SUPPORTING INFORMATION

Internal Loop-Helix Coupling in the Dynamics of the RNA Duplex $(GC^*C^*AGUUCGCUGGC)_2$

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PARAMETERS FOR 5-BROMOCYTOSINE

```
--5-Bromo CYTOSINE RNA - with 5' - Phosphate and 3' - O
5Br.dat
5Br  INT    0
CORRECT OMIT DU   BEG
 0.0
 1  DUMM  DU   M   0 -1 -2   0.00    0.00    0.00    0.0000
 2  DUMM  DU   M   1  0 -1   1.00    0.00    0.00    0.0000
 3  DUMM  DU   M   2  1  0   1.00   90.00    0.00    0.0000
 4  P     P    M   3  2  1   1.60  119.04  200.00    1.1662
 5  O1P   O2   E   4  3  2   1.48  109.61  150.00   -0.7760
 6  O2P   O2   E   4  3  2   1.48  109.58   20.00   -0.7760
 7  O5'   OS   M   4  3  2   1.60  101.43  -98.89   -0.4989
 8  C5'   CT   M   7  4  3   1.44  119.00  -39.22    0.0558
 9  H5'1  H1   E   8  7  4   1.09  109.50   60.00    0.0679
10  H5'2  H1   E   8  7  4   1.09  109.50  -60.00    0.0679
11  C4'   CT   M   8  7  4   1.52  110.00  180.00    0.1065
12  H4'   H1   E  11  8  7   1.09  109.50 -200.00    0.1174
13  O4'   OS   S  11  8  7   1.46  108.86  -86.31   -0.3548
14  C1'   CT   B  13 11  8   1.42  110.04  105.60   -0.0365
15  H1'   H2   E  14 13 11   1.09  109.50 -240.00    0.2029
16  N1    N*   S  14 13 11   1.49  108.10 -127.70   -0.1614
17  C6    CM   B  16 14 13   1.36  121.10   81.59    0.2839
18  H6    H4   E  17 16 14   1.08  120.00    0.00    0.1634
19  C5    CM   B  17 16 14   1.36  121.00  180.00   -0.5891
20  Br5   BR   E  19 17 16   1.89  120.00  180.00   -0.0453
21  C4    CA   B  19 17 16   1.43  116.90    0.00    1.0795
22  N4    N2   B  21 19 17   1.32  120.10  180.00   -1.0858
23  H41   H    E  22 21 19   1.01  117.70  180.00    0.47495
24  H42   H    E  22 21 19   1.01  120.27    0.00    0.47925
25  N3    NC   S  21 19 17   1.33  121.70    0.00   -0.8434
26  C2    C    S  25 21 19   1.36  120.50    0.00    0.8012
27  O2    O    E  26 25 21   1.24  122.40  180.00   -0.6076
28  C3'   CT   M  11  8  7   1.53  115.78 -329.11    0.2022
29  H3'   H1   E  28 11  8   1.09  109.50   30.00    0.0615
30  C2'   CT   B  28 11  8   1.53  102.80  -86.30    0.0670
31  H2'1  H1   E  30 28 11   1.09  109.50  120.00    0.0972
32  O2'   OH   S  30 28 11   1.43  109.50  240.00   -0.6139
33  HO'2  HO   E  32 30 28   0.96  107.00  180.00    0.4186
34  O3'   OS   M  28 11  8   1.42  116.52 -203.47   -0.5246

IMPROPER
C6  C2  N1  C1'
N1  N3  C2  O2
C4  H41 N4  H42
N1  C5  C6  H6
C6  C4  C5  Br5
N3  C5  C4  N4

LOOP CLOSING EXPLICIT
C1' C2'
C2  N1
```

PARAMETERS FOR 5-BROMOCYTOSINE (cont.)

Extra parameters for 5-bromocytosine

```
MASS
BR     79.90

NONB
 BR         2.3300  0.2700

BOND
CM BR  260.1   1.889

ANGL
CA CM BR    75.4     122.57
CM CM BR    75.4     121.03

DIHE
X  CA CM BR   4       10.20       180.0       2.0
X  CM CM BR   4       26.60       180.0       2.0

IMPR
CM CA CM BR         10.20       180.0       2.0
```

EQUILIBRATION PROTOCOL

Name	Length	Temp	RNA Force Constant	Na^+ Force Constant	Water Force Constant
min1	*	-	not minimized	not minimized	minimize
min2	*	-	minimize	minimize	minimize
md1	10 ps	100 K	100.0	100.0	0.0
md2	10 ps	100 K	100.0	0.0	0.0
md3	10 ps	100-300 K	100.0	0.0	0.0
md4	10 ps	300 K	50.0	0.0	0.0
md5	10 ps	300 K	25.0	0.0	0.0
md6	10 ps	300 K	10.0	0.0	0.0
md7	10 ps	300 K	5.0	0.0	0.0
md8	10 ps	300 K	2.0	0.0	0.0
md9	10 ps	300 K	1.0	0.0	0.0
production	4000 ps	300 K	0.0	0.0	0.0

* Steepest decent followed by conjugate gradient minimization

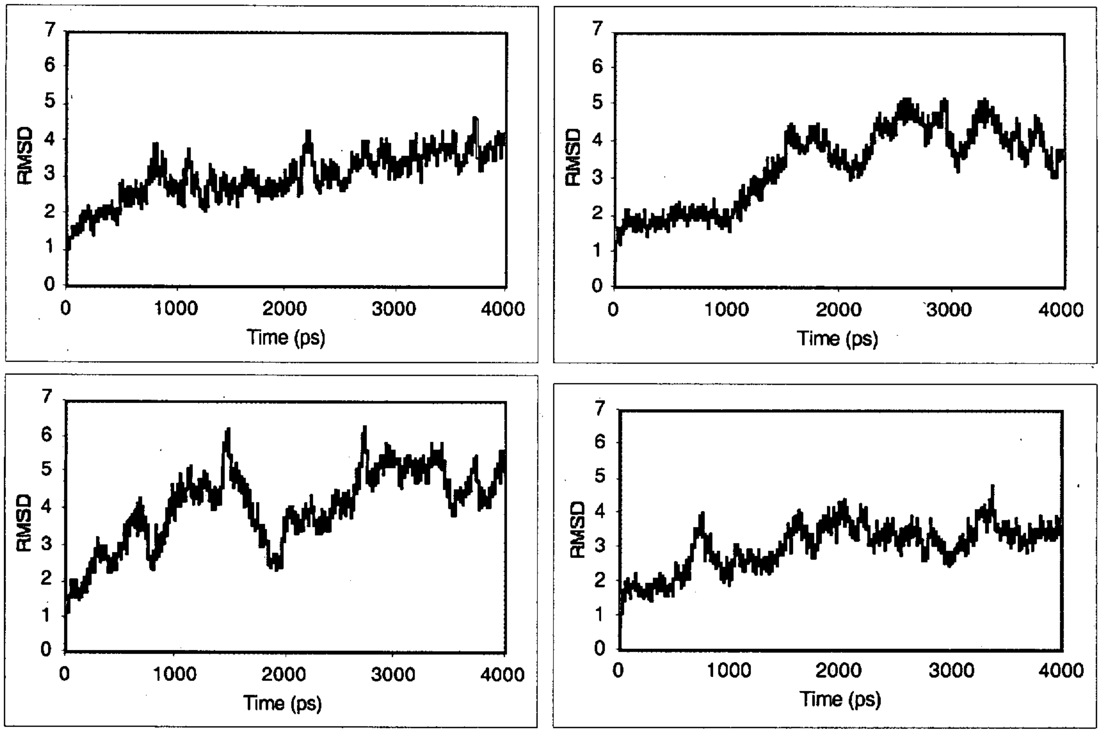

Figure S1. All atom RMS deviations (Å) for the three trajectories (I top left, II top right, III bottom left, Ia bottom right) with respect to their equilibrated starting structures.

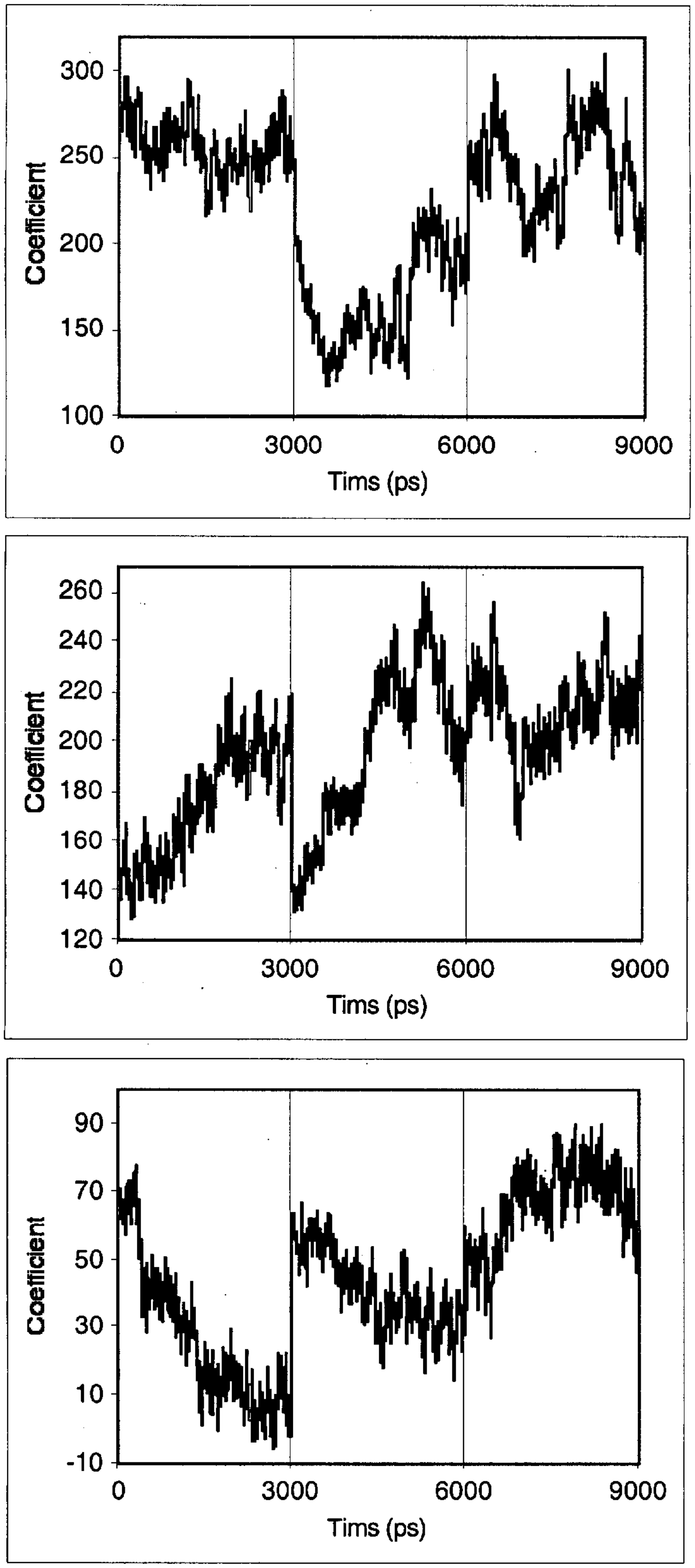

Figure S2. Time plots of the coefficients of the first three principal components (top to bottom) for the three separate trajectories (left to right within the individual plots).

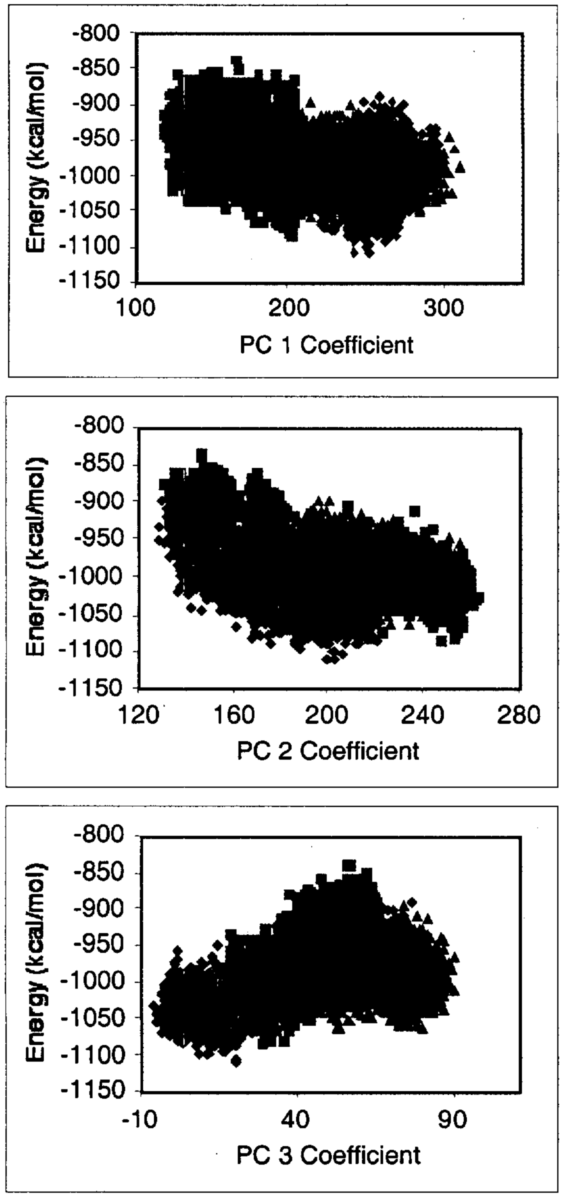

Figure S3. Plots of the forcefield energy as a function of the coefficient of the first three principal components (top to bottom) for the three separate trajectories (red, green, blue). Hydrogen positions were minimized while restraining heavy atom positions.

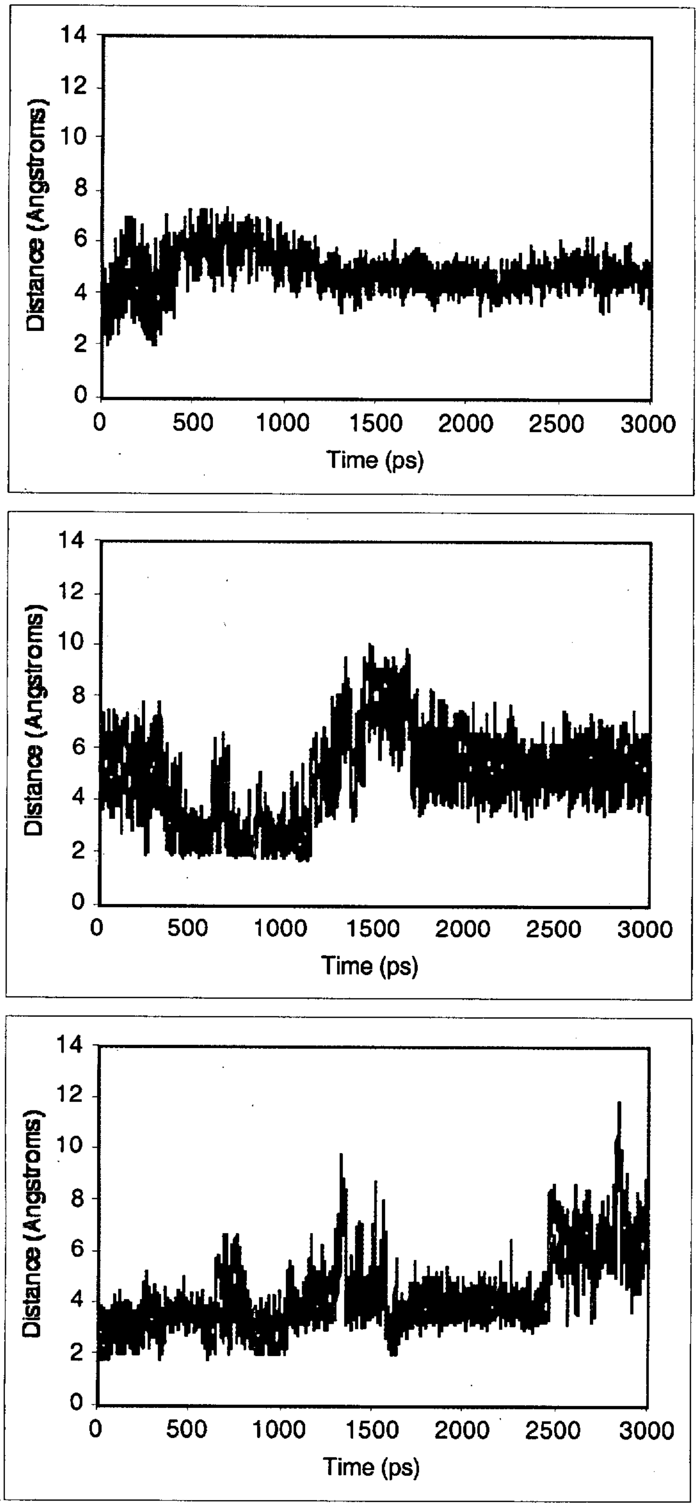

Figure S4. Intermolecular hydrogen bond lengths after removal of the first 1 ns from each trajectory for C8:C22 for the three trajectories (top to bottom). Curves are blue for C8(H42):C22(O2), and pink for C8(H42):C22(N3).

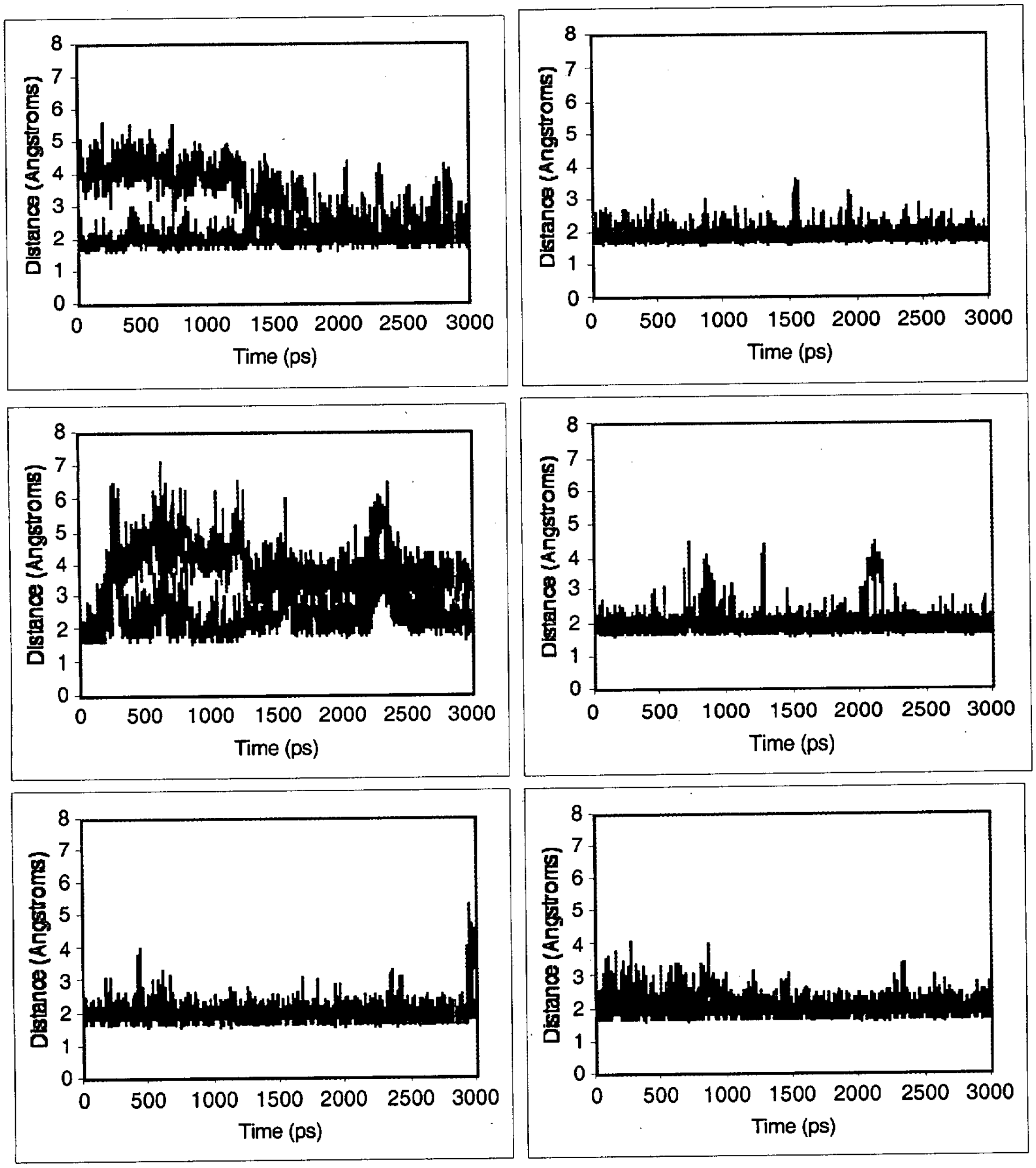

Figure S5. Hydrogen bond lengths after removal of the first 1 ns of each trajectory for the G:U wobble pairs (Pair 6:23 is left, and 9:20 is right) for trajectories I-III (top to bottom). The curves are blue for U(O2):G(H1) and pink for U(H3):G(O6).

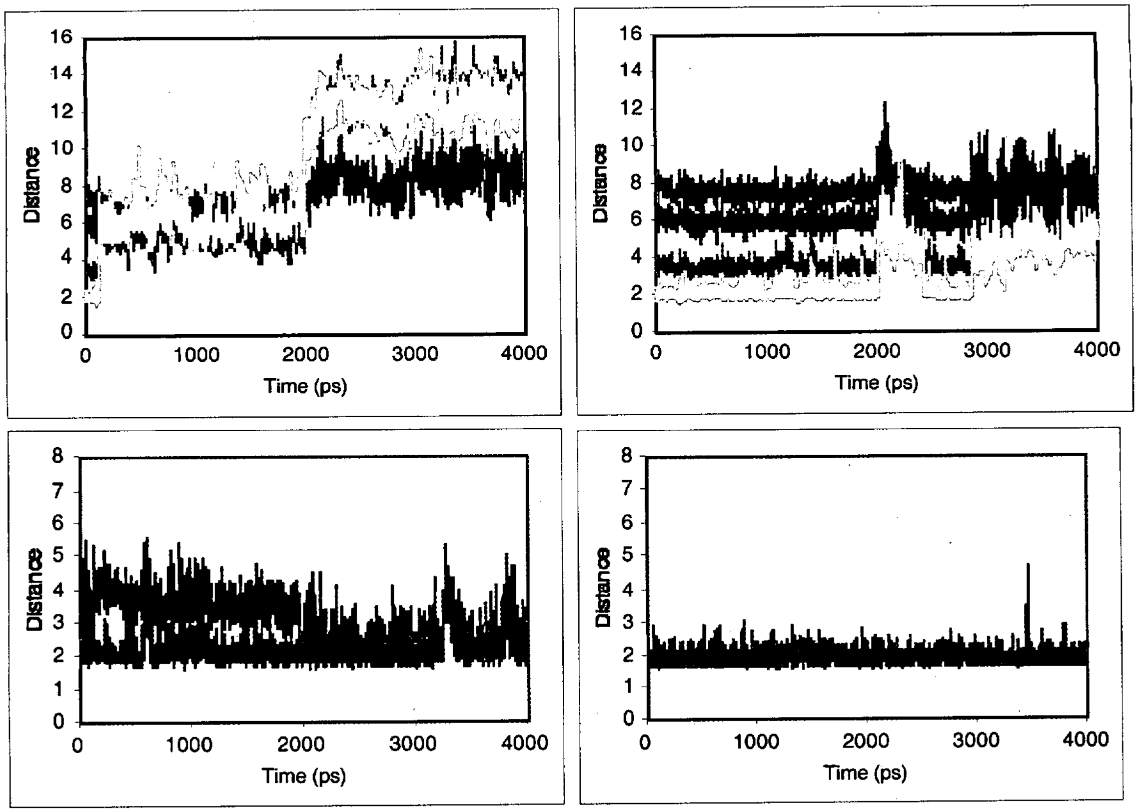

Figure S6. Hydrogen bond lengths from trajectory Ia. Time plots (ps) of H42 to O4 (cyan), H41 to O4 (yellow), H42 to O2 (magenta), and H41 to O2 (blue) distances (Å) for U7:C22 (top left) and C8:U21 (top right) base pairs. Time plots for the G:U wobble pairs (Pair 6:23 is bottom left, and 9:20 is bottom right) are blue for U(O2):G(H1) and pink for U(H3):G(O6). Distances in Å.