Supplementary material

S1 Theory

S1.1 The average frame

We consider an ensemble of n nucleic acid bases, each of which is modelled as a rigid body. The bases are numbered from 1 to n. The configuration of an arbitrary base a is given by a reference point $\mathbf{r}^a$ and a right-handed, orthonormal frame $\{\mathbf{d}_i^a\}$ $(i = 1, 2, 3)$, both attached to the base. There is now a well-established way of attaching a reference point and a frame to a base (1). The standard choice is such that if the base is included in the reference strand of the canonical B-DNA, then $\mathbf{d}_1$ points into the major groove, $\mathbf{d}_2$ points towards the backbone of the reference strand, and $\mathbf{d}_3 = \mathbf{d}_1 \times \mathbf{d}_2$ is the basepair normal pointing along the 5' to 3' direction of the reference strand. Notice that, although the definition is inspired by the double-stranded canonical B-DNA structure, the base-fixed reference point and frame depend only on the atomic coordinates of the base itself.

Let $\{\mathbf{e}_i\}$ denote a right-handed, orthonormal frame fixed in the lab. The configuration of the base a is uniquely defined by the component vector $r^a \in \mathbb{R}^3$ and the rotation matrix $R^a \in \mathbb{R}^{3\times 3}$, where $r_i^a = \mathbf{e}_i \cdot \mathbf{r}^a$ and $R_{ij}^a = \mathbf{e}_i \cdot \mathbf{d}_j^a$. Our goal is to replace the base-fixed points $\mathbf{r}^a$ by one point and the base-fixed frames $\{\mathbf{d}_i^a\}$ by one frame which would represent, in some sense, their respective means.

The appropriate average of the points $\mathbf{r}^a$ is their arithmetic mean $\overline{\mathbf{r}} = \frac{1}{n}\sum_{a=1}^n \mathbf{r}^a$, uniquely defined by its component vector $\overline{r}$, where $\overline{r}_i = \mathbf{e}_i \cdot \overline{\mathbf{r}}$. The component vector $\overline{r}$ is given by the arithmetic mean of the component vectors of the base-fixed points,

$$\overline{r} = \frac{1}{n}\sum_{a=1}^{n} r^a \tag{1}$$

The arithmetic mean has a variational property: it minimizes the sum of the squared Euclidean distances to the points $\mathbf{r}^a$.

The rotation matrices R^a, which represent the coordinate frames $\{\mathbf{d}_i^a\}$, are elements of the group of rotations. As the group of rotations is not a Euclidean space, the notion of mean or average of an ensemble of rotations is not obvious. Moakher (2) proposed two different notions of mean in the group of rotations, both based on a variational property analogous to the one satisfied by the arithmetic mean in the Euclidean space. Each of the two proposed means is represented by a rotation matrix which minimizes the squared distances to the given

matrices. The distance, however, is given by a different metrics in each case. The *mean rotation in the Euclidean sense* is based on the Euclidean distance: if R^1 and R^2 are two rotation matrices, their Euclidean distance is defined as $\mathrm{d}_F(R^1, R^2) = \|R^1 - R^2\|_F$, where $\|\cdot\|_F$ is the Frobenius norm which is induced by the Euclidean, or Frobenius, inner product $\langle R^1, R^2\rangle_F = \mathrm{tr}((R^1)^T R^2)$. Here tr means the trace of a matrix and the superscript T indicates the matrix transpose. The *mean rotation in the Riemannian sense* is based on the Riemannian distance $\mathrm{d}_R(R^1, R^2)$ between two rotations R^1 and R^2, which is the length of the shortest geodesic curve that connects R^1 and R^2. In the case of averaging just two matrices whose sum has a nonzero determinant, the two means coincide and can be calculated using an explicit formula (2).

For more than two matrices, the Riemannian mean cannot be given in a closed form. However, Moakher (2) has derived a formula to compute the Euclidean mean. Let R^a, $a = 1, \ldots, n$ be rotation matrices and $\overline{R}$ their arithmetic mean, $\overline{R} = \frac{1}{n}\sum_{a=1}^{n} R^a$. Let $\det \overline{R} \neq 0$ and define s such that $s = 1$ if $\det \overline{R} > 0$ and $s = -1$ if $\det \overline{R} < 0$. Then the Euclidean mean R of the matrices R^a, $a = 1, \ldots, n$ is given by

$$R = \overline{R} U \,\mathrm{diag}\left(\frac{1}{\sqrt{\Lambda_1}}, \frac{1}{\sqrt{\Lambda_2}}, \frac{s}{\sqrt{\Lambda_3}}\right) U^T \tag{2}$$

where $\Lambda_1 \geq \Lambda_2 \geq \Lambda_3 \geq 0$ are eigenvalues of the matrix $M = \overline{R}^T \overline{R}$ and the columns of U are unit eigenvectors of M corresponding to these eigenvalues, so that $M = U\mathrm{diag}(\Lambda_1, \Lambda_2, \Lambda_3)U^T$. For any three numbers d_1, d_2, d_3 we define $\mathrm{diag}(d_1, d_2, d_3)$ as the diagonal matrix D such that $D_{11} = d_1, D_{22} = d_2, D_{33} = d_3$. The case of $\det \overline{R} = 0$ is a singular one and will not be considered here.

The mean frame $\{\mathbf{d}_i\}$ of the base-fixed frames $\{\mathbf{d}_i^a\}$ can now be obtained. The frames $\{\mathbf{d}_i^a\}$ are represented by the rotation matrices R^a as described above, and their Euclidean mean R uniquely defines the mean frame $\{\mathbf{d}_i\}$ through the relation $R_{ij} = \mathbf{e}_i \cdot \mathbf{d}_j$.

S1.2 Bending measurement

We consider a nucleic acid structure represented as an ensemble of rigid bases. The configuration of each base is given by a reference point and a right-handed orthonormal frame fixed in the base, as described in Section S1.1. We now choose three groups of bases which we will call the initial, middle, and final group. Which bases belong to which group depends on the particular structure and the intentions of the researcher. In a double helical DNA oligomer, a natural choice would be to include several bases at one end into the initial group, while the final group would consist of several bases at the opposite end and the middle group would contain bases around the oligomer centre. Each group would include, for instance, bases in 2–3 consecutive base pairs. The middle group may coincide either with the initial or with the final group, so that only two distinct groups may be present. For instance, in the case of a V-shaped RNA motif, it may be natural to define two groups, each at the end of one of

the two arms forming the V. Notice that we make no assumption about the pairing of the bases.

For each group, the average frame is first computed as described in Section S1.1. We denote by $\{\mathbf{i}_i\}$ the mean frame of the initial group, by $\{\mathbf{m}_i\}$ the mean frame of the middle group and by $\{\mathbf{f}_i\}$ the one of the final group ($i = 1, 2, 3$). We then define the bending magnitude $\vartheta \in [0, \pi]$ by the relation $\cos\varphi = \mathbf{i}_3 \cdot \mathbf{f}_3$, or

$$\vartheta = \arccos(\mathbf{i}_3 \cdot \mathbf{f}_3) \tag{3}$$

Thus, the bending magnitude is the angle between the unit vectors $\mathbf{i}_3$ and $\mathbf{f}_3$. To assess the bending direction, we consider the mean frame $\{\mathbf{m}_i\}$ of the middle group. The projection $\mathbf{g}$ of the vector $\mathbf{f}_3 - \mathbf{i}_3$ onto the plane spanned by $\mathbf{m}_1$ and $\mathbf{m}_2$ is given by

$$\mathbf{g} = (\mathbf{f}_3 - \mathbf{i}_3) - [(\mathbf{f}_3 - \mathbf{i}_3) \cdot \mathbf{m}_3]\mathbf{m}_3$$

If $\mathbf{g} \neq \mathbf{0}$, we define the bending direction $\varphi \in [0, 2\pi)$ by the relations

$$\begin{aligned} \varphi &= \arccos\left(\frac{\mathbf{g} \cdot \mathbf{m}_1}{\|\mathbf{g}\|}\right) \quad \text{if} \quad (\mathbf{m}_1 \times \mathbf{g}) \cdot \mathbf{m}_3 \geq 0 \\ \varphi &= 2\pi - \arccos\left(\frac{\mathbf{g} \cdot \mathbf{m}_1}{\|\mathbf{g}\|}\right) \quad \text{if} \quad (\mathbf{m}_1 \times \mathbf{g}) \cdot \mathbf{m}_3 < 0 \end{aligned} \tag{4}$$

The bending direction is thus the oriented angle from $\mathbf{m}_1$ to the projection $\mathbf{g}$ of the vector $\mathbf{f}_3 - \mathbf{i}_3$ onto the plane spanned by $\mathbf{m}_1$ and $\mathbf{m}_2$. If $\mathbf{g} = \mathbf{0}$, the bending direction is not defined.

As discussed above, there is now a standard way of attaching a reference point and a frame to a base (1). Nevertheless, adjustments may be necessary depending on the particular situation. In the case of double helical B-DNA structures, for instance, the standard definition of the frame attached to a base in the complementary strand (1) can be formulated as follows: a frame is first attached as if the base was in the reference strand, then it is rotated by π rad (or 180 °) around $\mathbf{d}_1$. In this way the normals $\mathbf{d}_3$ of both bases in a pair point along the 5' to 3' direction of the reference strand. It is up to the researcher to make sensible choices in a nonstandard case, such as for an irregular RNA structure. Once the base-fixed frames are suitably defined, the procedure described above can be followed. We remark that the middle frame $\{\mathbf{m}_i\}$ may not represent a separate group of bases but may be the mean of the initial frame $\{\mathbf{i}_i\}$ and the final frame $\{\mathbf{f}_i\}$. This is analogous to the concept of intermediate frame proposed to define local conformational parameters (3).

We have not used the average reference points in our definition of global bending. They may nevertheless be useful in defining distances between groups of bases in a nucleic acids structure. For the sake of convenience, angular quantities reported in the paper are in degrees.

References

1. Olson,W.K., Bansal,M., Burley,S.K., Dickerson,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., and Berman,H.M. (2001) A standard reference frame for the description of nucleic acid base-pair geometry. *J. Mol. Biol.*, **313**, 229–237.

2. Moakher,M. (2002) Means and averaging in the group of rotations. *SIAM J. Matrix Anal. Appl.*, **24**, 1–16.

3. Dickerson,R.E., Bansal,M., Calladine,C.R., Diekmann,S., Hunter,W.N., Kennard,O., Lavery,R., Nelson,H.C.M., Olson,W.K., Saenger,W., Shakked,Z., Sklenar,H., Soumpasis,D.M., Tung,C.-S., von Kitzing,E., Wang,A.H.-J., and Zhurkin,V.B. (1989) Definitions and nomenclature of nucleic acid structure parameters. *J. Mol. Biol.*, **205**, 787–791.

S2 Trajectory filtering

Code	Snapshots with intact H-bonds [%]	Snapshots with canonical γ [%]	Admissible snapshots [%]
AT_short	72 (87, 57)	67 (81, 53)	62 (73, 51)
AT_short_neut	63 (78, 49)	58 (51, 66)	48 (50, 46)
AT_short_lowT	97 (95, 99)	100 (100, 100)	97 (95, 99)
AT_short_Na	64 (79, 49)	50 (68, 33)	47 (63, 32)
TA_short	81 (97, 65)	93 (94, 91)	76 (91, 61)
TA_short_neut	88 (96, 80)	36 (73, 0)	34 (70, 0)
TA_short_lowT	99 (98, 99)	100 (100, 100)	98 (98, 99)
TA_short_Na	58 (62, 54)	74 (82, 66)	44 (47, 40)
AT_long	90 (85, 95)	83 (87, 79)	75 (75, 75)
TA_long	93 (92, 95)	45 (76, 15)	42 (69, 14)

Table S1: Fraction of snapshots from the trajectories in which no conformational anomaly is observed anywhere in the oligomer. Anomalies examined include a broken intra-basepair H-bond (second column) and a flip of the backbone torsion angle γ into a non-canonical state (third column). Admissible snapshots (last column) are those in which neither of the two anomalies occur. Typically only these snapshots were used for the analysis. Values for the two halves of each trajectory are in parentheses. H-bonds of the 3' end pair in the TA_short_lowT simulation broke at 5 ns and at least one of them stayed broken until the end of the simulation. To be able to analyze this simulation, too, we allowed shapshots with a broken H-bond in the 3' end pair of TA_short_lowT to pass through the filtering. The values for this simulation in the Table do not include the broken H-bonds in the 3' end pair.

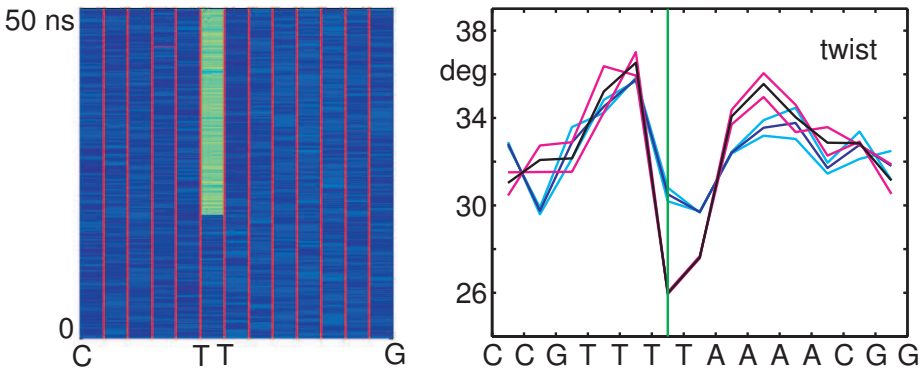

Figure S1: Illustration of the effect of a γ-flip on the DNA conformation. The TA_short_neut simulation exhibits just one γ-flip, which makes it possible to study the effect of a single flip in isolation. The left panel of the figure shows time series of γ in the complementary strand of TA_short_neut. The x-axis represents the backbone fragments, the y-axis indicates simulation time. The γ angles show canonical values ($g+$, blue), except in step 6 (TT) where the flip into the non-canonical t state (green) occurs at roughly 18 ns and lasts until the end of the simulation. The comparison of the intra-basepair and inter-basepair parameters averaged over the first 18 ns (no flip) and the last 18 ns of the trajectory shows that the flip affects all the parameters. The effect is strongest in the flipped step itself, where roll and twist decrease due to the flip by 4 °, tilt by 2 °, slide by 0.5 Å and shift by 0.3 Å. Other parameters are influenced to a lesser extent. Parameters in neighbouring steps change, too, so that the effect is nonlocal. In the right panel, profiles of twist averaged over 1-18 ns (blue) and over 32-50 ns (black) indicate that the flip affects twist values in the flipped step (vertical green line) and three neighbouring steps. The averages over the halves of the time intervals (1-9 ns and 9-18 ns, cyan, and 32-41 ns and 41-50 ns, magenta), confirm the effect.

S3 Conformational parameters

This section includes profiles of selected structural parameters averaged over the filtered trajectories and over the ensemble of NMR models. A complete list of parameters for the AT_short and TA_short simulations, averaged over the filtered trajectory and over its halves, is also provided.

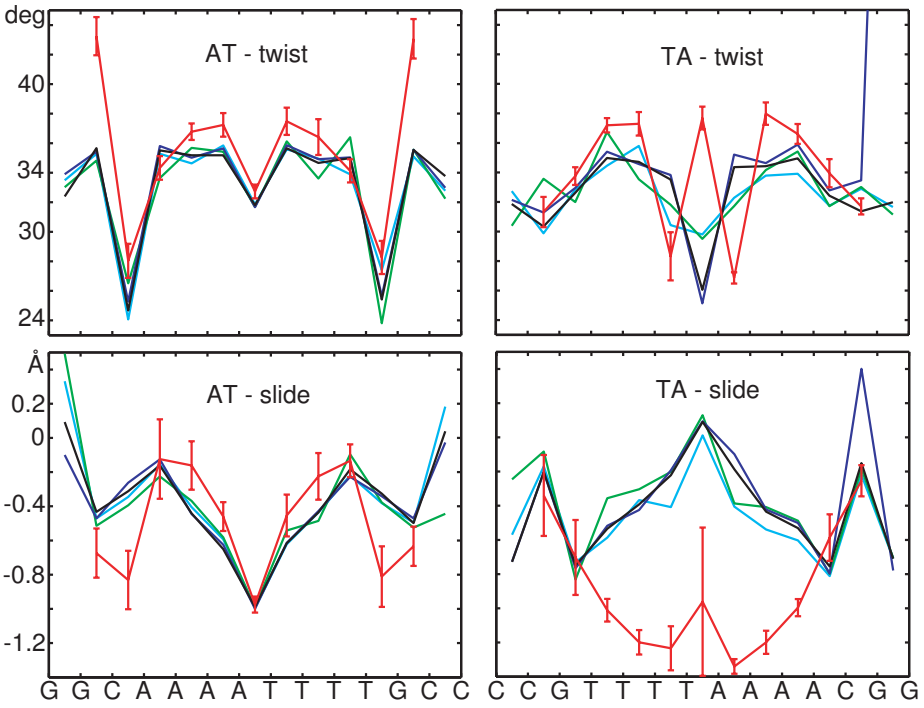

Figure S2: Average twist and slide profiles in the simulated and NMR structures. The lines connect vertices marking values for individual steps, placed in the middle of each indicated step. Values for AT_short (black), AT_short_lowT (blue), AT_short_Na (green), AT_short_neut (cyan) simulations, and NMR data AT_nmr (red) are shown. The colour coding for TA tracts is analogous. Error bars represent one standard deviation for the ensemble of NMR models. The anomalous values at the 3' end of TA_short_lowT (blue curves) are probably due to the broken end pair - see Section S2.

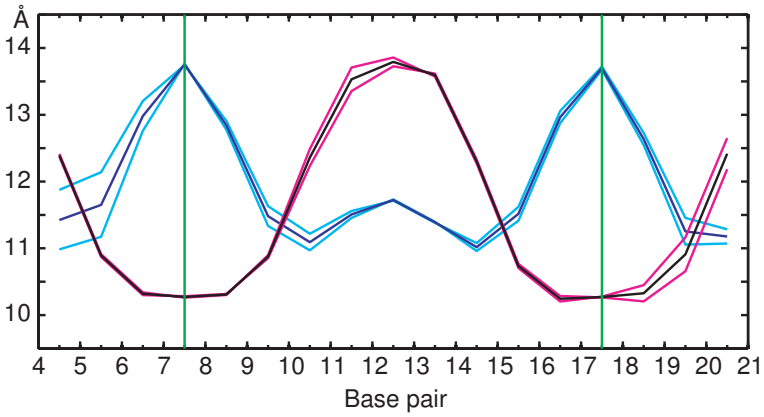

Figure S3: Average minor groove profiles of the simulated AT tract and TA tract tandems (AT_long and TA_long respectively). The base pair numbers are indicated on the x-axis. Averages over the whole filtered trajectories (black for the AT tandem, blue for the TA tandem) are shown together with the averages over the two halves of each trajectory (magenta and cyan for AT and TA, respectively). The narrowing of the minor groove within each AT tract, and widening in each TA tract is seen. The tract centres are indicated by vertical green lines. The two tracts in each dimer exhibit almost identical profiles. The values for the two trajectory halves are close to those for the whole trajectory for both simulations, indicating good convergence.

AT_short, intra basepair parameters

bp	Shear	Stretch	Stagger	Buckle	Propeller	Opening
1 G-C	-0.33	-0.10	0.02	0.09	3.02	0.10
	-0.32,-0.33	*-0.10,-0.10*	*0.02,0.01*	*0.41,-0.37*	*3.79,1.93*	*0.21,-0.05*
2 G-C	-0.16	-0.07	0.14	1.46	-7.64	-0.68
	-0.16,-0.17	*-0.07,-0.07*	*0.16,0.12*	*2.34,0.21*	*-7.37,-8.02*	*-0.68,-0.68*
3 C-G	0.13	-0.05	0.07	2.16	-5.72	-0.50
	0.13,0.14	*-0.05,-0.05*	*0.06,0.07*	*2.83,1.21*	*-6.14,-5.12*	*-0.56,-0.41*
4 A-T	0.03	-0.01	-0.19	8.97	-10.93	1.22
	0.03,0.04	*-0.01,-0.01*	*-0.19,-0.17*	*8.17,10.10*	*-11.40,-10.26*	*1.30,1.10*
5 A-T	0.10	0.00	-0.10	9.15	-17.23	0.83
	0.10,0.10	*0.00,0.00*	*-0.10,-0.10*	*8.94,9.45*	*-16.77,-17.88*	*0.81,0.87*
6 A-T	0.11	0.00	-0.02	4.48	-18.67	0.79
	0.11,0.11	*0.00,0.00*	*-0.02,-0.03*	*4.85,3.96*	*-18.42,-19.03*	*0.78,0.80*
7 A-T	0.10	0.01	0.16	0.05	-17.31	0.87
	0.10,0.10	*0.01,0.01*	*0.17,0.15*	*0.59,-0.72*	*-17.28,-17.34*	*0.90,0.82*
8 T-A	-0.11	0.01	0.15	-0.28	-17.30	0.87
	-0.11,-0.10	*0.01,0.01*	*0.15,0.14*	*0.48,-1.36*	*-17.43,-17.12*	*0.98,0.71*
9 T-A	-0.11	0.00	-0.02	-5.03	-18.33	0.68
	-0.11,-0.11	*0.00,0.00*	*-0.01,-0.04*	*-4.45,-5.85*	*-18.79,-17.67*	*0.74,0.60*
10 T-A	-0.10	0.00	-0.12	-8.73	-16.96	0.79
	-0.10,-0.10	*0.00,-0.00*	*-0.11,-0.14*	*-9.09,-8.21*	*-17.32,-16.45*	*0.63,1.02*
11 T-A	-0.04	-0.01	-0.20	-7.88	-10.90	1.12
	-0.04,-0.03	*-0.01,-0.01*	*-0.20,-0.22*	*-8.32,-7.27*	*-10.26,-11.79*	*1.19,1.02*
12 G-C	-0.14	-0.05	0.06	-2.25	-6.48	-0.42
	-0.13,-0.15	*-0.05,-0.06*	*0.07,0.04*	*-1.50,-3.30*	*-5.81,-7.42*	*-0.40,-0.46*
13 C-G	0.16	-0.06	0.15	-2.03	-8.33	-0.77
	0.16,0.15	*-0.07,-0.06*	*0.16,0.15*	*-1.33,-3.03*	*-8.98,-7.40*	*-0.83,-0.67*
14 C-G	0.32	-0.09	0.02	-0.31	2.27	0.09
	0.32,0.32	*-0.09,-0.09*	*0.03,0.01*	*-0.40,-0.18*	*1.90,2.81*	*0.09,0.09*

Table S2: Tables of intra and inter basepair parameters for the AT_short and TA_short simulations. Values for the whole trajectory (roman font) and values for the two halves of the trajectory (italics) are shown. The whole trajectory and its halves were filtered for broken intra-basepair hydrogen bonds and non-canonical flips of the backbone torsion angle γ, and the first nanosecond was omitted, as described in the main text. The values for the two trajectory halves are in general close to each other and close to the value for the whole trajectory, which indicates good convergence of the parameters.

AT_short, inter basepair parameters

bp step	Shift	Slide	Rise	Tilt	Roll	Twist
1 GG/CC	-0.69	0.09	3.42	-2.12	4.95	32.39
	-0.73,-0.64	*0.20,-0.06*	*3.42,3.43*	*-2.26,-1.90*	*5.20,4.60*	*32.22,32.63*
2 GC/GC	0.25	-0.43	3.36	0.44	0.50	35.66
	0.26,0.25	*-0.45,-0.41*	*3.37,3.36*	*0.56,0.28*	*0.50,0.50*	*35.38,36.07*
3 CA/TG	-0.10	-0.31	3.20	2.20	11.02	24.67
	-0.11,-0.09	*-0.32,-0.31*	*3.23,3.15*	*2.12,2.32*	*11.12,10.87*	*25.79,23.08*
4 AA/TT	-0.42	-0.16	3.32	-1.77	1.56	35.51
	-0.36,-0.51	*-0.20,-0.10*	*3.31,3.33*	*-1.70,-1.87*	*1.96,1.00*	*34.74,36.60*
5 AA/TT	-0.08	-0.44	3.40	-1.59	1.62	35.18
	-0.10,-0.05	*-0.43,-0.45*	*3.38,3.41*	*-1.62,-1.55*	*1.55,1.72*	*35.16,35.21*
6 AA/TT	-0.08	-0.65	3.34	-2.50	0.72	35.18
	-0.09,-0.06	*-0.65,-0.65*	*3.34,3.35*	*-2.50,-2.50*	*0.62,0.87*	*35.18,35.18*
7 AT/AT	-0.02	-0.99	3.30	0.10	-1.29	31.80
	-0.01,-0.04	*-0.98,-1.01*	*3.29,3.31*	*0.12,0.06*	*-1.39,-1.16*	*31.88,31.69*
8 TT/AA	0.13	-0.62	3.35	2.56	0.76	35.65
	0.12,0.15	*-0.63,-0.59*	*3.35,3.35*	*2.50,2.64*	*0.53,1.08*	*35.65,35.66*
9 TT/AA	0.06	-0.44	3.38	1.50	1.73	34.66
	0.05,0.08	*-0.45,-0.41*	*3.39,3.36*	*1.58,1.38*	*1.14,2.56*	*35.15,33.97*
10 TT/AA	0.38	-0.18	3.31	1.68	1.81	34.99
	0.42,0.33	*-0.15,-0.23*	*3.31,3.31*	*1.68,1.67*	*1.22,2.66*	*35.51,34.25*
11 TG/CA	0.13	-0.33	3.22	-2.15	11.01	25.41
	0.15,0.09	*-0.32,-0.33*	*3.19,3.26*	*-2.22,-2.06*	*10.64,11.55*	*24.40,26.84*
12 GC/GC	-0.30	-0.50	3.37	-0.54	0.70	35.54
	-0.36,-0.21	*-0.43,-0.59*	*3.37,3.36*	*-0.62,-0.42*	*0.12,1.52*	*36.05,34.83*
13 CC/GG	0.72	0.04	3.40	2.37	4.31	33.77
	0.73,0.71	*0.05,0.02*	*3.42,3.38*	*2.32,2.45*	*4.10,4.60*	*33.95,33.52*

TA_short, intra basepair parameters

bp	Shear	Stretch	Stagger	Buckle	Propeller	Opening
1 C-G	0.20	-0.08	-0.08	1.83	-14.68	-0.20
	0.20,0.21	*-0.08,-0.09*	*-0.04,-0.14*	*0.46,3.84*	*-14.93,-14.31*	*-0.26,-0.11*
2 C-G	0.16	-0.07	0.12	-3.78	-8.71	-0.39
	0.15,0.16	*-0.06,-0.08*	*0.14,0.09*	*-5.19,-1.71*	*-7.75,-10.12*	*-0.21,-0.65*
3 G-C	-0.13	-0.05	0.14	-1.08	-10.87	0.03
	-0.12,-0.15	*-0.05,-0.06*	*0.15,0.12*	*0.12,-2.85*	*-10.09,-12.02*	*0.08,-0.03*
4 T-A	-0.11	0.01	0.12	-2.32	-15.93	0.33
	-0.13,-0.09	*0.01,0.01*	*0.11,0.14*	*-1.39,-3.69*	*-16.27,-15.44*	*0.00,0.80*
5 T-A	-0.11	-0.00	-0.08	-4.94	-17.92	0.92
	-0.11,-0.11	*-0.00,-0.00*	*-0.07,-0.09*	*-4.81,-5.13*	*-18.12,-17.63*	*0.89,0.97*
6 T-A	-0.10	0.00	-0.11	-8.04	-15.76	0.94
	-0.10,-0.10	*0.00,0.00*	*-0.12,-0.11*	*-8.07,-7.99*	*-16.00,-15.40*	*0.95,0.93*
7 T-A	-0.07	0.00	-0.21	-4.58	-9.98	2.12
	-0.06,-0.07	*0.00,0.01*	*-0.21,-0.20*	*-4.76,-4.30*	*-9.96,-10.01*	*2.14,2.09*
8 A-T	0.08	0.01	-0.19	4.33	-9.51	2.05
	0.08,0.09	*0.01,0.01*	*-0.19,-0.18*	*4.35,4.31*	*-9.42,-9.65*	*2.20,1.83*
9 A-T	0.09	0.00	-0.11	7.51	-16.11	0.93
	0.09,0.10	*0.00,0.00*	*-0.12,-0.10*	*7.56,7.45*	*-15.97,-16.31*	*1.01,0.82*
10 A-T	0.11	-0.00	-0.08	4.51	-17.65	0.72
	0.11,0.12	*-0.00,-0.00*	*-0.09,-0.08*	*4.81,4.08*	*-17.55,-17.80*	*0.75,0.66*
11 A-T	0.11	0.01	0.14	2.76	-15.56	0.25
	0.11,0.10	*0.01,0.01*	*0.13,0.16*	*2.84,2.65*	*-15.70,-15.36*	*0.08,0.48*
12 C-G	0.13	-0.06	0.14	1.80	-11.17	-0.01
	0.13,0.14	*-0.05,-0.06*	*0.13,0.15*	*1.94,1.61*	*-11.20,-11.14*	*0.02,-0.06*
13 G-C	-0.15	-0.07	0.12	3.73	-9.38	-0.52
	-0.15,-0.15	*-0.07,-0.07*	*0.13,0.12*	*4.07,3.24*	*-9.20,-9.65*	*-0.46,-0.60*
14 G-C	-0.20	-0.08	-0.05	-2.09	-14.91	-0.43
	-0.20,-0.20	*-0.08,-0.08*	*-0.05,-0.05*	*-1.98,-2.25*	*-15.12,-14.58*	*-0.40,-0.47*

TA_short, inter basepair parameters

bp step	Shift	Slide	Rise	Tilt	Roll	Twist
1 GG/CC	-0.69	0.09	3.42	-2.12	4.95	32.39
	-0.73,-0.64	*0.20,-0.06*	*3.42,3.43*	*-2.26,-1.90*	*5.20,4.60*	*32.22,32.63*
1 CC/GG	-0.11	-0.73	3.50	-0.94	6.03	31.86
	-0.01,-0.25	*-0.69,-0.78*	*3.50,3.51*	*-0.61,-1.41*	*5.69,6.52*	*32.53,30.88*
2 CG/CG	0.01	-0.20	3.24	-0.56	8.77	30.34
	0.02,0.00	*-0.19,-0.22*	*3.19,3.32*	*-0.49,-0.66*	*8.51,9.15*	*28.68,32.77*
3 GT/AC	-0.12	-0.75	3.37	0.49	0.60	32.62
	-0.18,-0.03	*-0.71,-0.81*	*3.38,3.36*	*0.53,0.42*	*-0.13,1.67*	*33.33,31.58*
4 TT/AA	0.14	-0.53	3.33	2.46	1.92	34.98
	0.16,0.10	*-0.53,-0.54*	*3.34,3.30*	*2.36,2.60*	*1.75,2.16*	*35.25,34.59*
5 TT/AA	0.17	-0.39	3.39	1.19	2.47	34.71
	0.14,0.21	*-0.39,-0.40*	*3.39,3.38*	*1.19,1.18*	*2.45,2.52*	*34.60,34.88*
6 TT/AA	0.33	-0.22	3.27	1.44	2.25	33.52
	0.35,0.31	*-0.20,-0.26*	*3.27,3.27*	*1.45,1.43*	*2.27,2.22*	*33.69,33.27*
7 TA/TA	0.10	0.09	3.22	-0.09	11.19	26.05
	0.10,0.10	*0.11,0.07*	*3.21,3.22*	*-0.10,-0.07*	*11.49,10.75*	*25.87,26.31*
8 AA/TT	-0.42	-0.19	3.28	-1.43	1.72	34.36
	-0.41,-0.44	*-0.20,-0.16*	*3.28,3.28*	*-1.39,-1.49*	*1.90,1.45*	*34.15,34.66*
9 AA/TT	-0.14	-0.43	3.38	-1.13	2.45	34.42
	-0.15,-0.13	*-0.43,-0.45*	*3.38,3.39*	*-1.15,-1.10*	*2.60,2.22*	*34.30,34.61*
10 AA/TT	-0.13	-0.53	3.31	-2.57	1.56	34.96
	-0.16,-0.09	*-0.52,-0.55*	*3.31,3.30*	*-2.52,-2.64*	*1.66,1.42*	*35.07,34.80*
11 AC/GT	0.08	-0.75	3.37	-0.41	0.66	32.43
	0.11,0.03	*-0.73,-0.79*	*3.36,3.37*	*-0.40,-0.43*	*0.56,0.82*	*32.62,32.14*
12 CG/CG	0.02	-0.15	3.27	0.68	8.53	31.37
	0.01,0.05	*-0.16,-0.14*	*3.26,3.27*	*0.53,0.90*	*8.67,8.31*	*30.89,32.07*
13 GG/CC	0.10	-0.71	3.50	0.80	5.68	31.98
	0.08,0.14	*-0.71,-0.71*	*3.50,3.49*	*0.74,0.88*	*5.58,5.83*	*32.30,31.51*