CAPÍTOL V- ANNEX

1. PUBLICACIONS

Part del treball realitzat en aquesta tesi ha donat lloc a les següents publicacions:

1. Valls, N., Wright, G., Steiner, R. A., Murshudov, G. N. i Subirana, J. A. DNA variability in five crystal structures of d(CGCAATTGCG). *Acta Cryst.* **D60**, 680-685 (2004).
2. Valls, N., Usón, I., Gouyette, C. i Subirana, J. A. A cubic arrangement of DNA double helices based on nickel-guanine interactions. *J. Am. Chem. Soc*. **126**, 7812-7816 (2004).
3. Valls, N., Steiner, R. A., Wright, G., Murshudov, G. N. i Subirana, J. A. Variable role of ions in two drug intercalation complexes of DNA. *En preparació.*

2. PARÀMETRES CONFORMACIONALS

Tots els paràmetres conformacionals de les estructures resoltes s'han calculat amb el programa 3DNA. En alguns casos s'han eliminat les bases terminals que no formen part del dúplex.

2.1 ESTRUCTURA d(CGCAATTGCG)

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**********************************************************************
**********************************************************************
    3DNA (v1.5, Nov. 2002) by Xiang-Jun Lu at Wilma K. Olson's Lab.
**********************************************************************
1. The list of the parameters given below correspond to the 5' to 3' direction
   of strand I and 3' to 5' direction of strand II.

2. All angular parameters, except for the phase angle of sugar pseudo-
   rotation, are measured in degrees in the range of [-180, +180], and all
   displacements are measured in Angstrom units.
**********************************************************************
File name: duplex_nuria_r1.pdb
Date and time: Tue Jul 22 13:04:07 2003

Number of base-pairs: 8
Number of atoms: 328
**********************************************************************
**********************************************************************
RMSD of the bases (----- for WC bp, + for isolated bp, x for helix change)

            Strand I                    Strand II          Helix
   1   (0.020) A:...2_:[..G]G-----C[..C]:...9_:A (0.023)     |
   2   (0.022) A:...3_:[..C]C-----G[..G]:...8_:A (0.016)     |
   3   (0.022) A:...4_:[..A]A-----T[..T]:...7_:A (0.022)     |
   4   (0.010) A:...5_:[..A]A-----T[..T]:...6_:A (0.018)     |
   5   (0.018) A:...6_:[..T]T-----A[..A]:...5_:A (0.010)     |
   6   (0.022) A:...7_:[..T]T-----A[..A]:...4_:A (0.022)     |
   7   (0.016) A:...8_:[..G]G-----C[..C]:...3_:A (0.022)     |
   8   (0.023) A:...9_:[..C]C-----G[..G]:...2_:A (0.020)     |
**********************************************************************
Detailed H-bond information: atom-name pair and length [ON]
   1 G-----C  [3]  N2 - O2  2.71  N1 - N3  2.93  O6 - N4  2.95
   2 C-----G  [3]  O2 - N2  2.70  N3 - N1  2.88  N4 - O6  2.90
   3 A-----T  [2]  N1 - N3  2.83  N6 - O4  3.08
   4 A-----T  [2]  N1 - N3  2.90  N6 - O4  3.19
   5 T-----A  [2]  N3 - N1  2.90  O4 - N6  3.19
   6 T-----A  [2]  N3 - N1  2.83  O4 - N6  3.08
   7 G-----C  [3]  N2 - O2  2.70  N1 - N3  2.88  O6 - N4  2.90
   8 C-----G  [3]  O2 - N2  2.71  N3 - N1  2.93  N4 - O6  2.95
**********************************************************************
Overlap area in Angstrom^2 between polygons defined by atoms on successive
bases. Polygons projected in the mean plane of the designed base-pair step.

Values in parentheses measure the overlap of base ring atoms only. Those
outside parentheses include exocyclic atoms on the ring. Intra- and
inter-strand overlap is designated according to the following diagram:

                    i2  3'      5' j2
                       /|\      |
                        |       |
                Strand I |      | II
                        |       |
                        |       |
                        |      \|/
                    i1  5'      3' j1
```

```
     step      i1-i2        i1-j2        j1-i2        j1-j2        sum
   1 GC/GC  4.58( 2.46)  0.00( 0.00)  0.00( 0.00)  4.11( 1.99)  8.69( 4.44)
   2 CA/TG  0.66( 0.00)  0.00( 0.00)  0.13( 0.00)  1.82( 0.13)  2.61( 0.13)
   3 AA/TT  3.81( 2.42)  0.00( 0.00)  0.00( 0.00)  5.32( 0.13)  9.13( 2.55)
   4 AT/AT  5.41( 1.68)  0.00( 0.00)  0.00( 0.00)  5.41( 1.68) 10.82( 3.36)
   5 TT/AA  5.32( 0.13)  0.00( 0.00)  0.00( 0.00)  3.81( 2.42)  9.13( 2.55)
   6 TG/CA  1.82( 0.13)  0.00( 0.00)  0.13( 0.00)  0.66( 0.00)  2.60( 0.13)
   7 GC/GC  4.11( 1.99)  0.00( 0.00)  0.00( 0.00)  4.59( 2.46)  8.69( 4.45)
***************************************************************************
Origin (Ox, Oy, Oz) and mean normal vector (Nx, Ny, Nz) of each base-pair in
   the coordinate system of the given structure

      bp        Ox        Oy        Oz        Nx        Ny        Nz
    1 G-C       0.00      0.00      0.00      0.00      0.00      1.00
    2 C-G       0.17     -0.12      3.15      0.00      0.00      1.00
    3 A-T       0.05     -0.33      6.47      0.09      0.06      0.99
    4 A-T       0.56     -0.01      9.71      0.06      0.05      1.00
    5 T-A       1.18      0.28     12.95      0.09      0.00      1.00
    6 T-A       1.77      0.48     16.19      0.11      0.03      0.99
    7 G-C       1.56      0.42     19.51      0.01     -0.02      1.00
    8 C-G       1.59      0.56     22.67      0.01     -0.02      1.00
***************************************************************************
Local base-pair parameters
     bp        Shear    Stretch   Stagger    Buckle  Propeller  Opening
    1 G-C      -0.35     -0.16      0.04     -2.71     -1.19     -0.03
    2 C-G       0.26     -0.17      0.04      5.53     -5.60      0.89
    3 A-T      -0.15     -0.13     -0.11      3.80    -15.21      1.59
    4 A-T      -0.02     -0.06      0.08      1.31    -16.60      4.77
    5 T-A       0.02     -0.06      0.08     -1.28    -16.60      4.78
    6 T-A       0.15     -0.13     -0.11     -3.82    -15.20      1.59
    7 G-C      -0.26     -0.17      0.04     -5.51     -5.59      0.89
    8 C-G       0.35     -0.16      0.04      2.73     -1.22     -0.04
          ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.      0.00     -0.13      0.01      0.01     -9.65      1.81
      s.d.      0.24      0.05      0.08      3.93      6.91      1.94
***************************************************************************
Local base-pair step parameters
    step       Shift     Slide      Rise      Tilt      Roll     Twist
   1 GC/GC      0.13     -0.15      3.15      0.14     -0.04     31.85
   2 CA/TG     -0.41      0.00      3.30      1.70      6.08     33.24
   3 AA/TT      0.17     -0.25      3.28     -2.05     -0.48     36.16
   4 AT/AT      0.00     -0.44      3.29      0.01     -3.65     34.90
   5 TT/AA     -0.17     -0.25      3.28      2.03     -0.46     36.16
   6 TG/CA      0.41      0.00      3.30     -1.70      6.08     33.25
   7 GC/GC     -0.13     -0.15      3.15     -0.14     -0.05     31.84
         ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.      0.00     -0.18      3.25      0.00      1.07     33.91
      s.d.      0.27      0.16      0.07      1.54      3.65      1.85
***************************************************************************
Local base-pair helical parameters
    step       X-disp    Y-disp   h-Rise     Incl.       Tip   h-Twist
   1 GC/GC     -0.27     -0.22      3.15     -0.08     -0.25     31.85
   2 CA/TG     -0.99      0.98      3.23     10.51     -2.94     33.82
   3 AA/TT     -0.34     -0.56      3.27     -0.77      3.30     36.22
   4 AT/AT     -0.17      0.00      3.32     -6.07     -0.02     35.09
   5 TT/AA     -0.34      0.56      3.27     -0.74     -3.27     36.21
   6 TG/CA     -0.99     -0.98      3.23     10.51      2.94     33.83
   7 GC/GC     -0.27      0.22      3.15     -0.09      0.26     31.84
         ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.     -0.48      0.00      3.23      1.90      0.00     34.12
      s.d.      0.35      0.66      0.06      6.24      2.55      1.84
***************************************************************************
Structure classification:

This is a right-handed nucleic acid structure
***************************************************************************
lambda: virtual angle between C1'-YN1 or C1'-RN9 glycosidic bonds and the
        base-pair C1'-C1' line

C1'-C1': distance between C1' atoms for each base-pair
RN9-YN1: distance between RN9-YN1 atoms for each base-pair
RC8-YC6: distance between RC8-YC6 atoms for each base-pair

    bp     lambda(I) lambda(II)  C1'-C1'   RN9-YN1   RC8-YC6
   1 G-C      53.3      53.4      10.7       8.9       9.8
   2 C-G      55.1      54.2      10.6       8.9       9.8
   3 A-T      52.0      55.7      10.6       8.9       9.8
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   4 A-T      54.2      54.3      10.5       8.8       9.9
   5 T-A      54.4      54.1      10.5       8.8       9.9
   6 T-A      55.7      52.0      10.6       8.9       9.8
   7 G-C      54.2      55.1      10.6       8.9       9.8
   8 C-G      53.4      53.3      10.7       8.9       9.8
**************************************************************************
Classification of each dinucleotide step in a right-handed nucleic acid
structure: A-like; B-like; TA-like; intermediate of A and B, or other cases

    step       Xp      Yp      Zp     XpH     YpH     ZpH    Form
   1 GC/GC   -3.42    9.26   -0.63   -3.69    9.26   -0.64     B
   2 CA/TG   -3.06    8.98   -0.30   -4.04    8.89    1.31     B
   3 AA/TT   -3.19    9.08   -0.39   -3.49    9.07   -0.51     B
   4 AT/AT   -3.41    9.14   -0.36   -3.57    9.05   -1.28     B
   5 TT/AA   -3.19    9.08   -0.39   -3.49    9.07   -0.50     B
   6 TG/CA   -3.06    8.98   -0.30   -4.04    8.89    1.31     B
   7 GC/GC   -3.42    9.26   -0.63   -3.69    9.26   -0.65     B
**************************************************************************
Minor and major groove widths: direct P-P distances and refined P-P distances
   which take into account the directions of the sugar-phosphate backbones

   (Subtract 5.8 Angstrom from the values to take account of the vdw radii
    of the phosphate groups, and for comparison with FreeHelix and Curves.)

Ref: M. A. El Hassan and C. R. Calladine (1998). ``Two Distinct Modes of
     Protein-induced Bending in DNA.'' J. Mol. Biol., v282, pp331-343.

                Minor Groove        Major Groove
               P-P     Refined     P-P     Refined
   1 GC/GC     ---       ---       ---       ---
   2 CA/TG     ---       ---       ---       ---
   3 AA/TT     9.8       ---      18.7       ---
   4 AT/AT     9.0       9.0      16.9      16.9
   5 TT/AA     9.8       ---      18.7       ---
   6 TG/CA     ---       ---       ---       ---
   7 GC/GC     ---       ---       ---       ---
**************************************************************************
Global linear helical axis defined by equivalent C1' and RN9/YN1 atom pairs
Deviation from regular linear helix: 3.31(0.25)
Helix:     0.048   0.013   0.999
HETATM 9998  XS    X X 999       0.208   0.179  -0.254
HETATM 9999  XE    X X 999       1.329   0.472  22.923
Average and standard deviation of helix radius:
      P: 9.71(0.39), O4': 6.53(0.23),  C1': 6.06(0.20)

Global parameters based on C1'-C1' vectors:

disp.: displacement of the middle C1'-C1' point from the helix
angle: inclination between C1'-C1' vector and helix (subtracted from 90)
twist: helical twist angle between consecutive C1'-C1' vectors
rise:  helical rise by projection of the vector connecting consecutive
       C1'-C1' middle points onto the helical axis

     bp       disp.    angle     twist      rise
   1 G-C      2.69      0.07     28.38      3.54
   2 C-G      2.89     -2.33     35.50      3.53
   3 A-T      3.25     -3.42     35.47      3.07
   4 A-T      2.93     -3.26     34.59      2.92
   5 T-A      2.93     -3.27     35.47      3.08
   6 T-A      3.25     -3.43     35.49      3.53
   7 G-C      2.89     -2.33     28.38      3.54
   8 C-G      2.69      0.07      ---       ---
**************************************************************************
Main chain and chi torsion angles:

Note: alpha:   O3'(i-1)-P-O5'-C5'
      beta:    P-O5'-C5'-C4'
      gamma:   O5'-C5'-C4'-C3'
      delta:   C5'-C4'-C3'-O3'
      epsilon: C4'-C3'-O3'-P(i+1)
      zeta:    C3'-O3'-P(i+1)-O5'(i+1)

      chi for pyrimidines(Y): O4'-C1'-N1-C2
          chi for purines(R): O4'-C1'-N9-C4

Strand I
  base    alpha    beta   gamma   delta  epsilon   zeta    chi
   1 G     ---   -142.0    51.1   145.0   179.8   -95.6   -96.4
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2 C	-60.8	168.7	49.7	101.9	168.2	-92.5	-116.4
3 A	-47.8	-177.8	44.9	136.9	176.9	-96.8	-110.4
4 A	-47.2	177.9	42.0	127.8	179.1	-93.8	-111.5
5 T	-58.2	174.1	55.1	118.9	-178.3	-98.8	-121.1
6 T	-50.8	172.8	51.6	122.0	-173.5	-87.8	-110.1
7 G	-65.4	179.0	52.7	123.8	-161.4	-99.4	-108.4
8 C	-50.1	169.6	35.6	132.7	---	---	-104.6

Strand II

base	alpha	beta	gamma	delta	epsilon	zeta	chi
1 C	-50.1	169.6	35.6	132.7	---	---	-104.6
2 G	-65.3	179.0	52.7	123.8	-161.5	-99.3	-108.4
3 T	-50.8	172.8	51.7	121.9	-173.5	-87.8	-110.2
4 T	-58.1	174.1	55.1	118.8	-178.3	-98.8	-121.1
5 A	-47.2	177.9	42.1	127.7	179.1	-93.8	-111.5
6 A	-47.8	-177.8	44.9	137.0	176.9	-96.9	-110.4
7 C	-60.9	168.8	49.7	102.1	168.2	-92.5	-116.3
8 G	---	-142.0	51.0	145.1	179.8	-95.6	-96.5

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Sugar conformational parameters:

Note: v0: C4'-O4'-C1'-C2'
v1: O4'-C1'-C2'-C3'
v2: C1'-C2'-C3'-C4'
v3: C2'-C3'-C4'-O4'
v4: C3'-C4'-O4'-C1'

tm: amplitude of pseudorotation of the sugar ring
P: phase angle of pseudorotation of the sugar ring

Strand I

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 G	-10.3	26.6	-32.3	26.7	-10.6	32.3	180.3	C3'-exo
2 C	-37.4	27.4	-7.8	-13.7	31.8	36.6	102.2	O4'-endo
3 A	-25.4	35.3	-31.2	16.9	5.0	35.0	153.1	C2'-endo
4 A	-27.0	35.1	-28.4	13.2	8.4	33.9	146.7	C2'-endo
5 T	-37.8	38.9	-25.2	3.9	21.1	39.5	129.6	C1'-exo
6 T	-32.0	36.6	-27.6	9.9	13.7	36.3	139.6	C1'-exo
7 G	-37.0	40.2	-28.4	7.5	18.6	40.4	134.7	C1'-exo
8 C	-35.4	45.9	-38.1	18.4	10.9	45.1	147.8	C2'-endo

Strand II

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-35.4	45.9	-38.2	18.4	10.9	45.1	147.9	C2'-endo
2 G	-37.1	40.3	-28.5	7.6	18.6	40.4	134.8	C1'-exo
3 T	-32.0	36.5	-27.6	9.9	13.6	36.2	139.7	C1'-exo
4 T	-37.8	38.8	-25.2	3.9	21.1	39.5	129.6	C1'-exo
5 A	-26.9	35.1	-28.4	13.2	8.3	33.9	146.8	C2'-endo
6 A	-25.4	35.3	-31.2	16.9	5.0	35.0	153.1	C2'-endo
7 C	-37.4	27.4	-7.8	-13.7	31.8	36.7	102.2	O4'-endo
8 G	-10.3	26.5	-32.3	26.7	-10.5	32.3	180.2	C3'-exo

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Same strand P--P and C1'--C1' virtual bond distances

Strand I			Strand II		
base	P--P	C1'--C1'	base	P--P	C1'--C1'
1 G/C	6.3	4.5	1 C/G	6.5	4.7
2 C/A	6.6	5.2	2 G/T	6.7	4.8
3 A/A	6.9	4.8	3 T/T	6.7	4.9
4 A/T	6.8	4.8	4 T/A	6.8	4.8
5 T/T	6.7	4.9	5 A/A	6.9	4.8
6 T/G	6.7	4.8	6 A/C	6.6	5.2
7 G/C	6.5	4.7	7 C/G	6.4	4.5

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Helix radius (radial displacement of P, O4', and C1' atoms in local helix frame of each dimer)

	Strand I			Strand II		
step	P	O4'	C1'	P	O4'	C1'
1 GC/GC	9.7	6.3	5.8	10.2	6.7	6.2
2 CA/TG	10.3	7.8	7.1	9.3	6.1	5.6
3 AA/TT	9.2	6.0	5.6	10.3	6.9	6.5
4 AT/AT	9.7	6.3	5.9	9.7	6.3	5.9
5 TT/AA	10.3	6.9	6.5	9.2	6.0	5.6
6 TG/CA	9.3	6.1	5.6	10.3	7.8	7.1
7 GC/GC	10.2	6.7	6.2	9.7	6.3	5.8

****

Position (Px, Py, Pz) and local helical axis vector (Hx, Hy, Hz)

```
        for each dinucleotide step

     bp         Px         Py         Pz         Hx         Hy         Hz
   1 GC/GC      0.28       0.21       1.58       0.00       0.00       1.00
   2 CA/TG      1.43      -0.13       4.86      -0.05       0.18       0.98
   3 AA/TT     -0.18       0.22       8.13       0.08       0.00       1.00
   4 AT/AT      0.79       0.28      11.33       0.16       0.07       0.98
   5 TT/AA      1.41       1.00      14.55       0.05       0.05       1.00
   6 TG/CA      0.87      -0.61      17.78       0.13      -0.16       0.98
   7 GC/GC      1.24       0.47      21.09       0.01      -0.02       1.00
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2.2 ESTRUCTURA d(GAATTCG)

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****************************************************************************
****************************************************************************
    3DNA (v1.5, Nov. 2002) by Xiang-Jun Lu at Wilma K. Olson's Lab.
****************************************************************************
1. The list of the parameters given below correspond to the 5' to 3' direction
   of strand I and 3' to 5' direction of strand II.

2. All angular parameters, except for the phase angle of sugar pseudo-
   rotation, are measured in degrees in the range of [-180, +180], and all
   displacements are measured in Angstrom units.
****************************************************************************
File name: duplex_new.pdb
Date and time: Fri Dec 12 18:03:36 2003

Number of base-pairs: 6
Number of atoms: 240
****************************************************************************
****************************************************************************
RMSD of the bases (----- for WC bp, + for isolated bp, x for helix change)

            Strand I                    Strand II          Helix
   1   (0.024) A:...1_:[..G]G-----C[..C]:..12_:B (0.016)     |
   2   (0.016) A:...2_:[..A]A-----T[..T]:..11_:B (0.025)     |
   3   (0.028) A:...3_:[..A]A-----T[..T]:..10_:B (0.046)     |
   4   (0.026) A:...4_:[..T]T-----A[..A]:...9_:B (0.021)     |
   5   (0.032) A:...5_:[..T]T-----A[..A]:...8_:B (0.038)     |
   6   (0.019) A:...6_:[..C]C-----G[..G]:...7_:B (0.033)     |
****************************************************************************
Detailed H-bond information: atom-name pair and length [ON]
   1 G-----C  [3]  N2 - O2  2.72  N1 - N3  2.72  O6 - N4  2.66
   2 A-----T  [2]  N1 - N3  2.72  N6 - O4  2.66
   3 A-----T  [2]  N1 - N3  2.60  N6 - O4  2.72
   4 T-----A  [2]  N3 - N1  2.66  O4 - N6  2.69
   5 T-----A  [2]  N3 - N1  2.66  O4 - N6  2.68
   6 C-----G  [3]  O2 - N2  2.86  N3 - N1  2.82  N4 - O6  2.82
****************************************************************************
Overlap area in Angstrom^2 between polygons defined by atoms on successive
bases. Polygons projected in the mean plane of the designed base-pair step.

Values in parentheses measure the overlap of base ring atoms only. Those
outside parentheses include exocyclic atoms on the ring. Intra- and
inter-strand overlap is designated according to the following diagram:

                    i2  3'      5' j2
                       /|\      |
                        |       |
                Strand I |      | II
                        |       |
                        |       |
                        |      \|/
                    i1  5'      3' j1

     step      i1-i2        i1-j2        j1-i2        j1-j2        sum
   1 GA/TC  3.70( 1.13)  0.00( 0.00)  0.00( 0.00)  6.37( 1.69) 10.07( 2.82)
   2 AA/TT  2.58( 1.30)  0.00( 0.00)  0.00( 0.00)  4.89( 0.16)  7.47( 1.46)
   3 AT/AT  5.89( 2.09)  0.00( 0.00)  0.00( 0.00)  6.12( 2.43) 12.00( 4.52)
   4 TT/AA  4.51( 0.07)  0.00( 0.00)  0.00( 0.00)  2.95( 1.64)  7.46( 1.71)
   5 TC/GA  5.92( 1.28)  0.00( 0.00)  0.00( 0.00)  3.55( 1.07)  9.47( 2.34)
****************************************************************************
Origin (Ox, Oy, Oz) and mean normal vector (Nx, Ny, Nz) of each base-pair in
   the coordinate system of the given structure
```

```
      bp        Ox        Oy        Oz        Nx        Ny        Nz
    1 G-C     31.22      8.12     17.19     -0.58     -0.68      0.45
    2 A-T     28.83      6.65     19.37     -0.51     -0.67      0.53
    3 A-T     27.17      4.14     20.77     -0.50     -0.68      0.54
    4 T-A     25.86      1.38     22.31     -0.49     -0.65      0.58
    5 T-A     24.67     -0.97     24.23     -0.50     -0.65      0.57
    6 C-G     22.23     -2.52     26.42     -0.46     -0.62      0.63
***************************************************************************
Local base-pair parameters
     bp        Shear    Stretch   Stagger    Buckle  Propeller  Opening
    1 G-C       0.24     -0.29      0.02     -1.38      1.66     -3.10
    2 A-T       0.77     -0.29      0.10      0.84     -6.17     -9.09
    3 A-T       0.34     -0.33      0.04      2.51     -7.75     -5.37
    4 T-A      -0.46     -0.33      0.09     -0.97     -8.37     -6.62
    5 T-A      -0.74     -0.32      0.16      0.37     -7.88     -8.88
    6 C-G      -0.64     -0.21      0.09      1.31      2.33     -3.68
          ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.     -0.08     -0.29      0.08      0.44     -4.36     -6.12
      s.d.      0.62      0.05      0.05      1.45      4.98      2.54
***************************************************************************
Local base-pair step parameters
    step       Shift     Slide      Rise      Tilt      Roll     Twist
   1 GA/TC     -0.91      0.63      3.38     -5.44      3.32     34.86
   2 AA/TT     -0.11     -0.46      3.28     -0.05      0.58     35.73
   3 AT/AT     -0.13     -0.70      3.35     -1.08      2.20     25.98
   4 TT/AA      0.01     -0.49      3.23     -0.99     -0.03     36.59
   5 TC/GA      0.77      0.66      3.48      4.04      2.18     32.93
         ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.     -0.07     -0.07      3.34     -0.70      1.65     33.22
      s.d.      0.60      0.66      0.10      3.38      1.36      4.27
***************************************************************************
Local base-pair helical parameters
    step       X-disp    Y-disp   h-Rise     Incl.       Tip   h-Twist
   1 GA/TC      0.52      0.64      3.52      5.48      8.99     35.42
   2 AA/TT     -0.84      0.17      3.27      0.94      0.08     35.74
   3 AT/AT     -2.17     -0.02      3.28      4.88      2.39     26.09
   4 TT/AA     -0.78     -0.15      3.23     -0.05      1.57     36.60
   5 TC/GA      0.76     -0.62      3.58      3.81     -7.08     33.24
         ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.     -0.50      0.01      3.38      3.01      1.19     33.42
      s.d.      1.18      0.46      0.16      2.45      5.74      4.28
***************************************************************************
Structure classification:

This is a right-handed nucleic acid structure
***************************************************************************
lambda: virtual angle between C1'-YN1 or C1'-RN9 glycosidic bonds and the
        base-pair C1'-C1' line

C1'-C1': distance between C1' atoms for each base-pair
RN9-YN1: distance between RN9-YN1 atoms for each base-pair
RC8-YC6: distance between RC8-YC6 atoms for each base-pair

    bp     lambda(I) lambda(II)  C1'-C1'   RN9-YN1   RC8-YC6
   1 G-C      55.4      55.0      10.5       8.8       9.7
   2 A-T      52.1      46.0      10.8       8.9       9.7
   3 A-T      50.5      54.3      10.6       8.8       9.6
   4 T-A      49.8      51.0      10.7       8.8       9.6
   5 T-A      46.7      53.6      10.7       8.9       9.6
   6 C-G      54.1      56.0      10.6       9.0       9.8
***************************************************************************
Classification of each dinucleotide step in a right-handed nucleic acid
structure: A-like; B-like; TA-like; intermediate of A and B, or other cases

    step       Xp       Yp       Zp      XpH      YpH      ZpH    Form
   1 GA/TC   -2.47     8.89     0.05    -1.95     8.85     0.80      B
   2 AA/TT   -2.78     8.96    -0.20    -3.58     8.96    -0.06      B
   3 AT/AT   -2.92     9.03    -0.27    -5.03     9.02     0.47      B
   4 TT/AA   -2.76     8.90    -0.16    -3.50     8.90    -0.16      B
   5 TC/GA   -2.40     8.86    -0.01    -1.64     8.84     0.47      B
***************************************************************************
Minor and major groove widths: direct P-P distances and refined P-P distances
   which take into account the directions of the sugar-phosphate backbones

   (Subtract 5.8 Angstrom from the values to take account of the vdw radii
    of the phosphate groups, and for comparison with FreeHelix and Curves.)
```

```
Ref: M. A. El Hassan and C. R. Calladine (1998). ``Two Distinct Modes of
     Protein-induced Bending in DNA.'' J. Mol. Biol., v282, pp331-343.

                 Minor Groove        Major Groove
                P-P     Refined     P-P     Refined
   1 GA/TC       ---       ---       ---       ---
   2 AA/TT       ---       ---       ---       ---
   3 AT/AT      12.3       ---      16.6       ---
   4 TT/AA       ---       ---       ---       ---
   5 TC/GA       ---       ---       ---       ---
*****************************************************************************
Global linear helical axis defined by equivalent C1' and RN9/YN1 atom pairs
Deviation from regular linear helix: 3.29(0.30)
Helix:    -0.581  -0.568   0.582
HETATM 9998  XS    X X 999      31.802   7.469  17.442
HETATM 9999  XE    X X 999      22.309  -1.806  26.947
Average and standard deviation of helix radius:
      P: 9.64(0.30), O4': 6.86(0.40),  C1': 6.21(0.39)

Global parameters based on C1'-C1' vectors:

disp.: displacement of the middle C1'-C1' point from the helix
angle: inclination between C1'-C1' vector and helix (subtracted from 90)
twist: helical twist angle between consecutive C1'-C1' vectors
rise:  helical rise by projection of the vector connecting consecutive
       C1'-C1' middle points onto the helical axis

     bp       disp.    angle     twist      rise
   1 G-C      3.21      8.19     33.13      3.52
   2 A-T      3.43      4.22     37.81      3.20
   3 A-T      3.20      5.92     31.18      2.98
   4 T-A      3.12      5.63     38.04      3.11
   5 T-A      3.38      3.78     33.61      3.52
   6 C-G      3.09      7.45      ---       ---
*****************************************************************************
Main chain and chi torsion angles:

Note: alpha:   O3'(i-1)-P-O5'-C5'
      beta:    P-O5'-C5'-C4'
      gamma:   O5'-C5'-C4'-C3'
      delta:   C5'-C4'-C3'-O3'
      epsilon: C4'-C3'-O3'-P(i+1)
      zeta:    C3'-O3'-P(i+1)-O5'(i+1)

      chi for pyrimidines(Y): O4'-C1'-N1-C2
          chi for purines(R): O4'-C1'-N9-C4

Strand I
  base    alpha    beta   gamma   delta  epsilon   zeta    chi
   1 G     ---     ---     76.6   163.2  -135.2  -148.5   -96.3
   2 A    -78.1   123.8    79.5   128.1  -153.3  -117.7  -137.7
   3 A    -55.4   157.7    52.5   113.6   168.8   -83.4  -121.4
   4 T    -96.7  -176.7    85.7   120.5  -170.0  -104.7  -124.3
   5 T    -70.5  -174.7    54.8   123.9  -175.6   -98.2  -116.8
   6 C    -58.2   178.6    53.1   156.5    ---     ---    -91.7

Strand II
  base    alpha    beta   gamma   delta  epsilon   zeta    chi
   1 C    -56.7   179.9    52.9   154.5    ---     ---    -89.6
   2 T    -60.9   178.7    47.6   124.1  -175.8  -102.3  -117.2
   3 T    -86.4   179.7    74.2   121.4  -166.2  -107.3  -126.3
   4 A    -46.9   150.8    50.4   115.3   175.4   -86.2  -123.2
   5 A    -74.3   128.7    76.0   131.0  -154.5  -121.7  -135.7
   6 G     ---     ---     76.0   163.9  -137.5  -157.1   -95.4
*****************************************************************************
Sugar conformational parameters:

Note: v0: C4'-O4'-C1'-C2'
      v1: O4'-C1'-C2'-C3'
      v2: C1'-C2'-C3'-C4'
      v3: C2'-C3'-C4'-O4'
      v4: C3'-C4'-O4'-C1'

      tm: amplitude of pseudorotation of the sugar ring
      P:  phase angle of pseudorotation of the sugar ring

Strand I
 base       v0      v1      v2      v3      v4      tm       P    Puckering
```

1	G	-10.0	31.3	-40.8	35.5	-16.0	41.0	184.7	C3'-exo
2	A	-46.9	43.5	-26.2	-0.5	29.5	47.0	123.8	C1'-exo
3	A	-45.5	37.0	-17.7	-8.5	35.5	44.8	113.4	C1'-exo
4	T	-47.1	44.1	-25.0	-1.5	30.0	47.1	122.1	C1'-exo
5	T	-43.3	40.1	-22.3	-2.4	28.8	43.4	120.9	C1'-exo
6	C	-21.3	41.3	-44.4	33.2	-7.7	45.0	171.0	C2'-endo

Strand II

base		v0	v1	v2	v3	v4	tm	P	Puckering
1	C	-15.1	37.8	-44.6	37.1	-14.1	44.6	179.3	C2'-endo
2	T	-44.3	41.5	-23.2	-2.0	29.7	44.7	121.3	C1'-exo
3	T	-49.1	42.8	-24.0	-3.2	32.8	48.0	120.0	C1'-exo
4	A	-49.8	44.4	-25.2	-2.9	34.1	49.5	120.6	C1'-exo
5	A	-49.4	45.5	-28.4	0.9	30.0	49.3	125.2	C1'-exo
6	G	-12.9	35.5	-41.9	36.9	-15.1	41.9	181.6	C3'-exo

****

Same strand P--P and C1'--C1' virtual bond distances

	Strand I			Strand II		
	base	P--P	C1'--C1'	base	P--P	C1'--C1'
1	G/A	---	4.6	1 C/T	6.4	5.0
2	A/A	6.7	5.3	2 T/T	6.5	5.0
3	A/T	6.6	4.7	3 T/A	6.6	4.7
4	T/T	6.7	5.1	4 A/A	6.9	5.1
5	T/C	6.4	4.9	5 A/G	---	4.7

****

Helix radius (radial displacement of P, O4', and C1' atoms in local helix frame of each dimer)

		Strand I			Strand II		
	step	P	O4'	C1'	P	O4'	C1'
1	GA/TC	9.6	7.0	6.1	8.6	5.6	5.1
2	AA/TT	9.7	6.9	6.2	9.6	6.7	6.1
3	AT/AT	10.3	7.4	6.9	10.3	7.3	6.8
4	TT/AA	9.6	6.6	6.1	9.6	6.7	6.1
5	TC/GA	8.6	5.6	5.0	9.5	6.8	6.0

****

Position (Px, Py, Pz) and local helical axis vector (Hx, Hy, Hz) for each dinucleotide step

	bp	Px	Py	Pz	Hx	Hy	Hz
1	GA/TC	29.47	7.45	17.72	-0.63	-0.54	0.56
2	AA/TT	28.70	5.10	20.36	-0.51	-0.66	0.55
3	AT/AT	27.77	3.10	23.21	-0.57	-0.61	0.55
4	TT/AA	25.30	0.67	23.86	-0.50	-0.66	0.55
5	TC/GA	23.14	-2.27	24.61	-0.56	-0.53	0.63

2.3 ESTRUCTURES d(CGTACG)

Complex CGTACG/antraquinona

```
**************************************************************************
**************************************************************************
    3DNA (v1.5, Nov. 2002) by Xiang-Jun Lu at Wilma K. Olson's Lab.
**************************************************************************
1. The list of the parameters given below correspond to the 5' to 3' direction
   of strand I and 3' to 5' direction of strand II.

2. All angular parameters, except for the phase angle of sugar pseudo-
   rotation, are measured in degrees in the range of [-180, +180], and all
   displacements are measured in Angstrom units.
**************************************************************************
File name: cc4_3DNA.pdb
Date and time: Tue Feb 10 11:54:25 2004

Number of base-pairs: 5
Number of atoms: 202
**************************************************************************
**************************************************************************
RMSD of the bases (----- for WC bp, + for isolated bp, x for helix change)

            Strand I                    Strand II          Helix
   1   (0.018) A:...1_:[..G]G-----C[..C]:..10_:B (0.019)     |
   2   (0.015) A:...2_:[..T]T-----A[..A]:...9_:B (0.025)     |
   3   (0.027) A:...3_:[..A]A-----T[..T]:...8_:B (0.015)     |
   4   (0.011) A:...4_:[..C]C-----G[..G]:...7_:B (0.013)     |
   5   (0.013) A:...5_:[..G]G-**+-C[..C]:...6_:B (0.014)     |

Note: This structure contains 1[1] non-Watson-Crick base-pair.
**************************************************************************
Detailed H-bond information: atom-name pair and length [ON]
   1 G-----C  [3]  N2 - O2  2.65  N1 - N3  2.89  O6 - N4  2.89
   2 T-----A  [2]  N3 - N1  2.93  O4 - N6  3.07
   3 A-----T  [2]  N1 - N3  2.82  N6 - O4  2.78
   4 C-----G  [3]  O2 - N2  2.61  N3 - N1  2.71  N4 - O6  2.76
   5 G-**+-C  [0]
**************************************************************************
Overlap area in Angstrom^2 between polygons defined by atoms on successive
bases. Polygons projected in the mean plane of the designed base-pair step.

Values in parentheses measure the overlap of base ring atoms only. Those
outside parentheses include exocyclic atoms on the ring. Intra- and
inter-strand overlap is designated according to the following diagram:

                    i2  3'      5' j2
                       /|\      |
                        |       |
                Strand I |      | II
                        |       |
                        |       |
                        |      \|/
                    i1  5'      3' j1

     step      i1-i2        i1-j2        j1-i2        j1-j2        sum
   1 GT/AC  6.94( 2.79)  0.00( 0.00)  0.00( 0.00)  4.92( 3.27) 11.86( 6.06)
   2 TA/TA  0.98( 0.01)  0.00( 0.00)  0.00( 0.00)  0.58( 0.00)  1.57( 0.01)
   3 AC/GT  5.77( 4.02)  0.00( 0.00)  0.00( 0.00)  5.62( 1.41) 11.39( 5.43)
   4 CG/CG  4.04( 1.65)  0.00( 0.00)  0.00( 0.00)  0.00( 0.00)  4.04( 1.65)
**************************************************************************
Origin (Ox, Oy, Oz) and mean normal vector (Nx, Ny, Nz) of each base-pair in
   the coordinate system of the given structure

      bp         Ox         Oy         Oz         Nx         Ny         Nz
    1 G-C      19.84      12.42      10.01      -0.61      -0.79       0.03
    2 T-A      18.17       9.69       9.91      -0.65      -0.75       0.10
    3 A-T      16.58       6.89      10.34      -0.60      -0.79       0.12
    4 C-G      14.65       4.85      11.78      -0.66      -0.74       0.14
    5 G+C      14.68       1.23      20.21      -0.90       0.01       0.44
**************************************************************************
Local base-pair parameters
     bp        Shear    Stretch   Stagger    Buckle  Propeller  Opening
    1 G-C      -0.27      -0.13     -0.15    -11.49       5.41       2.21
```

```
    2 T-A      -0.07     -0.04      0.34     -0.66     -1.11      1.58
    3 A-T       0.17     -0.15     -0.16     -1.11      1.82     -4.48
    4 C-G       0.27     -0.30     -0.08     15.71     -1.56     -0.13
    5 G+C      -0.29     22.36      3.95      4.33    -89.81     91.56
         ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.     -0.04      4.35      0.78      1.35    -17.05     18.15
      s.d.      0.25     10.07      1.79      9.87     40.77     41.12
*********************************************************************************
Local base-pair step parameters
    step       Shift     Slide      Rise      Tilt      Roll     Twist
   1 GT/AC     -0.15     -0.50      3.16     -4.31      2.79     24.40
   2 TA/TA     -0.05     -0.52      3.21      4.05      0.39     38.90
   3 AC/GT      0.87     -0.65      2.97     -2.85      4.20     27.31
   4 CG/CG     -0.95     -8.15      4.09      4.82     49.50     12.91
         ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.     -0.07     -2.46      3.36      0.43     14.22     25.88
      s.d.      0.74      3.79      0.50      4.68     23.57     10.68
*********************************************************************************
Local base-pair helical parameters
    step       X-disp    Y-disp   h-Rise     Incl.       Tip   h-Twist
   1 GT/AC     -1.97     -0.88      3.06      6.51     10.06     24.92
   2 TA/TA     -0.83      0.55      3.18      0.59     -6.06     39.10
   3 AC/GT     -2.25     -2.41      2.74      8.81      5.97     27.77
   4 CG/CG     -6.97      0.86     -6.86     76.01     -7.40     51.28
         ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.     -3.00     -0.47      0.53     22.98      0.64     35.77
      s.d.      2.72      1.50      4.93     35.52      8.69     12.02
*********************************************************************************
Structure classification:

This nucleic acid structure is *unusual*
*********************************************************************************
lambda: virtual angle between C1'-YN1 or C1'-RN9 glycosidic bonds and the
        base-pair C1'-C1' line

C1'-C1': distance between C1' atoms for each base-pair
RN9-YN1: distance between RN9-YN1 atoms for each base-pair
RC8-YC6: distance between RC8-YC6 atoms for each base-pair

    bp     lambda(I) lambda(II)  C1'-C1'   RN9-YN1   RC8-YC6
   1 G-C      51.6      54.7      10.7       8.9       9.8
   2 T-A      56.3      57.1      10.5       8.9       9.9
   3 A-T      52.0      49.3      10.9       9.0       9.8
   4 C-G      56.3      51.2      10.5       8.7       9.6
   5 G+C      93.1     171.0      19.8      21.4      23.4
*********************************************************************************
Classification of each dinucleotide step in a right-handed nucleic acid
structure: A-like; B-like; TA-like; intermediate of A and B, or other cases

    step       Xp       Yp       Zp      XpH      YpH      ZpH    Form
   1 GT/AC   -3.55     9.26    -0.29    -5.47     9.24     0.71
   2 TA/TA   -2.83     8.90     0.64    -3.57     8.89     0.71
   3 AC/GT   -2.50     9.02     0.97    -4.70     8.77     2.37
   4 CG/CG   -2.22     8.58     0.38    -8.65     2.10     8.12
*********************************************************************************
Minor and major groove widths: direct P-P distances and refined P-P distances
   which take into account the directions of the sugar-phosphate backbones

   (Subtract 5.8 Angstrom from the values to take account of the vdw radii
    of the phosphate groups, and for comparison with FreeHelix and Curves.)

Ref: M. A. El Hassan and C. R. Calladine (1998). ``Two Distinct Modes of
     Protein-induced Bending in DNA.'' J. Mol. Biol., v282, pp331-343.

                Minor Groove        Major Groove
               P-P     Refined     P-P     Refined
   1 GT/AC     ---       ---       ---       ---
   2 TA/TA     ---       ---       ---       ---
   3 AC/GT     ---       ---       ---       ---
   4 CG/CG     ---       ---       ---       ---
*********************************************************************************
Global linear helical axis defined by equivalent C1' and RN9/YN1 atom pairs
Deviation from regular linear helix: 2.81(1.14)
*********************************************************************************
Main chain and chi torsion angles:

Note: alpha:   O3'(i-1)-P-O5'-C5'
      beta:    P-O5'-C5'-C4'
```

```
      gamma:   O5'-C5'-C4'-C3'
      delta:   C5'-C4'-C3'-O3'
      epsilon: C4'-C3'-O3'-P(i+1)
      zeta:    C3'-O3'-P(i+1)-O5'(i+1)

      chi for pyrimidines(Y): O4'-C1'-N1-C2
          chi for purines(R): O4'-C1'-N9-C4
```

Strand I

base	alpha	beta	gamma	delta	epsilon	zeta	chi
1 G	---	-178.3	39.8	147.0	-168.6	-99.7	-112.2
2 T	-53.5	162.1	45.1	104.0	164.3	-81.8	-122.9
3 A	-73.7	-172.5	53.4	123.7	-173.6	-87.0	-113.8
4 C	-60.8	172.2	43.9	114.5	-156.5	-130.8	-118.9
5 G	79.3	153.5	-58.2	111.7	---	---	-70.0

Strand II

base	alpha	beta	gamma	delta	epsilon	zeta	chi
1 C	-69.8	175.4	50.2	131.6	---	---	-100.3
2 A	-64.4	-160.7	39.5	141.7	-166.3	-88.1	-113.5
3 T	-62.4	178.8	58.3	146.6	-173.5	-101.7	-123.6
4 G	68.1	134.4	45.4	81.4	-166.1	-75.8	-165.2
5 C	---	---	-165.8	146.3	-113.6	72.7	-119.2

****

Sugar conformational parameters:

```
Note: v0: C4'-O4'-C1'-C2'
      v1: O4'-C1'-C2'-C3'
      v2: C1'-C2'-C3'-C4'
      v3: C2'-C3'-C4'-O4'
      v4: C3'-C4'-O4'-C1'

      tm: amplitude of pseudorotation of the sugar ring
      P:  phase angle of pseudorotation of the sugar ring
```

Strand I

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 G	-17.0	29.2	-31.4	22.3	-3.4	32.1	168.0	C2'-endo
2 T	-39.1	28.7	-9.0	-13.3	32.3	37.9	103.7	O4'-endo
3 A	-29.6	29.6	-19.0	2.5	16.7	30.5	128.5	C1'-exo
4 C	-43.4	34.2	-12.7	-11.8	34.8	42.3	107.4	O4'-endo
5 G	18.4	-24.1	20.4	-10.6	-4.8	23.6	329.8	C2'-exo

Strand II

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-45.2	48.5	-35.6	10.8	21.5	49.2	136.3	C1'-exo
2 A	-15.7	28.2	-29.3	21.6	-3.9	29.9	168.5	C2'-endo
3 T	-24.7	37.4	-36.7	22.3	1.5	39.1	159.9	C2'-endo
4 G	-3.4	-20.4	35.0	-37.8	26.1	38.2	23.5	C3'-endo
5 C	-18.3	34.6	-37.1	27.7	-6.0	37.6	170.4	C2'-endo

****

Same strand P--P and C1'--C1' virtual bond distances

Strand I			Strand II		
base	P--P	C1'--C1'	base	P--P	C1'--C1'
1 G/T	6.7	4.6	1 C/A	6.4	4.8
2 T/A	6.8	5.0	2 A/T	7.0	5.3
3 A/C	6.4	4.5	3 T/G	6.1	5.6
4 C/G	6.3	7.4	4 G/C	---	8.9

****

Helix radius (radial displacement of P, O4', and C1' atoms in local helix frame of each dimer)

	Strand I			Strand II		
step	P	O4'	C1'	P	O4'	C1'
1 GT/AC	10.0	7.0	6.3	11.5	8.2	7.6
2 TA/TA	10.3	7.3	6.7	8.9	6.5	5.8
3 AC/GT	8.5	5.9	5.2	11.6	10.0	9.1
4 CG/CG	12.7	11.6	11.6	5.7	7.8	7.4

****

Position (Px, Py, Pz) and local helical axis vector (Hx, Hy, Hz) for each dinucleotide step

bp	Px	Py	Pz	Hx	Hy	Hz
1 GT/AC	18.74	11.14	12.04	-0.74	-0.66	-0.07
2 TA/TA	17.73	8.23	10.99	-0.64	-0.74	0.20
3 AC/GT	13.22	7.97	10.83	-0.66	-0.75	-0.05
4 CG/CG	12.78	8.60	18.39	-0.64	0.11	-0.76

Complex CGTACG/acridina

```
**************************************************************************
**************************************************************************
    3DNA (v1.5, Nov. 2002) by Xiang-Jun Lu at Wilma K. Olson's Lab.
**************************************************************************
1. The list of the parameters given below correspond to the 5' to 3' direction
   of strand I and 3' to 5' direction of strand II.

2. All angular parameters, except for the phase angle of sugar pseudo-
   rotation, are measured in degrees in the range of [-180, +180], and all
   displacements are measured in Angstrom units.
**************************************************************************
File name: b6_3DNA.pdb
Date and time: Fri Feb 13 13:16:17 2004

Number of base-pairs: 5
Number of atoms: 202
**************************************************************************
**************************************************************************
RMSD of the bases (----- for WC bp, + for isolated bp, x for helix change)

            Strand I                   Strand II          Helix
   1   (0.033) A:...1_:[..G]G-----C[..C]:..10_:B (0.019)     |
   2   (0.016) A:...2_:[..T]T-----A[..A]:...9_:B (0.032)     |
   3   (0.019) A:...3_:[..A]A-----T[..T]:...8_:B (0.015)     |
   4   (0.013) A:...4_:[..C]C-----G[..G]:...7_:B (0.014)     |
   5   (0.017) A:...5_:[..G]G-**--C[..C]:...6_:B (0.014)     |

Note: This structure contains 1[1] non-Watson-Crick base-pair.
**************************************************************************
Detailed H-bond information: atom-name pair and length [ON]
   1 G-----C  [3]  N2 - O2  2.81  N1 - N3  2.92  O6 - N4  2.84
   2 T-----A  [2]  N3 - N1  2.87  O4 - N6  2.99
   3 A-----T  [2]  N1 - N3  2.92  N6 - O4  2.91
   4 C-----G  [3]  O2 - N2  2.78  N3 - N1  2.91  N4 - O6  2.97
   5 G-**--C  [0]
**************************************************************************
Overlap area in Angstrom^2 between polygons defined by atoms on successive
bases. Polygons projected in the mean plane of the designed base-pair step.

Values in parentheses measure the overlap of base ring atoms only. Those
outside parentheses include exocyclic atoms on the ring. Intra- and
inter-strand overlap is designated according to the following diagram:

                    i2  3'      5' j2
                       /|\       |
                        |        |
                Strand I |       | II
                        |        |
                        |        |
                        |       \|/
                    i1  5'      3' j1

     step      i1-i2        i1-j2        j1-i2        j1-j2        sum
   1 GT/AC  6.84( 2.68)  0.00( 0.00)  0.00( 0.00)  4.57( 2.84) 11.41( 5.52)
   2 TA/TA  0.89( 0.00)  0.00( 0.00)  0.00( 0.00)  0.79( 0.00)  1.68( 0.00)
   3 AC/GT  5.68( 3.95)  0.00( 0.00)  0.00( 0.00)  5.28( 1.25) 10.96( 5.20)
   4 CG/CG  2.28( 0.64)  0.00( 0.00)  0.00( 0.00)  0.00( 0.00)  2.28( 0.64)
**************************************************************************
Origin (Ox, Oy, Oz) and mean normal vector (Nx, Ny, Nz) of each base-pair in
   the coordinate system of the given structure

      bp        Ox        Oy        Oz        Nx        Ny        Nz
    1 G-C      19.47     12.58     10.02     -0.57     -0.82      0.03
    2 T-A      17.86      9.87     10.06     -0.60     -0.80      0.09
    3 A-T      16.38      6.85     10.33     -0.56     -0.82      0.12
    4 C-G      14.48      4.81     11.84     -0.63     -0.76      0.15
    5 G-C      14.33      1.16     20.48     -0.02     -1.00      0.07
**************************************************************************
Local base-pair parameters
     bp        Shear    Stretch   Stagger    Buckle  Propeller  Opening
    1 G-C      -0.32     -0.18     -0.13     -9.83      5.85     -0.87
    2 T-A       0.10     -0.16      0.18      0.65     -0.81      1.48
    3 A-T       0.12     -0.06     -0.20     -0.79      0.10     -4.38
    4 C-G       0.31     -0.10     -0.20     17.19     -3.20      0.42
    5 G-C     -13.06     18.75     -0.92    -49.31     55.72    174.05
```

```
          ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.     -2.57      3.65     -0.26     -8.42     11.53     34.14
      s.d.      5.87      8.44      0.40     24.85     24.92     78.24
*******************************************************************************
Local base-pair step parameters
    step       Shift     Slide      Rise      Tilt      Roll     Twist
   1 GT/AC     -0.06     -0.32      3.14     -3.23      2.76     26.94
   2 TA/TA     -0.21     -0.52      3.33      2.90      0.94     36.75
   3 AC/GT      0.95     -0.65      2.95     -1.93      5.35     28.34
   4 CG/CG      5.51     -6.12      4.48     26.35    -28.58    -40.05
          ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.      1.55     -1.90      3.48      6.02     -4.88     13.00
      s.d.      2.69      2.82      0.69     13.80     15.90     35.63
*******************************************************************************
Local base-pair helical parameters
    step       X-disp    Y-disp   h-Rise     Incl.       Tip   h-Twist
   1 GT/AC     -1.33     -0.65      3.08      5.87      6.87     27.27
   2 TA/TA     -0.95      0.73      3.29      1.48     -4.58     36.87
   3 AC/GT     -2.34     -2.28      2.71     10.80      3.88     28.89
   4 CG/CG      7.29      6.58     -2.25     33.72     31.08    -55.25
          ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.      0.67      1.10      1.71     12.97      9.31      9.45
      s.d.      4.45      3.86      2.65     14.35     15.30     43.33
*******************************************************************************
Structure classification:

This nucleic acid structure is *unusual*
*******************************************************************************
lambda: virtual angle between C1'-YN1 or C1'-RN9 glycosidic bonds and the
        base-pair C1'-C1' line

C1'-C1': distance between C1' atoms for each base-pair
RN9-YN1: distance between RN9-YN1 atoms for each base-pair
RC8-YC6: distance between RC8-YC6 atoms for each base-pair

     bp     lambda(I) lambda(II)  C1'-C1'   RN9-YN1   RC8-YC6
   1 G-C       50.6      57.0       10.7       8.9       9.8
   2 T-A       54.6      53.5       10.5       8.8       9.8
   3 A-T       52.1      50.3       10.9       9.0       9.9
   4 C-G       55.8      54.3       10.6       8.9       9.8
   5 G-C       96.0     169.2       19.8      21.4      23.5
*******************************************************************************
Classification of each dinucleotide step in a right-handed nucleic acid
structure: A-like; B-like; TA-like; intermediate of A and B, or other cases

     step       Xp       Yp       Zp      XpH      YpH      ZpH     Form
   1 GT/AC   -3.47     9.16    -0.23    -4.73     9.14     0.66      B
   2 TA/TA   -2.85     8.93     0.44    -3.73     8.92     0.65      B
   3 AC/GT   -2.50     9.04     0.85    -4.77     8.73     2.51
   4 CG/CG   -3.66     7.50     0.97     3.85     5.32     6.67
*******************************************************************************
Minor and major groove widths: direct P-P distances and refined P-P distances
   which take into account the directions of the sugar-phosphate backbones

   (Subtract 5.8 Angstrom from the values to take account of the vdw radii
    of the phosphate groups, and for comparison with FreeHelix and Curves.)

Ref: M. A. El Hassan and C. R. Calladine (1998). ``Two Distinct Modes of
     Protein-induced Bending in DNA.'' J. Mol. Biol., v282, pp331-343.

                Minor Groove        Major Groove
               P-P     Refined     P-P     Refined
   1 GT/AC     ---       ---       ---       ---
   2 TA/TA     ---       ---       ---       ---
   3 AC/GT     ---       ---       ---       ---
   4 CG/CG     ---       ---       ---       ---
*******************************************************************************
Global linear helical axis defined by equivalent C1' and RN9/YN1 atom pairs
Deviation from regular linear helix: 3.02(1.08)
*******************************************************************************
Main chain and chi torsion angles:

Note: alpha:   O3'(i-1)-P-O5'-C5'
      beta:    P-O5'-C5'-C4'
      gamma:   O5'-C5'-C4'-C3'
      delta:   C5'-C4'-C3'-O3'
      epsilon: C4'-C3'-O3'-P(i+1)
      zeta:    C3'-O3'-P(i+1)-O5'(i+1)
```

chi for pyrimidines(Y): O4'-C1'-N1-C2
chi for purines(R): O4'-C1'-N9-C4

Strand I

base	alpha	beta	gamma	delta	epsilon	zeta	chi
1 G	---	-174.6	48.4	143.1	-178.9	-95.4	-108.6
2 T	-54.9	167.7	51.4	107.4	174.2	-89.8	-121.1
3 A	-63.4	-171.3	43.0	134.6	-169.0	-98.5	-108.5
4 C	-60.3	166.3	46.0	104.4	-165.2	-92.8	-117.8
5 G	-65.2	-144.4	46.8	82.9	---	---	-78.9

Strand II

base	alpha	beta	gamma	delta	epsilon	zeta	chi
1 C	-71.2	178.4	48.5	128.4	---	---	-94.9
2 A	-63.6	-165.5	45.6	135.8	-168.5	-87.0	-113.1
3 T	-66.9	-176.7	63.4	140.4	178.6	-95.6	-121.5
4 G	71.3	141.2	53.3	83.0	-169.8	-76.9	-160.2
5 C	---	---	-27.0	155.7	-116.6	54.9	-114.0

****

Sugar conformational parameters:

Note: v0: C4'-O4'-C1'-C2'
v1: O4'-C1'-C2'-C3'
v2: C1'-C2'-C3'-C4'
v3: C2'-C3'-C4'-O4'
v4: C3'-C4'-O4'-C1'

tm: amplitude of pseudorotation of the sugar ring
P: phase angle of pseudorotation of the sugar ring

Strand I

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 G	-13.9	26.3	-28.6	21.1	-4.7	28.9	170.7	C2'-endo
2 T	-40.0	35.7	-17.0	-5.8	28.7	39.7	115.4	C1'-exo
3 A	-23.4	31.5	-27.3	14.3	5.7	31.2	151.1	C2'-endo
4 C	-43.3	29.5	-6.8	-17.6	38.4	42.4	99.3	O4'-endo
5 G	-0.3	-20.8	33.2	-33.8	21.5	35.1	18.8	C3'-endo

Strand II

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-37.2	42.3	-32.0	11.9	15.7	41.9	139.8	C1'-exo
2 A	-22.4	32.6	-31.2	18.2	2.5	33.7	157.8	C2'-endo
3 T	-21.3	33.1	-32.2	20.4	0.5	34.1	160.8	C2'-endo
4 G	-7.8	-16.7	32.5	-38.4	29.6	37.8	30.5	C3'-endo
5 C	-18.3	40.8	-46.2	37.1	-12.0	46.3	176.0	C2'-endo

****

Same strand P--P and C1'--C1' virtual bond distances

	Strand I			Strand II	
base	P--P	C1'--C1'	base	P--P	C1'--C1'
1 G/T	6.8	4.5	1 C/A	6.5	4.8
2 T/A	6.6	5.1	2 A/T	6.9	5.2
3 A/C	6.4	4.6	3 T/G	6.3	5.6
4 C/G	6.1	7.2	4 G/C	---	8.8

****

Helix radius (radial displacement of P, O4', and C1' atoms in local helix frame of each dimer)

	Strand I			Strand II		
step	P	O4'	C1'	P	O4'	C1'
1 GT/AC	9.7	6.7	6.0	10.9	7.6	7.0
2 TA/TA	10.5	7.5	6.9	8.8	6.4	5.7
3 AC/GT	8.6	6.1	5.4	11.5	9.9	9.0
4 CG/CG	12.4	11.3	11.1	7.0	5.6	6.0

****

Position (Px, Py, Pz) and local helical axis vector (Hx, Hy, Hz) for each dinucleotide step

bp	Px	Py	Pz	Hx	Hy	Hz
1 GT/AC	18.46	11.37	11.45	-0.68	-0.73	-0.03
2 TA/TA	17.56	8.24	11.24	-0.61	-0.77	0.17
3 AC/GT	13.06	7.92	10.93	-0.66	-0.75	-0.04
4 CG/CG	22.47	-0.08	15.01	-0.36	-0.73	-0.58

2.4 ESTRUCTURA d(CAATTAATTG)

```
**************************************************************************
**************************************************************************
    3DNA (v1.5, Nov. 2002) by Xiang-Jun Lu at Wilma K. Olson's Lab.
**************************************************************************
1. The list of the parameters given below correspond to the 5' to 3' direction
   of strand I and 3' to 5' direction of strand II.

2. All angular parameters, except for the phase angle of sugar pseudo-
   rotation, are measured in degrees in the range of [-180, +180], and all
   displacements are measured in Angstrom units.
**************************************************************************
File name: last_3_3DNA.pdb
Date and time: Fri Jun 11 10:49:43 2004

Number of base-pairs: 10
Number of atoms: 404
**************************************************************************
**************************************************************************
RMSD of the bases (----- for WC bp, + for isolated bp, x for helix change)

            Strand I                    Strand II          Helix
   1   (0.009) A:...1_:[CYT]C-----G[GUA]:..20_:A (0.016)     |
   2   (0.024) A:...2_:[ADE]A-----T[THY]:..19_:A (0.009)     |
   3   (0.016) A:...3_:[ADE]A-----T[THY]:..18_:A (0.013)     |
   4   (0.010) A:...4_:[THY]T-----A[ADE]:..17_:A (0.027)     |
   5   (0.008) A:...5_:[THY]T-----A[ADE]:..16_:A (0.016)     |
   6   (0.014) A:...6_:[ADE]A-----T[THY]:..15_:A (0.012)     |
   7   (0.016) A:...7_:[ADE]A-----T[THY]:..14_:A (0.010)     |
   8   (0.009) A:...8_:[THY]T-----A[ADE]:..13_:A (0.013)     |
   9   (0.010) A:...9_:[THY]T-----A[ADE]:..12_:A (0.014)     |
  10   (0.018) A:..10_:[GUA]G-----C[CYT]:..11_:A (0.012)     |
**************************************************************************
Detailed H-bond information: atom-name pair and length [ON]
   1 C-----G  [3]  O2 - N2  2.84  N3 - N1  2.90  N4 - O6  2.86
   2 A-----T  [2]  N1 - N3  2.70  N6 - O4  2.65
   3 A-----T  [2]  N1 - N3  2.95  N6 - O4  3.17
   4 T-----A  [2]  N3 - N1  2.89  O4 - N6  3.67
   5 T-----A  [2]  N3 - N1  2.82  O4 - N6  2.98
   6 A-----T  [2]  N1 - N3  2.81  N6 - O4  2.67
   7 A-----T  [2]  N1 - N3  2.70  N6 - O4  2.71
   8 T-----A  [2]  N3 - N1  3.02  O4 - N6  3.25
   9 T-----A  [2]  N3 - N1  2.88  O4 - N6  3.18
  10 G-----C  [3]  N2 - O2  2.89  N1 - N3  2.90  O6 - N4  2.92
**************************************************************************
Overlap area in Angstrom^2 between polygons defined by atoms on successive
bases. Polygons projected in the mean plane of the designed base-pair step.

Values in parentheses measure the overlap of base ring atoms only. Those
outside parentheses include exocyclic atoms on the ring. Intra- and
inter-strand overlap is designated according to the following diagram:

                    i2  3'      5' j2
                       /|\      |
                        |       |
                Strand I |      | II
                         |       |
                         |       |
                         |      \|/
                    i1  5'      3' j1

     step      i1-i2        i1-j2        j1-i2        j1-j2        sum
   1 CA/TG  0.68( 0.00)  0.00( 0.00)  0.33( 0.00)  1.97( 0.04)  2.98( 0.04)
   2 AA/TT  3.56( 2.35)  0.00( 0.00)  0.00( 0.00)  4.48( 0.00)  8.03( 2.35)
   3 AT/AT  5.68( 2.23)  0.00( 0.00)  0.00( 0.00)  6.78( 3.39) 12.46( 5.62)
   4 TT/AA  4.98( 0.11)  0.00( 0.00)  0.00( 0.00)  3.31( 2.01)  8.29( 2.12)
   5 TA/TA  0.65( 0.00)  0.00( 0.00)  0.15( 0.14)  0.80( 0.00)  1.60( 0.14)
   6 AA/TT  2.35( 1.24)  0.00( 0.00)  0.00( 0.00)  5.42( 0.37)  7.77( 1.61)
   7 AT/AT  5.22( 1.57)  0.00( 0.00)  0.00( 0.00)  6.72( 3.37) 11.94( 4.93)
   8 TT/AA  4.02( 0.00)  0.00( 0.00)  0.00( 0.00)  4.67( 3.16)  8.69( 3.16)
   9 TG/CA  6.25( 1.40)  0.00( 0.00)  0.00( 0.00)  1.64( 0.00)  7.89( 1.40)
**************************************************************************
Origin (Ox, Oy, Oz) and mean normal vector (Nx, Ny, Nz) of each base-pair in
   the coordinate system of the given structure

      bp        Ox        Oy        Oz        Nx        Ny        Nz
```

```
    1 C-G      -1.16     36.68      9.04     -0.46     -0.85     -0.26
    2 A-T      -3.05     33.43      8.06     -0.43     -0.90     -0.08
    3 A-T      -4.24     30.41      8.21     -0.46     -0.88     -0.11
    4 T-A      -5.17     27.73      8.36     -0.53     -0.84     -0.08
    5 T-A      -6.67     24.79      8.40     -0.51     -0.85     -0.14
    6 A-T      -8.65     21.51      8.68     -0.53     -0.84     -0.11
    7 A-T     -10.60     18.97      8.60     -0.51     -0.85     -0.17
    8 T-A     -12.84     16.35      8.28     -0.48     -0.87     -0.10
    9 T-A     -14.78     13.87      8.14     -0.46     -0.87     -0.14
   10 G-C     -15.34     10.37      9.39     -0.50     -0.85     -0.18
***************************************************************************
Local base-pair parameters
     bp        Shear    Stretch   Stagger    Buckle  Propeller  Opening
    1 C-G      -0.66     -0.10     -0.40     14.69    -17.70      0.12
    2 A-T       0.33     -0.31     -0.55     -4.48    -18.79     -1.77
    3 A-T      -0.93     -0.25     -0.29     -5.24    -22.66      0.99
    4 T-A       0.20      0.05     -0.01      9.73    -22.92     10.20
    5 T-A       0.18     -0.12     -0.04      8.36     -9.20      2.94
    6 A-T       0.38     -0.17     -0.38    -10.23    -18.87     -4.38
    7 A-T       0.05     -0.28     -0.21    -11.38    -16.19     -3.12
    8 T-A       0.40      0.01      0.25    -14.33    -12.56      0.77
    9 T-A      -0.24     -0.05      0.12     -5.87    -13.84      1.49
   10 G-C       0.48     -0.09      0.22      8.16    -13.30     -0.93
          ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.      0.02     -0.13     -0.13     -1.06    -16.60      0.63
      s.d.      0.48      0.12      0.28     10.31      4.44      4.02
***************************************************************************
Local base-pair step parameters
    step       Shift     Slide      Rise      Tilt      Roll     Twist
   1 CA/TG     -0.37      0.09      3.87     -1.16     10.81     43.33
   2 AA/TT      0.38     -0.38      3.20     -2.28     -0.94     26.48
   3 AT/AT     -0.08     -0.66      2.76     -2.52      4.46     36.73
   4 TT/AA     -0.19     -0.44      3.27     -2.95     -1.88     36.16
   5 TA/TA     -0.39     -0.65      3.77      2.12      0.45     37.92
   6 AA/TT     -0.19     -0.46      3.16     -2.86      2.69     34.64
   7 AT/AT     -0.25     -0.61      3.40     -2.54     -3.71     34.00
   8 TT/AA     -0.54     -0.23      3.09      0.83      2.41     31.43
   9 TG/CA      0.83      1.99      3.09      2.76     -2.05     41.62
          ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.     -0.09     -0.15      3.29     -0.96      1.36     35.81
      s.d.      0.43      0.84      0.35      2.26      4.41      5.08
***************************************************************************
Local base-pair helical parameters
    step       X-disp    Y-disp   h-Rise     Incl.       Tip   h-Twist
   1 CA/TG     -1.06      0.36      3.80     14.37      1.54     44.60
   2 AA/TT     -0.58     -1.41      3.17     -2.04      4.97     26.60
   3 AT/AT     -1.54     -0.16      2.66      7.03      3.98     37.08
   4 TT/AA     -0.45     -0.11      3.29     -3.02      4.75     36.32
   5 TA/TA     -1.07      0.91      3.73      0.68     -3.25     37.98
   6 AA/TT     -1.15     -0.10      3.12      4.50      4.79     34.86
   7 AT/AT     -0.42      0.00      3.46     -6.31      4.31     34.28
   8 TT/AA     -0.84      1.13      3.05      4.44     -1.53     31.53
   9 TG/CA      3.00     -0.89      3.04     -2.88     -3.88     41.76
          ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
      ave.     -0.46     -0.03      3.26      1.87      1.74     36.11
      s.d.      1.35      0.80      0.36      6.39      3.67      5.30
***************************************************************************
Structure classification:

This is a right-handed nucleic acid structure
***************************************************************************
lambda: virtual angle between C1'-YN1 or C1'-RN9 glycosidic bonds and the
        base-pair C1'-C1' line

C1'-C1': distance between C1' atoms for each base-pair
RN9-YN1: distance between RN9-YN1 atoms for each base-pair
RC8-YC6: distance between RC8-YC6 atoms for each base-pair

    bp     lambda(I) lambda(II)  C1'-C1'   RN9-YN1   RC8-YC6
   1 C-G      49.2      55.7      10.8       9.0       9.9
   2 A-T      55.3      50.1      10.6       8.8       9.7
   3 A-T      49.3      56.8      10.5       8.8       9.8
   4 T-A      57.8      53.3      10.4       8.8       9.9
   5 T-A      57.2      53.4      10.5       8.8       9.8
   6 A-T      55.4      48.9      10.7       8.9       9.8
   7 A-T      52.6      50.0      10.6       8.8       9.6
   8 T-A      59.9      51.3      10.6       8.9       9.9
   9 T-A      52.5      55.6      10.6       8.9       9.9
```

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  10 G-C      54.5      50.5      10.8       9.0       9.9
**************************************************************************
Classification of each dinucleotide step in a right-handed nucleic acid
structure: A-like; B-like; TA-like; intermediate of A and B, or other cases

    step       Xp      Yp      Zp     XpH     YpH     ZpH    Form
   1 CA/TG   -3.31    8.34   -0.74   -4.28    8.29    1.20     B
   2 AA/TT   -3.46    8.86   -1.18   -4.04    8.82   -1.47     B
   3 AT/AT   -3.70    8.98   -0.47   -5.13    8.97    0.59     B
   4 TT/AA   -3.55    8.88   -0.44   -3.97    8.85   -0.89     B
   5 TA/TA   -3.14    8.74   -0.36   -4.14    8.75   -0.25     B
   6 AA/TT   -3.07    8.90   -0.29   -4.22    8.90    0.36     B
   7 AT/AT   -3.17    8.93   -0.15   -3.59    8.86   -1.11     B
   8 TT/AA   -3.20    9.05   -0.56   -3.99    9.07    0.11     B
   9 TG/CA   -2.35    8.69   -0.93    0.46    8.64   -1.33     B
**************************************************************************
Minor and major groove widths: direct P-P distances and refined P-P distances
   which take into account the directions of the sugar-phosphate backbones

   (Subtract 5.8 Angstrom from the values to take account of the vdw radii
    of the phosphate groups, and for comparison with FreeHelix and Curves.)

Ref: M. A. El Hassan and C. R. Calladine (1998). ``Two Distinct Modes of
     Protein-induced Bending in DNA.'' J. Mol. Biol., v282, pp331-343.

                 Minor Groove        Major Groove
                P-P     Refined     P-P     Refined
   1 CA/TG       ---       ---       ---       ---
   2 AA/TT       ---       ---       ---       ---
   3 AT/AT       9.4       ---      18.9       ---
   4 TT/AA       9.4       9.4      19.7      19.5
   5 TA/TA       9.7       9.6      19.2      19.2
   6 AA/TT       9.9       9.8      20.0      19.9
   7 AT/AT      10.6       ---      18.4       ---
   8 TT/AA       ---       ---       ---       ---
   9 TG/CA       ---       ---       ---       ---
**************************************************************************
Global linear helical axis defined by equivalent C1' and RN9/YN1 atom pairs
Deviation from regular linear helix: 3.26(0.28)
Helix:    -0.490  -0.860  -0.143
HETATM 9998  XS    X X 999      -2.233  36.512  10.252
HETATM 9999  XE    X X 999     -16.610  11.252   6.061
Average and standard deviation of helix radius:
      P: 9.95(1.32), O4': 6.93(1.31),  C1': 6.46(1.33)

Global parameters based on C1'-C1' vectors:

disp.: displacement of the middle C1'-C1' point from the helix
angle: inclination between C1'-C1' vector and helix (subtracted from 90)
twist: helical twist angle between consecutive C1'-C1' vectors
rise:  helical rise by projection of the vector connecting consecutive
       C1'-C1' middle points onto the helical axis

     bp       disp.    angle     twist      rise
   1 C-G      3.25     -0.57     37.36      3.30
   2 A-T      4.19     -3.13     33.61      3.03
   3 A-T      4.07     -3.71     32.25      3.54
   4 T-A      4.67     -4.52     34.97      3.06
   5 T-A      4.50     -2.67     36.26      2.90
   6 A-T      4.14     -2.97     36.41      3.13
   7 A-T      3.82     -3.78     32.41      3.12
   8 T-A      3.53     -3.36     34.77      3.63
   9 T-A      3.51     -3.56     37.69      3.67
  10 G-C      3.07      0.81      ---       ---
**************************************************************************
Main chain and chi torsion angles:

Note: alpha:   O3'(i-1)-P-O5'-C5'
      beta:    P-O5'-C5'-C4'
      gamma:   O5'-C5'-C4'-C3'
      delta:   C5'-C4'-C3'-O3'
      epsilon: C4'-C3'-O3'-P(i+1)
      zeta:    C3'-O3'-P(i+1)-O5'(i+1)

      chi for pyrimidines(Y): O4'-C1'-N1-C2
          chi for purines(R): O4'-C1'-N9-C4

Strand I
```

base	alpha	beta	gamma	delta	epsilon	zeta	chi
1 C	---	---	41.6	144.6	160.9	-81.1	-112.7
2 A	-96.0	-129.6	56.9	157.1	-167.0	-126.7	-84.8
3 A	-46.3	152.5	45.1	117.2	177.9	-88.9	-118.5
4 T	-47.5	-152.5	19.6	151.3	178.8	-97.8	-93.9
5 T	-50.8	-176.2	35.3	134.2	164.8	-99.9	-100.5
6 A	-76.7	-178.3	65.5	133.3	-156.2	-122.4	-114.2
7 A	-60.2	162.6	49.4	120.2	172.2	-94.9	-131.6
8 T	-81.6	-172.1	75.8	105.3	179.2	-77.5	-132.3
9 T	-61.7	-163.2	27.8	125.2	-177.7	-99.8	-99.1
10 G	-68.7	175.0	61.6	137.3	---	---	-85.2

Strand II

base	alpha	beta	gamma	delta	epsilon	zeta	chi
1 G	52.6	94.8	-13.2	134.8	---	---	-86.9
2 T	-39.8	157.4	13.9	153.3	-161.1	-177.1	-85.4
3 T	-71.0	177.4	61.9	124.6	-130.7	-145.8	-116.8
4 A	-69.4	179.5	66.8	107.7	178.7	-75.9	-139.8
5 A	-138.3	-139.5	111.2	105.1	-179.3	-92.8	-143.5
6 T	21.1	98.4	29.7	108.5	161.4	-100.7	-117.8
7 T	-44.8	141.7	48.4	122.7	-158.0	-166.7	-115.1
8 A	-70.5	-168.3	47.6	150.1	-149.9	-144.5	-88.2
9 A	-81.9	152.7	50.5	144.7	173.9	-95.0	-91.8
10 C	---	---	-147.5	157.5	-107.9	-172.4	-99.0

****

Sugar conformational parameters:

Note: v0: C4'-O4'-C1'-C2'
v1: O4'-C1'-C2'-C3'
v2: C1'-C2'-C3'-C4'
v3: C2'-C3'-C4'-O4'
v4: C3'-C4'-O4'-C1'

tm: amplitude of pseudorotation of the sugar ring
P: phase angle of pseudorotation of the sugar ring

Strand I

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 C	-17.6	33.0	-35.3	25.8	-5.5	35.9	169.9	C2'-endo
2 A	-13.7	34.1	-41.3	34.6	-13.2	41.3	180.0	C2'-endo
3 A	-45.7	43.6	-24.2	-1.5	29.4	45.9	121.7	C1'-exo
4 T	-7.1	26.6	-35.1	32.1	-15.9	35.4	187.6	C3'-exo
5 T	-28.8	37.6	-32.6	16.4	7.5	37.6	150.2	C2'-endo
6 A	-32.9	41.6	-33.8	15.7	10.5	40.6	146.3	C2'-endo
7 A	-42.7	36.6	-18.4	-5.8	30.6	41.9	116.0	C1'-exo
8 T	-31.9	22.7	-6.0	-11.9	27.3	31.1	101.2	O4'-endo
9 T	-19.1	23.3	-19.2	8.9	6.3	23.2	146.0	C2'-endo
10 G	-28.8	35.5	-28.4	13.0	9.7	34.6	145.1	C2'-endo

Strand II

base	v0	v1	v2	v3	v4	tm	P	Puckering
1 G	-18.9	28.6	-27.1	17.0	1.1	29.0	159.2	C2'-endo
2 T	-28.0	46.7	-46.6	32.0	-2.6	48.4	164.4	C2'-endo
3 T	-51.1	50.4	-31.5	3.3	30.0	52.2	127.1	C1'-exo
4 A	-54.8	43.2	-17.2	-13.3	42.9	53.0	109.0	C1'-exo
5 A	-49.9	39.7	-16.3	-11.9	39.4	48.6	109.6	C1'-exo
6 T	-48.2	40.1	-18.7	-8.0	34.1	46.3	113.8	C1'-exo
7 T	-47.9	49.6	-31.9	5.4	26.5	50.0	129.6	C1'-exo
8 A	-30.8	44.6	-42.6	26.2	2.8	45.8	158.4	C2'-endo
9 A	-11.1	26.7	-31.8	26.1	-9.5	31.8	178.7	C2'-endo
10 C	-24.4	44.1	-44.8	32.2	-5.0	45.9	167.2	C2'-endo

****

Same strand P--P and C1'--C1' virtual bond distances

Strand I			Strand II		
base	P--P	C1'--C1'	base	P--P	C1'--C1'
1 C/A	---	5.2	1 G/T	6.8	5.0
2 A/A	6.2	4.4	2 T/T	6.5	4.9
3 A/T	6.8	5.4	3 T/A	6.7	5.0
4 T/T	6.5	4.9	4 A/A	6.9	4.9
5 T/A	6.7	4.8	5 A/T	6.6	5.1
6 A/A	6.9	5.0	6 T/T	6.7	4.9
7 A/T	6.8	5.0	7 T/A	6.7	4.5
8 T/T	6.6	5.4	8 A/A	7.1	4.7
9 T/G	6.2	4.8	9 A/C	---	5.5

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Helix radius (radial displacement of P, O4', and C1' atoms in local helix frame of each dimer)

	Strand I			Strand II		
	step	P	O4'	C1'	P	O4'	C1'
1	CA/TG	9.4	7.3	6.6	9.2	6.6	6.0
2	AA/TT	8.6	5.3	4.9	10.9	7.6	7.2
3	AT/AT	10.1	7.3	6.7	10.6	7.3	6.7
4	TT/AA	9.6	6.3	6.0	9.8	6.8	6.1
5	TA/TA	10.4	7.4	7.0	8.9	6.3	5.7
6	AA/TT	9.8	6.8	6.2	9.9	7.1	6.5
7	AT/AT	9.3	6.3	5.8	9.8	6.5	6.1
8	TT/AA	11.0	7.8	7.3	8.8	5.9	5.4
9	TG/CA	8.0	4.8	4.5	9.4	6.5	6.2

****

Position (Px, Py, Pz) and local helical axis vector (Hx, Hy, Hz)
for each dinucleotide step

	bp	Px	Py	Pz	Hx	Hy	Hz
1	CA/TG	-1.62	34.54	9.32	-0.64	-0.76	-0.11
2	AA/TT	-5.01	32.46	8.36	-0.39	-0.91	-0.17
3	AT/AT	-5.77	29.49	9.20	-0.52	-0.83	-0.22
4	TT/AA	-6.31	26.46	8.34	-0.45	-0.89	-0.07
5	TA/TA	-8.76	23.83	8.83	-0.55	-0.82	-0.16
6	AA/TT	-9.92	20.50	7.61	-0.43	-0.90	-0.10
7	AT/AT	-11.65	17.65	8.05	-0.59	-0.80	-0.08
8	TT/AA	-14.00	15.33	6.89	-0.41	-0.91	-0.09
9	TG/CA	-17.51	12.99	10.09	-0.43	-0.88	-0.22