.530739000	0.453201000	0.454957000
6	3.781861000	1.013320000	0.671369000	6	-3.659257000	-0.878637000	0.436028000
6	2.605494000	1.152451000	-0.148235000	6	-4.866801000	-1.510900000	-0.028232000
7	2.073438000	0.104606000	-0.789226000	6	-5.862468000	-0.697093000	-0.445377000
6	2.639803000	-1.129134000	-0.686450000	7	-5.723074000	0.665029000	-0.425170000
7	2.020629000	2.330102000	-0.272848000	8	-4.466057000	2.485943000	0.029758000
1	1.175703000	2.426579000	-0.853195000	7	-2.649860000	-1.614345000	0.865385000
1	2.410870000	3.151635000	0.210835000	1	-1.789363000	-1.160735000	1.203748000
1	4.215656000	1.865322000	1.195273000	1	-2.723634000	-2.641429000	0.861077000
1	5.214229000	-0.372059000	1.369653000	1	-4.973035000	-2.595495000	-0.042911000
8	2.176461000	-2.120758000	-1.262343000	1	-6.794289000	-1.133196000	-0.805103000
1	4.162728000	-2.217873000	0.153681000	1	-6.453552000	1.289477000	-0.731274000
6	-2.643622000	-1.146960000	0.661825000	7	3.555675000	0.410485000	-0.437710000
7	-3.768504000	-1.275823000	-0.114143000	6	4.545942000	1.259270000	0.002659000
6	-4.323707000	-0.203145000	-0.773383000	7	5.698989000	0.653128000	0.435027000
6	-3.793612000	1.027128000	-0.672008000	6	5.853430000	-0.713671000	0.417598000
6	-2.613031000	1.261234000	0.123314000	6	4.867701000	-1.520399000	-0.011788000
1	-5.209910000	-0.354162000	-1.389117000	6	3.617587000	-0.975278000	-0.482686000
7	-2.117490000	0.123009000	0.743362000	1	6.792015000	-1.150978000	0.758406000
1	-4.261096000	1.859208000	-1.197531000	1	5.015171000	-2.599367000	-0.004603000
1	-1.272684000	0.239306000	1.321377000	8	2.666777000	-1.627963000	-0.907159000
8	-2.048170000	2.343380000	0.264672000	1	2.682148000	0.847128000	-0.766434000
8	-2.130035000	-2.080996000	1.257671000	8	4.382168000	2.469019000	0.007096000
1	-4.158519000	-2.202456000	-0.180592000	1	6.429812000	1.267362000	0.757195000
5'_G3' 3'_G_5'				5'_G_3' 3'_G5'			
7	-0.801910000	-1.772834000	0.392393000	6	-3.796196000	-0.938090000	0.197644000
6	-1.462077000	-0.936078000	1.306879000	6	-2.506918000	-0.825643000	0.771280000
6	-2.477998000	-0.181694000	0.672271000	7	-2.116962000	0.518649000	0.890329000
7	-3.364690000	0.755201000	1.205695000	6	-2.887569000	1.606401000	0.502151000
6	-4.081714000	1.127746000	0.174763000	7	-4.089047000	1.498531000	-0.040403000
7	-3.738960000	0.505691000	-1.007104000	6	-4.476790000	0.197356000	-0.159176000

6	-2.695885000	-0.341109000	-0.671372000	7	-5.685063000	-0.217345000	-0.692492000
7	-2.050052000	-1.157015000	-1.551338000	7	-4.549361000	-2.075423000	-0.097620000
6	-1.095219000	-1.857822000	-0.961360000	6	-5.650608000	-1.593212000	-0.617634000
1	-4.880509000	1.866223000	0.245387000	1	-6.470128000	-2.225914000	-0.961477000
1	-0.042918000	-2.368737000	0.753687000	8	-1.748428000	-1.717017000	1.157946000
7	-0.346126000	-2.718074000	-1.652437000	1	-1.190454000	0.711532000	1.295868000
1	0.387599000	-3.261346000	-1.175204000	7	-2.327512000	2.800253000	0.702838000
1	-0.501211000	-2.840044000	-2.663960000	1	-1.388026000	2.863913000	1.119065000
8	-1.114516000	-0.929992000	2.489751000	1	-2.834651000	3.656651000	0.441177000
1	-4.139588000	0.623563000	-1.923605000	1	-6.414359000	0.378942000	-1.048779000
6	1.461945000	0.935792000	1.307250000	6	2.506529000	-0.825568000	-0.771292000
7	0.801906000	1.772696000	0.392735000	6	3.796407000	-0.938404000	-0.197576000
6	1.095201000	1.858202000	-0.960957000	6	4.476304000	0.197193000	0.159109000
7	2.050020000	1.157634000	-1.550662000	7	4.089093000	1.498101000	0.040345000
6	2.695913000	0.341318000	-0.671545000	6	2.887357000	1.606034000	-0.502245000
7	3.739045000	-0.505444000	-1.006973000	7	2.117442000	0.518622000	-0.890290000
6	4.081927000	-1.128117000	0.174643000	7	5.685307000	-0.216830000	0.692533000
7	3.364450000	-0.755295000	1.205274000	7	2.327418000	2.799705000	-0.702969000
6	2.478271000	0.181052000	0.672335000	1	2.835131000	3.657468000	-0.441273000
1	0.043058000	2.368258000	0.753560000	1	1.388013000	2.864204000	-1.119189000
1	4.880501000	-1.866300000	0.244820000	6	5.651035000	-1.593326000	0.617756000
7	0.346145000	2.718653000	-1.651762000	7	4.549433000	-2.074994000	0.097718000
8	1.114286000	0.929416000	2.490062000	1	6.469453000	-2.225465000	0.961489000
1	0.501601000	2.840457000	-2.663203000	8	1.748072000	-1.717317000	-1.157916000
1	-0.387212000	3.261216000	-1.174594000	1	1.190784000	0.712421000	-1.295857000
1	4.139547000	-0.622921000	-1.923580000	1	6.414540000	0.379595000	1.048717000
		5' _G3'				5'G_3'	
		3'U_5'				3'_U5'	
6	1.453143000	1.103103000	-0.812199000	7	-4.237919000	-2.044506000	0.096657000
6	2.535078000	0.673886000	-0.006528000	6	-3.567856000	-0.826607000	0.214225000
6	2.794226000	-0.666364000	0.115286000	6	-4.341693000	0.198333000	-0.265085000
7	2.135531000	-1.719003000	-0.446149000	7	-5.527700000	-0.370612000	-0.697906000
6	1.119381000	-1.320110000	-1.193969000	6	-5.385609000	-1.718556000	-0.444207000
7	0.780236000	0.011877000	-1.385514000	6	-2.277044000	-0.544035000	0.723761000
1	-0.025678000	0.215425000	-1.994427000	7	-1.989991000	0.828853000	0.651827000
7	3.454350000	1.420829000	0.732086000	6	-2.850595000	1.795391000	0.150851000
6	4.230772000	0.514179000	1.271427000	7	-4.053179000	1.528275000	-0.331501000
7	3.897300000	-0.783155000	0.944370000	8	-1.442980000	-1.318222000	1.198023000
1	5.068322000	0.764119000	1.922921000	1	-1.071513000	1.142395000	0.996541000
8	1.061747000	2.249816000	-1.039974000	7	-2.379671000	3.042939000	0.173821000
7	0.347877000	-2.200715000	-1.832780000	1	-1.438264000	3.231048000	0.545635000
1	-0.434152000	-1.871943000	-2.417232000	1	-2.958175000	3.818577000	-0.180770000
1	0.533932000	-3.210330000	-1.742396000	1	-6.160911000	-2.449144000	-0.673784000
1	4.338758000	-1.641618000	1.231647000	1	-6.309121000	0.117896000	-1.104246000
7	-2.069476000	0.446290000	1.036075000	6	6.098166000	-0.692163000	0.469287000
6	-2.540849000	-0.834450000	1.219918000	7	5.838976000	0.646318000	0.286034000
7	-3.621781000	-1.186335000	0.450599000	6	4.653009000	1.090599000	-0.243085000
6	-4.186856000	-0.314231000	-0.451405000	7	3.741090000	0.111488000	-0.566715000
6	-3.710907000	0.932418000	-0.606930000	6	3.910134000	-1.256997000	-0.409019000
6	-2.579433000	1.393812000	0.159879000	6	5.187294000	-1.627848000	0.150460000
1	-4.185309000	1.603989000	-1.321780000	1	5.416896000	-2.679421000	0.316137000
1	-1.258218000	0.728522000	1.604871000	1	7.059498000	-1.000082000	0.880813000
8	-2.019756000	-1.587545000	2.027717000	1	2.844382000	0.425647000	-0.965443000
1	-5.036281000	-0.640640000	-1.050759000	8	3.022141000	-2.037260000	-0.744980000
8	-2.064858000	2.506706000	0.077609000	8	4.396858000	2.271558000	-0.416464000

1	-3.974028000	-2.121311000	0.580671000	1	6.512976000	1.356491000	0.523848000
		5' _U3'				5' _U_3'	
		3' _U_5'				3' _U5'	
7	2.121957000	0.141309000	-0.744310000	6	1.266471000	1.256578000	0.584116000
6	2.619633000	1.275116000	-0.118316000	6	0.791115000	0.084486000	1.278975000
6	3.801018000	1.034380000	0.674759000	6	1.449625000	-1.082419000	1.191213000
6	4.328874000	-0.196770000	0.767725000	7	2.602633000	-1.198064000	0.448955000
7	3.771617000	-1.265123000	0.103018000	6	3.125923000	-0.137401000	-0.247539000
6	2.646138000	-1.130347000	-0.670981000	7	2.427828000	1.045573000	-0.145124000
1	1.276689000	0.262086000	-1.320785000	1	1.062892000	-1.955572000	1.717967000
8	2.056134000	2.358901000	-0.252817000	1	-0.114507000	0.147851000	1.882909000
1	5.216118000	-0.353137000	1.382362000	8	0.727291000	2.360865000	0.590939000
1	4.270646000	1.863285000	1.205108000	1	2.805457000	1.853216000	-0.661357000
8	2.130750000	-2.059701000	-1.271545000	8	4.146343000	-0.211016000	-0.913365000
1	4.160476000	-2.192634000	0.163753000	1	3.032317000	-2.109300000	0.434885000
7	-2.121859000	0.141250000	0.744431000	7	-1.469974000	0.113362000	-1.023727000
6	-2.646134000	-1.129978000	0.670925000	6	-1.390856000	-1.230537000	-0.733966000
7	-3.771622000	-1.265122000	-0.103091000	7	-2.263297000	-1.684709000	0.223460000
6	-4.329149000	-0.197193000	-0.768055000	6	-3.163168000	-0.847868000	0.842666000
6	-3.800829000	1.034461000	-0.674483000	6	-3.215458000	0.461248000	0.545460000
6	-2.619782000	1.275045000	0.118210000	6	-2.335792000	1.030969000	-0.445863000
1	-5.215758000	-0.353184000	-1.381961000	1	-3.846118000	-1.254371000	1.588067000
1	-4.270130000	1.862719000	-1.204406000	1	-3.931795000	1.101314000	1.059512000
8	-2.056430000	2.358863000	0.252600000	8	-2.318798000	2.208924000	-0.795464000
1	-1.276631000	0.262235000	1.320866000	1	-0.822821000	0.472676000	-1.740254000
8	-2.130500000	-2.059705000	1.271724000	8	-0.582312000	-1.950246000	-1.299215000
1	-4.160289000	-2.192724000	-0.163674000	1	-2.213109000	-2.667489000	0.439797000

Table S21. DNA monomer geometries with methyls.

A				C			
6	0.000000000	0.000000000	0.000000000	7	0.000000000	0.000000000	0.000000000
7	0.000000000	0.000000000	1.341221000	6	0.000000000	0.000000000	1.356121000
6	1.163683000	0.000000000	1.984372000	7	1.221571000	0.000000000	2.025896000
7	2.387107000	0.005668000	1.499817000	6	2.392418000	0.005277000	1.338404000
6	2.354173000	0.007209000	0.154351000	6	2.415501000	0.003044000	-0.021742000
6	1.251605000	-0.000804000	-0.649967000	6	1.149889000	0.007398000	-0.686377000
7	1.608534000	0.008938000	-1.986677000	7	1.090613000	0.012272000	-2.008993000
6	2.907946000	0.005799000	-1.960973000	1	0.177590000	0.010410000	-2.483447000
7	3.431396000	0.008566000	-0.696493000	1	1.958907000	0.017629000	-2.562074000
7	-1.169624000	-0.001271000	-0.661125000	1	3.353272000	-0.001707000	-0.576984000
1	-2.056441000	-0.000995000	-0.138036000	8	-1.045191000	-0.007242000	2.018242000
1	-1.178593000	-0.002918000	-1.691165000	1	3.332902000	0.011565000	1.888372000
1	3.522855000	0.001507000	-2.861563000	6	1.185044000	-0.000158000	3.488685000
1	1.094243000	-0.005701000	3.071891000	1	2.202836000	-0.000881000	3.879306000
6	4.830410000	0.008911000	-0.295497000	1	0.646512000	-0.880386000	3.840349000
1	4.856559000	0.011266000	0.795231000	1	0.647827000	0.880784000	3.840572000
1	5.340034000	0.898503000	-0.668707000				
1	5.339312000	-0.882815000	-0.664578000				
G				T			
7	0.000000000	0.000000000	0.000000000	6	-1.214692000	-0.759953000	-0.006379000
6	0.000000000	0.000000000	1.308158000	7	0.016270000	-1.385091000	-0.000448000
7	1.258675000	0.000000000	1.871004000	6	1.248163000	-0.772558000	0.003697000
6	2.132417000	-0.004539000	0.806758000	6	1.191805000	0.668999000	0.001602000
6	1.355459000	-0.003881000	-0.337491000	6	0.009131000	1.314120000	-0.011095000
6	1.980206000	-0.008232000	-1.605284000	7	-1.174245000	0.618513000	-0.012622000
7	3.381157000	-0.008431000	-1.488253000	8	-2.258073000	-1.388727000	-0.007496000
6	4.076213000	0.001391000	-0.295421000	1	0.011794000	-2.414918000	0.000776000
7	3.488035000	-0.002194000	0.897742000	8	2.288388000	-1.442961000	0.010194000
7	5.409464000	0.004357000	-0.391114000	6	2.512833000	1.378979000	-0.001983000
1	5.859581000	-0.000225000	-1.317227000	1	3.317613000	0.649816000	-0.098019000
1	5.986551000	0.011125000	0.462265000	1	2.632130000	1.930121000	0.930382000
1	3.930532000	-0.016651000	-2.358656000	1	2.550252000	2.072471000	-0.841998000
8	1.465878000	-0.009880000	-2.723641000	1	-0.007787000	2.403508000	-0.020730000
1	-0.914929000	0.000424000	1.900904000	6	-2.461878000	1.320833000	0.016919000
6	1.616852000	0.043226000	3.278627000	1	-3.193913000	0.766131000	-0.569777000
1	2.525237000	-0.536755000	3.447676000	1	-2.818696000	1.386150000	1.044632000
1	1.797193000	1.075064000	3.583433000	1	-2.340254000	2.323750000	-0.391913000
1	0.807331000	-0.373196000	3.879783000				

Table S22. DNA monomer geometries with hydrogens.

A				C			
6	-1.231894000	-0.603278000	0.000391000	6	-1.177421000	-0.495416000	-0.001685000
7	-1.924864000	0.545053000	-0.000616000	7	0.066255000	-1.036083000	0.002050000
6	-1.260837000	1.696950000	0.001267000	6	1.154186000	-0.255178000	-0.000942000
7	0.037003000	1.914192000	-0.001549000	6	1.049220000	1.170476000	0.004351000
6	0.703972000	0.745211000	-0.002148000	6	-0.207342000	1.691581000	-0.001679000
6	0.175524000	-0.513102000	0.004227000	7	-1.304642000	0.891901000	-0.000857000
7	1.171780000	-1.473152000	-0.003786000	7	2.343518000	-0.836843000	-0.002303000
6	2.271025000	-0.779778000	0.001976000	1	2.414620000	-1.863325000	-0.001131000
7	2.065880000	0.573302000	-0.000676000	1	3.196930000	-0.261043000	-0.004237000
7	-1.891723000	-1.773635000	-0.000220000	1	1.932279000	1.809122000	0.012681000
1	-1.367214000	-2.660173000	0.002181000	1	-0.336733000	2.773357000	-0.007425000
1	-2.921264000	-1.783967000	-0.002692000	8	-2.201363000	-1.189975000	0.001448000
1	-1.882192000	2.592186000	0.006011000	1	-2.243969000	1.260085000	-0.003972000
1	3.262799000	-1.233144000	0.008194000				
1	2.754587000	1.308753000	-0.000044000				
G				T			
7	2.204753000	0.711868000	-0.004781000	6	-1.214692000	-0.759953000	-0.006379000
6	0.823904000	0.503237000	-0.000325000	7	0.016270000	-1.385091000	-0.000448000
6	-0.239683000	1.433980000	0.001463000	6	1.248163000	-0.772558000	0.003697000
7	-1.488129000	0.787441000	0.003441000	6	1.191805000	0.668999000	0.001602000
6	-1.672067000	-0.580077000	-0.002561000	6	0.009131000	1.314120000	-0.011095000
7	-0.671352000	-1.456643000	0.003471000	7	-1.174245000	0.618513000	-0.012622000
6	0.545865000	-0.852034000	0.004075000	8	-2.258073000	-1.388727000	-0.007496000
7	1.761209000	-1.499486000	0.001306000	1	0.011794000	-2.414918000	0.000776000
6	2.707231000	-0.495862000	-0.001467000	8	2.288388000	-1.442961000	0.010194000
1	3.779337000	-0.692160000	-0.001342000	6	2.512833000	1.378979000	-0.001983000
8	-0.194240000	2.664007000	-0.000288000	1	3.317613000	0.649816000	-0.098019000
1	-2.330541000	1.380656000	0.010147000	1	2.632130000	1.930121000	0.930382000
7	-2.939695000	-1.003925000	-0.004356000	1	2.550252000	2.072471000	-0.841998000
1	-3.711487000	-0.321121000	-0.001575000	1	-0.007787000	2.403508000	-0.020730000
1	-3.145267000	-2.012866000	-0.008275000	6	-2.461878000	1.320833000	0.016919000
1	1.902870000	-2.496812000	0.002673000	1	-3.193913000	0.766131000	-0.569777000
				1	-2.818696000	1.386150000	1.044632000
				1	-2.340254000	2.323750000	-0.391913000

Table S23. DNA intra-strand dimer geometries with methyls. The stacks are written 5' TO 3'.

AA				AC			
6	1.852840000	-1.624050000	-0.663783000	6	-0.737090000	-0.590636000	1.639634000
7	0.872942000	-1.636627000	-1.579489000	7	-1.388006000	-1.457138000	0.852936000
6	0.327707000	-0.483221000	-1.953888000	6	-2.394977000	-1.041596000	0.045224000
7	0.606360000	0.740763000	-1.559166000	7	-2.747430000	0.306196000	0.053493000
6	1.592539000	0.720697000	-0.643516000	6	-2.094599000	1.191584000	0.849391000
6	2.246119000	-0.370985000	-0.149846000	6	-1.083373000	0.796003000	1.668826000
7	3.206232000	-0.001997000	0.775529000	7	0.241185000	-1.050491000	2.404069000
6	3.101182000	1.292166000	0.832519000	1	0.483971000	-2.050171000	2.383676000
7	2.145339000	1.802083000	-0.003702000	1	0.758381000	-0.406886000	3.019002000
1	3.716422000	1.912913000	1.484706000	1	-0.562996000	1.502142000	2.315592000
1	-0.466215000	-0.563090000	-2.696089000	8	-3.015363000	-1.817578000	-0.692242000
7	2.410727000	-2.783315000	-0.276517000	1	-2.387282000	2.240869000	0.830726000
1	2.086166000	-3.671777000	-0.683162000	6	-3.838040000	0.720227000	-0.829808000
1	3.162737000	-2.782732000	0.427433000	1	-4.007853000	1.791758000	-0.722677000
6	1.810645000	3.210618000	-0.152203000	1	-4.743302000	0.168598000	-0.575448000
1	1.012088000	3.279313000	-0.892444000	1	-3.582307000	0.481397000	-1.862307000
1	1.460102000	3.627172000	0.793297000	7	1.324415000	1.999589000	-0.350662000
1	2.673880000	3.779050000	-0.501601000	6	2.397457000	1.983647000	0.498600000
7	-0.781720000	0.866139000	1.628771000	7	2.942040000	0.810654000	0.627666000
6	-1.363279000	1.899231000	1.096822000	6	2.167858000	-0.003684000	-0.179664000
7	-2.275292000	1.575689000	0.128984000	6	2.230459000	-1.380022000	-0.480906000
6	-2.269283000	0.205832000	0.050990000	7	1.314885000	-1.869155000	-1.330227000
7	-3.014805000	-0.561290000	-0.766347000	6	0.405570000	-1.044294000	-1.840669000
6	-2.749094000	-1.833561000	-0.563349000	7	0.245382000	0.247328000	-1.646651000
7	-1.893380000	-2.393617000	0.286490000	6	1.178101000	0.708328000	-0.792906000
6	-1.165149000	-1.602838000	1.089635000	7	3.153671000	-2.203985000	0.042422000
6	-1.358479000	-0.210250000	0.978422000	1	3.859441000	-1.836825000	0.696751000
1	-3.313094000	-2.531324000	-1.182551000	1	3.155142000	-3.202053000	-0.210410000
7	-0.298450000	-2.156086000	1.953221000	1	-0.312225000	-1.505236000	-2.518796000
1	-0.195388000	-3.180570000	1.994861000	1	2.761124000	2.871059000	1.017677000
1	0.263394000	-1.556956000	2.574398000	6	0.485505000	3.127069000	-0.728897000
1	-1.145545000	2.925005000	1.392657000	1	-0.268200000	2.753546000	-1.423719000
6	-3.070374000	2.522132000	-0.639217000	1	1.075933000	3.900953000	-1.221710000
1	-3.694109000	1.944119000	-1.322754000	1	-0.011138000	3.550725000	0.145306000
1	-3.710421000	3.113125000	0.017620000				
1	-2.427943000	3.188924000	-1.216313000				
AG				AT			
7	-2.857152000	0.605311000	-0.483977000	6	-1.115914000	1.101606000	1.256232000
6	-3.105454000	-0.682595000	-0.262062000	6	-0.686367000	-0.204858000	1.692014000
7	-2.371475000	-1.461447000	0.610127000	7	-1.364173000	-1.247003000	1.102705000
6	-1.288707000	-1.005758000	1.382346000	6	-2.376863000	-1.148342000	0.169525000
6	-1.030176000	0.364620000	1.152455000	7	-2.719875000	0.137420000	-0.192421000
6	-1.811562000	1.065296000	0.251646000	6	-2.096276000	1.237244000	0.342147000
7	-0.060570000	1.204601000	1.705159000	6	-0.398112000	2.267922000	1.867518000
6	-0.280226000	2.360275000	1.132931000	1	-1.093521000	2.844129000	2.477178000
7	-1.329998000	2.355258000	0.239055000	1	0.418396000	1.905756000	2.492594000
1	0.314356000	3.249121000	1.344748000	1	0.004303000	2.901566000	1.077256000
8	-0.709539000	-1.788926000	2.134990000	8	0.207077000	-0.419167000	2.521098000
1	-2.637097000	-2.451632000	0.702117000	1	-1.087896000	-2.197674000	1.386361000
7	-4.103113000	-1.298420000	-0.904059000	8	-2.922640000	-2.132294000	-0.297347000
1	-4.286338000	-2.297320000	-0.733942000	1	-2.397811000	2.234304000	0.022629000
1	-4.688640000	-0.773130000	-1.569310000	6	-3.824392000	0.265020000	-1.198875000
6	-1.759232000	3.420068000	-0.650064000	1	-4.241236000	-0.720285000	-1.408622000

1	-1.204941000	3.361436000	-1.587937000	1	-3.429943000	0.695648000	-2.119500000
1	-2.824474000	3.315404000	-0.861216000	1	-4.606269000	0.911831000	-0.800272000
1	-1.579449000	4.387336000	-0.178522000	7	1.348891000	1.708314000	-0.959415000
7	2.870463000	1.017757000	-0.182917000	6	2.401122000	1.940564000	-0.115740000
6	3.657824000	0.245053000	0.626965000	7	2.950428000	0.855510000	0.342586000
7	3.305200000	-1.005516000	0.656591000	6	2.201623000	-0.159503000	-0.226034000
6	2.203475000	-1.058019000	-0.178714000	6	2.280917000	-1.564681000	-0.135716000
6	1.361146000	-2.117052000	-0.576082000	7	1.389559000	-2.280448000	-0.837166000
7	0.364585000	-1.828621000	-1.426109000	6	0.487259000	-1.639720000	-1.574135000
6	0.221302000	-0.575857000	-1.847836000	7	0.313587000	-0.346745000	-1.746307000
7	0.936535000	0.490521000	-1.559965000	6	1.222170000	0.343417000	-1.032501000
6	1.927712000	0.169342000	-0.708039000	1	-0.210723000	-2.278723000	-2.114551000
1	-0.610164000	-0.407397000	-2.531824000	7	3.196791000	-2.200820000	0.613690000
1	4.501196000	0.641096000	1.193593000	1	3.211214000	-3.229832000	0.645196000
7	1.515309000	-3.379128000	-0.141908000	1	3.883971000	-1.658680000	1.156766000
1	0.871821000	-4.115990000	-0.462882000	1	2.746027000	2.941186000	0.146922000
1	2.277080000	-3.608915000	0.512284000	6	0.532590000	2.703241000	-1.638986000
6	3.001268000	2.435775000	-0.465474000	1	-0.212322000	2.166109000	-2.228023000
1	2.208961000	2.706544000	-1.165225000	1	1.142761000	3.315877000	-2.304371000
1	3.968296000	2.652760000	-0.922082000	1	0.024560000	3.345427000	-0.917966000
1	2.892984000	3.022986000	0.447858000				
CA				CC			
7	-2.202687000	-1.457934000	-0.084292000	6	3.307023000	0.123315000	0.472612000
6	-3.211707000	-0.872285000	0.609568000	6	2.756774000	-0.739933000	-0.525833000
6	-3.468768000	0.459275000	0.499834000	7	1.651769000	-0.407562000	-1.204547000
6	-2.632718000	1.203840000	-0.389834000	6	1.021827000	0.771087000	-0.973747000
7	-1.638486000	0.618024000	-1.068423000	7	1.541737000	1.630627000	-0.008675000
6	-1.398556000	-0.710792000	-0.941984000	6	2.660378000	1.301220000	0.686077000
8	-0.487267000	-1.279834000	-1.555608000	8	-0.000827000	1.105367000	-1.584668000
7	-2.825464000	2.502997000	-0.554845000	7	3.333892000	-1.900393000	-0.795011000
1	-2.218325000	3.037149000	-1.192719000	1	2.932118000	-2.521898000	-1.511341000
1	-3.582750000	2.980486000	-0.045307000	1	4.185114000	-2.182525000	-0.288129000
1	-3.829429000	-1.481897000	1.268979000	1	4.200698000	-0.149043000	1.034741000
1	-4.272555000	0.935250000	1.062150000	1	3.049076000	1.995335000	1.431158000
6	-1.973048000	-2.899758000	-0.020272000	6	0.837322000	2.893517000	0.214889000
1	-0.981229000	-3.105428000	0.381525000	1	-0.191417000	2.689979000	0.512817000
1	-2.023647000	-3.325201000	-1.022212000	1	1.347904000	3.463921000	0.991057000
1	-2.732162000	-3.351063000	0.618099000	1	0.807797000	3.464392000	-0.713401000
7	0.668322000	-0.397212000	1.571249000	6	-0.844146000	-0.080204000	1.646635000
6	1.199781000	-1.553903000	1.310338000	6	-1.848581000	0.721287000	1.200249000
7	2.201227000	-1.498388000	0.379112000	7	-2.683441000	0.322062000	0.206678000
6	2.312514000	-0.177075000	0.026447000	6	-2.531917000	-0.924958000	-0.395663000
7	3.173997000	0.353498000	-0.861618000	7	-1.535495000	-1.739101000	0.032565000
6	2.999289000	1.654797000	-0.942748000	6	-0.705985000	-1.352853000	1.010389000
7	2.134231000	2.433600000	-0.299882000	7	0.252304000	-2.185923000	1.385253000
6	1.289011000	1.875863000	0.580587000	8	-3.314316000	-1.253291000	-1.296180000
6	1.375462000	0.480886000	0.769305000	1	0.345192000	-3.103018000	0.928054000
1	3.660657000	2.170618000	-1.639097000	1	0.904097000	-1.915241000	2.134759000
7	0.411505000	2.651588000	1.237296000	1	-0.177645000	0.233179000	2.449940000
1	0.389680000	3.666939000	1.062624000	1	-1.986560000	1.704487000	1.648907000
1	-0.239811000	2.232310000	1.915881000	6	-3.768517000	1.174910000	-0.279461000
1	0.878741000	-2.479571000	1.787004000	1	-4.721373000	0.660160000	-0.154600000
6	2.878928000	-2.604603000	-0.276382000	1	-3.772193000	2.113109000	0.275753000
1	3.814817000	-2.230510000	-0.693266000	1	-3.632101000	1.368259000	-1.343650000
1	2.262707000	-2.998711000	-1.085441000				

1	3.091805000	-3.392373000	0.447309000				
CG				CT			
7	2.715287000	1.002478000	-0.295051000	7	1.555550000	1.544586000	-0.317528000
6	1.691280000	0.387238000	-1.011549000	6	2.673610000	1.263071000	0.398878000
7	1.626207000	-0.967362000	-1.023109000	6	3.298778000	0.059148000	0.294427000
6	2.530812000	-1.703852000	-0.366276000	6	2.726731000	-0.885131000	-0.614399000
6	3.588326000	-1.095671000	0.379811000	7	1.622473000	-0.599384000	-1.315199000
6	3.635753000	0.264075000	0.375811000	6	1.014146000	0.606632000	-1.193659000
1	4.430115000	0.771388000	0.923214000	7	3.282265000	-2.075760000	-0.775564000
1	4.320446000	-1.692289000	0.924668000	1	2.864816000	-2.755268000	-1.427350000
7	2.422602000	-3.022205000	-0.415512000	1	4.132355000	-2.323366000	-0.249119000
1	1.656827000	-3.456844000	-0.949832000	1	4.191887000	-0.174233000	0.874695000
1	3.104186000	-3.614155000	0.080618000	1	3.079418000	2.017805000	1.072469000
8	0.869848000	1.094138000	-1.608485000	8	-0.007242000	0.899271000	-1.827631000
6	2.805594000	2.459005000	-0.351094000	6	0.951734000	2.875283000	-0.292363000
1	3.691936000	2.779797000	0.196055000	1	1.540241000	3.520247000	0.360155000
1	1.916161000	2.908007000	0.090706000	1	-0.075256000	2.818468000	0.068418000
1	2.867233000	2.786643000	-1.388753000	1	0.926171000	3.287327000	-1.301158000
7	-0.151353000	0.709557000	1.676567000	6	-0.854931000	0.068869000	1.516671000
6	-0.431906000	1.942112000	1.339856000	6	-1.840157000	0.831204000	1.003609000
7	-1.512041000	2.061815000	0.491304000	7	-2.689305000	0.336150000	0.045424000
6	-1.947034000	0.773689000	0.273180000	6	-2.577209000	-0.949704000	-0.440229000
7	-3.001299000	0.417352000	-0.506267000	7	-1.552233000	-1.697447000	0.104203000
6	-3.195936000	-0.898460000	-0.525158000	6	-0.657899000	-1.287296000	1.065825000
7	-2.404311000	-1.796357000	0.162708000	6	0.103367000	0.561022000	2.560056000
6	-1.311459000	-1.449580000	0.976207000	1	0.869217000	-0.194637000	2.736193000
6	-1.109801000	-0.050915000	1.002588000	1	0.574942000	1.481116000	2.215094000
1	-2.631381000	-2.796306000	0.073129000	1	-0.435773000	0.753953000	3.487094000
1	0.138116000	2.799109000	1.699124000	1	-1.964046000	1.855348000	1.354213000
7	-4.193493000	-1.423341000	-1.243561000	6	-3.688894000	1.195745000	-0.594127000
1	-4.820530000	-0.807027000	-1.780509000	1	-3.917166000	2.025411000	0.074610000
1	-4.335178000	-2.443121000	-1.260441000	1	-4.590136000	0.614131000	-0.786873000
8	-0.678559000	-2.335641000	1.550308000	1	-3.304704000	1.576201000	-1.540338000
6	-1.950876000	3.242179000	-0.231917000	8	-3.324389000	-1.400724000	-1.290115000
1	-1.335632000	3.389579000	-1.120630000	1	-1.446262000	-2.660322000	-0.245375000
1	-2.988498000	3.097279000	-0.535905000	8	0.222556000	-2.052580000	1.478970000
1	-1.883817000	4.117495000	0.415684000				
GA				GC			
6	-1.684722000	0.571040000	0.583152000	6	2.610438000	1.992346000	-0.073860000
7	-0.654246000	0.671645000	1.463586000	7	3.079484000	0.881912000	0.434117000
6	-0.184378000	-0.517477000	1.831080000	6	2.228414000	-0.105067000	-0.067723000
7	-0.697815000	-1.714432000	1.375387000	6	2.236537000	-1.504349000	0.130889000
6	-1.760370000	-1.842036000	0.463616000	7	1.187012000	-2.128266000	-0.566147000
6	-2.254684000	-0.578903000	0.066568000	6	0.253911000	-1.474334000	-1.344394000
7	-3.288008000	-0.251031000	-0.813791000	7	0.250335000	-0.158130000	-1.537866000
6	-3.311267000	1.056796000	-0.801328000	6	1.259424000	0.464985000	-0.874062000
7	-2.364481000	1.629133000	0.022234000	7	1.503090000	1.820298000	-0.877855000
8	-2.132521000	-2.963810000	0.119865000	7	-0.672341000	-2.243661000	-1.924672000
1	-0.269800000	-2.581665000	1.730801000	1	-1.397237000	-1.817348000	-2.518824000
7	0.832462000	-0.603248000	2.694333000	1	-0.661055000	-3.263556000	-1.777767000
1	1.260441000	0.253484000	3.072591000	1	1.108909000	-3.152825000	-0.490072000
1	1.188145000	-1.526729000	2.981681000	8	3.008429000	-2.188092000	0.802985000
1	-4.016524000	1.643052000	-1.390277000	1	3.055171000	2.968094000	0.121264000
6	-2.146414000	3.038782000	0.288196000	6	0.714410000	2.834330000	-1.558934000
1	-1.362367000	3.119790000	1.042800000	1	-0.219148000	3.001372000	-1.039868000

1	-1.830414000	3.559470000	-0.617202000	1	0.485281000	2.522561000	-2.568470000
1	-3.056551000	3.503802000	0.670457000	1	1.254765000	3.769727000	-1.602667000
7	0.553926000	1.043537000	-1.780159000	6	-0.908205000	1.508764000	1.456248000
6	1.068891000	2.093451000	-1.213631000	6	-1.916977000	1.676988000	0.559245000
7	2.048593000	1.799431000	-0.304294000	7	-2.645034000	0.623538000	0.107879000
6	2.163181000	0.432137000	-0.305462000	6	-2.375216000	-0.671169000	0.545791000
7	3.008163000	-0.309586000	0.434924000	7	-1.372237000	-0.861781000	1.438408000
6	2.843061000	-1.587440000	0.169752000	6	-0.647500000	0.170975000	1.887392000
7	2.000266000	-2.173738000	-0.675281000	7	0.322908000	-0.073768000	2.754143000
6	1.171122000	-1.407733000	-1.400851000	1	0.504031000	-1.037556000	3.065637000
6	1.249701000	-0.011601000	-1.217312000	1	0.895747000	0.701214000	3.116248000
1	3.492374000	-2.265409000	0.723946000	8	-3.062581000	-1.604455000	0.112908000
1	0.751019000	3.110619000	-1.440489000	1	-0.327482000	2.352936000	1.827551000
7	0.316181000	-1.987482000	-2.258754000	1	-2.146015000	2.677849000	0.194781000
1	-0.322653000	-1.407323000	-2.820710000	6	-3.733749000	0.793251000	-0.854913000
1	0.299193000	-3.013305000	-2.355308000	1	-4.662983000	0.418815000	-0.425013000
6	2.791646000	2.715095000	0.544954000	1	-3.523011000	0.209237000	-1.751022000
1	3.645139000	2.172018000	0.953753000	1	-3.835201000	1.848533000	-1.109040000
1	3.151583000	3.564838000	-0.037182000				
1	2.170692000	3.075584000	1.366515000				
GG				GT			
7	1.152692000	2.416794000	-0.324362000	7	-1.536296000	-1.418034000	-1.275592000
6	0.071549000	2.418502000	-1.180040000	6	-2.630079000	-1.757075000	-0.506879000
7	-0.123117000	1.281420000	-1.796828000	7	-3.078496000	-0.783499000	0.242908000
6	0.898445000	0.458189000	-1.317364000	6	-2.227194000	0.285133000	-0.046232000
6	1.202267000	-0.888812000	-1.618874000	6	-1.279153000	-0.098338000	-0.978033000
7	2.329693000	-1.333588000	-0.906521000	7	-0.276506000	0.650260000	-1.508571000
6	3.063777000	-0.564873000	-0.025473000	6	-0.263393000	1.891335000	-1.029617000
7	2.773131000	0.700582000	0.263926000	7	-1.175245000	2.362615000	-0.107448000
6	1.683999000	1.149544000	-0.412986000	6	-2.217704000	1.606127000	0.456146000
7	4.107773000	-1.167186000	0.552468000	1	-3.080757000	-2.749337000	-0.522663000
1	4.323926000	-2.149145000	0.330332000	1	-1.085562000	3.344686000	0.191051000
1	4.696057000	-0.648445000	1.220420000	8	-2.970072000	2.129008000	1.278080000
1	2.630637000	-2.306945000	-1.053123000	7	0.659447000	2.764571000	-1.444772000
8	0.627312000	-1.660801000	-2.386154000	1	1.368843000	2.475835000	-2.132976000
1	-0.564993000	3.290728000	-1.329969000	1	0.661039000	3.726962000	-1.076405000
6	1.600083000	3.478665000	0.558154000	6	-0.892050000	-2.201256000	-2.314872000
1	2.635332000	3.278558000	0.839496000	1	-0.408252000	-3.087153000	-1.899806000
1	0.986951000	3.520576000	1.459957000	1	-0.138182000	-1.570635000	-2.789376000
1	1.548780000	4.438913000	0.042182000	1	-1.618271000	-2.513543000	-3.067357000
7	-0.968764000	0.431361000	1.481218000	6	0.612465000	-0.497551000	1.785146000
6	-1.972492000	0.064289000	0.641601000	7	1.390443000	0.600800000	1.500279000
6	-2.198511000	-1.177852000	0.075839000	6	2.407027000	0.671165000	0.568773000
6	-1.321955000	-2.247530000	0.367285000	7	2.641209000	-0.491369000	-0.135158000
7	-0.293959000	-1.846528000	1.238523000	6	1.913090000	-1.634803000	0.080834000
6	-0.139658000	-0.573949000	1.749121000	6	0.932321000	-1.667442000	1.003919000
7	-3.334532000	-1.138359000	-0.735447000	6	0.103114000	-2.887096000	1.276058000
6	-3.751437000	0.097536000	-0.636148000	1	-0.689201000	-2.638317000	1.982399000
7	-2.973473000	0.890417000	0.181374000	1	-0.339588000	-3.240571000	0.344915000
1	-4.635686000	0.468586000	-1.154192000	1	0.733648000	-3.668742000	1.698847000
1	0.397244000	-2.557944000	1.517334000	1	2.130784000	-2.528848000	-0.502635000
8	-1.357741000	-3.410973000	-0.032909000	8	-0.273241000	-0.439380000	2.647520000
7	0.906414000	-0.387421000	2.559965000	1	1.194437000	1.457998000	2.036337000
1	1.541653000	-1.171065000	2.770363000	8	3.046157000	1.692104000	0.386560000
1	1.077579000	0.539348000	2.974737000	6	3.661610000	-0.461681000	-1.184817000

6	-3.168641000	2.287889000	0.516126000	1	3.201519000	-0.312980000	-2.161925000
1	-3.054645000	2.917871000	-0.367652000	1	4.212184000	-1.402634000	-1.181379000
1	-2.414914000	2.565163000	1.255009000	1	4.342393000	0.364925000	-0.980387000
1	-4.160056000	2.445958000	0.943965000				
TA				TC			
6	1.019613000	0.896422000	-1.065659000	6	2.537435000	-0.758437000	-0.765445000
7	1.814951000	1.672117000	-0.247708000	6	3.074192000	0.163681000	0.205888000
6	2.925421000	1.167176000	0.382349000	6	2.440833000	1.319983000	0.484691000
6	3.283215000	-0.122840000	0.228231000	7	1.263098000	1.648453000	-0.139912000
6	2.514497000	-1.008569000	-0.612276000	6	0.675889000	0.824669000	-1.077928000
7	1.422432000	-0.417409000	-1.203947000	7	1.357967000	-0.347030000	-1.341422000
1	0.846139000	-1.015917000	-1.812851000	1	0.940806000	-0.977338000	-2.041264000
8	0.032098000	1.331992000	-1.630092000	8	3.055761000	-1.835390000	-1.082981000
8	2.775010000	-2.200948000	-0.811478000	1	2.869555000	2.004669000	1.216080000
1	3.526155000	1.819417000	1.015776000	6	4.364283000	-0.240486000	0.854240000
6	4.488385000	-0.722962000	0.888131000	1	5.101434000	0.552416000	0.724327000
1	5.370063000	-0.128790000	0.646127000	1	4.732733000	-1.156852000	0.391918000
1	4.629617000	-1.743171000	0.529733000	1	4.198936000	-0.411463000	1.917826000
1	4.343801000	-0.734318000	1.968296000	8	-0.368414000	1.104210000	-1.638979000
6	1.471783000	3.084794000	-0.074023000	6	0.551450000	2.886872000	0.194743000
1	2.300808000	3.714614000	-0.397076000	1	1.255417000	3.615330000	0.596678000
1	0.595950000	3.294069000	-0.688383000	1	-0.219252000	2.676236000	0.935974000
1	1.244551000	3.291252000	0.971949000	1	0.072888000	3.286025000	-0.699365000
7	-0.846050000	0.341427000	1.557001000	6	-0.992060000	-0.116834000	1.637011000
6	-1.487051000	1.454182000	1.358617000	6	-2.029744000	0.686971000	1.279735000
7	-2.538271000	1.332823000	0.490652000	7	-2.929185000	0.303944000	0.337477000
6	-2.562315000	0.013980000	0.112890000	6	-2.812506000	-0.928077000	-0.302323000
7	-3.432267000	-0.569728000	-0.732561000	7	-1.784001000	-1.744182000	0.037108000
6	-3.156086000	-1.849878000	-0.856762000	6	-0.890914000	-1.373814000	0.963734000
7	-2.190024000	-2.565554000	-0.288725000	7	0.095959000	-2.207928000	1.252151000
6	-1.338980000	-1.956004000	0.550837000	1	0.162279000	-3.113811000	0.768726000
6	-1.528222000	-0.577205000	0.779201000	1	0.796594000	-1.949292000	1.960727000
7	-0.359904000	-2.667839000	1.131984000	1	-0.273269000	0.183394000	2.399202000
1	0.296777000	-2.208596000	1.778786000	1	-2.142027000	1.658796000	1.759280000
1	-0.265434000	-3.674143000	0.931107000	8	-3.653572000	-1.241930000	-1.153784000
1	-3.815917000	-2.405800000	-1.523060000	6	-4.050378000	1.159377000	-0.052692000
1	-1.213704000	2.394081000	1.837167000	1	-4.020874000	2.089724000	0.525835000
6	-3.391693000	2.380956000	-0.045535000	1	-4.994199000	0.632091000	0.126973000
1	-3.617535000	3.111057000	0.732792000	1	-3.988960000	1.378729000	-1.124709000
1	-4.317592000	1.920212000	-0.392334000				
1	-2.908014000	2.876519000	-0.888338000				
TG				TT			
6	3.363925000	0.803829000	0.166992000	6	-2.829550000	-0.968750000	-0.325149000
6	3.498387000	-0.536873000	0.148318000	7	-2.922277000	0.325915000	0.140781000
6	2.540551000	-1.367049000	-0.541068000	6	-2.019587000	0.846622000	1.034237000
7	1.518788000	-0.668922000	-1.141708000	6	-0.997963000	0.102127000	1.500146000
6	1.342709000	0.700942000	-1.139241000	6	-0.817708000	-1.261501000	1.065068000
7	2.307518000	1.416395000	-0.460580000	7	-1.766434000	-1.697725000	0.169300000
8	2.591745000	-2.600664000	-0.611005000	1	-2.130226000	1.876791000	1.371362000
1	0.812714000	-1.224803000	-1.645241000	8	-3.624131000	-1.442477000	-1.117757000
8	0.400822000	1.232044000	-1.699837000	1	-1.674136000	-2.666750000	-0.166910000
1	4.104403000	1.410925000	0.687237000	8	0.093177000	-2.011750000	1.437848000
6	4.634847000	-1.255338000	0.811881000	6	0.018973000	0.622471000	2.471890000
1	4.585084000	-2.317487000	0.569836000	1	-0.463255000	0.830385000	3.426626000
1	5.581309000	-0.846869000	0.456456000	1	0.800695000	-0.123835000	2.615102000

1	4.566313000	-1.125426000	1.891795000	1	0.460373000	1.538729000	2.079979000
6	2.137651000	2.872440000	-0.404036000	6	-4.059130000	1.122602000	-0.333532000
1	3.103097000	3.346091000	-0.227007000	1	-3.822104000	2.182965000	-0.249847000
1	1.451527000	3.128950000	0.402939000	1	-4.939483000	0.896608000	0.267685000
1	1.715753000	3.227617000	-1.344049000	1	-4.273006000	0.871376000	-1.372136000
7	-0.399590000	0.716468000	1.630441000	6	0.688247000	0.616695000	-1.325729000
6	-0.856138000	1.905450000	1.331837000	7	1.281423000	1.557544000	-0.509484000
7	-1.981204000	1.892561000	0.534894000	6	2.455839000	1.309128000	0.156936000
6	-2.251793000	0.561280000	0.310085000	6	3.079848000	0.120296000	0.042036000
6	-1.279601000	-0.154997000	0.984443000	6	2.536338000	-0.922954000	-0.793502000
6	-1.295556000	-1.567533000	0.938488000	7	1.360832000	-0.585662000	-1.423238000
7	-2.369887000	-2.044903000	0.167585000	8	3.046010000	-2.037630000	-0.957970000
6	-3.304664000	-1.250520000	-0.465815000	1	0.939090000	-1.303328000	-2.030015000
7	-3.285057000	0.079082000	-0.428722000	6	4.365969000	-0.200708000	0.742675000
7	-4.256634000	-1.893079000	-1.149625000	1	4.198263000	-0.221574000	1.819349000
1	-4.984142000	-1.358017000	-1.645380000	1	4.727229000	-1.175164000	0.412296000
1	-4.262863000	-2.922295000	-1.181018000	1	5.109778000	0.560619000	0.505834000
1	-2.466687000	-3.064782000	0.067792000	1	2.889566000	2.084919000	0.787459000
8	-0.524832000	-2.369670000	1.465576000	8	-0.353204000	0.824367000	-1.922170000
1	-0.388230000	2.825416000	1.682788000	6	0.579759000	2.836059000	-0.350786000
6	-2.762549000	3.021456000	0.056103000	1	1.289377000	3.607402000	-0.052047000
1	-3.016661000	2.892360000	-0.986790000	1	-0.193322000	2.736217000	0.410889000
1	-2.204911000	3.941574000	0.162348000	1	0.105316000	3.111546000	-1.292479000
1	-3.682743000	3.111330000	0.616486000				

Table S24. DNA intra-strand dimer geometries with hydrogens. The stacks are written 5' TO 3'.

AA				AC			
7	2.251690000	1.937199000	-0.241262000	7	0.202912000	-0.182268000	-1.806686000
6	3.126744000	1.467033000	0.700090000	6	1.090260000	0.529590000	-1.087494000
7	3.116224000	0.173007000	0.820628000	7	1.287122000	1.887389000	-1.131901000
6	2.160588000	-0.236113000	-0.092427000	6	2.281685000	2.149796000	-0.229180000
6	1.674275000	-1.509707000	-0.453577000	7	2.731943000	1.089402000	0.372463000
7	0.730857000	-1.564054000	-1.405355000	6	1.974119000	0.061080000	-0.159086000
6	0.306073000	-0.430529000	-1.955338000	6	1.967318000	-1.330759000	0.068308000
7	0.679964000	0.807805000	-1.713833000	7	1.094718000	-2.067696000	-0.634804000
6	1.626682000	0.829393000	-0.757472000	6	0.289953000	-1.459138000	-1.500721000
1	-0.464589000	-0.543373000	-2.717506000	1	-0.398430000	-2.113387000	-2.035176000
7	2.110659000	-2.648330000	0.110528000	7	2.784882000	-1.934197000	0.947262000
1	1.721871000	-3.553240000	-0.189551000	1	2.739162000	-2.954714000	1.075797000
1	2.833808000	-2.615409000	0.843355000	1	3.456880000	-1.375454000	1.492505000
1	3.771762000	2.116584000	1.292735000	1	2.660536000	3.153453000	-0.033374000
1	2.082881000	2.892251000	-0.514351000	1	0.787823000	2.538332000	-1.716856000
7	-0.804912000	1.484589000	1.359038000	6	-1.114240000	0.282740000	1.446947000
6	-1.271065000	2.480932000	0.667328000	6	-1.361925000	1.592653000	0.930890000
7	-2.173188000	2.106790000	-0.291498000	6	-2.267627000	1.691228000	-0.079319000
6	-2.288373000	0.743586000	-0.186441000	7	-2.910634000	0.597090000	-0.561977000
7	-3.070357000	-0.061938000	-0.929375000	6	-2.655858000	-0.669226000	-0.040088000
6	-2.928357000	-1.312481000	-0.546669000	7	-1.754793000	-0.790525000	0.966109000
7	-2.157985000	-1.821783000	0.410029000	7	-0.241107000	0.105269000	2.426228000
6	-1.390557000	-0.993381000	1.134943000	1	0.265530000	0.912622000	2.815281000
1	-3.530537000	-2.037888000	-1.093975000	1	-0.069418000	-0.838619000	2.798144000
6	-1.452935000	0.382309000	0.830585000	8	-3.263874000	-1.641284000	-0.505170000
7	-0.609131000	-1.495018000	2.104873000	1	-0.850419000	2.469733000	1.326901000
1	-0.018094000	-0.866509000	2.667134000	1	-2.481979000	2.668418000	-0.510790000
1	-0.600773000	-2.509236000	2.287130000	1	-3.586102000	0.650850000	-1.309473000
1	-2.650298000	2.704142000	-0.936119000				
1	-1.041222000	3.458563000	0.748612000				
AG				AT			
7	3.396761000	-0.412605000	0.668572000	6	2.026485000	-0.011880000	-0.167846000
6	2.297673000	-0.659587000	-0.134729000	6	2.105093000	-1.321078000	0.350604000
6	1.501597000	-1.807177000	-0.330359000	7	1.309842000	-2.251722000	-0.197443000
7	0.492824000	-1.717139000	-1.209645000	6	0.497634000	-1.900238000	-1.189702000
6	0.295184000	-0.566644000	-1.846121000	7	0.336011000	-0.726560000	-1.762370000
7	0.963878000	0.563292000	-1.758468000	6	1.147074000	0.184112000	-1.192967000
6	1.968689000	0.441168000	-0.871447000	7	1.253685000	1.512673000	-1.521457000
7	2.874301000	1.408689000	-0.513512000	6	2.195267000	2.031830000	-0.674806000
6	3.694972000	0.826536000	0.414127000	7	2.693872000	1.158175000	0.148153000
7	1.710519000	-2.964150000	0.319928000	1	2.498510000	3.079220000	-0.689419000
1	1.099232000	-3.772980000	0.140518000	1	-0.125555000	-2.701190000	-1.586771000
1	2.482031000	-3.041339000	0.998070000	7	2.929250000	-1.663883000	1.354775000
1	-0.543330000	-0.558004000	-2.542089000	1	3.542135000	-0.954947000	1.782383000
1	4.520885000	1.352491000	0.894162000	1	2.947644000	-2.634851000	1.696752000
1	2.907418000	2.349412000	-0.872873000	1	0.758564000	1.977456000	-2.264840000
7	-0.060572000	1.804120000	1.336043000	6	-1.454485000	1.489073000	0.482966000
6	-0.993398000	0.838846000	0.949694000	6	-2.319079000	1.302728000	-0.533309000
6	-1.192267000	-0.478454000	1.421709000	7	-2.865606000	0.067431000	-0.777436000
7	-2.254936000	-1.109785000	0.751995000	6	-2.558700000	-1.035321000	-0.008287000
6	-3.022588000	-0.530415000	-0.238503000	7	-1.664587000	-0.806617000	1.018531000
7	-2.830367000	0.706791000	-0.687922000	6	-1.070373000	0.392401000	1.337971000

6	-1.805056000	1.334257000	-0.054669000	8	-3.036978000	-2.136549000	-0.214564000
7	-1.379714000	2.620626000	-0.300446000	1	-1.417095000	-1.616197000	1.604954000
6	-0.330434000	2.829142000	0.569374000	8	-0.281267000	0.474576000	2.287764000
8	-0.579189000	-1.089907000	2.296650000	6	-0.824152000	2.814771000	0.790223000
1	-2.477433000	-2.078150000	1.020786000	1	-0.334662000	3.200260000	-0.104066000
7	-3.993202000	-1.292396000	-0.752329000	1	-0.085813000	2.691701000	1.582864000
1	-4.601417000	-0.919186000	-1.495376000	1	-1.592075000	3.516011000	1.115570000
1	-4.132941000	-2.251931000	-0.405807000	1	-2.587696000	2.144724000	-1.170514000
1	0.225338000	3.765891000	0.614768000	1	-3.473847000	-0.111265000	-1.560872000
1	-1.768947000	3.254929000	-0.979335000				
CA				CC			
6	-3.204576000	-1.086063000	0.576329000	7	-1.464355000	-1.824385000	0.066464000
6	-3.386253000	0.261847000	0.540192000	6	-0.908700000	-1.028593000	-0.932756000
6	-2.522201000	1.003637000	-0.324693000	7	-1.454522000	0.188941000	-1.175652000
7	-1.573590000	0.398962000	-1.050408000	6	-2.511865000	0.619257000	-0.476358000
6	-1.408605000	-0.946122000	-0.997143000	6	-3.097101000	-0.177183000	0.557106000
7	-2.241422000	-1.690606000	-0.164894000	6	-2.535063000	-1.395630000	0.782219000
1	-3.846377000	-1.693556000	1.214351000	1	-3.951590000	0.174674000	1.135783000
1	-4.152816000	0.752340000	1.140710000	1	-2.953693000	-2.041396000	1.554076000
8	-0.540850000	-1.532792000	-1.655634000	7	-3.007481000	1.813794000	-0.758555000
7	-2.642369000	2.318507000	-0.418855000	1	-3.820476000	2.170938000	-0.236449000
1	-2.015149000	2.850233000	-1.039083000	1	-2.580465000	2.386831000	-1.500246000
1	-3.363218000	2.810652000	0.128206000	8	0.068324000	-1.453051000	-1.562081000
1	-2.169527000	-2.693572000	-0.082485000	1	-1.033828000	-2.723758000	0.220329000
7	0.710333000	-0.882808000	1.491380000	6	1.029057000	1.002234000	0.952473000
6	1.170424000	-2.052414000	1.161532000	7	1.857381000	1.302462000	-0.056069000
7	2.159330000	-2.004792000	0.216570000	6	2.777336000	0.405730000	-0.490373000
6	2.341118000	-0.675180000	-0.069285000	7	2.851608000	-0.835363000	0.138123000
7	3.218276000	-0.148265000	-0.944084000	6	2.017419000	-1.147766000	1.162861000
6	3.117495000	1.163305000	-0.954704000	6	1.089038000	-0.262633000	1.615832000
7	2.308391000	1.954950000	-0.257006000	1	2.093690000	-2.128285000	1.631669000
6	1.445792000	1.400431000	0.608513000	1	0.423757000	-0.506494000	2.443881000
6	1.454697000	-0.005197000	0.723306000	7	0.147031000	1.913746000	1.331978000
1	0.803864000	-2.982207000	1.595418000	1	0.110496000	2.824757000	0.855064000
7	0.624293000	2.188986000	1.320098000	1	-0.501894000	1.710131000	2.104829000
1	-0.039810000	1.772151000	1.987707000	8	3.556525000	0.653528000	-1.418996000
1	0.658278000	3.211725000	1.198552000	1	3.546862000	-1.478079000	-0.210355000
1	3.796916000	1.676759000	-1.635241000				
1	2.664588000	-2.772194000	-0.196960000				
CG				CT			
6	-3.674436000	-0.709450000	0.252637000	6	2.555625000	1.363075000	-0.530713000
6	-3.650214000	0.644469000	0.384894000	7	1.493848000	1.141072000	-1.346735000
6	-2.599975000	1.337668000	-0.294325000	6	0.939198000	-0.131147000	-1.466326000
7	-1.680086000	0.681421000	-1.012171000	7	1.476848000	-1.147165000	-0.746639000
6	-1.722107000	-0.669134000	-1.128557000	6	2.525373000	-0.938150000	0.059007000
7	-2.738595000	-1.366016000	-0.479260000	6	3.109351000	0.359295000	0.202083000
7	-2.514042000	2.656406000	-0.218602000	1	3.956579000	0.535186000	0.865475000
1	-1.753463000	3.152076000	-0.705070000	1	2.973732000	2.367238000	-0.460925000
1	-3.207778000	3.187610000	0.326979000	7	3.013304000	-1.966737000	0.734377000
1	-4.394771000	1.174892000	0.979123000	1	2.587179000	-2.898881000	0.632668000
1	-4.462416000	-1.279166000	0.745120000	1	3.819420000	-1.835431000	1.362104000
8	-0.886145000	-1.302947000	-1.784482000	8	-0.029584000	-0.293577000	-2.218567000
1	-2.739927000	-2.369121000	-0.587325000	1	1.069549000	1.873095000	-1.896292000
6	0.416991000	-2.403255000	1.078644000	6	-2.000547000	1.490031000	-0.141505000
7	0.113998000	-1.212722000	1.528204000	7	-2.830474000	0.511497000	-0.629298000

6	1.062276000	-0.376366000	0.934517000	6	-2.774494000	-0.790161000	-0.177195000
6	1.240174000	1.021709000	1.041110000	7	-1.825931000	-1.035309000	0.795550000
7	2.330496000	1.461640000	0.270384000	6	-0.956391000	-0.120690000	1.343406000
6	3.140309000	0.645779000	-0.494222000	6	-1.090966000	1.214286000	0.813317000
7	2.968051000	-0.669002000	-0.600431000	8	-0.146510000	-0.460733000	2.215193000
6	1.916622000	-1.114601000	0.135725000	1	-1.762744000	-2.001391000	1.146630000
7	1.502703000	-2.424574000	0.229038000	6	-0.156611000	2.243155000	1.376888000
1	-0.139901000	-3.299611000	1.352250000	1	-0.727803000	2.991872000	1.925027000
7	4.131901000	1.252458000	-1.154079000	1	0.387524000	2.723811000	0.563967000
1	4.771692000	0.699944000	-1.742913000	1	0.551307000	1.761203000	2.051533000
1	4.256252000	2.271498000	-1.074049000	1	-2.077847000	2.504233000	-0.532098000
1	2.540876000	2.469203000	0.276680000	8	-3.505384000	-1.667372000	-0.601819000
8	0.589760000	1.839137000	1.692289000	1	-3.521474000	0.690850000	-1.341111000
1	1.921692000	-3.215026000	-0.237367000				
GA				GC			
7	-3.225371000	0.146805000	-0.834842000	6	-2.050160000	0.027642000	-0.063804000
6	-2.200306000	-0.363008000	-0.035078000	7	-2.915913000	-1.061423000	0.057444000
6	-1.655306000	-1.665420000	0.029729000	6	-2.549817000	-1.865566000	-0.907147000
7	-0.624103000	-1.744000000	0.982136000	7	-1.497673000	-1.394508000	-1.664331000
6	-0.181638000	-0.693113000	1.759205000	6	-1.177994000	-0.171012000	-1.119240000
7	-0.699376000	0.531119000	1.704082000	7	-0.187639000	0.652582000	-1.552897000
6	-1.700675000	0.628590000	0.790262000	6	-0.102156000	1.766008000	-0.829839000
7	-2.416601000	1.770039000	0.506000000	7	-0.935937000	2.051847000	0.231801000
6	-3.312772000	1.401528000	-0.475481000	6	-1.964111000	1.214400000	0.698892000
1	-4.030397000	2.095239000	-0.913344000	1	-3.033305000	-2.823975000	-1.095921000
7	0.815589000	-0.965949000	2.606335000	7	0.820253000	2.688930000	-1.119502000
1	1.191334000	-0.225283000	3.214992000	1	1.473401000	2.536642000	-1.900809000
1	1.208412000	-1.917588000	2.650672000	1	0.877789000	3.553132000	-0.561167000
1	-0.163559000	-2.656810000	1.109750000	1	-0.794434000	2.948189000	0.719813000
8	-1.963258000	-2.668226000	-0.614151000	8	-2.643637000	1.568568000	1.662139000
1	-2.293701000	2.671400000	0.938641000	1	-1.044580000	-1.830845000	-2.451128000
7	0.572403000	1.806051000	-1.275346000	6	1.095052000	-2.139529000	0.356102000
6	1.020718000	2.685776000	-0.430621000	6	2.022822000	-1.936280000	-0.617792000
7	1.989843000	2.198640000	0.404035000	7	2.773643000	-0.805581000	-0.654449000
6	2.171045000	0.887314000	0.043180000	6	2.611104000	0.191169000	0.305188000
7	3.031870000	0.009010000	0.590796000	7	1.690043000	0.009961000	1.283898000
6	2.936247000	-1.156769000	-0.011117000	6	0.943523000	-1.101025000	1.326710000
7	2.145144000	-1.528796000	-1.013058000	1	2.166901000	-2.696339000	-1.384972000
6	1.298566000	-0.630448000	-1.539338000	1	0.496794000	-3.049688000	0.393921000
6	1.304128000	0.667573000	-0.987833000	7	0.056023000	-1.222915000	2.301562000
1	0.659513000	3.712930000	-0.390318000	1	-0.046410000	-0.475248000	3.001006000
1	3.603386000	-1.931711000	0.366731000	1	-0.531152000	-2.066582000	2.359128000
7	0.495348000	-0.993213000	-2.552390000	8	3.315983000	1.205882000	0.238974000
1	-0.156352000	-0.309930000	-2.963361000	1	3.467067000	-0.637989000	-1.367874000
1	0.530962000	-1.955565000	-2.919177000				
1	2.483208000	2.683047000	1.136933000				
GG				GT			
7	-3.458731000	-0.457889000	-0.781629000	6	2.472665000	1.798508000	-0.942943000
6	-2.318345000	-0.760443000	-0.034454000	7	2.873543000	1.050454000	0.052457000
6	-1.496810000	-1.910396000	-0.048254000	6	2.079128000	-0.094065000	-0.043823000
7	-0.440361000	-1.798105000	0.872582000	6	2.055619000	-1.258633000	0.756633000
6	-0.213775000	-0.709314000	1.689384000	7	1.088658000	-2.173506000	0.304277000
7	-0.991102000	0.370150000	1.708280000	6	0.254749000	-1.974906000	-0.776986000
6	-2.021206000	0.281265000	0.826148000	7	0.281660000	-0.882244000	-1.535406000
7	-2.981572000	1.245781000	0.617185000	6	1.212243000	0.015362000	-1.116493000

6	-3.808573000	0.729342000	-0.358309000	7	1.463350000	1.238244000	-1.697671000
1	-4.677060000	1.263968000	-0.742823000	1	2.898382000	2.778733000	-1.157113000
7	0.848760000	-0.789282000	2.496325000	1	0.995870000	-3.060727000	0.819873000
1	1.072911000	-0.010284000	3.131269000	7	-0.604011000	-2.962686000	-1.047820000
1	1.443669000	-1.630595000	2.483366000	1	-0.616059000	-3.810313000	-0.461922000
1	0.214939000	-2.590086000	0.942979000	1	-1.253559000	-2.876933000	-1.842155000
8	-1.598171000	-2.928111000	-0.733104000	8	2.741315000	-1.538236000	1.739832000
1	-3.045680000	2.132532000	1.090785000	1	0.995860000	1.619696000	-2.504319000
7	-0.134418000	1.994707000	-1.259920000	6	-1.210962000	1.903998000	0.240698000
6	0.126359000	2.923404000	-0.376293000	6	-2.101018000	1.610018000	-0.726997000
7	1.214392000	2.648530000	0.424761000	7	-2.777748000	0.415749000	-0.724306000
6	1.676916000	1.422729000	0.001029000	6	-2.581242000	-0.536361000	0.253814000
7	2.747449000	0.761992000	0.514227000	7	-1.657239000	-0.202132000	1.223664000
6	2.967750000	-0.398599000	-0.097408000	6	-0.936145000	0.966874000	1.302555000
7	2.185210000	-0.877470000	-1.129087000	1	-2.285669000	2.330598000	-1.523120000
6	1.075864000	-0.209767000	-1.676705000	8	-0.132869000	1.154043000	2.225195000
6	0.846851000	1.027028000	-1.032098000	1	-1.490695000	-0.899098000	1.963303000
1	-0.464555000	3.834663000	-0.282115000	8	-3.175522000	-1.599680000	0.267433000
7	3.984100000	-1.179594000	0.281807000	6	-0.440673000	3.190116000	0.282637000
1	4.605681000	-0.879893000	1.046756000	1	-1.126612000	4.019599000	0.452161000
1	4.145705000	-2.080353000	-0.190239000	1	0.077474000	3.334304000	-0.665356000
1	2.432690000	-1.793529000	-1.527926000	1	0.288755000	3.151223000	1.091953000
8	0.453182000	-0.728868000	-2.603021000	1	-3.450811000	0.171282000	-1.433917000
1	1.605355000	3.206182000	1.166991000				
TA				TC			
7	-1.841579000	-1.870758000	-0.300864000	6	-2.306082000	-1.368819000	0.666928000
6	-2.908200000	-1.299355000	0.347902000	6	-2.855620000	-0.207148000	0.261418000
6	-3.167270000	0.017687000	0.228764000	6	-2.260626000	0.560060000	-0.805948000
6	-2.336254000	0.863894000	-0.592968000	7	-1.118779000	0.002145000	-1.332319000
7	-1.294416000	0.206955000	-1.205465000	6	-0.521894000	-1.180050000	-0.940299000
6	-0.992319000	-1.136836000	-1.103005000	7	-1.160297000	-1.849780000	0.083036000
1	-0.676334000	0.775496000	-1.801976000	1	-2.777887000	-1.935147000	1.469550000
8	-0.042787000	-1.631446000	-1.683729000	8	-2.701524000	1.630368000	-1.241112000
8	-2.505915000	2.077387000	-0.760198000	1	-0.662224000	0.518911000	-2.097564000
1	-3.554658000	-1.920232000	0.967685000	8	0.494877000	-1.595708000	-1.466506000
6	-4.320966000	0.690389000	0.910309000	6	-4.107760000	0.359703000	0.860479000
1	-4.172209000	0.662729000	1.989612000	1	-4.901726000	-0.386527000	0.818987000
1	-5.246153000	0.171433000	0.657966000	1	-4.412012000	1.243847000	0.299281000
1	-4.385352000	1.727326000	0.578888000	1	-3.922153000	0.634669000	1.898618000
1	-1.726114000	-2.860892000	-0.150434000	1	-0.726673000	-2.713912000	0.368643000
7	0.919225000	-0.793418000	1.522853000	6	2.204768000	-0.981151000	1.388594000
6	1.472958000	-1.946168000	1.292610000	6	1.231230000	-0.068885000	1.654166000
7	2.527364000	-1.882626000	0.422355000	6	1.216753000	1.109941000	0.845654000
6	2.650443000	-0.560084000	0.078317000	7	2.127252000	1.309104000	-0.115980000
7	3.559388000	-0.022489000	-0.756626000	6	3.090878000	0.387292000	-0.362458000
6	3.381045000	1.277738000	-0.846554000	7	3.122406000	-0.771637000	0.410022000
1	4.078983000	1.798969000	-1.501979000	1	2.249634000	-1.899584000	1.972959000
7	2.474242000	2.049826000	-0.255179000	1	0.498396000	-0.229486000	2.444669000
6	1.582163000	1.485187000	0.573116000	7	0.295565000	2.040910000	1.039452000
6	1.666667000	0.090541000	0.765117000	1	-0.416546000	1.914273000	1.772066000
7	0.662136000	2.254096000	1.177568000	1	0.291702000	2.890185000	0.458557000
1	0.643862000	3.269535000	1.003005000	8	3.945959000	0.542564000	-1.243145000
1	-0.025366000	1.829499000	1.815961000	1	3.852084000	-1.435872000	0.199641000
1	1.130499000	-2.874650000	1.748441000				
1	3.108336000	-2.635799000	0.090091000				

TG				TT			
6	1.326262000	0.935554000	-1.226245000	6	-2.878211000	0.147838000	0.130519000
7	2.320783000	1.653472000	-0.594712000	6	-2.287571000	-1.097664000	-0.295820000
6	3.360642000	1.040196000	0.059248000	7	-1.152998000	-1.449888000	0.397604000
6	3.448651000	-0.303350000	0.114475000	6	-0.559446000	-0.740475000	1.423258000
6	2.457055000	-1.136583000	-0.521416000	7	-1.193313000	0.435277000	1.768409000
7	1.454992000	-0.437643000	-1.153479000	6	-2.331784000	0.864611000	1.132299000
6	4.565162000	-1.023092000	0.809760000	1	-2.800256000	1.798312000	1.442565000
1	4.476802000	-2.094652000	0.627620000	8	0.450832000	-1.132373000	1.979357000
1	5.522145000	-0.668234000	0.426065000	1	-0.699749000	-2.333533000	0.124062000
1	4.510152000	-0.831150000	1.881171000	8	-2.726096000	-1.817448000	-1.200765000
1	4.125917000	1.649025000	0.540091000	6	-4.110606000	0.596111000	-0.604365000
8	2.465113000	-2.373211000	-0.522808000	1	-3.893329000	0.731973000	-1.667120000
1	0.726003000	-0.995639000	-1.620711000	1	-4.495589000	1.535377000	-0.201316000
8	0.398601000	1.467263000	-1.809528000	1	-4.895831000	-0.161666000	-0.542360000
1	2.229004000	2.655951000	-0.648930000	1	-0.762146000	0.952924000	2.518343000
7	-0.391318000	1.165493000	1.549369000	6	1.126580000	0.366448000	-1.305015000
6	-0.809085000	2.351275000	1.187886000	7	2.079658000	-0.613988000	-1.152832000
7	-1.940531000	2.333438000	0.400123000	6	3.079492000	-0.650521000	-0.201466000
6	-2.258712000	1.001984000	0.251607000	7	3.097652000	0.414998000	0.673854000
7	-3.314107000	0.515870000	-0.452540000	6	2.184832000	1.437401000	0.598354000
6	-3.379841000	-0.812248000	-0.415337000	6	1.226706000	1.442010000	-0.348767000
7	-2.467754000	-1.602384000	0.255356000	1	2.235211000	2.256861000	1.314655000
6	-1.371218000	-1.120740000	0.991555000	6	0.285762000	2.602296000	-0.532790000
6	-1.306201000	0.290753000	0.958600000	1	0.382602000	3.326664000	0.279909000
1	-0.306835000	3.272415000	1.484008000	1	0.493606000	3.118692000	-1.474800000
7	-4.359062000	-1.458161000	-1.056155000	1	-0.750421000	2.265304000	-0.590513000
1	-2.600480000	-2.622231000	0.213189000	8	0.276990000	0.289603000	-2.201586000
1	-5.071800000	-0.926381000	-1.576294000	8	3.883858000	-1.563655000	-0.145012000
1	-4.401024000	-2.486689000	-1.030090000	1	2.043540000	-1.401046000	-1.816006000
8	-0.624157000	-1.918683000	1.557636000	1	3.826162000	0.388001000	1.370137000
1	-2.443645000	3.111547000	0.004958000				

Table S25. DNA inter-strand dimer geometries with methyls.

5'_A3' 3'_A_5'				5'_A3' 3'_C_5'			
7	-4.130170000	1.182138000	-0.311350000	6	-3.052354000	0.793526000	0.119526000
6	-4.780052000	0.108998000	-0.649707000	7	-4.192562000	1.257961000	-0.511697000
7	-4.139654000	-1.050224000	-0.304383000	6	-4.870154000	0.178366000	-0.764289000
6	-2.977915000	-0.666196000	0.316516000	7	-4.245659000	-0.968205000	-0.353756000
6	-2.992771000	0.698561000	0.310497000	6	-1.919861000	1.452068000	0.641857000
7	-2.029871000	-1.472709000	0.829417000	6	-3.064134000	-0.567757000	0.217443000
6	-1.057918000	-0.756662000	1.351977000	7	-2.121767000	-1.357680000	0.765427000
7	-0.922011000	0.564451000	1.417724000	7	-0.962361000	0.690744000	1.193467000
6	-1.884514000	1.342385000	0.898975000	6	-1.125458000	-0.628666000	1.219731000
1	-5.742587000	0.129885000	-1.159833000	1	-0.314422000	-1.188068000	1.686282000
1	-0.244420000	-1.330299000	1.796434000	7	-1.767811000	2.785828000	0.610295000
7	-1.759850000	2.677954000	0.960175000	1	-2.498227000	3.377933000	0.190306000
1	-2.494336000	3.282647000	0.566013000	1	-0.920141000	3.217464000	1.006616000
1	-0.929140000	3.098363000	1.401878000	1	-5.842349000	0.185098000	-1.256155000
6	-4.565032000	-2.422413000	-0.534720000	6	-4.696958000	-2.344834000	-0.487752000
1	-4.663696000	-2.623500000	-1.603603000	1	-4.853126000	-2.599736000	-1.538038000
1	-5.517478000	-2.621761000	-0.038728000	1	-5.623824000	-2.506210000	0.067221000
1	-3.799647000	-3.074724000	-0.116870000	1	-3.916500000	-2.983373000	-0.076565000
6	1.057761000	-0.756466000	-1.352011000	6	3.181057000	1.394937000	-0.528907000
7	0.922367000	0.564584000	-1.417570000	7	2.420815000	0.339975000	-0.847099000
6	1.884508000	1.341900000	-0.898979000	6	2.819690000	-0.920869000	-0.546300000
6	2.993002000	0.698643000	-0.310395000	7	4.042944000	-1.101238000	0.095257000
6	2.977661000	-0.666045000	-0.316590000	6	4.821609000	-0.037814000	0.419847000
7	2.030092000	-1.472653000	-0.829288000	7	2.740752000	2.603471000	-0.841587000
1	0.244694000	-1.330133000	-1.796286000	6	4.442390000	1.235294000	0.125630000
7	4.130355000	1.182434000	0.311426000	1	5.068957000	2.091590000	0.376614000
6	4.779768000	0.108638000	0.649608000	1	5.771288000	-0.207400000	0.927172000
7	4.139812000	-1.050784000	0.304481000	1	3.304761000	3.433556000	-0.609296000
1	5.743182000	0.129502000	1.160091000	1	1.834043000	2.714501000	-1.317371000
7	1.759560000	2.678214000	-0.960313000	8	2.139079000	-1.914970000	-0.827938000
1	0.929404000	3.097735000	-1.401798000	6	4.442140000	-2.473623000	0.407620000
1	2.494649000	3.282500000	-0.565916000	1	4.492378000	-3.061623000	-0.509041000
6	4.564737000	-2.422152000	0.534492000	1	3.700788000	-2.936756000	1.059447000
1	3.798200000	-3.074171000	0.118304000	1	5.415482000	-2.456983000	0.897731000
1	5.516039000	-2.622230000	0.036822000				
1	4.665309000	-2.622797000	1.603281000				
5'_A3' 3'_G_5'				5'_A3' 3'_T_5'			
7	1.994894000	-1.267605000	-1.080818000	6	3.389227000	0.457765000	0.243225000
6	1.027965000	-0.491336000	-1.520069000	7	4.602037000	0.795053000	-0.302628000
7	0.901109000	0.829801000	-1.438598000	6	5.153296000	-0.377801000	-0.742725000
6	1.868806000	1.538722000	-0.837194000	7	4.401673000	-1.416515000	-0.531548000
6	2.972517000	0.825976000	-0.324488000	6	3.287362000	-0.895946000	0.102122000
6	2.948329000	-0.529536000	-0.482044000	6	2.106765000	-1.492415000	0.591471000
7	4.107289000	-0.988066000	0.091708000	7	1.195658000	-0.685641000	1.156885000
6	4.755533000	0.121233000	0.563290000	6	1.446575000	0.618318000	1.226630000
7	4.113073000	1.229723000	0.346585000	7	2.495181000	1.292149000	0.806079000
1	0.210652000	-1.006497000	-2.025034000	1	0.669109000	1.216475000	1.702166000
1	5.718086000	0.078766000	1.072040000	1	6.128947000	-0.434900000	-1.224373000
7	1.753290000	2.873643000	-0.749605000	7	1.865972000	-2.811266000	0.516093000
1	0.925564000	3.346165000	-1.141415000	1	0.986340000	-3.196774000	0.889665000

1	2.491817000	3.425793000	-0.291130000	1	2.560227000	-3.438035000	0.085214000
6	4.556325000	-2.372322000	0.111487000	6	5.153478000	2.139654000	-0.379171000
1	3.714796000	-2.996359000	-0.185860000	1	4.420176000	2.817748000	0.059847000
1	4.883947000	-2.652511000	1.114259000	1	6.086867000	2.208244000	0.181509000
1	5.376907000	-2.528647000	-0.592865000	1	5.330954000	2.426107000	-1.416826000
6	-1.046165000	-0.902154000	1.182730000	6	-2.456601000	1.248100000	-0.564786000
7	-0.934476000	0.459436000	1.376569000	7	-2.192452000	-0.071085000	-0.877057000
6	-1.881320000	1.413711000	0.964891000	6	-3.004778000	-1.152882000	-0.628079000
6	-2.977053000	0.805490000	0.311487000	6	-4.246793000	-0.821157000	0.027096000
6	-3.000620000	-0.568608000	0.152159000	6	-4.536855000	0.453650000	0.353654000
7	-2.073635000	-1.474533000	0.561020000	7	-3.663942000	1.472993000	0.063753000
7	-4.171865000	-0.864538000	-0.508807000	8	-2.659188000	-2.293752000	-0.957170000
6	-4.789730000	0.351232000	-0.714660000	6	-5.161099000	-1.971390000	0.325521000
7	-4.124201000	1.374926000	-0.245371000	1	-5.358215000	-2.526387000	-0.591368000
1	-5.748589000	0.449986000	-1.223370000	1	-4.690337000	-2.631085000	1.054062000
8	-1.681201000	2.605632000	1.197943000	1	-6.099997000	-1.593991000	0.730916000
7	-0.041192000	-1.648287000	1.651604000	1	-5.477545000	0.679059000	0.855473000
1	-0.063360000	-2.671513000	1.538675000	1	-1.294946000	-0.264768000	-1.344024000
1	0.756077000	-1.199690000	2.125963000	8	-1.673632000	2.143281000	-0.827658000
1	-0.092183000	0.803541000	1.860040000	6	-4.009112000	2.849728000	0.431851000
6	-4.627567000	-2.187817000	-0.899662000	1	-3.208208000	3.499455000	0.078377000
1	-4.772531000	-2.242337000	-1.980825000	1	-4.099231000	2.940389000	1.514530000
1	-5.564144000	-2.440374000	-0.397075000	1	-4.949248000	3.138676000	-0.038456000
1	-3.899550000	-2.910419000	-0.534527000				
		5' _C3'				5' _C3'	
		3'C_5'				3'G_5'	
6	-4.914753000	0.058109000	-0.520053000	7	2.401004000	0.498428000	-0.921404000
6	-4.505989000	1.340140000	-0.320446000	6	2.790484000	-0.783860000	-0.713781000
6	-3.229178000	1.519248000	0.296974000	7	4.012151000	-1.019659000	-0.087075000
7	-2.481203000	0.473530000	0.671701000	6	4.798866000	0.011437000	0.314767000
6	-2.909103000	-0.796641000	0.465227000	6	4.428697000	1.305030000	0.114445000
7	-4.148560000	-0.995999000	-0.138789000	6	3.169413000	1.521665000	-0.526496000
8	-2.241523000	-1.782960000	0.800479000	7	2.737390000	2.753011000	-0.750085000
1	-5.122139000	2.188739000	-0.617044000	1	1.832652000	2.904517000	-1.216152000
7	-2.759825000	2.737263000	0.518326000	1	3.307738000	3.558561000	-0.457418000
1	-1.842499000	2.861779000	0.967471000	8	2.103257000	-1.750087000	-1.067339000
1	-3.313752000	3.559482000	0.240869000	1	5.061571000	2.135174000	0.427596000
1	-5.877078000	-0.127521000	-0.995959000	1	5.746413000	-0.202510000	0.808117000
6	-4.572792000	-2.379101000	-0.356561000	6	4.420134000	-2.413690000	0.092790000
1	-3.841677000	-2.895724000	-0.978740000	1	3.684994000	-2.943978000	0.698872000
1	-4.626872000	-2.903844000	0.597513000	1	4.471389000	-2.911746000	-0.875524000
1	-5.548921000	-2.378434000	-0.842058000	1	5.394800000	-2.438027000	0.579717000
7	2.481212000	0.473365000	-0.671420000	6	-1.112842000	-0.716751000	1.095503000
6	3.228412000	1.519233000	-0.297241000	7	-0.972662000	0.655147000	1.142634000
6	4.505715000	1.340681000	0.320402000	6	-1.911556000	1.579773000	0.652555000
6	4.914193000	0.058344000	0.520238000	6	-3.032466000	0.928468000	0.089646000
7	4.148598000	-0.995895000	0.139461000	6	-3.083997000	-0.454012000	0.076317000
6	2.909249000	-0.796794000	-0.464568000	7	-2.164161000	-1.330463000	0.558919000
7	2.759675000	2.737197000	-0.518688000	7	-4.275022000	-0.794090000	-0.525404000
1	3.313063000	3.560672000	-0.241637000	6	-4.875762000	0.405528000	-0.845185000
1	1.841445000	2.862185000	-0.968190000	7	-4.181699000	1.459243000	-0.500124000
1	5.121543000	2.190272000	0.616664000	7	-0.110854000	-1.429592000	1.619340000
1	5.877101000	-0.126334000	0.996401000	1	-0.153714000	-2.458368000	1.615193000
8	2.241288000	-1.782849000	-0.799701000	1	0.704816000	-0.949791000	2.027223000
6	4.574191000	-2.378870000	0.355378000	1	-0.113632000	1.031104000	1.569637000

6	-5.130259000	0.607602000	-0.829556000	1	-5.480214000	-2.917116000	-0.285751000
7	-4.608338000	-0.617179000	-0.470991000	1	-4.875479000	-2.797739000	1.382934000
8	-1.762293000	2.820051000	0.642236000	1	-6.350682000	-1.923399000	0.907081000
1	-0.303927000	0.993642000	1.505476000	8	-2.796420000	-2.491592000	-0.583839000
7	-0.467901000	-1.458157000	1.649335000	1	-1.588193000	-0.402286000	-1.133912000
1	0.383587000	-1.021096000	2.029147000	8	-2.184397000	2.004072000	-0.883482000
1	-0.581599000	-2.481459000	1.684771000	1	-5.922524000	0.395648000	0.815346000
1	-6.098855000	0.719991000	-1.317033000	6	-4.619726000	2.630854000	0.218057000
6	-5.192545000	-1.936228000	-0.648402000	1	-3.837543000	3.306208000	-0.115508000
1	-5.383921000	-2.134044000	-1.705249000	1	-5.529371000	2.811221000	-0.359309000
1	-4.480156000	-2.668255000	-0.271408000	1	-4.820831000	2.799372000	1.278273000
1	-6.127027000	-2.024380000	-0.089556000	6	3.254172000	-1.354793000	0.387381000
7	2.196482000	0.220000000	-0.959668000	7	2.522722000	-0.237220000	0.717205000
6	3.017705000	1.274976000	-0.635991000	6	2.906816000	1.078151000	0.548761000
6	4.253567000	0.888467000	0.000526000	7	4.153203000	1.259578000	-0.012885000
6	4.530242000	-0.407976000	0.242592000	6	4.951518000	0.203246000	-0.374971000
7	3.649204000	-1.397334000	-0.117996000	6	4.545207000	-1.067716000	-0.188886000
6	2.446897000	-1.119520000	-0.734914000	8	2.802025000	-2.489175000	0.588105000
8	2.684268000	2.438486000	-0.889724000	1	1.593873000	-0.398144000	1.131823000
6	5.177175000	2.007453000	0.378500000	6	5.374219000	-2.257572000	-0.571224000
1	4.709254000	2.621680000	1.147500000	1	6.268312000	-2.292935000	0.050582000
1	5.383645000	2.620332000	-0.498604000	1	5.662737000	-2.177670000	-1.619236000
1	6.110653000	1.594910000	0.761557000	1	4.793405000	-3.168331000	-0.423767000
1	1.302963000	0.452944000	-1.416233000	1	5.927571000	0.394904000	-0.819640000
8	1.656831000	-1.987658000	-1.059910000	8	2.189096000	2.007035000	0.874423000
1	5.466486000	-0.675309000	0.731989000	6	4.580985000	2.648982000	-0.203415000
6	4.006231000	-2.802421000	0.105084000	1	5.545588000	2.646684000	-0.708195000
1	3.143703000	-3.411556000	-0.148679000	1	4.670169000	3.155949000	0.758517000
1	4.847539000	-3.087318000	-0.531334000	1	3.849377000	3.187676000	-0.805627000
1	4.275279000	-2.956292000	1.152072000				
		5'A_3'				5'A_3'	
		3'_A5'				3'_C5'	
6	3.865669000	0.467330000	-0.135185000	7	-1.485785000	1.111730000	0.887199000
7	3.463929000	1.748863000	-0.217693000	6	-1.872854000	-0.169289000	0.976874000
6	2.257872000	1.814798000	-0.738982000	6	-3.151704000	-0.498065000	0.481473000
7	1.464773000	0.834340000	-1.160257000	6	-3.884354000	0.528982000	-0.039144000
6	1.892980000	-0.433192000	-1.063311000	7	-3.524173000	1.821462000	-0.144650000
6	3.173629000	-0.646782000	-0.512715000	6	-2.315083000	1.997651000	0.343866000
7	3.909879000	-1.795108000	-0.281887000	7	-5.069941000	-0.031968000	-0.444192000
6	5.014874000	-1.354393000	0.241211000	6	-4.977242000	-1.362384000	-0.137079000
7	5.062297000	0.008479000	0.358185000	7	-3.852616000	-1.689682000	0.426155000
7	1.099755000	-1.432622000	-1.484655000	1	-1.938416000	3.019106000	0.295877000
1	0.171426000	-1.222588000	-1.879489000	1	-5.771747000	-2.079795000	-0.345113000
1	1.419489000	-2.409033000	-1.412720000	7	-1.043060000	-1.073995000	1.522820000
1	1.848850000	2.820056000	-0.840265000	1	-1.331851000	-2.060194000	1.594062000
1	5.828395000	-2.008952000	0.557472000	1	-0.118769000	-0.781344000	1.869386000
6	6.134041000	0.836101000	0.890840000	6	-6.173722000	0.678548000	-1.072239000
1	5.810248000	1.873294000	0.817969000	1	-6.376718000	0.277154000	-2.067406000
1	6.328033000	0.593141000	1.937749000	1	-7.076772000	0.609818000	-0.461945000
1	7.050398000	0.703821000	0.311827000	1	-5.879346000	1.723277000	-1.160590000
6	-1.892698000	-0.433290000	1.063390000	7	2.886903000	0.076857000	-0.784559000
7	-1.464744000	0.834136000	1.160142000	6	3.882562000	0.920572000	-0.413828000
6	-2.257770000	1.814664000	0.738863000	7	5.055905000	0.383771000	0.110365000
7	-3.464153000	1.749046000	0.217399000	6	5.206565000	-0.958928000	0.244632000
6	-3.865832000	0.467161000	0.134982000	6	4.220687000	-1.823333000	-0.118277000

6	-3.173428000	-0.646619000	0.512759000	6	3.027863000	-1.248281000	-0.657680000
7	-3.910051000	-1.794802000	0.281779000	8	3.780999000	2.149170000	-0.518964000
7	-5.061936000	0.008289000	-0.358083000	7	2.026543000	-2.026004000	-1.039685000
6	-5.015258000	-1.354479000	-0.241455000	1	1.167147000	-1.607311000	-1.423232000
1	-5.828375000	-2.008828000	-0.557467000	1	2.107375000	-3.048853000	-0.953090000
7	-1.099800000	-1.432791000	1.484600000	1	4.334045000	-2.901508000	-0.003930000
1	-1.420105000	-2.409140000	1.412396000	1	6.137977000	-1.352890000	0.652243000
1	-0.172267000	-1.222541000	1.878990000	6	6.109927000	1.321574000	0.498331000
1	-1.848902000	2.819725000	0.840018000	1	6.416500000	1.912603000	-0.365065000
6	-6.133861000	0.836271000	-0.890090000	1	6.957754000	0.759486000	0.889646000
1	-7.048477000	0.708618000	-0.307111000	1	5.732534000	2.009598000	1.255123000
1	-6.332289000	0.589298000	-1.935228000				
1	-5.807386000	1.872888000	-0.822691000				
		5'A_3'				5'A_3'	
		3'_G5'				3'_T5'	
6	-3.939097000	0.352534000	0.201407000	6	3.369343000	0.515638000	0.470378000
7	-3.504580000	1.602891000	0.444651000	7	4.003162000	1.743320000	0.397180000
6	-2.299662000	1.570655000	0.972593000	6	5.144720000	1.470455000	-0.160971000
7	-1.534696000	0.524395000	1.269190000	7	5.311317000	0.142762000	-0.448010000
6	-1.995027000	-0.709129000	1.013484000	6	4.158284000	-0.476914000	-0.034659000
6	-3.277963000	-0.817764000	0.437944000	7	3.870410000	-1.788817000	-0.120722000
1	-1.865272000	2.543929000	1.199741000	6	2.672501000	-2.024414000	0.370294000
7	-5.144143000	-0.009077000	-0.347637000	7	1.794865000	-1.177775000	0.900161000
6	-5.133620000	-1.376475000	-0.402667000	6	2.110235000	0.123938000	0.970569000
7	-4.043039000	-1.908027000	0.063410000	7	1.231059000	0.989344000	1.502764000
1	-5.961841000	-1.964289000	-0.799806000	1	0.324098000	0.651133000	1.853622000
7	-1.230682000	-1.774193000	1.307635000	1	1.464664000	1.990998000	1.559173000
1	-1.575944000	-2.724966000	1.112983000	1	2.353088000	-3.065789000	0.337660000
1	-0.300076000	-1.639673000	1.727089000	1	5.898419000	2.227610000	-0.379719000
6	-6.192078000	0.904507000	-0.776848000	6	6.453825000	-0.513729000	-1.065036000
1	-5.844921000	1.916890000	-0.576185000	1	6.210719000	-1.571138000	-1.158346000
1	-7.114735000	0.724753000	-0.220902000	1	6.647819000	-0.100334000	-2.056971000
1	-6.386451000	0.796434000	-1.846063000	1	7.346466000	-0.403968000	-0.445323000
7	1.435404000	0.795197000	-1.004359000	6	-2.822908000	1.009488000	-0.681996000
6	1.759426000	-0.568660000	-1.114694000	7	-2.670537000	-0.355182000	-0.770654000
6	3.039816000	-0.839666000	-0.583000000	6	-3.590400000	-1.313762000	-0.396287000
6	3.790915000	0.192824000	-0.050274000	7	-4.776410000	-0.825424000	0.111926000
6	2.247813000	1.759367000	-0.445203000	6	-5.017001000	0.520982000	0.235347000
7	3.457183000	1.506427000	0.049049000	6	-4.090713000	1.427510000	-0.135251000
7	4.972740000	-0.367129000	0.382865000	6	-4.304612000	2.908099000	-0.026915000
6	4.868822000	-1.709751000	0.083108000	1	-5.248530000	3.102879000	0.482128000
7	3.741230000	-2.044141000	-0.488824000	1	-3.487854000	3.352890000	0.540615000
8	0.951717000	-1.343484000	-1.627086000	1	-4.333756000	3.344721000	-1.024346000
7	1.760430000	3.003792000	-0.427489000	1	-5.970628000	0.861141000	0.638207000
1	0.521231000	1.097814000	-1.369272000	8	-1.922542000	1.773533000	-1.049979000
1	0.826655000	3.196466000	-0.817881000	1	-1.777904000	-0.695416000	-1.156549000
1	2.317582000	3.770772000	-0.024153000	8	-3.364344000	-2.505793000	-0.510930000
1	5.657505000	-2.429171000	0.304125000	6	-5.803600000	-1.787563000	0.523981000
6	6.078496000	0.336694000	1.010573000	1	-6.052110000	-1.642887000	1.577543000
1	5.788506000	1.380562000	1.118882000	1	-6.702951000	-1.664059000	-0.083681000
1	6.977556000	0.277313000	0.392915000	1	-5.401558000	-2.785678000	0.378008000
1	6.290486000	-0.080729000	1.997234000				
		5'C_3'				5'C_3'	
		3'_C5'				3'_G5'	
6	2.982018000	-1.018203000	-0.718516000	6	5.331484000	-1.019610000	0.288734000

1	6.774851000	1.654119000	-0.118955000	1	-6.964649000	-0.976488000	1.134939000
1	6.090053000	1.706466000	1.527271000	1	-6.496854000	-2.299032000	0.035159000
1	5.438227000	2.766987000	0.255190000				

Table S26. DNA inter-strand dimer geometries with hydrogens.

5'_A3' 3'_A_5'				5'_A3' 3'_C_5'			
6	4.753253000	-0.189223000	0.821288000	6	-1.953896000	1.122438000	0.591646000
7	4.116418000	0.884582000	0.460005000	6	-3.070994000	0.465516000	0.035235000
6	3.002206000	0.400809000	-0.202402000	7	-4.194214000	0.932134000	-0.624205000
6	1.915613000	1.044083000	-0.830483000	6	-4.863389000	-0.146805000	-0.900892000
7	0.972789000	0.266780000	-1.383436000	7	-4.248873000	-1.294909000	-0.479719000
6	1.105762000	-1.054272000	-1.313126000	6	-3.083773000	-0.896288000	0.125485000
7	2.058654000	-1.770473000	-0.755771000	7	-2.155666000	-1.688151000	0.694601000
6	2.987127000	-0.963879000	-0.209231000	6	-1.172941000	-0.960537000	1.179693000
7	4.126165000	-1.348636000	0.453265000	7	-1.010795000	0.359170000	1.164950000
1	0.309235000	-1.627926000	-1.786430000	1	-5.821882000	-0.138456000	-1.418925000
7	1.792927000	2.380398000	-0.896193000	1	-0.374188000	-1.521584000	1.665078000
1	0.979200000	2.799930000	-1.367262000	7	-1.802667000	2.456510000	0.571385000
1	2.513322000	2.984672000	-0.475542000	1	-0.966590000	2.886905000	0.992884000
1	5.697658000	-0.168372000	1.366135000	1	-2.522134000	3.050094000	0.134908000
1	4.420626000	-2.297529000	0.620872000	1	-4.566936000	-2.245681000	-0.580039000
6	-1.105922000	-1.054680000	1.312917000	7	2.426940000	0.023042000	-0.784874000
7	-2.058410000	-1.770713000	0.755648000	6	2.819037000	-1.238982000	-0.480133000
6	-2.987386000	-0.964186000	0.208989000	7	4.024646000	-1.421505000	0.193419000
7	-4.126002000	-1.348196000	-0.453367000	6	4.792922000	-0.359018000	0.544732000
6	-4.753574000	-0.188965000	-0.821457000	6	4.420280000	0.915255000	0.247169000
7	-4.116321000	0.884166000	-0.459849000	6	3.176983000	1.077082000	-0.440502000
6	-3.002043000	0.400571000	0.202525000	7	2.743859000	2.286815000	-0.758526000
6	-1.915713000	1.044380000	0.830573000	1	3.300346000	3.116236000	-0.506557000
7	-0.972499000	0.266432000	1.383599000	1	1.850263000	2.399443000	-1.258145000
7	-1.793362000	2.379947000	0.896306000	1	5.038763000	1.770853000	0.519664000
1	-0.308946000	-1.628329000	1.786346000	1	5.728686000	-0.530326000	1.076732000
1	-0.979107000	2.800343000	1.367666000	8	2.147528000	-2.232275000	-0.785478000
1	-2.513190000	2.984651000	0.475987000	1	4.285472000	-2.373007000	0.404402000
1	-5.697114000	-0.168064000	-1.365914000				
1	-4.420132000	-2.297208000	-0.620880000				
5'_A3' 3'_G_5'				5'_A3' 3'_T_5'			
6	-4.763301000	0.221411000	-0.909306000	6	-5.200308000	0.044554000	-0.843897000
7	-4.108465000	1.177105000	-0.301894000	7	-4.452071000	1.087113000	-0.639767000
6	-2.985280000	0.535380000	0.224356000	6	-3.351796000	0.579725000	0.028193000
6	-1.909602000	1.052714000	0.981180000	6	-2.180975000	1.185917000	0.528949000
7	-0.983837000	0.047590000	1.311813000	7	-1.282763000	0.391043000	1.130679000
6	-1.097024000	-1.281239000	0.957726000	6	-1.536558000	-0.910915000	1.223563000
7	-2.105383000	-1.767338000	0.238867000	7	-2.576938000	-1.593042000	0.796012000
6	-3.011700000	-0.810765000	-0.093891000	6	-3.458115000	-0.770519000	0.196594000
7	-4.160641000	-1.016272000	-0.824622000	7	-4.659670000	-1.118802000	-0.366957000
1	-5.702936000	0.388140000	-1.435839000	1	-0.769848000	-1.499091000	1.728126000
1	-0.157059000	0.324838000	1.860614000	1	-6.165648000	0.091803000	-1.346918000
7	-0.113903000	-2.086837000	1.371262000	7	-1.937169000	2.502647000	0.429899000
1	-0.138395000	-3.089862000	1.139793000	1	-2.621584000	3.120346000	-0.028916000
1	0.668849000	-1.704288000	1.921580000	1	-1.065075000	2.895609000	0.813249000
8	-1.710478000	2.207581000	1.357570000	1	-5.043121000	-2.049512000	-0.408246000
1	-4.472254000	-1.894608000	-1.206927000	7	2.146290000	-0.270014000	-0.818291000
6	1.902625000	1.346831000	-0.664119000	6	2.954479000	0.816401000	-0.576050000
6	2.983077000	0.568314000	-0.199803000	6	4.182196000	0.498195000	0.111955000
7	4.101658000	0.880054000	0.552402000	6	4.463945000	-0.769387000	0.472182000

6	4.729178000	-0.252581000	0.661140000	7	3.596106000	-1.794214000	0.186412000
7	4.091167000	-1.293213000	0.042124000	6	2.402379000	-1.582257000	-0.471919000
6	2.956089000	-0.759570000	-0.514158000	8	1.538893000	-2.381515000	-0.786684000
7	2.019881000	-1.413648000	-1.226906000	1	1.258929000	-0.085947000	-1.307982000
6	1.073918000	-0.581933000	-1.606234000	8	2.617115000	1.950060000	-0.937049000
7	0.952439000	0.722153000	-1.376589000	6	5.091390000	1.654038000	0.404258000
1	5.672851000	-0.363446000	1.194365000	1	5.308196000	2.188780000	-0.520192000
1	0.271806000	-1.026852000	-2.195339000	1	4.606299000	2.329779000	1.108279000
7	1.792347000	2.663783000	-0.426413000	1	6.021209000	1.284927000	0.837270000
1	0.981940000	3.186893000	-0.789065000	1	5.393718000	-0.984443000	0.998301000
1	2.517597000	3.151623000	0.118119000	1	3.792572000	-2.748241000	0.448017000
1	4.376705000	-2.258096000	-0.009514000				
	5'_C3'				5'_C3'		
	3'_C_5'				3'_G_5'		
7	-2.494164000	0.119977000	0.622167000	7	2.407947000	0.267265000	-0.877874000
6	-3.233820000	1.165771000	0.233088000	6	3.167993000	1.254680000	-0.387200000
6	-4.498617000	0.987095000	-0.409742000	6	4.408100000	0.984986000	0.270776000
6	-4.903020000	-0.295282000	-0.617454000	6	4.768629000	-0.321715000	0.385180000
6	-2.917983000	-1.150224000	0.407050000	7	3.990457000	-1.316363000	-0.113496000
7	-4.145103000	-1.349445000	-0.221413000	6	2.787609000	-1.028797000	-0.754818000
1	-5.856289000	-0.480055000	-1.112595000	1	5.701283000	-0.576264000	0.887549000
1	-5.108467000	1.836626000	-0.718284000	1	5.034389000	1.786554000	0.661907000
7	-2.769597000	2.383780000	0.463612000	7	2.746104000	2.501334000	-0.531121000
1	-1.860466000	2.508858000	0.931220000	1	3.310394000	3.280203000	-0.163967000
1	-3.317400000	3.207199000	0.175519000	1	1.855288000	2.691384000	-1.009715000
8	-2.256777000	-2.136212000	0.755510000	8	2.107720000	-1.962820000	-1.197799000
1	-4.429343000	-2.306660000	-0.365796000	1	4.241983000	-2.290595000	-0.039295000
7	2.493916000	0.120081000	-0.622263000	7	-1.021955000	0.288301000	1.097413000
6	2.917667000	-1.150049000	-0.407157000	6	-1.943933000	1.251298000	0.651063000
7	4.144905000	-1.349286000	0.221354000	6	-3.050504000	0.648973000	0.010588000
6	4.903359000	-0.295102000	0.617586000	7	-4.181106000	1.227616000	-0.570100000
6	4.498605000	0.986886000	0.409725000	6	-4.868328000	0.205753000	-1.011265000
6	3.234288000	1.165870000	-0.232925000	7	-4.280401000	-1.017209000	-0.764413000
1	5.856060000	-0.480637000	1.112513000	6	-3.105762000	-0.728477000	-0.106295000
1	5.108731000	1.835545000	0.718362000	7	-2.202482000	-1.642782000	0.335631000
7	2.769388000	2.383840000	-0.463720000	6	-1.164845000	-1.075653000	0.945148000
1	1.861149000	2.508266000	-0.930990000	1	-5.822063000	0.311147000	-1.528207000
1	3.317683000	3.206114000	-0.175451000	8	-1.716843000	2.444853000	0.848270000
8	2.256891000	-2.136434000	-0.755440000	7	-0.180118000	-1.830255000	1.442557000
1	4.429138000	-2.306500000	0.365753000	1	-0.225913000	-2.855691000	1.361205000
				1	0.625184000	-1.385984000	1.907322000
				1	-0.174157000	0.627383000	1.574772000
				1	-4.616281000	-1.936035000	-1.004575000
	5'_C3'				5'_G3'		
	3'_T_5'				3'_G_5'		
7	2.179848000	-0.168139000	-0.690113000	7	0.961040000	0.454777000	-1.389175000
6	2.972620000	0.917969000	-0.400231000	6	1.895964000	1.350433000	-0.841382000
6	4.225791000	0.583284000	0.231787000	6	2.966348000	0.665962000	-0.222187000
6	4.543271000	-0.698317000	0.501255000	7	4.095171000	1.162435000	0.433907000
7	3.688392000	-1.721493000	0.173578000	6	4.740646000	0.088253000	0.809105000
6	2.472184000	-1.493972000	-0.436655000	7	4.126600000	-1.092279000	0.448066000
1	5.491944000	-0.926236000	0.986642000	6	2.980141000	-0.717056000	-0.215944000
6	5.119547000	1.737664000	0.573335000	7	2.065766000	-1.565448000	-0.754587000
1	6.068690000	1.362023000	0.955862000	6	1.062119000	-0.921375000	-1.344049000
1	5.298842000	2.335291000	-0.320117000	7	0.071793000	-1.603709000	-1.927485000

5'A_3' 3'_A5'				5'A_3' 3'_C5'			
6	-4.990639000	-1.245725000	-0.548303000	7	-3.835562000	-1.635852000	0.188904000
7	-5.030806000	0.117142000	-0.668016000	6	-3.164952000	-0.429196000	0.281381000
6	-3.866690000	0.576021000	-0.102207000	6	-1.920701000	-0.073425000	0.841954000
6	-3.199099000	-0.538072000	0.317094000	7	-1.558011000	1.216020000	0.773669000
7	-3.919801000	-1.686412000	0.041592000	6	-2.377851000	2.084670000	0.189622000
7	-3.470773000	1.857560000	0.004735000	7	-3.556180000	1.882971000	-0.360331000
6	-2.298955000	1.923523000	0.599003000	6	-3.892580000	0.582625000	-0.274873000
7	-1.533179000	0.943087000	1.068160000	7	-5.043192000	-0.003412000	-0.740704000
6	-1.954628000	-0.324451000	0.945183000	6	-4.936885000	-1.332155000	-0.430771000
7	-1.188730000	-1.323860000	1.414416000	1	-5.703633000	-2.066438000	-0.680011000
1	-1.503446000	-2.300276000	1.323045000	7	-1.100084000	-0.960850000	1.428615000
1	-5.783230000	-1.900302000	-0.913835000	1	-1.370234000	-1.953338000	1.483857000
1	-5.751998000	0.686115000	-1.082033000	1	-0.201432000	-0.648676000	1.822362000
1	-1.896920000	2.928788000	0.725142000	1	-2.021931000	3.114290000	0.162139000
1	-0.286364000	-1.113805000	1.865430000	1	-5.907009000	0.423180000	-1.251614000
6	1.954347000	-0.324600000	-0.945353000	6	3.079878000	-1.040356000	-0.540896000
7	1.533126000	0.942819000	-1.068215000	6	4.255996000	-1.590188000	0.058186000
6	2.298819000	1.923368000	-0.599132000	6	5.202645000	-0.705079000	0.472060000
7	3.470952000	1.857778000	-0.004664000	7	5.029357000	0.634273000	0.331793000
6	3.866827000	0.575899000	0.102279000	6	3.872758000	1.146258000	-0.251145000
6	3.198900000	-0.537900000	-0.317208000	7	2.916285000	0.281636000	-0.673307000
7	3.919977000	-1.686069000	-0.041446000	7	2.116867000	-1.839102000	-0.974532000
6	4.991013000	-1.245719000	0.548565000	1	1.269150000	-1.438592000	-1.401077000
1	5.783223000	-1.900050000	0.913872000	1	2.215792000	-2.860114000	-0.885083000
7	1.188778000	-1.324122000	-1.414359000	1	4.387202000	-2.665857000	0.176951000
1	0.287176000	-1.113894000	-1.864897000	1	6.120488000	-1.079330000	0.926351000
1	1.504057000	-2.300467000	-1.322612000	8	3.749527000	2.372554000	-0.359936000
7	5.030444000	0.117054000	0.667785000	1	5.719176000	1.305725000	0.633755000
1	1.896919000	2.928423000	-0.725208000				
1	5.751297000	0.686554000	1.081668000				
5'A_3' 3'_G5'				5'A_3' 3'_T5'			
7	5.117260000	0.171998000	0.648545000	6	-5.116073000	-1.502251000	-0.475020000
6	3.939866000	0.519779000	0.034429000	7	-5.317550000	-0.175120000	-0.741563000
6	3.320738000	-0.658878000	-0.265728000	6	-4.209303000	0.475761000	-0.259394000
7	4.086025000	-1.740527000	0.132594000	6	-3.409436000	-0.499269000	0.262313000
6	5.134150000	-1.196186000	0.675060000	7	-3.993318000	-1.746846000	0.132217000
1	5.949791000	-1.774768000	1.109994000	7	-3.966199000	1.798762000	-0.303417000
7	3.492897000	1.765616000	-0.209450000	6	-2.802723000	2.065731000	0.250334000
6	2.323202000	1.719277000	-0.810495000	7	-1.920895000	1.239085000	0.804262000
7	1.601310000	0.663701000	-1.174407000	6	-2.191070000	-0.074359000	0.831527000
6	2.072906000	-0.565032000	-0.916175000	7	-1.307123000	-0.919753000	1.387457000
7	1.351907000	-1.639444000	-1.277991000	1	-1.506075000	-1.930161000	1.411107000
1	1.706019000	-2.586675000	-1.081970000	1	-0.431123000	-0.557454000	1.789239000
1	0.445633000	-1.515635000	-1.750645000	1	-2.520726000	3.118348000	0.255454000
1	1.881610000	2.687812000	-1.043928000	1	-5.829982000	-2.280669000	-0.746307000
1	5.811448000	0.811458000	1.001234000	1	-6.105639000	0.257166000	-1.196800000
7	-1.506393000	0.822257000	0.918651000	6	2.844955000	-0.744480000	-0.596920000
6	-2.304897000	1.780861000	0.330640000	7	2.646800000	0.615539000	-0.663884000
7	-3.476117000	1.513097000	-0.241537000	6	3.511677000	1.597566000	-0.224814000
6	-3.785652000	0.190876000	-0.189456000	7	4.689142000	1.140434000	0.330145000
6	-3.045194000	-0.836745000	0.367050000	6	4.973015000	-0.198979000	0.436513000
6	-1.805777000	-0.550228000	0.981294000	6	4.099625000	-1.129318000	0.002000000

7	-4.926187000	-0.384499000	-0.705198000	1	1.761767000	0.932389000	-1.085537000
6	-4.810477000	-1.730787000	-0.426975000	8	1.992059000	-1.531598000	-1.024530000
7	-3.712374000	-2.053496000	0.205807000	8	3.247583000	2.783063000	-0.324988000
8	-1.013384000	-1.318661000	1.526194000	1	5.918114000	-0.513960000	0.878084000
1	-0.623035000	1.136217000	1.344748000	6	4.362525000	-2.603401000	0.089151000
7	-1.845421000	3.035428000	0.367973000	1	3.536441000	-3.090087000	0.606591000
1	-0.941575000	3.239359000	0.818460000	1	4.455558000	-3.015634000	-0.914724000
1	-2.394210000	3.798972000	-0.052964000	1	5.287479000	-2.775927000	0.639370000
1	-5.567958000	-2.461811000	-0.710276000	1	5.321901000	1.857557000	0.649013000
1	-5.674191000	0.097834000	-1.176982000				
	5'C_3'				5'C_3'		
	3'_C5'				3'_G5'		
6	-3.012538000	-0.828594000	0.576903000	6	5.348104000	-0.713830000	0.495838000
6	-4.166095000	-1.513288000	0.081558000	6	4.441250000	-1.650781000	0.107361000
6	-5.159521000	-0.741412000	-0.436601000	6	3.242750000	-1.169291000	-0.506340000
7	-5.050964000	0.610618000	-0.489309000	7	3.022084000	0.140240000	-0.675435000
6	-3.915182000	1.254988000	-0.004268000	6	3.939132000	1.057125000	-0.278385000
7	-2.913404000	0.505177000	0.518733000	7	5.116539000	0.611827000	0.318192000
1	-6.062070000	-1.219153000	-0.817646000	7	2.315928000	-2.020499000	-0.916989000
1	-4.245506000	-2.600125000	0.117632000	1	1.451722000	-1.670034000	-1.354187000
8	-3.852089000	2.488784000	-0.071769000	1	2.458479000	-3.033893000	-0.799437000
7	-2.007032000	-1.510764000	1.102061000	1	4.619426000	-2.716094000	0.256302000
1	-1.175585000	-1.014734000	1.453444000	1	6.280735000	-1.034751000	0.959775000
1	-2.055547000	-2.538116000	1.159512000	8	3.763162000	2.273458000	-0.421072000
1	-5.776463000	1.198688000	-0.871047000	1	5.776533000	1.320557000	0.601053000
7	2.913144000	0.504961000	-0.518935000	7	-1.522426000	0.973446000	0.720618000
6	3.915473000	1.254739000	0.004325000	6	-2.379120000	1.853805000	0.093457000
7	5.051274000	0.611077000	0.489429000	7	-3.549324000	1.495640000	-0.429212000
6	5.159572000	-0.741348000	0.436677000	6	-3.794339000	0.166845000	-0.284060000
6	4.166127000	-1.513024000	-0.081431000	7	-4.917956000	-0.492840000	-0.731458000
6	3.012537000	-0.828728000	-0.576850000	6	-4.731897000	-1.811284000	-0.370387000
1	6.062409000	-1.219277000	0.817926000	7	-3.605217000	-2.041092000	0.252640000
1	4.245210000	-2.599681000	-0.117609000	6	-2.993063000	-0.787038000	0.317642000
7	2.006818000	-1.511434000	-1.102078000	6	-1.754667000	-0.404294000	0.879269000
1	1.175600000	-1.014798000	-1.453367000	7	-1.979071000	3.127901000	0.037896000
1	2.056062000	-2.538364000	-1.159025000	1	-2.573224000	3.836233000	-0.416640000
8	3.851902000	2.488544000	0.071452000	1	-1.075671000	3.402189000	0.450331000
1	5.776300000	1.199495000	0.871530000	1	-0.645287000	1.354870000	1.102185000
				8	-0.914126000	-1.098194000	1.451356000
				1	-5.460171000	-2.593308000	-0.586004000
				1	-5.697627000	-0.077783000	-1.215787000
	5'C_3'				5'G_3'		
	3'_T5'				3'_G5'		
7	-5.377158000	0.463691000	-0.500417000	6	1.895964000	1.350433000	-0.841382000
6	-4.286230000	1.179736000	-0.012937000	6	2.966348000	0.665962000	-0.222187000
7	-3.239954000	0.495908000	0.513366000	7	4.095171000	1.162435000	0.433906000
6	-3.253728000	-0.841433000	0.572441000	6	4.740646000	0.088254000	0.809105000
6	-4.359788000	-1.598862000	0.074646000	7	4.126600000	-1.092279000	0.448066000
6	-5.399151000	-0.892477000	-0.446813000	6	2.980141000	-0.717056000	-0.215944000
1	-6.268265000	-1.427241000	-0.829826000	7	2.065766000	-1.565447000	-0.754587000
1	-4.369615000	-2.688527000	0.111461000	6	1.062119000	-0.921375000	-1.344049000
7	-2.208066000	-1.457518000	1.100854000	7	0.961039000	0.454778000	-1.389175000
1	-1.410999000	-0.909072000	1.454000000	1	5.681559000	0.123699000	1.358531000
1	-2.190923000	-2.485828000	1.159075000	7	0.071794000	-1.603711000	-1.927484000
8	-4.302001000	2.414994000	-0.081350000	1	0.087420000	-2.633802000	-1.928113000

Table S27. DNA H-bonding dimer geometries with methyls.

AT				GC			
6	2.540729000	1.138059000	0.026186000	7	4.652465000	-0.300170000	0.003821000
6	3.983127000	1.158057000	0.035913000	6	4.917918000	1.052861000	0.049946000
6	4.691080000	0.011067000	0.016893000	7	3.849576000	1.807015000	0.066827000
7	4.059787000	-1.207903000	-0.021938000	6	2.791680000	0.895235000	0.033331000
6	2.684837000	-1.320244000	-0.038262000	6	3.278426000	-0.399219000	-0.004755000
7	1.995459000	-0.124755000	-0.011009000	7	2.571237000	-1.558798000	-0.050081000
8	2.112367000	-2.395543000	-0.072788000	6	1.257106000	-1.349373000	-0.056359000
1	0.966853000	-0.182853000	-0.018984000	7	0.684331000	-0.095560000	-0.009779000
8	1.817245000	2.141046000	0.046717000	6	1.396423000	1.116138000	0.034737000
1	5.779897000	0.051395000	0.033048000	7	0.411153000	-2.383284000	-0.099280000
6	4.622164000	2.514135000	0.084041000	1	-0.605592000	-2.216884000	-0.096550000
1	5.703291000	2.410136000	-0.007574000	1	0.774611000	-3.346609000	-0.134772000
1	4.245393000	3.122969000	-0.737169000	1	-0.344112000	-0.043108000	-0.007193000
1	4.383183000	2.994739000	1.031811000	8	0.779010000	2.180595000	0.066734000
6	4.815961000	-2.463556000	-0.051079000	1	5.929794000	1.458000000	0.070062000
1	5.879366000	-2.229196000	-0.002660000	6	5.589812000	-1.409246000	-0.029554000
1	4.601233000	-3.014104000	-0.966986000	1	6.213677000	-1.417095000	0.865876000
1	4.536808000	-3.090407000	0.795815000	1	5.007261000	-2.331301000	-0.068433000
7	-0.953047000	-0.298378000	0.015951000	1	6.227750000	-1.350771000	-0.913116000
6	-1.618402000	-1.448344000	0.070880000	1	-0.874219000	2.385258000	-0.064800000
7	-2.915959000	-1.664656000	0.077130000	7	-1.890690000	2.544029000	-0.082137000
6	-3.582619000	-0.496401000	0.021782000	1	-2.261875000	3.503220000	-0.127250000
7	-4.943715000	-0.323231000	0.014165000	6	-2.722659000	1.514769000	-0.046061000
6	-5.148439000	1.028658000	-0.046137000	7	-2.203783000	0.281597000	0.012838000
7	-4.048511000	1.719486000	-0.083283000	6	-3.007844000	-0.809919000	0.046653000
6	-3.052800000	0.760354000	-0.029943000	8	-2.558888000	-1.961568000	0.101661000
6	-1.645329000	0.849944000	-0.036895000	7	-4.388587000	-0.625557000	0.026819000
1	-6.139026000	1.482125000	-0.061821000	6	-4.923698000	0.621004000	-0.030614000
1	-0.997237000	-2.342965000	0.117628000	6	-4.135859000	1.729514000	-0.062989000
7	-0.985265000	2.018014000	-0.091308000	1	-4.561799000	2.731975000	-0.100135000
1	0.045180000	2.028111000	-0.093562000	1	-6.007013000	0.735090000	-0.051313000
1	-1.508402000	2.904170000	-0.130557000	6	-5.231424000	-1.823752000	0.062672000
6	-5.935589000	-1.386913000	0.065683000	1	-5.005053000	-2.464615000	-0.789381000
1	-6.556513000	-1.294761000	0.958116000	1	-5.036409000	-2.390133000	0.973236000
1	-5.396150000	-2.334675000	0.100698000	1	-6.277185000	-1.518220000	0.031389000
1	-6.570339000	-1.367655000	-0.821558000				

Table S28. RNA H-bonding dimer geometries with methyls.

AU				GC			
6	-2.704511000	1.476872000	-0.150963000	6	-1.255570000	-1.349998000	0.028736000
7	-2.249129000	0.175204000	0.003504000	7	-0.683308000	-0.094959000	-0.008246000
6	-3.027428000	-0.955818000	0.109931000	6	-1.395946000	1.116762000	-0.030904000
7	-4.383675000	-0.751568000	0.055488000	6	-2.791759000	0.895299000	-0.018250000
6	-4.923924000	0.503732000	-0.105260000	6	-3.277888000	-0.399703000	0.008878000
6	-4.141677000	1.591779000	-0.200614000	7	-2.569355000	-1.559258000	0.032947000
1	-4.598412000	2.574046000	-0.317307000	7	-4.651353000	-0.300627000	0.015116000
1	-6.006390000	0.617627000	-0.156097000	6	-4.917889000	1.052319000	-0.011823000
8	-1.908305000	2.408235000	-0.244288000	7	-3.849587000	1.806973000	-0.030155000
1	-1.228347000	0.041639000	0.042087000	1	-5.929943000	1.456873000	-0.016946000
8	-2.520963000	-2.057890000	0.251919000	8	-0.779604000	2.181905000	-0.055988000
6	-5.230413000	-1.944894000	0.161069000	1	0.345577000	-0.041514000	-0.020460000
1	-5.033862000	-2.622729000	-0.669347000	7	-0.408131000	-2.383391000	0.050543000
1	-6.274328000	-1.633907000	0.126282000	1	-0.771199000	-3.346545000	0.077920000
1	-5.029978000	-2.463800000	1.098216000	1	0.608681000	-2.216449000	0.039719000
1	-0.160341000	2.179484000	0.221541000	6	-5.585093000	-1.406221000	0.040376000
7	0.866923000	2.100299000	0.231526000	1	-6.243051000	-1.367976000	0.911198000
1	1.447674000	2.943279000	0.348224000	1	-5.021438000	-2.341141000	0.070774000
6	1.450567000	0.895075000	0.092229000	1	-6.232118000	-1.418835000	-0.839341000
7	0.680873000	-0.193107000	-0.059986000	7	2.204471000	0.283801000	-0.054976000
6	1.265228000	-1.385245000	-0.209345000	6	2.722817000	1.516170000	0.013891000
7	2.554943000	-1.684015000	-0.219039000	6	4.135584000	1.729015000	0.074329000
6	3.287408000	-0.570929000	-0.057141000	6	4.921703000	0.618525000	0.072684000
6	2.845122000	0.713220000	0.096115000	7	4.386873000	-0.627229000	0.004850000
7	3.908492000	1.587676000	0.232219000	6	3.007227000	-0.809305000	-0.057658000
6	4.956259000	0.824345000	0.150388000	8	2.557513000	-1.960203000	-0.120771000
7	4.660052000	-0.496468000	-0.024848000	7	1.892750000	2.547266000	0.018230000
1	5.976339000	1.202813000	0.215251000	1	0.875945000	2.390515000	-0.030326000
1	0.586424000	-2.227892000	-0.340992000	1	2.263312000	3.507006000	0.070090000
6	5.574470000	-1.621045000	-0.153204000	1	4.561506000	2.731687000	0.119711000
1	6.227063000	-1.491808000	-1.017295000	1	6.004411000	0.731761000	0.126992000
1	4.970271000	-2.518450000	-0.290460000	6	5.228448000	-1.826831000	-0.001092000
1	6.182074000	-1.731772000	0.747579000	1	4.976147000	-2.463810000	0.846578000
				1	5.059214000	-2.396652000	-0.914659000
				1	6.273336000	-1.522754000	0.059650000

Table S29. DNA H-bonding dimer geometries with hydrogens.

AT				GC			
6	3.108113000	-0.583999000	-0.016616000	7	2.182900000	-0.045968000	0.021842000
6	1.699049000	-0.642654000	-0.028724000	6	2.717337000	-1.272416000	-0.038291000
7	1.031977000	0.520667000	0.020165000	6	4.133158000	-1.469453000	-0.051044000
6	1.722232000	1.655807000	0.076212000	6	4.906972000	-0.351272000	-0.013396000
6	3.665225000	0.660878000	0.035592000	7	4.356138000	0.888365000	0.045250000
7	3.024197000	1.843567000	0.087055000	6	2.973141000	1.055419000	0.060943000
7	4.082699000	-1.564841000	-0.065089000	1	5.991690000	-0.451769000	-0.030772000
6	5.197396000	-0.898299000	-0.024654000	1	4.571713000	-2.466422000	-0.089179000
7	5.022206000	0.457838000	0.033271000	8	2.509650000	2.201233000	0.117222000
1	1.120707000	2.563918000	0.119571000	7	1.898419000	-2.311895000	-0.079597000
7	1.013683000	-1.796009000	-0.084212000	1	0.879992000	-2.165874000	-0.065253000
1	-0.016719000	-1.783468000	-0.090308000	1	2.281708000	-3.266263000	-0.125778000
1	1.517364000	-2.693493000	-0.120449000	1	4.913721000	1.728667000	0.075125000
1	6.177830000	-1.373438000	-0.036094000	6	-1.297854000	1.541815000	-0.054930000
1	5.726995000	1.176985000	0.069283000	7	-0.709611000	0.295143000	-0.009456000
6	-3.935049000	-0.826943000	0.023405000	6	-1.406648000	-0.925458000	0.029790000
6	-4.617551000	0.335298000	0.000372000	6	-2.804544000	-0.721996000	0.024282000
7	-3.959484000	1.540054000	-0.037551000	6	-3.307301000	0.566367000	-0.012315000
6	-2.582347000	1.622140000	-0.048868000	7	-2.614514000	1.734795000	-0.052512000
6	-2.492534000	-0.838651000	0.019048000	7	-3.851068000	-1.646996000	0.052080000
7	-1.919512000	0.411830000	-0.017612000	6	-4.928690000	-0.906205000	0.033462000
1	-0.889855000	0.447305000	-0.021810000	1	0.319392000	0.255534000	-0.003583000
8	-1.791346000	-1.857264000	0.043479000	8	-0.776089000	-1.982196000	0.061283000
1	-5.707043000	0.318922000	0.012504000	7	-0.464752000	2.586312000	-0.092564000
8	-1.986261000	2.684557000	-0.082534000	1	0.553979000	2.432617000	-0.086858000
6	-4.603905000	-2.168591000	0.070760000	1	-0.840101000	3.545106000	-0.126952000
1	-5.682138000	-2.040981000	-0.025021000	7	-4.680016000	0.450145000	-0.008537000
1	-4.379063000	-2.653122000	1.019988000	1	-5.935484000	-1.323997000	0.049248000
1	-4.237559000	-2.786601000	-0.748310000	1	-5.340990000	1.209988000	-0.030590000
1	-4.443810000	2.423979000	-0.058276000				

Table S30. RNA H-bonding dimer geometries with hydrogens.

AU				GC			
7	2.226748000	0.083885000	0.028960000	6	4.907847000	-0.355124000	-0.034019000
6	2.693725000	-1.213862000	-0.123867000	6	4.135120000	-1.454878000	-0.170596000
6	4.132191000	-1.317738000	-0.157646000	6	2.709306000	-1.261978000	-0.115250000
6	4.905017000	-0.224064000	-0.050570000	7	2.175274000	-0.046877000	0.061300000
7	4.353462000	1.026656000	0.107459000	6	2.975828000	1.045695000	0.199890000
6	2.995174000	1.220473000	0.147179000	7	4.354978000	0.883991000	0.148315000
1	5.988821000	-0.329613000	-0.089523000	1	5.993036000	-0.456008000	-0.069690000
1	4.597669000	-2.296189000	-0.271828000	1	4.570781000	-2.443788000	-0.315494000
8	1.905727000	-2.150969000	-0.228651000	7	1.895098000	-2.293440000	-0.249474000
1	1.204610000	0.209605000	0.056408000	1	2.280827000	-3.238273000	-0.386430000
8	2.478777000	2.318278000	0.286417000	1	0.875911000	-2.151540000	-0.216862000
1	4.918998000	1.857690000	0.188843000	8	2.519678000	2.184112000	0.363059000
1	0.150949000	-1.936761000	0.218085000	1	4.914976000	1.716640000	0.252123000
7	-0.876935000	-1.865390000	0.216717000	7	-0.711420000	0.294725000	-0.047410000
1	-1.452531000	-2.713066000	0.324606000	6	-1.404046000	-0.919897000	0.083860000
6	-1.468129000	-0.664240000	0.074097000	6	-2.804826000	-0.715663000	0.079458000
7	-0.705073000	0.430160000	-0.066520000	6	-3.299923000	0.555908000	-0.048024000
6	-1.296766000	1.618245000	-0.219244000	7	-2.619264000	1.729579000	-0.175842000
7	-2.588527000	1.907260000	-0.242653000	6	-1.309529000	1.541475000	-0.164769000
6	-3.314275000	0.788212000	-0.092001000	7	-0.465999000	2.568127000	-0.279684000
6	-2.863983000	-0.492969000	0.062774000	1	0.550741000	2.402357000	-0.277178000
7	-3.922132000	-1.375831000	0.184548000	1	-0.830871000	3.527580000	-0.371476000
6	-4.974689000	-0.620237000	0.092979000	1	0.318246000	0.257481000	-0.057702000
7	-4.686589000	0.703263000	-0.075362000	8	-0.773353000	-1.973711000	0.192141000
1	-0.622956000	2.466373000	-0.340977000	7	-3.845886000	-1.639976000	0.181315000
1	-5.992525000	-1.006601000	0.145338000	6	-4.925743000	-0.901710000	0.113434000
1	-5.325349000	1.477155000	-0.167319000	7	-4.680393000	0.447704000	-0.028457000
				1	-5.931717000	-1.318567000	0.164916000
				1	-5.333455000	1.211105000	-0.098156000

Full Citations for Truncated References (5a and 12)

- (5) (a) Olson, W. K.; Bansal, M.; Burley, S. K.; Dikerson, R. E.; Gerstein, M.; Harvey, S. C.; Heinemann, U.; Lu, X.-J.; Neidle, S.; Shakked, Z.; Sklenar, H.; Suzuki, M.; Tung, C.-S.; Westhof, E.; Wolberger, C.; Berman, H. M. *J. Mol. Biol.* **2001**, *313*, 229, 237.
- (12) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision A.1*, Gaussian, Inc., Wallingford CT, 2009.