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Limits of RNA 2′-OH Mimicry by Fluorine: Crystal Structure of *Bacillus halodurans* RNase H Bound to a 2′-FRNA:DNA Hybrid

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Supporting Information

ABSTRACT: RNase H1 cleaves the RNA strand of RNA:DNA hybrids. Replacement of RNA 2′-hydroxyls by fluorine (FRNA) is commonly used to stabilize aptamers and siRNAs. However, FRNA:DNA hybrids fail to elicit RNase H activity. The underlying reasons are unclear, as 2′-OH groups are not directly involved in cleavage. We determined the crystal structure of *Bacillus halodurans* RNase H bound to a FRNA:DNA hybrid. The structure points to dynamic (slippage of the FRNA:DNA hybrid relative to the enzyme), geometric (different curvatures of FRNA:DNA and RNA:DNA hybrids), and electronic reasons (Mg^{2+} absent from the active site of the FRNA:DNA complex) for the loss of RNaseH activity.

Ribonuclease H (RNase H) hydrolyzes the RNA of RNA:DNA hybrid duplexes endonucleolytically, resulting in cleavage products with 5′-phosphate and 3′-hydroxyl termini.[1−4] RNases H are divided into types 1, called RNase HI (prokaryotes) and RNase H1 (eukaryotes), and 2, called RNase HII (prokaryotes) and RNase H2 (eukaryotes).[5] Human RNase H1 is a single protein and appears to play a role in mitochondrial DNA replication.[6] Human RNase H2 consists of three subunits, and mutations in these cause Aicardi-Goutiéres syndrome, a neurological disorder.[7]

Crystal structures of RNA:DNA hybrids bound to the catalytic domains of *Bacillus halodurans* RNase HI (*Bh*RNase H)[8] and human RNase H1 (*Hs*RNase H)[9] revealed shared features in terms of the active site, recognition, and duplex conformation, as well as differences between the enzymes from prokaryotes and eukaryotes. The structural data are consistent with a two-metal ion mechanism (Mg^{2+}) in both cases, with conserved residues involved in metal ion coordination [D71, E109, D132, E188, and D192 in *Bh*RNase H (Figure 1) and D145, E186, D210, and D274 in *Hs*RNase H]. The specificity of the enzymes for the hybrid duplex is grounded in A- and B-form conformations of the RNA and DNA strands, respectively, that result in a unique width of the minor groove, the site contacted by RNase H. Five consecutive ribose 2′-hydroxyl groups that are contacted by four amino acids in the complex of *Bh*RNase H allow the enzyme to distinguish between RNA and DNA.[8] The scissile phosphate group is accommodated at the active site and is engaged in direct interactions with metal ions A (production of the hydroxy anion nucleophile) and B (leaving group stabilization) (Figure 1). A phosphate group of the DNA strand 2 bp from the scissile phosphate (in the RNA 5′-direction) is lodged at the so-called

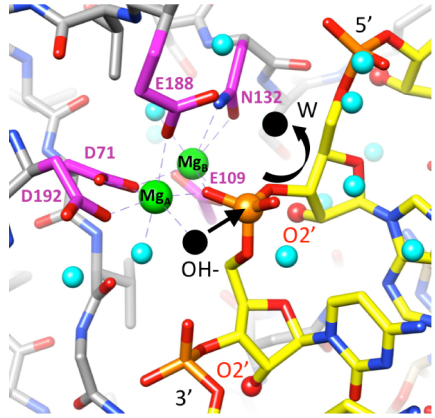

Figure 1. Active site of *Bh*RNase H bound to an RNA:DNA hybrid (Protein Data Bank entry 1zbi[8]). Mg^{2+} ions are colored green, RNA carbons yellow, with the phosphorus atom of the scissile phosphate shown as a sphere, side chain carbons of Glu and Asp coordinated to Mg^{2+} magenta, and waters cyan, exept for those involved in nucleophilic attack and leaving group protonation (black spheres and arrows, respectively).

phosphate binding pocket, such that the enzyme bridges RNA and DNA across the minor groove. In the structure of the *Hs*RNase H substrate complex, the enzyme establishes more extensive interactions with the DNA compared with the structure of the bacterial complex and the conformation of the DNA strand varies between the B- and A-forms near a basic protrusion that is missing in *Bh*RNase H.[8,9]

The mechanism of RNase H cleavage was further probed by crystal structures of product complexes with different *Bh*RNase H mutant proteins.[10] Accordingly, the two metal ions are separated by ∼4 Å upon binding of the enzyme to the hybrid duplex. $Mg^{2+}{}_A$ shows the standard octahedral coordination geometry and activates and orients a water molecule for nucleophilic attack (Figure 1). Unlike that of metal ion A, the coordination of $Mg^{2+}{}_B$ is irregular, but following formation of the pentacovalent transition state, concomitant shortening of the distance between the two metal ions to ∼3.5 Å, and finally release of the 5′-phosphate and 3′-hydroxyl groups, $Mg^{2+}{}_B$ reaches a regular octahedral coordination state that involves two water molecules.[10] E188, the fifth acidic amino acid at the active site of

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*Bh*RNase H, facilitates efficient product release. Importantly, with respect to a potential role of RNA 2′-hydroxyl groups in RNase H activity, only one 2′-oxygen is situated in the proximity of the active site [E109 (Figure 1)]. However, the structural analyses do not directly implicate 2′-hydroxyl groups in the cleavage mechanism.[4,8,10]

RNase H is considered a key player in antisense oligonucleotide (AON)-mediated degradation of RNA.[11−14] However, most chemically modified AONs paired with RNA as well as all-RNA and -DNA duplexes do not elicit cleavage by RNase H and function as competitive inhibitors instead.[15−17] Phosphorothioate-DNA (PS-DNA)[18] and 2′-deoxy-2′-fluoro-arabinonucleic acid (FANA)[19] are two of only a handful of modifications that are tolerated in fully modified AONs opposite RNA by RNase H. Thus, the enzyme is unable to cleave RNA bound to complementary, fully 2′-modified AONs.[20,21] A common strategy for circumventing this limitation is the use of gapmer AONs with various 2′ modifications in the wings combined with a central PS-DNA window that permits RNase H action.[14,22,23] Whereas the effects of modifications in the DNA (antisense) strand on RNase H activity have been studied extensively, the consequences of an altered RNA (sense) strand have been assessed for only a limited number of analogues, e.g., oligo-2′-deoxy-2′-fluoro-ribonucleotide (FRNA)[11] and oligo-2′-*O*-methyl-ribonucleotide.[15] Considering that ribose 2′-hydroxyl groups do not seem to participate in cleavage action, it is unclear why FRNA is not tolerated in the sense strand of the hybrid duplex (Figure 2).[11] Conversely, extensive 2′-F modification of both

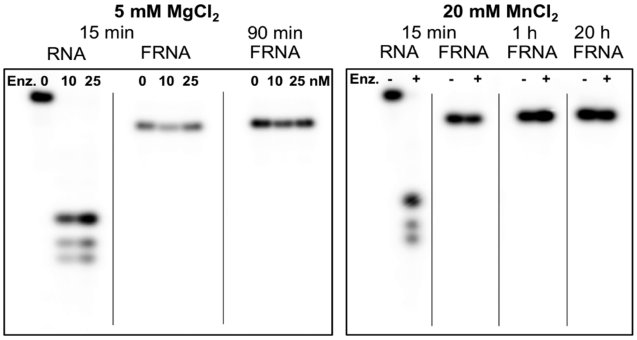

Figure 2. RNase H cleavage assays with RNA:DNA and FRNA:DNA duplexes in the presence of Mg^{2+} or Mn^{2+}. The reaction conditions were as follows: 50 nM RNA(FRNA):DNA (FRNA/RNA = 5′-GACACCUGAUUC-3′), 0−25 nM RNase H, 50 mM Tris-HCl (pH 7.9), 50 mM NaCl, 1 mM DTT, 20 μg/mL BSA, and 4% glycerol.

sense and antisense strands of siRNA duplexes and opposite the cleavage site in the target RNA does not hamper the activity of the RISC Ago2 enzyme in the RNAi pathway.[24]

To gain a better understanding of the origins of the inability of RNase H to process FRNA paired to DNA, we determined the crystal structure of *Bh*RNase H bound to an FRNA:DNA dodecamer duplex. The sequence of the hybrid duplex matches that in the structure of the complex with native RNA:DNA[8] (Figure 3A). As in the case of that structure, we used the D132N mutant of the enzyme that prevents cleavage of RNA even in the presence of both Mg^{2+} ions (Figure 1). The FRNA strand was synthesized following published protocols.[25] Crystals of the complex with FRNA:DNA were grown under conditions that differ from those used for the complex with the native substrate. In particular, the pH of the crystallization condition [0.4 M ammonium phosphate (pH 5)] (Supporting Information) is

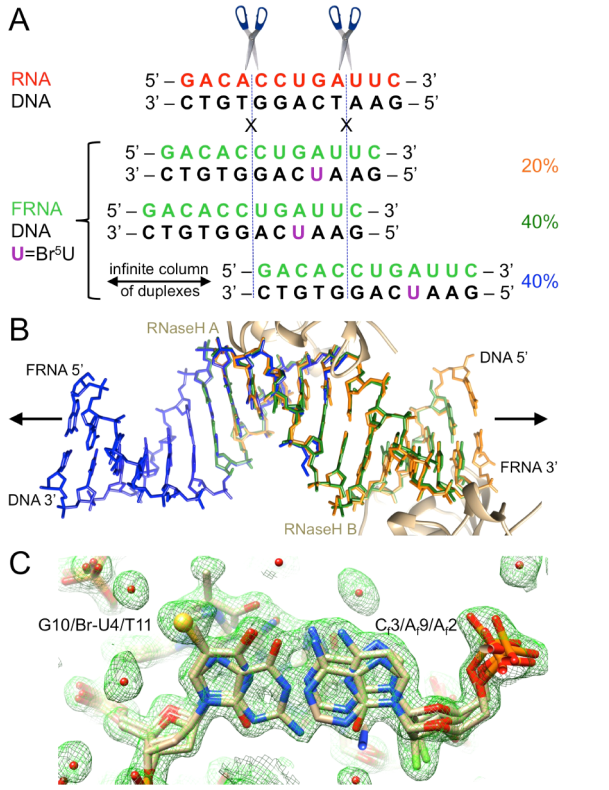

Figure 3. (A) Sequence of RNA(red):DNA[8] and FRNA(green):DNA hydrids in RNase H cocrystals. Relative shifts of FRNA:DNA duplexes and occupancies in the P1 unit cell are indicated. Scissors mark scissile phosphates in RNA, and X marks the lack of cleavage with FRNA. (B) Unit cell content and relative orientations of the three duplexes in the FRNA:DNA complex. (C) Quality of the final Fourier $2F_o - F_c$ sum electron density (∼1σ threshold). Adjacent pairs with overlaid base triples bound to RNaseH A (B) are depicted. The bromine of U4 is shown as a yellow sphere.

reduced by ∼2 units compared to that of the complex with RNA:DNA[8] [Tris-HCl (pH 7.5)]. The structure of the FRNA:DNA complex was phased by molecular replacement, using the apo form of *Bh*RNase H (D132N mutant) as the search model, and refined to a resolution of 1.50 Å (Table S1).

The triclinic P1 unit cell contains two RNase H molecules and a single duplex and therefore matches the contents of the asymmetric unit of the crystal with the native substrate that is of monoclinic space group *C*2. However, the position of the FRNA:DNA duplex is 3-fold disordered, with occupancies of 0.4, 0.4, and 0.2 for individual orientations along the helical stack, as established by a Br^5U modification in the DNA strand (Figure 3 and Figure S1). Slipping by the FRNA:DNA duplex likely has its origin in the weakened ability of RNase H to hold on to the FRNA strand compared with RNA. Among side chains interacting with RNA 2′-OH groups, active site E109 is the only one that establishes a direct H-bond with a 2′-OH [from the ribose that carries the leaving group O3′ (Figure 1)]. Fluorine is unable to act as a donor, and thus, the stabilizing effect of the interaction in the complex with RNA substrate is lost. The distances between E109(Oε2) and F2′ range from 3.02 to 3.39 Å (RNase H A) and from 2.99 to 3.35 Å [RNase H B (for a detailed list of all F2′ contacts, see Table S2)]. By comparison, the corresponding distances between E109 and O2′ in the structure of the D132N mutant with RNA are 2.75 and 2.90 Å, and in the structure of the D192N mutant with RNA, they are 2.78 and 2.81

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Å.[8] When examining these interactions, one needs to keep in mind the smaller size of fluorine relative to oxygen, and the fact that despite short distances involving fluorine in some cases (Table S2), there is no stabilizing effect.

Both RNase H molecules per unit cell accommodate three superimposed FRNA strands at their active site. The particular shifts between individual duplexes result in overlays of various combinations of Watson−Crick base pairs. Thus, fC:dG/fC:dG, fU:dA/fC:dG, and fU:dA/fU:dA flank the scissile phosphate at the active site of RNase H B (Figure 3A,B). However, at other steps, two purines are combined with a pyrimidine in one strand, two pyrimidines with a single purine in the other, etc. The particular sequence of the 12mer studied precludes conservation of a particular base pair as a result of the shifts between duplexes. Unlike the significant geometric deviations between individual overlaid bases in some cases, the sugar−phosphate backbones of both FRNA and DNA display only minimal differences (Figure 3B,C and Figure S1). Therefore, phosphate groups from individual duplexes are nearly perfectly superimposed at the active sites. In the case of RNase H A, only two duplexes contribute a phosphate because the enzyme molecule binds at the transition between adjacent (symmetry-related) "blue" duplexes. The other RNase H molecule (B) binds at a site that features superimposed phosphates from the FRNA strands of blue, green, and orange duplexes (Figure 3).

Replacement of the 2′-hydroxyl group with fluorine preserves the preference of the ribose for a C3′-*endo* conformation, and both RNA and FRNA duplexes adopt an overall A-form geometry.[26] However, inspection of the structures of the *Bh*RNase H complexes with native RNA:DNA and FRNA:DNA hybrids reveals virtually identical conformations of the protein, but subtle differences between the conformations of the two duplex types. An overlay of the structures shows slightly different curvatures of the FRNA and RNA strands as well as the DNA portions (Figure 4). In addition, corresponding base pairs in the two duplexes (green FRNA:DNA) do not overlap in the superimposed structures in many cases. The root-mean-square deviation (rmsd) for phosphorus atoms is ∼1.9 Å. Inclusion of all atoms reduces the rmsd to ∼1.5 Å (Figure S2). Comparing only the P atoms of the FRNA and RNA strands gives an rmsd of ∼1.3 Å, and the rmsd for DNA P atoms alone is ∼2.0 Å. To gain a better understanding of the geometrical differences between the two duplexes, we calculated helical parameters using Curves[27] (Figure S3 and Tables S3−S6). Among global base pair axis parameters, both *x*- and *y*-displacements show a difference of ∼0.3 Å (−3.85/−0.17 Å, FRNA:DNA; −4.15/0.20 Å, RNA:DNA). The inclination angle is 3° in both cases. The helical rise and twist are also similar: 3.13 Å and 31° for FRNA and 3.15 Å and 30° for RNA, respectively. Conversely, there is a sizable difference in overall axis bend (angle between terminal base pairs) of 10° between the FRNA:DNA and RNA:DNA duplexes (0° and 10°, respectively). However, the deviating curvatures that are also visible in Figure 4 appear not to be of much consequence for the dimensions of the minor groove. Thus, in the FRNA:DNA duplex, the minor groove width (8.3 Å) and depth (2.1 Å) are comparable to the corresponding values in the RNA:DNA duplex (8.4 and 2.4 Å, respectively). Average distances between phosphorus atoms from opposite strands roughly normal to the minor groove (14.1 Å, FRNA; 14.3 Å, RNA) are also consistent with similar widths.

The two-metal ion mechanism is key to the endonucleolytic activity of RNase H. Crystallization with the D132N mutant prevents cleavage in the presence of Mg^{2+}, although both metal

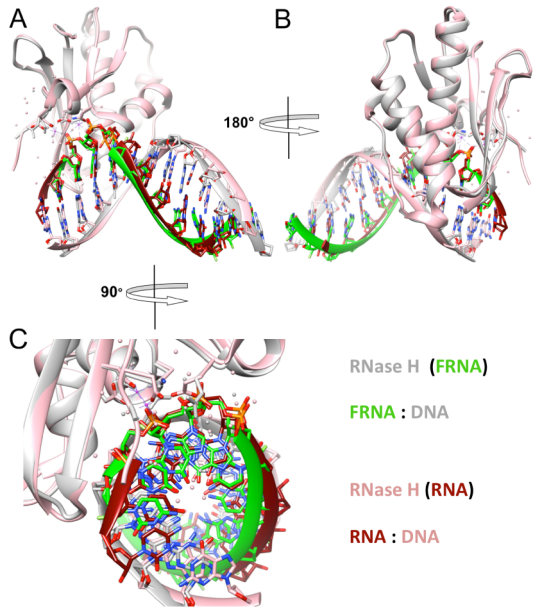

Figure 4. Comparison between the crystal structures of *Bh*RNase H in complex with FRNA:DNA and RNA:DNA[8] hybrids. Superimpositions using both protein and nucleic acid components of the two complexes are (A) viewed across the major and minor grooves, with the FRNA/RNA strands in the foreground, (B) rotated around the vertical by 180°, with the DNA strands in the foreground, and (C) rotated around the vertical by 90° relative to panel A and viewed along the stacking direction.

ions are still present in the crystal structure with the native RNA:DNA hybrid (Figure 1).[8] However, in the structure of the complex with the FRNA:DNA hybrid, these metal ions are missing at the active site of RNase H (Figure 5A), despite a Mg^{2+} concentration used in the crystallizations [5 mM (see the Supporting Information)] that matches that leading to growth of crystals with the native hybrid.[8] Comparison with the corresponding active site in the complex with the RNA:DNA hybrid reveals that many water molecules in and around the active site assume similar positions (Figure 5A). At the location formerly occupied by metal ion A, both E188 and D192 in the FRNA:DNA complex display altered orientations compared to the RNA:DNA complex. E188 is detached from the FRNA backbone in the former, and D192 has shifted somewhat closer to the FRNA phosphate as a result of the missing metal ion (Figure 5A). Similarly, inspection of the adjacent metal ion B site shows that D71 and N132 have inched closer to the FRNA backbone in the absence of Mg^{2+}. F2′ (FRNA) and O2′ (RNA) are 3.0 and 2.9 Å from Oε2 of E109, respectively, in the two structures, but the average distance between carboxylate oxygens of D71 and OP1 of the scissile phosphate (2.94 Å) is 0.5 Å shorter in the structure with the FRNA:DNA hybrid compared to that of the native complex (3.45 Å). In addition, Nδ of N132 is 0.2 Å closer to OP1 in the structure with the FRNA:DNA hybrid (3.0 Å) than in the native complex (3.2 Å). At the active site of the second RNase H molecule (RNase H A), metal ion A is also absent, but we assigned Na^{+} to site B in the complex with the FRNA:DNA hybrid (Figure 5B).

In summary, the crystal structure of *Bh*RNase H in complex with an FRNA:DNA hybrid duplex reveals three key differences from the complex with the RNA:DNA hybrid. These concern the RNase H−hybrid interaction (3-fold disordered FRNA:-DNA hybrid vs single orientation of the RNA:DNA hybrid),

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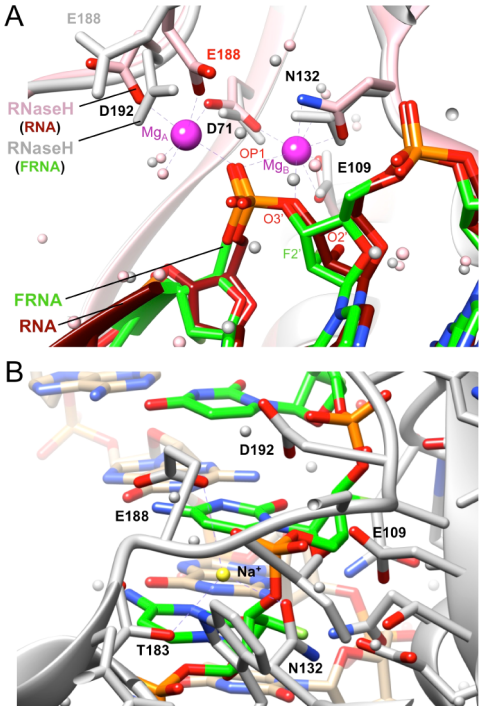

Figure 5. Active site configurations in the *Bh*RNase H complex with the FRNA:DNA hybrid. (A) The FRNA 5′-UpU-3′ step lodged at the active site of RNase H B (see Figure 3), with the overlaid RNA 5′-ApU-3′ step, bound at the active site of RNase H in the structure of the complex with the native RNA:DNA hybrid.[8] No metal ions are observed in the complex with the FRNA:DNA hybrid at that site, whereas the complex with the RNA:DNA hybrid features two Mg^{2+} ions (magenta spheres). The color code matches that in Figure 4, and dashed lines indicate coordination geometries of Mg^{2+}. (B) The FRNA 5′-CpC-3′ step lodged at the active site of RNase H A. Metal ion A is absent, and the site formerly occupied by Mg^{2+}_B in the RNA:DNA complex [5′-ApU-3′ (panel A and Figure 1)] is now taken by a Na^+ ion (yellow; dashed lines indicate coordination).

duplex conformation (deviating strand curvatures), and stereoelectronics (absence vs presence of two Mg^{2+} ions, respectively). Although the latter observation alone can explain the lack of FRNA cleavage (Figure 2), it is likely that the differences in protein binding and duplex conformation due to replacement of 2′-OH with 2′-F also lead to inhibition of RNase H. Our structural data show that fluorine cannot mimic the hydroxyl group with regard to the need by RNase H to properly hold on to the RNA backbone to execute cleavage. The conformational differences between the FRNA:DNA and RNA:DNA hybrids, although subtle, are perhaps surprising given the well-established notion that both 2′-ribonucleotides and 2′-deoxy-2′-fluororibonucleotides prefer the C3′-*endo* sugar pucker. However, the lack of FRNA processing is not caused by the direct involvement of fluorine in the cleavage mechanism, as neither OH (RNA) nor F (FRNA) lies close to the water nucleophile and the higher electronegativity of F relative to that of O is expected to facilitate nucleophilic attack at the phosphate and 3′-OH leaving group stabilization.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.biochem.6b00849.

Methods and materials, Figures S1 (electron density), S2 (structural superimpositions), and S3 (helical geometry graphs), and Tables S1 (crystallographic data), S2 (F2′−vs O2′−protein contacts), and S3−S6 (FRNA:DNA and RNA:DNA duplex geometries calculated with Curves) (PDF)

Accession Codes

The Protein Data Bank entry for the complex is 5SWM.

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Notes

The authors declare no competing financial interest.

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Supporting Information

Limits of RNA 2′-OH Mimicry by Fluorine: Crystal Structure of *Bacillus halodurans* RNase H Bound to a 2′F-RNA:DNA Hybrid

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_Bh_RNase H expression and purification

The Asp132→Asn mutant of *Bh*RNase H (Met58 to Lys196) was expressed in *E. coli* and purified as previously described.[1,2]

FRNA synthesis and purification

All reagents and solutions used for oligonucleotide synthesis were purchased from commercial sources. The standard phosphoramidites and solid supports were used for incorporation of dA, dG, dT, and dC residues. 2′-F A^{Bz}, 2′-F G_{ibu}, 2′-F U and 2′-F C^{Bz} phosphoramidites were used for the synthesis of 2′-F oligonucleotide. A 0.1 M solution of phosphoramidites in anhydrous acetonitrile (CH_3CN) was used for the synthesis. The modified oligonucleotides were synthesized on VIMAD UnyLinker^{TM} solid support. Dichloroacetic acid (6%) in toluene was used as detritylating reagent. 1M 4,5-Dicyanoimidazole in the presence of 0.1 M *N*-methylimidazole in CH_3CN was used as activator for coupling reaction. The synthesis of modified oligonucleotides was performed on an ÄKTAOligopilot synthesizer (GE Healthcare Bioscience) synthesizer on a 40 μmol scale using the procedures described below.

A solid support preloaded with the Unylinker^{TM} was loaded into a synthesis column after closing the column bottom outlet and acetonitrile (CH_3CN) was added to form slurry. The swelled support-bound Unylinker^{TM} was treated with a detritylating reagent containing 6% dichloroacetic acid in toluene to provide the free hydroxyl groups. During the coupling step, four equivalents of phosphoramidite solutions were delivered and the coupling was allowed to carry out for 6 min. All other steps in the protocol supplied by the manufacturer were used without modification. Phosphate diester linkages were incorporated *via* oxidation of phosphite triesters using a solution of *tert*-butyl hydroperoxide/CH_3CN/water (10:87:3) for a contact time of 12 min. After the desired sequence was assembled, the solid-support bound oligonucleotide was treated with 1:1 triethylamine: acetonitrile to remove cyanoethyl protecting groups from the phosphotriester linkages. The solid-support bound oligonucleotide was suspended in ammonia (28-30 wt%) and heated at 55^{o}C for 2 h followed by keeping at ambient temperature over 24 h. The unbound oligonucleotide was then filtered and the support was rinsed and filtered with water:ethanol (1:1) followed by water. Filtrate and washing combined together and purified by HPCL on a strong anion exchange column (GE Healthcare Bioscience, Source 30Q, 30 μm, 2.54 x 8 cm, A = 100 mM ammonium acetate in 30% aqueous CH_3CN, B = 1.5 M NaBr in A, 0-40%

of B in 60 min, flow 14 mL min^{-1}). The fractions containing full length oligonucleotides were pooled together and diluted with water to get the acetonitrile concentration to 10% and desalted by HPLC on reverse phase column to yield the oligonucleotides in an isolated yield of 20-25% based on solid-support loading. The oligonucleotides were characterized by ion-pair-HPLC-MS analysis with Agilent 1100 MSD system.

Crystallization experiments

Protein and FRNA:DNA solutions were mixed in a 1:1 molar ratio in the presence of 5 mM $MgCl_2$ and crystallization experiments were performed by the sitting drop vapor diffusion technique using the Crystal Screen conditions (Hampton Research, Aliso Viejo, CA).[3] Initial sitting-drop vapor diffusion crystallization experiments were carried out with a 96-well crystallization plate (CrystalQuick plate , Greiner Bio-One GmbH) and using an automated mosquito Crystal (TTP Labtech). Briefly, 200 nL complex solution was mixed with an equal amount of reservoir solution and equilibrated against 70 μL reservoir wells. The crystallization hits were then used to set-up 2 μL drops using the sitting drop vapor diffusion method in a CombiClover 4 chamber plate (Molecular Dimensions) at 18°C. Crystals appeared in droplets that were mixed and equilibrated with 0.4 M ammonium phosphate monobasic in about 1-3 days. Crystals were mounted in nylon loops, cryo-protected in reservoir solution containing 35% glycerol and frozen in liquid nitrogen.

X-ray data collection, structure determination and refinement

Diffraction data were collected at a wavelength of 0.91836 Å with a Dectris Eiger 9M detector on the 21-ID-D beam line of the Life Sciences Collaborative Access Team (LS-CAT) at the Advanced Photon Source, Argonne National Laboratory (Argonne, IL). Diffraction data were integrated and scaled with the program HKL2000.[5] The structure was determined with the Molecular Replacement (MR) technique using the program MOLREP[6,7] and the *Bh*RNase H structure with PDB ID 3D0P[2] as the search model. Initial refinement was carried out with the program REFMAC.[8] Manual rebuilding of some protein residues was performed in COOT[9] and water molecules were added gradually and isotropic/TLS refinement was continued with the program REFMAC. A summary of crystallographic parameters is provided in **Table S1**. All crystallographic figures were generated using the program Chimera.[10] Examples of the quality of

the final 2Fo-Fc omit electron density around selected base pairs are depicted in **Figure S2** and refinement statistics are summarized in **Table S1**.

Data deposition

Atomic coordinates and structure factor data for the *Bh*RNase H complex with FRNA:DNA have been deposited in the Protein Data Bank (http://www.rcsb.org, entry code 5SWM).

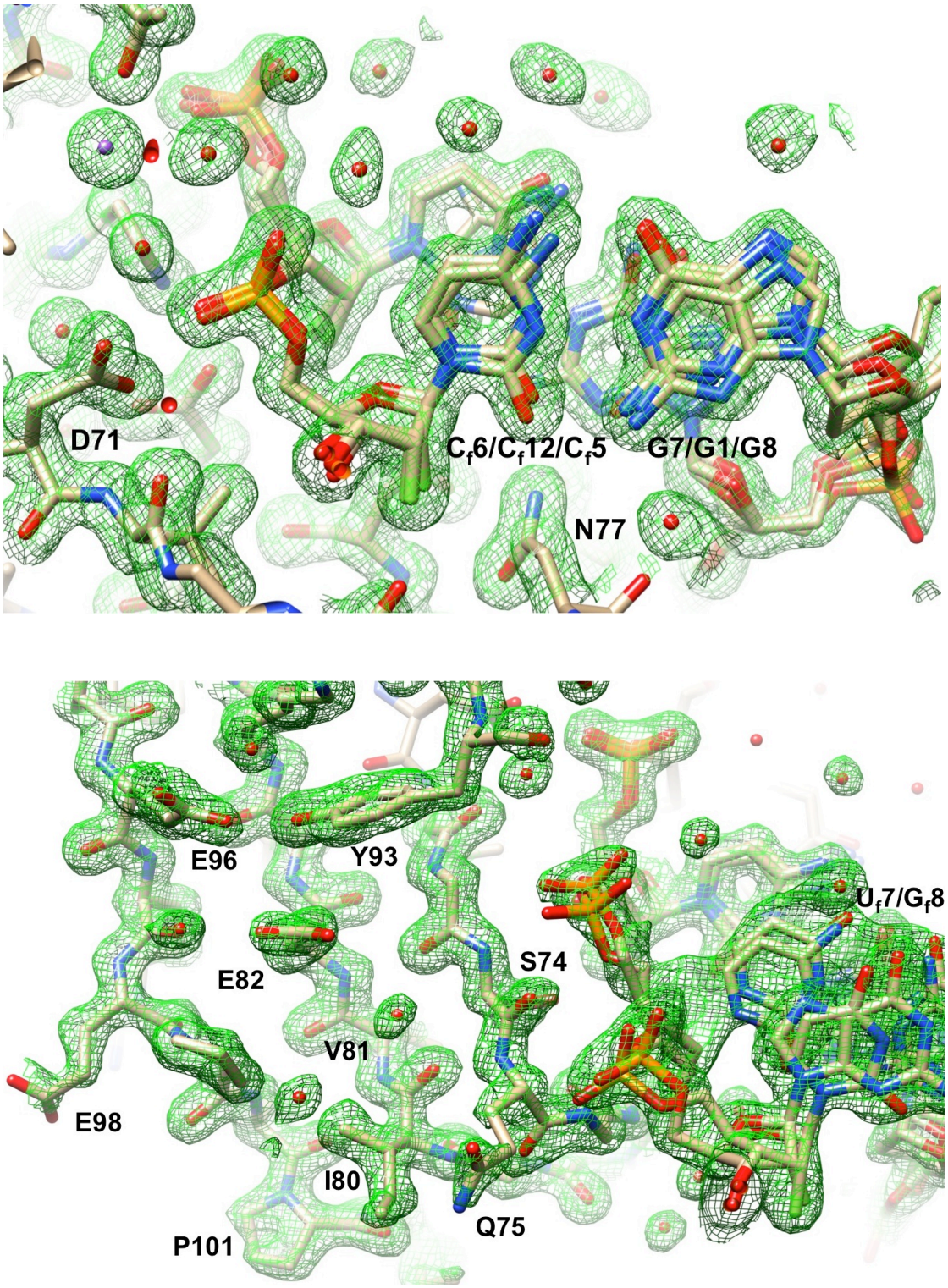
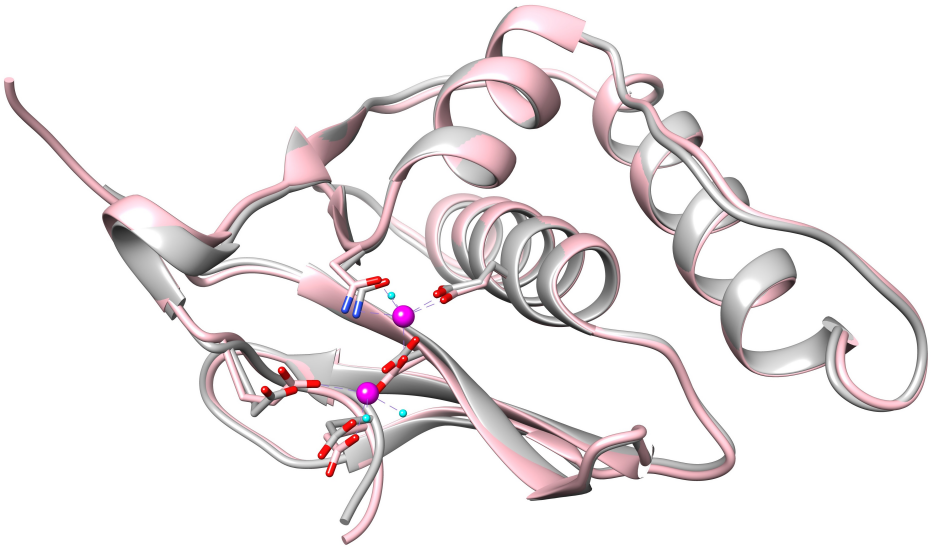


Figure S1. Quality of the final Fourier electron Fourier 2Fo-Fc sum electron density (1σ threshold) in two different regions of the unit cell. Selected residues are labeled.

A



B

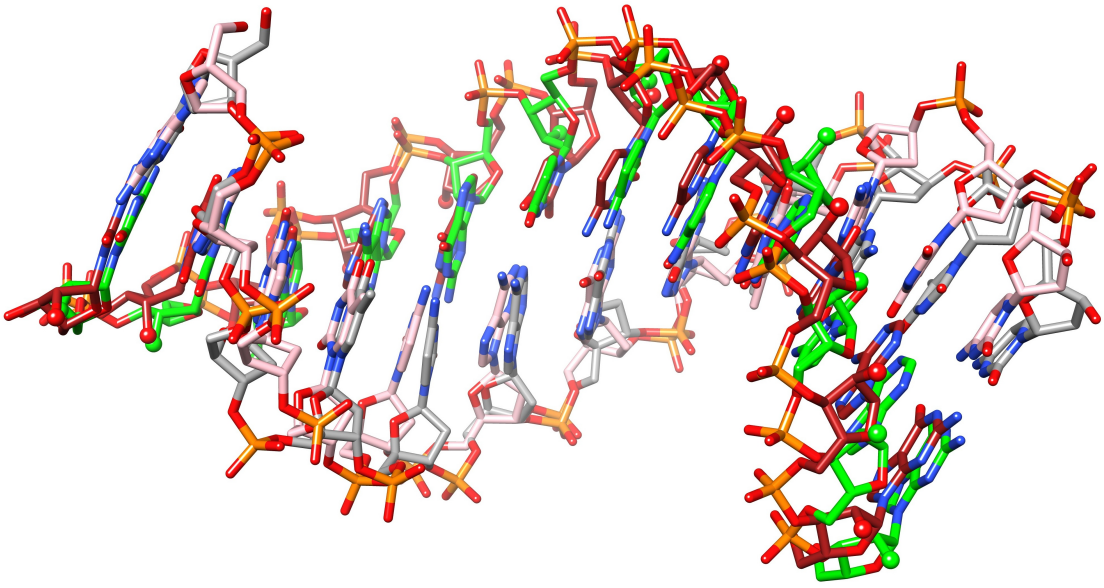


Figure S2. Overlays of complexes between *Bh*RNase H and FRNA:DNA and RNA:DNA. (A) Superimposition of the *Bh*RNase H molecules from the complexes with FNA:DNA (gray) and RNA:DNA (pink, PDB ID 1ZBI[1]). N- and C-Termini are at the top, left, and at the bottom, center, respectively. Only the protein in complex with RNA:DNA features bound Mg^{2+} ions (magenta spheres). (B) Superimposition of FRNA(green):DNA(gray) and RNA(brown):DNA (pink) hybrid duplexes. 2′-Fluorine and 2′-hydroxyl oxygen atoms are highlighted with light green and red spheres, respectively.

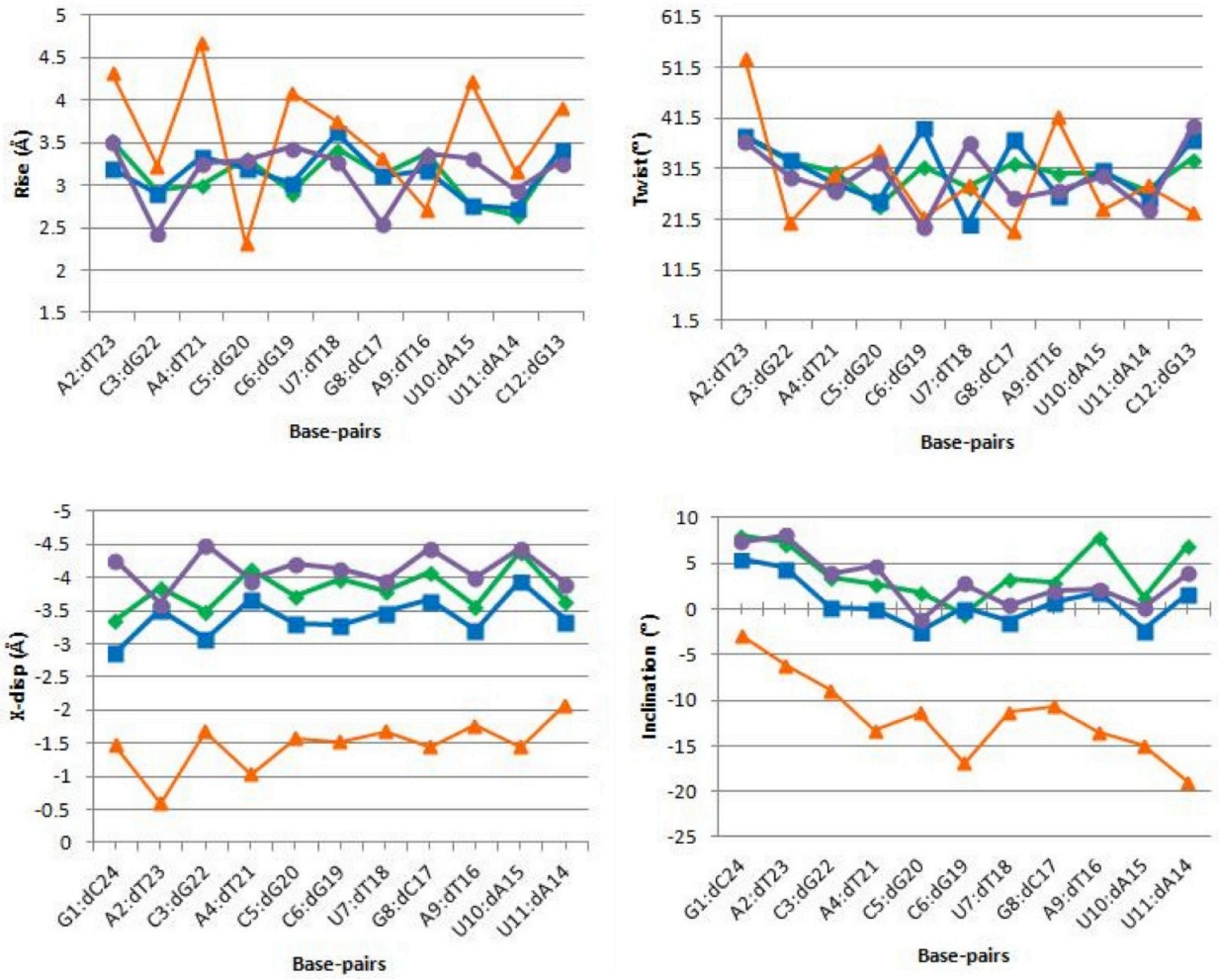


Figure S3. Comparison of the helical parameters rise, twist, x-displacement and inclination for the three FRNA:DNA hybrids (green, duplex A; blue, duplex B; orange, duplex C) and the native RNA:DNA hybrid (PDB ID 1ZBI,[1] purple). All parameters were calculated with the program Curves[11] (see also **Tables S3** to **S6**).

Table S1. Crystal data, X-ray data collection and refinement parameters.

Complex	***Bh*RNase-H : FRNA-DNA**
Data collection	
Wavelength [Å]	0.91836
Space group	*P*1
Resolution (outer shell) [Å]	50.00 - 1.50 (1.55 - 1.50)
Unit cell constants *a, b, c* [Å]; α, β, γ [°]	37.47, 44.50, 62.17; 84.42, 89.90, 65.10
Unique reflections	55,661 (4,620)
Completeness [%]	95.7 (79.8)
I/σ(I)	46.0 (10.6)
R-merge	0.067 (0.130)
Redundancy	6.1 (3.8)
Refinement	
Phasing method	Molecular Replacement
R-work	0.161 (0.153)
R-free	0.185 (0.183)
Number of amino acids	266
Number of protein atoms	2,133
Number of nucleic acid atoms	1,584[a]
Average B-factor, protein atoms [$Å^2$]	17.8
Average B-factor, nucleic acid atoms [$Å^2$]	14.3
Average B-factor, water / Na^+ /Cl^- ions [$Å^2$]	30.8 / 21.5 / 26.4
Wilson B-factor [$Å^2$]	13.5

R.m.s.d. bond lengths [Å]	0.023
R.m.s.d. bond angles [°]	2.1
Ramachandran plot: No of favored / allowed residues / outliers	Chain A: 129 / 0 / 0 Chain B: 131 / 0 / 0
PDB ID code	5SWM

[a]The FRNA:DNA hybrid duplex has multiple occupancies and hence the number of listed atoms appears higher.

Table S2. FRNA 2′-F/phosphate backbone : *Bh*RNase H vs. RNA 2′-OH : *Bh*RNase H contacts.

DNA – FRNA* base- pairs (Orientation A, green duplex)	FRNA : protein contacts G1.A → C12.A; 0.4 occupancy		DNA – FRNA* base- pairs (Orientation B, blue duplex)	FRNA : protein contacts G1.B → C12.B; 0.4 occupancy		DNA – FRNA base- pairs (Orientation C, orange duplex)	FRNA : protein contacts G1.C → C12.C; 0.2 occupancy	
	Contact	**Dist. [Å]**		**Contact**	**Dist. [Å]**		**Contact**	**Dist. [Å]**
G1 – **C12**	**OP1** : D71-OD1 **OP1** : D71-OD2 **OP1** : D192-OD1	3.31 2.59 3.44	G1 – **C12**			G1 – **C12**	**F2′** :G76-NH **OP1** : S74-O **OP1** : S74-NH	2.53 2.66 2.59
A2 – **U11**	**F2′** : E109-OE2	3.35	A2 – **U11**			A2 – **U11**	**OP1** : D71-OD1 **OP1** : D71-OD2	3.50 2.96
A3 – **U10**	**OP1** : T183-OG1 **F2′** : Q134-NH **F2′** : N132-O	2.47 3.10 3.19	A3 – **U10**			A3 – **U10**	**F2′** : E109-OE2 **OP1** : T183-OG1 **OP1** : K180-NZ	3.00 2.65 2.50
5-Br-U4 – **A9**			5-Br-U4 – **A9**			5-Br-U4 – **A9**	**F2′** : Q134-NH **F2′** : N132-O	2.91 3.02
C5 –**G8**			C5 –**G8**			C5 –**G8**		
A6 – **U7**	**OP1** : #G76-NH **F2′** : #G76-NH	3.48 3.06	A6 – **U7**	**OP1** : S74-NH **F2′** : G76-NH **F2′** : N77-NH **O3′** : G76-NH	3.18 2.97 3.40 2.72	A6 – **U7**		
G7 – **C6**			G7 – **C6**	**F2′** : S74-OG **OP1** : D71-OD1 **OP1** : D71-OD2 **OP1** : N132-OD1	3.12 3.09 2.60 2.94	G7 – **C6**	**OP1** : #G76-NH **O3′** : #G76-NH	2.67 2.54
G8 – **C5**			G8 – **C5**	**OP1** : T183-OG1 **OP1** : N132-O **OP1** : K180-NZ	2.71 3.29 2.73	G8 – **C5**		
T9 – **A4**			T9 – **A4**	**F2′** :E109-OE2 **F2′** : Q134-NH **F2′** : N132-O	2.98 3.27 3.03	T9 – **A4**		
G10 – **C3**			G10 – **C3**			G10 – **C3**		
T11 – **A2**			T11 – **A2**			T11 – **A2**		
C12 – **G1**			C12 – **G1**			C12 – **G1**		

FRNA residues are highlighted in bold green, and their respective atoms in bold. Only interactions with one of the two RNase H molecules contacting the duplexes are listed (residues A9.A to C12.A, A4.B to U7.B and U10.C to C12.C). For the analysis of contacts involving some of the FRNA residues in duplex C, a symmetry-related RNase H molecule (#) was used.

Table S2 continued: RNA 2′-OH/phosphate backbone: *Bh*RNase H contacts based on the complex with RNA:DNA (PDB ID 1ZBI).[1]

DNA - RNA base- pairs	RNA : protein contacts G1 → C12	
	Contact	Dist. [Å]
G1 – C12		
A2 – U11	**O2′** : G76-NH **OP1** : S74-NH	3.06 2.86
A3 – U10	**O2′** : S74-OG	2.64
T4 – A9	**O2′** : E109-OE2 **OP1** : K180-NZ **OP1** : T183-OG	2.75 2.44 2.72
C5 – G8	**O2′** : N132-O **O2′** : Q134-NH	2.75 3.13
A6 – U7	**O2′** : 134Q-OE1	2.69
G7 – C6		
G8 – C5		
T9 – A4		
G10 – C3		
T11 – A2		
C12 – G1		

Table S3. Curves output for FRNA:DNA duplex A (green molecule, 40% occupancy, Figure 3 – main paper).

```
   ***********************************              **************
   ******  CURVES 5.3 R.L. 1998  *****              *  16 Aug 16 *
   ***********************************              **************


  FILE : 5SWM_A.pdb                          LIS  : green
  dna  :                                     axin :
  axout:                                     daf  :
  PDB  : green

  acc  :    0.000  wid  :    0.750

  maxn :   500  ior  :     0  ibond:     0  splin:     3  break:    -1
  nleve:     3  nbac :     7

  ends :     F  supp :     T  COMB :     T  DINU :     T  mini :     T
  rest :     F  line :     F  zaxe :     F  FIT  :     T  test :     F
  GRV  :     T  old  :     T  axonl:     F

  Least squares fitting of standard bases ...

   Str   Pos  Base          Rms (ang)

    1 :   1)  GA     1      0.074
    1 :   2)  AA     2      0.065
    1 :   3)  CA     3      0.054
    1 :   4)  AA     4      0.069
    1 :   5)  CA     5      0.046
    1 :   6)  CA     6      0.056
    1 :   7)  UA     7      0.061
    1 :   8)  GA     8      0.092
    1 :   9)  AA     9      0.076
    1 :  10)  UA    10      0.051
    1 :  11)  UA    11      0.057
    1 :  12)  CA    12      0.044
    2 :   1)  CB    24      0.024
    2 :   2)  TB    23      0.054
    2 :   3)  GB    22      0.029
    2 :   4)  TB    21      0.036
    2 :   5)  GB    20      0.038
    2 :   6)  GB    19      0.045
    2 :   7)  AB    18      0.042
    2 :   8)  CB    17      0.041
    2 :   9)  TB    16      0.048
    2 :  10)  AB    15      0.058
    2 :  11)  AB    14      0.047
    2 :  12)  GB    13      0.071

  Strand=    2 Nucleo=   24 Atoms =  495 Units =   24

  Input   1) Xdisp=    0.00 Ydisp=    0.00 Inclin=    0.00 Tip=    0.00

  Combined strands have   12 levels ...

  Strand  1 has  12 bases (5'-3'): GACACCUGAUUC
  Strand  2 has  12 bases (3'-5'): CTGTGGACTAAG
```

```
FIRST SUM=  124.073 CPTS:    2.793   2.259   4.597 114.424

MINIMISATION: ACC =  0.100E-05 MAXN=  500 NVAR=   48

STEP    1 SUM=  124.073 DEL=  0.000E+00
STEP    2 SUM=  104.719 DEL= -0.194E+02
STEP    3 SUM=   76.151 DEL= -0.286E+02
STEP    4 SUM=   50.192 DEL= -0.260E+02
STEP    5 SUM=   60.660 DEL=  0.105E+02
STEP    6 SUM=   39.386 DEL= -0.213E+02
STEP    7 SUM=   32.079 DEL= -0.731E+01
STEP    8 SUM=   28.642 DEL= -0.344E+01
STEP    9 SUM=   24.106 DEL= -0.454E+01
STEP   10 SUM=   20.151 DEL= -0.396E+01
STEP   11 SUM=   20.929 DEL=  0.778E+00
STEP   12 SUM=   18.349 DEL= -0.258E+01
STEP   13 SUM=   15.419 DEL= -0.293E+01
STEP   14 SUM=   12.128 DEL= -0.329E+01
STEP   15 SUM=   34.885 DEL=  0.228E+02
STEP   16 SUM=   11.759 DEL= -0.231E+02
STEP   17 SUM=   11.668 DEL= -0.914E-01
STEP   18 SUM=   11.492 DEL= -0.175E+00
STEP   19 SUM=   10.585 DEL= -0.907E+00
STEP   20 SUM=   10.332 DEL= -0.253E+00
STEP   21 SUM=   10.029 DEL= -0.303E+00
STEP   22 SUM=    9.567 DEL= -0.462E+00
STEP   23 SUM=    9.710 DEL=  0.143E+00
STEP   24 SUM=    9.367 DEL= -0.343E+00
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STEP   26 SUM=    9.282 DEL= -0.158E+00
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STEP   29 SUM=    9.069 DEL= -0.621E-01
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STEP   32 SUM=    8.911 DEL= -0.376E-03
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STEP   34 SUM=    8.793 DEL= -0.704E-01
STEP   35 SUM=    8.691 DEL= -0.102E+00
STEP   36 SUM=    8.896 DEL=  0.205E+00
STEP   37 SUM=    8.666 DEL= -0.230E+00
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STEP   40 SUM=    8.693 DEL=  0.159E+00
STEP   41 SUM=    8.492 DEL= -0.201E+00
STEP   42 SUM=    8.419 DEL= -0.733E-01
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```

```
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STEP   73 SUM=    8.044 DEL= -0.565E-12
STEP   74 SUM=    8.044 DEL= -0.888E-14
STEP   75 SUM=    8.044 DEL=  0.000E+00

FINAL SUM=    8.044 CPTS:    2.099   2.995   0.960   1.991

GRA= 0.10E-07-0.69E-09 0.27E-08-0.22E-08-0.13E-07 0.35E-08-0.63E-08 0.66E-08
GRA= 0.12E-07-0.15E-07 0.57E-08 0.18E-08 0.94E-09 0.39E-08-0.47E-09-0.19E-08
GRA=-0.27E-08 0.83E-08 0.62E-08-0.65E-09-0.12E-07-0.15E-07 0.13E-08-0.11E-07
GRA=-0.64E-09-0.98E-09-0.99E-08 0.50E-08 0.98E-10-0.72E-09 0.58E-08-0.40E-08
GRA=-0.20E-08 0.11E-07-0.59E-08 0.90E-08-0.15E-07 0.18E-08 0.87E-08-0.15E-08
GRA= 0.13E-07 0.45E-08-0.72E-08 0.70E-08-0.20E-08-0.13E-07-0.40E-08-0.81E-08

----------------------------
|A| Global axis parameters |
----------------------------

  1) U:   -0.994  -0.061  -0.092  P:   13.647  -2.032  18.825  D:    0.821
  2) U:   -0.998   0.034  -0.054  P:   10.108  -2.022  18.898  D:    0.922
  3) U:   -0.997   0.076  -0.026  P:    7.183  -1.541  19.023  D:    0.817
  4) U:   -0.998  -0.004   0.058  P:    4.186  -1.599  18.910  D:    1.028
  5) U:   -0.996  -0.014   0.085  P:    0.896  -1.986  19.420  D:    0.711
  6) U:   -0.995   0.026   0.100  P:   -1.982  -2.058  20.013  D:    0.654
  7) U:   -0.996  -0.008   0.090  P:   -5.379  -2.341  20.502  D:    0.623
  8) U:   -0.993  -0.031   0.110  P:   -8.490  -2.352  20.760  D:    0.898
  9) U:   -0.999   0.017   0.042  P:  -11.872  -2.568  20.841  D:    0.727
 10) U:   -1.000  -0.003  -0.022  P:  -14.634  -2.625  21.108  D:    0.582
 11) U:   -0.996  -0.019  -0.082  P:  -17.267  -2.512  20.779  D:    0.262
 12) U:   -0.993  -0.043  -0.107  P:  -20.637  -2.649  20.271

---------------------------------
|B| Global Base-Axis Parameters |
---------------------------------

  1st strand      Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) GA    1      -3.41    -0.22     1.47    -9.75   1   0
  2) AA    2      -3.87     0.31     0.83   -14.26   2  21
  3) CA    3      -3.54     0.18     1.74   -12.49   3 -16
  4) AA    4      -4.08     0.44    -3.88   -13.34   2  29
  5) CA    5      -3.72    -0.19    -3.81    -9.69   3  -6
  6) CA    6      -4.13     0.10    -2.52   -10.33   3  -3
  7) UA    7      -3.67    -0.50    -2.74    -6.98   4 -25
  8) GA    8      -3.90    -0.09     0.20   -10.34   1  12
  9) AA    9      -3.61    -0.29     1.52   -12.50   2  22
```

```
 10) UA   10      -4.41    -0.08    -3.49   -14.52   4 -24
 11) UA   11      -3.58    -0.44     7.20    -9.62   4 -18
 12) CA   12      -4.43    -0.26    -1.47   -10.49   3   0

  2nd strand      Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) CB   24      -3.31     0.36    14.47    -1.47   3   0
  2) TB   23      -3.85    -0.14    13.63    -2.18   4 -21
  3) GB   22      -3.45     0.09     5.16     2.42   1  16
  4) TB   21      -4.18    -0.04     9.46    -3.44   4 -29
  5) GB   20      -3.72     0.34     7.41     5.14   1   6
  6) GB   19      -3.81    -0.10     1.31    -0.64   1   3
  7) AB   18      -3.95     0.25     9.32     4.57   2  25
  8) CB   17      -4.26     0.03     5.72     2.91   3 -12
  9) TB   16      -3.51     0.28    14.19    -3.51   4 -22
 10) AB   15      -4.35    -0.01     6.17    -2.18   2  24
 11) AB   14      -3.69     0.38     6.84     0.56   2  18
 12) GB   13      -4.06     0.10     2.16     1.35   1   0

---------------------------------------
|C| Global Base pair-Axis Parameters |
---------------------------------------

  Strand 1 with strand 2 ...

  Duplex          Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) G  1-C 24    -3.36    -0.29     7.97    -4.14   1   0
  2) A  2-T 23    -3.86     0.22     7.23    -6.04   2  21
  3) C  3-G 22    -3.49     0.05     3.45    -7.45   3 -16
  4) A  4-T 21    -4.13     0.24     2.79    -4.95   2  29
  5) C  5-G 20    -3.72    -0.26     1.80    -7.42   3  -6
  6) C  6-G 19    -3.97     0.10    -0.61    -4.85   3  -3
  7) U  7-A 18    -3.81    -0.37     3.29    -5.77   4 -25
  8) G  8-C 17    -4.08    -0.06     2.96    -6.63   1  12
  9) A  9-T 16    -3.56    -0.29     7.86    -4.49   2  22
 10) U 10-A 15    -4.38    -0.04     1.34    -6.17   4 -24
 11) U 11-A 14    -3.64    -0.41     7.02    -5.09   4 -18
 12) C 12-G 13    -4.24    -0.18     0.34    -5.92   3   0

  Average:        -3.85    -0.11     3.79    -5.74

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|D| Global Base-Base Parameters |
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  Strand 1 with strand 2 ...

  Duplex          Shear    Stretch  Stagger  Buckle   Propel  Opening  Bc  Tc
                  (Sx)      (Sy)     (Sz)    (kappa)  (omega) (sigma)

  1) G  1-C 24    -0.11     0.14    -0.33   -13.00   -11.22     1.78   1   0
  2) A  2-T 23    -0.02     0.17    -0.44   -12.80   -16.45     6.70   2  21
  3) C  3-G 22    -0.09     0.27     0.21    -3.42   -10.08     3.80   3 -16
  4) A  4-T 21     0.10     0.39    -0.66   -13.34   -16.77     5.07   2  29
  5) C  5-G 20    -0.00     0.14     0.20   -11.22    -4.55     2.65   3  -6
  6) C  6-G 19    -0.32    -0.00     0.29    -3.83   -10.97    -0.51   3  -3
  7) U  7-A 18     0.28    -0.25     0.13   -12.06    -2.41    -2.92   4 -25
  8) G  8-C 17     0.36    -0.05     0.24    -5.51    -7.43    -1.30   1  12
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  9) A  9-T 16    -0.10    -0.01    -0.52   -12.67   -16.01    -0.77   2  22
 10) U 10-A 15    -0.06    -0.09     0.08    -9.66   -16.71    -0.06   4 -24
 11) U 11-A 14     0.11    -0.06    -0.38     0.36    -9.07     1.30   4 -18
 12) C 12-G 13    -0.37    -0.16     0.31    -3.63    -9.14    -3.28   3   0

  Average:        -0.02     0.04    -0.07    -8.40   -10.90     1.04
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|E| Global Inter-Base Parameters |
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1st strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) G 1/A 2	-0.47	0.86	3.48	-3.50	-9.69	40.34	2
3) A 2/C 3	0.26	0.27	3.26	-1.86	1.08	31.57	-6
4) C 3/A 4	-0.65	0.06	2.56	-2.51	5.00	31.73	9
5) A 4/C 5	0.55	-1.04	3.75	0.98	5.06	23.18	-6
6) C 5/C 6	-0.22	0.01	2.96	0.08	1.54	30.44	-1
7) C 6/U 7	0.23	-0.86	3.35	-0.11	1.30	26.74	-3
8) U 7/G 8	-0.18	0.46	3.17	3.84	-4.87	33.45	-9
9) G 8/A 9	0.27	0.06	3.01	0.25	2.49	30.75	2
10) A 9/U 10	-1.05	0.21	3.06	-7.17	1.14	30.94	7
11) U 10/U 11	0.99	-0.53	2.42	10.45	8.51	27.93	-4
12) U 11/C 12	-0.69	0.08	3.75	-8.75	1.11	31.20	-2

2nd strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 24/T 23	-0.56	-0.83	3.58	-3.69	4.46	35.42	-2
3) T 23/G 22	0.33	-0.17	2.62	-11.24	5.29	34.46	6
4) G 22/T 21	-0.84	0.07	3.43	7.41	-11.70	30.46	-9
5) T 21/G 20	0.65	0.79	2.89	-1.14	7.16	25.61	6
6) G 20/G 19	0.10	-0.16	2.88	-7.31	-7.96	33.60	1
7) G 19/A 18	-0.38	0.61	3.50	8.12	7.26	29.15	3
8) A 18/C 17	-0.25	-0.26	3.07	-2.70	-0.16	31.83	9
9) C 17/T 16	0.73	-0.01	3.76	7.41	-11.07	30.21	-2
10) T 16/A 15	-1.09	-0.29	2.47	-10.19	-1.84	30.23	7
11) A 15/A 14	0.82	0.57	2.88	0.44	-0.87	26.56	4
12) A 14/G 13	-0.21	-0.18	3.06	-4.77	-1.19	35.78	2

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|F| Global Inter-Base pair Parameters |
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Strand 1 with strand 2 ...

Duplex	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) G 1/A 2	-0.52	0.85	3.53	-3.60	-7.08	37.88	2
3) A 2/C 3	0.30	0.22	2.94	-6.55	-2.11	33.01	-6
4) C 3/A 4	-0.75	-0.01	3.00	2.45	8.35	31.09	9
5) A 4/C 5	0.60	-0.91	3.32	-0.08	-1.05	24.39	-6
6) C 5/C 6	-0.06	0.09	2.92	-3.61	4.75	32.02	-1
7) C 6/U 7	-0.08	-0.73	3.43	4.01	-2.98	27.94	-3
8) U 7/G 8	-0.22	0.36	3.12	0.57	-2.36	32.64	-9
9) G 8/A 9	0.50	0.03	3.38	3.83	6.78	30.48	2
10) A 9/U 10	-1.07	0.25	2.77	-8.68	1.49	30.59	7
11) U 10/U 11	0.90	-0.55	2.65	5.45	4.69	27.24	-4
12) U 11/C 12	-0.45	0.13	3.41	-6.76	1.15	33.49	-2

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  Average:        -0.08    -0.03     3.13    -1.18     1.06    30.98

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|G| Local Inter-Base Parameters |
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  1st strand      Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) G  1/A  2     0.19    -1.59     3.25     4.69    -8.50    40.42   2
  3) A  2/C  3     0.85    -1.69     3.14     5.34     1.83    31.18  -6
  4) C  3/A  4    -0.14    -2.07     3.02     5.00     4.32    31.49   9
  5) A  4/C  5     1.18    -2.86     3.49     5.61     3.41    22.57  -6
  6) C  5/C  6     0.32    -2.22     2.99     5.30    -0.09    30.06  -1
  7) C  6/U  7     0.75    -2.81     3.00     3.90     0.00    26.32  -3
  8) U  7/G  8     0.42    -1.78     3.03     8.69    -5.42    32.56  -9
  9) G  8/A  9     0.97    -1.86     3.21     6.16     3.01    30.04   2
 10) A  9/U 10    -0.13    -1.98     3.39     0.35     0.69    31.79   7
 11) U 10/U 11     1.55    -2.40     2.50    15.82     9.15    25.30  -4
 12) U 11/C 12     0.29    -1.88     4.01    -2.96     2.69    32.12  -2

  2nd strand      Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) C 24/T 23    -0.59    -0.58     3.48    -4.57     4.01    35.54  -2
  3) T 23/G 22     0.34    -1.53     2.86   -10.76     0.35    34.30   6
  4) G 22/T 21    -0.86    -1.65     4.04     6.88    15.37    29.76  -9
  5) T 21/G 20     0.78    -2.01     3.34    -0.76    -3.21    25.13   6
  6) G 20/G 19     0.34    -1.86     3.13    -5.81    10.20    33.76   1
  7) G 19/A 18    -0.27    -2.19     3.63     8.84    -4.39    29.03   3
  8) A 18/C 17     0.07    -1.63     3.19    -0.54     4.20    31.88   9
  9) C 17/T 16     0.69    -1.36     4.39     7.14    15.92    29.28  -2
 10) T 16/A 15    -1.08    -1.27     2.94   -11.36     7.10    28.80   7
 11) A 15/A 14     0.84    -2.02     3.39     0.04     3.90    25.97   4
 12) A 14/G 13     0.05    -1.97     3.35    -3.95     3.99    35.62   2

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|H| Local Inter-Base pair Parameters |
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  Strand 1 with strand 2 ...

  Duplex          Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) G  1/A  2    -0.18    -1.07     3.42     0.35    -2.04    38.64   2
  3) A  2/C  3     0.57    -1.58     3.01    -2.75     1.55    32.76  -6
  4) C  3/A  4    -0.44    -1.87     3.56     6.22     9.76    31.10   9
  5) A  4/C  5     0.97    -2.40     3.45     2.28     0.22    23.45  -6
  6) C  5/C  6     0.33    -2.04     3.06    -0.15     5.16    32.19  -1
  7) C  6/U  7     0.25    -2.52     3.35     6.40    -2.21    27.49  -3
  8) U  7/G  8     0.24    -1.71     3.11     4.02    -0.68    32.49  -9
  9) G  8/A  9     0.87    -1.65     3.79     6.66     9.43    30.22   2
 10) A  9/U 10    -0.65    -1.59     3.22    -5.52     4.03    30.75   7
 11) U 10/U 11     1.23    -2.23     2.97     7.93     6.60    25.60  -4
 12) U 11/C 12     0.14    -1.92     3.67    -3.47     3.34    33.98  -2

  Average:         0.30    -1.87     3.33     2.00     3.20    30.79

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|I| Global Axis Curvature |
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  Duplex          Ax      Ay     Ainc    Atip    Adis    Angle   Path   Dc

 2) G  1/A  2   -0.02    0.34   -2.85   -5.18    0.34    5.91    3.54   2
 3) A  2/C  3   -0.07    0.39   -2.77   -0.69    0.40    2.86    2.97  -6
 4) C  3/A  4   -0.11   -0.20    3.11    5.85    0.23    6.62    3.00   9
 5) A  4/C  5    0.19   -0.41    0.91    1.42    0.45    1.68    3.35  -6
 6) C  5/C  6    0.19   -0.28   -1.20    2.19    0.34    2.49    2.94  -1
 7) C  6/U  7   -0.24   -0.26    0.11   -2.06    0.35    2.06    3.44  -3
 8) U  7/G  8    0.06    0.05    0.90   -1.50    0.07    1.75    3.12  -9
 9) G  8/A  9   -0.02    0.26   -1.07    4.64    0.26    4.76    3.39   2
10) A  9/U 10   -0.25    0.00   -2.16    3.17    0.25    3.83    2.78   7
11) U 10/U 11    0.16   -0.18   -0.24    3.61    0.24    3.61    2.66  -4
12) U 11/C 12    0.16   -0.10   -0.08    1.98    0.19    1.98    3.41  -2

Overall axis bend ... UU=    1.36 PP=   10.07


  Duplex       Offset   L.Dir  ... wrt end-to-end vector

 1) G  1         0.00    0.00
 2) A  2         0.11   16.83
 3) C  3         0.61  -53.51
 4) A  4         0.68  -64.84
 5) C  5         0.28 -127.30
 6) C  6         0.59  149.91
 7) U  7         0.87   99.63
 8) G  8         1.00   68.46
 9) A  9         0.94   28.52
10) U 10         1.09   -2.24
11) U 11         0.65  -19.18
12) C 12         0.00    0.00

  Path length=    34.59  End-to-end=    34.32  Shortening=     0.79 %

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|J| Backbone Parameters |
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  1st strand   C1'-C2' C2'-C3'  Phase   Ampli   Pucker    C1'   C2'   C3'

  1)GA    1    -27.53   34.95    5.01   35.86  C3'-endo  106.2 103.1 102.4
  2)AA    2    -34.16   39.82  358.60   40.60  C2'-exo   105.4 103.0 100.4
  3)CA    3    -27.58   39.43   14.51   41.61  C3'-endo  105.4 103.9  98.9
  4)AA    4    -33.12   42.30    6.08   43.43  C3'-endo  105.5 101.9  99.9
  5)CA    5    -25.86   45.98   24.81   51.34  C3'-endo  104.6 103.6  96.9
  6)CA    6    -32.29   46.50   13.95   49.03  C3'-endo  107.2  99.5  98.1
  7)UA    7    -30.04   36.53  358.01   36.47  C2'-exo   105.3 102.8 104.3
  8)GA    8    -25.28   38.69   16.49   40.91  C3'-endo  105.6 102.2 102.4
  9)AA    9    -25.97   44.96   24.97   50.57  C3'-endo  104.7 104.0  96.1
 10)UA   10    -31.30   44.50   11.91   46.29  C3'-endo  105.8  99.5 100.9
 11)UA   11    -16.19   36.76   33.76   45.05  C3'-endo  107.6 103.1 100.0
 12)CA   12    -22.49   35.40   18.94   38.06  C3'-endo  106.8 103.7 101.5

  Torsions       Chi    Gamma   Delta   Epsil   Zeta    Alpha   Beta
                 C1'-N  C5'-C4' C4'-C3' C3'-O3' O3'-P   P-O5'  O5'-C5'

  1)GA    1   -176.79   56.06   87.44 -142.47  -78.32  -66.28  172.66
  2)AA    2   -158.00   53.19   85.25 -144.62  -74.13  -59.59  157.73
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  3)CA    3   -166.38   59.89   79.98 -157.66  -70.06  -65.96  178.31
  4)AA    4   -153.81   49.57   78.26 -149.42  -52.27  -96.05  172.08
  5)CA    5   -159.74   94.36   66.93 -166.73  -70.88  -68.84  173.97
  6)CA    6   -160.34   56.53   65.96 -164.62  -50.62 -162.33  163.03
  7)UA    7   -177.26  158.66   84.54 -144.32  -70.79  -78.74  168.05
  8)GA    8   -154.48   75.76   80.25 -136.56  -70.46  -71.71  157.54
  9)AA    9   -156.00   76.43   68.60 -165.18  -77.13  -68.97  171.73
 10)UA   10   -162.14   58.21   74.27 -141.19  -49.90 -110.74  157.75
 11)UA   11   -162.94  115.95   70.88 -151.08  -75.13  -62.17  169.24
 12)CA   12   -161.21   58.16   85.36  ......  ......  ......  ......


  2nd strand   C1'-C2' C2'-C3'  Phase   Ampli   Pucker    C1'   C2'   C3'

  1)CB   24     33.94  -34.43  165.40   36.28  C2'-endo  106.0 102.1 103.3
  2)TB   23     30.49  -25.58  148.64   30.64  C2'-endo  105.9 103.7 104.2
  3)GB   22      0.89   21.74   56.66   40.96  C4'-exo   107.1 103.8 101.2
  4)TB   21     40.73  -28.52  135.66   41.16  C1'-exo   104.6 102.0 103.6
  5)GB   20     31.12  -33.65  171.14   34.70  C2'-endo  106.2 102.8 103.5
  6)GB   19    -33.23   37.61  357.36   38.87  C2'-exo   107.4 101.7 101.2
  7)AB   18     41.19  -26.85  130.68   42.54  C1'-exo   104.1 101.4 103.9
  8)CB   17     35.11  -31.47  154.48   35.67  C2'-endo  105.9 102.3 103.6
  9)TB   16     17.50    1.50   87.24   33.07  O1'-endo  106.4 106.2 103.1
 10)AB   15     41.05  -32.67  144.49   41.15  C2'-endo  104.9 101.0 104.0
 11)AB   14     33.41  -26.92  145.18   33.49  C2'-endo  106.2 103.0 104.8
 12)GB   13    -25.38   22.78  336.33   25.67  C2'-exo   108.3 104.5 103.9

  Torsions       Chi    Gamma   Delta   Epsil   Zeta    Alpha   Beta
                 C1'-N  C5'-C4' C4'-C3' C3'-O3'  O3'-P   P-O5'  O5'-C5'

  1)CB   24    -99.33   38.13  141.42  ......  ......  ......  ......
  2)TB   23   -120.71   42.76  129.60 -176.42  -81.15  -66.32 -167.46
  3)GB   22   -162.82 -170.12   79.68 -173.07  -64.30  -54.51 -173.83
  4)TB   21   -117.01   48.81  130.94 -163.70  -97.29  122.93 -165.09
  5)GB   20   -129.76   46.55  144.04 -176.90  -89.76  -70.37 -169.56
  6)GB   19   -175.11 -142.52   92.44 -141.82  -82.95  -45.45  176.86
  7)AB   18   -123.73   55.29  127.50 -166.55 -119.43   88.40 -154.41
  8)CB   17   -121.74   64.64  135.35 -175.56  -84.29  -91.47 -172.78
  9)TB   16   -138.70  179.14   99.91  174.03  -77.96  -79.30 -164.49
 10)AB   15   -110.71   45.10  132.69 -176.53  -83.45  137.09  177.17
 11)AB   14   -131.50   52.29  126.79  178.99  -93.16  -59.61 -168.51
 12)GB   13   -173.71 -150.90  111.61 -134.72  -71.56  -67.76  178.59


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|K| Groove parameters |
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Atom defining backbone: P      12 levels,  3 sub-levels

 Levels          Minor groove                Major groove
    i  n      Width    Depth  Angle       Width    Depth  Angle    Diam

G   1  0        --       --     --    G     --       --     --       --
    1  1        --       --     --          --       --     --       --
    1  2        --       --     --          --       --     --       --
    1  3        --       --     --          --       --     --       --
A   2  0        --       --     --    A     --       --     --       --
    2  1        --       --     --          --       --     --       --
    2  2      7.50     3.26    32           --       --     --     20.42
C   3  0      7.89     3.59    23    C     --       --     --     20.97
```

	3	1	8.62	2.98	24		--	--	--	21.32
	3	2	9.12	2.11	40		--	--	--	21.32
	3	3	8.80	2.06	44		--	--	--	21.07
A	4	0	8.35	2.05	47	A	--	--	--	20.77
	4	1	7.96	2.36	42		14.66	3.63	74	20.12
	4	2	7.66	2.70	37		15.06*	5.33	66	20.21
	4	3	7.54	2.92	35		16.10*	3.08	72	20.69
C	5	0	7.62	3.13	30	C	11.25	8.94	27	21.08
	5	1	7.97	2.99	27		11.96	8.99	31	21.46
	5	2	8.25	2.66	25		12.87	8.33	41	21.59
C	6	0	8.35	2.12	25	C	13.91	7.69	47	21.54
	6	1	8.53	1.86	26		14.80	7.17	50	21.50
	6	2	8.73	1.77	27		15.43	10.16	14	21.51
	6	3	8.79	1.74	32		15.00	2.35	75	21.48
U	7	0	8.80	2.04	35	U	14.60	1.39	79	21.34
	7	1	8.77	2.37	38		14.47	10.22	16	20.85
	7	2	8.73	2.58	39		13.98	10.25	19	19.88
	7	3	8.65	2.66	36		13.38	10.21	24	19.49
G	8	0	8.53	2.58	37	G	12.37	9.60	33	19.49
	8	1	8.38	2.64	37		11.64	9.27	35	19.80
	8	2	8.23	2.79	34		--	--	--	20.43
	8	3	8.13	3.10	31		--	--	--	21.27
A	9	0	8.35	3.24	30	A	--	--	--	21.87
	9	1	9.10	2.38	32		--	--	--	21.91
	9	2	9.09	1.64	47		--	--	--	21.22
U	10	0	8.68	1.66	45	U	--	--	--	20.38
	10	1	8.18	2.29	37		--	--	--	19.94
	10	2	--	--	--		--	--	--	20.19
U	11	0	--	--	--	U	--	--	--	--
	11	1	--	--	--		--	--	--	--
	11	2	--	--	--		--	--	--	--
	11	3	--	--	--		--	--	--	--
C	12	0	--	--	--	C	--	--	--	--

Table S4. Curves output for RNA:DNA duplex B (blue molecule, 40% occupancy, Figure 3 – main paper).

```
    ************************************              **************
    ******  CURVES 5.3 R.L. 1998  *****               *  16 Aug 16 *
    ************************************              **************


  FILE : 5SWM_B.pdb                          LIS  : blue
  dna  :                                     axin :
  axout:                                     daf  :
  PDB  : blue

  acc  :    0.000  wid  :    0.750

  maxn :   500  ior  :     0  ibond:     0  splin:     3  break:    -1
  nleve:     3  nbac :     7

  ends :     F  supp :     T  COMB :     T  DINU :     T  mini :     T
  rest :     F  line :     F  zaxe :     F  FIT  :     T  test :     F
  GRV  :     T  old  :     T  axonl:     F

  Least squares fitting of standard bases ...

   Str   Pos  Base          Rms (ang)

    1 :   1)  GC     1      0.071
    1 :   2)  AC     2      0.064
    1 :   3)  CC     3      0.034
    1 :   4)  AC     4      0.061
    1 :   5)  CC     5      0.023
    1 :   6)  CC     6      0.042
    1 :   7)  UC     7      0.068
    1 :   8)  GC     8      0.071
    1 :   9)  AC     9      0.070
    1 :  10)  UC    10      0.054
    1 :  11)  UC    11      0.051
    1 :  12)  CC    12      0.052
    2 :   1)  CD    12      0.021
    2 :   2)  TD    11      0.048
    2 :   3)  GD    10      0.034
    2 :   4)  TD     9      0.041
    2 :   5)  GD     8      0.070
    2 :   6)  GD     7      0.043
    2 :   7)  AD     6      0.026
    2 :   8)  CD     5      0.023
    2 :   9)  UD     4      0.065
    2 :  10)  AD     3      0.042
    2 :  11)  AD     2      0.051
    2 :  12)  GD     1      0.055

  Strand=    2 Nucleo=   24 Atoms =  495 Units =   24

  Input   1) Xdisp=    0.00 Ydisp=    0.00 Inclin=    0.00 Tip=    0.00

  Combined strands have   12 levels ...

  Strand  1 has  12 bases (5'-3'): GACACCUGAUUC
  Strand  2 has  12 bases (3'-5'): CTGTGGACUAAG

  FIRST SUM=  119.763 CPTS:    4.068   1.499   5.083 109.112
```

```
MINIMISATION: ACC =  0.100E-05 MAXN=  500 NVAR=   48

STEP    1 SUM=  119.763 DEL=  0.000E+00
STEP    2 SUM=   99.466 DEL= -0.203E+02
STEP    3 SUM=   71.568 DEL= -0.279E+02
STEP    4 SUM=   47.789 DEL= -0.238E+02
STEP    5 SUM=   54.051 DEL=  0.626E+01
STEP    6 SUM=   37.275 DEL= -0.168E+02
STEP    7 SUM=   31.404 DEL= -0.587E+01
STEP    8 SUM=   28.272 DEL= -0.313E+01
STEP    9 SUM=   24.364 DEL= -0.391E+01
STEP   10 SUM=   20.902 DEL= -0.346E+01
STEP   11 SUM=   27.509 DEL=  0.661E+01
STEP   12 SUM=   20.016 DEL= -0.749E+01
STEP   13 SUM=   18.432 DEL= -0.158E+01
STEP   14 SUM=   15.838 DEL= -0.259E+01
STEP   15 SUM=   13.952 DEL= -0.189E+01
STEP   16 SUM=   18.862 DEL=  0.491E+01
STEP   17 SUM=   13.542 DEL= -0.532E+01
STEP   18 SUM=   13.715 DEL=  0.173E+00
STEP   19 SUM=   13.373 DEL= -0.343E+00
STEP   20 SUM=   13.084 DEL= -0.289E+00
STEP   21 SUM=   12.798 DEL= -0.287E+00
STEP   22 SUM=   12.211 DEL= -0.586E+00
STEP   23 SUM=   15.740 DEL=  0.353E+01
STEP   24 SUM=   12.138 DEL= -0.360E+01
STEP   25 SUM=   12.045 DEL= -0.936E-01
STEP   26 SUM=   11.886 DEL= -0.159E+00
STEP   27 SUM=   12.240 DEL=  0.354E+00
STEP   28 SUM=   11.849 DEL= -0.391E+00
STEP   29 SUM=   11.789 DEL= -0.594E-01
STEP   30 SUM=   11.701 DEL= -0.881E-01
STEP   31 SUM=   11.654 DEL= -0.470E-01
STEP   32 SUM=   11.576 DEL= -0.781E-01
STEP   33 SUM=   11.562 DEL= -0.142E-01
STEP   34 SUM=   11.533 DEL= -0.288E-01
STEP   35 SUM=   11.504 DEL= -0.285E-01
STEP   36 SUM=   11.451 DEL= -0.530E-01
STEP   37 SUM=   11.302 DEL= -0.150E+00
STEP   38 SUM=   13.202 DEL=  0.190E+01
STEP   39 SUM=   11.284 DEL= -0.192E+01
STEP   40 SUM=   11.264 DEL= -0.197E-01
STEP   41 SUM=   11.229 DEL= -0.355E-01
STEP   42 SUM=   11.163 DEL= -0.654E-01
STEP   43 SUM=   11.074 DEL= -0.893E-01
STEP   44 SUM=   10.993 DEL= -0.814E-01
STEP   45 SUM=   11.017 DEL=  0.245E-01
STEP   46 SUM=   10.964 DEL= -0.536E-01
STEP   47 SUM=   10.970 DEL=  0.621E-02
STEP   48 SUM=   10.953 DEL= -0.164E-01
STEP   49 SUM=   10.954 DEL=  0.747E-03
STEP   50 SUM=   10.952 DEL= -0.265E-02
STEP   51 SUM=   10.952 DEL=  0.172E-04
STEP   52 SUM=   10.951 DEL= -0.518E-03
STEP   53 SUM=   10.951 DEL= -0.380E-04
STEP   54 SUM=   10.951 DEL= -0.222E-03
STEP   55 SUM=   10.951 DEL= -0.104E-03
STEP   56 SUM=   10.951 DEL= -0.112E-03
STEP   57 SUM=   10.951 DEL=  0.555E-05
STEP   58 SUM=   10.951 DEL= -0.232E-04
```

```
STEP   59 SUM=   10.950 DEL= -0.164E-04
STEP   60 SUM=   10.950 DEL= -0.200E-04
STEP   61 SUM=   10.950 DEL= -0.188E-04
STEP   62 SUM=   10.950 DEL= -0.348E-06
STEP   63 SUM=   10.950 DEL= -0.236E-05
STEP   64 SUM=   10.950 DEL= -0.733E-06
STEP   65 SUM=   10.950 DEL= -0.138E-06
STEP   66 SUM=   10.950 DEL= -0.430E-07
STEP   67 SUM=   10.950 DEL=  0.150E-08
STEP   68 SUM=   10.950 DEL= -0.773E-08
STEP   69 SUM=   10.950 DEL= -0.596E-09
STEP   70 SUM=   10.950 DEL= -0.283E-09
STEP   71 SUM=   10.950 DEL= -0.951E-11
STEP   72 SUM=   10.950 DEL= -0.279E-11
STEP   73 SUM=   10.950 DEL= -0.757E-12
STEP   74 SUM=   10.950 DEL= -0.195E-12
STEP   75 SUM=   10.950 DEL= -0.249E-13
STEP   76 SUM=   10.950 DEL=  0.000E+00

FINAL SUM=   10.950 CPTS:    2.511   4.747   1.068   2.625

GRA= 0.10E-07-0.36E-07 0.30E-08-0.34E-08 0.11E-07-0.15E-07-0.42E-08 0.68E-08
GRA=-0.23E-08 0.19E-07 0.43E-08-0.45E-09 0.18E-07-0.36E-08 0.78E-08 0.46E-08
GRA= 0.21E-08 0.13E-07-0.41E-09-0.67E-08-0.13E-10-0.18E-07 0.98E-09-0.11E-08
GRA=-0.97E-08 0.18E-07-0.47E-08-0.43E-08-0.11E-08-0.85E-08 0.41E-08-0.15E-08
GRA= 0.10E-07-0.80E-08-0.61E-08 0.49E-08 0.22E-07-0.32E-08-0.38E-08-0.52E-09
GRA=-0.12E-07-0.75E-08 0.12E-07 0.12E-07 0.16E-08 0.32E-07-0.73E-08-0.10E-07

----------------------------
|A| Global axis parameters |
----------------------------

  1) U:   -0.989   0.025   0.149  P:   32.208  -2.588  21.131  D:    0.944
  2) U:   -0.995  -0.001   0.104  P:   28.998  -2.692  21.198  D:    1.022
  3) U:   -0.998  -0.007   0.064  P:   26.092  -2.924  21.303  D:    1.265
  4) U:   -0.999   0.025  -0.032  P:   22.768  -2.496  21.584  D:    0.926
  5) U:   -0.996   0.045  -0.079  P:   19.603  -2.238  21.068  D:    0.961
  6) U:   -0.985   0.088  -0.145  P:   16.629  -2.283  20.455  D:    1.357
  7) U:   -0.987   0.063  -0.147  P:   13.130  -1.441  19.740  D:    0.940
  8) U:   -0.989   0.038  -0.145  P:   10.054  -1.241  19.339  D:    1.289
  9) U:   -0.997  -0.028  -0.072  P:    6.889  -1.264  19.114  D:    1.203
 10) U:   -1.000   0.009   0.025  P:    4.132  -1.467  18.686  D:    0.636
 11) U:   -0.996   0.004   0.089  P:    1.414  -1.550  18.980  D:    0.406
 12) U:   -0.989   0.012   0.149  P:   -1.948  -1.403  19.573

---------------------------------
|B| Global Base-Axis Parameters |
---------------------------------

  1st strand      Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) GC    1      -2.92    -0.27    -1.97    -8.60   1   0
  2) AC    2      -3.79     0.44     0.40   -10.06   2  21
  3) CC    3      -3.12     0.11     1.45   -12.45   3 -16
  4) AC    4      -3.66     0.23    -4.71   -11.72   2  29
  5) CC    5      -3.39    -0.39    -5.84    -9.33   3  -6
  6) CC    6      -3.24     0.31    -2.38   -12.19   3  -3
  7) UC    7      -3.50    -0.77    -8.04    -2.73   4 -25
  8) GC    8      -3.46     0.20    -2.81    -8.47   1  12
  9) AC    9      -3.22    -0.44    -1.37   -11.43   2  22
```

```
 10) UC   10      -3.84    -0.04    -3.90   -10.60   4 -24
 11) UC   11      -3.33    -0.51     2.75    -9.05   4 -18
 12) CC   12      -3.71    -0.15    -5.06    -9.10   3   0

  2nd strand      Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) CD   12      -2.83     0.35    12.86    -1.58   3   0
  2) TD   11      -3.24    -0.20     8.56     0.13   4 -21
  3) GD   10      -3.06     0.16    -1.13    -0.98   1  16
  4) TD    9      -3.69    -0.08     4.63    -2.00   4 -29
  5) GD    8      -3.25     0.57     0.93     1.66   1   6
  6) GD    7      -3.33    -0.28     2.59    -0.58   1   3
  7) AD    6      -3.46     0.32     5.30     2.34   2  25
  8) CD    5      -3.85    -0.07     4.36     4.34   3 -12
  9) UD    4      -3.23     0.38     5.12    -6.91   4 -22
 10) AD    3      -4.05     0.05    -0.65    -0.74   2  24
 11) AD    2      -3.37     0.66     0.69    -1.40   2  18
 12) GD    1      -3.79     0.12     3.95     0.73   1   0

---------------------------------------
|C| Global Base pair-Axis Parameters |
---------------------------------------

  Strand 1 with strand 2 ...

  Duplex          Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) G  1-C 12    -2.88    -0.31     5.45    -3.51   1   0
  2) A  2-T 11    -3.52     0.32     4.48    -5.10   2  21
  3) C  3-G 10    -3.09    -0.02     0.16    -5.73   3 -16
  4) A  4-T  9    -3.67     0.16    -0.04    -4.86   2  29
  5) C  5-G  8    -3.32    -0.48    -2.46    -5.49   3  -6
  6) C  6-G  7    -3.28     0.29     0.10    -5.81   3  -3
  7) U  7-A  6    -3.48    -0.55    -1.37    -2.53   4 -25
  8) G  8-C  5    -3.66     0.14     0.78    -6.40   1  12
  9) A  9-U  4    -3.22    -0.41     1.87    -2.26   2  22
 10) U 10-A  3    -3.95    -0.04    -2.27    -4.93   4 -24
 11) U 11-A  2    -3.35    -0.59     1.72    -3.83   4 -18
 12) C 12-G  1    -3.75    -0.13    -0.56    -4.91   3   0

  Average:        -3.43    -0.14     0.65    -4.61

---------------------------------
|D| Global Base-Base Parameters |
---------------------------------

  Strand 1 with strand 2 ...

  Duplex          Shear    Stretch  Stagger  Buckle   Propel  Opening  Bc  Tc
                  (Sx)      (Sy)     (Sz)    (kappa)  (omega) (sigma)

  1) G  1-C 12    -0.09     0.08    -0.38   -14.83   -10.18     1.97   1   0
  2) A  2-T 11    -0.54     0.24    -0.37    -8.16    -9.94     2.95   2  21
  3) C  3-G 10    -0.07     0.27     0.13     2.57   -13.43     3.74   3 -16
  4) A  4-T  9     0.03     0.14    -0.31    -9.34   -13.72     4.33   2  29
  5) C  5-G  8    -0.14     0.19     0.26    -6.78    -7.67     4.61   3  -6
  6) C  6-G  7     0.09     0.03    -0.36    -4.98   -12.77     2.89   3  -3
  7) U  7-A  6    -0.03    -0.44     0.19   -13.34    -0.38    -5.25   4 -25
  8) G  8-C  5     0.39     0.13     0.19    -7.16    -4.13    -1.44   1  12
```

```
  9) A  9-U  4     0.01    -0.06    -0.01    -6.48   -18.34    -0.30   2  22
 10) U 10-A  3     0.21     0.01     0.56    -3.25   -11.34     2.30   4 -24
 11) U 11-A  2     0.04     0.15    -0.19     2.06   -10.46     4.15   4 -18
 12) C 12-G  1     0.08    -0.03     0.03    -9.01    -8.37    -1.14   3   0

  Average:        -0.00     0.06    -0.02    -6.56   -10.06     1.57
```

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|E| Global Inter-Base Parameters |
-----------------------------------
```

1st strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) G 1/A 2	-0.96	1.07	3.20	-0.37	-2.59	38.59	2
3) A 2/C 3	0.60	-0.07	3.15	-0.87	-1.07	33.74	-6
4) C 3/A 4	-0.64	-0.33	3.12	-5.92	6.57	28.99	9
5) A 4/C 5	0.57	-0.82	3.48	0.52	4.79	25.42	-6
6) C 5/C 6	0.52	0.68	2.71	7.92	-1.80	38.65	-1
7) C 6/U 7	-0.75	-1.42	3.89	-6.01	10.89	16.52	-3
8) U 7/G 8	0.01	1.03	3.11	5.48	-4.31	39.23	-9
9) G 8/A 9	0.36	-0.58	3.07	1.07	2.70	26.86	2
10) A 9/U 10	-0.93	0.12	3.06	-6.15	5.54	32.57	7
11) U 10/U 11	0.63	-0.60	2.35	7.73	5.10	26.95	-4
12) U 11/C 12	-0.16	0.32	3.52	-5.79	2.77	34.61	-2

2nd strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 12/T 11	-0.51	-0.91	3.18	-7.04	2.84	37.61	-2
3) T 11/G 10	0.12	0.10	2.66	-11.60	-2.42	32.96	6
4) G 10/T 9	-0.74	0.21	3.55	6.00	-6.86	28.40	-9
5) T 9/G 8	0.74	0.87	2.91	-2.05	1.26	25.14	6
6) G 8/G 7	0.29	-0.84	3.33	6.12	-3.30	40.38	1
7) G 7/A 6	-0.63	0.95	3.35	2.35	1.50	24.66	3
8) A 6/C 5	-0.42	-0.46	3.11	-0.70	0.56	35.42	9
9) C 5/U 4	0.74	0.39	3.27	0.39	-16.91	25.72	-2
10) U 4/A 3	-1.13	-0.06	2.49	-9.39	1.46	29.97	7
11) A 3/A 2	0.80	0.74	3.11	2.42	-4.22	25.10	4
12) A 2/G 1	-0.19	-0.50	3.30	5.28	-0.68	39.90	2

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|F| Global Inter-Base pair Parameters |
----------------------------------------
```

Strand 1 with strand 2 ...

Duplex	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) G 1/A 2	-0.73	0.99	3.19	-3.71	-2.71	38.10	2
3) A 2/C 3	0.36	-0.09	2.91	-6.23	0.68	33.35	-6
4) C 3/A 4	-0.69	-0.27	3.34	0.04	6.72	28.70	9
5) A 4/C 5	0.66	-0.84	3.20	-0.76	1.76	25.28	-6
6) C 5/C 6	0.41	0.76	3.02	7.02	0.75	39.51	-1
7) C 6/U 7	-0.69	-1.18	3.62	-1.83	4.70	20.59	-3
8) U 7/G 8	-0.21	0.75	3.11	2.39	-2.44	37.32	-9
9) G 8/A 9	0.55	-0.49	3.17	0.73	9.80	26.29	2
10) A 9/U 10	-1.03	0.09	2.77	-7.77	2.04	31.27	7
11) U 10/U 11	0.71	-0.67	2.73	5.07	4.66	26.03	-4
12) U 11/C 12	-0.18	0.41	3.41	-0.25	1.73	37.26	-2

```
  Average:        -0.08    -0.05     3.13    -0.48     2.52    31.24

---------------------------------
|G| Local Inter-Base Parameters |
---------------------------------

  1st strand      Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) G  1/A  2    -0.49    -1.22     3.24     5.62    -2.97    38.18   2
  3) A  2/C  3     1.01    -2.00     3.13     5.63    -0.37    33.26  -6
  4) C  3/A  4     0.02    -2.13     3.47     0.65     5.71    29.68   9
  5) A  4/C  5     1.19    -2.70     3.22     5.26     2.33    25.00  -6
  6) C  5/C  6     0.98    -1.72     2.55    14.75    -4.46    36.70  -1
  7) C  6/U  7    -0.16    -2.78     3.78    -3.80     9.27    17.29  -3
  8) U  7/G  8     0.43    -1.59     3.08     8.90    -7.59    38.67  -9
  9) G  8/A  9     0.95    -2.21     3.21     5.60     1.80    26.46   2
 10) A  9/U 10    -0.12    -2.01     3.36     0.28     4.06    33.31   7
 11) U 10/U 11     1.12    -2.30     2.40    12.13     4.73    25.40  -4
 12) U 11/C 12     0.67    -1.86     3.58     0.05     2.06    35.10  -2

  2nd strand      Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) C 12/T 11    -0.44    -0.49     3.28    -7.26     4.07    37.16  -2
  3) T 11/G 10     0.15    -1.71     2.84   -11.50     4.40    32.90   6
  4) G 10/T  9    -0.83    -1.76     3.92     4.90     7.69    28.40  -9
  5) T  9/G  8     0.86    -2.18     3.17    -2.13     0.10    24.97   6
  6) G  8/G  7     0.41    -1.40     3.42     6.37     4.52    40.32   1
  7) G  7/A  6    -0.58    -2.12     3.60     2.67     0.25    24.47   3
  8) A  6/C  5    -0.13    -1.50     3.35     1.41     2.45    35.14   9
  9) C  5/U  4     0.70    -1.74     3.78    -0.15    18.72    25.47  -2
 10) U  4/A  3    -1.15    -1.70     2.84   -11.17    -0.11    29.15   7
 11) A  3/A  2     0.86    -2.34     3.35     1.82     4.24    25.14   4
 12) A  2/G  1     0.05    -1.82     3.54     4.82     2.41    39.81   2

---------------------------------------
|H| Local Inter-Base pair Parameters |
---------------------------------------

  Strand 1 with strand 2 ...

  Duplex          Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) G  1/A  2    -0.46    -0.85     3.27    -0.72     0.75    37.91   2
  3) A  2/C  3     0.57    -1.83     3.01    -2.86     2.30    33.20  -6
  4) C  3/A  4    -0.37    -1.93     3.73     2.83     6.61    29.26   9
  5) A  4/C  5     1.01    -2.42     3.21     1.52     1.38    24.95  -6
  6) C  5/C  6     0.73    -1.56     3.01    10.74     0.12    38.79  -1
  7) C  6/U  7    -0.39    -2.43     3.71    -0.54     4.80    20.46  -3
  8) U  7/G  8     0.15    -1.56     3.20     5.02    -2.68    37.20  -9
  9) G  8/A  9     0.83    -1.99     3.49     2.73    10.25    26.49   2
 10) A  9/U 10    -0.67    -1.84     3.14    -5.51     2.07    31.34   7
 11) U 10/U 11     1.03    -2.31     2.88     6.99     4.63    25.36  -4
 12) U 11/C 12     0.35    -1.83     3.57     2.45     2.19    37.56  -2

  Average:         0.25    -1.87     3.29     2.06     2.95    31.14

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```

```
|I| Global Axis Curvature |
---------------------------

  Duplex          Ax      Ay     Ainc    Atip    Adis    Angle   Path   Dc

 2) G  1/A  2   -0.10    0.36   -2.74   -1.13    0.37    2.96    3.21   2
 3) A  2/C  3   -0.06    0.25   -1.92    1.32    0.26    2.33    2.92  -6
 4) C  3/A  4   -0.11   -0.45    0.24    5.84    0.46    5.85    3.36   9
 5) A  4/C  5    0.30   -0.21    1.65    2.40    0.37    2.91    3.22  -6
 6) C  5/C  6    0.37   -0.01    4.46    1.07    0.37    4.59    3.04  -1
 7) C  6/U  7   -0.49   -0.35   -0.35    1.43    0.60    1.47    3.67  -3
 8) U  7/G  8   -0.03    0.06    0.24    1.43    0.07    1.45    3.11  -9
 9) G  8/A  9    0.11    0.06   -0.37    5.65    0.13    5.67    3.17   2
10) A  9/U 10   -0.30   -0.27   -3.62    4.71    0.40    5.94    2.80   7
11) U 10/U 11    0.11   -0.13    1.08    3.56    0.17    3.72    2.73  -4
12) U 11/C 12    0.22   -0.04    2.02    2.81    0.22    3.46    3.42  -2

Overall axis bend ... UU=    0.72 PP=    9.81


  Duplex       Offset   L.Dir  ... wrt end-to-end vector

 1) G  1         0.00    0.00
 2) A  2         0.30   17.08
 3) C  3         0.71  -22.01
 4) A  4         0.91  -15.48
 5) C  5         0.52  -35.62
 6) C  6         0.24 -146.05
 7) U  7         0.71   55.94
 8) G  8         0.97   23.06
 9) A  9         0.97    5.08
10) U 10         1.17   -7.46
11) U 11         0.75  -25.00
12) C 12         0.00    0.00

  Path length=    34.65  End-to-end=    34.21  Shortening=     1.26 %

--------------------------
|J| Backbone Parameters |
--------------------------

  1st strand   C1'-C2' C2'-C3'  Phase   Ampli   Pucker    C1'   C2'   C3'

  1)GC    1    -24.26   33.42   11.06   34.53  C3'-endo  105.5 105.6 100.7
  2)AC    2    -35.31   40.73  357.81   41.36  C2'-exo   104.2 104.4  99.2
  3)CC    3    -29.95   37.70    3.73   38.28  C3'-endo  105.5 103.6 101.5
  4)AC    4    -27.05   38.84   12.72   40.58  C3'-endo  107.5 100.7 102.7
  5)CC    5    -28.96   35.14  359.87   35.53  C2'-exo   105.8 103.6 103.4
  6)CC    6    -35.35   46.47    9.47   48.58  C3'-endo  106.3 100.9  95.8
  7)UC    7    -23.70   27.15  355.13   27.66  C2'-exo   107.0 103.3 105.1
  8)GC    8    -30.67   40.16    7.84   41.55  C3'-endo  106.2 101.9 100.3
  9)AC    9    -23.23   39.96   23.62   44.23  C3'-endo  104.8 104.4  98.9
 10)UC   10    -26.58   41.58   18.03   44.64  C3'-endo  106.5 100.3 101.8
 11)UC   11    -13.40   30.56   34.44   38.23  C3'-endo  106.3 104.5  99.6
 12)CC   12    -23.72   35.54   16.92   37.75  C3'-endo  105.5 106.0  98.1

  Torsions       Chi    Gamma   Delta   Epsil   Zeta    Alpha   Beta
                 C1'-N  C5'-C4' C4'-C3' C3'-O3'  O3'-P   P-O5'  O5'-C5'

  1)GC    1   -175.47   56.47   88.10 -137.35  -89.36  -59.02  173.00
  2)AC    2   -161.23   35.27   89.25 -157.07  -67.86  -56.86  166.95
```

```
  3)CC    3   -159.94   59.72   81.05 -162.30  -56.02  -76.32 -174.07
  4)AC    4   -153.27   52.76   77.49 -166.57  -53.32  152.44  178.05
  5)CC    5   -169.88 -176.07   88.27 -150.65  -64.61  -64.25  170.46
  6)CC    6   -151.93   48.37   66.85 -160.19  -78.93  135.17 -150.70
  7)UC    7    176.69 -158.98   94.38 -130.89  -73.83  -73.94  163.83
  8)GC    8   -153.66   62.00   77.59 -148.95  -61.52  -72.65  162.66
  9)AC    9   -156.73   78.12   73.13 -170.99  -67.21  -89.89 -173.96
 10)UC   10   -161.01   65.98   75.34 -148.60  -51.64 -128.41  152.23
 11)UC   11   -176.66  132.39   73.13 -147.16  -70.93  -56.95  166.48
 12)CC   12   -166.23   51.61   82.13  ......  ......  ......  ......


  2nd strand   C1'-C2' C2'-C3'  Phase   Ampli   Pucker    C1'   C2'   C3'

  1)CD   12     31.85  -34.88  172.05   35.88  C2'-endo  106.2 102.2 103.3
  2)TD   11     32.33  -21.08  130.20   33.51  C1'-exo   105.4 104.1 104.3
  3)GD   10      0.21   23.43   55.41   42.72  C4'-exo   107.1 103.2 101.7
  4)TD    9     40.09  -29.77  140.25   40.10  C1'-exo   105.0 101.5 103.5
  5)GD    8     18.58   -9.35  117.20   21.13  C1'-exo   107.1 106.0 104.8
  6)GD    7      4.17   17.83   61.30   38.23  C4'-exo   107.6 104.3 102.6
  7)AD    6     41.66  -28.49  134.13   42.40  C1'-exo   104.5 101.2 103.5
  8)CD    5     40.66  -30.63  140.90   40.73  C1'-exo   105.0 101.3 103.7
  9)UD    4     14.91    5.12   80.86   33.91  O1'-endo  105.7 107.1 103.3
 10)AD    3     40.40  -29.78  138.95   40.61  C1'-exo   104.6 101.8 103.7
 11)AD    2     29.19  -20.13  133.58   29.90  C1'-exo   105.7 104.5 104.8
 12)GD    1    -23.46   19.74  329.74   23.47  C2'-exo   107.7 105.1 104.4

  Torsions       Chi    Gamma   Delta   Epsil   Zeta    Alpha   Beta
                 C1'-N  C5'-C4' C4'-C3' C3'-O3'  O3'-P   P-O5'  O5'-C5'

  1)CD   12    -94.95   36.56  145.09  ......  ......  ......  ......
  2)TD   11   -133.74   58.61  122.50 -172.62  -92.78  -57.07 -168.29
  3)GD   10   -170.30 -155.91   77.16 -162.59  -72.68  -61.07  174.73
  4)TD    9   -129.63   45.64  137.80 -147.99 -107.06   99.85 -150.52
  5)GD    8   -160.95   51.66  118.58 -174.72  -75.80  -66.66 -170.42
  6)GD    7   -175.16 -145.22   91.16 -147.37  -96.15  -71.54  170.64
  7)AD    6   -125.83   47.98  130.08 -160.41 -115.01  106.33 -148.85
  8)CD    5   -129.68   69.89  133.43 -163.56 -108.18  -66.38  172.78
  9)UD    4   -149.10 -177.05   96.53 -170.78  -87.18  -78.72 -176.88
 10)AD    3   -125.41   45.78  131.28 -171.14  -85.39  134.04 -179.10
 11)AD    2   -152.03   56.89  123.47 -173.29  -88.83  -60.21 -170.95
 12)GD    1   -171.04 -165.28  114.90 -143.23  -67.73  -81.28 -178.15


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|K| Groove parameters |
------------------------

Atom defining backbone: P      12 levels,  3 sub-levels

 Levels          Minor groove                Major groove
    i  n      Width    Depth  Angle       Width    Depth  Angle    Diam

G   1  0        --       --     --    G     --       --     --       --
    1  1        --       --     --          --       --     --       --
    1  2        --       --     --          --       --     --       --
    1  3        --       --     --          --       --     --       --
A   2  0        --       --     --    A     --       --     --       --
    2  1        --       --     --          --       --     --     19.54
    2  2        --       --     --          --       --     --     20.06
C   3  0      8.26     3.21    28    C     --       --     --     20.42
```

	3	1	8.78	2.74	29		--	--	--	20.62
	3	2	9.09	2.02	42		--	--	--	20.61
	3	3	8.83	1.98	47		12.12	5.71	66	20.17
A	4	0	8.41	2.03	47	A	12.83	5.81	67	19.97
	4	1	8.02	2.32	46		13.69	4.06	73	19.79
	4	2	7.70	2.67	41		14.96	1.95	77	19.99
	4	3	7.58	2.94	38		15.91	1.48	76	20.39
C	5	0	7.66	3.17	31	C	10.91	8.85	27	20.73
	5	1	7.99	3.32	26		11.14	8.29	34	20.84
	5	2	8.36	3.30	25		11.91	7.89	36	20.91
	5	3	8.49	3.16	29		13.25	7.21	41	20.97
C	6	0	8.53	2.74	34	C	14.48	6.20	47	21.05
	6	1	8.65	2.19	38		14.71	9.37	8	21.09
	6	2	8.80	2.03	37		14.63	9.64	9	20.99
	6	3	8.90	1.84	41		14.57	9.96	7	20.79
U	7	0	8.97	1.91	42	U	14.39	10.15	6	20.56
	7	1	8.98	2.26	42		13.92	10.23	10	20.19
	7	2	8.89	2.60	36		13.38	10.27	15	19.68
	7	3	8.69	2.69	34		12.58	9.71	29	19.48
G	8	0	8.55	2.70	31	G	11.45	9.45	32	19.59
	8	1	8.52	2.56	35		--	--	--	19.95
	8	2	8.57	2.66	34		--	--	--	20.43
	8	3	8.62	2.76	35		--	--	--	20.94
A	9	0	8.81	2.77	36	A	--	--	--	21.35
	9	1	9.23	2.21	36		--	--	--	21.55
	9	2	9.14	1.67	45		--	--	--	21.21
U	10	0	8.73	1.73	44	U	--	--	--	20.47
	10	1	8.24	2.30	41		--	--	--	19.88
	10	2	--	--	--		--	--	--	20.04
U	11	0	--	--	--	U	--	--	--	--
	11	1	--	--	--		--	--	--	--
	11	2	--	--	--		--	--	--	--
	11	3	--	--	--		--	--	--	--
C	12	0	--	--	--	C	--	--	--	--

Table S5. Curves output for RNA:DNA duplex C (orange molecule, 20% occupancy, Figure 3 – main paper).

```
    ************************************              **************
    ******  CURVES 5.3 R.L. 1998  *****              *  16 Aug 16 *
    ************************************              **************


  FILE : 5SWM.pdb                           LIS  : orange
  dna  :                                    axin :
  axout:                                    daf  :
  PDB  : orange

  acc  :    0.000  wid  :    0.750

  maxn :   500  ior  :     0  ibond:     0  splin:     3  break:    -1
  nleve:     3  nbac :     7

  ends :     F  supp :     T  COMB :     T  DINU :     T  mini :     T
  rest :     F  line :     F  zaxe :     F  FIT  :     T  test :     F
  GRV  :     T  old  :     T  axonl:     F

  Least squares fitting of standard bases ...

   Str   Pos  Base          Rms (ang)

    1 :   1)  CC     1      1.844
    1 :   2)  AC     2      0.067
    1 :   3)  CC     3      0.041
    1 :   4)  AC     4      0.059
    1 :   5)  CC     5      0.031
    1 :   6)  CC     6      0.047
    1 :   7)  UC     7      0.071
    1 :   8)  CC     8      1.833
    1 :   9)  AC     9      0.061
    1 :  10)  UC    10      0.054
    1 :  11)  UC    11      0.058
    1 :  12)  CC    12      0.038
    2 :   1)  CD    12      0.019
    2 :   2)  TD    11      0.023
    2 :   3)  GD    10      0.058
    2 :   4)  TD     9      0.030
    2 :   5)  GD     8      0.022
    2 :   6)  GD     7      0.027
    2 :   7)  AD     6      0.020
    2 :   8)  CD     5      0.032
    2 :   9)  UD     4      0.064
    2 :  10)  AD     3      0.025
    2 :  11)  AD     2      0.025
    2 :  12)  GD     1      0.043

  Strand=    2 Nucleo=   24 Atoms =  495 Units =   24

  Input   1) Xdisp=    0.00 Ydisp=    0.00 Inclin=    0.00 Tip=    0.00

  Combined strands have   12 levels ...

  Strand  1 has  12 bases (5'-3'): CACACCUCAUUC
  Strand  2 has  12 bases (3'-5'): CTGTGGACUAAG

  FIRST SUM=  266.231 CPTS:   15.005  31.518  18.416 201.292
```

```
MINIMISATION: ACC =  0.100E-05 MAXN=  500 NVAR=   48

STEP    1 SUM=  266.231 DEL=  0.000E+00
STEP    2 SUM=  227.671 DEL= -0.386E+02
STEP    3 SUM=  189.171 DEL= -0.385E+02
STEP    4 SUM=  198.687 DEL=  0.952E+01
STEP    5 SUM=  152.881 DEL= -0.458E+02
STEP    6 SUM=  108.354 DEL= -0.445E+02
STEP    7 SUM=   98.418 DEL= -0.994E+01
STEP    8 SUM=   87.530 DEL= -0.109E+02
STEP    9 SUM=   78.106 DEL= -0.942E+01
STEP   10 SUM=   70.786 DEL= -0.732E+01
STEP   11 SUM=   66.117 DEL= -0.467E+01
STEP   12 SUM=   62.654 DEL= -0.346E+01
STEP   13 SUM=   63.011 DEL=  0.357E+00
STEP   14 SUM=   61.007 DEL= -0.200E+01
STEP   15 SUM=   58.728 DEL= -0.228E+01
STEP   16 SUM=   55.937 DEL= -0.279E+01
STEP   17 SUM=   82.891 DEL=  0.270E+02
STEP   18 SUM=   55.704 DEL= -0.272E+02
STEP   19 SUM=   55.440 DEL= -0.264E+00
STEP   20 SUM=   54.968 DEL= -0.472E+00
STEP   21 SUM=   54.211 DEL= -0.757E+00
STEP   22 SUM=   59.452 DEL=  0.524E+01
STEP   23 SUM=   54.015 DEL= -0.544E+01
STEP   24 SUM=   53.717 DEL= -0.299E+00
STEP   25 SUM=   53.340 DEL= -0.376E+00
STEP   26 SUM=   53.038 DEL= -0.302E+00
STEP   27 SUM=   52.625 DEL= -0.413E+00
STEP   28 SUM=   51.983 DEL= -0.642E+00
STEP   29 SUM=   51.153 DEL= -0.830E+00
STEP   30 SUM=   50.922 DEL= -0.231E+00
STEP   31 SUM=   50.497 DEL= -0.425E+00
STEP   32 SUM=   49.512 DEL= -0.985E+00
STEP   33 SUM=   71.316 DEL=  0.218E+02
STEP   34 SUM=   49.476 DEL= -0.218E+02
STEP   35 SUM=   49.406 DEL= -0.701E-01
STEP   36 SUM=   48.975 DEL= -0.431E+00
STEP   37 SUM=   49.935 DEL=  0.960E+00
STEP   38 SUM=   48.847 DEL= -0.109E+01
STEP   39 SUM=   49.226 DEL=  0.380E+00
STEP   40 SUM=   48.821 DEL= -0.405E+00
STEP   41 SUM=   48.773 DEL= -0.480E-01
STEP   42 SUM=   48.636 DEL= -0.137E+00
STEP   43 SUM=   48.590 DEL= -0.462E-01
STEP   44 SUM=   48.543 DEL= -0.465E-01
STEP   45 SUM=   48.525 DEL= -0.177E-01
STEP   46 SUM=   48.505 DEL= -0.203E-01
STEP   47 SUM=   48.496 DEL= -0.896E-02
STEP   48 SUM=   48.492 DEL= -0.453E-02
STEP   49 SUM=   48.488 DEL= -0.317E-02
STEP   50 SUM=   48.487 DEL= -0.141E-02
STEP   51 SUM=   48.487 DEL= -0.235E-03
STEP   52 SUM=   48.487 DEL= -0.177E-04
STEP   53 SUM=   48.487 DEL= -0.214E-05
STEP   54 SUM=   48.487 DEL= -0.672E-06
STEP   55 SUM=   48.487 DEL= -0.411E-06
STEP   56 SUM=   48.487 DEL= -0.609E-07
STEP   57 SUM=   48.487 DEL= -0.136E-07
STEP   58 SUM=   48.487 DEL= -0.119E-08
```

```
STEP   59 SUM=   48.487 DEL= -0.217E-09
STEP   60 SUM=   48.487 DEL= -0.239E-10
STEP   61 SUM=   48.487 DEL= -0.201E-11
STEP   62 SUM=   48.487 DEL= -0.924E-13
STEP   63 SUM=   48.487 DEL= -0.711E-14
STEP   64 SUM=   48.487 DEL=  0.000E+00

FINAL SUM=   48.487 CPTS:   10.567  24.629   8.936   4.355

GRA=-0.51E-08-0.35E-08 0.55E-09 0.33E-09 0.17E-08-0.10E-07-0.51E-09-0.12E-08
GRA= 0.43E-08 0.78E-09-0.71E-09-0.24E-09 0.12E-07-0.16E-07-0.12E-08 0.21E-08
GRA=-0.13E-07 0.17E-07-0.19E-09-0.40E-09-0.10E-07 0.40E-08-0.16E-08 0.17E-09
GRA= 0.47E-08-0.65E-08-0.13E-09 0.40E-11 0.87E-08-0.93E-08 0.26E-08-0.42E-09
GRA= 0.80E-08 0.63E-10-0.17E-09-0.19E-08-0.96E-08-0.52E-08-0.14E-08 0.47E-09
GRA=-0.22E-08 0.13E-08 0.60E-09-0.16E-08 0.16E-08 0.11E-07 0.20E-08 0.15E-08

----------------------------
|A| Global axis parameters |
----------------------------

  1) U:   -0.934  -0.198  -0.298  P:   11.119   1.480  17.404  D:    3.131
  2) U:   -0.939  -0.279  -0.203  P:    7.045   0.309  16.587  D:    6.284
  3) U:   -0.957  -0.282   0.067  P:    4.022  -0.661  16.185  D:    4.364
  4) U:   -0.916  -0.237   0.323  P:   -0.232  -2.261  17.227  D:    3.351
  5) U:   -0.901  -0.225   0.370  P:   -2.250  -3.052  18.064  D:    4.917
  6) U:   -0.913  -0.090   0.398  P:   -5.748  -4.346  19.870  D:    4.401
  7) U:   -0.893   0.063   0.447  P:   -8.913  -4.492  21.924  D:    3.445
  8) U:   -0.921   0.163   0.354  P:  -11.817  -4.231  23.513  D:    6.226
  9) U:   -0.963   0.268   0.031  P:  -14.451  -3.603  23.606  D:    5.011
 10) U:   -0.956   0.213  -0.199  P:  -18.383  -2.217  23.055  D:    4.437
 11) U:   -0.928   0.108  -0.356  P:  -21.157  -1.260  21.772  D:    2.921
 12) U:   -0.900   0.037  -0.434  P:  -24.601  -0.977  19.931

----------------------------------
|B| Global Base-Axis Parameters |
----------------------------------

  1st strand      Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) CC    1      -2.48    -2.55    -0.12   -22.25   3   0
  2) AC    2      -0.56    -0.46   -12.27   -13.43   2  29
  3) CC    3      -1.86    -1.03   -14.74   -22.89   3 -16
  4) AC    4      -0.95    -0.22   -38.71    -0.96   2  29
  5) CC    5      -1.53    -0.59    -9.89   -12.89   3  -6
  6) CC    6      -1.93    -0.60   -21.87    -4.50   3  -3
  7) UC    7      -2.06    -0.54   -22.43   -10.36   4 -17
  8) CC    8      -2.13    -2.55   -16.10   -14.71   3 -12
  9) AC    9      -1.83    -0.65   -16.90    -6.67   2  30
 10) UC   10      -1.34    -0.89   -25.86    -4.92   4 -24
 11) UC   11      -1.95    -0.95   -24.11    -1.40   4 -18
 12) CC   12      -2.56    -0.31   -21.96    -4.55   3   0

  2nd strand      Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) CD   12      -0.48     0.10    -5.58     9.82   3   0
  2) TD   11      -0.62     0.31    -0.20     4.66   4 -21
  3) GD   10      -1.48     0.64    -3.08     3.11   1  16
  4) TD    9      -1.12     1.08    11.98    -4.14   4 -29
  5) GD    8      -1.61     0.51   -13.02     2.84   1   6
```

```
  6) GD    7      -1.11     0.92   -11.92    -1.19   1   3
  7) AD    6      -1.31     0.93    -0.12    -5.78   2  25
  8) CD    5      -0.77     0.07    -5.31    -0.45   3 -12
  9) UD    4      -1.70     0.68   -10.14    -3.32   4 -22
 10) AD    3      -1.53     1.35    -4.05     6.91   2  24
 11) AD    2      -2.21     1.04   -13.88    -1.48   2  18
 12) GD    1       0.07     1.92    -6.98     1.66   1   0

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|C| Global Base pair-Axis Parameters |
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  Strand 1 with strand 2 ...

  Duplex          Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) C  1-C 12    -1.48    -1.32    -2.85   -16.04   3   0
  2) A  2-T 11    -0.59    -0.38    -6.23    -9.04   2  29
  3) C  3-G 10    -1.67    -0.83    -8.91   -13.00   3 -16
  4) A  4-T  9    -1.04    -0.65   -13.36     1.59   2  29
  5) C  5-G  8    -1.57    -0.55   -11.45    -7.87   3  -6
  6) C  6-G  7    -1.52    -0.76   -16.90    -1.66   3  -3
  7) U  7-A  6    -1.68    -0.74   -11.28    -2.29   4 -17
  8) C  8-C  5    -1.45    -1.31   -10.71    -7.13   3 -12
  9) A  9-U  4    -1.77    -0.66   -13.52    -1.67   2  30
 10) U 10-A  3    -1.44    -1.12   -14.96    -5.92   4 -24
 11) U 11-A  2    -2.08    -1.00   -19.00     0.04   4 -18
 12) C 12-G  1    -1.25    -1.11   -14.47    -3.11   3   0

  Average:        -1.46    -0.87   -11.97    -5.51

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|D| Global Base-Base Parameters |
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  Strand 1 with strand 2 ...

  Duplex          Shear    Stretch  Stagger  Buckle   Propel  Opening  Bc  Tc
                  (Sx)      (Sy)     (Sz)    (kappa)  (omega) (sigma)

  1) C  1-C 12    -2.00    -2.46    -0.91     5.46   -12.43   -38.91   3   0
  2) A  2-T 11     0.07    -0.15    -1.18   -12.07    -8.77     0.92   2  29
  3) C  3-G 10    -0.38    -0.39    -0.62   -11.67   -19.77    -3.23   3 -16
  4) A  4-T  9     0.17     0.86    -0.67   -50.69    -5.10     5.65   2  29
  5) C  5-G  8     0.08    -0.08    -0.72     3.13   -10.05     7.10   3  -6
  6) C  6-G  7    -0.81     0.32     0.52    -9.95    -5.69     6.77   3  -3
  7) U  7-A  6    -0.75     0.39    -0.56   -22.32   -16.13     7.49   4 -17
  8) C  8-C  5    -1.36    -2.48    -0.14   -10.79   -15.16   -26.71   3 -12
  9) A  9-U  4    -0.13     0.04    -0.15    -6.76    -9.99     4.21   2  30
 10) U 10-A  3     0.19     0.46     0.29   -21.81     1.99     4.13   4 -24
 11) U 11-A  2     0.26     0.09     0.15   -10.24    -2.87     3.34   4 -18
 12) C 12-G  1    -2.63     1.61    -0.14   -14.98    -2.89    26.39   3   0

  Average:        -0.61    -0.15    -0.34   -13.56    -8.91    -0.24

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|E| Global Inter-Base Parameters |
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  1st strand      Shift    Slide     Rise     Tilt     Roll    Twist   Dc
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```
                  (Dx)     (Dy)      (Dz)     (tau)    (rho)  (Omega)

  2) C  1/A  2     2.19     2.24      4.18   -14.02    15.68    73.10   9
  3) A  2/C  3    -1.46    -0.69      3.50    -6.93     5.50    18.50  -6
  4) C  3/A  4     0.97     0.38      4.66   -23.37    37.03    34.52   9
  5) A  4/C  5    -0.73    -0.60      2.28    30.42    -9.56    35.52  -6
  6) C  5/C  6    -0.96    -0.46      4.71   -12.72    16.30    21.50  -1
  7) C  6/U  7    -0.32    -0.43      3.21     4.11     2.19    28.34  -3
  8) U  7/C  8    -0.32    -2.17      3.53     5.06     3.53     1.83  -2
  9) C  8/A  9     0.72     2.03      2.71    -2.41    27.65    57.11   9
 10) A  9/U 10     0.60    -0.67      4.43    -8.96    15.37    23.48   7
 11) U 10/U 11    -0.58    -0.70      3.08     3.29    14.34    27.61  -4
 12) U 11/C 12    -0.48     0.34      3.76     5.01     2.41    34.40  -2

  2nd strand      Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)      (Dz)     (tau)    (rho)  (Omega)

  2) C 12/T 11     0.13     0.07      4.45     3.51   -12.02    33.27  -2
  3) T 11/G 10    -1.01     0.45      2.95    -7.33   -16.50    22.64   6
  4) G 10/T  9     0.41     0.87      4.71    15.66   -22.35    25.64  -9
  5) T  9/G  8    -0.64    -0.34      2.33   -23.41     4.61    34.07   6
  6) G  8/G  7    -0.07     0.86      3.47     0.37   -11.94    21.82   1
  7) G  7/A  6    -0.39     0.50      4.29    16.47   -12.63    27.63   3
  8) A  6/C  5     0.28    -0.70      3.11    -6.47    -2.56    36.03   9
  9) C  5/U  4    -0.51     0.48      2.72    -6.45   -22.48    26.19  -2
 10) U  4/A  3     0.28     1.09      3.99     6.10    -3.39    23.56   7
 11) A  3/A  2    -0.65     0.33      3.22    -8.28   -19.21    28.40   4
 12) A  2/G  1     2.40     1.18      4.05     9.76    -2.43    11.35   2

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|F| Global Inter-Base pair Parameters |
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  Strand 1 with strand 2 ...

  Duplex          Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)      (Dz)     (tau)    (rho)  (Omega)

  2) C  1/A  2     1.16     1.08      4.31    -5.25    13.85    53.19   9
  3) A  2/C  3    -1.24    -0.57      3.22    -7.13    11.00    20.57  -6
  4) C  3/A  4     0.69    -0.24      4.68    -3.86    29.69    30.08   9
  5) A  4/C  5    -0.68    -0.13      2.31     3.50    -7.08    34.79  -6
  6) C  5/C  6    -0.51    -0.66      4.09    -6.18    14.12    21.66  -1
  7) C  6/U  7    -0.35    -0.47      3.75    10.29     7.41    27.98  -3
  8) U  7/C  8    -0.02    -0.74      3.32    -0.71     3.05    18.93  -2
  9) C  8/A  9     0.10     0.77      2.71    -4.43    25.07    41.65   9
 10) A  9/U 10     0.44    -0.88      4.21    -1.43     9.38    23.52   7
 11) U 10/U 11    -0.62    -0.51      3.15    -2.50    16.77    28.00  -4
 12) U 11/C 12     0.96    -0.42      3.91     7.39     2.42    22.88  -2

  Average:        -0.01    -0.25     3.61    -0.94    11.43    29.39

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|G| Local Inter-Base Parameters |
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  1st strand      Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)      (Dz)     (tau)    (rho)  (Omega)

  2) C  1/A  2     4.69    -0.52      3.10     8.93     6.06    74.43   9
  3) A  2/C  3    -0.16    -1.90      3.74     0.01     0.95    22.47  -6
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  4) C  3/A  4     2.35    -2.79     3.73   -14.11    18.47    42.38   9
  5) A  4/C  5    -0.34    -2.08     1.80    34.41   -22.31    31.41  -6
  6) C  5/C  6     0.01    -2.43     4.53    -8.48     9.94    24.58  -1
  7) C  6/U  7     0.28    -2.51     2.70     8.34    -9.02    28.43  -3
  8) U  7/C  8     0.35    -3.41     2.88     5.22     2.36     3.23  -2
  9) C  8/A  9     2.66    -1.05     2.94     6.57    10.09    60.03   9
 10) A  9/U 10     1.35    -2.94     3.84    -5.51     5.89    27.53   7
 11) U 10/U 11    -0.01    -2.74     2.42     5.18     1.65    29.32  -4
 12) U 11/C 12     0.03    -2.40     3.29     7.40   -11.50    33.53  -2

  2nd strand      Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) C 12/T 11     0.81    -0.69     4.44     8.65    10.32    32.91  -2
  3) T 11/G 10    -0.45    -0.92     3.27    -5.58    15.86    23.55   6
  4) G 10/T  9     0.67    -1.12     5.25    15.43    23.85    25.05  -9
  5) T  9/G  8    -0.00    -0.48     2.43   -22.85    -4.29    34.55   6
  6) G  8/G  7     0.27    -2.17     3.26     0.20     6.94    23.02   1
  7) G  7/A  6    -0.27    -1.57     4.27    13.93     9.74    29.53   3
  8) A  6/C  5     0.45    -0.07     3.28    -7.47     1.22    36.01   9
  9) C  5/U  4    -0.33    -1.48     2.92    -5.35    18.77    28.52  -2
 10) U  4/A  3     0.78    -2.16     4.12     6.21     0.64    24.78   7
 11) A  3/A  2     0.19    -1.83     3.29    -7.02    14.42    30.33   4
 12) A  2/G  1     2.70    -2.07     3.82     8.98     0.63    12.24   2

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|H| Local Inter-Base pair Parameters |
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  Strand 1 with strand 2 ...

  Duplex          Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) C  1/A  2     2.77    -0.95     3.92     8.37     8.03    53.98   9
  3) A  2/C  3    -0.35    -1.38     3.52    -2.68     8.51    23.81  -6
  4) C  3/A  4     1.52    -2.05     4.59     0.36    21.93    33.15   9
  5) A  4/C  5    -0.17    -1.32     2.17     5.73   -12.78    33.25  -6
  6) C  5/C  6     0.08    -2.29     3.87    -4.24     8.20    23.82  -1
  7) C  6/U  7     0.09    -2.10     3.53    11.75     0.02    30.05  -3
  8) U  7/C  8     0.27    -1.74     3.27    -1.09     1.37    19.53  -2
  9) C  8/A  9     1.17    -1.39     3.00     0.27    13.90    44.63   9
 10) A  9/U 10     1.07    -2.53     4.00     0.22     3.02    25.62   7
 11) U 10/U 11     0.10    -2.33     2.88    -0.61     8.36    30.38  -4
 12) U 11/C 12     1.37    -2.40     3.47     8.90    -5.57    23.41  -2

  Average:         0.72    -1.86     3.47     2.45     5.00    31.06

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|I| Global Axis Curvature |
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  Duplex           Ax       Ay      Ainc     Atip     Adis     Angle   Path   Dc

 2) C  1/A  2     0.27     0.14    -1.87     6.85     0.30     7.10    4.32   9
 3) A  2/C  3    -0.16    -0.12    -4.46    14.96     0.20    15.61    3.20  -6
 4) C  3/A  4     0.06    -0.42     0.60    15.10     0.43    15.11    4.66   9
 5) A  4/C  5    -0.15    -0.23     1.60     2.38     0.27     2.86    2.32  -6
 6) C  5/C  6    -0.56    -0.45    -0.73     7.91     0.72     7.95    4.14  -1
 7) C  6/U  7    -0.19    -0.49     4.67     8.04     0.53     9.30    3.78  -3
 8) U  7/C  8    -0.25    -0.17    -1.28     7.89     0.30     7.99    3.32  -2
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 9) C  8/A  9    0.42    0.13   -1.62   19.61    0.44   19.68    2.71   9
10) A  9/U 10    0.11   -0.42    0.01   13.62    0.44   13.62    4.21   7
11) U 10/U 11    0.03   -0.64    1.54   10.82    0.64   10.93    3.20  -4
12) U 11/C 12    0.12   -0.30    2.86    5.57    0.33    6.26    3.92  -2

Overall axis bend ... UU=   15.73 PP=   25.90


  Duplex       Offset   L.Dir  ... wrt end-to-end vector

 1) C  1         0.00    0.00
 2) A  2         1.42   65.40
 3) C  3         2.39   50.84
 4) A  4         3.12   42.49
 5) C  5         3.62   21.02
 6) C  6         4.82   17.71
 7) U  7         5.52    6.96
 8) C  8         6.07   16.29
 9) A  9         5.48  -40.78
10) U 10         3.92  -54.31
11) U 11         2.14  -72.32
12) C 12         0.00    0.00

  Path length=    39.78  End-to-end=    35.89  Shortening=     9.76 %

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|J| Backbone Parameters |
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  1st strand   C1'-C2' C2'-C3'  Phase   Ampli   Pucker    C1'   C2'   C3'

  1)CC    1    -22.28   35.29   17.94   37.35  C3'-endo  105.7 103.7 102.9
  2)AC    2    -35.32   44.48    3.61   44.84  C3'-endo  103.9 103.7  99.2
  3)CC    3    -26.09   37.38   12.99   39.24  C3'-endo  106.7 100.9 102.9
  4)AC    4    -29.80   32.00  349.30   32.80  C2'-exo   104.6 104.8 103.4
  5)CC    5    -25.54   38.70   17.18   41.43  C3'-endo  106.5 102.3 100.5
  6)CC    6    -34.00   26.49  326.60   33.18  C2'-exo   107.1 103.7 102.4
  7)UC    7    -37.96   33.77  335.03   38.15  C2'-exo   104.2 103.4 102.3
  8)CC    8    -27.98   36.77    7.05   37.47  C3'-endo  105.9 104.0 101.6
  9)AC    9    -28.89   39.14   10.00   40.69  C3'-endo  106.1 102.1 101.0
 10)UC   10    -28.76   35.65  359.66   35.54  C2'-exo   104.7 103.8 104.6
 11)UC   11    -22.31   35.93   20.97   39.25  C3'-endo  107.0 103.9  99.5
 12)CC   12    -31.39   41.87   10.49   43.80  C3'-endo  104.7 103.8  98.4

  Torsions       Chi    Gamma   Delta   Epsil   Zeta    Alpha   Beta
                C1'-N  C5'-C4' C4'-C3' C3'-O3'  O3'-P   P-O5'  O5'-C5'

  1)CC    1   -157.99   94.62   78.02 -144.12  -72.49  -63.81  169.11
  2)AC    2   -157.42   53.31   82.27 -154.01  -83.98  -36.97  162.97
  3)CC    3   -156.50   41.71   80.14 -151.62  -68.01  134.95 -169.06
  4)AC    4    161.54 -168.02   95.97 -134.64  -79.55  -80.10  164.78
  5)CC    5   -147.89   72.40   78.87 -176.16  -68.16  123.62  171.24
  6)CC    6   -164.60 -134.02  110.03 -150.41  -64.41   49.58 -158.41
  7)UC    7   -162.04  -88.90   99.89 -149.29  -59.80  -59.71  164.15
  8)CC    8   -146.47   54.63   85.39 -150.99  -81.95  -54.72  170.77
  9)AC    9   -153.76   46.04   80.71 -148.70  -74.12  126.74 -157.96
 10)UC   10    176.69 -158.75   88.79 -147.99  -72.15  -81.70  173.53
 11)UC   11   -173.83   72.82   77.61 -165.58  -60.53  -61.53 -168.55
 12)CC   12   -148.92   44.02   81.67  ......  ......  ......  ......
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2nd strand		C1'-C2'	C2'-C3'	Phase	Ampli	Pucker	C1'	C2'	C3'
1)CD	12	31.58	-34.68	172.23	35.66	C2'-endo	106.2	102.2	103.2
2)TD	11	26.47	-8.42	104.80	34.86	O1'-endo	106.0	104.1	104.4
3)GD	10	37.88	-33.41	152.65	38.38	C2'-endo	105.0	101.7	103.7
4)TD	9	30.37	-12.06	109.71	37.33	C1'-exo	105.4	103.8	104.6
5)GD	8	32.98	-20.26	127.78	34.40	C1'-exo	106.2	103.3	104.0
6)GD	7	34.49	-16.05	114.95	39.83	C1'-exo	105.0	103.2	103.8
7)AD	6	28.24	-33.84	179.86	34.49	C2'-endo	106.5	102.7	103.2
8)CD	5	22.24	-2.10	93.72	36.03	O1'-endo	105.7	104.2	103.9
9)UD	4	37.05	-21.82	123.90	40.04	C1'-exo	103.7	102.2	104.8
10)AD	3	31.72	-35.82	174.52	36.63	C2'-endo	106.3	101.9	103.2
11)AD	2	-33.37	38.57	357.37	39.50	C2'-exo	106.4	101.2	102.2
12)GD	1	16.50	5.80	81.17	38.07	O1'-endo	105.8	104.3	103.5

Torsions		Chi C1'-N	Gamma C5'-C4'	Delta C4'-C3'	Epsil C3'-O3'	Zeta O3'-P	Alpha P-O5'	Beta O5'-C5'
1)CD	12	-101.41	60.02	146.28	.....	.....	.....	.....
2)TD	11	-128.07	-158.04	109.19	170.09	-90.28	-81.04	-148.58
3)GD	10	-107.44	52.55	135.63	-165.12	-90.55	105.28	-169.59
4)TD	9	-105.60	57.24	110.14	174.83	-91.08	-63.92	-166.61
5)GD	8	-148.29	-119.15	119.10	-147.74	-93.52	-72.29	165.24
6)GD	7	-142.64	74.65	109.11	-156.66	-96.81	78.75	-159.36
7)AD	6	-93.08	37.29	149.23	171.69	-96.07	-72.60	173.92
8)CD	5	-140.54	-170.47	99.16	-174.14	-81.56	-63.75	-161.28
9)UD	4	-123.94	65.42	116.40	-174.91	-83.72	125.72	-177.85
10)AD	3	-120.37	61.66	147.09	-174.27	-88.08	-88.39	-169.58
11)AD	2	-171.02	164.25	88.03	-156.26	-68.44	-53.20	-174.92
12)GD	1	-116.24	-134.24	85.03	142.68	-34.89	160.18	117.59

|K| Groove parameters

Atom defining backbone: P 12 levels, 3 sub-levels

Levels			Minor groove			Major groove			
	i	n	Width	Depth	Angle	Width	Depth	Angle	Diam
C	1	0	--	--	--	C --	--	--	--
	1	1	--	--	--	--	--	--	--
	1	2	--	--	--	--	--	--	--
	1	3	--	--	--	--	--	--	17.90
	1	4	--	--	--	--	--	--	18.35
A	2	0	--	--	--	A --	--	--	18.32
	2	1	--	--	--	--	--	--	18.29
	2	2	--	--	--	--	--	--	18.24
	2	3	9.18	1.50	66	--	--	--	18.40
C	3	0	8.71	1.57	63	C --	--	--	18.74
	3	1	8.32	1.90	61	--	--	--	18.93
	3	2	7.91	2.22	60	--	--	--	19.04
	3	3	7.62	2.60	53	14.96	1.91	63	19.00
	3	4	7.51	2.93	49	15.61	-0.63	65	18.85
	3	5	7.52	3.19	46	12.76*	6.37	42	18.69
A	4	0	7.70	3.43	44	A 12.05*	6.74	35	18.64
	4	1	8.09	3.48	41	11.43	7.64	22	18.69
	4	2	8.38	2.88	51	13.12	7.13	24	18.75
C	5	0	8.36	2.94	52	C 13.97	9.08	-5	18.88
	5	1	8.32	2.93	54	13.92	9.18	-7	19.11

	5	2	8.29	2.90	54		13.91	9.28	−6	19.28
	5	3	8.24	2.89	52		13.85	9.44	−10	19.38
	5	4	8.16	2.81	52		13.70	9.44	−11	19.44
C	6	0	8.04	2.89	49	C	13.57	9.41	−11	19.52
	6	1	7.90	3.02	50		13.24	9.41	−6	19.65
	6	2	7.72	3.11	52		12.93	9.51	−7	19.64
	6	3	7.53	3.23	49		12.65	9.54	7	19.39
U	7	0	7.58	3.15	48	U	11.48	8.92	14	19.02
	7	1	7.83	3.15	45		10.69	8.98	16	18.68
	7	2	8.20	3.04	43		10.33	8.91	20	18.47
	7	3	8.52	2.66	49		10.27	9.12	23	18.37
C	8	0	8.73	2.37	51	C	10.54	8.93	29	18.34
	8	1	9.12	1.95	51		11.82	8.53	38	18.52
	8	2	9.24	1.61	61		13.02	3.79	61	18.87
A	9	0	8.78	1.86	59	A	13.54	1.21	68	19.26
	9	1	8.42	2.02	60		13.74	−1.24	74	19.50
	9	2	8.02	2.20	55		--	--	--	19.72
	9	3	7.71	2.40	51		--	--	--	19.64
	9	4	7.60	2.61	48		--	--	--	18.83
U	10	0	7.63	2.88	43	U	--	--	--	18.16
	10	1	7.61	3.04	39		--	--	--	18.08
	10	2	--	--	--		--	--	--	18.15
	10	3	--	--	--		--	--	--	18.34
U	11	0	--	--	--	U	--	--	--	18.63
	11	1	--	--	--		--	--	--	18.98
	11	2	--	--	--		--	--	--	--
	11	3	--	--	--		--	--	--	--
	11	4	--	--	--		--	--	--	--
C	12	0	--	--	--	C	--	--	--	--

Table S6. Curves output for RNA:DNA duplex.[1]

```
 ************************************        *************
 ****** CURVES 5.3 R.L. 1998 *****          * 24 Jun 16 *
 ************************************        *************

FILE : 1zbi_.pdb                          LIS  : ref
dna  :                                    axin :
axout:                                    daf  :
PDB  : ref

acc  :    0.000  wid  :    0.750

maxn :   500  ior  :     0  ibond:     0  splin:     3  break:    -1
nleve:     3  nbac :     7

ends :     F  supp :     T  COMB :     T  DINU :     T  mini :     T
rest :     F  line :     F  zaxe :     F  FIT  :     T  test :     F
GRV  :     T  old  :     T  axonl:     F

Least squares fitting of standard bases ...

 Str   Pos  Base          Rms (ang)

  1 :   1)  GC     1      0.026
  1 :   2)  AC     2      0.036
  1 :   3)  CC     3      0.013
  1 :   4)  AC     4      0.021
  1 :   5)  CC     5      0.008
  1 :   6)  CC     6      0.029
  1 :   7)  UC     7      0.021
  1 :   8)  GC     8      0.035
  1 :   9)  AC     9      0.018
  1 :  10)  UC    10      0.012
  1 :  11)  UC    11      0.021
  1 :  12)  CC    12      0.031
  2 :   1)  CD    24      0.024
  2 :   2)  TD    23      0.052
  2 :   3)  GD    22      0.022
  2 :   4)  TD    21      0.023
  2 :   5)  GD    20      0.064
  2 :   6)  GD    19      0.032
  2 :   7)  AD    18      0.041
  2 :   8)  CD    17      0.013
  2 :   9)  TD    16      0.026
  2 :  10)  AD    15      0.039
  2 :  11)  AD    14      0.060
  2 :  12)  GD    13      0.055

Strand=    2 Nucleo=   24 Atoms =  495 Units =   24

Input   1) Xdisp=    0.00 Ydisp=    0.00 Inclin=    0.00 Tip=    0.00

Combined strands have   12 levels ...

Strand  1 has  12 bases (5'-3'): GACACCUGAUUC
Strand  2 has  12 bases (3'-5'): CTGTGGACTAAG

FIRST SUM=  139.564 CPTS:    3.301   0.678   3.678 131.908
```

```
MINIMISATION: ACC =  0.100E-05 MAXN=  500 NVAR=   48

STEP    1 SUM=  139.564 DEL=  0.000E+00
STEP    2 SUM=  116.267 DEL= -0.233E+02
STEP    3 SUM=   82.196 DEL= -0.341E+02
STEP    4 SUM=   63.692 DEL= -0.185E+02
STEP    5 SUM=   51.697 DEL= -0.120E+02
STEP    6 SUM=   40.792 DEL= -0.109E+02
STEP    7 SUM=   40.532 DEL= -0.260E+00
STEP    8 SUM=   35.274 DEL= -0.526E+01
STEP    9 SUM=   29.759 DEL= -0.552E+01
STEP   10 SUM=   24.950 DEL= -0.481E+01
STEP   11 SUM=   29.593 DEL=  0.464E+01
STEP   12 SUM=   23.328 DEL= -0.626E+01
STEP   13 SUM=   21.123 DEL= -0.221E+01
STEP   14 SUM=   17.336 DEL= -0.379E+01
STEP   15 SUM=   13.296 DEL= -0.404E+01
STEP   16 SUM=   49.511 DEL=  0.362E+02
STEP   17 SUM=   12.115 DEL= -0.374E+02
STEP   18 SUM=   22.174 DEL=  0.101E+02
STEP   19 SUM=   12.003 DEL= -0.102E+02
STEP   20 SUM=   11.812 DEL= -0.191E+00
STEP   21 SUM=   11.619 DEL= -0.193E+00
STEP   22 SUM=   11.623 DEL=  0.396E-02
STEP   23 SUM=   11.428 DEL= -0.195E+00
STEP   24 SUM=   11.485 DEL=  0.571E-01
STEP   25 SUM=   11.344 DEL= -0.140E+00
STEP   26 SUM=   11.232 DEL= -0.113E+00
STEP   27 SUM=   11.082 DEL= -0.149E+00
STEP   28 SUM=   11.758 DEL=  0.675E+00
STEP   29 SUM=   11.059 DEL= -0.698E+00
STEP   30 SUM=   11.017 DEL= -0.420E-01
STEP   31 SUM=   10.921 DEL= -0.961E-01
STEP   32 SUM=   10.756 DEL= -0.165E+00
STEP   33 SUM=   11.208 DEL=  0.453E+00
STEP   34 SUM=   10.721 DEL= -0.488E+00
STEP   35 SUM=   10.661 DEL= -0.601E-01
STEP   36 SUM=   10.595 DEL= -0.653E-01
STEP   37 SUM=   10.664 DEL=  0.683E-01
STEP   38 SUM=   10.546 DEL= -0.118E+00
STEP   39 SUM=   10.510 DEL= -0.365E-01
STEP   40 SUM=   10.447 DEL= -0.623E-01
STEP   41 SUM=   10.386 DEL= -0.615E-01
STEP   42 SUM=   10.354 DEL= -0.321E-01
STEP   43 SUM=   10.306 DEL= -0.476E-01
STEP   44 SUM=   10.220 DEL= -0.859E-01
STEP   45 SUM=   10.061 DEL= -0.159E+00
STEP   46 SUM=   10.148 DEL=  0.868E-01
STEP   47 SUM=    9.956 DEL= -0.191E+00
STEP   48 SUM=    9.966 DEL=  0.100E-01
STEP   49 SUM=    9.917 DEL= -0.491E-01
STEP   50 SUM=    9.923 DEL=  0.607E-02
STEP   51 SUM=    9.910 DEL= -0.132E-01
STEP   52 SUM=    9.914 DEL=  0.339E-02
STEP   53 SUM=    9.908 DEL= -0.536E-02
STEP   54 SUM=    9.908 DEL= -0.273E-03
STEP   55 SUM=    9.907 DEL= -0.782E-03
STEP   56 SUM=    9.907 DEL=  0.152E-03
STEP   57 SUM=    9.907 DEL= -0.644E-03
STEP   58 SUM=    9.906 DEL= -0.292E-03
```

```
STEP   59 SUM=    9.906 DEL= -0.149E-03
STEP   60 SUM=    9.906 DEL= -0.741E-04
STEP   61 SUM=    9.906 DEL= -0.848E-04
STEP   62 SUM=    9.906 DEL= -0.663E-04
STEP   63 SUM=    9.906 DEL= -0.418E-04
STEP   64 SUM=    9.906 DEL= -0.242E-04
STEP   65 SUM=    9.906 DEL=  0.874E-06
STEP   66 SUM=    9.906 DEL= -0.897E-05
STEP   67 SUM=    9.906 DEL= -0.857E-06
STEP   68 SUM=    9.906 DEL= -0.596E-06
STEP   69 SUM=    9.906 DEL= -0.513E-07
STEP   70 SUM=    9.906 DEL= -0.756E-07
STEP   71 SUM=    9.906 DEL= -0.259E-07
STEP   72 SUM=    9.906 DEL= -0.323E-08
STEP   73 SUM=    9.906 DEL= -0.539E-09
STEP   74 SUM=    9.906 DEL= -0.593E-10
STEP   75 SUM=    9.906 DEL= -0.231E-10
STEP   76 SUM=    9.906 DEL= -0.373E-12
STEP   77 SUM=    9.906 DEL= -0.177E-11
STEP   78 SUM=    9.906 DEL= -0.240E-12
STEP   79 SUM=    9.906 DEL= -0.110E-12
STEP   80 SUM=    9.906 DEL= -0.178E-14
STEP   81 SUM=    9.906 DEL=  0.000E+00

FINAL SUM=    9.906 CPTS:    2.123   3.907   1.521   2.355

GRA= 0.84E-09-0.34E-08 0.25E-08-0.13E-08-0.27E-08 0.27E-08-0.45E-08 0.28E-08
GRA= 0.45E-08 0.99E-10 0.14E-08 0.47E-09 0.52E-09-0.51E-08-0.27E-08 0.15E-08
GRA=-0.20E-08-0.13E-08 0.36E-08-0.59E-09 0.26E-08-0.56E-09 0.96E-09-0.68E-09
GRA= 0.40E-09 0.15E-08 0.97E-09-0.26E-08-0.30E-08-0.93E-09-0.30E-08-0.27E-08
GRA= 0.81E-08-0.14E-08 0.11E-08-0.70E-09-0.93E-09 0.84E-09-0.13E-08-0.23E-09
GRA=-0.13E-08 0.88E-09 0.18E-09 0.88E-09 0.24E-10 0.44E-09 0.12E-08 0.19E-08

-----------------------------
|A| Global axis parameters |
-----------------------------

  1) U:    0.015  -0.988  -0.155  P:   24.719  19.210  67.346  D:    0.377
  2) U:    0.006  -0.993  -0.116  P:   24.575  15.702  67.075  D:    1.139
  3) U:    0.069  -0.997  -0.033  P:   24.283  13.274  66.750  D:    1.079
  4) U:    0.109  -0.994   0.011  P:   24.634  10.033  66.917  D:    1.195
  5) U:    0.143  -0.989  -0.029  P:   25.172   6.768  67.277  D:    1.382
  6) U:    0.149  -0.988  -0.035  P:   26.080   3.404  67.689  D:    0.697
  7) U:    0.065  -0.995  -0.071  P:   26.423   0.143  67.454  D:    1.538
  8) U:   -0.119  -0.990  -0.072  P:   26.641  -2.398  67.215  D:    0.864
  9) U:   -0.211  -0.973  -0.090  P:   25.982  -5.703  67.143  D:    0.723
 10) U:   -0.170  -0.982  -0.087  P:   25.116  -8.906  66.939  D:    0.625
 11) U:   -0.167  -0.977  -0.133  P:   24.476 -11.757  66.531  D:    0.286
 12) U:   -0.151  -0.974  -0.170  P:   24.167 -14.992  66.088

---------------------------------
|B| Global Base-Axis Parameters |
---------------------------------

  1st strand      Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) GC    1      -4.21     0.29     8.36   -12.04   1   0
  2) AC    2      -3.55     0.49     2.00   -15.45   2  21
  3) CC    3      -4.41     0.57     1.08   -13.82   3 -16
  4) AC    4      -3.96     0.05    -2.41   -10.04   2  29
```

```
  5) CC    5      -4.14     0.70    -3.35    -9.45   3  -6
  6) CC    6      -4.11    -0.16     1.42   -12.03   3  -3
  7) UC    7      -3.92     0.58    -3.24   -10.50   4 -25
  8) GC    8      -4.43     0.27    -1.01   -11.26   1  12
  9) AC    9      -3.97    -0.06    -7.76    -9.79   2  22
 10) UC   10      -4.52     0.22    -7.64    -7.46   4 -24
 11) UC   11      -3.96    -0.48     0.56   -10.29   4 -18
 12) CC   12      -4.22     0.30    -5.21    -9.37   3   0

  2nd strand      Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) CD   24      -4.33    -0.45     6.37     1.76   3   0
  2) TD   23      -3.67    -0.07    14.14     2.18   4 -21
  3) GD   22      -4.58    -0.52     6.72     1.61   1  16
  4) TD   21      -3.99    -0.10    11.95     6.85   4 -29
  5) GD   20      -4.27    -0.49     0.88     9.30   1   6
  6) GD   19      -4.16     0.26     4.14     3.95   1   3
  7) AD   18      -3.97    -0.05     4.06     6.65   2  25
  8) CD   17      -4.44    -0.13     5.05     1.79   3 -12
  9) TD   16      -4.05     0.03    12.15     2.63   4 -22
 10) AD   15      -4.38    -0.35     7.95     7.36   2  24
 11) AD   14      -3.86     0.32     7.16     1.99   2  18
 12) GD   13      -4.43    -0.61    10.79     4.92   1   0

---------------------------------------
|C| Global Base pair-Axis Parameters |
---------------------------------------

  Strand 1 with strand 2 ...

  Duplex          Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) G  1-C 24    -4.27     0.37     7.37    -6.90   1   0
  2) A  2-T 23    -3.61     0.28     8.07    -8.81   2  21
  3) C  3-G 22    -4.49     0.54     3.90    -7.72   3 -16
  4) A  4-T 21    -3.97     0.08     4.77    -8.45   2  29
  5) C  5-G 20    -4.21     0.59    -1.23    -9.37   3  -6
  6) C  6-G 19    -4.14    -0.21     2.78    -7.99   3  -3
  7) U  7-A 18    -3.95     0.31     0.41    -8.58   4 -25
  8) G  8-C 17    -4.44     0.20     2.02    -6.52   1  12
  9) A  9-T 16    -4.01    -0.05     2.19    -6.21   2  22
 10) U 10-A 15    -4.45     0.28     0.15    -7.41   4 -24
 11) U 11-A 14    -3.91    -0.40     3.86    -6.14   4 -18
 12) C 12-G 13    -4.33     0.45     2.79    -7.14   3   0

  Average:        -4.15     0.20     3.09    -7.60

---------------------------------
|D| Global Base-Base Parameters |
---------------------------------

  Strand 1 with strand 2 ...

  Duplex          Shear    Stretch  Stagger  Buckle   Propel  Opening  Bc  Tc
                  (Sx)      (Sy)     (Sz)    (kappa)  (omega) (sigma)

  1) G  1-C 24     0.12    -0.16    -0.03     1.99   -10.28    -2.18   1   0
  2) A  2-T 23     0.12     0.42    -0.39   -12.14   -13.27     6.46   2  21
  3) C  3-G 22     0.17     0.06    -0.03    -5.64   -12.21     0.29   3 -16
```

```
  4) A  4-T 21     0.03    -0.04    -0.24   -14.36    -3.19    -1.38   2  29
  5) C  5-G 20     0.14     0.22    -0.01    -4.24    -0.15     2.09   3  -6
  6) C  6-G 19     0.05     0.11    -0.27    -2.72    -8.08     0.90   3  -3
  7) U  7-A 18     0.06     0.53     0.04    -7.30    -3.84     8.82   4 -25
  8) G  8-C 17     0.01     0.14    -0.33    -6.06    -9.47     1.28   1  12
  9) A  9-T 16     0.08    -0.02    -0.39   -19.91    -7.15    -1.84   2  22
 10) U 10-A 15    -0.14    -0.13     0.12   -15.59    -0.10     0.38   4 -24
 11) U 11-A 14    -0.11    -0.16     0.01    -6.60    -8.31     0.02   4 -18
 12) C 12-G 13     0.21    -0.31     0.11   -16.00    -4.45    -2.60   3   0

  Average:         0.06     0.05    -0.12    -9.05    -6.71     1.02

-----------------------------------
|E| Global Inter-Base Parameters |
-----------------------------------

  1st strand      Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) G  1/A  2     0.50     0.42     3.33    -8.63    -3.69    41.38   2
  3) A  2/C  3    -1.25     0.21     2.61    -2.36     7.44    26.92  -6
  4) C  3/A  4     0.66    -0.50     3.15    -2.30     6.98    26.44   9
  5) A  4/C  5     0.19     0.47     3.42     0.67    -1.98    34.56  -6
  6) C  5/C  6     0.22    -1.49     3.32     4.89    -3.05    19.38  -1
  7) C  6/U  7     0.18     0.79     3.44    -8.70     4.87    40.46  -3
  8) U  7/G  8    -0.80    -0.23     2.37     2.77     9.81    21.95  -9
  9) G  8/A  9     0.45    -0.55     3.34    -5.08     6.66    25.65   2
 10) A  9/U 10    -0.49     0.03     3.57    -1.80     0.85    31.16   7
 11) U 10/U 11     0.65    -0.84     2.89     7.86    -0.16    23.11  -4
 12) U 11/C 12    -0.21     0.99     3.33    -5.65     3.23    38.46  -2

  2nd strand      Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) C 24/T 23     0.50     0.16     3.69     5.50     0.70    32.74  -2
  3) T 23/G 22    -1.30    -0.58     2.26    -8.86    -6.39    33.10   6
  4) G 22/T 21     0.80     0.40     3.36     6.42     2.05    28.10  -9
  5) T 21/G 20     0.08    -0.21     3.19    -9.45     5.02    31.09   6
  6) G 20/G 19     0.31     1.38     3.57     3.38    -4.88    20.56   1
  7) G 19/A 18     0.17    -0.37     3.14    -4.12    -0.64    32.54   3
  8) A 18/C 17    -0.75    -0.15     2.74     1.53   -15.44    29.50   9
  9) C 17/T 16     0.38     0.39     3.40     8.77    -4.34    28.76  -2
 10) T 16/A 15    -0.27    -0.13     3.06    -6.12     6.20    28.93   7
 11) A 15/A 14     0.62     0.81     3.01    -1.13    -8.05    23.47   4
 12) A 14/G 13    -0.53    -1.15     3.22     3.75     0.62    41.09   2

----------------------------------------
|F| Global Inter-Base pair Parameters |
----------------------------------------

  Strand 1 with strand 2 ...

  Duplex          Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) G  1/A  2     0.50     0.13     3.51    -1.56    -2.19    37.06   2
  3) A  2/C  3    -1.27     0.40     2.44    -5.61     6.92    30.01  -6
  4) C  3/A  4     0.73    -0.45     3.26     2.06     2.47    27.27   9
  5) A  4/C  5     0.14     0.34     3.30    -4.39    -3.50    32.82  -6
  6) C  5/C  6     0.27    -1.43     3.45     4.14     0.91    19.97  -1
  7) C  6/U  7     0.17     0.58     3.29    -6.41     2.76    36.50  -3
```

```
  8) U  7/G  8    -0.77    -0.04     2.56     2.15    12.63    25.72  -9
  9) G  8/A  9     0.42    -0.47     3.37     1.84     5.50    27.21   2
 10) A  9/U 10    -0.38     0.08     3.32    -3.96    -2.67    30.05   7
 11) U 10/U 11     0.63    -0.82     2.95     3.37     3.94    23.29  -4
 12) U 11/C 12    -0.37     1.07     3.27    -0.95     1.31    39.78  -2

  Average:         0.01    -0.06     3.15    -0.85     2.55    29.97
```

```
----------------------------------
|G| Local Inter-Base Parameters |
----------------------------------
```

```
  1st strand      Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) G  1/A  2     1.03    -2.01     3.36     1.60     0.24    42.07   2
  3) A  2/C  3    -0.68    -1.56     3.32     4.63     8.15    26.48  -6
  4) C  3/A  4     1.19    -2.46     3.17     3.26     6.58    26.40   9
  5) A  4/C  5     0.50    -2.12     3.11     6.43    -3.72    33.80  -6
  6) C  5/C  6     0.70    -2.91     3.18     8.34    -3.33    18.17  -1
  7) C  6/U  7     0.74    -2.11     3.55    -0.35     4.32    41.41  -3
  8) U  7/G  8    -0.39    -1.91     3.19     7.34     8.96    21.34  -9
  9) G  8/A  9     1.04    -2.68     3.37    -0.14     4.66    26.45   2
 10) A  9/U 10    -0.06    -2.71     3.17     2.77    -3.35    30.60   7
 11) U 10/U 11     1.09    -2.69     2.82    11.18    -1.51    21.84  -4
 12) U 11/C 12     0.47    -1.89     3.38     1.18     1.65    38.91  -2

  2nd strand      Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) C 24/T 23     0.38    -1.73     4.02     6.30     5.02    32.13  -2
  3) T 23/G 22    -1.27    -1.31     3.02    -7.76    12.12    31.94   6
  4) G 22/T 21     0.88    -1.83     3.93     8.26     2.57    26.70  -9
  5) T 21/G 20     0.45    -1.66     3.20    -4.61    -1.47    32.21   6
  6) G 20/G 19     0.67    -2.74     3.60     5.69     5.68    20.08   1
  7) G 19/A 18     0.53    -1.66     3.46    -1.30     2.86    32.47   3
  8) A 18/C 17    -0.52    -1.77     3.70     3.17    17.58    28.60   9
  9) C 17/T 16     0.45    -1.91     4.11     9.65     8.54    27.42  -2
 10) T 16/A 15    -0.04    -1.42     3.27    -3.49    -1.02    29.18   7
 11) A 15/A 14     0.88    -2.07     3.42     0.75    10.98    23.02   4
 12) A 14/G 13    -0.42    -1.27     3.66     5.92     5.80    39.98   2
```

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|H| Local Inter-Base pair Parameters |
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```
  Strand 1 with strand 2 ...

  Duplex          Shift    Slide     Rise     Tilt     Roll    Twist   Dc
                  (Dx)     (Dy)     (Dz)     (tau)    (rho)  (Omega)

  2) G  1/A  2     0.73    -1.87     3.70     4.03     2.56    37.35   2
  3) A  2/C  3    -0.99    -1.41     3.19    -1.47    10.43    29.42  -6
  4) C  3/A  4     1.05    -2.17     3.56     5.75     4.54    26.32   9
  5) A  4/C  5     0.47    -1.89     3.16     0.93    -2.52    32.95  -6
  6) C  5/C  6     0.69    -2.83     3.39     7.09     1.19    19.24  -1
  7) C  6/U  7     0.64    -1.87     3.51    -0.86     3.62    36.94  -3
  8) U  7/G  8    -0.44    -1.85     3.44     5.49    13.35    25.18  -9
  9) G  8/A  9     0.76    -2.32     3.77     4.78     6.56    27.02   2
 10) A  9/U 10    -0.05    -2.05     3.28    -0.35    -2.17    29.72   7
 11) U 10/U 11     0.99    -2.40     3.13     6.05     4.79    22.89  -4
```

```
 12) U 11/C 12     0.02    -1.59     3.55     3.56     3.72    39.51  -2

  Average:         0.35    -2.02     3.43     3.18     4.19    29.68

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|I| Global Axis Curvature |
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  Duplex          Ax      Ay     Ainc    Atip    Adis    Angle   Path   Dc

 2) G  1/A  2   -0.16    0.22   -2.27   -0.28    0.28    2.28    3.52   2
 3) A  2/C  3   -0.39    0.13   -1.44    5.82    0.41    5.99    2.47  -6
 4) C  3/A  4    0.21    0.02    1.19    3.20    0.21    3.41    3.26   9
 5) A  4/C  5    0.37   -0.18    1.62   -2.58    0.41    3.04    3.33  -6
 6) C  5/C  6    0.20   -0.63    0.12   -0.47    0.66    0.48    3.51  -1
 7) C  6/U  7   -0.02    0.06   -4.04    3.34    0.06    5.24    3.29  -3
 8) U  7/G  8   -0.28    0.07    0.55   10.58    0.29   10.59    2.56  -9
 9) G  8/A  9   -0.01   -0.23    1.67    5.18    0.23    5.45    3.37   2
10) A  9/U 10    0.05   -0.25   -1.91   -1.47    0.25    2.42    3.32   7
11) U 10/U 11    0.10   -0.14   -0.34    2.68    0.17    2.70    2.95  -4
12) U 11/C 12    0.05    0.22    0.12    2.31    0.22    2.31    3.28  -2

Overall axis bend ... UU=    9.58 PP=    4.56


  Duplex       Offset   L.Dir  ... wrt end-to-end vector

 1) G  1         0.00    0.00
 2) A  2         0.17   31.05
 3) C  3         0.51   -6.57
 4) A  4         0.11   43.64
 5) C  5         0.76   95.10
 6) C  6         1.86   74.72
 7) U  7         2.17   26.81
 8) G  8         2.36   -0.45
 9) A  9         1.81  -19.32
10) U 10         1.06  -37.40
11) U 11         0.41  -45.60
12) C 12         0.00    0.00

  Path length=    34.86  End-to-end=    34.23  Shortening=     1.82 %

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|J| Backbone Parameters |
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  1st strand   C1'-C2' C2'-C3'  Phase   Ampli   Pucker    C1'   C2'   C3'

  1)GC    1    -27.67   39.58   12.89   41.37  C3'-endo  106.6 101.3 101.5
  2)AC    2    -27.76   38.83   11.35   40.37  C3'-endo  106.9 101.1 102.0
  3)CC    3    -25.13   37.89   16.16   40.19  C3'-endo  107.2 101.2 102.0
  4)AC    4    -31.98   40.85    4.97   41.84  C3'-endo  106.0 100.9 101.3
  5)CC    5    -26.94   41.11   16.28   43.47  C3'-endo  106.7 100.6 101.8
  6)CC    6    -26.52   36.77   10.57   38.11  C3'-endo  107.3 101.4 102.8
  7)UC    7    -27.86   40.38   13.28   42.18  C3'-endo  107.0 100.6 101.9
  8)GC    8    -22.27   39.13   24.23   43.66  C3'-endo  107.6 100.8 101.2
  9)AC    9    -32.55   40.80    3.42   41.72  C3'-endo  106.2 100.5 101.4
 10)UC   10    -26.57   41.55   18.29   44.58  C3'-endo  106.8 100.5 100.7
 11)UC   11    -20.74   37.26   25.08   41.78  C3'-endo  107.3 101.6 101.8
 12)CC   12    -25.68   40.53   18.63   43.48  C3'-endo  106.9 100.9 101.2
```

```
 Torsions       Chi    Gamma   Delta   Epsil   Zeta    Alpha   Beta
              C1'-N  C5'-C4' C4'-C3' C3'-O3'  O3'-P   P-O5'  O5'-C5'

 1)GC    1   -171.80   44.77   82.44 -156.12  -64.37  -67.08 -177.07
 2)AC    2   -159.24   52.67   84.65 -152.65  -75.61  -61.65  176.33
 3)CC    3   -152.85   44.92   81.09 -166.58  -61.47  152.36 -170.82
 4)AC    4   -177.16 -179.43   83.99 -138.54  -77.94  -56.04  161.90
 5)CC    5   -163.69   50.51   78.31 -144.11  -53.36 -122.01  134.70
 6)CC    6   -175.51  147.99   84.60 -141.45  -70.13  -61.94 -179.29
 7)UC    7   -157.05   42.39   79.59 -151.47  -72.92  -58.29  173.79
 8)GC    8   -151.75   46.77   78.59 -176.22  -62.37  155.05 -172.82
 9)AC    9    179.51 -178.88   84.42 -141.96  -69.91  -59.58  174.73
10)UC   10   -165.67   46.99   75.69 -148.28  -55.23 -109.58  149.99
11)UC   11   -176.53  127.58   79.59 -140.64  -80.84  -60.82  166.71
12)CC   12   -162.15   51.44   74.50  ......  ......  ......  ......


 2nd strand   C1'-C2' C2'-C3'  Phase   Ampli   Pucker    C1'   C2'   C3'

 1)CD   24     34.30  -33.65  162.46   35.98  C2'-endo  105.2 102.7 102.8
 2)TD   23     31.29  -15.87  117.33   35.46  C1'-exo   104.4 104.5 104.5
 3)GD   22     39.23  -32.87  148.99   39.38  C2'-endo  104.6 101.4 103.0
 4)TD   21     33.27  -27.31  146.70   33.43  C2'-endo  105.3 103.0 104.2
 5)GD   20     37.70  -24.25  130.16   38.86  C1'-exo   104.3 103.0 103.4
 6)GD   19     35.10  -32.97  158.92   36.17  C2'-endo  105.7 102.2 103.3
 7)AD   18     29.78  -14.69  116.09   34.16  C1'-exo   104.4 105.1 104.6
 8)CD   17     36.49  -28.54  143.22   36.57  C1'-exo   104.7 102.6 103.6
 9)TD   16     33.91  -23.82  135.20   34.49  C1'-exo   105.1 103.3 104.3
10)AD   15     33.43  -26.27  143.58   33.45  C1'-exo   105.4 103.4 104.1
11)AD   14     28.53  -25.49  154.14   28.93  C2'-endo  106.5 104.0 104.6
12)GD   13     33.53  -30.50  156.38   34.13  C2'-endo  106.1 102.8 103.6

 Torsions       Chi    Gamma   Delta   Epsil   Zeta    Alpha   Beta
              C1'-N  C5'-C4' C4'-C3' C3'-O3'  O3'-P   P-O5'  O5'-C5'

 1)CD   24   -120.74   44.08  142.23  ......  ......  ......  ......
 2)TD   23   -137.01 -166.85  115.24 -177.53  -93.43  -54.23 -168.24
 3)GD   22   -122.07   45.46  136.00 -169.88  -90.67  120.39 -173.08
 4)TD   21   -120.47   48.90  133.79 -176.51 -101.96  -57.77 -173.74
 5)GD   20   -129.05   36.95  121.74 -176.62 -113.96  -51.80 -179.27
 6)GD   19   -116.89   45.07  139.81  179.63  -91.12  -64.42 -167.02
 7)AD   18   -148.10 -161.58  116.30 -170.03  -92.34  -66.08 -167.15
 8)CD   17   -125.73   44.08  129.94 -164.58  -89.54  114.51 -176.74
 9)TD   16   -120.98   44.34  125.44 -176.58  -95.52  -57.36 -172.63
10)AD   15   -121.48   37.38  130.66 -178.94 -105.29  -45.44  175.80
11)AD   14   -125.34   42.22  138.46  179.91  -94.61  -58.72 -164.48
12)GD   13   -120.17   41.61  139.95  175.50 -102.56  -60.88 -165.83


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|K| Groove parameters |
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Atom defining backbone: P      12 levels,  3 sub-levels

 Levels          Minor groove                Major groove
   i  n      Width    Depth  Angle       Width    Depth  Angle    Diam

G  1  0       --       --     --    G     --       --     --       --
   1  1       --       --     --          --       --     --       --
   1  2       --       --     --          --       --     --       --
```

	1	3	--	--	--		--	--	--	--
A	2	0	--	--	--	A	--	--	--	--
	2	1	--	--	--		--	--	--	--
	2	2	9.28	1.75	43		--	--	--	--
C	3	0	8.78	1.68	39	C	--	--	--	19.63
	3	1	8.32	2.07	39		--	--	--	20.11
	3	2	7.97	2.48	35		13.66	3.57	77	20.44
	3	3	7.81	2.77	34		14.66*	3.22	75	20.90
A	4	0	7.87	3.04	29	A	16.28	0.91	78	21.34
	4	1	8.10	3.16	23		13.86	6.54	56	21.57
	4	2	8.27	2.93	25		15.55	7.10	49	21.64
	4	3	8.25	2.74	27		17.09	2.75	69	21.64
C	5	0	8.17	2.36	29	C	18.02*	3.75	64	21.58
	5	1	8.17	2.10	34		12.38	9.62	15	21.53
	5	2	8.21	2.06	35		12.32	9.77	12	21.46
	5	3	8.21	2.12	37		12.39	9.97	12	21.42
C	6	0	8.19	2.31	37	C	12.53	10.21	11	21.46
	6	1	8.20	2.42	41		12.98	10.57	14	21.61
	6	2	8.34	2.48	41		12.96	10.66	26	21.76
	6	3	8.73	2.35	40		12.71	10.74	33	21.84
U	7	0	9.18	2.12	40	U	12.16	10.71	36	21.88
	7	1	9.48	1.67	43		11.57	11.00	35	21.83
	7	2	9.26	1.65	43		11.03	11.26	31	21.37
G	8	0	8.69	1.76	43	G	--	--	--	21.31
	8	1	8.18	2.14	42		--	--	--	21.33
	8	2	7.79	2.55	37		--	--	--	21.37
	8	3	7.66	2.72	38		--	--	--	21.40
A	9	0	7.82	2.95	34	A	--	--	--	21.34
	9	1	8.15	2.89	29		--	--	--	21.23
	9	2	8.44	2.66	28		--	--	--	21.06
	9	3	8.55	2.36	29		--	--	--	20.82
U	10	0	8.65	2.09	29	U	--	--	--	20.51
	10	1	--	--	--		--	--	--	20.22
	10	2	--	--	--		--	--	--	--
U	11	0	--	--	--	U	--	--	--	--
	11	1	--	--	--		--	--	--	--
	11	2	--	--	--		--	--	--	--
	11	3	--	--	--		--	--	--	--
C	12	0	--	--	--	C	--	--	--	--

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