STRUCTURAL STUDIES OF SYNTHETIC BASE ANALOGS IN OLIGODEOXYNUCLEOTIDES

By

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To my amazing daughter Liliana

and

To my beloved husband Michał

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CHAPTER I

INTRODUCTION

Structure and Stability of DNA molecule

In 1953 James D. Watson and Francis Crick proposed what is now the first correct structure of double-helix DNA (*1*). It was based on the single fiber diffraction image of DNA taken by Raymond Gosling while working as a graduate student under the supervision of Rosalind Franklin in 1952. It was published in the same issue of *Nature* as the first publication of this more clarified X-ray image of DNA (*2*). In 1962, after Franklin's death, Watson, Crick, and Wilkins jointly received the Nobel Prize in Physiology or Medicine *"for their discoveries concerning the molecular structure of nucleic acids and its significance for information transfer in living material"* (*3*).

Deoxyribonucleic acid (DNA) is a linear polymer built up from nucleotides. A DNA molecule has two strands that wind around a central axis and form a right-handed helix. The two strands of DNA are antiparallel. Each nucleotide (monomer unit) has a deoxyribose – the sugar, phosphate and heterocyclic base. The sugar is connected by a *β*–glycosyl bond to one of the four bases: adenine (A), cytosine (C), guanine (G) and thymine (T) (*4*) (Figure 1). The sequence in which nucleotides are connected in DNA constitutes a form of genetic information that can be efficiently decoded and copied. Adenine and guanine are purines, and cytosine and thymine are pyrimidines. The linkage between nucleotides is a phosphodiester bond. The terminal residue whose C5′ is not connected to another nucleotide is called the 5′ end, and the terminal residue whose C3′ is

not connected to another nucleotide is called the 3′ end (Figure 2a). The surface of the double helix has major and minor grooves (Figure 2b). There are three most common forms of DNA: A, B and Z form. The A and B forms are right-handed helices while the Z form is a left-handed helix (*5*). A-DNA is similar to B-DNA but there is a slight increase in the number of base pairs per rotation (resulting in a tighter rotation angle), and smaller rise/turn. B form DNA is most common in vitro under physiological conditions. Z-form DNA has a structure that repeats every two base pairs. Certain conditions can promote Z form DNA, such as an alternating sequence poly(dGC)$_2$, and high salt concentration (*6*). Two DNA strands interact by forming hydrogen bonds. Each base is hydrogen bonded to a base in the opposite strand to form a planar base pair. In B-form DNA there are two types of base pairs: C:G and A:T, called Watson-Crick base pairs (Figure 3). Two components are largely responsible for the stability of the DNA molecule: hydrogen bonding between bases and stacking interactions. Base stacking is a major stabilizing factor in double-helix DNA. Base-stacking contributes to the dependence of the duplex stability on its sequence (*7*).

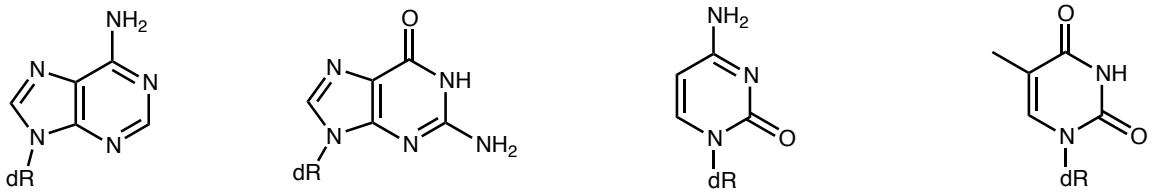


Figure 1. Chemical structures of DNA bases.

(a) (b)

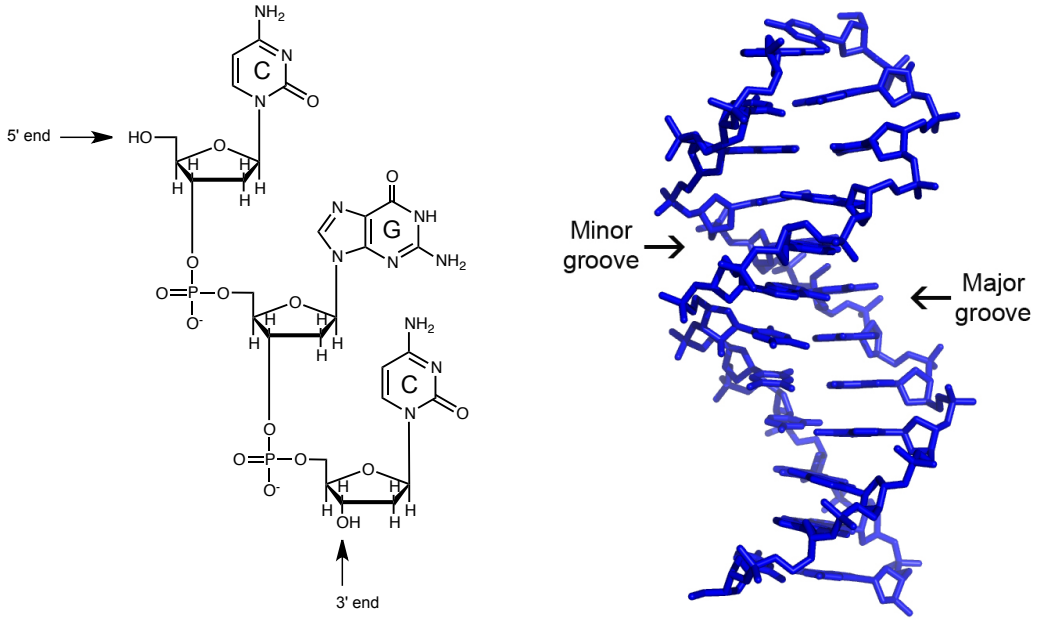


Figure 2. (a) Polynucleotide 5′-CGC-3′ sequence showing bases connected to sugars by *β*–glycosyl bonds and phosphodiester bonds between sugars. (b) B-form DNA structure with major and minor grooves shown, PDB code 436D.

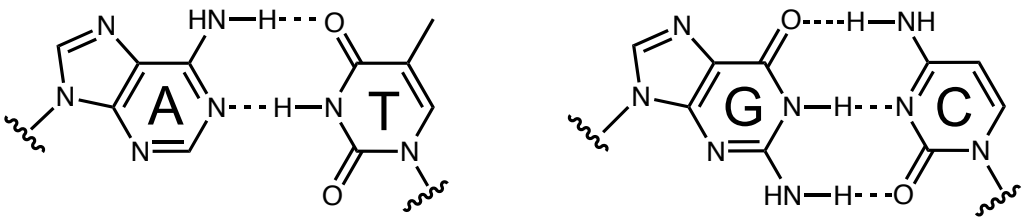


Figure 3. Watson-Crick base pairing (a) A:T base pair has two hydrogen bonds (b) G:C base pair has three hydrogen bonds.

Structure of Dickerson-Drew Dodecamer Duplex

In 1980 the first single-crystal structure of B-form DNA was reported by Dickerson et al. (*8*) The sequence used in the crystallization was the self-complementary [5′-$C^1G^2C^3G^4A^5A^6T^7T^8C^9G^{10}C^{11}G^{12}$-3′]•[5′-$C^{13}G^{14}C^{15}G^{16}A^{17}A^{18}T^{19}T^{20}C^{21}G^{22}C^{23}G^{24}$-3′] dodecamer called now the "Dickerson-Drew dodecamer" (DDD) duplex. The two strands of the DDD duplex were not symmetry-related in the crystal. Therefore, each of the nucleotides was uniquely numbered. The original structure was reported at 1.9 Å resolution and due to resolution, did not provided structural details. It was crystallized later by Egli and co-workers and revisited at atomic 1.1 Å resolution (*9*). The DDD duplex has cation binding sites, where Mg^{2+} or Ca^{2+} interact with the DNA molecule. Mg^{2+} ions are located near end-to-end overlaps between duplexes in the crystal lattice. One of the Mg^{2+} ions is responsible for the kink of the DNA molecule at one end into major groove. The ion contacts the N7 and O^6 edges of residues G^2 and G^{22} from opposite strands via coordinated waters. It was shown that the replacement of the N7 atom with C-H group on G^{22} removes the cation binding site in DDD and the kink is not present (Figure 4,6) (*10*).

The DDD sequence is one of the most studied fragments of DNA. The crystal packing of the DDD molecules allows a stable conformation of the DNA and good diffracting crystals. The sequence is also excellent to study by NMR, because it is a self-complementary duplex, and having 24 bases in the duplex we only observe signal from 12 bases (two strands are the same in the solution), which simplifies NMR analysis. In the crystal structure of the unmodified DDD duplex, we also observe inner and outer water spines in the minor groove of DNA (*9*). Cations play important roles in crystal

formation and stabilization of the DDD duplex. Structure of 7-deaza-dG is shown in Figure 5.

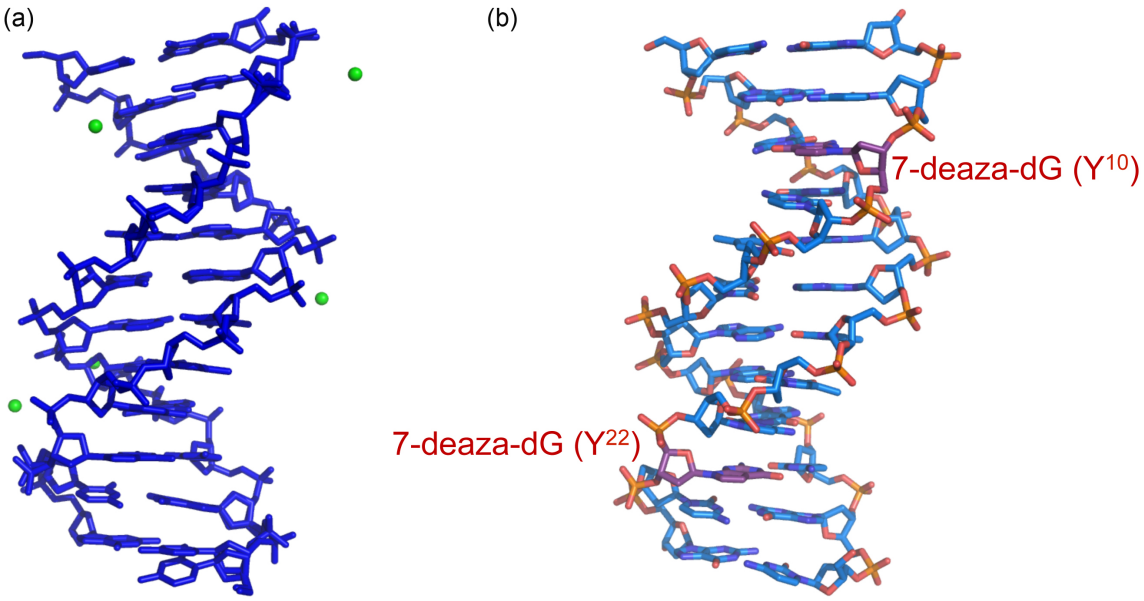
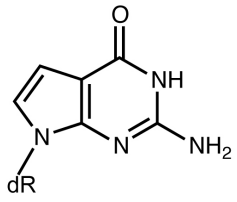


Figure 4. (a) Structure of unmodified DDD duplex, PDB code 436D with five Mg^{2+} ions (shown as green spheres). (b) Structure of 7-deaza-dG modified DDD, PDB code 2QEG.



7-deaza-dG

Figure 5. Chemical structure of 7-deaza-dG.

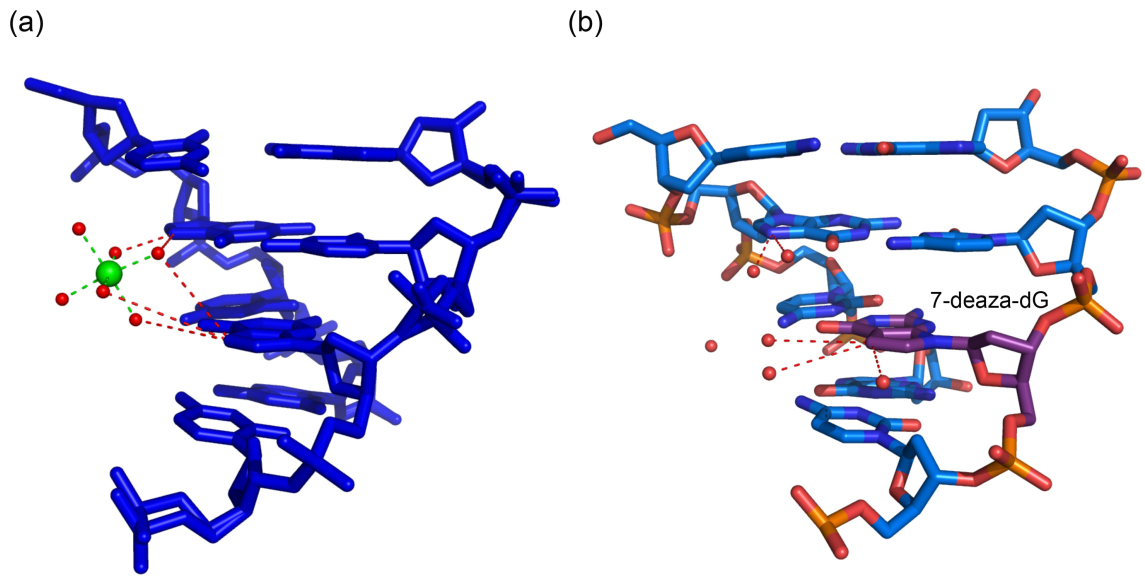


Figure 6. (a) Close view of the interactions between the Mg^{2+} ion and the unmodified DDD duplex, PDB code 436D. Mg^{2+} ion (green sphere) is coordinated by six water molecules (red spheres). The Mg^{2+} ion interacts via coordinated waters with N7 atoms of G^{2} and G^{22} nucleotides. This interaction is responsible for a kink of DNA into major groove. (b) Close view of the interactions between water molecules (red spheres) and the 7-deaza-dG modified DDD duplex, PDB code 2QEG. Modified base G^{22} (in purple) disrupts Mg^{2+} binding site in DNA and the kink associated with it is not observed.

Use of crystallography to solve nucleic acid structures

X-rays, or Röntgen rays were discovered by Röntgen in 1895 and for this discovery he received first Nobel Prize in Physics in 1901. X-ray crystallography is an experimental technique used to determine the arrangement of atoms within the crystal. X-rays are diffracted by crystals, because they have the proper wavelength (in the

Ångström range, ~10^{-8} cm) to be scattered by the electron cloud of an atom of comparable size. Based on the diffraction pattern obtained from X-ray scattering of the crystal, the electron density can be reconstructed. Additional phase information must be extracted either from the diffraction data or from supplementing diffraction experiments to complete the reconstruction. A model is then progressively built into the experimental electron density, refined against the data and the result is a final structure (Figure 7). X-ray crystallography has no size limit, and larger complexes can be analyzed by X-ray crystallography than by NMR spectroscopy. One of the difficulties in X-ray crystallography is fact that method requires a single crystal, which will diffract well. Many DNA sequences as well as proteins do not produce good crystals. Another challenge is phasing.

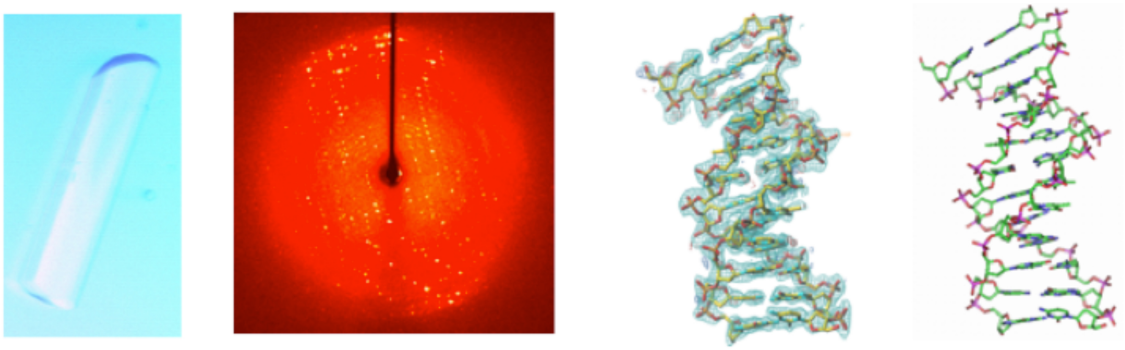


Figure 7. Process to obtain a crystal structure of DNA. First a single crystal is needed, which is mounted on a goniometer and gradually rotated while being bombarded with X-rays, producing a diffraction pattern of regularly spaced spots known as reflections. The two-dimensional images taken at different rotations are converted into a three-dimensional model of the density of electrons within the crystal using the mathematical method of Fourier transform, combined with chemical data known for the sample. Then the structure is refined to give a final crystal structure.

In the calculation step going from diffraction pattern to obtain electron density, ρ (xyz) for all x, y, z in the unit cell we have $|F_{hkl}|$, which we measured in the experiment, but we still need phase information ϕ_{hkl} (the phase problem):

$$\rho(xyz) = \frac{1}{V}\sum_{h}\sum_{k}\sum_{l} | F_{hkl} | \exp[-2\pi \cdot i(hx + ky + lz) + i\varphi_{hkl}] \qquad (1)$$

We record the position (the triple index hkl) and intensity, I_{hkl}, of each reflection and the measured intensities are proportional to the coefficients of the electron density equation:

$$I_{hkl} \propto | F_{hkl} |^2 \qquad (2)$$

The structure factor $|F_{hkl}|$ is complex and can be represented by the Argand diagram (Figure 8). F_{hkl} = A +iB. We measure $|F_{hkl}|$ in the experiment, but we still need ϕ_{hkl}, phases.

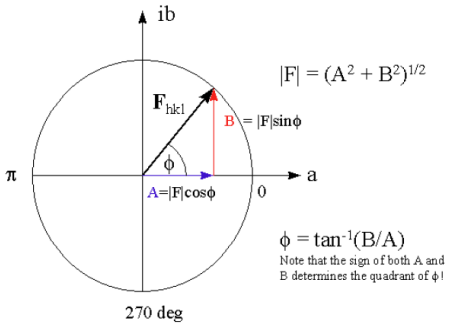


Figure 8. Argand diagram, vector representation of F_{hkl}.

There are a few methods available to solve phasing problem. One is the molecular replacement method (*11*). It can be used when a known model or structure of similar molecule in known. The model is then a source of the initial phases. The model is repositioned to obtain the best agreement with the experimental data. Phases are then calculated from the model using the structure factor equation and combined with the experimental data.

Another phasing method for DNA and proteins is called a multiple/single wavelength anomalous diffraction (MAD/SAD) (*12*). The sources of phases are the

anomalous intensity differences. The positions of anomalous scatterers are identified from anomalous difference Patterson maps. Heavy metal derivatives are used MAD/SAD data diffraction. Heavy atoms may be covalently attached to the modified DNA or protein. For example 5-Br-uridine is used instead of thymine for nucleic acids and methionine is replaced by selenomethionine in proteins. Other heavy atom used in crystallization conditions for nucleic acids are Ba^{2+} or Sr^{2+} salts. If the resolution of the crystal is higher than 1.4 Å direct methods to obtain phasing can be used by exploiting known phase relationships between certain groups of reflections (*13*).

CHAPTER II

ALTERING THE ELECTROSTATIC POTENTIAL IN THE MAJOR GROOVE: THERMODYNAMIC AND STRUCTURAL CHARACTERIZATION OF 7-DEAZA-2'-DEOXYADENOSINE:DT BASE PAIRING IN DNA*

Introduction

Nucleoside analogs containing pyrrolopyrimidine bases (*14, 15*), or 7-deaza-purines (Figure 8), are used as isosteric analogs of adenine and guanine in biochemical and biophysical studies (*16-20*). The 7-deazapurines are also used to study the effects of site-specific alteration of the electrostatic potential of the DNA major groove, where it has been shown for 7-deazaguanine that there is a significant alteration in DNA hydration and cation binding (*16, 21*). The 7-deazaadenosine base was identified in the antibiotic tubercidin, a ribonucleoside isolated from various species of *Streptomyces* (*15, 22-24*). The incorporation of 7-deaza-dA into DNA hinders the processing of the double helix by proteins, e.g., restriction endonucleases (*25*). It slightly reduces the bending of DNA in oligodeoxynucleotides containing $d(GGCA_6C)\cdot d(CCGT_6G)$ tracts (*26, 27*). The preparation of phosphoramidites containing 7-deaza-dA has been described by Seela et al. (*28, 29*). There remains a paucity of quantitative data as to how substitution of adenine with

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7-deaza-dA alters the structure and thermodynamics of the DNA double helix. Thermal denaturation of (7-deaza-dA)$_{11}$A•T$_{12}$ as compared to dA$_{12}$•dT$_{12}$ led to the conclusion that destabilization induced by 7-deaza-dA was associated with an unfavorable entropy change (*30*). Pope et al. (*31*) conducted a high-angle X-ray fiber diffraction study of poly[d(7-deaza-dA-T)]•poly[d(7-deaza-dA-T)]. They suggested that replacement of dA by 7-deaza-dA caused slight alterations to the structure of A-DNA, but greater perturbations to B-DNA. When 7-deaza-dG was incorporated into the Dickerson-Drew dodecamer (DDD) (*32, 33*) it had minimal effect on the overall conformation determined by NMR or crystallography (Figure 4b) (*10, 16*). However, duplex stability was reduced adjacent to the modification site due to a loss of enthalpic stabilization.

Moreover, 7-deaza-dG caused a reduction in hydration and cation binding. This was attributed to the elimination of a high affinity major groove cation binding site (*10*). Clearly, while 7-deaza-dG was an isostere of dG, it altered the ensemble of DNA, water and salts, and thermodynamic stability of the DDD (*16*).

In studies presented herein, an adenine at position A^6 in the DDD (*32, 33*) has been replaced by 7-deaza-dA (*28, 29*) to form the DDD-1 duplex [5′-d(C^{1}G^{2}C^{3}G^{4}A^5<u>Y</u>^{6}T^{7}T^{8}C^{9}G^{10}C^{11}G^{12})-3′]$_2$ (<u>Y</u>=7-deaza-dA) (Chart 1). Crystallography has been used to determine the structure of the DDD-1 duplex. A combination of thermal melting studies monitored by UV absorbance, differential scanning calorimetry (DSC), and NMR studies have been performed. The corresponding decamer DD-1, [5′-d(G^{1}C^{2}G^{3}A^4<u>Y</u>^{5}T^{6}T^{7}C^{8}G^{9}C^{10})-3′]$_2$, which does not form an intramolecular hairpin at low salt concentrations, was also used in thermodynamic studies. We demonstrate that 7-deaza-dA has minimal effect upon base pairing geometry and conformation of the

DDD. However, the 7-deaza-dA:dT base pair is thermodynamically destabilized, which is primarily attributed to unfavorable enthalpy terms dominated by less favorable stacking interactions, resulting from changes in the base electrostatics and electronic dipole-dipole interactions. There is also a net release of electrorestricted waters from the duplex.

Materials and Methods

Sample preparation

The oligodeoxynucleotides 5′-CGCGAYTTCGCG-3′ (DDD-1) and 5′-GCGAYTTCGC-3′, (DD-1), Y = 7-deaza-dA, were synthesized by the University of Nebraska Medical Center Eppley Institute Molecular Biology Shared Resource. The 7-deaza-dA phosphoramidite was obtained commercially (Glen Research, Sterling, VA, U.S.A.). The oligodeoxynucleotides were purified using semipreparative reverse-phase HPLC (Phenomenex, Phenyl-Hexyl, 5 μm, 250mm × 10.0 mm) equilibrated with 0.1M triethylammonium acetate (pH 7.0). The unmodified oligodeoxynucleotides, 5′-CGCGAATTCGCG-3′ (DDD) and 5′-GCGAATTCGC-3′ (DD), were synthesized by the Midland Reagent Company (Midland, TX) and purified by anion-exchange HPLC. The oligodeoxynucleotides were desalted using Sephadex G-25, lyophilized, and characterized by MALDI-TOF-MS. The oligodeoxynucleotides were dissolved in the appropriate buffers. The concentrations of single-stranded oligodeoxynucleotides were determined by UV absorbance at 260 nm using extinction coefficients of 1.11×10^5 M^{-1} cm^{-1} (dodecamers) and 9.5×10^4 M^{-1} cm^{-1} (decamers) (*34*) and assuming similar extinction coefficients for 7-deaza-dA and dA. The oligodeoxynucleotides were annealed

by heating to 80 °C for 15 min and then cooling to room temperature.

Temperature–Unfolding Profiles (Melting Curves)

The thermodynamic parameters for the temperature-induced unfolding reactions of the duplexes were measured using a VP-DSC differential scanning calorimeter (Microcal, Inc., Northampton, MA, U.S.A.). The heat capacity profile for each DNA solution was measured against a buffer solution. The experimental curves were normalized for the heating rate, and a buffer vs. buffer scan was subtracted using the program Origin (v. 5.0; Microcal, Inc.). The resulting monophasic or biphasic curves were analyzed by deconvolution with the Microcal software; their integration ($\int \Delta C_p \mathrm{d}T$) yielded the molar unfolding enthalpy (ΔH_{cal}), which was independent of the nature of the transition (*35, 36*). The molar entropy (ΔS_{cal}) was obtained similarly, using $\int (\Delta C_{\mathrm{p}} / T)\mathrm{d}T$. The free energy change at any temperature T was obtained with the Gibbs equation: $\Delta G°(T) = \Delta H_{\mathrm{cal}} - T\Delta S_{\mathrm{cal}}$. Absorption versus temperature profiles (UV melts) for each duplex were measured at either 260 or 275 nm using a thermoelectrically controlled UV-vis Aviv 14DS (Aviv Biomedical, Inc., Lakewood, NJ) or Lambda 40-Perkin-Elmer (Perkin-Elmer, Inc., Waltham, MA) spectrophotometers. The temperature was scanned at heating rates of 0.75–1.00 °C/min. Melting curves as a function of strand concentration (7–70 μM) were obtained to check the molecularity of each oligodeoxynucleotide (i.e., hairpin vs duplex). Additional melting curves were obtained as a function of salt (*37*) and osmolyte concentrations (*38-40*) to determine the differential binding of counterions (Δn_{Na^+}) and waters (Δn_{w}), which accompanied the helix-to-coil transitions (*41, 42*). For duplexes that melted via biphasic transitions only the T_{M} of the duplex → random coil

transition was used for the calculations. In the determination of Δn_{Na+}, UV melts were measured in the salt range of 10–200 mM NaCl at pH 7.0, whereas in the determination of Δn_w, UV melts were measured in the ethylene glycol concentration range of 0.5 – 4.0 mM at pH 7.0 and 10 mM NaCl. The osmolalites of the solutions were obtained with a UIC vapor pressure osmometer, Model 830 (Jolliet, IL, U.S.A.). These osmolalities were then converted into water activities, a_w, using the relationship $\ln a_w = -(\text{Osm}/M_w)$, where Osm is the solution osmolality and M_w is the molality of H_2O, 55.5 mol/kg (*43*).

Circular Dichroism

Circular dichroism (CD) measurements were conducted on an Aviv model 202SF CD spectropolarimeter (Aviv Biomedical, Inc., Lakewood, NJ). To approach 100% duplex formation the spectrum of each sample was obtained using a strain-free 1cm quartz cell at low temperatures. Typically, 1 OD of a duplex DNA was dissolved in 1 mL of 10 mM sodium phosphate buffer (pH 7.0). The reported spectra correspond to an average of three scans from 220 to 350 nm at a wavelength step of 1 nm.

Nuclear Magnetic Resonance (NMR) Spectroscopy

Modified and unmodified duplexes were prepared at 0.3 mM and 1.8 mM concentrations, respectively. The samples were prepared in 10 mM NaH_2PO_4, 0.1 M NaCl, and 50 μM Na_2EDTA (pH 7.0). The samples were exchanged with D_2O and dissolved in 0.5 mL of 99.99% D_2O to observe nonexchangeable protons. For the observation of exchangeable protons, the samples were dissolved in 0.5 mL of 9:1 H_2O/D_2O. ^1H NMR spectra for unmodified and modified oligodeoxynucleotides were

recorded at 600 and 800 MHz. Chemical shifts were referenced to water. Data were processed using TOPSPIN software (Bruker Biospin Inc., Billerica, MA). The NOESY (*44, 45*) and DQF-COSY (*46*) spectra of samples in D_2O were collected at 15 °C at 800 MHz; NOESY experiments were conducted at a mixing time of 250 ms. The NOESY spectra of the modified and unmodified sample in H_2O were collected at 5 °C at 600 MHz, with a 250 ms mixing time. These experiments were performed with a relaxation delay of 2.0 s. Water suppression was performed using the WATERGATE pulse sequence (*47*).

Crystallization and Data Collection

Crystallization trials were performed with the Nucleic Acid Mini-screen (Hampton Research, Aliso Viejo, CA) (*48*). The hanging drop vapor diffusion technique was used. Droplets, with a volume of 2 μL, of a 1:1 mixture of sample and mini-screen buffer were equilibrated against 0.75 mL of 35% 2-methyl-2,4-pentanediol (MPD) at 18 °C. The crystal used for data collection was grown in 10% MPD, 40 mM sodium cacodylate (pH 6.0), 12 mM spermine tetra-HCl, and 80 mM NaCl. The single crystal was mounted in a nylon loop and frozen in liquid nitrogen. Diffraction data were collected at low temperature in a cold nitrogen stream on beamline 21-ID-F at LSCAT, APS (Argonne National Laboratory, Argonne, IL). Separate data sets for high and low resolution reflections were collected. All data were processed with the program HKL2000 (*49*).

Crystal Structure Determination and Refinement

The diffraction data were processed in space group $P2_12_12_1$ (orthorhombic). Phasing was carried out by the molecular replacement method using the program MOLREP in the CCP4 suite (*50*). The DDD sequence with PDB entry 355D (*51*) was used as the starting model. Initial refinements of the model were performed with the CNS program (*52*), setting aside 5% randomly selected reflections for calculating the R_{free}. Rigid body refinement and simulated annealing were performed. Multiple rounds of coordinate refinements and simulated annealing led to an improved model for which sum ($2F_o$-F_c) and difference (F_o-F_c) Fourier electron density maps were generated. At a later stage solvent water molecules were added on the basis of Fourier $2F_o$-F_c sum and F_o-F_c difference electron density maps. Water molecules were accepted based on the standard distances and B-factor criteria. Further structure refinement was performed using the program SHELX (*53*), and REFMAC in CCP4 (*50*). One Mg^{2+} ion and four Na^+ ions were identified in the electron density maps based on their low B-factors and the characteristic Mg^{2+} octahedral and Na^+ tetrahedral coordination geometries. Geometry and topology files were generated for the 7-deaza-dA modified bases and anisotropic temperature factor refinement was performed afterward. The program TURBOFRODO (*54*) was used to display electron density maps. The helicoidal parameters of the 7-deaza-dA-modified DDD were analyzed using the program CURVES (version 5.3) (*55*).

Data Deposition

Complete structure factor and final coordinates were deposited in the Protein Data Bank (www.rcsb.org): PDB ID code 3OPI.

Results

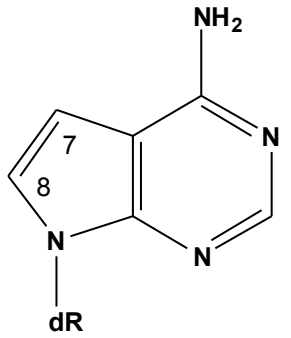
Crystallography

The 7-deaza-dA-modified DDD-1 diffracted at a resolution of 1.1 Å. The two strands of the DDD-1 duplex were not symmetry-related in the crystal. Therefore, each of the nucleotides was uniquely numbered (Chart 1). Minimal perturbation of the DNA duplex was observed at the 7-deaza-dA site (Figure 9) (*9*). The 7-deaza-dA bases were in the *anti* conformation about the glycosyl bonds and Watson–Crick base pairing was maintained at base pairs Y^6•T^{19} and Y^{18}•T^7 (Figure 10). Waters formed the anticipated minor groove inner spine of hydration (Figure 11), similar to the situation in the DDD (*9, 32, 33*). The replacement of N7-dA with a carbon atom in 7-deaza-dA^6 did not alter Mg^{2+} binding in the crystal, e.g., as indicated by a comparison to the high resolution structure of the DDD obtained by Tereshko and Egli (*9*). One Mg^{2+} ion was present per asymmetric unit, but two Mg^{2+} ions interacted with each DNA molecule as a consequence of the crystallographic 2_1 symmetry. This Mg^{2+} interacted via six coordinated waters with the G^2 and G^{22} nucleotides in the major groove (Figure 9). It also interacted via coordinated waters with the Y^6 and T^7 phosphate oxygens from an adjacent DNA molecule. It did not interact directly with the Y^6 7-deaza-dA base (Figure 9 and 12). Instead, it stabilized a contact between DNA molecules. The sum electron density contoured at the 1.0 σ level

for the G^4, A^5 and Y^6 nucleotides suggested two conformations of the phosphate backbone (Figure 12). These were each refined with occupancy 0.5. It is likely that these were due to this Mg^{2+}-mediated lattice contact between DNA molecules.

Chart 1. (a) Structure of 7-deaza-dA. (b) Sequences and numbering of the nucleotides for unmodified DD, 7-deaza-dA DD, unmodified DDD, 7-deaza-dA DDD (NMR) and 7-deaza-dA DDD (X-ray) duplexes. In solution, the two strands exhibit pseudo-dyad symmetry. In the crystal structure, the two strands were not symmetry related and the nucleotides were individually numbered.

(a)



7-deaza-dA

(b)

DD

5'-G^1 $C^2$$G^3$$A^4$$A^5$$T^6$$T^7$$C^8$$G^9$$C^{10}$-3'
3'-$C^{10}$$G^9$$C^8$$T^7$$T^6$$A^5$$A^4$$G^3$$C^2$$G^1$ -5'

7-deaza-dA DD (DD-1)

5'-G^1 $C^2$$G^3$$A^4$$Y^5$$T^6$$T^7$$C^8$$G^9$$C^{10}$-3'
3'-$C^{10}$$G^9$$C^8$$T^7$$\overline{T^6}$$\underline{Y^5}$$A^4$$G^3$$C^2$$G^1$ -5'

DDD

5'-C^1 G^2 C^3 G^4 A^5 A^6 T^7 T^8 C^9 $G^{10}$$C^{11}$$G^{12}$-3'
3'-$G^{12}$$C^{11}$$G^{10}$$C^9$ T^8 T^7 A^6 A^5 G^4 C^3 G^2 C^1 -5'

7-deaza-dA DDD (NMR) (DDD-1)

5'-C^1 G^2 C^3 G^4 A^5 $\underline{Y^6}$ T^7 T^8 C^9 $G^{10}$$C^{11}$$G^{12}$-3'
3'-$G^{12}$$C^{11}$$G^{10}$$C^9$ T^8 $\overline{T^7}$ $\underline{Y^6}$ A^5 G^4 C^3 G^2 C^1 -5'

7-deaza-dA DDD (Xray)

5'-C^1 G^2 C^3 G^4 A^5 $\underline{Y^6}$ T^7 T^8 C^9 $G^{10}$$C^{11}$$G^{12}$-3'
3'-$G^{24}$$C^{23}$$G^{22}$$C^{21}$$T^{20}$$\overline{T^{19}}$$\underline{Y^{18}}$$A^{17}$$G^{16}$$C^{15}$$G^{14}$$C^{13}$-5'

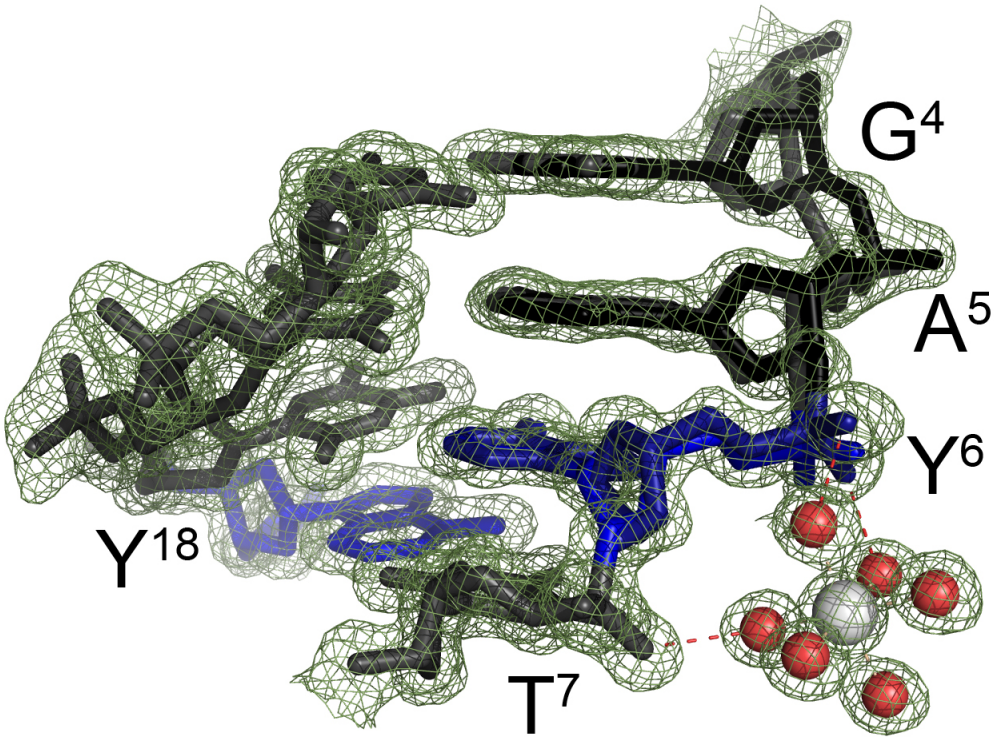


Figure 9. Sum electron density contoured at the 1.0 σ level (green meshwork) surrounding the DDD-1 duplex in the region of the G^4, A^5 and Y^6 nucleotides, where the phosphate groups display two alternative conformations. Bases G^4 and A^5 are shown in grey (one phosphate conformation) and black (second phosphate conformation). Modified base Y^6 is in blue (one phosphate conformation) and navy (second phosphate group conformation). Mg^{2+} ion (white sphere) is coordinated by six water molecules (red spheres). The Mg^{2+} ion interacts via coordinated waters with phosphate oxygens of one conformer of Y^6 only (second conformation of the phosphate backbone is shown in navy) and T^7 residue. Similar interactions are observed in the unmodified DDD duplex (PDB entry 355D). This interaction does not involve the N7 atom of the Y^6 and is maintained for the 7-deaza-dA base.

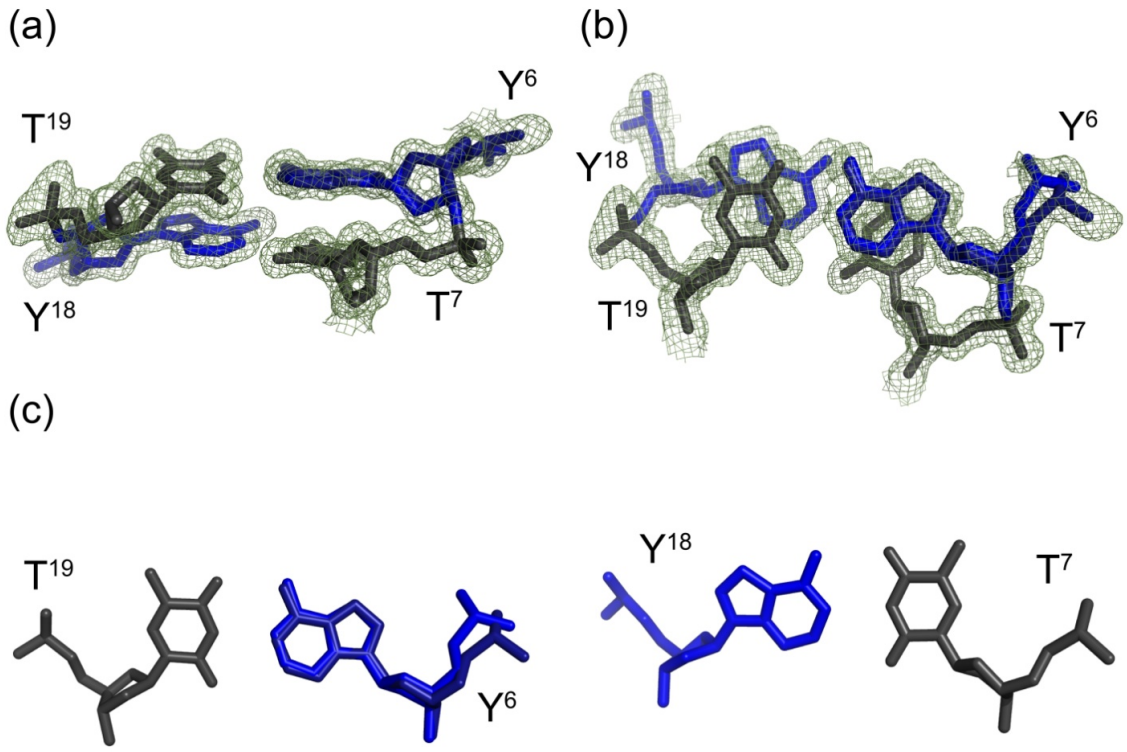


Figure 10. Sum electron density contoured at the 1.0 σ level (green meshwork) around modified Y^6•T^{19} and Y^{18}•T^7 base pairs, viewed. (a) from the side and (b) from the top approximately the named to base pairs, revealing stacking interactions. (c) Watson-Crick base pairing of 7-deaza-dA•dT. Y^6 and Y^{18} bases are shown in blue.

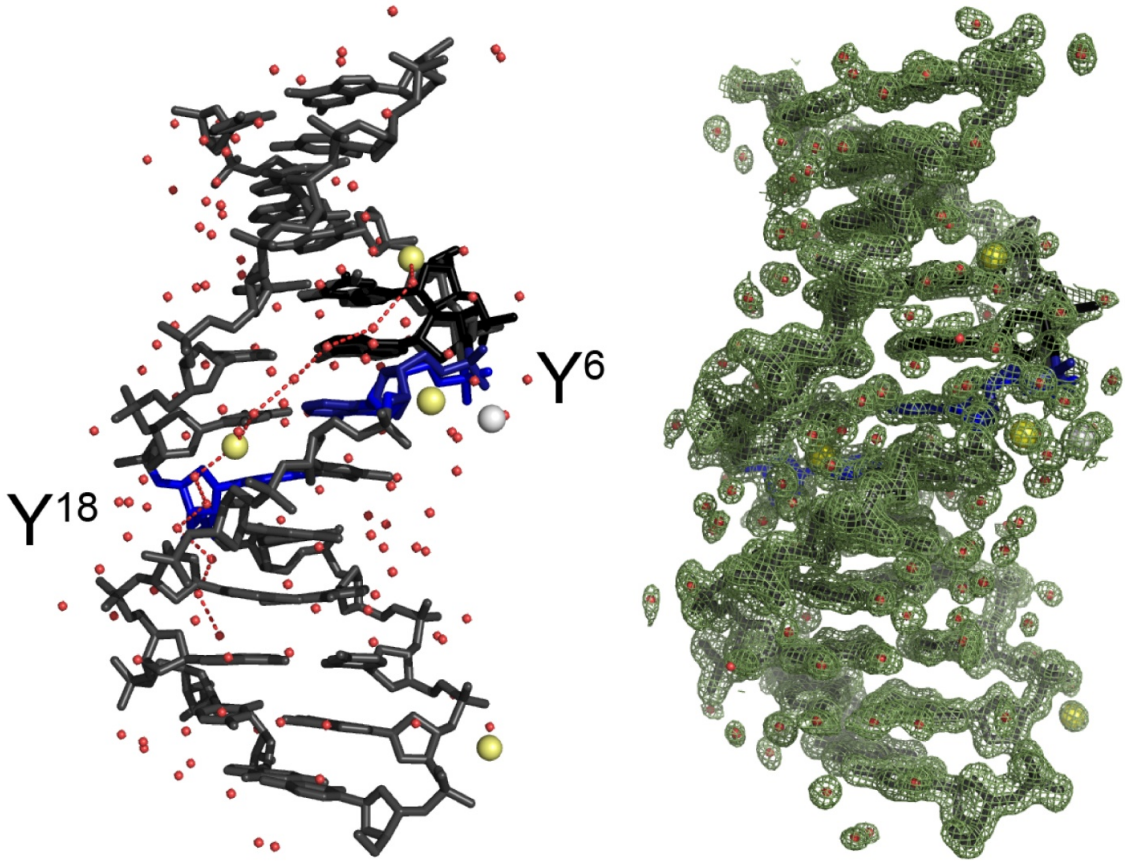


Figure 11. Stick model of the crystal structure of 7-deaza-dA modified DDD-1 (left side) and electron density shown at 1.0 σ level around the duplex (right side). Modified bases Y^6 and Y^{18} are shown in blue, Mg^{2+} ion is shown as white sphere, 133 water molecules are shown as red spheres and four Na^+ ions as yellow spheres. Red dash line shows water inner spine in the minor groove of DNA duplex. It contains water and sodium molecules (from the bottom end): HOH 426, HOH 444, HOH 438, HOH 442, HOH 412, HOH 441, NA 400, HOH 450, HOH 413, HOH 451, HOH 432, HOH 519, NA 402.

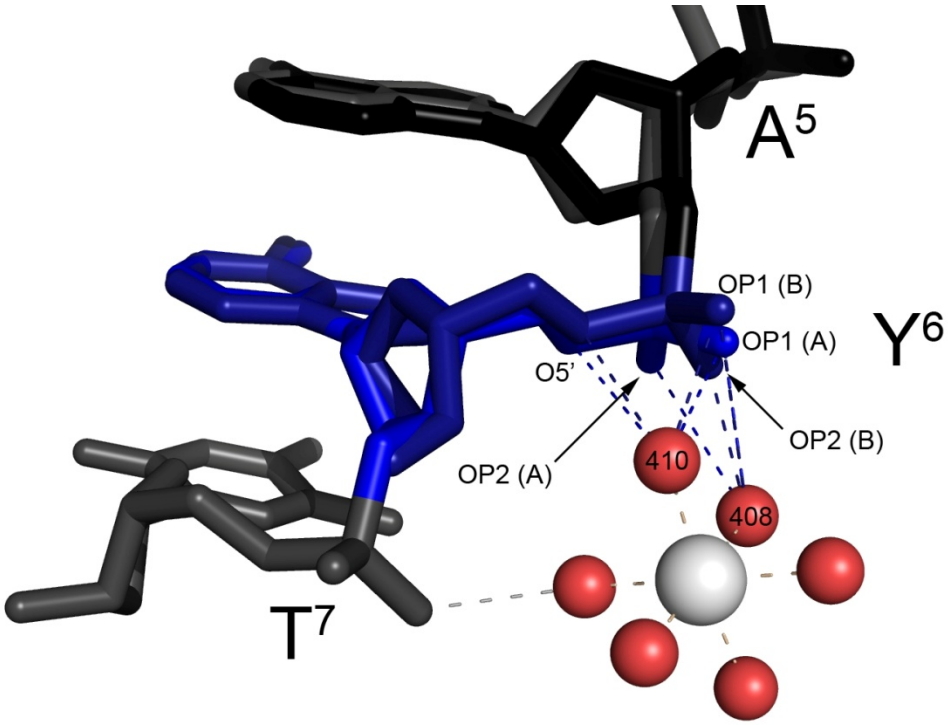


Figure 12. Interactions between Mg^{2+} ion and DDD-1 duplex are indicated by dash lines. Modified base Y^6 is in blue (one phosphate conformation, A) and navy (second phosphate group conformation, B). Mg^{2+} ion (white sphere) is coordinated by six water molecules (red spheres). The Mg^{2+} ion interacts via coordinated waters with phosphate oxygens of two conformers of Y^6 and T^7 nucleotides. Distances between water molecules coordinated to Mg^{2+} ion and Y^6 nucleotide are shown below:

HOH 410	OP1 (A)	3.55 Å
HOH 410	OP1 (B)	2.73 Å
HOH 410	O5' (A)	4.06 Å
HOH 410	O5' (B)	3.44 Å
HOH 408	OP1 (A)	2.85 Å
HOH 408	OP1 (B)	3.53 Å
HOH 408	OP2 (A)	4.04 Å
HOH 408	OP2 (B)	2.77 Å

Helicoidal analyses indicated that the rise, roll, and twist parameters of the DDD-1 duplex were unaffected by these two backbone conformations (Figure 13). The difference between the two conformations primarily involved torsion angle α (5'-PO-C5-C4-3') (Figure 14). Smaller variations were observed in other torsion and glycosyl angles of the G^4, A^5 and Y^6 nucleotides (Figure 15). In all, 133 waters and four Na^+ ions, of which one was observed at the 5'-ApT-3' step (*9*), were assigned per asymmetric unit. A summary of crystal data and data collection statistics is given in Table 1.

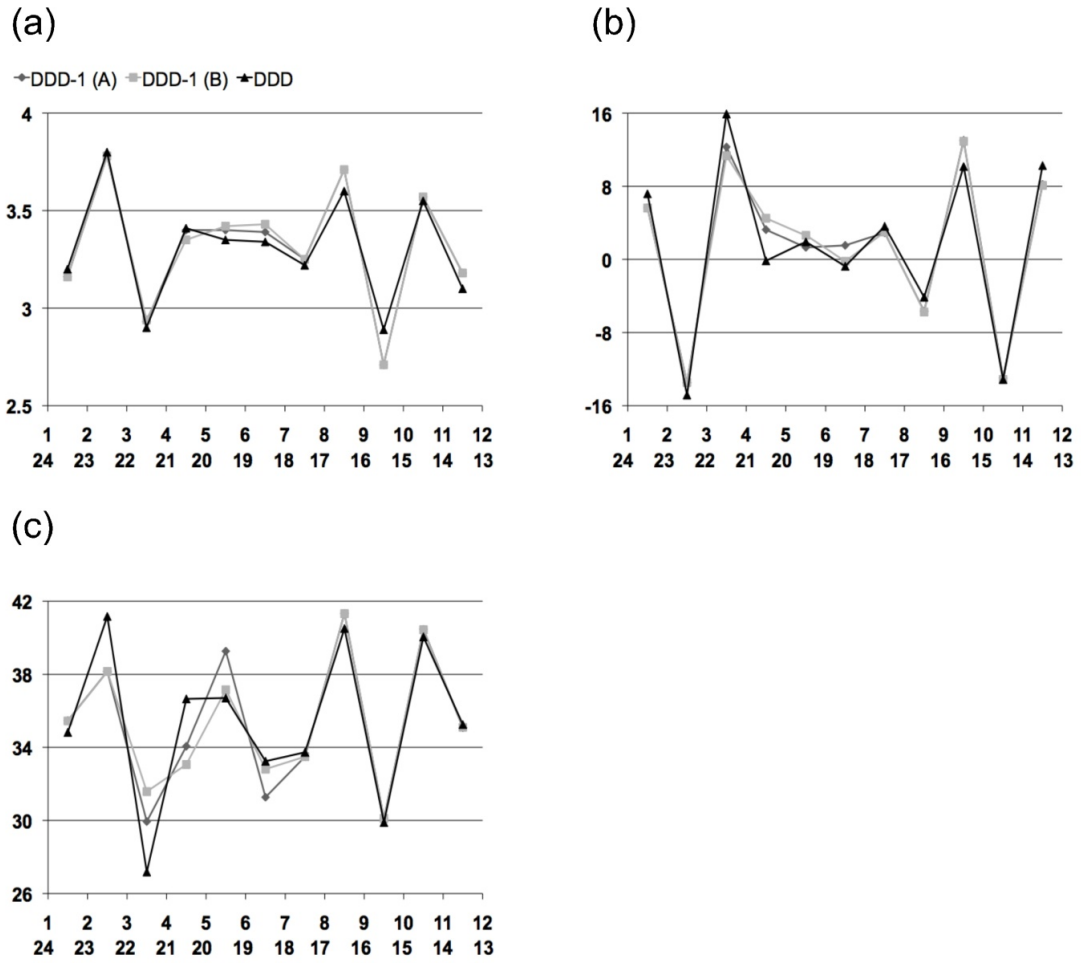


Figure 13. Interbase pair parameters: (a) helical rise, (b) roll and (c) twist for the DDD-1(A) (with one phosphate backbone conformation for the G^4, A^5 and Y^6), DDD-1 (B) (with second phosphate conformation for the G^4, A^5 and Y^6), DDD (PDB entry 355D) duplexes.

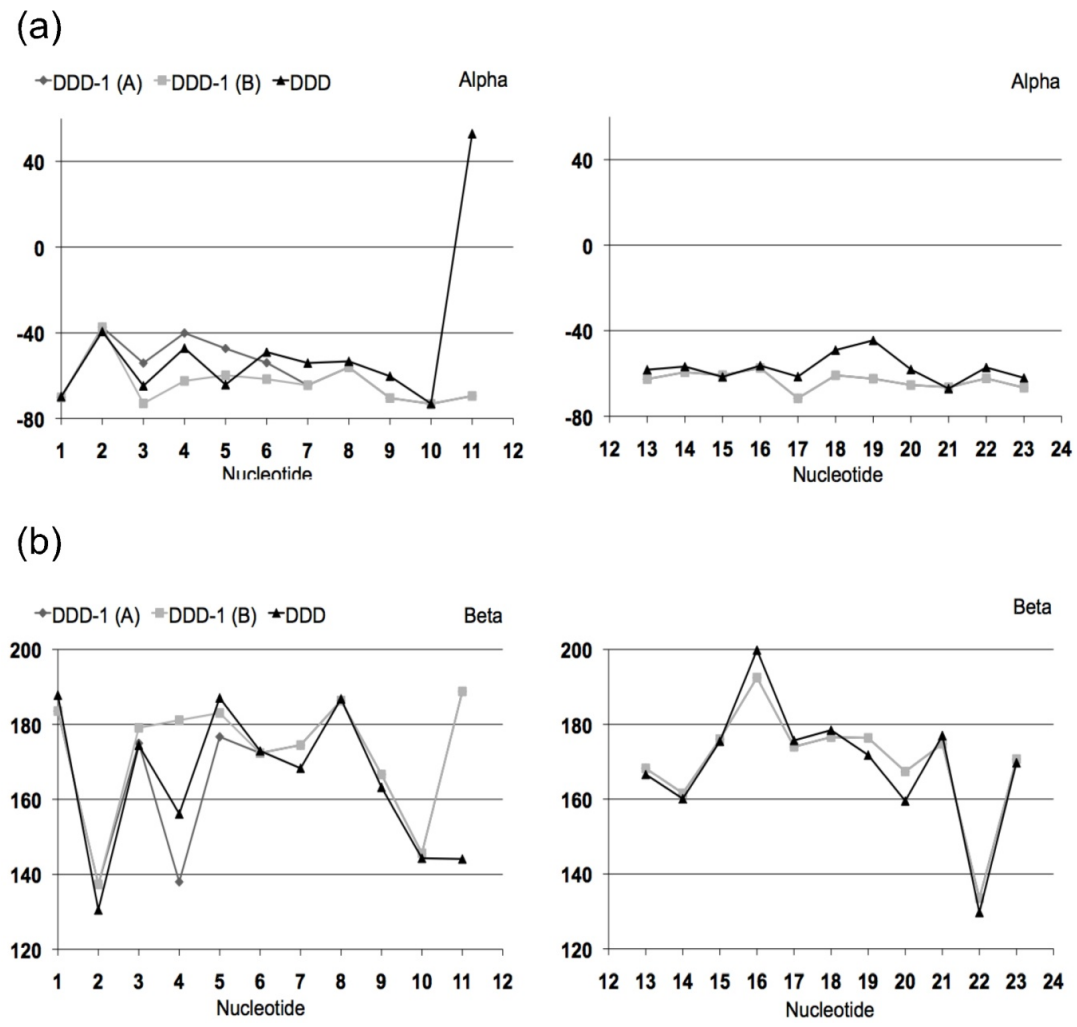


Figure 14. Comparison of backbone torsion angles (a) α and (b) β in the crystal structures of the DDD-1(A) (with one phosphate backbone conformation for the G^4, A^5 and Y^6), DDD-1 (B) (with second phosphate conformation for the G^4, A^5 and Y^6), DDD (PDB entry 355D) duplexes.

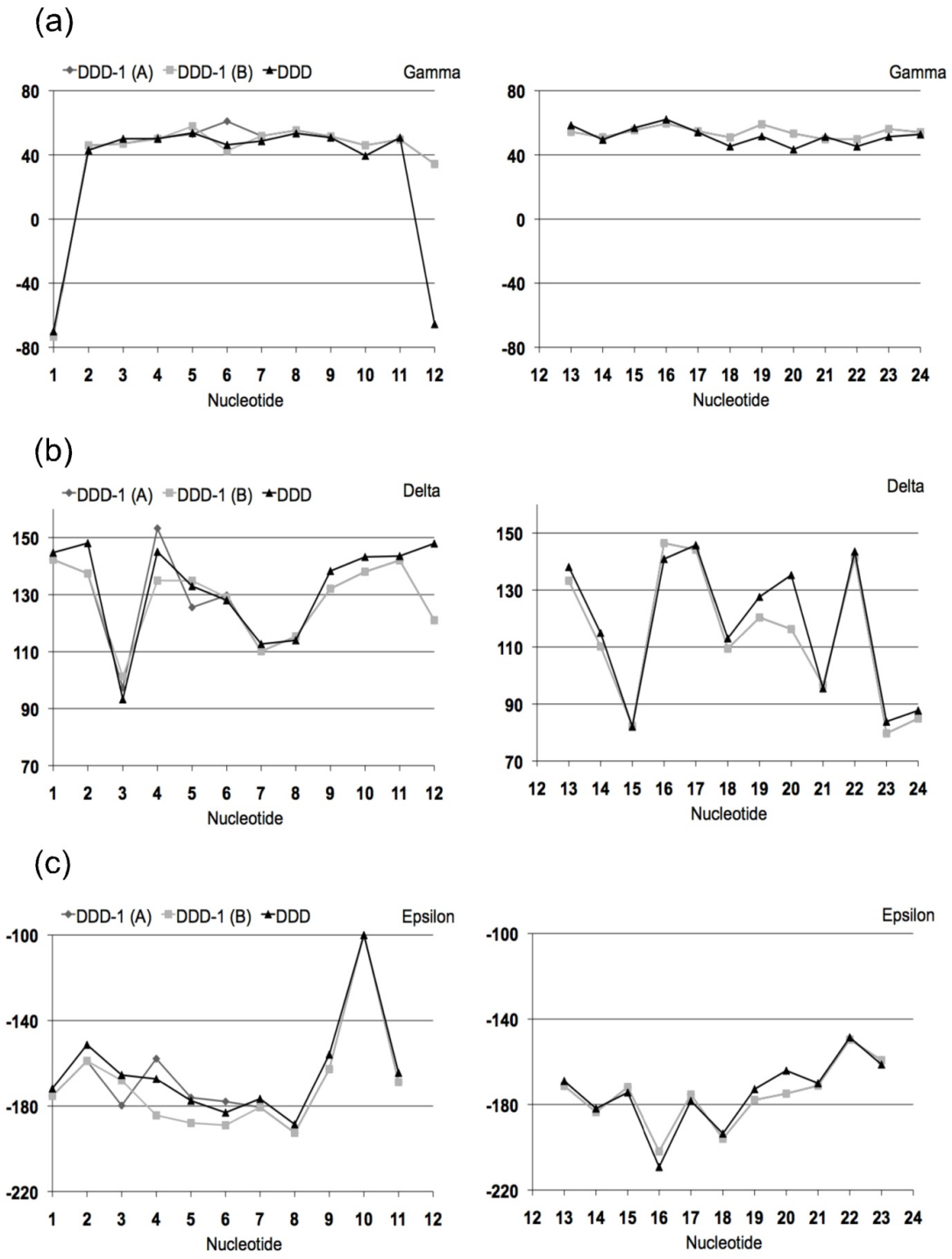


Figure 15. Comparison of (a) γ, (b) δ, (c) ε, (d) χ and (e) ζ angles in the crystal structures of the DDD-1(A) (with one phosphate backbone conformation for the G^4, A^5 and Y^6), DDD-1 (B) (with second phosphate conformation for the G^4, A^5 and Y^6), DDD (PDB entry 355D) duplexes.

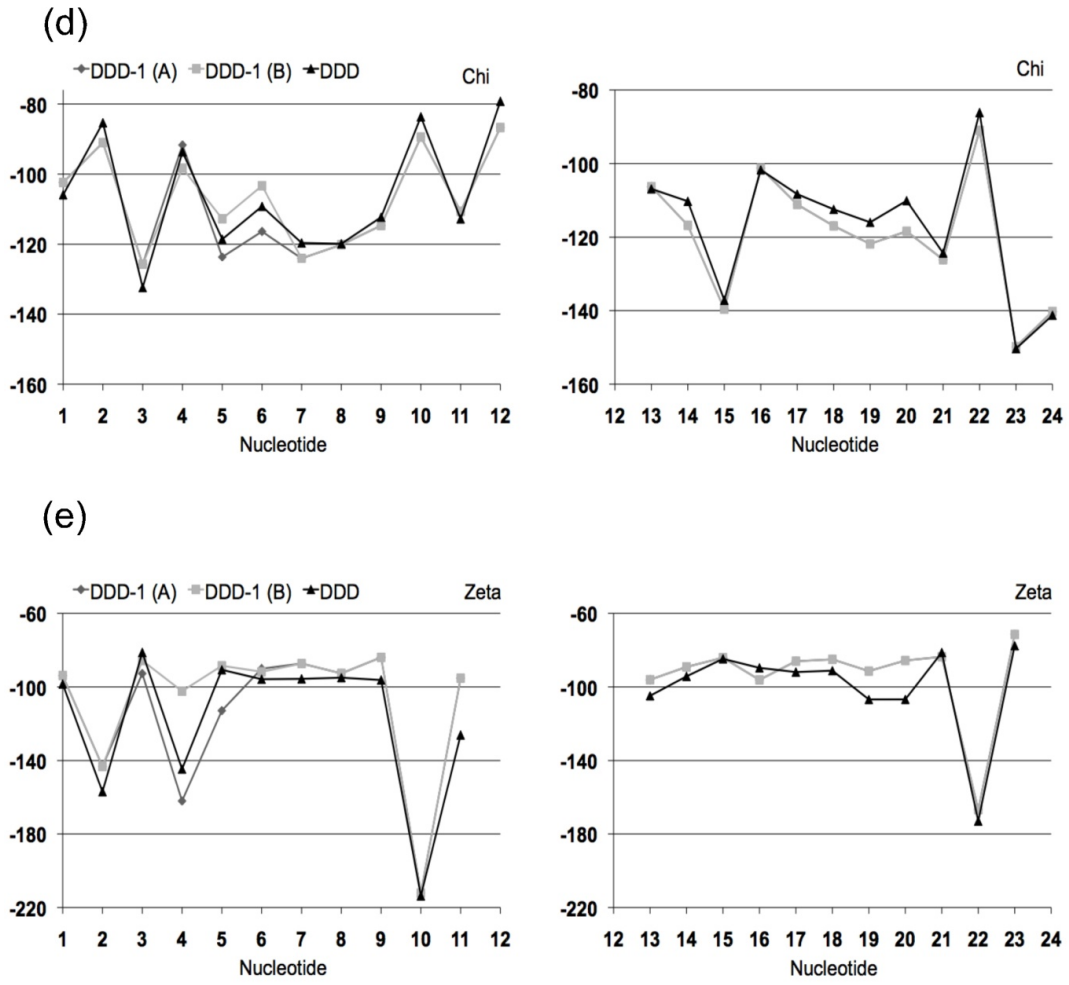


Figure 15-Continuation. Comparison of (a) γ, (b) δ, (c) ε, (d) χ and (e) ζ angles in the crystal structures of the DDD-1(A) (with one phosphate backbone conformation for the G^4, A^5 and Y^6), DDD-1 (B) (with second phosphate conformation for the G^4, A^5 and Y^6), DDD (PDB entry 355D) duplexes.

Table 1. Crystal Data, Data Collection, and Refinement Statistics.

Space group	Orthorhombic $P2_12_12_1$
Cell parameters (Å)	a=25.64, b=40.31, c=65.93
Temperature of data collection (° C)	-170
Wavelength (Å)	0.9785
Max resolution (Å)	1.1
Unique reflections	27920
Completeness all/1.14-1.10 Å (%)	97.8/95.8
Redundancy all/1.14-1.1 Å	10.6/6.9
I/σ (I) all/1.14-1.1 Å	61.26/4.8
R_{merge} all/1.14-1.10 Å	0.048/0.394
R_{work}	0.161
R_{free}	0.195
Number of DNA atoms	486
Number of water molecules	133
Number of ions	1 Mg^{2+} 4 Na^{+}
r.m.s. distances (Å)	0.024
r.m.s. angles (°)	1.95

Circular Dichroism

The CD spectra of the DDD and DDD-1 dodecamers are shown in Figure 16. These experiments were performed at 16 mM [Na^+]. In both instances, a positive Cotton effect was observed, centered near 280 nm. In both instances, a negative Cotton effect was centered at 250 nm. These were characteristic of a right-handed helix in the B-DNA family. There was an 18% decrease in the intensity of the 250 nm band for DDD-1 relative to DDD. CD experiments with the decamers DD and DD-1 revealed a similar trend. The decreased intensity of the 250 nm band for DD-1 relative to DD was 10% (Figure 16).

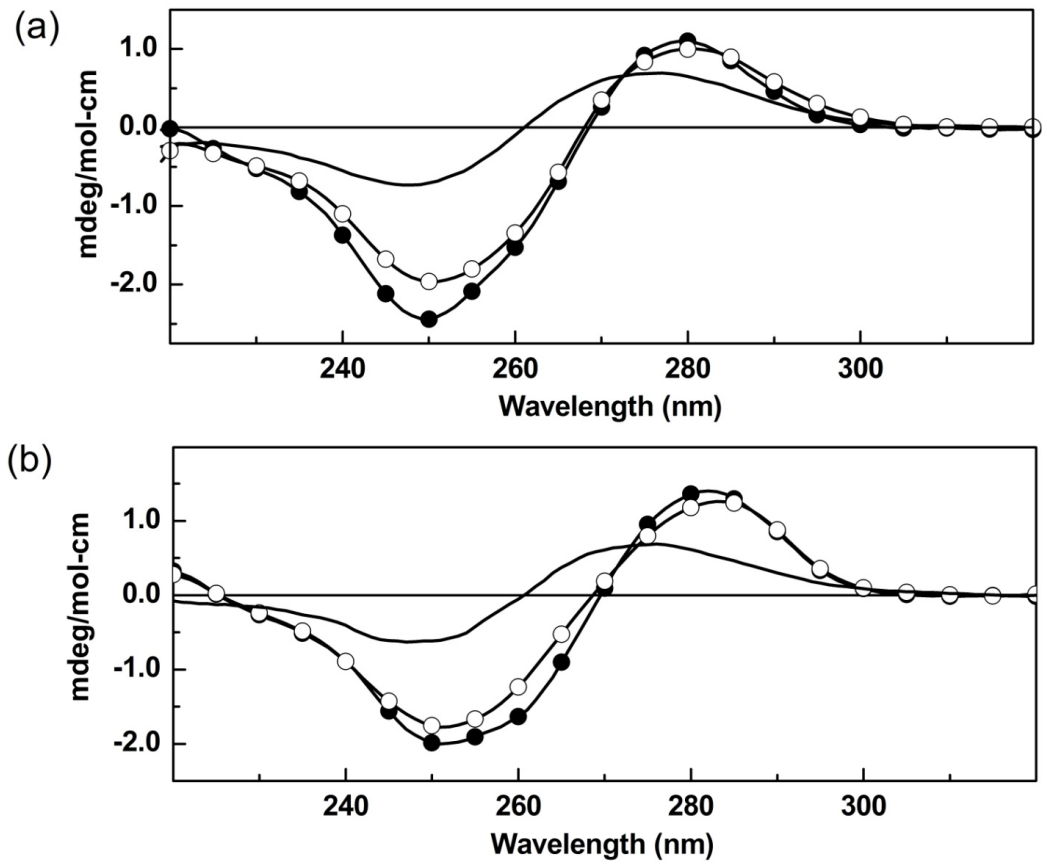


Figure 16. CD spectra of duplexes in 10 mM sodium phosphate buffer (pH 7.0) at 4 ºC, ~10 μM strand concentration: (a) DDD (●) and DDD-1 (O) and (b) DD (●) and DD-1 (O). The spectra without symbols are the spectra of the unmodified DDD and DD at 90 ºC.

Nuclear Magnetic Resonance Spectroscopy

In solution, the pseudo dyad symmetry of the DNA duplex results in the symmetry-related resonances from the two strands being isochronous (*56, 57*); thus, the NMR resonances are labeled for nucleotides 1–12. The 7-deaza-dA H7 and H8 protons were assigned from a combination of COSY and NOESY spectra, which established the presence of the 7-deaza-dA base at position Y^6 in the DDD-1 duplex (Figure 17). The upfield chemical shift of 1.07 ppm observed for Y^6 H8 relative to A^6 H8 in the DDD was attributed primarily to different electron distributions in the pyrrolopyrimidine vs. purine bases, not to a conformational change in the DDD-1 duplex. The nonexchangeable DNA protons were assigned using standard methods (*58, 59*). All sequential NOEs between the aromatic and anomeric protons of the DDD-1 duplex were observed (Figure 17). The imino proton region of the NOESY spectrum of the DDD-1 duplex is shown in Figure 18. The sequential connectivity of the base imino protons was obtained from base pairs G^2•C^{11} → C^3•G^{10} → G^4•C^9 → A^5•T^8 → Y^6•T^7 (*60*). Cross peaks from A^5 H2 to T^8 N3H and Y^6 H2 to T^7 N3H were observed. For the imino protons, the greatest downfield shift of 0.49 ppm was observed for the T^7 imino proton. The imino resonances of the terminal base pairs C^1•G^{12} were missing. This was attributed to rapid exchange with water.

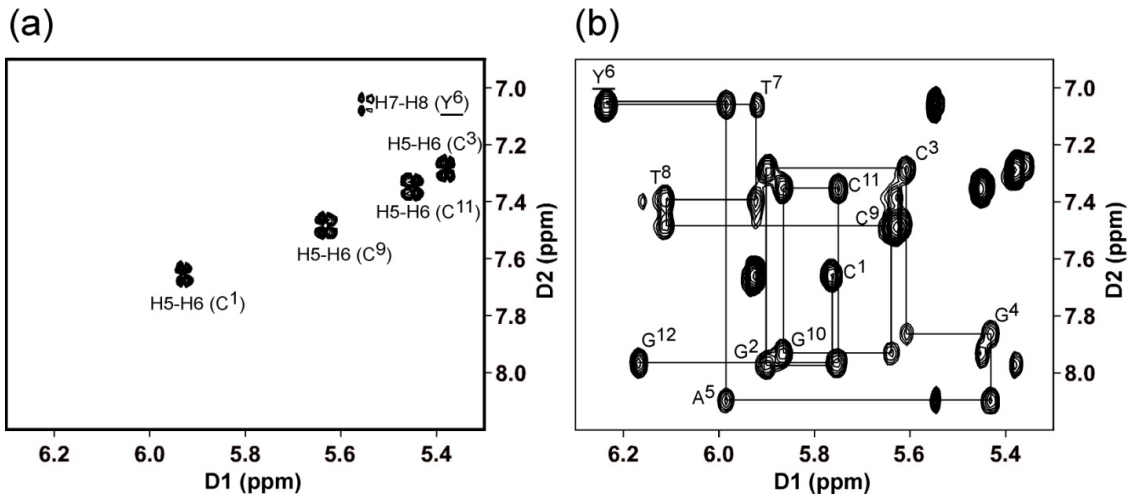


Figure 17. The 7-deaza-dA modified DDD-1 duplex. (a) The expanded plot of a DQF-COSY spectrum of DDD-1 duplex shows four cross peaks corresponding to four cytosine H5-H6 proton interactions (C^1, C^3, C^9, C^{11}) and one cross peak corresponding to the H7-H8 proton interactions of the 7-deaza-dA (b) The expanded plot of the NOESY spectrum of the DDD-1 duplex showing sequential NOEs between the aromatic and anomeric protons.

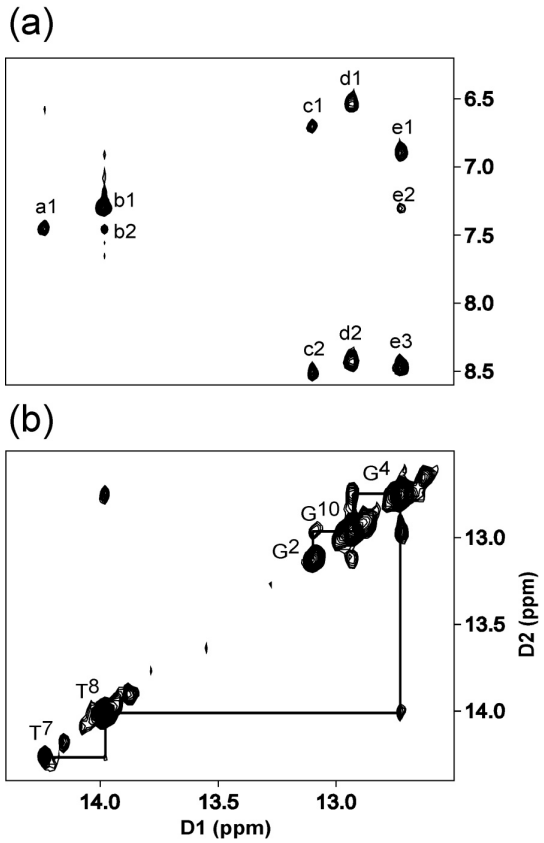


Figure 18. (a) Interstrand NOE cross peaks between opposite bases: a1, T^7N3H → Y^6 H2; b1, T^8 N3H → A^5 H2; b2, T^8 N3H → Y^6 H2; c1, G^2 N1H → C^{11} N^2H2; c2, G^2 N1H → C^{11} N^2H1; d1, G^{10} N1H → C^3 N^2H2; d2, G^{10} N1H → C^3 N^2H1; e1, G^4 N1H → C^9 N^2H2; e2, G^4 N1H → A^5 H2; e3, G^4 N1H → C^9 N^2H1. (b) NOE connectivity for the imino protons for the base pairs G^2•C^{11} to Y^6•T^7. The experiments were carried out at a mixing time of 250 ms and 600 MHz at 5 °C.

Unfolding studies – NMR

Spectra of the DDD-1 and DDD duplexes were collected as a function of temperature, over the range 5–65 °C (Figure 19). At 15 °C, for the 7-deaza-dA-modified duplex, the T^7 imino resonance began to broaden, compared with the other peaks and

with the unmodified DDD. At 45 °C, the T^7 peak completely broadened. These observations indicated that the T^7 imino proton was in enhanced exchange with the solvent and indicated a destabilization of the $Y^6 \bullet T^7$ base pair.

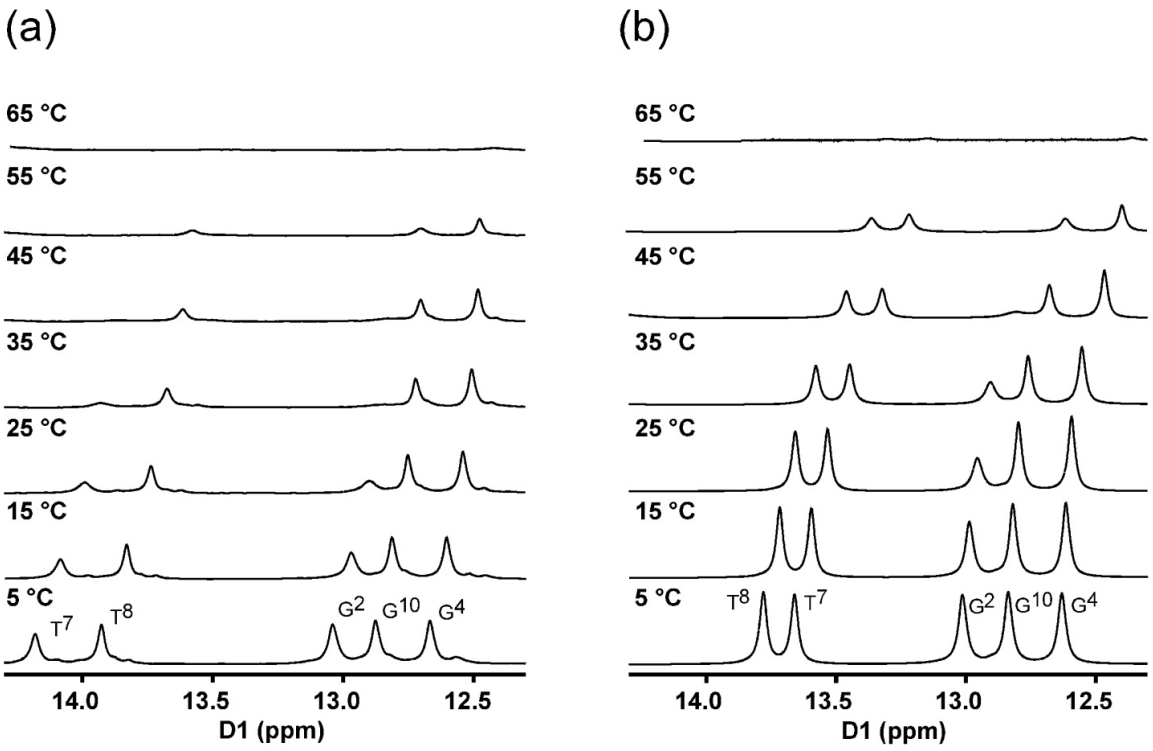


Figure 19. ^{1}H NMR of imino proton resonances as a function of temperature. (a) 7-deaza-dA DDD-1 duplex. (b) Unmodified DDD duplex. Modified and unmodified duplexes were prepared at 0.3 mM and 1.8 mM concentration respectively. The samples were prepared in 10 mM NaH_2PO_4, 0.1 M NaCl, 50 μM Na_2EDTA at pH 7.0.

Unfolding Studies – UV Melting

The unfolding of duplexes was studied by temperature-dependent UV spectroscopy. Absorption spectra at low and high temperatures revealed a greater hyperchromic effect at 260 nm for DDD and DD and at 275 nm for DDD-1 and DD-1. These were chosen as optimum wavelengths used for all UV melting studies. Typical melting curves of dodecamer and decamer duplexes are shown in Figure 20. In 10 mM NaCl, dodecamers (DDD and DDD-1) unfolded in broad biphasic transitions, whereas decamers (DD and DD-1) unfolded via monophasic transitions. The overall sequential melting behavior corresponded to duplex → hairpin and hairpin → random coil transitions, while the corresponding decamers, which formed less stable hairpins, melted through a single duplex random coil transition. The T_M values were determined by taking the first derivative of the melting curves, and shape analysis of these curves are reported in Table 2. Incorporation of 7-deaza-dA was destabilizing for both dodecamer and decamer. The T_M of the first transition for the dodecamer DDD-1 relative to DDD was unchanged in 16 mM Na^+ (low salt) and 8.2 °C lower in 116 mM Na^+ (high salt) concentrations. At higher salt concentration both melting transitions overlapped and only one transition was observed. The T_M of the modified DD-1 was lower than that for DD by 3.4 °C in low salt and by 5.5 °C in high salt.

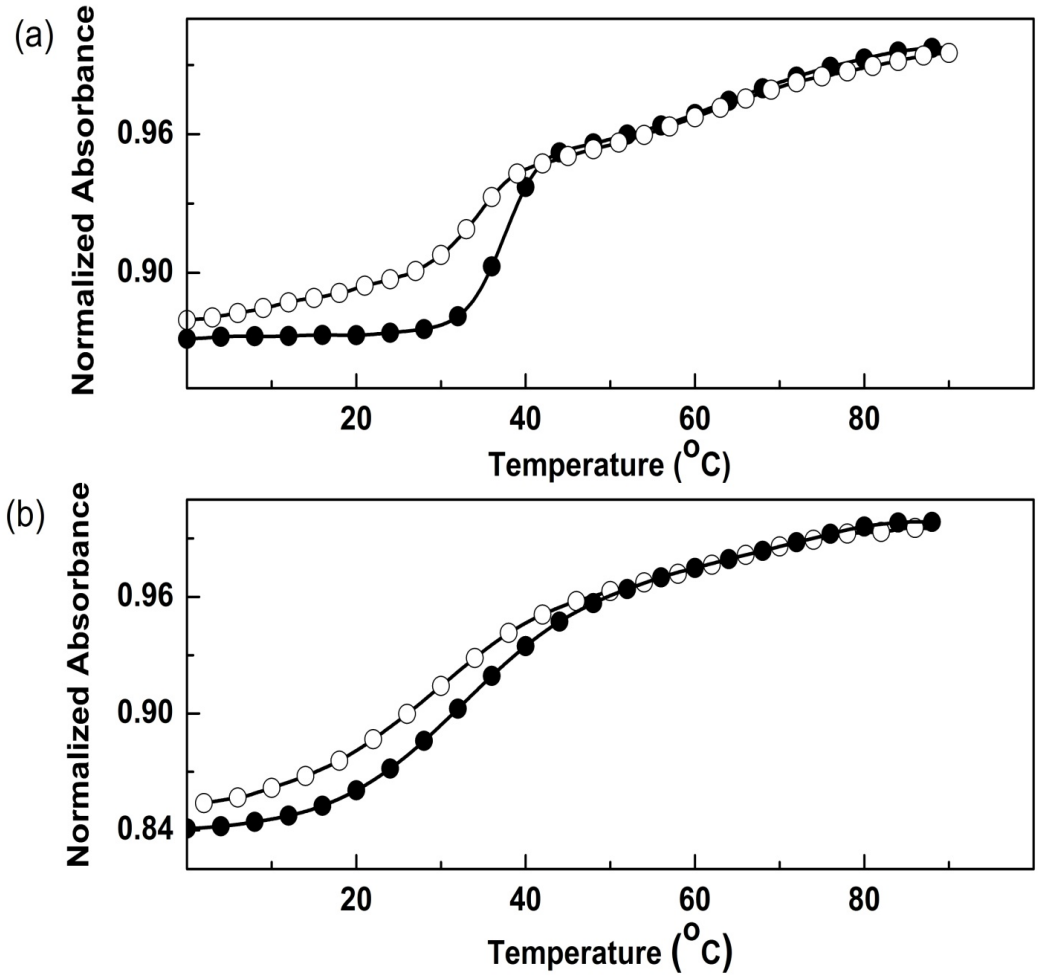


Figure 20. UV melting curves in 10 mM sodium phosphate buffer (pH 7.0) ~ 40 μM total strand concentration for (a) DDD (●) at 260 nm and DDD-1 (O) at 275 nm; (b) DD (●) at 260 nm and DD-1 (O) at 275 nm.

Table 2. Thermodynamic Profiles for the Formation of Duplexes at 20°C.[a]

Oligodeoxynucleotide	NaCl [b]	T_M [c]	$\Delta G°$ [d,e]	ΔH [e]	$T\Delta S$ [e]	Δn_{Na+} [f]	Δn_w [f]
DDD	10	33.3	-6.9	-116.0	-109.1	-2.3 ± 0.2	-38.0 ± 2.0
	100	57.7	-15.5	-109.5	-94.0	-1.8 ± 0.1	-30.0 ± 2.0
DDD-1	10	34.5	-4.6	-76.0	-71.4	-1.4 ± 0.1	-19.0 ± 2.0
	100	49.5	-10.4	-74.0	-63.6	-1.1 ± 0.1	-15.0 ± 2.0
DD	10	29.5	-5.6	-80.1	-74.5	-2.2 ± 0.2	-30.0 ± 4.0
	100	53.0	-8.2	-72.3	-64.1	-1.7 ± 0.1	-22.0 ± 3.0
DD-1	10	26.1	-3.8	-56.4	-52.6	-1.5 ± 0.2	-17.0 ± 2.0
	100	47.5	-5.7	-54.1	-48.4	-1.3 ± 0.1	-14.0 ± 2.0

[a]Parameters are measured from UV (T_M) and DSC melting curves in 10 mM sodium phosphate buffer (pH 7.0). The observed standard deviations are: T_M (± 0.5), ΔH_{cal} (± 3%), $\Delta G°_{20}$ (± 5%), $T\Delta S_{cal}$ (± 3%). [b]Salt concentration in mM. [c] °C. [d] Determined at 20 °C. [e]kcal/mol. [f] per mol DNA.

DSC of the 7-deaza-dA-Modified Duplexes

The DSC melting curves for the DDD and DDD-1 dodecamers and the DD and DD-1 decamers are shown in Figure 21, and the thermodynamic profiles are listed in Table 2. At the lower salt concentration (16 mM Na^+), the helix–coil transition was biphasic for the dodecamers. The DDD unfolded via a broad first transition and a sharper second transition. The biphasic DSC thermogram of DDD-1 revealed a broad peak with a shoulder for the first transition at lower temperature that could not be resolved. At increased salt concentration, the dodecamers unfolded via monophasic transitions. This was attributed to higher screening by salt on the duplex phosphates, relative to the phosphates of the hairpin. This shifts the duplex transition to higher temperatures,

confirming the helix → hairpin → random coil transitions of each dodecamer duplex, which was observed in the UV melting studies. For the decamers, the helix–coil transitions were monophasic, confirming their unfolding through a duplex to random coil transition as seen in the UV studies. Enthalpies were determined by deconvolution of the DSC graphs; however, only the model-independent enthalpies of the duplex → random coil transitions are reported in Table 2.

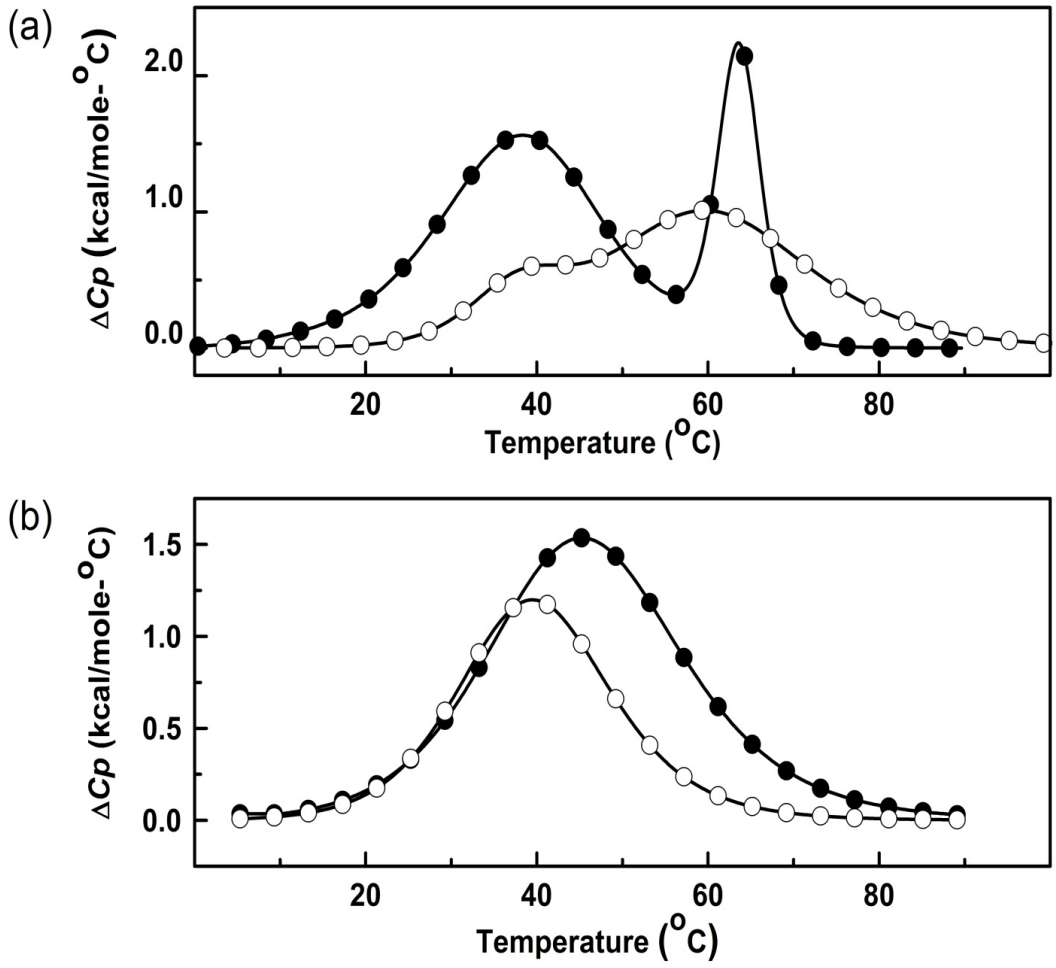


Figure 21. DSC curves in 10 mM sodium phosphate buffer (pH 7.0): (a) DDD (●) and DDD-1 (O) at ~200 μM (b) DD (●) and DD-1 (O) at ~300 μM.

The dA to 7-deaza-dA substitution was destabilizing at both low and high salt concentrations. Analysis of thermograms of dodecamers revealed decreased endothermic enthalpies of 40.0 and 35.5 kcal/mol for DDD-1 relative to DDD in 10 and 100mM NaCl, respectively (Table 3). For decamers, endothermic enthalpies of 80.1 kcal/mol for DD and a reduced unfolding enthalpy of 56.4 kcal/mol for DD-1 (Table 3) were obtained at low salt. At the higher salt concentration, the $\Delta\Delta H$ was 18.2 kcal/mol for DD vs. DD-1.

Table 3. Differential Thermodynamic Profiles for Pairs of Dodecamer and Decamer Duplexes.

NaCl[a]	$\Delta\Delta H$ [c]	$\Delta\Delta G°$ [b,c]	$\Delta(T\Delta S)$ [c]	$\Delta\Delta n_{Na+}$ [d]	$\Delta\Delta n_w$ [d]
Substitution of dA[6] with 7-deaza-dA in DDD (DDD-1 minus DDD)					
10	40.0	2.3	37.7	0.9	19.0
100	35.5	5.1	30.4	0.7	15.0
Substitution of dA[5] with 7-deaza-dA in DD (DD-1 minus DD)					
10	23.7	1.8	21.9	0.7	13.0
100	18.2	2.5	15.7	0.4	8.0

[a] Salt concentration in mM. [b] Determined at 20 °C. [c] kcal/mol. [d] per mol DNA.

Thermodynamic Profiles for the Formation of Each Duplex

The thermodynamic data is provided in Table 2. The favorable Gibbs free energies, indicating spontaneous formation of each duplex, resulted from compensation of favorable enthalpy and unfavorable entropy contributions. The favorable enthalpies arose from the formation of base pairs and base pair stacks, uptake of electrostricted

waters, and release of structural waters, whereas the unfavorable entropy terms included the ordering of two strands to form a duplex, condensation of counterions, and immobilization of waters.

Relative to the unmodified oligodeoxynucleotides, the 7-deaza-dA modified oligodeoxy-nucleotides were destabilized at low and high salt concentrations. The inclusion of two 7-deaza-dA modifications in DDD-1 yielded a decrease in ΔG of 2.3 and 5.1 kcal/mol in 10 and 100 mM NaCl, respectively, whereas in decamers ΔG decreases of 1.8 and 2.5 kcal/mol in low and high salt, respectively, were observed following two 7-deaza-dA substitutions.

Differential Association of Water Molecules

T_M dependencies on water activity were studied to determine the thermodynamic association of water molecules to DNA duplexes. By increasing concentrations of the osmolyte ethylene glycol from 0.5 to 4.0 m the activity of water was decreased. The UV melting curves showed that the T_Ms of the dodecamers (DDD and DDD-1) and decamers (DD and DD-1) decreased linearly with increasing osmolyte concentrations (i.e., decreasing activity of water). The T_M dependence on water activity of dodecamers and decamers are shown in Figure 22. The slopes of these lines, $\partial T_M/\partial \log a_w$, in conjunction with the $\Delta H/RT_M^2$ term, were used to obtain the differential association of water molecules. The Δn_w values for the formation of each duplex in 10 mM NaCl are shown in Table 2. Water uptake values, expressed as mol H_2O per mol duplex, measured in low salt, were 38 (DDD) and 19 (DDD-1) for dodecamers, and 30 (DD) and 17 (DD-1) for

decamers. At the higher salt concentration (116 mM Na^+), Δn_w values followed a similar trend. Lower Δn_w values at this salt concentration (Table 2) were due to increased screening of the water dipoles at higher salt concentration. The overall effect, and assuming that the random coil states of all the duplexes behave similarly at higher temperature, was that the substitution of 7-deaza-dA into duplex DNA caused a decreased association of water molecules. For instance, there was a $\Delta\Delta n_w$ of 19 and 15 between DDD and DDD-1 at 10 mM and 100 mM NaCl, respectively, and $\Delta\Delta n_w$ of 13 and 8 between the pair of decamer duplexes at low and high salt, respectively (Table 3). Parameters used to calculate differential water binding for dodecamers are shown in Table 4.

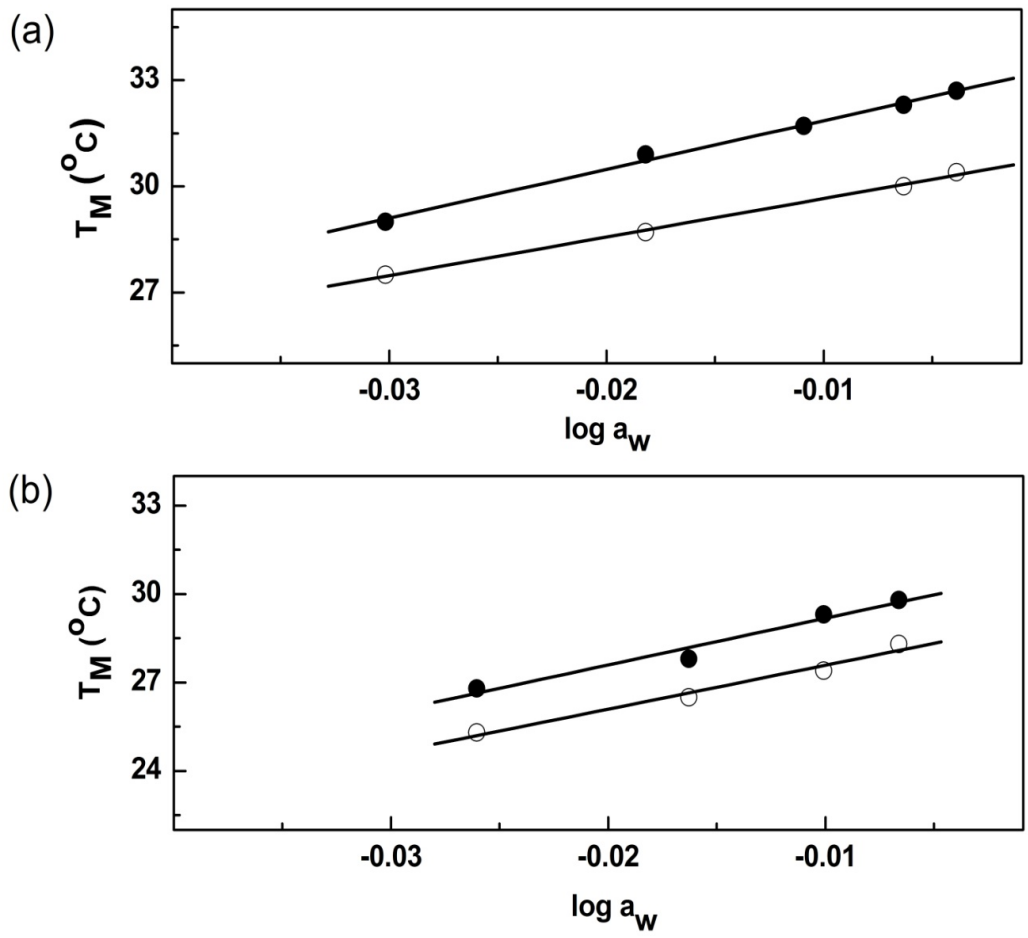


Figure 22. T_M dependence on osmolyte concentration (as a function of ethylene glycol) for duplexes in 10 mM sodium phosphate buffer (pH 7.0), ~ 5μM strand concentration for (a) DDD (●) and DDD-1 (○) and ~ 7μM strand concentration for (b) DD (●) and DD-1 (○).

Table 4. Parameters used to calculate differential water binding for dodecamers.[a]

Oligodeoxynucleotide	NaCl (mM)	$\Delta H_{cal}/RT_M^2$ (°C)	$\partial T_M/\partial \log a_w$ (°C)	Δn_w (mol^{-1}) DNA
DDD	10	0.62		
	100	0.50	7.49	-53.0 ± 5.0
	100 (EG)	0.40		
7-deaza-dA DDD	10	0.40		
	100	0.32	7.41	-26.0 ± 4.0
	100 (EG)	0.28		

[a]The slopes of T_M vs log a_w were obtained by least-square analysis. The values of $\Delta H/RT_M^2$ represent an average of three determinations in each salt concentration while $\partial T_M/\log a_w$ was determined at 100 mM sodium phosphate buffer (pH 7.0).

Differential Association of Counterions

UV melting curves at salt concentrations ranging from 16 to 216 mM [Na^+] were measured to examine the thermodynamic association of counterions with the DNA duplexes. The T_M values of the DDD and DDD-1 dodecamers, and DD and DD-1 decamers increased linearly with salt concentration (Figure 23), consistent with the expectation that the duplex states should have higher charge density parameters. The T_M dependence on salt concentration for dodecamers and decamers are shown in Figure 23, panels a and b, respectively. The slopes of these lines, $\partial T_M/\partial \log[Na^+]$, in conjunction with the experimentally determined $\Delta H/RT_M^2$ terms, allowed measurement of differential counterion binding. The Δn_{Na^+} values for the formation of each duplex, from the association of two complementary strands, in low and high salt are shown in Table 2.

In low salt, the Na^+ uptake as measured in mol Na^+ per mol duplex was 2.3 for the DDD dodecamer and 1.4 for the DDD-1 dodecamer, and 2.2 for the DD dodecamer and 1.5 for the DD-1 decamer. The Δn_{Na^+} values at the higher salt concentration of 116 mM showed a similar trend; however, the values were lower due to the higher screening of the phosphates by salt (Table 2).

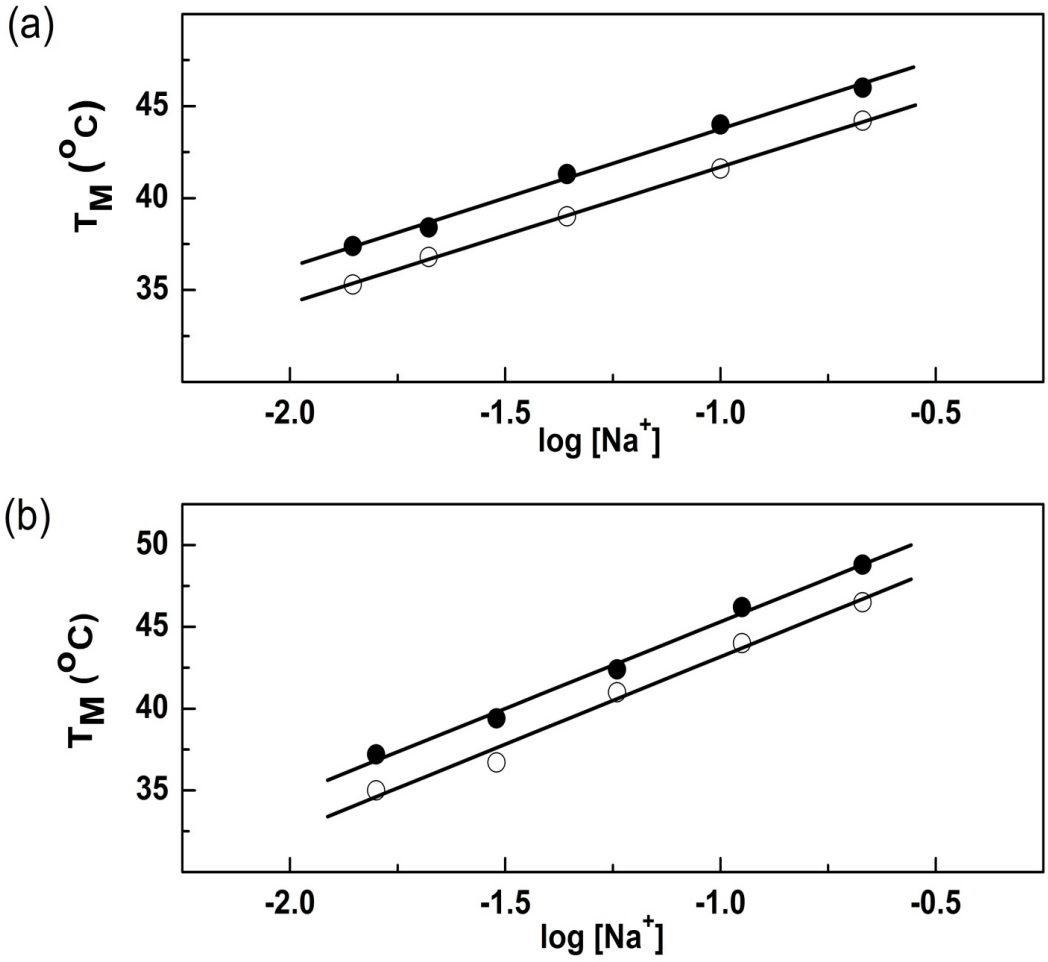


Figure 23. T_M dependence on salt concentration for duplexes in 10 mM sodium phosphate buffer (pH 7.0), ~ 5μM strand concentration for (a) DDD (●) and DDD-1 (○) and ~ 7μM strand concentration for (b) DD (●) and DD-1 (○).

The average differential Na^+ uptake as measured in mol Na^+ per mol phosphate was estimated as 0.094 (DDD and DD) in this range of salt concentration, which was consistent with the fact that these oligodeoxynucleotides were not behaving electrostatically as long polyelectrolytes (*61*). However, the main effect, assuming that the random coil states of the different single strand oligodeoxynucleotides were thermodynamically similar at higher temperatures, was that the introduction of 7-deaza-dA into the duplex DNA caused a slightly decreased association of counterions. For instance, there was a $\Delta\Delta n_{Na}^+$ of 0.9 and 0.7 between DDD and DDD-1 at 10 and 100 mM NaCl, respectively, and $\Delta\Delta n_{Na}^+$ of 0.7 and 0.4 between the pair of decamer duplexes at low and high salt, respectively (Table 3). Parameters used to calculate differential counterion binding for dodecamers are presented in Table 5.

Table 5. Parameters Used to Calculate Differential Counterion Binding for Dodecamers.[a]

Oligodeoxynucleotide	NaCl (mM)	$\Delta H_{cal}/RT_M^2$ (°C)	$\partial T_M/\partial \log[Na^+]$ (°C)	Δn_{Na+} (mol^{-1}) DNA
DDD	10	0.62	7.49	-2.3 ± 0.15
	100	0.50		-1.8 ± 0.12
7-deaza-dA DDD-1	10	0.40	7.41	-1.4 ± 0.14
	100	0.32		-1.1 ± 0.12

[a] Data obtained in 10 mM sodium phosphate at pH 7.0 adjusted to the desired ionic strength with NaCl.

Discussion

It has been assumed that 7-deaza-dA, an isostere for dA in duplex DNA, does not substantially perturb the duplex, and thus provides a good model for dA. However, in light of suggestions that 7-deaza-dA introduces a large structural perturbation to the B-form of poly(dA-dT)•poly(dA-dT) (*31*), it was of interest to provide a comprehensive characterization of B-DNA with a 7-deaza-dA modification. The Dickerson–Drew dodecamer (*32, 33*) provides a well-characterized system suitable for detailed crystallographic analysis (*9*), as well as NMR analysis (*57, 62, 63*), The present studies provide the first high-resolution crystallographic data for the substitution of adenine with 7-deaza-dA in duplex DNA.

Structure of the 7-Deaza-dA:dT Base Pair

The structure of the 7-deaza-dA:dT base pair in the DDD duplex reveals that 7-deaza-dA has minimal effect on duplex conformation (Figure 9) and base pair geometry (Figure 10) as compared to a canonical dA:dT base pair. Substitution of 7-deaza-dA changes the electronegative N7-dA atom to a carbon atom, which alters the electrostatics of the nucleobase. Consistent with this expectation, the downfield shift of the T^7 imino resonance (Figure 19) is attributed to stronger hydrogen bonding with the more electronegative 7-deaza-dA N1 nitrogen. Thus, the observed destabilization of 7-deaza-dA does not result from a decrease in H-bonding but must be due to other changes induced by the perturbation of the electrostatic potential in the major groove. Other NMR chemical shift perturbations are minimal, which indicates that the modification does not affect the structure at the flanking nucleotides. Our results differ

from those of Pope et al. (*31*), who suggested that replacement of dA by 7-deaza-dA caused perturbations to B-DNA for the poly[d(7-deaza-dA-T)]•poly[d(7-deaza-dA-T)] duplex. The physical properties of poly(dA-dT) differ from the DDD, and it may be of interest to look for structural perturbations induced by 7-deaza-dA in other sequences.

7-Deaza-dA Enthalpically Destabilizes the DDD

The 7-deaza-dA substitution thermodynamically destabilizes the DDD-1 and DD-1 duplexes, compared to the unmodified DDD and DD duplexes. This is evidenced by the $\Delta\Delta G$ values (computed as the average of 10 and 100 mM [Na^+], Table 3). At 20 °C, $\Delta\Delta G$ is decreased by 3.7 kcal/mol for DDD-1 and by 2.2 kcal/mol for DD-1. In both cases, the major contributor to the reduced $\Delta\Delta G$ values is the enthalpy term, which drops 37.8 kcal/mol for DDD-1 and 20.9 kcal/mol for DD-1 (Table 3). The differential $\Delta\Delta H$ values at different salt concentrations suggest the presence of heat capacity effects. The heat capacity values were 0.8 kcal/K mol (DDD) and –0.08 kcal/K mol (DDD-1), and –0.5 kcal/K mol (DD) and –0.2 kcal/K mol (DD-1). These may be due to exposures of nonpolar groups to solvent and/or to changes in structural hydration between the random coil and duplex states of DDD-1 and DD-1 (*64*). The present data lead to a different conclusion than did studies of $(7\text{-deaza-dA})_{11}A\bullet T_{12}$ as compared to $dA_{12}\bullet dT_{12}$, conducted by Seela and Thomas (*30*). They concluded that destabilization induced by 7-deaza-dA was minimal and was associated with an unfavorable entropy change (*30*). It should be noted, however, that the DDD presents a different sequence context than does the A-tract $dA_{12}\bullet dT_{12}$ sequence (*65*).

Base Stacking Effects

The most significant contribution to the unfavorable $\Delta\Delta H$ term (Table 3) of 32.7 kcal/mol for DDD-1 (17.6 kcal/mol for DD-1) results from a reduction of stacking enthalpy in the modified duplexes, attributed to less favorable π–π interactions involving the pyrrolopyrimidine ring of 7-deaza-dA and the neighboring base pairs vs. adenine. In the CD spectra, the intensities of the negative bands near 250 nm are thought to track base stacking contributions. The band intensities at 250 nm are consistent with reduced base stacking in DDD-1 and DD-1 at low temperature (Figure 16). There is an 18% decrease in the intensity of the 250 nm band for DDD-1 relative to DDD. The decreased intensity of the 250 nm band for DD-1 relative to DD is 10%. However, changes in the electronic structure of 7-deaza-dA may modulate the relative optical dipole orientations responsible for the CD bands. Exchange-mediated line broadening of DNA imino protons is often associated with the rate-limiting formation of an open state of the base pair in which the imino proton is freed from its hydrogen bond and is accessible to the base that catalyzes the proton exchange (*66-70*). The increased broadening of the $Y^6 \bullet T^7$ base pair thymine N3 imino resonance (Figure 19) is consistent with this model, which correlates with reduced stacking enthalpy of the DDD-1 duplex relative to the DDD duplex. However, the possibility that base pair opening is not rate-limiting cannot be ruled out, with the line broadening reflecting a more rapid hydrogen exchange catalysis for the substituted duplex (*71*). In this regard, the C7–H on the 7-deaza-dA (as compared to the: N7 on the natural dA) would be anticipated to exhibit a reduced electrostatic repulsion with hydroxide or phosphate base catalyst.

Duplex Hydration

The unfavorable $\Delta\Delta H$ term observed upon incorporation of 7-deaza-dA is partially attributed to reduced hydration of the modified duplexes. This may, in part, be due to the more hydrophobic major groove edge of 7-deaza-dA as compared to dA. Thus, 7-deaza-dA substitution results in a $\Delta\Delta n_W$ of 17 H_2O per mol DNA for DDD-1 and 11 H_2O per mol DNA for DD-1 (obtained by averaging the data obtained in 10 and 100 mM NaCl, Table 3). This "translates" into a reduction of approximately 9 H_2O per mol DNA per 7-deaza-dA nucleotide for the DDD-1 duplex and 6 H_2O per mol DNA per 7-deaza-dA nucleotide for the DD-1 duplex, assuming localized effects. A release of 17 water molecules from the DDD-1 duplex (11 water molecules from the DD-1) accounts for an unfavorable enthalpy term $\Delta\Delta H$ of 5.1 kcal/mol (3.3 kcal/mol for the DD-1) (*72*). The release of waters indicates increases in the volumes of the modified systems, i.e, positive $\Delta\Delta V$ terms. Since $\Delta\Delta G$ is also positive, this indicates release of electrostricted waters from DDD-1 and DD-1 (*73*). There may also be a compensating increase of structural water due to the more hydrophobic major groove edge of 7-deaza-dA. Another way to interpret the data is that the displacement of water by ethylene glycol, used in the osmotic stress experiments, near 7-deaza-dA will be more facile than at dA because of the reduced electrostatic interaction with solvent. In any case, similar reductions in hydration were observed for DNA modified with 7-deaza-dG nucleotides (*16*).

Cation Binding

The introduction of the 7-deaza-dA:dT pair into the DDD causes a decrease in the differential association of cations. This is reflected in the $\Delta\Delta n_{Na^+}$ of 0.9 and 0.7 between

DDD and DDD-1 at 10 and 100 mM NaCl, respectively, and $\Delta\Delta n_{Na^+}$ of 0.7 and 0.4 between the pair of decamer duplexes at low and high salt, respectively. The reduced uptake of Na^+ is not attributed to the loss of a major groove high affinity cation binding site near the 7-deaza-dA nucleotide. High-resolution crystallographic structures of the DDD (*32, 33*) provide insight into the sequence-dependent distribution of waters and counterions in B-DNA (*9, 51, 74-83*). When the DDD was crystallized in the presence of Tl^+, no high-occupancy cation binding sites were observed in the major groove near A^6. Likewise, Tereshko and Egli (*9*) did not observe a high affinity cation site near A^6. In the present crystallographic unit cell two Mg^{2+} ions interact with the DNA, but they are not associated with the major groove edge of either Y^6 or Y^{18} (Figure 9 and 12). This is consistent with the notion that cation binding in A-T tracts occurs in the minor groove (*79*). It seems possible that the thermodynamically measured decrease in the association of cations could be due to the disruption of nonspecific cation binding, particularly in the minor groove. In any case, the contribution to the large $\Delta\Delta H$ term for the release of counterions is anticipated to be negligible since counterion release contributes predominantly to the $\Delta(T\Delta S)$ term (*84*). In contrast, the major groove high-affinity cation sites in the DDD were associated with the major groove edge of dG nucleotides (*80*). Indeed, the incorporation of 7-deaza-dG into the DDD was accompanied by changes in hydration and major groove cation organization (*16*).

Summary

Introduction of the 7-deaza-dA:T base pair into the DDD has minimal effect upon base pairing geometry and DNA conformation, as evidenced by a combination of

crystallographic and NMR studies. The 7-deaza-dA retains Watson–Crick hydrogen bonding, but the 7-deaza-dA:dT base pair is thermodynamically destabilized. A detailed analysis reveals that this is due to primarily to unfavorable enthalpy terms, which are dominated by less favorable stacking interactions, resulting from changes in the base electrostatics and electronic dipole–dipole interactions. There is also a net release of electrostricted waters from the duplex. The introduction of the 7-deaza-dA:dT pair into the DDD causes a decreased association of cations, which is reflected in the $T\Delta S$ term.

Acknowledgments

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CHAPTER III

RECOGNITION OF 0^6-BENZYL-2'-DEOXYGUANOSINE BY A PERIMIDINONE-DERIVED SYNTHETIC NUCLEOSIDE (dPER): A UNIQUE DNA INTERSTRAND STACKING INTERACTION

Introduction

Use of NMR in structure refinement of nucleic acids

Nuclear Magnetic Resonance (NMR) Spectroscopy is a principal technique used to determine three-dimentional structures of small molecules, proteins, and nucleic acids in solution. Nuclear magnetic resonance is based upon the magnetic properties of certain atomic nuclei when they are exposed to magnetic fields (*85*). The most important nuclei for biomolecular NMR are: protons (^{1}H), carbons (^{13}C), nitrogens (^{15}N) and phosphorus (^{31}P). Nuclear Magnetic Resonance was discovered in 1946, but the real application to macromolecules started after two major two major breakthroughs in the 1970s: Fourier transformation (FT) NMR, allowing rapid recording of NMR signals, and two-dimensional NMR spectroscopy, dramatically increasing spectral resolution. These advances and the development of stable magnets at higher fields led to extensive investigations using NMR to determine the three-dimensional structures of macro-molecules. X-ray crystallography is one of methods for structure determination, but NMR provides complementary structural information in a more physiologically relevant solution environment. Moreover, since some biomolecules are difficult to crystallize,

NMR can be used as an alternative method for obtaining three-dimensional structures. NMR allows structural studies in solution, which avoids experimental artifacts such as crystal packing. NMR spectroscopy can provide information about protein dynamics, flexibility, and folding/unfolding transitions (*86*).

For structural elucidations of nucleic acids, two 2D NMR experiments are important. In the ^{1}H homonuclear correlation spectroscopy (COSY) experiment, interactions (scalar couplings) through bonds between protons are observed, up to three bonds. Of the DNA bases, cytosine has two hydrogens (H5 and H6) connected by three bonds, which give cross peaks in the COSY spectrum. Those cross peaks are used to identify the cytosine cross peaks in the sequence. In the COSY spectrum cross peaks between sugar protons within one nucleotide are also observed. From the COSY spectrum *J* coupling constants between atoms can be calculated. They provide geometric information between the atoms in molecule. The most useful are vicinal scalar coupling constants, ^{3}J, between atoms separated from each other by three covalent bonds. The relation of the vicinal coupling constant and the dihedral angle θ is defined by Karplus equation:

$$^{3}J(\theta) = A\cos^{2}\theta + B\cos\theta + C \quad (4)$$

In this equation, *A*, *B*, and *C* are coefficients for various types of couplings, and θ is the dihedral angle. Those torsion angles are used as back-bone and sugar restraints for restrained molecular dynamics (rMD) calculations (*86*).

The most important experiment is ^{1}H homonuclear Nuclear Overhauser Effect spectroscopy (NOESY) experiment (*44, 45*). In the NOESY spectrum, dipole-dipole interactions are observed between nuclei. Dipolar interactions are through space effects in which one nuclear magnetic dipole interacts with the local field of the second nuclear dipole. NOEs are the most important NMR parameters for structure determination because they provide short-range as well as long-range distance information between pairs of hydrogen atoms separated by less than 5 Å. The intensity of an NOE (I) is related to the distance r between the proton pair, $I = f(\tau_c) < r^{-6} >$ in which $f(\tau_c)$ is a function of the rotational correlation time τ_c of the molecule. Because of variable τ_c for different molecules, it is common to use intensity I (or cross-peak volume) to obtain qualitative distance information. The more intense cross peak that is observed, the shorter is the distance between the two hydrogens. The r^{-6} distance dependence is key to structural refinement. For a rigid molecule the distances and angles are constant and if we assume isotropic rotational tumbling with time constant τ_c, we obtain:

$$J_{ij}^{n}(\omega) = \frac{1}{4\pi} \times \frac{1}{r^6} \left(\frac{\tau_c}{1 + \omega^2 \tau_c^2} \right) \quad (5)$$

This is the simplest motional model for relaxation, in which ω is the proton Larmor frequency, τ_c is the correlation time and r is the distance between spins i and j. If we can measure the cross-peak intensities accurately for a small mixing time, we have as a linear approximation to $\exp(-\mathbf{R}\tau_m)_{ij}$, $i \neq j$:

$$I_{ij} = - R_{ij}\tau_m \qquad (6)$$

and the intensities (I) are directly proportional to the relaxation rates (R).

In NOESY spectra some problems exist such as overlapped peaks, and the intensities of the peaks at short mixing times may be influenced by noise such that longer distances may be significantly underestimated, often by more than 1 Å. Assigning deliberately conservative distance bound, can offset these difficulties. This however, can entail a significant loss of information (*87*).

Steps for NMR solution structure determination are shown in Figure 24. Experimental constraints used in restrained molecular dynamics (rMD) calculation are determined from NMR experiments. First, NOESY and COSY spectra for DNA samples are collected. In order to see non-exchangeable hydrogens D_2O solution is used for data collection. For exchangeable hydrogens 90% H_2O/10% D_2O solution is used. The NOESY spectrum can be assigned based on the H6/H8-H1' region, in which sequential connectivities between aromatic hydrogens and deoxyribose H1' hydrogens can be assigned (Figure 25). The COSY spectrum is used to confirm the cytosine positions in the sequence. Standard procedures for assignment of non-exchangeable hydrogens in the NOESY spectrum of DNA are established (*58, 88*). Dipolar interactions between the aromatic hydrogen of the 5'-nucleotide gives a cross peak to its sugar H1' proton, the sugar H1' then gives a cross peak to the 3'-nucleotide's aromatic hydrogen. Using this method, interactions from the 5' to the 3' end of the DNA strand can be assigned. Figure 26 shows sequential assignment of protons in H6/H8-H1' region of the NOESY spectrum.

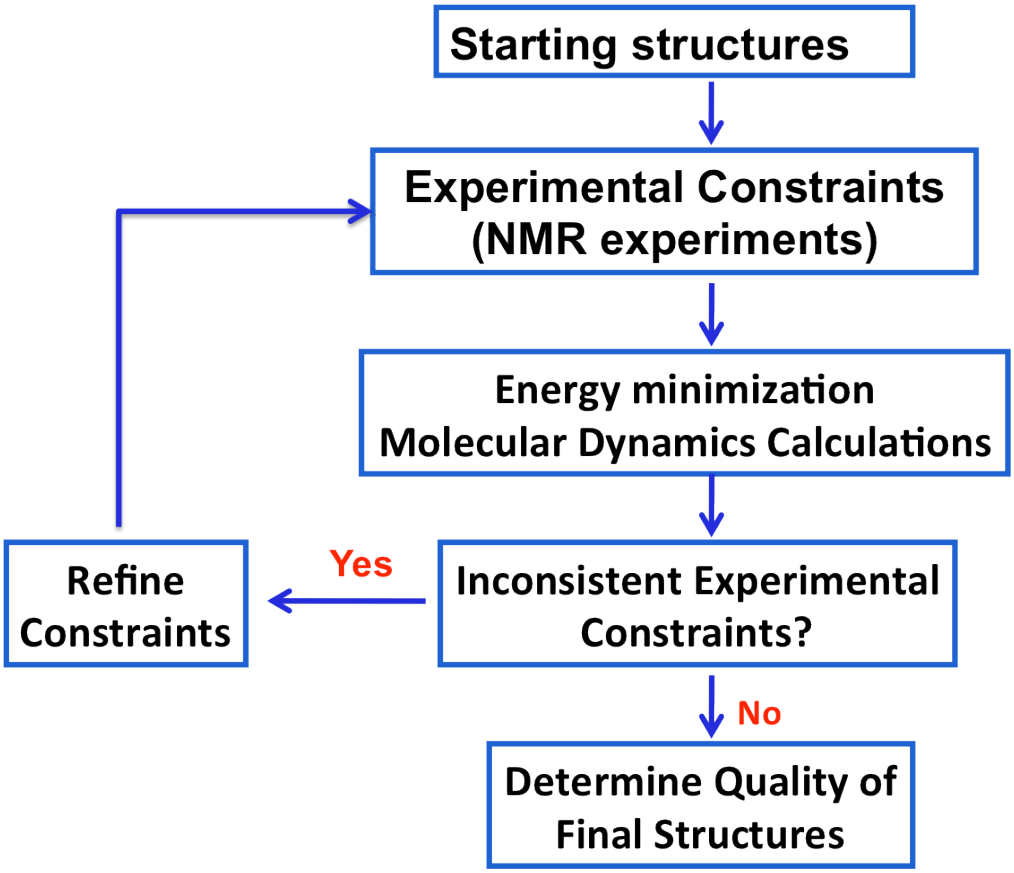


Figure 24. Overview of a solution structure determination process.

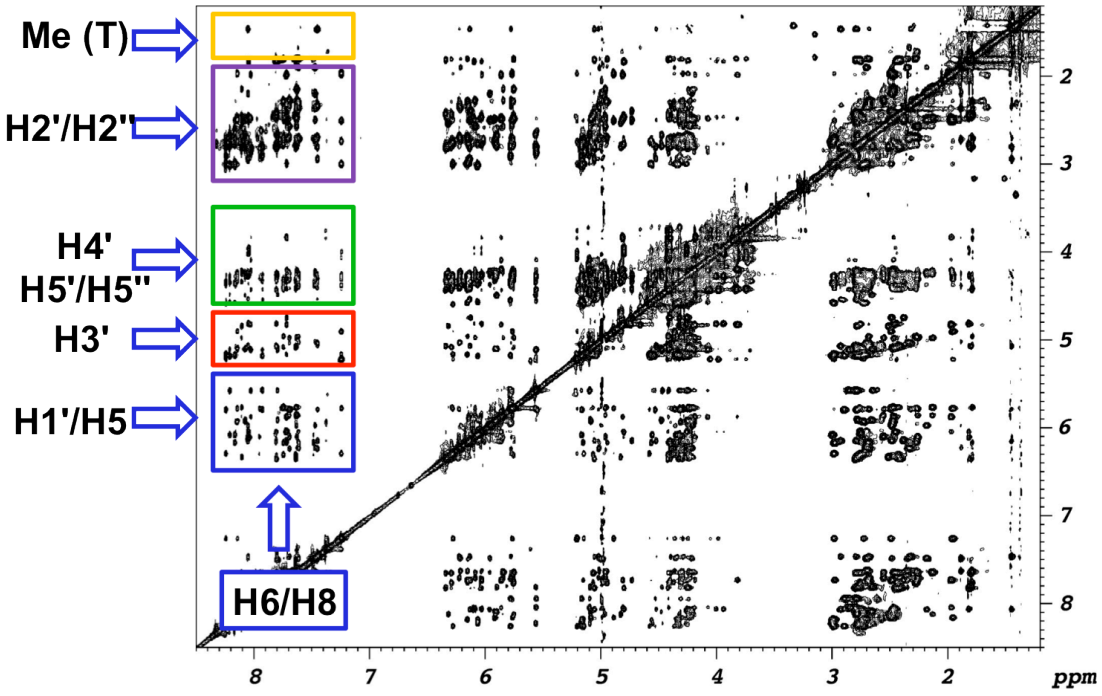


Figure 25. NOESY spectrum of DNA duplex with selected regions of interactions between base and sugar hydrogens. Region H6/H8 to H1' is shown in blue rectangular.

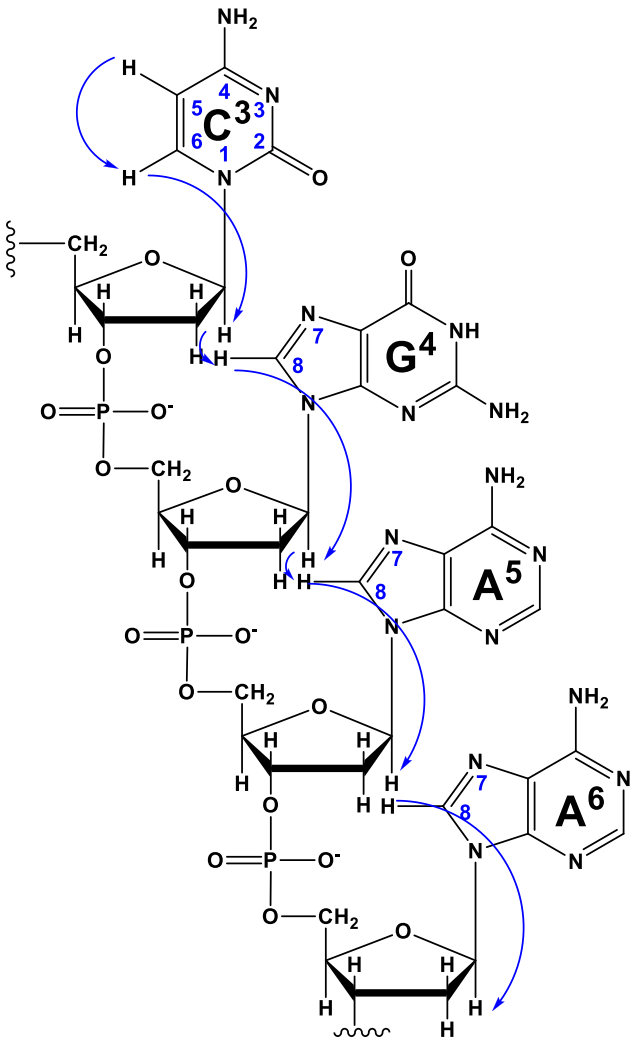


Figure 26. Sequential assignment of H6/H8 aromatic hydrogen to sugar H1' from 5' (top) to 3' (bottom) end of the DNA strand.

The SPARKY (*89*) program can be used for assignments and integrations of the cross peaks. It also generates output files for restrained molecular dynamics calculations. When the entire spectrum is assigned, cross peak volumes are measured and converted to distance restraints for rMD calculations using the program MARDIGRAS (*90*).

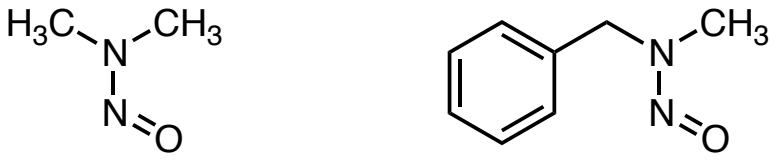
In the NOESY spectrum collected in 90% H_2O/10% D_2O solution we can see cross peaks between imino and amino protons within the duplex are observed. The sequential connectivity of the base imino protons can be obtained using established methods (*60*). This data provides information about base-stacking and base-pairing in the DNA duplex. Experimental NMR restraints are used along with empirical restraints for restrained molecular dynamics (rMD) calculations.

For rMD calculations, a model of DNA is used as a starting structure. It can be created by a graphical program such as INSIGHT II (Accelrys Inc., San Diego, CA), Coot (*91*), Pymol (*92*), or MOE (*93*). The model may also be obtained from the PDB databank (www.rcsb.org). Next, the model is energy minimized, and then restrained molecular dynamics calculations using a simulated annealing protocol are used (*94*). The program AMBER (*95*) with the parm99 force field can be used for calculations. Force constants are applied for all restraints. Coupling of the molecule to the bath temperature is used to control the temperature during simulated annealing. A typical simulating annealing protocol is as follows. First, the system is heated from 0 to 600 K, then kept at 600 K and slowly cooled from 600 K to 0 K. This allows the molecule to sample conformational space in order to find the conformation with the lowest energy of the molecule, consistent with the experimental restraints. Structure coordinates are saved after each cycle, and are subjected to potential energy minimization. Refined structures calculated from the different starting structures are chosen based on the lowest deviations from the experimental distance and dihedral restraints and energy minimized. They may be averaged to obtain an average structure. Complete relaxation matrix analysis (CORMA) (*96, 97*) is used to compare intensities calculated from these emergent

structures with the distance restraints. Helicoidal analysis is performed using the CURVES+ web server (*98*).

O^6-Benzyl-2'-Deoxyguanosine Adduct - *DNA Alkylation Product of Guanine*

DNA is constantly exposed to chemicals which can covalently modify its structure (*99*). There are endogenous and exogenous sources of alkylating agents. Food-derived nitrosamines like *N*-nitrosodimethylamine or *N*-nitrosobenzylmethylamine are examples of exogenous alkylating agents (Figure 27). Other examples of exogenous alkylating agents include tobacco-specific nitrosamines and chemotherapeutic agents such as temozolomide and streptozotocin (*100*).



NDMA
N-nitrosodimethylamine

NBzMA
N-nitrosobenzylmethylamine

Figure 27. Chemical structures of two examples of nitrosoamines.

Alkylating agents can modify all the bases and the DNA backbone (*101-103*). The adducts formed can be mutagenic or toxic, and therefore need to be efficiently removed. The N7 position on guanine is the most vulnerable site on DNA. The N3 and O^6 positions on guanine can be alkylated as well as can the N7 and N3 positions on adenine (Figure 28). The products of alkylation on different bases vary, depending on the alkylating agent.

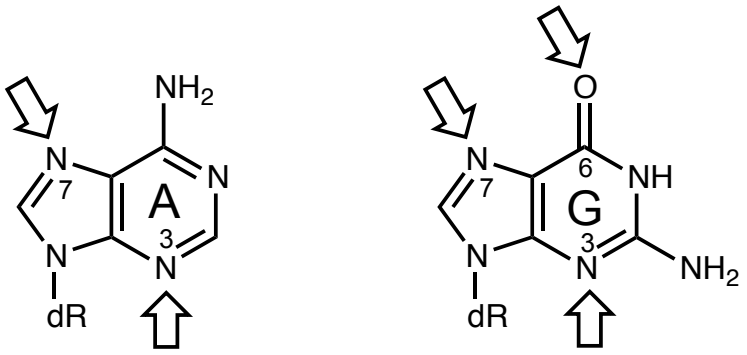


Figure 28. Alkylation sites on adenine (left) and guanine (right) bases.

Guanine O^6 position alkylation products (O^6-Alkyl-dG), such as O^6-methylguanine or O^6-benzylguanine are genotoxic (*104-106*) and mutagenic. O^6-Alkyl-G pairs with thymine to give G:C to A:T transition mutations (*107, 108*). Those adducts are repaired by the O^6-alkylguanine-DNA alkyltransferase family of proteins (*109-111*). Examples of O^6-alkyl-dG adducts are shown in Figure 29. The cytotoxic effects of alkylation damage on the O^6 position of guanine are used in cancer therapy. The family of nitrosoureas and O^6-(2-chloroethylating) agents such as carmustine (BCNU) are used as antitumor drugs (*112*).

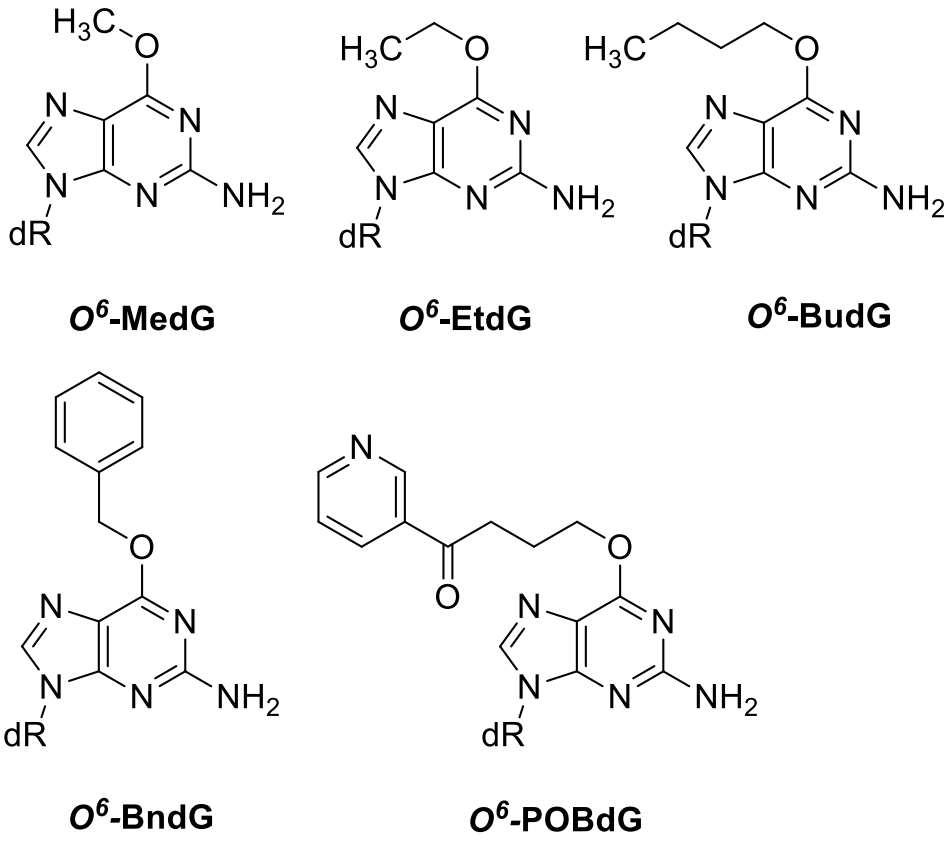


Figure 29. Chemical structures of O^6-Alkyl-dG adducts.

No structure of O^6-Bn-dG in DNA duplex has been reported to date. In the structural analysis of an O^6-Bn-dG modified template•primer complexed with the Y-family polymerase Dpo4, O^6-Bn-dG was observed to form a wobble base pair when placed opposite dC and a pseudo-Watson-Crick hydrogen bonding pattern when placed opposite dT (Figure 30).(*113*) The benzyl ring of the O^6-Bn-dG modified base was located in the major groove of DNA. It had a slightly different conformation for each structure.

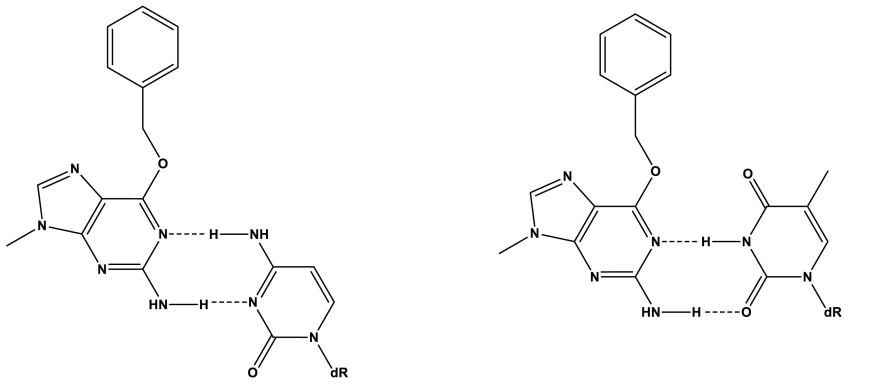


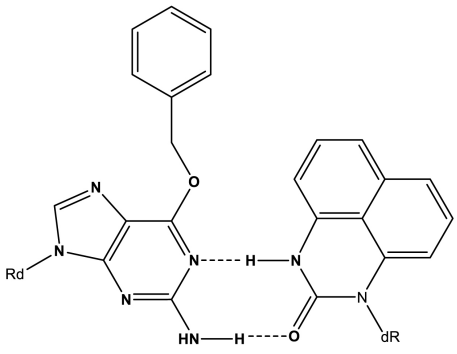
Figure 30. Schematic representation of base pairs observed when O^6-Bn-dG was placed opposite dC and dT in the complex with Dpo4 polymerase.

Synthetic Nucleosides as Chemical Probes

The development of synthetic nucleotides as chemical probes enabling site-specific reporting of damaged DNA is of considerable interest (*114-123*). They can be selectively designed to be specific for particular type of damage. The pyrene nucleoside triphosphate (dPTP) was shown to be efficiently and specifically inserted by DNA polymerases opposite sites that lack DNA bases (abasic sites). The probe can be used to sequence abasic lesions in DNA (*116*). Another example is adenosine-1,3-diazaphenoxazine (Adap) derivative, which can selectively recognize 8-oxo-dG in DNA by potential hydrogen bonding interactions (*124*).

Gong and Sturla (*125*) reported that the synthetic nucleobase 1-[(2*R*,4*S*,5*R*)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-2-yl)-1*H*-perimidin-2(3*H*)-one] (dPer; Figure 31) could

discern the O^6-benzyldeoxyguanosine base (O^6-Bn-dG), formed from guanosine when DNA is exposed to *N*-benzylmethyl-nitrosamine. Understanding the chemical interactions that dictate modified duplex stability is critical to further using nucleosides such as dPer to study these mutagenic lesions. Gong and Sturla (*125*) evaluated the recognition of O^6-Bn-dG by dPer by comparing thermal stabilities of DNA duplexes containing O^6-Bn-dG or dPer paired opposite each other or natural bases. They demonstrated that a duplex containing the O^6-Bn-dG:dPer pair was more stable than any pairing of the damaged base opposite a natural base, or of dPer opposite a natural base (Figure 32). It was hypothesized that this enhanced stability was due to a combination of stacking and hydrophobic interactions with the benzyl ring of the DNA adduct, combined with potential hydrogen bonding interactions between the anti conformation of Per and the N1 and N^2 nitrogen atoms of the alkylated guanine (Figure 31).



O^6-Bn-dG:*anti*-dPer

Figure 31. Proposed schematic interactions between *O*^{6}-Bn-dG and dPer bases.

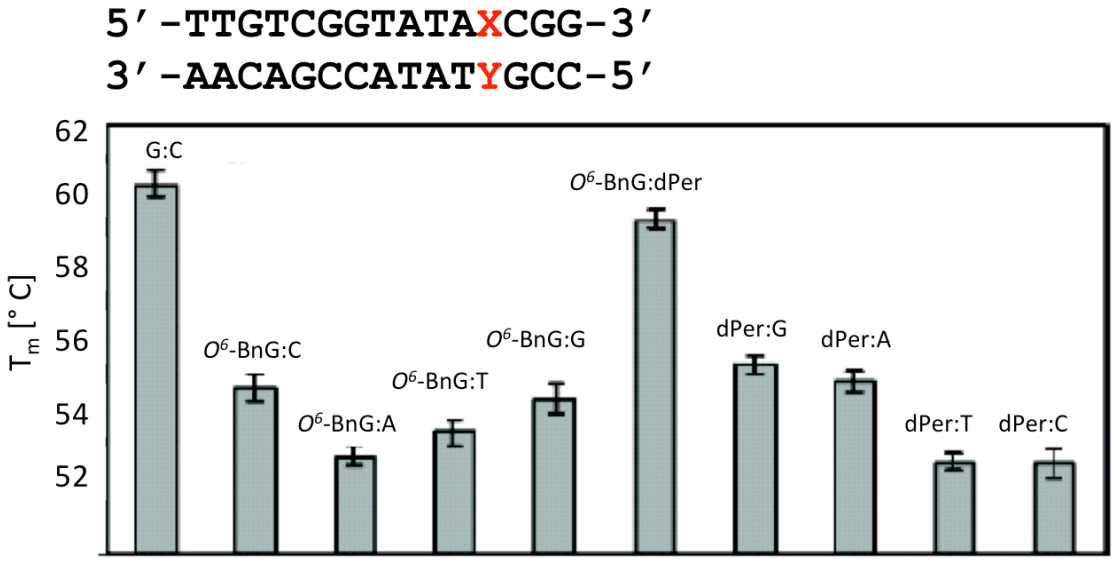


Figure 32. UV thermal stabilities of natural, damaged and dPer DNA. Adapted with permission from Gong, J.; Sturla, S. J. *J. Am. Chem. Soc.* **2007**, *129*, 4882-4883. Copyright (2007) American Chemical Society.

Project Statement

My work explains how dPer distinguishes between dG and O^6-Bn-dG in DNA on the basis of structures of correspondingly modified Dickerson-Drew dodecamers (DDD) (*8*). The crystal structure of the modified DDD, in which guanine at position G^4 has been replaced by O^6-Bn-G and a cytosine C^9 has been replaced with Per to form the modified O^6-Bn-dG•dPer (DDD-XY) duplex [5′-d($C^1G^2C^3\underline{X}^4A^5A^6T^7T^8\underline{Y}^9G^{10}C^{11}G^{12}$)-3′]$_2$ ($\underline{X}$ = O^6-Bn-dG, $\underline{Y}$ = dPer) (Chart 2), reveals that dPer intercalates into the duplex and adopts the *syn* conformation about the glycosyl bond. This interaction provides a binding pocket that allows the benzyl group of O^6-Bn-dG to intercalate between Per and thymine of the 3'-neighbor A•T base pair. NMR data for the O^6-Bn-dG•dPer interaction corroborate the crystallographic results, leading to the conclusion that a similar intercalative recognition mechanism applies in solution. In contrast to the O^6-Bn-dG•dPer structure, the structure of the modified DDD in which cytosine at position C^9 was replaced with Per to form the modified duplex dG•dPer (DDD-GY) [5'-d($C^1G^2C^3G^4A^5A^6T^7T^8\underline{Y}^9G^{10}C^{11}G^{12}$)-3′]$_2$ ($\underline{Y}$ = dPer), reveals that dPer adopts the *anti* conformation about the glycosyl bond and forms a less stable wobble pair with undamaged guanine.

Materials and Methods

Oligodeoxynucleotide Synthesis

The unmodified 5′-dCGCGAATTCGCG-3′ (DDD) was synthesized by the Midland Reagent Company (Midland, TX) and purified by anion-exchange HPLC. The modified oligodeoxynucleotides were synthesized using an ABI 394 DNA synthesizer (Applied Biosystems, Foster City, CA) or a Mermade 9 DNA synthesizer

(Bioautomation, Irving, TX) using β-cyanoethyl phosphoramidite chemistry. The dPer phosphoramidite was prepared and purified as reported (*125*). The synthesis and purification of the O^6-Bn-dG phosphoramidite was performed as described (*126*). The yields of the stepwise coupling reactions were monitored by trityl cation response. The oligodeoxynucleotides were removed from the resin by treating with 18 M (saturated) ammonium hydroxide for 1.5 h at 25 ºC. After filtration, the resulting solutions were heated at 55 ºC for 6 h to deprotect the oligodeoxynucleotides. All oligodeoxynucleotides were purified by semi-preparative reverse-phase HPLC (Phenomenex, Phenyl-Hexyl, 5 μm, 250 mm × 10.0 mm) equilibrated with 0.1 M triethylammonium acetate (pH 7.0). The oligodeoxynucleotides were desalted with Sephadex G-25, and characterized by matrix-assisted laser-desorption-ionization time-of-flight (MALDI-TOF) mass spectrometry. The concentrations of single-stranded oligodeoxynucleotides were estimated by UV absorbance at 260 nm on the basis of an extinction coefficient of 1.11×10^5 M^{-1} cm^{-1}, which was not adjusted for the presence of the modified bases (*34*). The oligodeoxynucleotides were annealed by heating to 80 °C for 15 min and then cooled to room temperature.

UV Melting Curves

Melting temperatures were measured with a Varian Cary 100 Bio spectrophotometer operated at 260 nm. The buffer used for measurements contained 10 mM sodium phosphate, 50 μM Na_2EDTA, 0.1 M NaCl (pH 7). The temperature was increased from 10 to 80 °C at a rate of 0.5 °C/min. Melting temperatures were calculated

from first-order derivatives of the absorbance vs. temperature profiles. The concentration of DNA was 1.5 μM.

Crystallization and Data Collection for O^6-BnG•dPer Duplex

Crystallization trials were performed with the Nucleic Acid Mini-screen (*48*) (Hampton Research, Aliso Viejo, CA). The hanging drop vapor diffusion technique was used. DNA was desalted and prepared in water at 1.2 mM concentration. Droplets with volume 2 μL of a 1:1 mixture of sample and mini-screen buffer were equilibrated against 0.75 mL of 35% 2-methyl-2,4-pentanediol (MPD) at 18 °C. Two crystals were obtained, and found to be suitable for data collection. The first was crystalized from 10 % MPD, 40 mM sodium cacodylate (pH 7.0), 12 mM spermine tetra-HCl, and 80 mM KCl, 20 mM $BaCl_2$. The second was crystallized from 10 % MPD, 40 mM sodium cacodylate (pH 7.0), 12 mM spermine tetra-HCl, 40 mM LiCl and 80 mM $SrCl_2$. Crystals were mounted in nylon loops and frozen in liquid nitrogen. Diffraction data were collected at low temperature in a cold nitrogen stream on beamline 21-ID-F at LS-CAT, APS (Argonne National Laboratory, Argonne, IL) for both crystals. Single anomalous dispersion (SAD) data was collected on the 21-ID-D beamline for the first crystal at the energy corresponding to absorption peak for the Ba atom. All data were processed with the program HKL2000 (*49*) and XDS (*127*).

Crystal Structure Determination and Refinement for the DDD-XY Duplex

The PHENIX (*128*) software was used to calculate phases and initial placing of the model into the electron density map from the SAD data for the first crystal, which

was crystallized with $BaCl_2$. Then, initial refinement of the model was performed with the CNS (*52*) program, setting aside 5% randomly selected reflections for calculating the R_{free}. Rigid body refinement and simulated annealing were performed. After several cycles of refinement the emergent model was used as the starting model for phasing by molecular replacement methods for a data set obtained from the second crystal. Multiple rounds of coordinate refinements and simulated annealing led to an improved model for which sum ($2F_o$-F_c) and difference (F_o-F_c) Fourier electron density maps were generated. At a later stage solvent water molecules were added on the basis of Fourier $2F_o$–F_c sum and F_o–F_c difference electron density maps. Water molecules were accepted based on the standard distances and B-factor criteria. Further structure refinement was performed using the program REFMAC in CCP4 (*50*). Geometry and topology files were generated for the O^6-Bn-dG and dPer modified bases and anisotropic temperature factor refinement was performed afterward. The programs TURBO-FRODO (*54*) and COOT (*91*) were used to display electron density maps. Helicoidal analysis was performed using the CURVES+ web server (*98*).

NMR Spectroscopy

The DDD-XY and DDD-GY modified duplexes were prepared at concentrations of 0.56 mM and 0.53 mM, respectively. The samples were prepared in 10 mM NaH_2PO_4, 0.1 M NaCl, and 50 μM Na_2EDTA (pH 7.0). To observe non-exchangeable protons, the samples were exchanged with D_2O. The DDD-GY duplex was dissolved in D_2O. The DDD-XY duplex was dissolved in 9:1 D_2O/CD_3CN. The presence of CD_3CN in the DDD-XY sample sharpened the resonances from the adduct protons. For the observation

of exchangeable protons, the samples were dissolved in 9:1 H_2O/D_2O. ^1H NMR spectra for DDD-XY duplex were recorded at 900 MHz at 10 °C and 500 MHz at 7 °C. ^1H NMR spectra for DDD-GY duplex were recorded at 800 MHz in D_2O at 10 °C and 600 MHz in 9:1 H_2O/D_2O at 5 °C. Chemical shifts were referenced to water. Data were processed using TOPSPIN software (Bruker Biospin Inc., Billerica, MA). The NOESY (*44, 45*) and DQF-COSY (*46*) spectra in D_2O were collected at 10 °C; NOESY experiments were conducted at a mixing time of 250 ms with a relaxation delay of 2.0 s. The NOESY spectra of the modified samples in H_2O were collected with a 250 ms mixing time, with a relaxation delay of 1.5 s. Water suppression was performed using the WATERGATE pulse sequence (*47*).

Solution Structural Refinement for the DDD-XY Duplex

Experimental Restraints

The NOESY spectrum was processed using the TOPSPIN software (Bruker Biospin Inc., Billerica, MA) and the spectral data were evaluated using the program SPARKY (*129*) to obtain the cross peak assignments. The intensities of cross peaks were measured by volume integrations. Experimental intensities were combined with intensities obtained from complete relaxation matrix analysis of starting model to generate a hybrid intensity matrix (*96, 97*). The intensities were converted to distances with the program MARDIGRAS (*90*), which refined the hybrid intensity matrix. Calculations were performed using 250 ms mixing time and 2, 3, and 4 ns isotropic correlation times. Evaluation of the resulting distance data allowed creation of upper and

lower bound distance restraints that were used in restrained molecular dynamics (rMD) calculations. Additional empirical base pair, backbone and deoxyribose pseudorotation restraints for base pairs not proximal to the sites of modification were obtained from canonical values derived from B-DNA (*130*).

Restrained Molecular Dynamics (rMD) Calculations

An unmodified B type DNA model was used as a starting structure. The cytosine at position C^9 in each strand was replaced by dPer with INSIGHT II (Accelrys Inc., San Diego, CA). Partial charges for Per were calculated with the B3LYP/6-31G* basis set in GAUSSIAN (*131*). The starting structure was energy minimized for 1000 cycles. A simulated annealing protocol (*94*) was used. The program AMBER (*95*) was used for calculations with the parm99 force field. Force constants of 32 kcal mol^{-1} $Å^{-2}$ were applied for distance restraints. The generalized Born model (*132*) was used for solvation. The salt concentration in all calculations was 0.1 M. Coupling of the molecule to the bath temperature was used to control the temperature during simulated annealing. First, calculations were performed for 20 ps (20000 steps) by the following protocol: During steps 0 – 1000, the system was heated from 0 to 600 K with a coupling of 0.5 ps. During steps 1001-2000, the system was kept at 600 K. The system was then cooled from 600 K to 100 K during steps 2001 – 18000 with a coupling of 4 ps. Further cooling from 100 K to 0 K occurred during steps 18001 – 20000 with a coupling of 1 ps. After initial cycles of refinement a longer 100 ps (100000 steps) calculation was performed by the following protocol: During steps 0 – 5000 the system was heated from 0 to 600 K with a coupling of 0.5 ps. During steps 5001 – 10000 the system was kept at 600 K. The system was

cooled from 600 K to 100 K during steps 10001 – 90000 with a coupling of 4 ps. Additional cooling from 100 K to 0 K occurred during steps 90001 – 100000 with a coupling of 1 ps. Structure coordinates were saved after each cycle, and were subjected to potential energy minimization. Nine refined structures calculated from the different starting structures were chosen based on the lowest deviations from the experimental distance and dihedral restraints and energy minimized to obtain an average structure. Complete relaxation matrix analysis (CORMA) (*96, 97*) was used to compare intensities calculated from these emergent structures with the distance restraints. Helicoidal analysis was performed using the CURVES+ web server (*98*).

Data Deposition

The complete structure factor and final coordinates were deposited in the Protein Data Bank (www.rcsb.org): the PDB ID code for the DDD-XY duplex is 4HQI and for the DDD-GY duplex the PDB ID code is 2M11.

Results

Thermodynamic Studies

The unfolding of the DDD-XY and DDD-GY duplexes was examined by UV spectroscopy. The T_M values were determined by taking the first derivative of the temperature-dependent UV melting curves. The melting temperature for the DDD-GY duplex was 28 °C and for the DDD-XY duplex was 33 °C. Thus, for the DDD-XY duplex, the presence of the dPer base complementary to O^6-Bn-dG increased the T_M of by

5 ºC as compared to the DDD-GY duplex, in agreement with the model that dPer thermodynamically discerns the presence of O^6-Bn-dG (*125*).

Structural Studies of the DDD-XY Duplex

Crystallography

For both crystals, the diffraction data were processed in space group $P2_12_12_1$ (orthorhombic). It was not possible to obtain the crystallographic phase data utilizing molecular replacement approaches. Instead, the experimental phases were obtained from single-wavelength anomalous dispersion (SAD) data obtained for the first crystal, which was crystallized from $BaCl_2$. The crystal diffracted to 1.95 Å. The SAD data enabled the experimental phases to be obtained and to perform the initial placing model into an electron density map. The processing and refinement parameters are shown in Table 6.

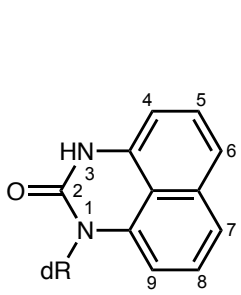
Table 6. Crystal and Data Collection Statistics for the Second Crystal. It was used to obtain phases for O^6-Bn-dG•dPer duplex.

Space group	Orthorhombic $P2_12_12_1$
Cell parameters (Å)	a= 26.410, b=37.320, c=77.630
Temperature of data collection (° C)	-170
Wavelength (Å)	1.605
Min resolution (Å)	26.9
Max resolution (Å)	1.95
Unique reflections (observed)	5861
Completeness all(%)/1.98-1.95 Å	99.0/98.0
I/σ (I) all/1.98-1.95 Å	20.34/4.34
R_{merge} all/1.98-1.95 Å	0.082/0.629
R_{work}	0.356
R_{free}	0.392
Number of DNA atoms	427
Number of water molecules	14
Number of ions	4 Ba^{2+}

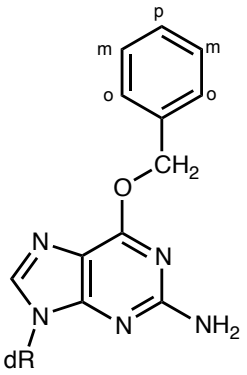
After initial refinement, the resulting structure was used as a starting model for molecular replacement phasing with the diffraction data set from the second crystal, which diffracted up to 1.7 Å in the presence of $SrCl_2$. Multiple rounds of coordinate refinements and simulated annealing led to an improved model for which sum ($2F_o$-F_c)

and difference (F_o-F_c) Fourier electron density maps were generated. At a later stage 49 water molecules were added on the basis of Fourier $2F_o$–F_c sum and F_o–F_c difference electron density maps. These waters were accepted based on the standard distances and B-factor criteria. One Sr^{2+} ion was identified in the electron density map based on its low B-factor and the characteristic geometry, as well as one spermine molecule. The cell parameters (a = 26.520, b= 36.968, c = 77.743, α = 90.0, β = 90.0, γ = 90.0, Table 7) were atypical for the DDD duplex. The volume of the unit cell was greater. The overall refined crystallographic structure of the DDD-XY duplex is shown with waters, Sr^{2+}, and a spermine molecule in Figure 33. While no electron density was observed for the 5'-terminal bases C^1 and C^{13}, and thus their positions could not be determined with certainty, the 3'-terminal bases G^{12} and G^{24} rotated out of the duplex toward the major groove of adjacent molecules. The crystal data collection and refinement statistics are compiled in Table 7. Structures of modified bases and sequences used in the study are shown in Chart 2.

(a)



dPer (Y)



O^6-Bn-dG (X)

(b)

DDD	5'-C^1 G^2 C^3 G^4 A^5 A^6 T^7 T^8 C^9 $G^{10}C^{11}G^{12}$-3' 3'-$G^{12}C^{11}G^{10}C^9$ T^8 T^7 A^6 A^5 G^4 C^3 G^2 C^1 -5'
DDD-GY (NMR)	5'-C^1 G^2 C^3 G^4 A^5 A^6 T^7 T^8 **Y^9** $G^{10}C^{11}G^{12}$-3' 3'-$G^{12}C^{11}G^{10}$**Y^9** T^8 T^7 A^6 A^5 G^4 C^3 G^2 C^1 -5'
DDD-XY (NMR)	5'-C^1 G^2 C^3 **X^4** A^5 A^6 T^7 T^8 **Y^9** $G^{10}C^{11}G^{12}$-3' 3'-$G^{12}C^{11}G^{10}$**Y^9** T^8 T^7 A^6 A^5 **X^4** C^3 G^2 C^1 -5'
DDD-XY (crystallography)	5'-C^1 G^2 C^3 **X^4** A^5 A^6 T^7 T^8 **Y^9** $G^{10}C^{11}G^{12}$-3' 3'-$G^{24}C^{23}G^{22}$**Y^{21}**$T^{20}T^{19}A^{18}A^{17}$**X^{16}**$C^{15}G^{14}C^{13}$-5'

Chart 2. (a) Structures of O^6-Bn-dG and dPer. (b) Sequences and numbering of the Dickerson-Drew dodecamers (DDD) for the DDD-XY, DDD-XY (crystallography) and DDD-GY duplexes. For the NMR studies, the two strands of dodecamer exhibit pseudo-dyad symmetry in solution, and thus both strands are numbered identically from nucleotides C^1 to G^{12}. For the crystallographic studies, the two strands are not symmetry related in the crystalline lattice and the nucleotides are individually numbered from C^1 to G^{12} in the first strand and from C^{13} to G^{24} in the complementary strand.

Table 7. Crystal and Data Collection, Refinement Statistics.

Space group	Orthorhombic $P2_12_12_1$
Cell parameters (Å)	a= 26.384, b=36.774, c=77.653
Temperature of data collection (° C)	-170
Wavelength (Å)	0.97857
Min resolution (Å)	30.0
Max resolution (Å)	1.7
Unique reflections (all)	8811
Unique reflections (observed)	8236
Completeness all/1.76-1.70 Å (%)	93.4/61.1
Redundancy all/1.76-1.70 Å	6.4/4.0
I/σ (I) all/1.76-1.70 Å	52.33/5.65
R_{merge} all/1.76-1.70 Å	0.044/0.228
R_{work}	0.259
R_{free}	0.298
Number of DNA atoms	481
Number of water molecules	49
Number of ions	1 Sr^{2+}
r.m.s. distances (Å)	0.011
r.m.s. angles (°)	1.652

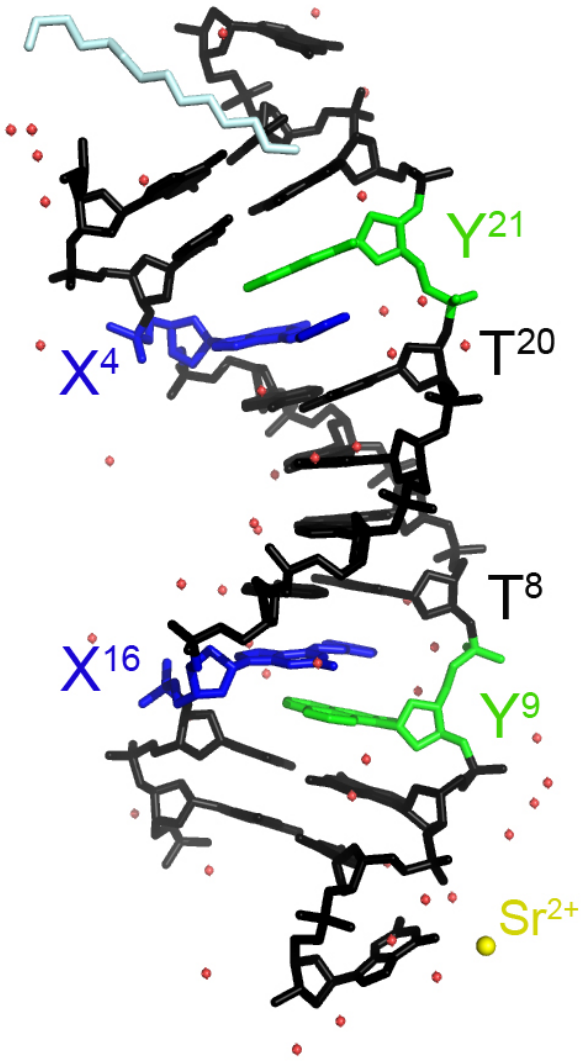


Figure 33. Structure of the *O*^{6}-Bn-dG•dPer (DDD-XY) duplex with water molecules (red spheres) and Sr^{2+} ion (yellow sphere) and spermine molecule (light blue). The benzyl groups of *O*^{6}-Bn-dG (shown in blue) intercalate between the thymine and dPer bases (shown in green) from the opposite strand. The dPer bases are in the *syn* conformation about the glycosyl bond. Electron density for bases C^1 and C^{13} was not visible. Bases G^{12}

and G^{24} flipped out from the duplex. The intercalated structures unwind the duplex as compared to the unmodified DDD.

Figure 34 shows an expanded view of the crystallographic electron density map of the DDD-XY duplex in the region of the C^3•G^{22}, X^4•Y^{21} and A^5•T^{20} base pairs. Both the O^6-Bn-G and Per bases fit well into the electron density map. The aromatic Per base was inserted into the helix and created an intercalated binding pocket into which the benzyl ring of the O^6-Bn-dG base was inserted. The benzyl ring of the O^6-Bn-G base also formed a stacking interaction with T^{20} of the 5'-neighbor A^5•T^{20} base pair. The crystallographic structure was not consistent with the notion that dPer might recognize the O^6-Bn-dG base via hydrogen bonding interactions between the NH proton and the keto oxygen of dPer, and N1 and N_2H of O^6-Bn-dG. (*125*) The simultaneous insertion of both dPer and the benzyl ring of the O^6-Bn-dG base unwound the duplex at the site of the O^6-Bn-dG base, such that the helical rise between neighboring base pairs C^3•G^{22} and A^5•T^{20} was increased to 9.5 Å, as compared to the anticipated rise of about 6.5 Å in B-DNA (Figure 35). For the interbase pair parameters, the biggest change in twist was observed for base pairs C^3•G^{22} and X^4•Y^{21} by 40 ° (Figure 35). It was -15 °, where for the unmodified duplex it was 25 °. It confirms unwinding of the DNA molecule. For the roll the biggest change is observed for base pairs C^3•G^{22} and X^4•Y^{21} as well as C^{15}•G^{10} and X^{16}•Y^9 by almost 90 °, which is consisted with the intercalated structure. The O^6-Bn-dG remained in the *anti* conformation and the Per base adopted the *syn* conformation about the respective glycosyl bonds. The greatest changes were observed for backbone angles α and γ of dPer bases by ~ 210 ° compared to the unmodified duplex (Figures 36 and 37). χ angle for

dPer bases is in range 60-80 °, which is consistent with the *syn* conformation of the Per base (Figures 38).

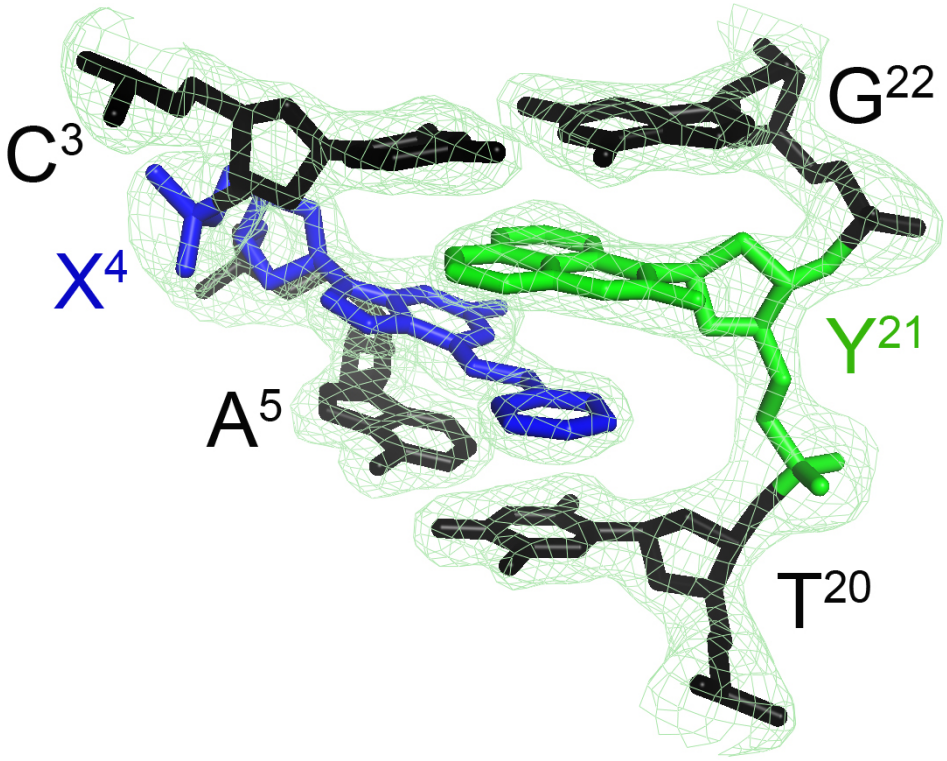


Figure 34. The electron density for the crystal structure of the DDD-XY duplex in the region of the C^3•G^{22}, X^4•Y^{21} and A^5•T^{20} base pairs. The dPer base recognizes the benzyl group of O^6-Bn-dG (X^4) via a stacking interaction, such that the benzyl ring intercalates between the T^{20} and Y^{21} bases.

The intercalated structure of the Per base, which was located between O^6-Bn-G and the 5' neighbor cytosine in both strands, affected the ζ angles of the C^3 and C^{15} cytosines by

90 ° (Figure 38). Watson-Crick base pairing interactions at the neighbor base pairs C^3•G^{22} and A^5•T^{20} were not disturbed. Figure 39 further illustrates the stacking interactions observed between the benzyl ring of O^6-Bn-dG and dPer. Effectively, the presence of dPer "trapped" the benzyl ring of O^6-Bn-dG between the dPer base and T^{20}, providing a mechanism whereby dPer specifically recognized the O^6-Bn-dG DNA damage.

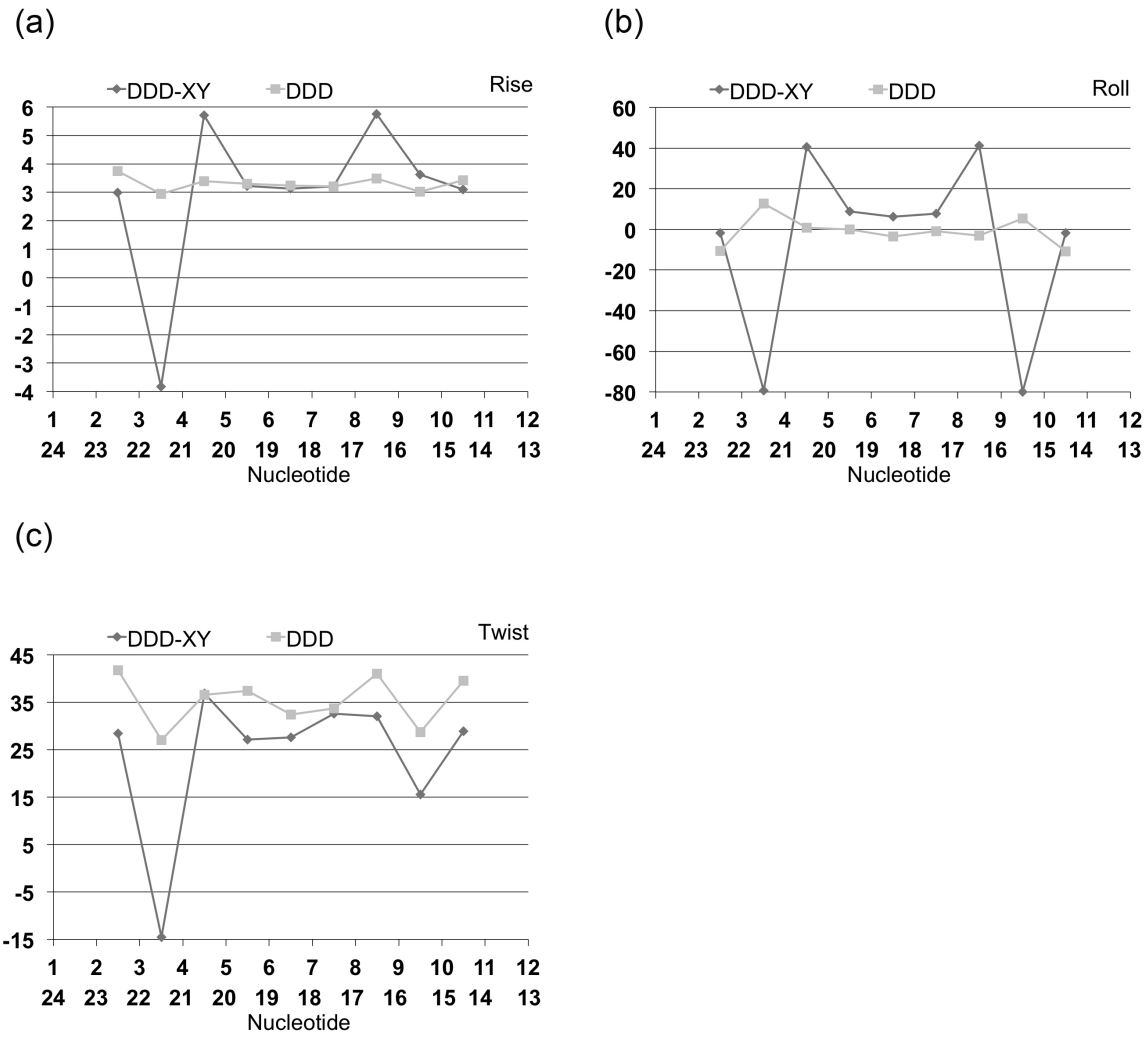


Figure 35. Interbase pair parameters: (a) helical rise, (b) roll and (c) twist for the DDD-XY, DDD (PDB entry 355D) duplexes.

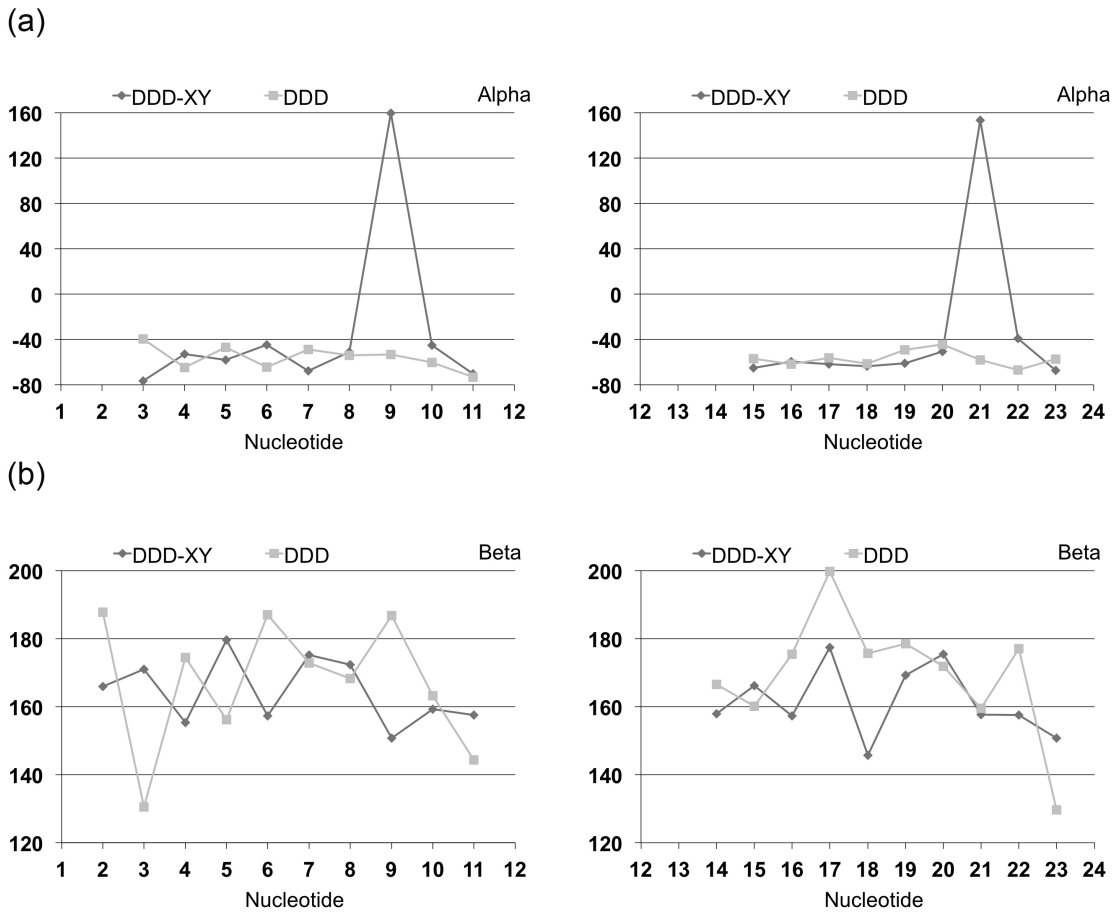


Figure 36. Comparison of backbone torsion angles (a) α and (b) β in the crystal structures of the DDD-XY, DDD (PDB entry 355D) duplexes.

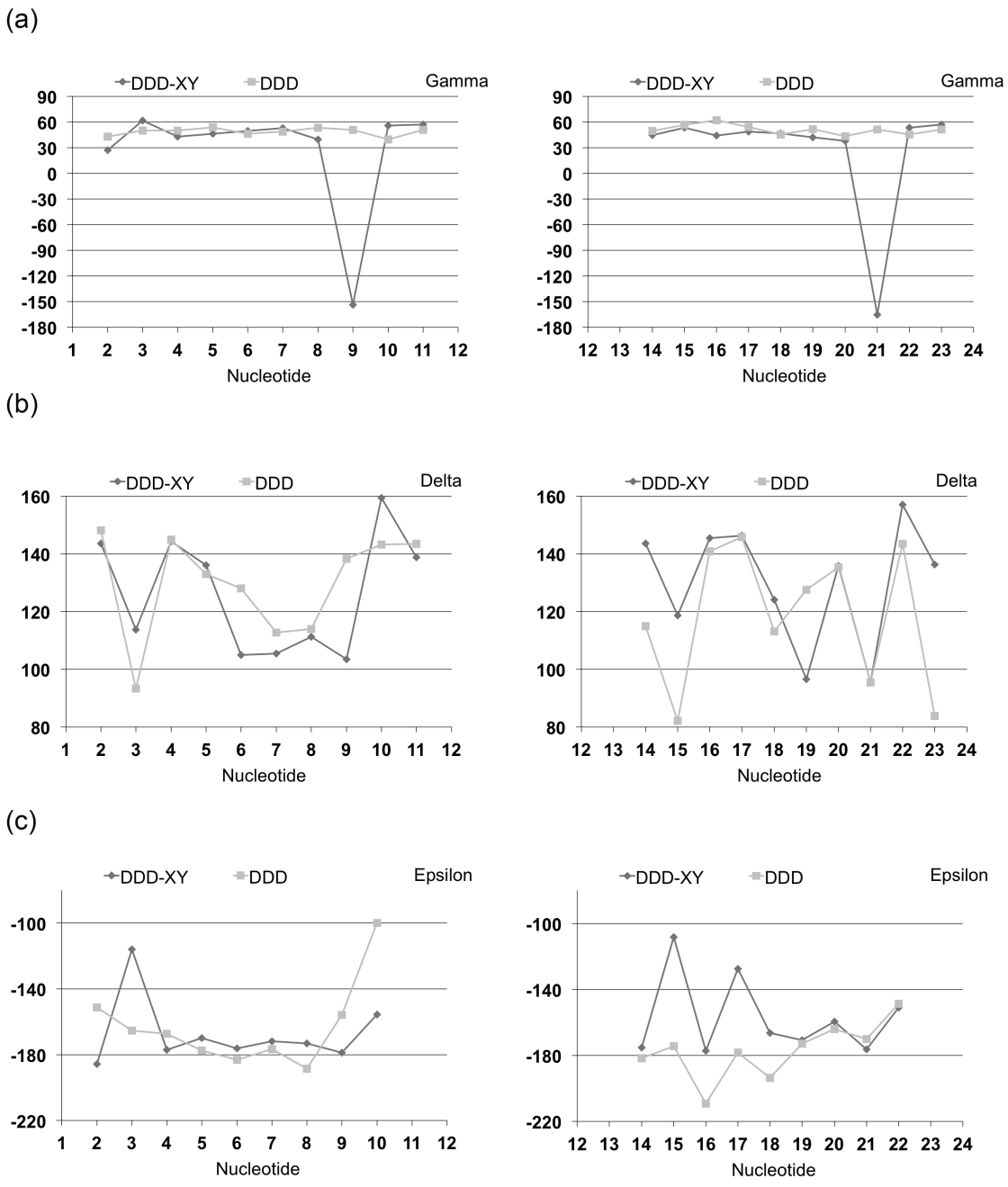


Figure 37. Comparison of (a) γ, (b) δ, (c) ε angles in the crystal structures of the DDD-XY, DDD (PDB entry 355D) duplexes.

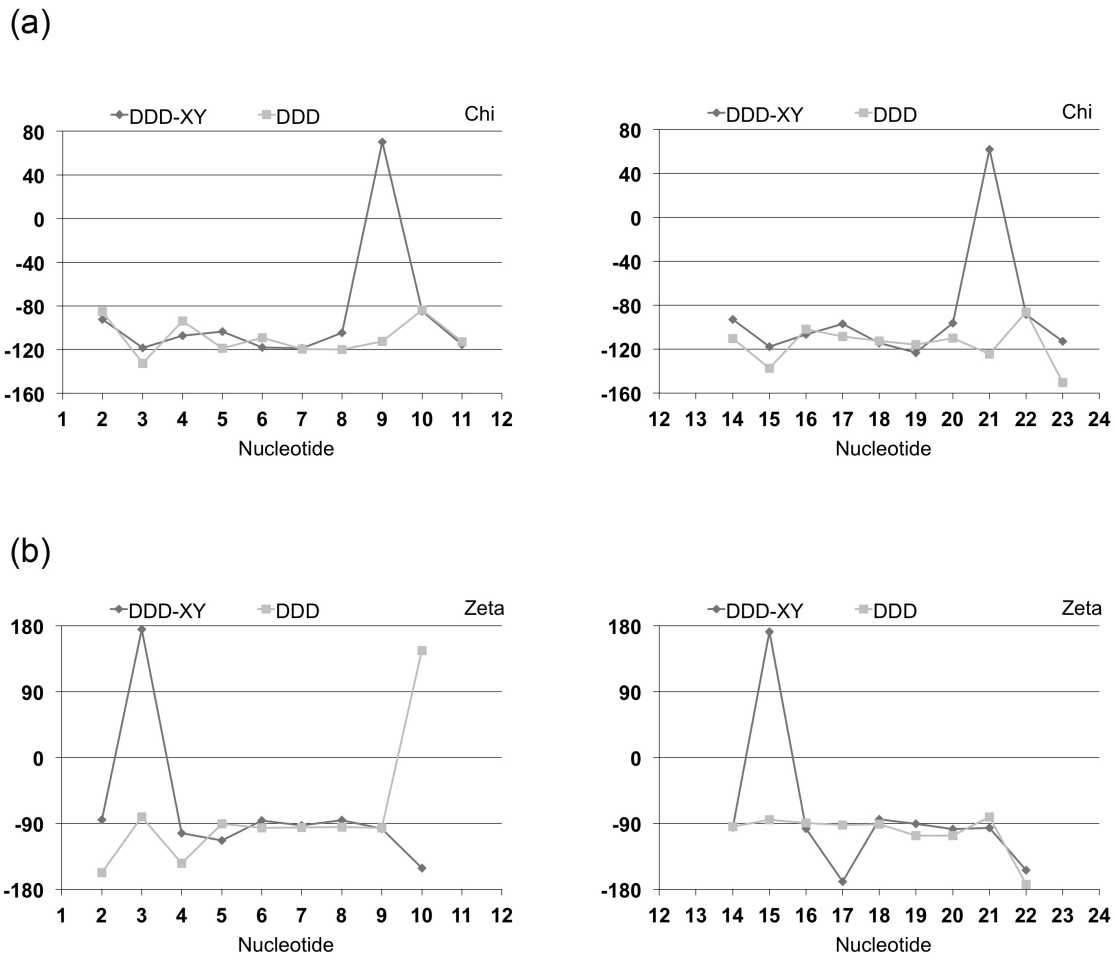


Figure 38. Comparison of (a) χ and (b) ζ angles in the crystal structures of the DDD-XY, DDD (PDB entry 355D) duplexes.

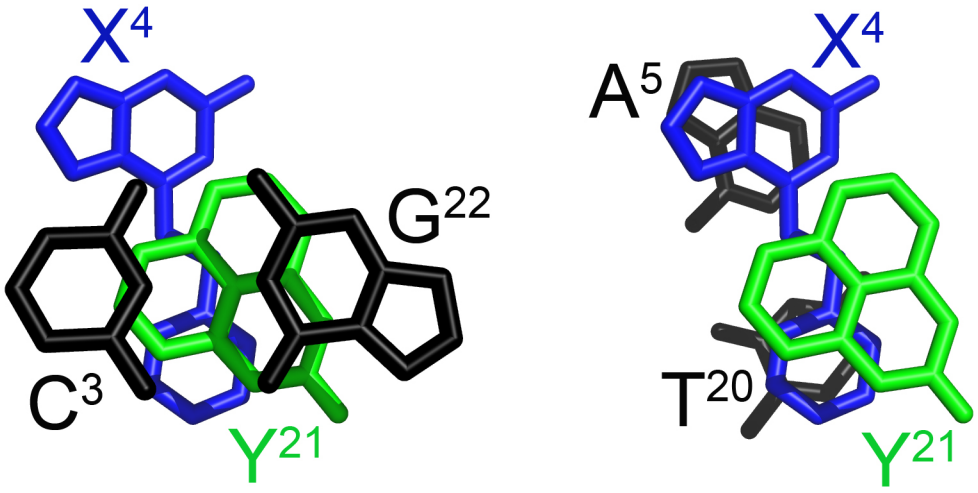


Figure 39. Stacking interaction for the *O*^{6}-Bn-dG•dPer (DDD-XY) duplex as determined from the crystallographic data. View at C^{3}•G^{22} base pair (in black) and X^{4}•Y^{21} shown is blue and green, respectively (left). View at X^{4}•Y^{21} (in blue and green, respectively) and A^{5}•T^{20} base pair (in black) (right). The benzyl ring of *O*^{6}-Bn-dG (X^{4}) is stabilized by intercalation between T^{20} and Y^{21} (dPer) bases.

NMR Spectroscopy

The *O*^{6}-Bn-dG•dPer duplex was also examined by NMR spectroscopy, to determine whether the crystallographic structural determination was re-capitulated in solution. The non-exchangeable DNA protons were assigned using standard methods (*58, 59*). The sequential NOE connectivity between base aromatic and deoxyribose H1' protons is shown in Figure 40. At the *O*^{6}-Bn-dG•dPer base pair, the C^{3} H6→C^{3} H1' NOE

was broadened. The C^3 H1'→X^4 H8 NOE was very weak; it is not observed in Figure 40. A weak, broad NOE was observed between X^4 H8 and X^4 H1'. A weak NOE was observed between X^4 H1' and A^5 H8. The T^7 H1'→T^8 H6, T^8 H6→T^8 H1', T^8 H1'→Y^9 H8, Y^9 H8→Y^9 H1', and Y^9 H1'→G^{10} H8 NOEs were weak. The Y^9 H8 resonance was broadened compared to other DNA cross peaks. The broad cross peaks of the bases next to Y^9•X^4 were related to rotation of the benzyl group of the X^4 base. The very weak cross peak T^8 H1'→Y^9 H8 indicated an increased distance between both bases.

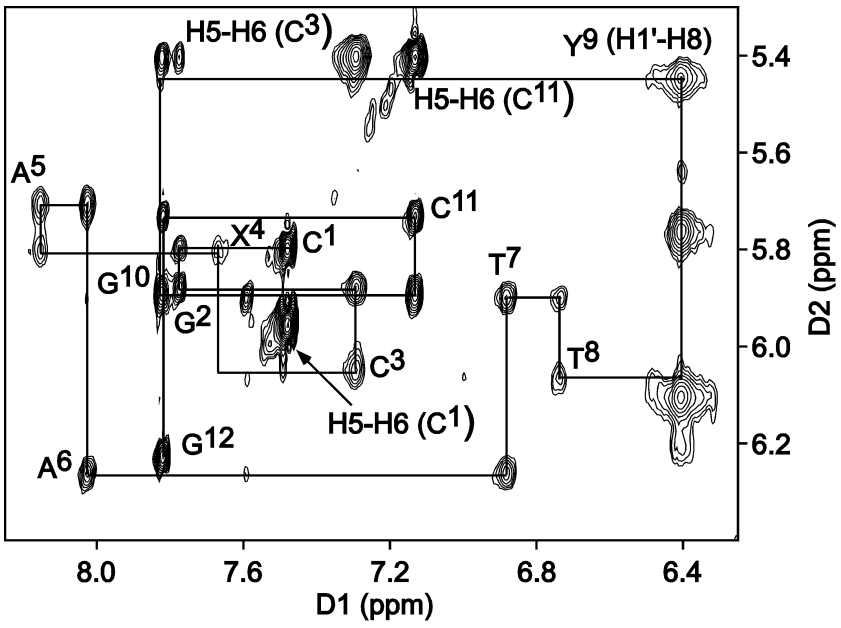


Figure 40. Expansion of a NOESY spectrum of the *O*^{6}-Bn-dG•dPer modified DDD-XY duplex showing sequential NOEs between the aromatic and anomeric protons from C^1 to G^{12}.

The imino and amino proton regions of the NOESY spectrum of the DDD-XY duplex are shown in Figure 41. The imino proton of Y^9 could not be identified. This was attributed to rapid exchange with solvent. Thus, no NOE was observed from the G^{10} N1H imino proton to the Y^9 imino proton, and likewise, no cross peak from the Y^9 imino proton to the T^8 N3H imino proton. The sequential connectivity of the base imino protons (*60*) was obtained from base pairs $G^2 \bullet C^{11} \rightarrow C^3 \bullet G^{10}$. Additionally, the sequential connectivity was observed from base pairs $A^5 \bullet T^8 \rightarrow A^6 \bullet T^7$. The imino resonance of the terminal base pair $C^1 \bullet G^{12}$ was not observed. This was also attributed to rapid exchange with solvent. The region of the spectrum showing NOEs between the base imino protons and the base amino and adenine H2 protons showed no cross peaks for $X^4 \bullet Y^9$ (Figure 41a). The anticipated cross peaks for base pairs $G^2 \bullet C^{11}$, $C^3 \bullet G^{10}$, $A^5 \bullet T^8$, and $A^6 \bullet T^7$ were observed, indicating that Watson-Crick hydrogen bonding was present at these base pairs. However, the A^5 H2 $\rightarrow$ T^8 N3H NOE (a, Figure 41a) was weak as compared to the A^6 H2$\rightarrow T^7$ N3H NOE (d, Figure 41a). The cross peaks between the C^3 amino protons and G^{10} N1H imino proton were similar in intensity to the corresponding NOEs for the $G^2 \bullet C^{11}$ base pair. However, the G^{10} N3H was shifted upfield as compared to the unmodified duplex. ^{1}H NMR spectra of the DDD-XY duplex were collected as a function of temperature. In Figure 42 the G^{10} N1H resonance was shifted upfield to 12 ppm compared to the G^2 N3H resonance. The T^8 N3H resonance was broadened compared to the T^7 N3H resonance and to the unmodified duplex.

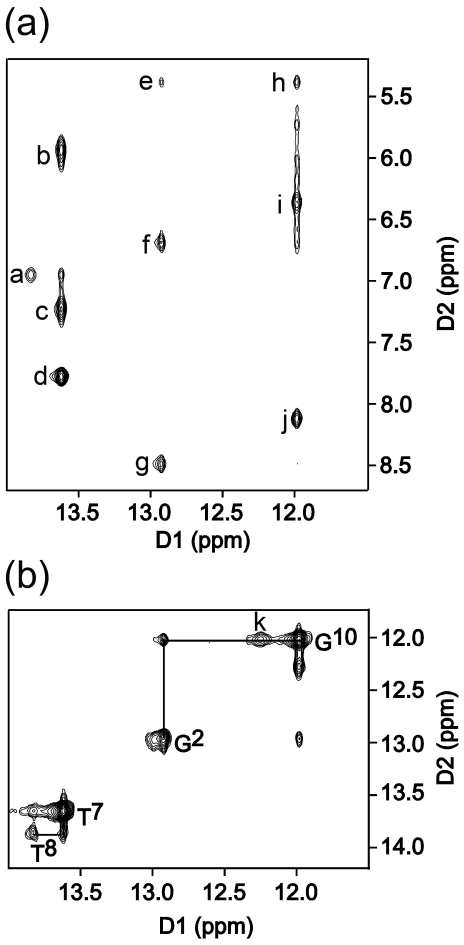


Figure 41. (a) Interstrand NOE cross peaks between complementary bases for the DDD-XY duplex: a, A^5 H2→T^8 N3H; b, A^5 N^6H2→T7 N3H; c, A^6 N^2H2→T^7 N3H; d, A^6 H2→T^7 N3H; e, C^{11} H5→G^2 N1H; f, C^{11} N^2H1→G^2 N1H; g, C^{11} N^2H2→G^2 N1H; h, C^3 H5→G^{10} N1H; i, C^3 N^2H1→G^{10} N1H; j, C^3 N^2H2→G^{10} N1H. (b) NOE connectivity of O^6-Bn-dG•dPer (DDD-XY) duplex, for the imino protons for the base pairs G^2•C^{11}, C^3•G^{10}, X^4•Y^9, A^5•T^8, A^5•T^7. Cross peaks between T^8 N3H→T^7 N3H and G^2 N1H→G^{10} N1H were present. There is no cross-peak between T^8→Y^9 and Y^9→G^{10}. G^{10} N1H has a cross-peak with peak which is not visible on the diagonal and could not be assigned (k). The experiment was carried out at a mixing time of 250 ms and 600 MHz at 7 °C.

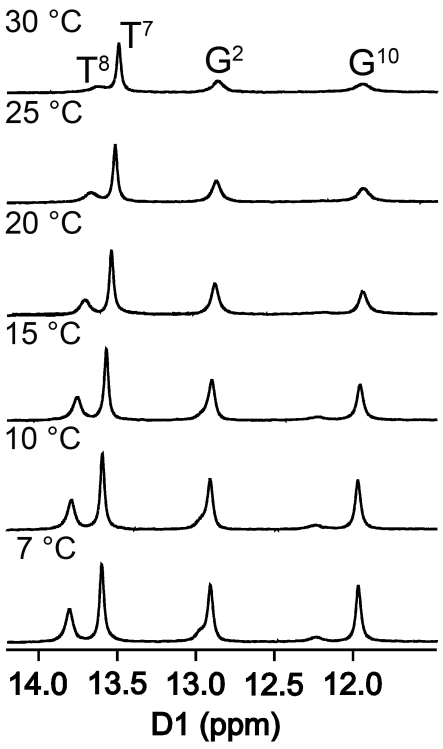


Figure 42. ^{1}H NMR spectra showing the imino proton resonances for the DDD-XY duplex as a function of temperature. Note that the imine nitrogen of the O^6-Bn-dG nucleotide X^4 is not protonated at neutral pH. The individual nucleotides are identified as superscripts.

The O^6-Bn-dG benzyl protons were observed as three broad signals between 6.6 and 7.4 ppm (Figure 43). All gave cross peaks with methylene (CH_2) hydrogens of X^4 base (1c, 2c, 4c, 5c, 6c, Figure 43c). This indicated that rotation of the benzyl ring was rapid on the NMR time scale. The resonance located farthest downfield at 7.3 ppm was assigned as arising from X^4 H_{meta}, while the resonance located farthest upfield was assigned as arising

from X^4 H_{ortho}. The X^4 H_{para} proton was assigned at 7 ppm. Cross-peaks were observed between H_{ortho}→H_{meta} (1d, Figure 11d), H_{meta}→H_{para} (2d, Figure 43d), H_{ortho}→H_{para} (3d, Figure 43d). Interstrand cross peaks between benzyl ring of X^4 and methyl group, H2', H2" of T^8 were observed (1a, 2a, 1b, 2b, 3b, 4b, Figure 43). A weak cross peak between Y^9 H9 and X^4 H_{ortho} was observed (7d, Figure 43d).

The dPer (Y^9) resonances were observed upfield from the benzyl ring protons of O^6-Bn-dG (X^4). Cross peaks between dPer hydrogens are shown in Figure 43d (4d-6d, 8d-14d). Additional cross peaks between dPer base and its sugar were identified (5b-8b, 8c-11c, Figure 43). Only one weak interstrand cross peak was identified between C^3 H2' and Y^9 H6 (7b, Figure 43b). In the NOESY spectrum additional cross peaks were observed, which were assigned to the modified bases.

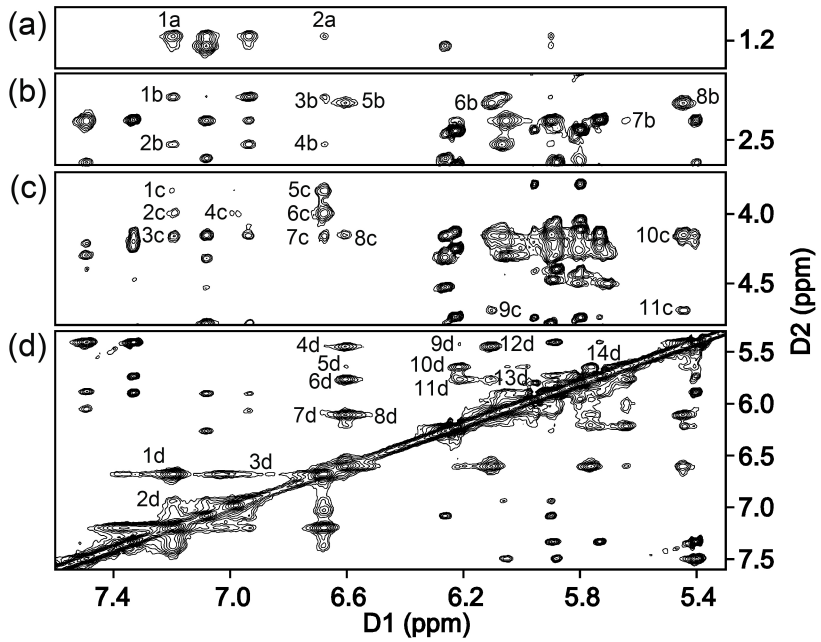


Figure 43. Adduct cross peak assignments for the DDD-XY duplex: (a) 1a, T^8 Me→X^4 H_{meta}; 2a T^8 Me→X^4 H_{ortho}; (b) 1b, T^8 H2'→X^4 H_{meta}; 2b, T^8 H2"→X^4 H_{meta}; 3b, T^8 H2'→X^4 H_{ortho}; 4b, T^8 H2"→X^4 H_{ortho}; 5b, Y^9 H2'/H2"→Y^9 H8; 6b, Y^9 H2'/H2"→Y^9 H9; 7b, C^3 H2'→Y^9 H6; 8b, Y^9 H2'/H2"→Y^9 H1'; (c) 1c, X^4 Hm_1→X^4 H_{meta}; 2c, X^4 Hm_2→X^4 H_{meta}; 3c, Y^9 H4'→X^4 H_{meta}; 4c, X^4 Hm_2→X^4 H_{para}; 5c, X^4 Hm_1→X^4 H_{ortho}; 6c, X^4 Hm_2→X^4 H_{ortho}; 7c, Y^9 H4'→X^4 H_{ortho}; 8c, Y^9 H4' →Y^9 H8; 9c, Y^9 H3'→Y^9 H9; 10c, Y^9 H4'→Y^9 H1'; 11c, Y^9 H3'→Y^9 H1'; (d) 1d, X^4 H_{ortho}→X^4 H_{meta}; 2d, X^4 H_{para}→X^4 H_{meta}; 3d, X^4 H_{ortho}→X^4 H_{para}; 4d, Y^9 H1'→Y^9 H8; 5d, Y^9 H6→Y^9 H8; 6d, Y^9 H7→Y^9 H8; 7d, Y^9 H9→X^4 H_{ortho}; 8d, Y^9 H9→Y^9 H8; 9d, Y^9 H4→Y^9 H5; 10d, Y^9 H6→Y^9 H5; 11d, Y^9 H7→Y^9 H5; 12d, Y^9 H1'→Y^9 H9; 13d, Y^9 H7→Y^9 H9.

Structure of the DDD-GY Duplex Determined by NMR

To determine the basis by which the dPer nucleotide selectively recognized the O^6-Bn-dG adduct vs. unmodified dG, the structure of the dPer nucleotide placed complementary to dG (DDD-GY) was also determined. The dG•dPer duplex was not amenable to crystallographic analysis. However, it was possible to complete a solution structural determination by NMR. Assignments between aromatic protons of the base to deoxyribose H1' protons are shown in Figure 44.

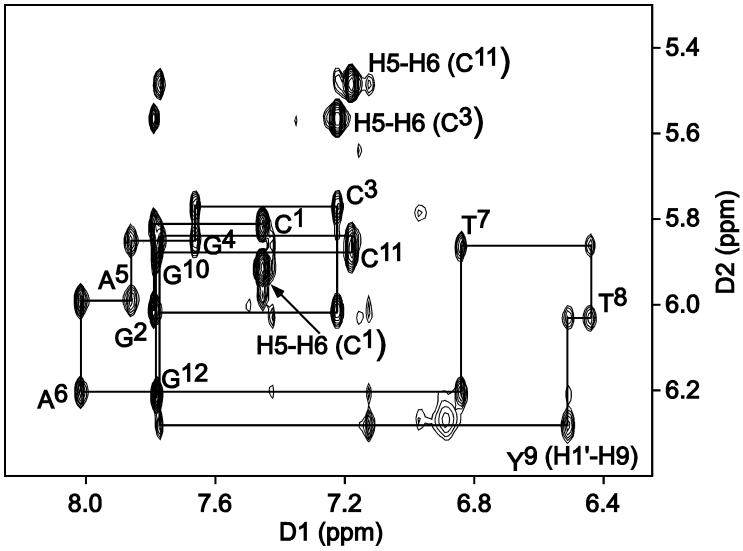


Figure 44. Expansion of a NOESY spectrum of the dG•dPer modified DDD-GY duplex showing sequential NOEs between the aromatic and anomeric protons from C^1 to G^{12}.

At the site of the G^4•Y^9 base pair, the C^3 H6→C^3 H1', C^3 H1'→G^4 H8, G^4 H8→G^4 H1', G^4 H1'→A^5 H8, and A^5 H8→A^5 H1' cross peaks were all observed and were of normal intensities. Also, the T^8 H6→T^8 H1', T^8 H1'→Y^9 H9, Y^9 H9→Y^9 H1', Y^9

H1'→G^{10} H8, and G^{10} H8→G^{10} H1' NOEs were observed and were of normal intensities. There was a small chemical shift difference compared to unmodified duplex for the T^8 and Y^9 bases.

The region of the NOESY spectrum showing the sequential NOEs between the base imino protons showed a strong cross peak between the G^4 N1H imino proton and the imino proton of the Y^9 dPer base (u, Figure 45b). The sequential connectivity of the base imino protons was thus obtained from base pairs G^2•C^{11} → C^3•G^{10} → G^4•Y^9 → A^5•T^8 → A^6•T^7 (Figure 45b). The region of the NOESY spectrum showing NOEs between the base imino and amino protons and adenine H2 protons showed cross peaks for base pairs A^5•T^8, A^6•T^7, G^2•C^{11}, G^{10}•C^3 and it showed that G^4 and Y^9 formed a base pair (k, l, m, n, Figure 45a). The G^{10} cross peak had a similar chemical shift as compared to G^2. The G^4 N1H and Y^9 HN resonances were shifted upfield to 10.25 and 10.7 ppm.

In Figure 46 two additional resonances were observed, which were assigned to the guanine G^4 and dPer Y^9 bases. These were smaller and broadened as compared to the other imino resonances. The chemical shift for guanine G^{10} N1H imino proton remained similar to that of the G^2 N1H imino proton. They remained sharp even at higher temperatures. The resonances for the DDD-GY duplex remained sharper at higher temperatures as compared to DDD-XY duplex, which confirmed that the DDD-GY duplex was more stable as compared to DDD-GY duplex. The thymine T^8 N3H imino resonance was smaller as compared to the T^7 N3H imino resonance, but it remained sharper at higher temperatures as compared to the T^8 N3H imino resonance in the DDD-XY duplex (Figure 42).

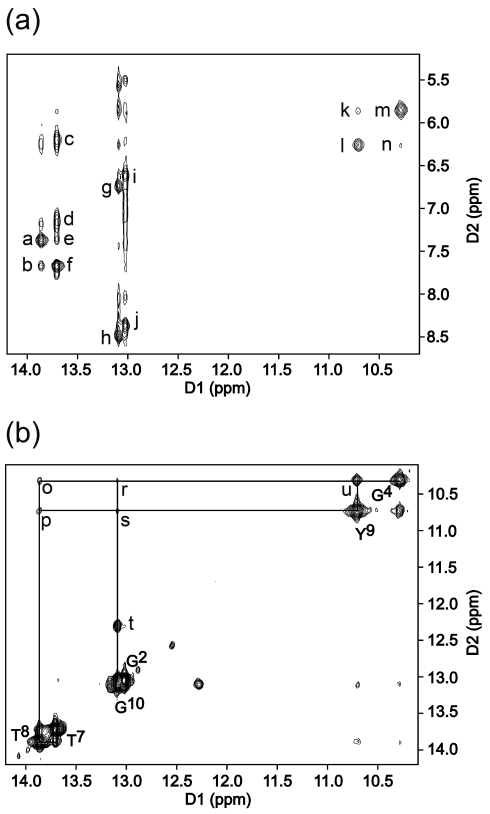


Figure 45. (a) Interstrand NOE cross peaks between opposite bases for DDD-GY duplex: a, A^5 H2→T^8 N3H; b, A^6 H2→T8 N3H; c, A^6 H1'→T^7 N3H; d, A^6 N^6H2→T^7 N3H; e, A^5 H2→T^7 N3H; f, A^6 H2→T^7 N3H; g, C^3 N^2H1→G^{10} N1H; h, C^3 N^2H2→G^{10} N1H; i, C^{11} N^2H1→G^2 N1H; j, C^{11} N^2H2→G^2 N1H; k, G^4 H1'→Y^9 HN; l, Y^9 H1'→Y^9 HN; m, G^4 H1'→G^4 N1H; n, Y^9 H1'→G^4 N1H. (b) NOE connectivity of G•dPer (DDD-GY) duplex, for the imino protons for the base pairs G^2•C^{11}, C^3•G^{10}, G^4•Y^9, A^5•T^8, A^5•T^7. Cross-peaks between T^8 N3H→T^7 N3H, T^8 N3H→Y^9 HN (p), T^8 N3H→G^4 N1H (o), Y^9 HN→G^{10} N1H (s), G^4 N1H→G^{10} N1H (r), G^2 N1H→G^{10} N1H and Y^9 HN→G^4 N1H (u) were present. G^{10} N1H has a cross-peak with a peak which is not observed on diagonal and could not be assigned (t). There is no break in connectivity between bases, but the T^8→Y^9 and Y^9→G^{10} cross-peaks are weak compared to other cross-peaks. The experiment was carried out at a mixing time of 250 ms and 500 MHz at 5 °C.

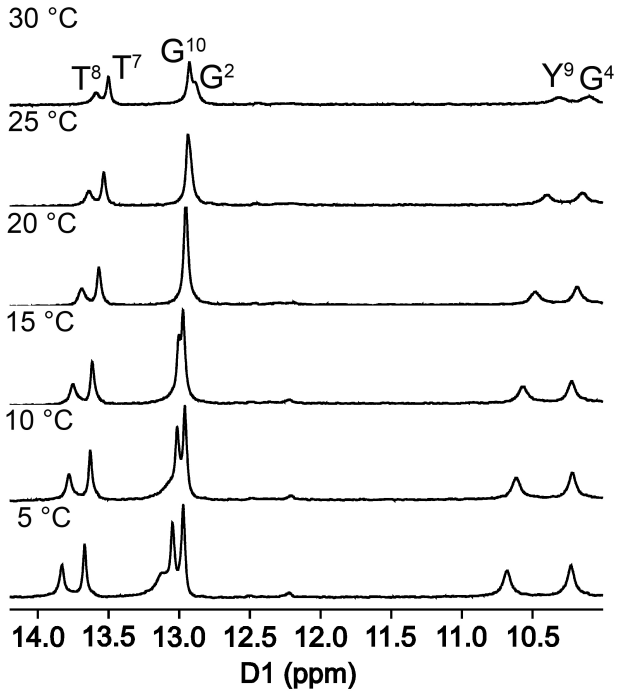


Figure 46. ^{1}H NMR spectra showing the imino proton resonances for the DDD-GY duplex as a function of temperature. The individual nucleotides are identified as superscripts.

The assignment of the dPer aromatic protons H4, H5, H6, H7, H8, and H9 is shown in Figure 47. These protons were observed between 6.2 and 7.4 ppm. The cross peak between T^{8} H1'→ Y^{9} H9 was identified (10d, Figure 47d). Based on the intensities of cross peaks H8, H7 were identified. They both give cross peaks to H9 (1d, 3d, Figure 47d). The H6 cross peak was identified based on close distance to H8 and H7 and H5 (2d, 4d, 6d, Figure 47d). The H5 proton showed a cross peak to H4 (7d, Figure 47d). This peak was broad and shifted upfield to 6.2 ppm. This was attributed to the proximity of the

NH imino hydrogen. H9 and H8 gave cross peaks to T^8 H2' (1a, 4a, Figure 47a). H6 and H5 gave cross peaks to the T^8 methyl group (2a, 3a, Figure 47a). Additional cross peaks between H9, H8, H7 and its deoxyribose, and to T^8 deoxyribose protons were assigned (Figure 47c).

The average structure of dG•dPer (DDD-GY) duplex was determined using a simulated annealing rMD protocol, restrained by experimental distance restraints determined from NOEs. Table 8 shows the number of restraints used for structure calculations. Nine structures were energy minimized and superimposed to obtain the average structure (Figure 48 and 49). Figure 49 shows these superimposed nine structures and the average structure. The latter is in good agreement with the experimental restraints confirmed by CORMA (*133*) analysis. Table 9 shows the structural statistics. Figure 50 shows an expanded view of the DDD-GY duplex in the region of the C^3•G^{10}, G^4•Y^9 and A^5•T^8 base pairs. The modified dPer Y^9 base formed a wobble base pair interaction with the complementary guanine G^4, involving two hydrogen bonds (Figure 51). The dPer ring was oriented in the major groove in DNA and adopted the *anti* conformation about the glyosyl bond. It did not disrupt neighbor base pairs. The dPer base had stacking interactions with its 5' neighbor T^8, but it did not stack well with its 3' neighbor G^{10} (Figure 52). The guanine opposite dPer, G^4 stacked with its 3' neighbor A^5 well, but not with C^3. Helicoidal analysis confirmed that the dPer•dG modified base pair did not disrupt the structure of the duplex significantly (Figures 53-56). The ζ angle of the dPer base was the most changed compared to the unmodified duplex (by ~ 50 °), which agree with less stacking interactions between dPer (Y^9) and the 3' neighbor guanine (G^{10}) (Figure 56).

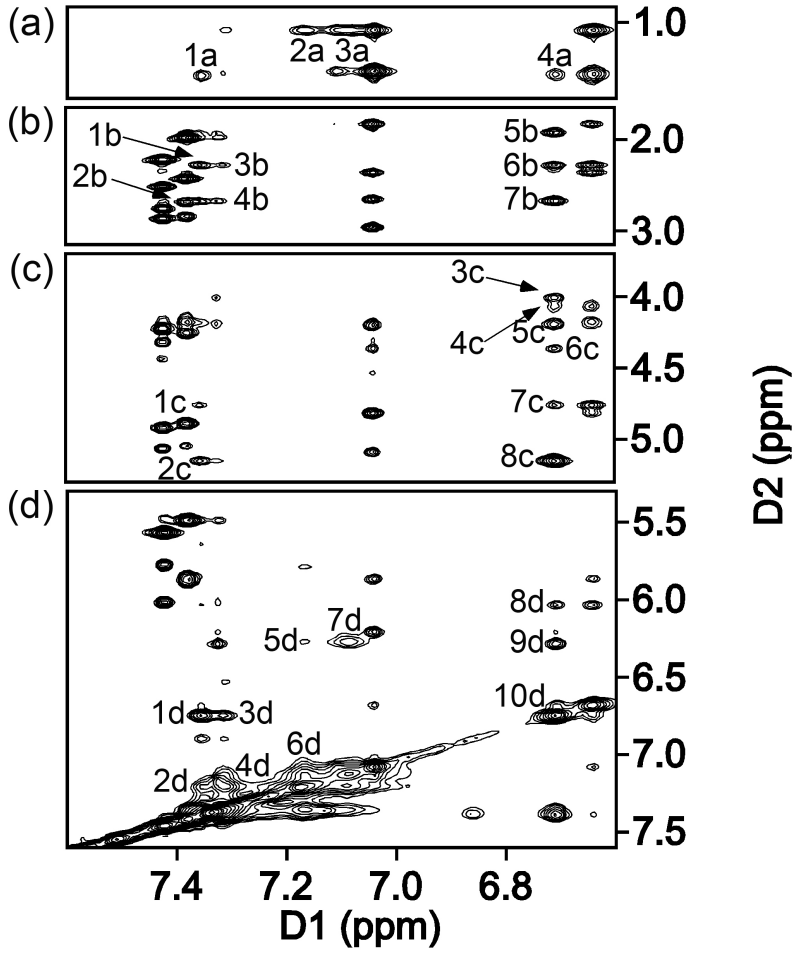


Figure 47. Adduct cross peaks assignment for DDD-GY duplex: (a) 1a, T^8 H2'→Y^9 H8; 2a, T^8 Me→Y^9 H6; 3a, T^8 Me→Y^9 H5; 4a, T^8 H2'→Y^9 H9; (b) 1b, T^8 H2"→Y^9 H8; 2b Y^9 H2"→Y^9 H8; 3b, T^8 H2"→Y^9 H7; 4b, Y^9 H2"→Y^9 H7; 5b, Y^9 H2'→Y^9 H9; 6b, T^8 H2"→Y^9 H9; 7b, Y^9 H2"→Y^9 H9; (c) 1c, T^8 H3'→Y^9 H8; 2c, Y^9 H3'→Y^9 H8; 3c, Y^9 H5"→Y^9 H9; 4c, T^8 H5"→Y^9 H9; 5c, Y^9 H5'→Y^9 H9; 6c, Y^9 H4'→Y^9 H9; 7c, T^8 H3'→Y^9 H9; 8c, Y^9 H3'→Y^9 H9; (d) 1d, Y^9 H9→Y^9 H8; 3d, Y^9 H9→Y^9 H7; 2d, Y^9 H6→Y^9 H8; 4d, Y^9 H6→Y^9 H7; 6d, Y^9 H5→Y^9 H6; 5d, Y^9 H4→Y^9 H6; 7d, Y^9 H4→Y^9 H5; 10d, T^8 H6→Y^9 H9; 9d, Y^9 H1'→Y^9 H9; 8d, T^8 H1'→Y^9 H9.

Table 8. NMR Restraints Used for the DDD-GY Structure Calculations.

NMR restraints	
NOE restraints	
Internucleotide	75
Intranucleotide	78
Total	153
Backbone torsion angle restraints	100
H-bonding restraints	50
Deoxyribose restraints	18
Total number of restraints	321

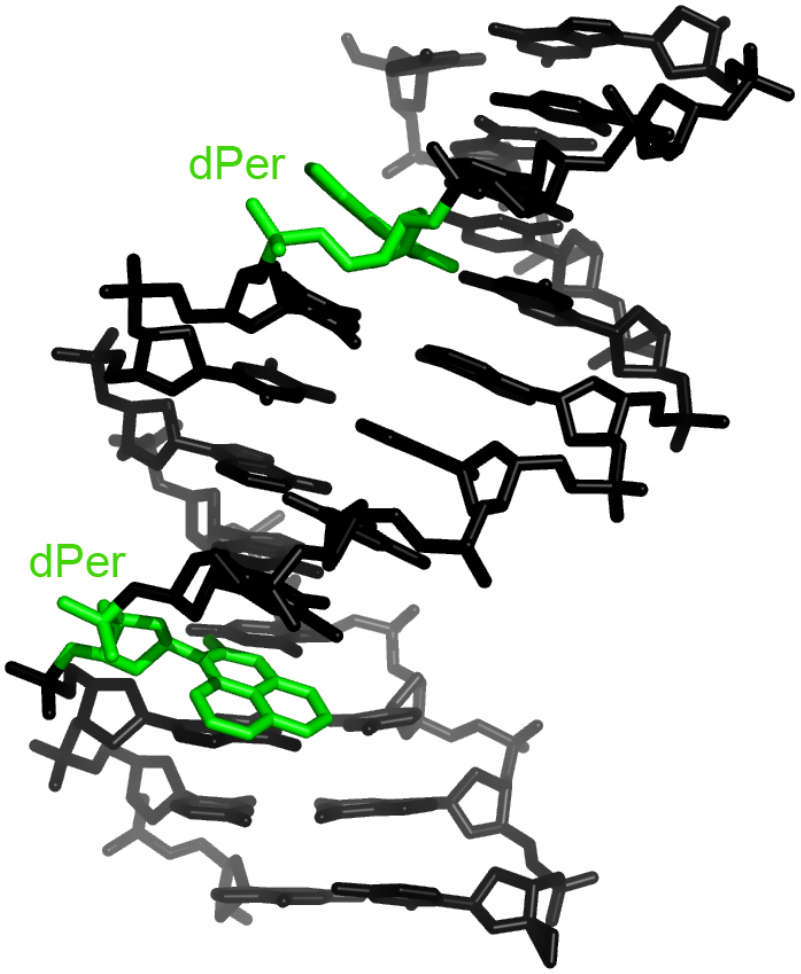


Figure 48. The average structure obtained from a series of rMD calculations for the DDD-GY duplex. dPer bases are shown in green. The dPer base is in the *anti* conformation about the glycosyl bond and it forms wobble pair with the complementary dG. The dPer ring is oriented in the major groove. Hydrogens are omitted on the picture for clarity.

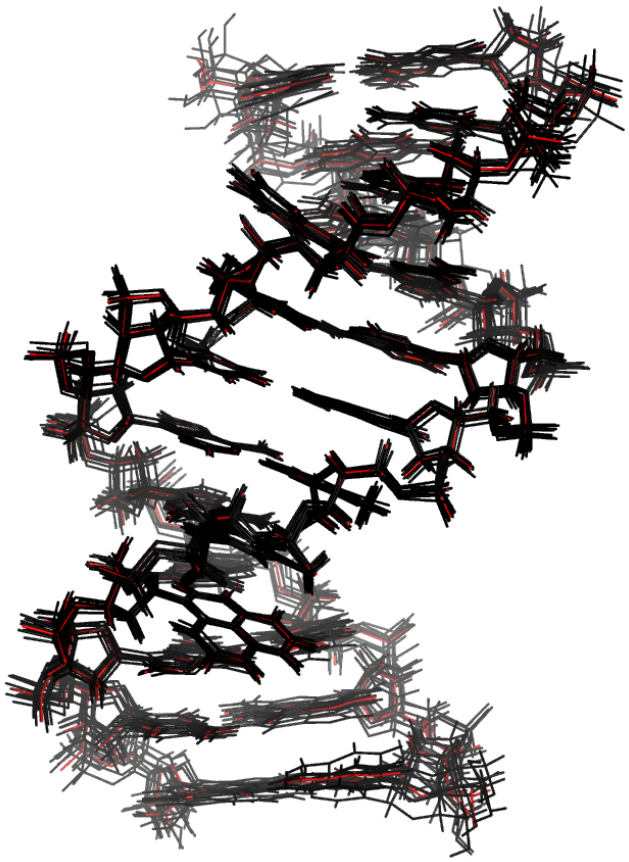


Figure 49. The superimposed 9 structures obtained from a series of rMD calculations for the DDD-GY duplex. The average structure obtained from 9 structures is shown in red.

Table 9. Structural Statistics for the DDD-GY Duplex.

Average structure (obtained from 9 structures)			
RMS pairwise difference between structures	0.705		
RMS difference from average structure	0.470		
CORMA analysis for average structure[a]			
	Intranucleotide	Internucleotide	Total
Rx[b]	0.102	0.103	0.102
Average error[c]			0.017

[a] The mixing time was 250 ms. [b] Rx is 6th root R factor: $\Sigma[((Io)_i^{1/6})-((Ic)_i^{1/6})/\Sigma((Io)_i^{1/6})]$.

[c] Average error: $\Sigma(Ic-Io)/n$, where Ic are NOE intensities calculated from refined structure, Io are experimental NOE intensities.

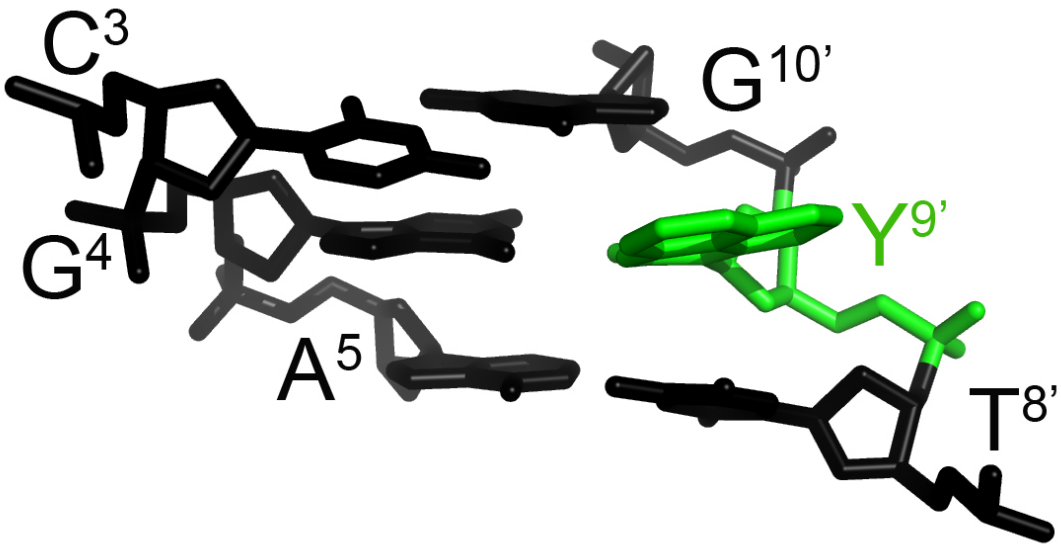


Figure 50. The average structure emergent from rMD calculations of DDD-GY duplex in the region of the C^3•G^{10}, G^4•Y^9 and A^5•T^8 base pairs. Base Y^9 is shown in green. The dPer (Y^9) forms wobble pair with the complementary dG (G^4). The dPer ring is oriented in the major groove. It does not disrupt neighbor base pairs.

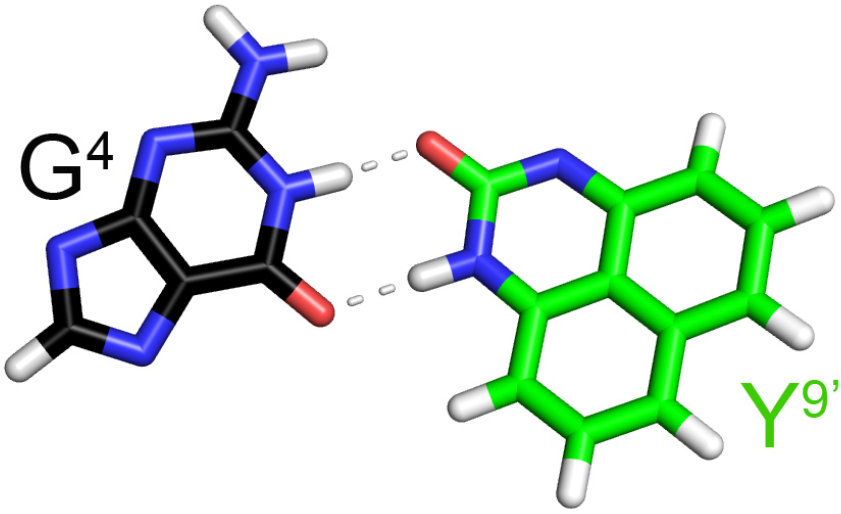


Figure 51. Average structure of the dG•dPer (DDD-GY) modified duplex as determined by NMR spectroscopy, showing G^4 forms a wobble base pair with the complementary dPer (Y^9) base. The anticipated hydrogen bonds are indicated as grey dashed lines.

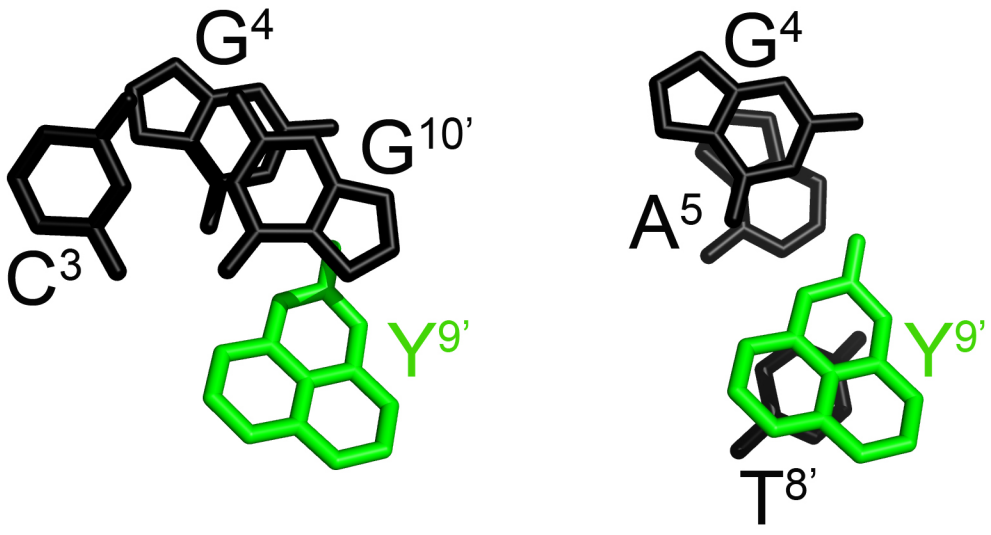


Figure 52. Stacking interactions for the dG•dPer (DDD-GY) duplex. (a) View from the C^3•G^{10} base pair (in black) and G^4•Y^9, shown in green. (b) View from the A^5•T^8 base pair (in black) and G^4 • Y^9 (in black and green, respectively). The dPer ring is oriented in the major groove. dPer (Y^9) base has a stacking interaction with T^8 base.

Discussion

O^6-Bn-dG (*105, 134, 135*) is formed following cellular exposures to *N*-benzylmethyl-nitrosamine (*136, 137*). It is mutagenic, causing G→T transversions but also G→C transversions and G→A transitions (*138, 139*). Sturla and coworkers showed that the dPer synthetic nucleotide (Chart 2) forms an orthogonal and thermodynamically stable base pair with O^6-Bn-dG (*125*). The present thermal melting studies comparing the DDD-XY and DDD-GY duplexes confirm, in a different sequence context, the earlier report, and the 5º C increase in the T_M of the DDD-XY duplex as compared to the DDD-GY duplex is consistent with the notion that dPer is a stable pairing partner for O^6-Bn-dG (*125*). Gong and Sturla (*125*) proposed that thermodynamic stabilization may

arise from a combination of π-π stacking interactions between the benzyl moiety of O^6-Bn-dG and the naphthyl moiety of dPer, and hydrogen bonding between the bases (*125*). However, no high resolution structural information has been available to test this model.

dPer Recognizes O^6-Bn-dG via a Stacking Interaction

New crystallographic data obtained in this study reveal that dPer recognizes O^6-Bn-dG via a stacking interaction between the dPer base and the benzyl group of O^6-Bn-dG (Figures 34 and 39). Electron density maps clearly show the insertion of the dPer base into the DNA, providing a binding pocket for the benzyl group of O^6-Bn-dG to intercalate between dPer and thymine of the 3'-neighbor A•T base pair. NMR data described here for the O^6-Bn-dG•dPer interaction corroborate the crystallographic results, leading to the conclusion that the intercalative recognition mechanism applies in solution. Furthermore, the absence of the dPer imino resonance indicates that the Y^9 imino proton is in enhanced exchange with the solvent, consistent with a lack of involvement in a base pairing interaction.

The chemical shifts of the dPer (Y^9) base resonances, observed in the 5.5-6.4 ppm range in the spectrum shown in Figure 43, are consistent with the insertion of dPer into the duplex and π–π stacking with the benzyl group of O^6-Bn-dG. In contrast, for the DDD-GY duplex, which lacks the O^6-Bn-dG lesion, the chemical shifts for the dPer protons are observed 6.6-7.4 ppm, i.e., further downfield, suggesting reduced stacking interactions. The NMR analysis shows a weak NOE interaction between the H9 proton of the dPer base and the deoxyribose H1' proton, consistent with dPer adopting the *syn*

glycosyl torsion angle, which accommodates for a π–π stacking interaction with the benzyl group of the O^6-Bn-dG. Modified Per base is almost symmetric. In addition, broad and overlapped cross peaks from NOESY spectrum of dPer base in DDD-XY duplex did not allowed with confidence to conform *syn* or anti conformation. However, in the crystal structure at 1.7 Å resolution, originally Per was inserted in *anti* conformation, but it did not fit well into electron density and an additional electron density was observed on the other side of the base. Base on this observation base was flipped into *syn* conformation and low R factor conformed correct placement of the base. The *syn*-glycosyl conformation of the dPer nucleoside was observed when it was not incorporated into DNA (*125*).

Base stacking interactions are of central importance in stabilizing nucleic acid duplexes (*140-143*). Those interactions contribute to the dependence of the duplex stability on its sequence (*144*). Lagenegger et al. (*145*) synthesized oligomers containing pyrene molecules. The modified bases were designed to pair through hydrophobic and packing forces, not to form hydrogen-bonding interactions. Upon annealing of both strands pyrenes formed an interstrand stacked structure for which the stability was almost equal to the unmodified duplex. Maleyshev et al. (*146*) determined the structure of the unnatural base pair in DNA. The NMR solution structure of dMMO2–d5SICS pair showed that modified bases were not in one plane, but formed an intercalated structure.

Duplexes containing O^6-Bn-dG:C are destabilized relative to those containing a G:C base pair (*125*); however, the structural consequences associated with placing O^6-Bn-dG into native DNA are not known, and attempts to characterize the structure of the lesion in this DDD were unsuccessful. NMR spectra of the O^6-Bn-dG-modified DDD

showed severe spectral broadening, which suggested that the lesion induced conformational disorder into the duplex. However, in a previous structural analysis of an O^6-Bn-dG modified template•primer complexed with the Y-family polymerase Dpo4, O^6-Bn-dG was observed to form a wobble base pair when placed opposite dC and a pseudo Watson-Crick hydrogen bonding pattern when placed opposite T (*113*).

The NMR analysis performed in this study provides information regarding solution dynamics of the O^6-Bn-dG•dPer interaction. The observation that the benzyl protons of the O^6-Bn-dG are observed as three broadened resonances (Figure 43) is consistent with rapid rotation of the benzyl ring in solution on the ms timescale of the NMR experiment, and probably on the time scale of DNA breathing motions. Further, this dynamic behavior probably accounts for the line broadening at base pairs C^3•G^{10} and X^4•Y^9 in the NMR spectrum (Figures 40 and 43). The intercalation of the flipping benzyl ring between Per and T^8 is consistent with line broadening observed both for T^8 and dPer protons. Similar flipping of the styrenyl moiety was observed previously in the *S*(61,2)-*R*-(N^6-Adenyl)styrene Oxide Adduct, when placed in DNA duplex based on the NOESY spectrum (*147*).

The simultaneous insertion of Per and the benzyl group of O^6-Bn-dG into the duplex unwinds the duplex at the recognition site (Figure 33, 34), as suggested by the weak sequential NOE connectivity cross-peak observed between C^3 H1' and X^4 H8. Additionally, the weak cross peak T^8 H1'→Y^9 H8 is also consistent with an increased distance between these bases. It seems likely that this distortion explains the greater volume of the crystallographic unit cell (Table 7) as compared to the canonical Dickerson-Drew dodecamer, and that these changes in the crystal packing of the

O^6-Bn-dG•dPer duplex may also explain why initial attempts to phase crystallographic data by the molecular replacement method failed. The electron density for the two 5'-terminal nucleotides C^1 and C^{13} was not visible, suggesting that these bases are disordered in the crystal. These terminal bases may be unable to fit into the lattice due to the unwinding of the dodecamer with the modified bases.

dPer Pairs with Guanine via a Wobble Base Pairing Interaction

The present results also reveal formation of a wobble pair between dPer and dG, with dPer oriented in the *anti* conformation with respect to the glycosyl bond, involving Per and the N1 and N^2 nitrogen atoms of the guanine (Figure 50). The presence of these hydrogen bonds is confirmed by the NMR data, which shows that the sequential connectivity of the base imino protons from base pairs C^3•G^{10} → G^4•Y^9 → A^5•T^8 is observed (Figure 45b). Moreover, the region of the spectrum showing NOEs between the base imino and amino protons (Figure 45a) is consistent with the notion that G^4 and Y^9 form a wobble-like base pair. Notably, the stability imparted by this wobble interaction is lower than that from the dPer•O^6-Bn-dG intercalative interaction, thus providing a basis for specificity. The presence of the wobble-pair interaction, however, may suggest a limitation in the selectivity of dPer for O^6-Bn-dG over G. Thus, although the stabilization of the wobble pair is smaller than the intercalated pair, it nonetheless participates in favorable H-bonding interactions and is not as disfavored as possible.

Summary

The synthetic base Per selectively distinguishes between dG and O^6-Bn-dG in DNA by an intercalative binding mode. The presence of the modified pair provides a binding pocket that allows the benzyl group of O^6-Bn-dG to intercalate between dPer and thymine of the 3'-neighbor A•T base pair. The binding of the benzyl group in this pocket is dynamic on the NMR time-scale and is captured in the face-to-face stack in the crystal structure. In contrast to the probe:adduct pair, dPer forms a less stable pair with dG, which is nonetheless minimally stabilized by a wobble-type H-bonding interaction. The new insight gained in this study furthers our understanding of alternative chemical interactions in DNA duplexes and their relationship with duplex thermodynamic stability. From the perspective of designing adduct-directed chemical probes, it provides information that may be applied to design modifications that could further stabilize the probe:adduct stacking interactions and/or destabilize the probe:G wobble interaction. There are currently limited examples of synthetic nucleotides that pair with bulky adducts, and the data presented here provide a first insight into a chemical basis of adduct recognition.

Acknowledgements

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of the Advanced Photon Source was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. The LS-CAT Sector 21 is supported by the Michigan Economic Development Corporation and the Michigan Technology Tri-Corridor for (Grant 085P1000817).

APPENDIX A

PDB COORDINATE FILES

File A-1: Crystal structure of 7-deaza-2'-deoxyadenosine modification in B-form DNA (PDB code 3OPI).

```
HEADER    DNA                                     01-SEP-10   3OPI
TITLE     7-DEAZA-2'-DEOXYADENOSINE MODIFICATION IN B-FORM DNA
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: DNA (5'-D(*CP*GP*CP*GP*AP*(7DA)P*TP*TP*CP*GP*CP*G)-3');
COMPND   3 CHAIN: A, B;
COMPND   4 ENGINEERED: YES
SOURCE    MOL_ID: 1;
SOURCE   2 SYNTHETIC: YES
KEYWDS    B-DNA, DODECAMER, 7-DEAZA-DEOXYADENOSINE, 7-DEAZA-DA, DNA
EXPDTA    X-RAY DIFFRACTION
AUTHOR    E.A.KOWAL,M.GANGULY,P.S.PALLAN,L.A.MARKY,B.GOLD,M.EGLI,M.P.STONE
REVDAT   2   28-DEC-11 3OPI    1       JRNL
REVDAT   1   31-AUG-11 3OPI    0
JRNL        AUTH   E.A.KOWAL,M.GANGULY,P.S.PALLAN,L.A.MARKY,B.GOLD,M.EGLI,
JRNL        AUTH 2 M.P.STONE
JRNL        TITL   ALTERING THE ELECTROSTATIC POTENTIAL IN THE MAJOR GROOVE:
JRNL        TITL 2 THERMODYNAMIC AND STRUCTURAL CHARACTERIZATION OF
JRNL        TITL 3 7-DEAZA-2'-DEOXYADENOSINE:DT BASE PAIRING IN DNA.
JRNL        REF    J.PHYS.CHEM.B                 V. 115 13925 2011
JRNL        REFN                   ISSN 1089-5647
JRNL        PMID   22059929
JRNL        DOI    10.1021/JP207104W
REMARK   2
REMARK   2 RESOLUTION.    1.10 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC 5.0
REMARK   3   AUTHORS     : MURSHUDOV,VAGIN,DODSON
REMARK   3
REMARK   3    REFINEMENT TARGET : NULL
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 1.10
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 34.40
REMARK   3   DATA CUTOFF            (SIGMA(F)) : NULL
REMARK   3   COMPLETENESS FOR RANGE        (%) : NULL
REMARK   3   NUMBER OF REFLECTIONS             : 27920
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD           : NULL
REMARK   3   FREE R VALUE TEST SET SELECTION   : RANDOM
REMARK   3   R VALUE     (WORKING + TEST SET) : NULL
REMARK   3   R VALUE            (WORKING SET) : 0.161
REMARK   3   FREE R VALUE                      : 0.195
REMARK   3   FREE R VALUE TEST SET SIZE   (%) : NULL
REMARK   3   FREE R VALUE TEST SET COUNT       : 2162
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REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           : NULL
REMARK   3   BIN RESOLUTION RANGE HIGH       (A) : 1.10
REMARK   3   BIN RESOLUTION RANGE LOW        (A) : 1.14
REMARK   3   REFLECTION IN BIN     (WORKING SET) : NULL
REMARK   3   BIN COMPLETENESS (WORKING+TEST) (%) : 97.90
REMARK   3   BIN R VALUE           (WORKING SET) : 0.1610
REMARK   3   BIN FREE R VALUE SET COUNT          : 2162
REMARK   3   BIN FREE R VALUE                    : 0.1950
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```
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REMARK   3   PROTEIN ATOMS            : 0
REMARK   3   NUCLEIC ACID ATOMS       : 486
REMARK   3   HETEROGEN ATOMS          : 5
REMARK   3   SOLVENT ATOMS            : 133
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REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : NULL
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) : NULL
REMARK   3    B22 (A**2) : NULL
REMARK   3    B33 (A**2) : NULL
REMARK   3    B12 (A**2) : NULL
REMARK   3    B13 (A**2) : NULL
REMARK   3    B23 (A**2) : NULL
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REMARK   3  ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3   ESU BASED ON R VALUE                            (A): NULL
REMARK   3   ESU BASED ON FREE R VALUE                       (A): NULL
REMARK   3   ESU BASED ON MAXIMUM LIKELIHOOD                 (A): NULL
REMARK   3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): NULL
REMARK   3
REMARK   3 CORRELATION COEFFICIENTS.
REMARK   3   CORRELATION COEFFICIENT FO-FC      : NULL
REMARK   3   CORRELATION COEFFICIENT FO-FC FREE : NULL
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES        COUNT    RMS    WEIGHT
REMARK   3   BOND LENGTHS REFINED ATOMS        (A):  NULL ;  NULL ;  NULL
REMARK   3   BOND LENGTHS OTHERS               (A):  NULL ;  NULL ;  NULL
REMARK   3   BOND ANGLES REFINED ATOMS   (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   BOND ANGLES OTHERS          (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   TORSION ANGLES, PERIOD 1    (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   TORSION ANGLES, PERIOD 2    (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   TORSION ANGLES, PERIOD 3    (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   TORSION ANGLES, PERIOD 4    (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   CHIRAL-CENTER RESTRAINTS       (A**3):  NULL ;  NULL ;  NULL
REMARK   3   GENERAL PLANES REFINED ATOMS      (A):  NULL ;  NULL ;  NULL
REMARK   3   GENERAL PLANES OTHERS             (A):  NULL ;  NULL ;  NULL
REMARK   3   NON-BONDED CONTACTS REFINED ATOMS (A):  NULL ;  NULL ;  NULL
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REMARK   3   NON-BONDED TORSION OTHERS         (A):  NULL ;  NULL ;  NULL
REMARK   3   H-BOND (X...Y) REFINED ATOMS      (A):  NULL ;  NULL ;  NULL
REMARK   3   H-BOND (X...Y) OTHERS             (A):  NULL ;  NULL ;  NULL
REMARK   3   POTENTIAL METAL-ION REFINED ATOMS (A):  NULL ;  NULL ;  NULL
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REMARK   3   SYMMETRY VDW REFINED ATOMS        (A):  NULL ;  NULL ;  NULL
REMARK   3   SYMMETRY VDW OTHERS               (A):  NULL ;  NULL ;  NULL
REMARK   3   SYMMETRY H-BOND REFINED ATOMS     (A):  NULL ;  NULL ;  NULL
REMARK   3   SYMMETRY H-BOND OTHERS            (A):  NULL ;  NULL ;  NULL
REMARK   3   SYMMETRY METAL-ION REFINED ATOMS  (A):  NULL ;  NULL ;  NULL
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REMARK   3   MAIN-CHAIN BOND OTHER ATOMS    (A**2):  NULL ;  NULL ;  NULL
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REMARK   3   SIDE-CHAIN BOND REFINED ATOMS  (A**2):  NULL ;  NULL ;  NULL
REMARK   3   SIDE-CHAIN ANGLE REFINED ATOMS (A**2):  NULL ;  NULL ;  NULL
REMARK   3
REMARK   3 ANISOTROPIC THERMAL FACTOR RESTRAINTS.    COUNT   RMS   WEIGHT
REMARK   3   RIGID-BOND RESTRAINTS          (A**2):  NULL ;  NULL ;  NULL
REMARK   3   SPHERICITY; FREE ATOMS         (A**2):  NULL ;  NULL ;  NULL
REMARK   3   SPHERICITY; BONDED ATOMS       (A**2):  NULL ;  NULL ;  NULL
REMARK   3
REMARK   3  NCS RESTRAINTS STATISTICS
REMARK   3   NUMBER OF DIFFERENT NCS GROUPS : NULL
REMARK   3
REMARK   3  TLS DETAILS
REMARK   3   NUMBER OF TLS GROUPS  : NULL
REMARK   3
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REMARK   3   ION PROBE RADIUS   : NULL
REMARK   3   SHRINKAGE RADIUS   : NULL
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REMARK   3  OTHER REFINEMENT REMARKS: NULL
REMARK   4
REMARK   4 3OPI COMPLIES WITH FORMAT V. 3.30, 13-JUL-11
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 23-SEP-10.
REMARK 100 THE RCSB ID CODE IS RCSB061410.
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REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        : 20-OCT-07
REMARK 200  TEMPERATURE           (KELVIN) : 100
REMARK 200  PH                             : 6.0
REMARK 200  NUMBER OF CRYSTALS USED        : 1
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REMARK 200  SYNCHROTRON              (Y/N) : Y
REMARK 200  RADIATION SOURCE               : APS
REMARK 200  BEAMLINE                       : 21-ID-F
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REMARK 200  WAVELENGTH OR RANGE        (A) : 0.9785
REMARK 200  MONOCHROMATOR                  : NULL
REMARK 200  OPTICS                         : NULL
REMARK 200
REMARK 200  DETECTOR TYPE                  : CCD
REMARK 200  DETECTOR MANUFACTURER          : MARMOSAIC 225 MM CCD
REMARK 200  INTENSITY-INTEGRATION SOFTWARE : HKL-2000
REMARK 200  DATA SCALING SOFTWARE          : HKL-2000
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : 27920
REMARK 200  RESOLUTION RANGE HIGH      (A) : 1.100
REMARK 200  RESOLUTION RANGE LOW       (A) : 50.000
REMARK 200  REJECTION CRITERIA  (SIGMA(I)) : 165.400
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REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE     (%) : 97.8
REMARK 200  DATA REDUNDANCY                : 10.600
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REMARK 200  R SYM                      (I) : NULL
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET  : 61.3000
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REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 1.10
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 1.14
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REMARK 200  DATA REDUNDANCY IN SHELL       : 6.90
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REMARK 200  R SYM FOR SHELL            (I) : NULL
REMARK 200  <I/SIGMA(I)> FOR SHELL         : NULL
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REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT
REMARK 200 SOFTWARE USED: CCP4-MOLREP
REMARK 200 STARTING MODEL: PDB ENTRY 355D
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REMARK 200 REMARK: NULL
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REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS   (%): 47.10
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 2.33
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REMARK 280 CRYSTALLIZATION CONDITIONS: DROPLETS CONTAINING 0.6 MM
REMARK 280  OLIGONUCLEOTIDE, 5% 2-METHYL-2,4-PENTANEDIOL (MPD), 20 MM SODIUM
REMARK 280  CACODYLATE, 6 MM SPERMINE TETRAHYDROCHLORIDE, 40 MM NACL WERE
REMARK 280  EQUILIBRATED AGAINST A RESERVOIR OF 0.75 ML OF 35% MPD, PH 6.0,
REMARK 280  VAPOR DIFFUSION, HANGING DROP, TEMPERATURE 291K
REMARK 290
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```
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 21 21 21
REMARK 290
REMARK 290      SYMOP   SYMMETRY
REMARK 290     NNNMMM   OPERATOR
REMARK 290       1555   X,Y,Z
REMARK 290       2555   -X+1/2,-Y,Z+1/2
REMARK 290       3555   -X,Y+1/2,-Z+1/2
REMARK 290       4555   X+1/2,-Y+1/2,-Z
REMARK 290
REMARK 290     WHERE NNN -> OPERATOR NUMBER
REMARK 290           MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
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REMARK 290 RELATED MOLECULES.
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REMARK 290   SMTRY2   1  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   1  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   2 -1.000000  0.000000  0.000000       12.81750
REMARK 290   SMTRY2   2  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   2  0.000000  0.000000  1.000000       32.96400
REMARK 290   SMTRY1   3 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   3  0.000000  1.000000  0.000000       20.15500
REMARK 290   SMTRY3   3  0.000000  0.000000 -1.000000       32.96400
REMARK 290   SMTRY1   4  1.000000  0.000000  0.000000       12.81750
REMARK 290   SMTRY2   4  0.000000 -1.000000  0.000000       20.15500
REMARK 290   SMTRY3   4  0.000000  0.000000 -1.000000        0.00000
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REMARK 300 THIS ENTRY. THE REMARK MAY ALSO PROVIDE INFORMATION ON
REMARK 300 BURIED SURFACE AREA.
REMARK 350
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW.  BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: DIMERIC
REMARK 350 SOFTWARE DETERMINED QUATERNARY STRUCTURE: DIMERIC
REMARK 350 SOFTWARE USED: PISA
REMARK 350 TOTAL BURIED SURFACE AREA: 3090 ANGSTROM**2
REMARK 350 SURFACE AREA OF THE COMPLEX: 4150 ANGSTROM**2
REMARK 350 CHANGE IN SOLVENT FREE ENERGY: -30.0 KCAL/MOL
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REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT3   1  0.000000  0.000000  1.000000        0.00000
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
REMARK 500  ATM1  RES C  SSEQI   ATM2  RES C  SSEQI           DISTANCE
REMARK 500   OP2  7DA A   106     O    HOH A   465             1.90
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
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REMARK 500 EXPECTED VALUES NUCLEIC ACID: CLOWNEY ET AL 1996
REMARK 500
REMARK 500  M RES CSSEQI ATM1   RES CSSEQI ATM2   DEVIATION
REMARK 500     DC A 103   O3'    DC A 103   C3'    -0.048
REMARK 500     DG A 102   O3'    DC A 103   P      -0.107
REMARK 500     DG A 104   N3     DG A 104   C4      0.055
REMARK 500     DG A 104   C4     DG A 104   C5     -0.051
REMARK 500     DG A 104   C6     DG A 104   N1      0.063
REMARK 500     DG A 104   C5     DG A 104   N7      0.045
REMARK 500     DG A 104   C2     DG A 104   N2      0.065
REMARK 500     DA A 105   C6     DA A 105   N1     -0.044
REMARK 500     DG A 112   C5'    DG A 112   C4'     0.079
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REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
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REMARK 500 EXPECTED VALUES NUCLEIC ACID: CLOWNEY ET AL 1996
REMARK 500
REMARK 500  M RES CSSEQI ATM1   ATM2   ATM3
REMARK 500     DG A 104   O5' -  C5' -  C4' ANGL. DEV. =  -6.5 DEGREES
REMARK 500     DG A 104   C8  -  N9  -  C4  ANGL. DEV. =   2.5 DEGREES
REMARK 500     DG A 104   C5  -  C6  -  O6  ANGL. DEV. =  -3.9 DEGREES
REMARK 500     DG A 110   O4' -  C1' -  N9  ANGL. DEV. =   1.8 DEGREES
REMARK 500     DG B 216   O4' -  C1' -  N9  ANGL. DEV. =   4.1 DEGREES
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: PLANAR GROUPS
REMARK 500
REMARK 500 PLANAR GROUPS IN THE FOLLOWING RESIDUES HAVE A TOTAL
REMARK 500 RMS DISTANCE OF ALL ATOMS FROM THE BEST-FIT PLANE
REMARK 500 BY MORE THAN AN EXPECTED VALUE OF 6*RMSD, WITH AN
REMARK 500 RMSD 0.02 ANGSTROMS, OR AT LEAST ONE ATOM HAS
REMARK 500 AN RMSD GREATER THAN THIS VALUE
REMARK 500 (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER;
REMARK 500 SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500  M RES CSSEQI        RMS     TYPE
REMARK 500     DC A 109         0.06    SIDE CHAIN
REMARK 500     DC B 223         0.09    SIDE CHAIN
REMARK 500
REMARK 500 REMARK: NULL
REMARK 620
REMARK 620 METAL COORDINATION
REMARK 620 (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER;
REMARK 620 SSEQ=SEQUENCE NUMBER; I=INSERTION CODE):
REMARK 620
REMARK 620 COORDINATION ANGLES FOR:  M RES CSSEQI METAL
REMARK 620                              MG A 301  MG
REMARK 620 N RES CSSEQI ATOM
REMARK 620 1 HOH A 410   O
REMARK 620 2 HOH A 408   O    91.4
REMARK 620 3 HOH A 407   O    93.0  87.6
REMARK 620 N                   1     2
REMARK 620
REMARK 620 COORDINATION ANGLES FOR:  M RES CSSEQI METAL
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REMARK 620                              NA B 403  NA
REMARK 620 N RES CSSEQI ATOM
REMARK 620 1  DC B 215   OP1
REMARK 620 2 HOH B 533   O    93.5
REMARK 620 N                   1
REMARK 620
REMARK 620 COORDINATION ANGLES FOR:  M RES CSSEQI METAL
REMARK 620                              NA A 400  NA
REMARK 620 N RES CSSEQI ATOM
REMARK 620 1  DT A 107   O2
REMARK 620 2  DT B 219   O2   80.1
REMARK 620 3 HOH B 441   O   113.7  96.6
REMARK 620 4 HOH B 450   O    94.0 109.9 144.8
REMARK 620 N                   1     2     3
REMARK 620
REMARK 620 COORDINATION ANGLES FOR:  M RES CSSEQI METAL
REMARK 620                              NA A 401  NA
REMARK 620 N RES CSSEQI ATOM
REMARK 620 1 HOH A 443   O
REMARK 620 2  DT A 107   OP1 106.6
REMARK 620 N                   1
REMARK 620
REMARK 620 COORDINATION ANGLES FOR:  M RES CSSEQI METAL
REMARK 620                              NA A 402  NA
REMARK 620 N RES CSSEQI ATOM
REMARK 620 1 HOH A 484   O
REMARK 620 2 HOH A 519   O   103.7
REMARK 620 N                   1
REMARK 800
REMARK 800 SITE
REMARK 800 SITE_IDENTIFIER: AC1
REMARK 800 EVIDENCE_CODE: SOFTWARE
REMARK 800 SITE_DESCRIPTION: BINDING SITE FOR RESIDUE MG A 301
REMARK 800
REMARK 800 SITE_IDENTIFIER: AC2
REMARK 800 EVIDENCE_CODE: SOFTWARE
REMARK 800 SITE_DESCRIPTION: BINDING SITE FOR RESIDUE NA A 400
REMARK 800
REMARK 800 SITE_IDENTIFIER: AC3
REMARK 800 EVIDENCE_CODE: SOFTWARE
REMARK 800 SITE_DESCRIPTION: BINDING SITE FOR RESIDUE NA A 401
REMARK 800
REMARK 800 SITE_IDENTIFIER: AC4
REMARK 800 EVIDENCE_CODE: SOFTWARE
REMARK 800 SITE_DESCRIPTION: BINDING SITE FOR RESIDUE NA A 402
REMARK 800
REMARK 800 SITE_IDENTIFIER: AC5
REMARK 800 EVIDENCE_CODE: SOFTWARE
REMARK 800 SITE_DESCRIPTION: BINDING SITE FOR RESIDUE NA B 403
DBREF  3OPI A  101   112  PDB    3OPI     3OPI           101    112
DBREF  3OPI B  213   224  PDB    3OPI     3OPI           213    224
SEQRES   1 A   12   DC  DG  DC  DG  DA 7DA  DT  DT  DC  DG  DC  DG
SEQRES   1 B   12   DC  DG  DC  DG  DA 7DA  DT  DT  DC  DG  DC  DG
MODRES 3OPI 7DA A  106   DA
MODRES 3OPI 7DA B  218   DA
HET    7DA  A 106      42
HET    7DA  B 218      21
HET     MG  A 301       1
HET     NA  A 400       1
HET     NA  A 401       1
HET     NA  A 402       1
HET     NA  B 403       1
HETNAM     7DA 7-DEAZA-2'-DEOXYADENOSINE-5'-MONOPHOSPHATE
HETNAM      MG MAGNESIUM ION
HETNAM      NA SODIUM ION
FORMUL   1  7DA    2(C11 H15 N4 O6 P)
FORMUL   3   MG    MG 2+
FORMUL   4   NA    4(NA 1+)
FORMUL   8  HOH   *133(H2 O)
LINK         O3'A DA A 105                 P  A7DA A 106     1555   1555  1.72
LINK         O3'B DA A 105                 P  B7DA A 106     1555   1555  1.56
LINK         O3'A7DA A 106                 P    DT A 107     1555   1555  1.66
LINK         O3'B7DA A 106                 P    DT A 107     1555   1555  1.51
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LINK         O3'  DA B 217                P    7DA B 218     1555   1555  1.56
LINK         O3' 7DA B 218                P     DT B 219     1555   1555  1.56
LINK        MG    MG A 301                O   HOH A 410     1555   1555  2.08
LINK        MG    MG A 301                O   HOH A 408     1555   1555  2.09
LINK        MG    MG A 301                O   HOH A 407     1555   1555  2.09
LINK         OP1  DC B 215               NA    NA B 403     1555   1555  2.68
LINK         O2   DT A 107               NA    NA A 400     1555   1555  2.73
LINK        NA    NA A 401                O   HOH A 443     1555   1555  2.73
LINK         OP1  DT A 107               NA    NA A 401     1555   1555  2.75
LINK        NA    NA B 403                O   HOH B 533     1555   1555  2.78
LINK         O2   DT B 219               NA    NA A 400     1555   1555  2.78
LINK        NA    NA A 400                O   HOH B 441     1555   1555  2.79
LINK        NA    NA A 402                O   HOH A 484     1555   1555  2.87
LINK        NA    NA A 400                O   HOH B 450     1555   1555  2.88
LINK        NA    NA A 402                O   HOH A 519     1555   1555  3.02
SITE     1 AC1  6 HOH A 406  HOH A 407  HOH A 408  HOH A 409
SITE     2 AC1  6 HOH A 410  HOH B 405
SITE     1 AC2  6  DT A 107   DT A 108   DT B 219   DT B 220
SITE     2 AC2  6 HOH B 441  HOH B 450
SITE     1 AC3  4  DT A 107  HOH A 409  HOH A 419  HOH A 443
SITE     1 AC4  5  DG A 104   DA A 105   DG A 112  HOH A 484
SITE     2 AC4  5 HOH A 519
SITE     1 AC5  5  DC A 101  HOH A 440   DG B 214   DC B 215
SITE     2 AC5  5 HOH B 533
CRYST1   25.635   40.310   65.928  90.00  90.00  90.00 P 21 21 21    8
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.039009  0.000000  0.000000        0.00000
SCALE2      0.000000  0.024808  0.000000        0.00000
SCALE3      0.000000  0.000000  0.015168        0.00000
ATOM      1  O5'  DC A 101     -17.790  -5.366  56.580  1.00 16.37           O
ANISOU    1  O5'  DC A 101     2010   1580   2630     71    145   -141       O
ATOM      2  C5'  DC A 101     -18.494  -6.541  56.907  1.00 14.62           C
ANISOU    2  C5'  DC A 101     1839   1390   2323     57     18    132       C
ATOM      3  C4'  DC A 101     -17.542  -7.703  56.860  1.00 13.62           C
ANISOU    3  C4'  DC A 101     1634   1519   2022    208    -61     45       C
ATOM      4  O4'  DC A 101     -18.167  -8.865  57.434  1.00 13.28           O
ANISOU    4  O4'  DC A 101     1785   1476   1785    -50    -84    -26       O
ATOM      5  C3'  DC A 101     -17.159  -8.104  55.486  1.00 14.17           C
ANISOU    5  C3'  DC A 101     1585   1767   2029    141     59    213       C
ATOM      6  O3'  DC A 101     -15.750  -8.487  55.494  1.00 15.83           O
ANISOU    6  O3'  DC A 101     1815   2030   2168    106    157    -22       O
ATOM      7  C2'  DC A 101     -18.087  -9.269  55.156  1.00 13.75           C
ANISOU    7  C2'  DC A 101     1817   1654   1751   -139   -103    -11       C
ATOM      8  C1'  DC A 101     -18.253  -9.932  56.500  1.00 13.14           C
ANISOU    8  C1'  DC A 101     1793   1543   1656      4    -57    -89       C
ATOM      9  N1   DC A 101     -19.505 -10.624  56.771  1.00 11.24           N
ANISOU    9  N1   DC A 101     1472   1311   1484    133   -125     34       N
ATOM     10  C2   DC A 101     -19.470 -11.840  57.476  1.00 11.67           C
ANISOU   10  C2   DC A 101     1460   1436   1537    132   -187    -16       C
ATOM     11  O2   DC A 101     -18.361 -12.308  57.775  1.00 13.17           O
ANISOU   11  O2   DC A 101     1555   1428   2020    110    -47    228       O
ATOM     12  N3   DC A 101     -20.634 -12.457  57.797  1.00 11.19           N
ANISOU   12  N3   DC A 101     1472   1371   1407    169   -110      6       N
ATOM     13  C4   DC A 101     -21.784 -11.909  57.451  1.00 11.57           C
ANISOU   13  C4   DC A 101     1468   1361   1565     49    -72     12       C
ATOM     14  N4   DC A 101     -22.892 -12.530  57.806  1.00 12.75           N
ANISOU   14  N4   DC A 101     1642   1535   1665    193    -41     35       N
ATOM     15  C5   DC A 101     -21.843 -10.672  56.735  1.00 12.50           C
ANISOU   15  C5   DC A 101     1532   1601   1617    234   -152     54       C
ATOM     16  C6   DC A 101     -20.702 -10.064  56.440  1.00 12.47           C
ANISOU   16  C6   DC A 101     1503   1536   1699    142   -144    -20       C
ATOM     17  P    DG A 102     -14.937  -8.876  54.182  1.00 17.24           P
ANISOU   17  P    DG A 102     1948   2208   2392    -81    199    -28       P
ATOM     18  OP1  DG A 102     -13.517  -8.493  54.431  1.00 20.98           O
ANISOU   18  OP1  DG A 102     1827   2881   3262   -425    174   -210       O
ATOM     19  OP2  DG A 102     -15.646  -8.366  53.025  1.00 19.40           O
ANISOU   19  OP2  DG A 102     2302   2525   2544    -60    388   -153       O
ATOM     20  O5'  DG A 102     -15.040 -10.463  54.079  1.00 16.07           O
ANISOU   20  O5'  DG A 102     1892   1883   2328    192    -31   -201       O
ATOM     21  C5'  DG A 102     -14.350 -11.271  55.009  1.00 16.33           C
ANISOU   21  C5'  DG A 102     1414   2251   2537    129    -91    -80       C
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ATOM     22  C4'  DG A 102     -14.554 -12.693  54.623  1.00 15.14           C
ANISOU   22  C4'  DG A 102     1288   2157   2307    -48    219   -117       C
ATOM     23  O4'  DG A 102     -15.902 -13.131  54.938  1.00 15.32           O
ANISOU   23  O4'  DG A 102     1330   2532   1956     55    147    -88       O
ATOM     24  C3'  DG A 102     -14.367 -12.991  53.141  1.00 14.75           C
ANISOU   24  C3'  DG A 102     1530   1930   2143    238    156   -239       C
ATOM     25  O3'  DG A 102     -13.620 -14.225  53.098  1.00 19.04           O
ANISOU   25  O3'  DG A 102     1906   2461   2866    762    983     76       O
ATOM     26  C2'  DG A 102     -15.798 -13.159  52.610  1.00 15.24           C
ANISOU   26  C2'  DG A 102     1515   2203   2071    -67    414   -116       C
ATOM     27  C1'  DG A 102     -16.459 -13.783  53.837  1.00 13.35           C
ANISOU   27  C1'  DG A 102     1334   1829   1908     98    129    -30       C
ATOM     28  N9   DG A 102     -17.881 -13.608  53.933  1.00 12.32           N
ANISOU   28  N9   DG A 102     1344   1664   1670    120     90    -55       N
ATOM     29  C8   DG A 102     -18.624 -12.548  53.523  1.00 12.33           C
ANISOU   29  C8   DG A 102     1434   1495   1754    131      1   -209       C
ATOM     30  N7   DG A 102     -19.906 -12.668  53.805  1.00 11.64           N
ANISOU   30  N7   DG A 102     1350   1579   1491    -12     47   -128       N
ATOM     31  C5   DG A 102     -19.995 -13.882  54.481  1.00 10.83           C
ANISOU   31  C5   DG A 102     1318   1387   1408    130    -69   -107       C
ATOM     32  C6   DG A 102     -21.100 -14.571  55.040  1.00 10.52           C
ANISOU   32  C6   DG A 102     1234   1445   1318    104   -129   -154       C
ATOM     33  O6   DG A 102     -22.278 -14.214  55.057  1.00 11.09           O
ANISOU   33  O6   DG A 102     1267   1418   1528     75    -98    -79       O
ATOM     34  N1   DG A 102     -20.744 -15.778  55.609  1.00 10.36           N
ANISOU   34  N1   DG A 102     1216   1415   1305     30   -128   -163       N
ATOM     35  C2   DG A 102     -19.466 -16.283  55.656  1.00 10.55           C
ANISOU   35  C2   DG A 102     1213   1394   1401     25   -124   -153       C
ATOM     36  N2   DG A 102     -19.305 -17.449  56.238  1.00 11.50           N
ANISOU   36  N2   DG A 102     1343   1554   1473     54   -133   -151       N
ATOM     37  N3   DG A 102     -18.410 -15.652  55.155  1.00 11.47           N
ANISOU   37  N3   DG A 102     1339   1545   1473     58    -71   -141       N
ATOM     38  C4   DG A 102     -18.760 -14.472  54.573  1.00 11.46           C
ANISOU   38  C4   DG A 102     1373   1384   1596     58     61   -134       C
ATOM     39  P    DC A 103     -12.799 -14.735  51.951  1.00 17.32           P
ANISOU   39  P    DC A 103     1898   2235   2445    107    641    -79       P
ATOM     40  OP1  DC A 103     -11.375 -14.565  52.179  1.00 27.38           O
ANISOU   40  OP1  DC A 103     2181   4210   4009   -457   1120   -698       O
ATOM     41  OP2  DC A 103     -13.354 -14.245  50.702  1.00 27.29           O
ANISOU   41  OP2  DC A 103     3325   4104   2937    782    929   -558       O
ATOM     42  O5'  DC A 103     -13.058 -16.257  52.015  1.00 21.49           O
ANISOU   42  O5'  DC A 103     3475   2378   2311   -286    594   -192       O
ATOM     43  C5'  DC A 103     -13.191 -17.006  53.211  1.00 16.57           C
ANISOU   43  C5'  DC A 103     1799   2022   2474     92     75    216       C
ATOM     44  C4'  DC A 103     -14.333 -17.962  53.037  1.00 14.19           C
ANISOU   44  C4'  DC A 103     1625   1947   1820     66   -115   -109       C
ATOM     45  O4'  DC A 103     -15.545 -17.233  53.075  1.00 14.47           O
ANISOU   45  O4'  DC A 103     1621   2058   1818     46   -256   -391       O
ATOM     46  C3'  DC A 103     -14.321 -18.731  51.731  1.00 17.55           C
ANISOU   46  C3'  DC A 103     2483   2025   2157    317   -218   -214       C
ATOM     47  O3'A DC A 103     -13.792 -19.996  51.761  0.50 24.47           O
ANISOU   47  O3'A DC A 103     3020   2929   3345    -23    178   -510       O
ATOM     48  O3'B DC A 103     -13.786 -20.041  52.178  0.50 23.35           O
ANISOU   48  O3'B DC A 103     2431   3030   3411    371    224   -481       O
ATOM     49  C2'  DC A 103     -15.755 -18.782  51.335  1.00 18.73           C
ANISOU   49  C2'  DC A 103     2263   2390   2463    240   -145   -562       C
ATOM     50  C1'  DC A 103     -16.505 -18.070  52.447  1.00 15.98           C
ANISOU   50  C1'  DC A 103     1713   2047   2310    124   -480   -310       C
ATOM     51  N1   DC A 103     -17.586 -17.187  52.000  1.00 14.54           N
ANISOU   51  N1   DC A 103     1545   2046   1932     93   -305   -272       N
ATOM     52  C2   DC A 103     -18.901 -17.415  52.363  1.00 12.96           C
ANISOU   52  C2   DC A 103     1705   1756   1462     37   -186   -294       C
ATOM     53  O2   DC A 103     -19.166 -18.426  52.977  1.00 13.82           O
ANISOU   53  O2   DC A 103     1709   1790   1749    157   -251   -300       O
ATOM     54  N3   DC A 103     -19.849 -16.503  51.998  1.00 12.66           N
ANISOU   54  N3   DC A 103     1440   1893   1475     94   -282   -350       N
ATOM     55  C4   DC A 103     -19.516 -15.446  51.277  1.00 13.13           C
ANISOU   55  C4   DC A 103     1594   1868   1526     65   -133   -259       C
ATOM     56  N4   DC A 103     -20.456 -14.573  50.983  1.00 13.99           N
ANISOU   56  N4   DC A 103     1779   1819   1717    127   -163   -170       N
ATOM     57  C5   DC A 103     -18.145 -15.220  50.841  1.00 14.87           C
ANISOU   57  C5   DC A 103     1637   2144   1865    102    -41   -163       C
ATOM     58  C6   DC A 103     -17.266 -16.121  51.228  1.00 14.95           C
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ANISOU   58  C6   DC A 103     1622   2073   1983     -8   -272   -319       C
ATOM     59  P  A DG A 104     -13.725 -20.908  50.414  0.50 17.70           P
ANISOU   59  P  A DG A 104     2345   2224   2155     65    436   -312       P
ATOM     60  P  B DG A 104     -13.284 -21.198  51.207  0.50 16.55           P
ANISOU   60  P  B DG A 104     1625   2213   2448    439    -29   -324       P
ATOM     61  OP1A DG A 104     -12.590 -21.825  50.633  0.50 20.12          O
ANISOU   61  OP1A DG A 104     1722   2685   3234     25    690  -1006       O
ATOM     62  OP1B DG A 104     -12.404 -22.102  51.991  0.50 21.85          O
ANISOU   62  OP1B DG A 104     2152   2329   3820    663     -7   -697       O
ATOM     63  OP2A DG A 104     -13.791 -20.076  49.202  0.50 23.65          O
ANISOU   63  OP2A DG A 104     3325   2867   2793    184    717   -759       O
ATOM     64  OP2B DG A 104     -12.756 -20.600  49.952  0.50 17.86          O
ANISOU   64  OP2B DG A 104     1498   2468   2819    -98    483   -373       O
ATOM     65  O5'A DG A 104     -15.040 -21.742  50.441  0.50 16.17          O
ANISOU   65  O5'A DG A 104     2236   1971   1937    296    -90   -353       O
ATOM     66  O5'B DG A 104     -14.677 -21.970  50.886  0.50 17.21          O
ANISOU   66  O5'B DG A 104     2106   2264   2167    541    -23   -151       O
ATOM     67  C5'A DG A 104     -15.360 -22.485  51.508  0.50 16.38          C
ANISOU   67  C5'A DG A 104     2111   2122   1988    307   -156    -79       C
ATOM     68  C5'B DG A 104     -15.288 -22.792  51.920  0.50 18.25          C
ANISOU   68  C5'B DG A 104     1995   2708   2231    153   -117    -56       C
ATOM     69  C4'A DG A 104     -16.684 -22.981  51.174  0.50 15.60          C
ANISOU   69  C4'A DG A 104     1906   1918   2102    -12    269   -290       C
ATOM     70  C4'B DG A 104     -16.605 -23.449  51.508  0.50 15.60          C
ANISOU   70  C4'B DG A 104     1539   2131   2257    149   -289     50       C
ATOM     71  O4'A DG A 104     -17.526 -21.809  51.094  0.50 12.74          O
ANISOU   71  O4'A DG A 104     1466   1634   1739     10     92   -110       O
ATOM     72  O4'B DG A 104     -17.686 -22.489  51.454  0.50 14.74          O
ANISOU   72  O4'B DG A 104     1739   2151   1708    168   -330    167       O
ATOM     73  C3'A DG A 104     -16.687 -23.618  49.750  0.50 14.83          C
ANISOU   73  C3'A DG A 104     1768   1922   1943    179    346   -257       C
ATOM     74  C3'B DG A 104     -16.629 -24.203  50.188  0.50 16.02          C
ANISOU   74  C3'B DG A 104     1850   2119   2115    520   -277     96       C
ATOM     75  O3'A DG A 104     -17.705 -24.604  49.651  0.50 19.08          O
ANISOU   75  O3'A DG A 104     2100   2313   2836     81    550   -533       O
ATOM     76  O3'B DG A 104     -17.292 -25.420  50.416  0.50 17.69          O
ANISOU   76  O3'B DG A 104     1671   2297   2751    250   -450    144       O
ATOM     77  C2'A DG A 104     -17.069 -22.450  48.901  0.50 16.89          C
ANISOU   77  C2'A DG A 104     1993   2218   2206    -21    333   -264       C
ATOM     78  C2'B DG A 104     -17.445 -23.274  49.259  0.50 16.19          C
ANISOU   78  C2'B DG A 104     2166   2193   1792    142   -325   -125       C
ATOM     79  C1'A DG A 104     -18.102 -21.822  49.824  0.50 13.58          C
ANISOU   79  C1'A DG A 104     1769   1716   1671    -40     74   -156       C
ATOM     80  C1'B DG A 104     -18.397 -22.567  50.220  0.50 14.79          C
ANISOU   80  C1'B DG A 104     1817   2035   1765    -82     26     11       C
ATOM     81  N9 A DG A 104     -18.472 -20.514  49.448  0.50 12.92           N
ANISOU   81  N9 A DG A 104     1214   1954   1738   -102    106   -153       N
ATOM     82  N9 B DG A 104     -18.715 -21.207  49.769  0.50 12.19           N
ANISOU   82  N9 B DG A 104     1571   1456   1604   -199   -219    -83       N
ATOM     83  C8 A DG A 104     -17.741 -19.541  48.821  0.50 14.37          C
ANISOU   83  C8 A DG A 104     2042   1850   1565    118   -210   -143       C
ATOM     84  C8 B DG A 104     -17.847 -20.343  49.144  0.50 12.95          C
ANISOU   84  C8 B DG A 104     1944   1616   1359    -91     33   -112       C
ATOM     85  N7 A DG A 104     -18.443 -18.452  48.632  0.50 14.44          N
ANISOU   85  N7 A DG A 104     1692   2048   1745     44   -226   -200       N
ATOM     86  N7 B DG A 104     -18.349 -19.177  48.856  0.50 12.95          N
ANISOU   86  N7 B DG A 104     1469   1891   1560    275   -190   -342       N
ATOM     87  C5 A DG A 104     -19.705 -18.806  49.212  0.50 15.00          C
ANISOU   87  C5 A DG A 104     1625   2626   1448    195   -225   -747       C
ATOM     88  C5 B DG A 104     -19.653 -19.221  49.310  0.50 13.06          C
ANISOU   88  C5 B DG A 104     1578   1899   1485     24   -234   -440       C
ATOM     89  C6 A DG A 104     -20.892 -18.118  49.316  0.50 14.65          C
ANISOU   89  C6 A DG A 104     1635   2487   1444   -140   -206   -630       C
ATOM     90  C6 B DG A 104     -20.715 -18.187  49.227  0.50 14.41          C
ANISOU   90  C6 B DG A 104     1591   2455   1428     38   -134   -617       C
ATOM     91  O6 A DG A 104     -21.066 -17.010  48.928  0.50 14.43          O
ANISOU   91  O6 A DG A 104     1211   2606   1664   -217     66   -555       O
ATOM     92  O6 B DG A 104     -20.696 -17.038  48.757  0.50 14.53          O
ANISOU   92  O6 B DG A 104     1340   2619   1562   -110    279   -651       O
ATOM     93  N1 A DG A 104     -21.953 -18.876  49.960  0.50 13.22          N
ANISOU   93  N1 A DG A 104     1364   2194   1462   -177   -146   -512       N
ATOM     94  N1 B DG A 104     -21.873 -18.620  49.769  0.50 14.13          N
ANISOU   94  N1 B DG A 104     1465   2334   1569   -129    -81   -608       N
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ATOM     95  C2 A DG A 104     -21.837 -20.135  50.426  0.50 15.84           C
ANISOU   95  C2 A DG A 104     1922   2433   1662    256   -176   -774       C
ATOM     96  C2 B DG A 104     -22.007 -19.873  50.326  0.50 12.83           C
ANISOU   96  C2 B DG A 104     1564   1858   1453    188   -200   -443       C
ATOM     97  N2 A DG A 104     -22.972 -20.719  51.016  0.50 13.90           N
ANISOU   97  N2 A DG A 104     1718   1795   1769    397   -415   -221       N
ATOM     98  N2 B DG A 104     -23.203 -20.184  50.808  0.50 11.37           N
ANISOU   98  N2 B DG A 104     1415   1328   1577    236   -186   -173       N
ATOM     99  N3 A DG A 104     -20.706 -20.792  50.316  0.50 15.98           N
ANISOU   99  N3 A DG A 104     1709   2716   1647     87   -280   -582       N
ATOM    100  N3 B DG A 104     -21.061 -20.833  50.411  0.50 14.83           N
ANISOU  100  N3 B DG A 104     1467   2404   1763    203   -204   -686       N
ATOM    101  C4 A DG A 104     -19.690 -20.041  49.701  0.50 13.26           C
ANISOU  101  C4 A DG A 104     1343   2053   1640    -48   -328   -482       C
ATOM    102  C4 B DG A 104     -19.910 -20.451  49.895  0.50 15.51           C
ANISOU  102  C4 B DG A 104     1799   2499   1592   -226   -124   -374       C
ATOM    103  P  A DA A 105     -17.700 -25.829  48.549  0.50 23.79           P
ANISOU  103  P  A DA A 105     2959   2839   3241    156    656   -635       P
ATOM    104  P  B DA A 105     -17.608 -26.442  49.262  0.50 21.07           P
ANISOU  104  P  B DA A 105     3050   2252   2700    967    114   -189       P
ATOM    105  OP1A DA A 105     -16.864 -26.917  49.086  0.50 26.39           O
ANISOU  105  OP1A DA A 105     2910   3849   3267    211    -36   -151       O
ATOM    106  OP1B DA A 105     -17.508 -27.790  49.837  0.50 24.13           O
ANISOU  106  OP1B DA A 105     2356   3012   3799    -36    -86    334       O
ATOM    107  OP2A DA A 105     -17.424 -25.304  47.190  0.50 26.49           O
ANISOU  107  OP2A DA A 105     3180   3239   3643   -232   -266   -658       O
ATOM    108  OP2B DA A 105     -16.788 -26.104  48.040  0.50 22.80           O
ANISOU  108  OP2B DA A 105     3139   2433   3090    621    370   -709       O
ATOM    109  O5'A DA A 105     -19.190 -26.311  48.539  0.50 19.50           O
ANISOU  109  O5'A DA A 105     2180   2310   2917   -117    230   -541       O
ATOM    110  O5'B DA A 105     -19.161 -26.166  49.008  0.50 19.47           O
ANISOU  110  O5'B DA A 105     2878   2292   2224   -284    164   -584       O
ATOM    111  C5'A DA A 105     -19.908 -26.399  49.714  0.50 16.47           C
ANISOU  111  C5'A DA A 105     1846   1982   2430   -156   -292    -22       C
ATOM    112  C5'B DA A 105     -20.054 -26.439  50.127  0.50 18.65           C
ANISOU  112  C5'B DA A 105     2124   2514   2445    -25   -214   -229       C
ATOM    113  C4'A DA A 105     -21.251 -25.874  49.445  0.50 17.75           C
ANISOU  113  C4'A DA A 105     1849   1985   2910   -183  -1037   -347       C
ATOM    114  C4'B DA A 105     -21.515 -26.192  49.842  0.50 18.86           C
ANISOU  114  C4'B DA A 105     2348   2095   2724   -111   -126   -225       C
ATOM    115  O4'A DA A 105     -21.109 -24.466  49.139  0.50 18.81           O
ANISOU  115  O4'A DA A 105     2794   1968   2384    225   -649   -369       O
ATOM    116  O4'B DA A 105     -21.781 -24.780  49.601  0.50 15.14           O
ANISOU  116  O4'B DA A 105     1907   1949   1895    -79   -309   -214       O
ATOM    117  C3'A DA A 105     -21.896 -26.549  48.249  0.50 21.23           C
ANISOU  117  C3'A DA A 105     2794   2681   2591   -118   -398   -113       C
ATOM    118  C3'B DA A 105     -22.104 -26.966  48.688  0.50 16.47           C
ANISOU  118  C3'B DA A 105     2109   1739   2407   -228     41     -2       C
ATOM    119  O3'A DA A 105     -23.158 -27.087  48.586  0.50 27.43           O
ANISOU  119  O3'A DA A 105     3789   1802   4831   -334   -793   -272       O
ATOM    120  O3'B DA A 105     -23.397 -27.500  49.132  0.50 14.30           O
ANISOU  120  O3'B DA A 105     1613   2033   1786    -94   -401    196       O
ATOM    121  C2'A DA A 105     -21.978 -25.441  47.228  0.50 18.28           C
ANISOU  121  C2'A DA A 105     2683   1616   2647   -716   -469   -139       C
ATOM    122  C2'B DA A 105     -22.184 -25.879  47.575  0.50 14.34           C
ANISOU  122  C2'B DA A 105     2048   1526   1874   -247     44    262       C
ATOM    123  C1'A DA A 105     -21.956 -24.150  48.101  0.50 19.90           C
ANISOU  123  C1'A DA A 105     3130   2132   2299    102   -370    271       C
ATOM    124  C1'B DA A 105     -22.496 -24.611  48.359  0.50 11.70           C
ANISOU  124  C1'B DA A 105     1398   1326   1719   -246   -258   -154       C
ATOM    125  N9 A DA A 105     -21.442 -22.885  47.469  0.50 16.94           N
ANISOU  125  N9 A DA A 105     2109   2362   1964    355   -231     60       N
ATOM    126  N9 B DA A 105     -21.957 -23.380  47.758  0.50 13.22           N
ANISOU  126  N9 B DA A 105     1603   1537   1880   -181    122     33       N
ATOM    127  C8 A DA A 105     -20.176 -22.644  46.959  0.50 16.83           C
ANISOU  127  C8 A DA A 105     2521   1850   2023    426   -235    264       C
ATOM    128  C8 B DA A 105     -20.688 -23.175  47.277  0.50 12.79           C
ANISOU  128  C8 B DA A 105     1400   1697   1763   -133     26    157       C
ATOM    129  N7 A DA A 105     -20.006 -21.422  46.459  0.50 16.13           N
ANISOU  129  N7 A DA A 105     2337   2213   1577    304   -439   -449       N
ATOM    130  N7 B DA A 105     -20.495 -21.986  46.829  0.50 13.54           N
ANISOU  130  N7 B DA A 105     2041   1578   1526   -105     98    -62       N
ATOM    131  C5 A DA A 105     -21.236 -20.824  46.657  0.50 12.36           C
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ANISOU  131  C5 A DA A 105     1536   1828   1331    117   -217   -233       C
ATOM    132  C5 B DA A 105     -21.705 -21.353  47.001  0.50 11.06           C
ANISOU  132  C5 B DA A 105     1373   1431   1396   -208   -185    -82       C
ATOM    133  C6 A DA A 105     -21.731 -19.538  46.354  0.50 12.87           C
ANISOU  133  C6 A DA A 105     2094   1494   1300   -223    -71   -156       C
ATOM    134  C6 B DA A 105     -22.150 -20.057  46.699  0.50 11.74           C
ANISOU  134  C6 B DA A 105     1563   1635   1262   -164   -101   -138       C
ATOM    135  N6 A DA A 105     -21.016 -18.561  45.759  0.50 14.06           N
ANISOU  135  N6 A DA A 105     2076   1766   1500   -291   -270   -385       N
ATOM    136  N6 B DA A 105     -21.374 -19.110  46.155  0.50 12.91           N
ANISOU  136  N6 B DA A 105     1794   1739   1372   -204     37   -215       N
ATOM    137  N1 A DA A 105     -22.977 -19.285  46.659  0.50 11.96           N
ANISOU  137  N1 A DA A 105     1847   1515   1181   -297     93   -184       N
ATOM    138  N1 B DA A 105     -23.415 -19.782  46.984  0.50 11.36           N
ANISOU  138  N1 B DA A 105     1527   1450   1338   -267     35   -110       N
ATOM    139  C2 A DA A 105     -23.717 -20.221  47.252  0.50 12.45           C
ANISOU  139  C2 A DA A 105     2072   1285   1373   -199   -151    -96       C
ATOM    140  C2 B DA A 105     -24.194 -20.684  47.548  0.50 12.45           C
ANISOU  140  C2 B DA A 105     1469   1560   1702   -404    227    -51       C
ATOM    141  N3 A DA A 105     -23.381 -21.447  47.622  0.50 13.52           N
ANISOU  141  N3 A DA A 105     1911   1765   1459    -69    -66     57       N
ATOM    142  N3 B DA A 105     -23.903 -21.931  47.892  0.50 13.28           N
ANISOU  142  N3 B DA A 105     1715   1671   1659   -193    168    -64       N
ATOM    143  C4 A DA A 105     -22.128 -21.704  47.288  0.50 14.01           C
ANISOU  143  C4 A DA A 105     2202   1560   1561   -120     39    -44       C
ATOM    144  C4 B DA A 105     -22.632 -22.201  47.576  0.50 11.84           C
ANISOU  144  C4 B DA A 105     1474   1679   1344     32   -138   -208       C
HETATM  145  P  A7DA A 106     -23.587 -27.869  47.112  0.50 18.90           P
ANISOU  145  P  A7DA A 106     2113   1979   3087    116   -947   -452       P
HETATM  146  P  B7DA A 106     -24.355 -28.197  48.120  0.50 12.91           P
ANISOU  146  P  B7DA A 106     1549   1582   1773   -156   -242   -140       P
HETATM  147  OP1A7DA A 106     -24.054 -29.121  47.806  0.50 23.28           O
ANISOU  147  OP1A7DA A 106     2948   2646   3249   -146   -749    188       O
HETATM  148  OP1B7DA A 106     -25.209 -29.023  49.063  0.50 15.31           O
ANISOU  148  OP1B7DA A 106     1731   2060   2023     64   -710   -629       O
HETATM  149  OP2A7DA A 106     -22.774 -27.893  45.858  0.50 25.07           O
ANISOU  149  OP2A7DA A 106     3039   2751   3735   -332  -1286   -791       O
HETATM  150  OP2B7DA A 106     -23.672 -28.990  47.005  0.50 11.78           O
ANISOU  150  OP2B7DA A 106     1506    940   2027   -237   -367   -266       O
HETATM  151  O5'A7DA A 106     -24.784 -26.898  46.794  0.50 15.58           O
ANISOU  151  O5'A7DA A 106     1746   1897   2277     22   -707   -458       O
HETATM  152  O5'B7DA A 106     -25.284 -27.135  47.462  0.50 12.74           O
ANISOU  152  O5'B7DA A 106     1488   1865   1485   -240     30    -24       O
HETATM  153  N9 A7DA A 106     -25.117 -23.514  44.860  0.50 11.96           N
ANISOU  153  N9 A7DA A 106     1402   1705   1435    -84   -118    -58       N
HETATM  154  N9 B7DA A 106     -25.094 -23.658  44.906  0.50 12.14           N
ANISOU  154  N9 B7DA A 106     1484   1712   1414   -179    -65    -75       N
HETATM  155  C4 A7DA A 106     -24.892 -22.212  44.446  0.50 11.58           C
ANISOU  155  C4 A7DA A 106     1539   1524   1336   -167    -93    -70       C
HETATM  156  C4 B7DA A 106     -24.967 -22.333  44.500  0.50 11.80           C
ANISOU  156  C4 B7DA A 106     1505   1538   1440   -287   -114   -115       C
HETATM  157  N3 A7DA A 106     -25.755 -21.197  44.408  0.50 11.44           N
ANISOU  157  N3 A7DA A 106     1327   1598   1421     -9     24   -152       N
HETATM  158  N3 B7DA A 106     -25.910 -21.391  44.473  0.50 11.99           N
ANISOU  158  N3 B7DA A 106     1533   1568   1453   -189     -5   -175       N
HETATM  159  C2 A7DA A 106     -25.212 -20.076  43.924  0.50 12.83           C
ANISOU  159  C2 A7DA A 106     1672   1635   1567   -287    -56   -366       C
HETATM  160  C2 B7DA A 106     -25.467 -20.211  44.007  0.50 10.63           C
ANISOU  160  C2 B7DA A 106     1272   1428   1339   -301    -10   -100       C
HETATM  161  N1 A7DA A 106     -23.967 -19.895  43.482  0.50 11.97           N
ANISOU  161  N1 A7DA A 106     1532   1646   1367   -275     -8   -274       N
HETATM  162  N1 B7DA A 106     -24.242 -19.898  43.577  0.50 10.71           N
ANISOU  162  N1 B7DA A 106     1303   1483   1281   -185     34   -246       N
HETATM  163  C6 A7DA A 106     -23.140 -20.944  43.557  0.50 10.70           C
ANISOU  163  C6 A7DA A 106     1307   1496   1262   -136    -64   -268       C
HETATM  164  C6 B7DA A 106     -23.319 -20.879  43.639  0.50 12.14           C
ANISOU  164  C6 B7DA A 106     1555   1729   1329   -133    -57   -371       C
HETATM  165  N6 A7DA A 106     -21.848 -20.705  43.152  0.50 12.33           N
ANISOU  165  N6 A7DA A 106     1491   1715   1477   -220     12   -323       N
HETATM  166  N6 B7DA A 106     -22.042 -20.503  43.235  0.50 11.41           N
ANISOU  166  N6 B7DA A 106     1365   1649   1320      5      1   -500       N
HETATM  167  C5 A7DA A 106     -23.562 -22.186  44.034  0.50 10.81           C
ANISOU  167  C5 A7DA A 106     1379   1563   1162    -67      9   -146       C
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HETATM  168  C5 B7DA A 106     -23.639 -22.185  44.101  0.50 12.16           C
ANISOU  168  C5 B7DA A 106     1550   1763   1304    -70    -73   -174       C
HETATM  169  C7 A7DA A 106     -22.967 -23.451  44.220  0.50 12.03           C
ANISOU  169  C7 A7DA A 106     1453   1614   1503   -121   -211   -172       C
HETATM  170  C7 B7DA A 106     -22.943 -23.410  44.275  0.50 13.42           C
ANISOU  170  C7 B7DA A 106     1669   1798   1631   -126   -143   -190       C
HETATM  171  C8 A7DA A 106     -23.977 -24.235  44.741  0.50 11.43           C
ANISOU  171  C8 A7DA A 106     1377   1530   1435    -60   -107    -47       C
HETATM  172  C8 B7DA A 106     -23.898 -24.292  44.781  0.50 14.21           C
ANISOU  172  C8 B7DA A 106     1633   1992   1772    -55    -45   -229       C
HETATM  173  C2'A7DA A 106     -26.905 -25.252  44.817  0.50 10.63           C
ANISOU  173  C2'A7DA A 106     1159   1405   1471     51     39     63       C
HETATM  174  C2'B7DA A 106     -26.646 -25.655  44.973  0.50 12.11           C
ANISOU  174  C2'B7DA A 106     1490   1439   1670   -256   -397    224       C
HETATM  175  C5'A7DA A 106     -25.724 -26.573  47.767  0.50 15.42           C
ANISOU  175  C5'A7DA A 106     1910   1773   2175   -219   -256   -242       C
HETATM  176  C5'B7DA A 106     -26.164 -26.332  48.253  0.50 12.53           C
ANISOU  176  C5'B7DA A 106     1826   1713   1219     56     90   -134       C
HETATM  177  C4'A7DA A 106     -26.694 -25.576  47.214  0.50 12.56           C
ANISOU  177  C4'A7DA A 106     1668   1610   1491   -150    -50     89       C
HETATM  178  C4'B7DA A 106     -26.970 -25.472  47.364  0.50 12.96           C
ANISOU  178  C4'B7DA A 106     1526   1796   1600   -335   -346     52       C
HETATM  179  O4'A7DA A 106     -25.954 -24.439  46.810  0.50 12.05           O
ANISOU  179  O4'A7DA A 106     1588   1633   1355   -351    -70    -26       O
HETATM  180  O4'B7DA A 106     -26.173 -24.379  46.894  0.50 13.72           O
ANISOU  180  O4'B7DA A 106     1904   1861   1445   -461   -140   -137       O
HETATM  181  C1'A7DA A 106     -26.357 -24.030  45.481  0.50 12.28           C
ANISOU  181  C1'A7DA A 106     1552   1677   1434   -362    -96    -46       C
HETATM  182  C1'B7DA A 106     -26.342 -24.261  45.472  0.50 12.04           C
ANISOU  182  C1'B7DA A 106     1477   1639   1460   -309    -30    -20       C
HETATM  183  C3'A7DA A 106     -27.485 -26.083  46.000  0.50 11.15           C
ANISOU  183  C3'A7DA A 106     1356   1432   1446   -309   -133    139       C
HETATM  184  C3'B7DA A 106     -27.448 -26.267  46.154  0.50 13.57           C
ANISOU  184  C3'B7DA A 106     1461   2068   1624   -372   -136    132       C
HETATM  185  O3'A7DA A 106     -28.911 -25.827  46.252  0.50 12.07           O
ANISOU  185  O3'A7DA A 106     1629   1553   1403   -143     -7     -5       O
HETATM  186  O3'B7DA A 106     -28.869 -26.038  46.080  0.50 12.72           O
ANISOU  186  O3'B7DA A 106     1661   1612   1558   -168   -190    -36       O
ATOM    187  P    DT A 107     -29.935 -26.363  45.060  1.00 12.51           P
ANISOU  187  P    DT A 107     1492   1643   1615   -138    -44    110       P
ATOM    188  OP1  DT A 107     -31.227 -26.528  45.793  1.00 14.01           O
ANISOU  188  OP1  DT A 107     1605   1796   1920   -159     73    319       O
ATOM    189  OP2  DT A 107     -29.439 -27.465  44.236  1.00 13.09           O
ANISOU  189  OP2  DT A 107     1579   1739   1653   -171   -180    184       O
ATOM    190  O5'  DT A 107     -30.022 -25.095  44.103  1.00 12.75           O
ANISOU  190  O5'  DT A 107     1637   1577   1629    -97     22    129       O
ATOM    191  C5'  DT A 107     -30.395 -23.834  44.651  1.00 14.05           C
ANISOU  191  C5'  DT A 107     1670   1790   1876     67    297    159       C
ATOM    192  C4'  DT A 107     -30.226 -22.777  43.611  1.00 13.12           C
ANISOU  192  C4'  DT A 107     1491   1777   1715   -218    166    249       C
ATOM    193  O4'  DT A 107     -28.834 -22.620  43.329  1.00 12.75           O
ANISOU  193  O4'  DT A 107     1533   1742   1569   -174     86     52       O
ATOM    194  C3'  DT A 107     -30.908 -23.084  42.290  1.00 12.82           C
ANISOU  194  C3'  DT A 107     1499   1578   1793    -30    -13    264       C
ATOM    195  O3'  DT A 107     -32.007 -22.179  42.171  1.00 14.84           O
ANISOU  195  O3'  DT A 107     1606   1991   2039      1    164    377       O
ATOM    196  C2'  DT A 107     -29.818 -22.895  41.232  1.00 13.59           C
ANISOU  196  C2'  DT A 107     1611   1823   1730    -70     84     55       C
ATOM    197  C1'  DT A 107     -28.757 -22.128  41.980  1.00 12.45           C
ANISOU  197  C1'  DT A 107     1646   1629   1454    -87    109    134       C
ATOM    198  N1   DT A 107     -27.374 -22.335  41.539  1.00 11.24           N
ANISOU  198  N1   DT A 107     1432   1438   1400   -103     -1    -55       N
ATOM    199  C2   DT A 107     -26.635 -21.249  41.076  1.00 11.45           C
ANISOU  199  C2   DT A 107     1479   1454   1417   -156      5     -7       C
ATOM    200  O2   DT A 107     -27.133 -20.142  40.944  1.00 12.28           O
ANISOU  200  O2   DT A 107     1568   1424   1672   -177    121    -18       O
ATOM    201  N3   DT A 107     -25.336 -21.516  40.763  1.00 11.55           N
ANISOU  201  N3   DT A 107     1595   1420   1373   -117     23   -168       N
ATOM    202  C4   DT A 107     -24.709 -22.715  40.850  1.00 11.51           C
ANISOU  202  C4   DT A 107     1413   1577   1384   -199    -39   -127       C
ATOM    203  O4   DT A 107     -23.518 -22.800  40.541  1.00 11.91           O
ANISOU  203  O4   DT A 107     1448   1622   1453   -101    -31    -68       O
ATOM    204  C5   DT A 107     -25.526 -23.834  41.278  1.00 11.36           C
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ANISOU  204  C5   DT A 107     1475   1411   1430   -129    -26   -124       C
ATOM    205  C7   DT A 107     -24.929 -25.194  41.367  1.00 13.07           C
ANISOU  205  C7   DT A 107     1622   1629   1713   -161    -65   -123       C
ATOM    206  C6   DT A 107     -26.794 -23.573  41.607  1.00 11.50           C
ANISOU  206  C6   DT A 107     1534   1437   1396   -229    -18    -45       C
ATOM    207  P    DT A 108     -32.998 -22.119  40.950  1.00 15.73           P
ANISOU  207  P    DT A 108     1595   2031   2351    -97    -87    349       P
ATOM    208  OP1  DT A 108     -34.292 -21.497  41.425  1.00 18.81           O
ANISOU  208  OP1  DT A 108     1557   2496   3091    112    157    300       O
ATOM    209  OP2  DT A 108     -33.035 -23.450  40.342  1.00 18.08           O
ANISOU  209  OP2  DT A 108     1707   2677   2483    120   -435    171       O
ATOM    210  O5′  DT A 108     -32.283 -21.139  39.935  1.00 14.67           O
ANISOU  210  O5′  DT A 108     1781   1726   2064   -113    -52    137       O
ATOM    211  C5′  DT A 108     -32.105 -19.817  40.315  1.00 14.55           C
ANISOU  211  C5′  DT A 108     1866   1770   1889    -22     71    225       C
ATOM    212  C4′  DT A 108     -31.294 -19.094  39.277  1.00 14.03           C
ANISOU  212  C4′  DT A 108     1573   1901   1856     47    162    297       C
ATOM    213  O4′  DT A 108     -29.969 -19.633  39.240  1.00 13.54           O
ANISOU  213  O4′  DT A 108     1525   1848   1770     77     78    124       O
ATOM    214  C3′  DT A 108     -31.861 -19.160  37.847  1.00 15.02           C
ANISOU  214  C3′  DT A 108     1883   1814   2008    113    -26    271       C
ATOM    215  O3′  DT A 108     -32.208 -17.854  37.482  1.00 15.17           O
ANISOU  215  O3′  DT A 108     1760   1917   2086    235    133    379       O
ATOM    216  C2′  DT A 108     -30.698 -19.768  37.047  1.00 15.06           C
ANISOU  216  C2′  DT A 108     1776   2064   1880    136   -251     93       C
ATOM    217  C1′  DT A 108     -29.515 -19.501  37.907  1.00 12.56           C
ANISOU  217  C1′  DT A 108     1607   1653   1510   -123    188    -29       C
ATOM    218  N1   DT A 108     -28.378 -20.409  37.745  1.00 11.93           N
ANISOU  218  N1   DT A 108     1549   1450   1533   -114     63    -22       N
ATOM    219  C2   DT A 108     -27.142 -19.926  37.393  1.00 11.08           C
ANISOU  219  C2   DT A 108     1434   1381   1393   -208    -21    -48       C
ATOM    220  O2   DT A 108     -26.949 -18.749  37.112  1.00 12.00           O
ANISOU  220  O2   DT A 108     1618   1354   1586   -110     14     13       O
ATOM    221  N3   DT A 108     -26.137 -20.852  37.347  1.00 11.01           N
ANISOU  221  N3   DT A 108     1515   1300   1368   -147     40    -49       N
ATOM    222  C4   DT A 108     -26.246 -22.199  37.608  1.00 10.78           C
ANISOU  222  C4   DT A 108     1510   1292   1292   -223    -20     93       C
ATOM    223  O4   DT A 108     -25.241 -22.913  37.570  1.00 11.21           O
ANISOU  223  O4   DT A 108     1541   1270   1448   -176     58    -41       O
ATOM    224  C5   DT A 108     -27.557 -22.682  37.940  1.00 11.40           C
ANISOU  224  C5   DT A 108     1524   1360   1446   -193    -50    -21       C
ATOM    225  C7   DT A 108     -27.781 -24.152  38.188  1.00 13.32           C
ANISOU  225  C7   DT A 108     1820   1489   1752   -321   -106     76       C
ATOM    226  C6   DT A 108     -28.551 -21.783  37.993  1.00 12.22           C
ANISOU  226  C6   DT A 108     1629   1445   1568   -264   -139    103       C
ATOM    227  P    DC A 109     -32.567 -17.398  35.991  1.00 16.58           P
ANISOU  227  P    DC A 109     1880   2204   2214    216     -8    366       P
ATOM    228  OP1  DC A 109     -33.474 -16.215  36.108  1.00 19.72           O
ANISOU  228  OP1  DC A 109     2107   2617   2769    486      6    544       O
ATOM    229  OP2  DC A 109     -33.002 -18.540  35.168  1.00 18.17           O
ANISOU  229  OP2  DC A 109     1900   2561   2441    113   -289    402       O
ATOM    230  O5′  DC A 109     -31.167 -16.900  35.405  1.00 15.21           O
ANISOU  230  O5′  DC A 109     1834   1974   1969     33    100    250       O
ATOM    231  C5′  DC A 109     -30.434 -15.881  36.080  1.00 14.88           C
ANISOU  231  C5′  DC A 109     1928   1805   1919    128    226    -60       C
ATOM    232  C4′  DC A 109     -29.246 -15.488  35.255  1.00 13.89           C
ANISOU  232  C4′  DC A 109     1779   1576   1920    371    234     13       C
ATOM    233  O4′  DC A 109     -28.323 -16.599  35.185  1.00 13.59           O
ANISOU  233  O4′  DC A 109     1879   1522   1762    256     49     27       O
ATOM    234  C3′  DC A 109     -29.581 -15.134  33.789  1.00 14.04           C
ANISOU  234  C3′  DC A 109     2009   1549   1775    185    186    238       C
ATOM    235  O3′  DC A 109     -28.920 -13.906  33.512  1.00 15.07           O
ANISOU  235  O3′  DC A 109     2102   1531   2091    314    254    164       O
ATOM    236  C2′  DC A 109     -29.049 -16.300  32.982  1.00 13.36           C
ANISOU  236  C2′  DC A 109     1920   1438   1718     28     70     62       C
ATOM    237  C1′  DC A 109     -27.930 -16.810  33.802  1.00 12.45           C
ANISOU  237  C1′  DC A 109     1719   1427   1583    114    170   -117       C
ATOM    238  N1   DC A 109     -27.611 -18.248  33.735  1.00 11.68           N
ANISOU  238  N1   DC A 109     1520   1307   1608     13     35     30       N
ATOM    239  C2   DC A 109     -26.301 -18.669  33.477  1.00 11.34           C
ANISOU  239  C2   DC A 109     1494   1393   1422     -4    -12    -81       C
ATOM    240  O2   DC A 109     -25.423 -17.856  33.129  1.00 11.46           O
ANISOU  240  O2   DC A 109     1478   1294   1581     22    145     23       O
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ATOM    241  N3   DC A 109     -26.007 -20.007  33.603  1.00 11.10           N
ANISOU  241  N3   DC A 109     1567   1248   1399    -11     57    -15       N
ATOM    242  C4   DC A 109     -26.971 -20.873  33.962  1.00 10.74           C
ANISOU  242  C4   DC A 109     1435   1349   1295   -100    -77    -36       C
ATOM    243  N4   DC A 109     -26.615 -22.147  34.132  1.00 11.36           N
ANISOU  243  N4   DC A 109     1579   1310   1423   -139     17      3       N
ATOM    244  C5   DC A 109     -28.310 -20.467  34.175  1.00 12.50           C
ANISOU  244  C5   DC A 109     1635   1511   1603   -125    -60     -6       C
ATOM    245  C6   DC A 109     -28.578 -19.143  34.086  1.00 12.44           C
ANISOU  245  C6   DC A 109     1692   1407   1627   -106    -27     -1       C
ATOM    246  P    DG A 110     -29.267 -12.959  32.301  1.00 17.10           P
ANISOU  246  P    DG A 110     2458   1663   2377    483    418    301       P
ATOM    247  OP1  DG A 110     -28.718 -11.611  32.647  1.00 20.41           O
ANISOU  247  OP1  DG A 110     3449   1571   2732    516    829     54       O
ATOM    248  OP2  DG A 110     -30.660 -13.105  31.973  1.00 21.17           O
ANISOU  248  OP2  DG A 110     3051   2502   2490    439    228    789       O
ATOM    249  O5'  DG A 110     -28.468 -13.556  31.093  1.00 15.81           O
ANISOU  249  O5'  DG A 110     2204   1726   2076    397    426    250       O
ATOM    250  C5'  DG A 110     -27.114 -13.464  31.041  1.00 15.43           C
ANISOU  250  C5'  DG A 110     2205   1414   2241     -6    413     52       C
ATOM    251  C4'  DG A 110     -26.554 -14.367  29.989  1.00 15.28           C
ANISOU  251  C4'  DG A 110     2316   1410   2077    297    285    116       C
ATOM    252  O4'  DG A 110     -26.669 -15.734  30.450  1.00 14.19           O
ANISOU  252  O4'  DG A 110     1969   1498   1922    148    126    134       O
ATOM    253  C3'  DG A 110     -27.265 -14.332  28.634  1.00 15.90           C
ANISOU  253  C3'  DG A 110     2349   1735   1957    331    552    168       C
ATOM    254  O3'  DG A 110     -26.291 -14.345  27.585  1.00 16.05           O
ANISOU  254  O3'  DG A 110     2385   1577   2133    319    319    465       O
ATOM    255  C2'  DG A 110     -28.024 -15.635  28.597  1.00 15.77           C
ANISOU  255  C2'  DG A 110     2039   1822   2129    445    133    287       C
ATOM    256  C1'  DG A 110     -27.004 -16.510  29.330  1.00 13.79           C
ANISOU  256  C1'  DG A 110     1938   1600   1698    302     89    158       C
ATOM    257  N9   DG A 110     -27.464 -17.832  29.753  1.00 13.18           N
ANISOU  257  N9   DG A 110     1797   1449   1759    251     74    172       N
ATOM    258  C8   DG A 110     -28.728 -18.293  30.092  1.00 14.02           C
ANISOU  258  C8   DG A 110     1813   1791   1723    228    127     47       C
ATOM    259  N7   DG A 110     -28.734 -19.533  30.438  1.00 13.01           N
ANISOU  259  N7   DG A 110     1626   1678   1637    129   -115    -76       N
ATOM    260  C5   DG A 110     -27.392 -19.945  30.341  1.00 12.16           C
ANISOU  260  C5   DG A 110     1670   1522   1425     37     39   -101       C
ATOM    261  C6   DG A 110     -26.766 -21.205  30.546  1.00 11.61           C
ANISOU  261  C6   DG A 110     1714   1376   1320     28     53   -113       C
ATOM    262  O6   DG A 110     -27.256 -22.248  30.917  1.00 12.64           O
ANISOU  262  O6   DG A 110     1739   1466   1595     17    113    -61       O
ATOM    263  N1   DG A 110     -25.420 -21.146  30.301  1.00 11.41           N
ANISOU  263  N1   DG A 110     1654   1338   1342      6     21    -25       N
ATOM    264  C2   DG A 110     -24.719 -20.029  29.891  1.00 11.92           C
ANISOU  264  C2   DG A 110     1760   1322   1446    121    158    -29       C
ATOM    265  N2   DG A 110     -23.421 -20.180  29.653  1.00 12.09           N
ANISOU  265  N2   DG A 110     1621   1376   1596    101     82     33       N
ATOM    266  N3   DG A 110     -25.279 -18.848  29.704  1.00 11.91           N
ANISOU  266  N3   DG A 110     1672   1311   1543    197     87     42       N
ATOM    267  C4   DG A 110     -26.618 -18.898  29.929  1.00 12.57           C
ANISOU  267  C4   DG A 110     1781   1378   1614    270     57    -71       C
ATOM    268  P    DC A 111     -25.822 -13.077  26.821  1.00 17.54           P
ANISOU  268  P    DC A 111     2574   1762   2328    493    383    394       P
ATOM    269  OP1  DC A 111     -25.933 -11.905  27.703  1.00 19.38           O
ANISOU  269  OP1  DC A 111     2949   1601   2812    560    606     93       O
ATOM    270  OP2  DC A 111     -26.505 -13.019  25.520  1.00 21.25           O
ANISOU  270  OP2  DC A 111     2960   2349   2762    416    274    230       O
ATOM    271  O5'  DC A 111     -24.323 -13.451  26.502  1.00 17.05           O
ANISOU  271  O5'  DC A 111     2500   1772   2207    177    385    329       O
ATOM    272  C5'  DC A 111     -23.383 -13.448  27.492  1.00 16.56           C
ANISOU  272  C5'  DC A 111     2058   1705   2529     26    356    -55       C
ATOM    273  C4'  DC A 111     -22.339 -14.559  27.254  1.00 16.13           C
ANISOU  273  C4'  DC A 111     2384   1586   2156     18    357   -136       C
ATOM    274  O4'  DC A 111     -22.967 -15.850  27.441  1.00 15.14           O
ANISOU  274  O4'  DC A 111     2292   1507   1954    -25    265    -31       O
ATOM    275  C3'  DC A 111     -21.744 -14.606  25.862  1.00 16.17           C
ANISOU  275  C3'  DC A 111     2026   1821   2295    117    499   -216       C
ATOM    276  O3'  DC A 111     -20.402 -14.929  25.988  1.00 19.33           O
ANISOU  276  O3'  DC A 111     2187   2572   2583     27    443   -426       O
ATOM    277  C2'  DC A 111     -22.565 -15.689  25.148  1.00 15.69           C
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ANISOU  277  C2′  DC A 111     2358   1628   1974   -122    311     69       C
ATOM    278  C1′  DC A 111     -22.744 -16.698  26.252  1.00 14.51           C
ANISOU  278  C1′  DC A 111     2084   1586   1842    -37    168   -112       C
ATOM    279  N1   DC A 111     -23.896 -17.565  26.197  1.00 13.41           N
ANISOU  279  N1   DC A 111     1859   1446   1788    156    206      5       N
ATOM    280  C2   DC A 111     -23.726 -18.939  26.470  1.00 12.22           C
ANISOU  280  C2   DC A 111     1776   1403   1462    146    124    -30       C
ATOM    281  O2   DC A 111     -22.566 -19.374  26.611  1.00 12.60           O
ANISOU  281  O2   DC A 111     1665   1369   1753     21    163     77       O
ATOM    282  N3   DC A 111     -24.812 -19.710  26.559  1.00 12.23           N
ANISOU  282  N3   DC A 111     1577   1528   1541    100     84    -21       N
ATOM    283  C4   DC A 111     -26.051 -19.193  26.412  1.00 12.52           C
ANISOU  283  C4   DC A 111     1684   1621   1449    280      1    -72       C
ATOM    284  N4   DC A 111     -27.099 -19.970  26.596  1.00 13.31           N
ANISOU  284  N4   DC A 111     1727   1619   1708    148     80    -75       N
ATOM    285  C5   DC A 111     -26.234 -17.798  26.105  1.00 13.94           C
ANISOU  285  C5   DC A 111     1904   1607   1784    288    124    -63       C
ATOM    286  C6   DC A 111     -25.141 -17.054  26.031  1.00 14.25           C
ANISOU  286  C6   DC A 111     1868   1699   1847    182      4     10       C
ATOM    287  P    DG A 112     -19.389 -14.810  24.748  1.00 24.07           P
ANISOU  287  P    DG A 112     2604   2782   3760   -289   1101   -511       P
ATOM    288  OP1  DG A 112     -18.126 -14.391  25.381  1.00 26.16           O
ANISOU  288  OP1  DG A 112     2566   2795   4576   -100    852  -1072       O
ATOM    289  OP2  DG A 112     -20.014 -13.942  23.681  1.00 34.43           O
ANISOU  289  OP2  DG A 112     4205   4893   3982    -54   1211   -157       O
ATOM    290  O5′  DG A 112     -19.307 -16.207  24.107  1.00 25.37           O
ANISOU  290  O5′  DG A 112     3783   2734   3123    733    695   -418       O
ATOM    291  C5′  DG A 112     -18.724 -17.190  24.726  1.00 21.95           C
ANISOU  291  C5′  DG A 112     3193   2558   2587   1030    132    677       C
ATOM    292  C4′  DG A 112     -18.601 -18.420  23.725  1.00 14.58           C
ANISOU  292  C4′  DG A 112     1825   1748   1966    263    160    -33       C
ATOM    293  O4′  DG A 112     -19.710 -19.328  23.704  1.00 23.20           O
ANISOU  293  O4′  DG A 112     1866   4500   2446   -610     64    797       O
ATOM    294  C3′  DG A 112     -18.369 -17.989  22.284  1.00 14.79           C
ANISOU  294  C3′  DG A 112     1752   1810   2056    267    315     -1       C
ATOM    295  O3′  DG A 112     -17.152 -18.536  21.794  1.00 15.76           O
ANISOU  295  O3′  DG A 112     1747   2101   2139    209    281    105       O
ATOM    296  C2′  DG A 112     -19.580 -18.501  21.521  1.00 14.77           C
ANISOU  296  C2′  DG A 112     1926   1731   1956     90    336     13       C
ATOM    297  C1′  DG A 112     -20.214 -19.551  22.417  1.00 15.51           C
ANISOU  297  C1′  DG A 112     1736   2155   2001      6    296    357       C
ATOM    298  N9   DG A 112     -21.659 -19.506  22.587  1.00 13.09           N
ANISOU  298  N9   DG A 112     1499   1702   1770    286     93     76       N
ATOM    299  C8   DG A 112     -22.502 -18.404  22.568  1.00 14.39           C
ANISOU  299  C8   DG A 112     1692   1832   1944    194     62    170       C
ATOM    300  N7   DG A 112     -23.728 -18.703  22.854  1.00 13.88           N
ANISOU  300  N7   DG A 112     1633   1770   1868    156     16    -44       N
ATOM    301  C5   DG A 112     -23.716 -20.065  23.091  1.00 12.47           C
ANISOU  301  C5   DG A 112     1586   1561   1589    286     16    -85       C
ATOM    302  C6   DG A 112     -24.740 -20.983  23.437  1.00 12.16           C
ANISOU  302  C6   DG A 112     1287   1748   1584    154     65    -43       C
ATOM    303  O6   DG A 112     -25.965 -20.715  23.608  1.00 14.00           O
ANISOU  303  O6   DG A 112     1491   1945   1880    367     41    -92       O
ATOM    304  N1   DG A 112     -24.293 -22.283  23.580  1.00 12.42           N
ANISOU  304  N1   DG A 112     1490   1725   1501    211     29    -50       N
ATOM    305  C2   DG A 112     -22.985 -22.691  23.403  1.00 11.31           C
ANISOU  305  C2   DG A 112     1211   1642   1442    194    112    -78       C
ATOM    306  N2   DG A 112     -22.749 -23.983  23.523  1.00 12.66           N
ANISOU  306  N2   DG A 112     1448   1729   1631     82    125     14       N
ATOM    307  N3   DG A 112     -22.010 -21.837  23.073  1.00 12.58           N
ANISOU  307  N3   DG A 112     1450   1726   1603    167    202    190       N
ATOM    308  C4   DG A 112     -22.437 -20.569  22.935  1.00 12.61           C
ANISOU  308  C4   DG A 112     1499   1756   1534     40    206    150       C
TER     309        DG A 112
ATOM    310  O5′  DC B 213     -29.959 -28.966  24.000  1.00 28.15           O
ANISOU  310  O5′  DC B 213     2516   3751   4429   -392   -234   -457       O
ATOM    311  C5′  DC B 213     -29.207 -29.755  23.110  1.00 23.21           C
ANISOU  311  C5′  DC B 213     2420   2817   3581   -482    -58    169       C
ATOM    312  C4′  DC B 213     -27.761 -29.708  23.523  1.00 18.87           C
ANISOU  312  C4′  DC B 213     2156   2250   2763   -333   -268    109       C
ATOM    313  O4′  DC B 213     -27.245 -28.372  23.328  1.00 17.22           O
ANISOU  313  O4′  DC B 213     2015   2247   2279     -2   -130    -37       O
ATOM    314  C3′  DC B 213     -27.447 -30.092  24.968  1.00 16.44           C
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ANISOU  314  C3′  DC B 213     1833   1909   2503   -177      6    164       C
ATOM    315  O3′  DC B 213    -26.341 -30.999  24.969  1.00 18.69           O
ANISOU  315  O3′  DC B 213     2353   2150   2597    -50     46    -10       O
ATOM    316  C2′  DC B 213    -27.132 -28.782  25.679  1.00 17.83           C
ANISOU  316  C2′  DC B 213     2213   2025   2534   -394    354     53       C
ATOM    317  C1′  DC B 213    -26.646 -27.898  24.524  1.00 16.22           C
ANISOU  317  C1′  DC B 213     1800   2150   2210    -65    110   -105       C
ATOM    318  N1   DC B 213    -27.006 -26.460  24.595  1.00 14.88           N
ANISOU  318  N1   DC B 213     1559   2021   2070    -67    170    -48       N
ATOM    319  C2   DC B 213    -26.030 -25.460  24.327  1.00 14.17           C
ANISOU  319  C2   DC B 213     1508   1976   1899    114    -22   -154       C
ATOM    320  O2   DC B 213    -24.858 -25.809  24.134  1.00 14.33           O
ANISOU  320  O2   DC B 213     1491   1929   2024     68    142     65       O
ATOM    321  N3   DC B 213    -26.406 -24.170  24.307  1.00 12.52           N
ANISOU  321  N3   DC B 213     1245   1817   1694     65     57     -4       N
ATOM    322  C4   DC B 213    -27.682 -23.849  24.544  1.00 13.72           C
ANISOU  322  C4   DC B 213     1539   1888   1785    120     80   -123       C
ATOM    323  N4   DC B 213    -27.997 -22.559  24.510  1.00 14.28           N
ANISOU  323  N4   DC B 213     1457   2110   1857    107      3     -9       N
ATOM    324  C5   DC B 213    -28.678 -24.846  24.786  1.00 15.61           C
ANISOU  324  C5   DC B 213     1507   2093   2331     62    118    140       C
ATOM    325  C6   DC B 213    -28.319 -26.114  24.791  1.00 16.34           C
ANISOU  325  C6   DC B 213     1656   2215   2338    -28    107   -157       C
ATOM    326  P    DG B 214    -25.854 -31.772  26.265  1.00 19.44           P
ANISOU  326  P    DG B 214     2450   2011   2923   -155     59    351       P
ATOM    327  OP1  DG B 214    -25.311 -33.071  25.798  1.00 21.26           O
ANISOU  327  OP1  DG B 214     2952   1966   3159    -43     62    -14       O
ATOM    328  OP2  DG B 214    -26.911 -31.748  27.328  1.00 23.06           O
ANISOU  328  OP2  DG B 214     2644   3055   3062   -547    448    378       O
ATOM    329  O5′  DG B 214    -24.678 -30.827  26.771  1.00 16.27           O
ANISOU  329  O5′  DG B 214     1935   1809   2437   -173     72    182       O
ATOM    330  C5′  DG B 214    -23.547 -30.615  25.982  1.00 15.54           C
ANISOU  330  C5′  DG B 214     2171   1554   2179    117    241   -113       C
ATOM    331  C4′  DG B 214    -22.720 -29.498  26.509  1.00 13.65           C
ANISOU  331  C4′  DG B 214     1868   1409   1909    200    108     52       C
ATOM    332  O4′  DG B 214    -23.490 -28.298  26.373  1.00 13.87           O
ANISOU  332  O4′  DG B 214     1771   1568   1929    214    147     38       O
ATOM    333  C3′  DG B 214    -22.393 -29.619  27.987  1.00 15.20           C
ANISOU  333  C3′  DG B 214     2002   1605   2169    184     36   -178       C
ATOM    334  O3′  DG B 214    -21.012 -29.897  28.101  1.00 14.28           O
ANISOU  334  O3′  DG B 214     1860   1567   1997    395     14     87       O
ATOM    335  C2′  DG B 214    -22.840 -28.289  28.613  1.00 14.09           C
ANISOU  335  C2′  DG B 214     1971   1546   1836    326    170     22       C
ATOM    336  C1′  DG B 214    -23.052 -27.404  27.416  1.00 13.61           C
ANISOU  336  C1′  DG B 214     1664   1517   1990    285    142    176       C
ATOM    337  N9   DG B 214    -24.119 -26.420  27.583  1.00 12.96           N
ANISOU  337  N9   DG B 214     1529   1414   1980     59    146     84       N
ATOM    338  C8   DG B 214    -25.392 -26.694  27.978  1.00 13.74           C
ANISOU  338  C8   DG B 214     1687   1477   2055     59    229     39       C
ATOM    339  N7   DG B 214    -26.164 -25.639  27.978  1.00 13.20           N
ANISOU  339  N7   DG B 214     1669   1542   1802     51     81     77       N
ATOM    340  C5   DG B 214    -25.316 -24.592  27.589  1.00 12.49           C
ANISOU  340  C5   DG B 214     1570   1605   1571     59     19    -74       C
ATOM    341  C6   DG B 214    -25.581 -23.221  27.448  1.00 10.88           C
ANISOU  341  C6   DG B 214     1310   1350   1473    205     12    -89       C
ATOM    342  O6   DG B 214    -26.657 -22.627  27.615  1.00 12.35           O
ANISOU  342  O6   DG B 214     1511   1562   1619    222      0   -113       O
ATOM    343  N1   DG B 214    -24.455 -22.504  27.084  1.00 11.30           N
ANISOU  343  N1   DG B 214     1456   1428   1408    208     53    -52       N
ATOM    344  C2   DG B 214    -23.221 -23.057  26.858  1.00 11.00           C
ANISOU  344  C2   DG B 214     1417   1353   1409    142    141    -48       C
ATOM    345  N2   DG B 214    -22.249 -22.239  26.486  1.00 12.26           N
ANISOU  345  N2   DG B 214     1513   1560   1584    104    232     14       N
ATOM    346  N3   DG B 214    -22.963 -24.372  26.960  1.00 11.70           N
ANISOU  346  N3   DG B 214     1409   1431   1605     97    170    -28       N
ATOM    347  C4   DG B 214    -24.062 -25.054  27.368  1.00 10.98           C
ANISOU  347  C4   DG B 214     1336   1204   1631    126     60      0       C
ATOM    348  P    DC B 215    -20.275 -30.011  29.517  1.00 14.40           P
ANISOU  348  P    DC B 215     2068   1545   1857    366     58    140       P
ATOM    349  OP1  DC B 215    -19.107 -30.891  29.255  1.00 16.51           O
ANISOU  349  OP1  DC B 215     2389   1679   2204    673    -87    -90       O
ATOM    350  OP2  DC B 215    -21.253 -30.430  30.558  1.00 16.98           O
ANISOU  350  OP2  DC B 215     2422   1862   2166    254    179    275       O
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ATOM    351  O5′  DC B 215     -19.797 -28.518  29.854  1.00 13.91           O
ANISOU  351  O5′  DC B 215     2122   1474   1689    324    264     46       O
ATOM    352  C5′  DC B 215     -18.922 -27.883  28.952  1.00 13.82           C
ANISOU  352  C5′  DC B 215     1843   1620   1785    199    270    -25       C
ATOM    353  C4′  DC B 215     -18.968 -26.385  29.203  1.00 13.34           C
ANISOU  353  C4′  DC B 215     1672   1760   1634     54    111     87       C
ATOM    354  O4′  DC B 215     -20.292 -25.943  28.994  1.00 13.42           O
ANISOU  354  O4′  DC B 215     1827   1453   1816    290     26    130       O
ATOM    355  C3′  DC B 215     -18.677 -25.904  30.598  1.00 12.86           C
ANISOU  355  C3′  DC B 215     1622   1723   1539    281    -67      1       C
ATOM    356  O3′  DC B 215     -17.278 -25.841  30.764  1.00 15.09           O
ANISOU  356  O3′  DC B 215     1965   1885   1881    339     39     43       O
ATOM    357  C2′  DC B 215     -19.341 -24.513  30.610  1.00 16.25           C
ANISOU  357  C2′  DC B 215     2005   1789   2377    408    -99   -124       C
ATOM    358  C1′  DC B 215     -20.469 -24.691  29.666  1.00 13.55           C
ANISOU  358  C1′  DC B 215     1897   1365   1884    263    123    -22       C
ATOM    359  N1   DC B 215     -21.824 -24.701  30.266  1.00 12.40           N
ANISOU  359  N1   DC B 215     1716   1381   1613     35     60     27       N
ATOM    360  C2   DC B 215     -22.574 -23.554  30.213  1.00 11.19           C
ANISOU  360  C2   DC B 215     1582   1211   1456    133     46     11       C
ATOM    361  O2   DC B 215     -22.013 -22.523  29.771  1.00 12.76           O
ANISOU  361  O2   DC B 215     1710   1402   1735     49    111    -30       O
ATOM    362  N3   DC B 215     -23.838 -23.542  30.624  1.00 11.61           N
ANISOU  362  N3   DC B 215     1662   1271   1478     31     69     -4       N
ATOM    363  C4   DC B 215     -24.338 -24.640  31.178  1.00 12.70           C
ANISOU  363  C4   DC B 215     1842   1455   1528     43     -4     62       C
ATOM    364  N4   DC B 215     -25.611 -24.628  31.570  1.00 13.44           N
ANISOU  364  N4   DC B 215     1919   1552   1636    -45    156     89       N
ATOM    365  C5   DC B 215     -23.567 -25.861  31.323  1.00 14.29           C
ANISOU  365  C5   DC B 215     2120   1438   1870     -5     33    123       C
ATOM    366  C6   DC B 215     -22.330 -25.852  30.850  1.00 13.41           C
ANISOU  366  C6   DC B 215     1885   1493   1714     91     86    186       C
ATOM    367  P    DG B 216     -16.615 -25.549  32.202  1.00 16.43           P
ANISOU  367  P    DG B 216     2014   2074   2152    479   -190     27       P
ATOM    368  OP1  DG B 216     -15.230 -26.033  32.132  1.00 19.97           O
ANISOU  368  OP1  DG B 216     2054   2716   2815    380   -175     31       O
ATOM    369  OP2  DG B 216     -17.467 -26.054  33.333  1.00 17.71           O
ANISOU  369  OP2  DG B 216     2389   2202   2139    354   -281    221       O
ATOM    370  O5′  DG B 216     -16.630 -23.964  32.326  1.00 15.24           O
ANISOU  370  O5′  DG B 216     1951   1896   1943    258     -4    -79       O
ATOM    371  C5′  DG B 216     -15.946 -23.146  31.418  1.00 16.00           C
ANISOU  371  C5′  DG B 216     1730   2198   2151    249    416   -108       C
ATOM    372  C4′  DG B 216     -16.238 -21.694  31.752  1.00 14.60           C
ANISOU  372  C4′  DG B 216     1544   2084   1917     26     80     33       C
ATOM    373  O4′  DG B 216     -17.659 -21.442  31.662  1.00 13.90           O
ANISOU  373  O4′  DG B 216     1611   1806   1865    155    180    -65       O
ATOM    374  C3′  DG B 216     -15.836 -21.229  33.158  1.00 16.56           C
ANISOU  374  C3′  DG B 216     2100   2124   2068    108    136   -188       C
ATOM    375  O3′  DG B 216     -15.441 -19.861  33.018  1.00 16.89           O
ANISOU  375  O3′  DG B 216     1928   2229   2261   -123    201   -426       O
ATOM    376  C2′  DG B 216     -17.128 -21.424  33.968  1.00 14.99           C
ANISOU  376  C2′  DG B 216     1753   2067   1874    172    200    -60       C
ATOM    377  C1′  DG B 216     -18.211 -21.129  32.934  1.00 13.22           C
ANISOU  377  C1′  DG B 216     1633   1688   1701    103     86     -5       C
ATOM    378  N9   DG B 216     -19.443 -21.849  33.194  1.00 12.64           N
ANISOU  378  N9   DG B 216     1690   1420   1692    -64    124    -37       N
ATOM    379  C8   DG B 216     -19.605 -23.118  33.702  1.00 13.84           C
ANISOU  379  C8   DG B 216     1733   1731   1795    245    137     58       C
ATOM    380  N7   DG B 216     -20.847 -23.453  33.893  1.00 13.12           N
ANISOU  380  N7   DG B 216     1731   1523   1729     82    130    100       N
ATOM    381  C5   DG B 216     -21.554 -22.327  33.527  1.00 11.46           C
ANISOU  381  C5   DG B 216     1634   1318   1400     69    147      5       C
ATOM    382  C6   DG B 216     -22.936 -22.073  33.573  1.00 11.15           C
ANISOU  382  C6   DG B 216     1563   1343   1330     29    146   -136       C
ATOM    383  O6   DG B 216     -23.836 -22.832  33.936  1.00 11.35           O
ANISOU  383  O6   DG B 216     1582   1292   1436    -54     69     -9       O
ATOM    384  N1   DG B 216     -23.234 -20.766  33.168  1.00 10.55           N
ANISOU  384  N1   DG B 216     1493   1177   1338    -30    163    -62       N
ATOM    385  C2   DG B 216     -22.305 -19.851  32.722  1.00 10.97           C
ANISOU  385  C2   DG B 216     1501   1345   1322      0    113    -68       C
ATOM    386  N2   DG B 216     -22.780 -18.644  32.382  1.00 11.97           N
ANISOU  386  N2   DG B 216     1776   1293   1477    -31    170     -7       N
ATOM    387  N3   DG B 216     -21.021 -20.108  32.617  1.00 11.51           N
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ANISOU  387  N3   DG B 216     1510   1280   1582     36    180    -63       N
ATOM    388  C4   DG B 216     -20.692 -21.337  33.083  1.00 11.54           C
ANISOU  388  C4   DG B 216     1367   1545   1469    199    125   -126       C
ATOM    389  P    DA B 217     -15.397 -18.748  34.186  1.00 17.39           P
ANISOU  389  P    DA B 217     1878   2400   2328   -259      9   -308       P
ATOM    390  OP1  DA B 217     -14.246 -17.907  33.882  1.00 19.74           O
ANISOU  390  OP1  DA B 217     1837   2844   2819   -502    144   -424       O
ATOM    391  OP2  DA B 217     -15.403 -19.398  35.523  1.00 21.10           O
ANISOU  391  OP2  DA B 217     2201   2923   2891   -183   -360   -462       O
ATOM    392  O5'  DA B 217     -16.783 -17.983  34.042  1.00 15.83           O
ANISOU  392  O5'  DA B 217     1730   2181   2103   -297    186   -300       O
ATOM    393  C5'  DA B 217     -17.103 -17.369  32.805  1.00 16.62           C
ANISOU  393  C5'  DA B 217     1989   2117   2207   -387    492    -12       C
ATOM    394  C4'  DA B 217     -18.294 -16.457  32.979  1.00 14.60           C
ANISOU  394  C4'  DA B 217     1748   1685   2112   -497    535   -140       C
ATOM    395  O4'  DA B 217     -19.469 -17.207  33.329  1.00 14.45           O
ANISOU  395  O4'  DA B 217     1919   1793   1777   -386    431   -200       O
ATOM    396  C3'  DA B 217     -18.173 -15.382  34.077  1.00 15.06           C
ANISOU  396  C3'  DA B 217     1853   1757   2111   -287    309    -25       C
ATOM    397  O3'  DA B 217     -18.823 -14.209  33.647  1.00 15.58           O
ANISOU  397  O3'  DA B 217     1899   1718   2303   -426    395    -62       O
ATOM    398  C2'  DA B 217     -18.845 -16.028  35.288  1.00 14.34           C
ANISOU  398  C2'  DA B 217     1876   1629   1943   -515    271   -116       C
ATOM    399  C1'  DA B 217     -19.934 -16.829  34.666  1.00 13.69           C
ANISOU  399  C1'  DA B 217     1782   1601   1818   -376    424   -127       C
ATOM    400  N9   DA B 217     -20.266 -18.095  35.328  1.00 12.12           N
ANISOU  400  N9   DA B 217     1525   1495   1581   -207    233   -132       N
ATOM    401  C8   DA B 217     -19.417 -19.101  35.637  1.00 13.32           C
ANISOU  401  C8   DA B 217     1678   1624   1757   -353     89   -137       C
ATOM    402  N7   DA B 217     -20.010 -20.178  36.140  1.00 12.79           N
ANISOU  402  N7   DA B 217     1734   1498   1626    -57    -27   -192       N
ATOM    403  C5   DA B 217     -21.354 -19.820  36.152  1.00 11.67           C
ANISOU  403  C5   DA B 217     1409   1551   1473     16    125   -210       C
ATOM    404  C6   DA B 217     -22.515 -20.525  36.551  1.00 10.89           C
ANISOU  404  C6   DA B 217     1564   1289   1281   -132     84    -79       C
ATOM    405  N6   DA B 217     -22.508 -21.787  37.032  1.00 11.91           N
ANISOU  405  N6   DA B 217     1636   1467   1421   -134     99    -76       N
ATOM    406  N1   DA B 217     -23.675 -19.890  36.465  1.00 10.81           N
ANISOU  406  N1   DA B 217     1482   1320   1302   -136    114   -134       N
ATOM    407  C2   DA B 217     -23.699 -18.633  35.989  1.00 10.71           C
ANISOU  407  C2   DA B 217     1506   1211   1349   -230     20   -113       C
ATOM    408  N3   DA B 217     -22.684 -17.891  35.557  1.00 11.20           N
ANISOU  408  N3   DA B 217     1489   1309   1457   -281    202   -134       N
ATOM    409  C4   DA B 217     -21.538 -18.542  35.675  1.00 11.25           C
ANISOU  409  C4   DA B 217     1441   1372   1459   -268    136    -91       C
HETATM  410  P   7DA B 218     -18.853 -12.851  34.405  1.00 17.01           P
ANISOU  410  P   7DA B 218     2138   1788   2533   -448    237    -69       P
HETATM  411  OP1 7DA B 218     -19.055 -11.718  33.456  1.00 20.32           O
ANISOU  411  OP1 7DA B 218     2767   1906   3046   -616    463    506       O
HETATM  412  OP2 7DA B 218     -17.685 -12.872  35.294  1.00 21.21           O
ANISOU  412  OP2 7DA B 218     2775   2367   2916      7    -67   -610       O
HETATM  413  O5' 7DA B 218     -20.090 -13.004  35.411  1.00 15.70           O
ANISOU  413  O5' 7DA B 218     2142   1614   2207   -239    307   -112       O
HETATM  414  N9  7DA B 218     -22.129 -15.978  38.333  1.00 13.51           N
ANISOU  414  N9  7DA B 218     1915   1535   1682   -384    200   -216       N
HETATM  415  C4  7DA B 218     -22.901 -17.040  38.798  1.00 12.25           C
ANISOU  415  C4  7DA B 218     1739   1440   1473   -363     55   -320       C
HETATM  416  N3  7DA B 218     -24.219 -17.096  38.895  1.00 12.07           N
ANISOU  416  N3  7DA B 218     1663   1418   1501   -271    140   -170       N
HETATM  417  C2  7DA B 218     -24.629 -18.265  39.384  1.00 12.20           C
ANISOU  417  C2  7DA B 218     1789   1561   1284   -275    158   -220       C
HETATM  418  N1  7DA B 218     -23.910 -19.306  39.768  1.00 11.42           N
ANISOU  418  N1  7DA B 218     1552   1491   1294   -259     56   -138       N
HETATM  419  C6  7DA B 218     -22.582 -19.207  39.637  1.00 12.13           C
ANISOU  419  C6  7DA B 218     1727   1544   1337   -197    -40   -352       C
HETATM  420  N6  7DA B 218     -21.853 -20.285  39.991  1.00 13.12           N
ANISOU  420  N6  7DA B 218     1635   1853   1495   -378     82   -386       N
HETATM  421  C5  7DA B 218     -22.001 -18.013  39.152  1.00 11.69           C
ANISOU  421  C5  7DA B 218     1581   1505   1352   -417    118   -306       C
HETATM  422  C7  7DA B 218     -20.643 -17.552  38.889  1.00 13.50           C
ANISOU  422  C7  7DA B 218     1683   1747   1697   -396     63   -234       C
HETATM  423  C8  7DA B 218     -20.839 -16.306  38.395  1.00 14.50           C
ANISOU  423  C8  7DA B 218     1922   1770   1815   -455     48   -198       C
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HETATM  424  C2' 7DA B 218     -22.156 -13.470  38.420  1.00 16.17           C
ANISOU  424  C2' 7DA B 218     2393   1484   2265   -438    283   -475       C
HETATM  425  C5' 7DA B 218     -21.371 -12.991  34.913  1.00 15.37           C
ANISOU  425  C5' 7DA B 218     2139   1679   2021   -276    373    -32       C
HETATM  426  C4' 7DA B 218     -22.357 -13.294  36.011  1.00 13.87           C
ANISOU  426  C4' 7DA B 218     1920   1398   1951   -322    421    -40       C
HETATM  427  O4' 7DA B 218     -22.223 -14.659  36.408  1.00 14.53           O
ANISOU  427  O4' 7DA B 218     2191   1413   1915   -399    288    -99       O
HETATM  428  C1' 7DA B 218     -22.656 -14.740  37.772  1.00 14.69           C
ANISOU  428  C1' 7DA B 218     1914   1734   1931   -451    433   -240       C
HETATM  429  C3' 7DA B 218     -22.164 -12.423  37.261  1.00 17.24           C
ANISOU  429  C3' 7DA B 218     2482   1761   2305   -489    524   -116       C
HETATM  430  O3' 7DA B 218     -23.251 -11.519  37.337  1.00 17.86           O
ANISOU  430  O3' 7DA B 218     2811   1617   2357   -157    711   -143       O
ATOM    431  P    DT B 219     -23.733 -10.661  38.544  1.00 19.92           P
ANISOU  431  P    DT B 219     3013   1811   2742   -277    529   -370       P
ATOM    432  OP1  DT B 219     -24.433  -9.454  38.082  1.00 23.06           O
ANISOU  432  OP1  DT B 219     3947   1408   3407   -100   1013   -158       O
ATOM    433  OP2  DT B 219     -22.583 -10.610  39.376  1.00 20.37           O
ANISOU  433  OP2  DT B 219     3024   2006   2709    240    859     -3       O
ATOM    434  O5'  DT B 219     -24.650 -11.595  39.355  1.00 17.58           O
ANISOU  434  O5'  DT B 219     2554   1811   2315   -428    520   -305       O
ATOM    435  C5'  DT B 219     -25.784 -12.109  38.763  1.00 17.21           C
ANISOU  435  C5'  DT B 219     2642   1762   2132    -67    360     45       C
ATOM    436  C4'  DT B 219     -26.446 -13.039  39.721  1.00 15.04           C
ANISOU  436  C4'  DT B 219     2223   1593   1899    -54    316    -13       C
ATOM    437  O4'  DT B 219     -25.618 -14.176  40.024  1.00 14.82           O
ANISOU  437  O4'  DT B 219     2204   1634   1791    106    158   -142       O
ATOM    438  C3'  DT B 219     -26.869 -12.432  41.061  1.00 16.26           C
ANISOU  438  C3'  DT B 219     2070   1979   2127    238    333      3       C
ATOM    439  O3'  DT B 219     -28.258 -12.603  41.161  1.00 19.32           O
ANISOU  439  O3'  DT B 219     2370   2692   2278    469    524    331       O
ATOM    440  C2'  DT B 219     -26.110 -13.275  42.112  1.00 15.52           C
ANISOU  440  C2'  DT B 219     2155   1857   1883    126    282   -256       C
ATOM    441  C1'  DT B 219     -25.843 -14.568  41.388  1.00 14.17           C
ANISOU  441  C1'  DT B 219     2091   1600   1689     -9    149   -150       C
ATOM    442  N1   DT B 219     -24.677 -15.338  41.818  1.00 12.94           N
ANISOU  442  N1   DT B 219     1766   1586   1564   -290    150   -235       N
ATOM    443  C2   DT B 219     -24.862 -16.633  42.268  1.00 11.88           C
ANISOU  443  C2   DT B 219     1637   1455   1419    -71     34   -260       C
ATOM    444  O2   DT B 219     -25.967 -17.133  42.421  1.00 13.53           O
ANISOU  444  O2   DT B 219     1692   1677   1770   -107    134    -96       O
ATOM    445  N3   DT B 219     -23.733 -17.302  42.544  1.00 11.87           N
ANISOU  445  N3   DT B 219     1565   1545   1400   -224     -1   -288       N
ATOM    446  C4   DT B 219     -22.463 -16.860  42.401  1.00 12.35           C
ANISOU  446  C4   DT B 219     1652   1582   1456   -147    -68   -347       C
ATOM    447  O4   DT B 219     -21.520 -17.596  42.634  1.00 12.86           O
ANISOU  447  O4   DT B 219     1577   1670   1639   -259    -50   -301       O
ATOM    448  C5   DT B 219     -22.326 -15.479  41.940  1.00 13.79           C
ANISOU  448  C5   DT B 219     1832   1708   1700   -322    -56   -433       C
ATOM    449  C7   DT B 219     -20.961 -14.874  41.761  1.00 15.98           C
ANISOU  449  C7   DT B 219     2006   1879   2185   -559    -66   -232       C
ATOM    450  C6   DT B 219     -23.440 -14.804  41.663  1.00 13.66           C
ANISOU  450  C6   DT B 219     1893   1680   1616   -306    110   -366       C
ATOM    451  P    DT B 220     -29.099 -12.075  42.368  1.00 24.96           P
ANISOU  451  P    DT B 220     3124   3148   3210   1157    825    668       P
ATOM    452  OP1  DT B 220     -30.453 -11.827  41.875  1.00 30.97           O
ANISOU  452  OP1  DT B 220     3317   5048   3399   1208    496   1616       O
ATOM    453  OP2  DT B 220     -28.321 -11.030  43.018  1.00 23.43           O
ANISOU  453  OP2  DT B 220     3294   2945   2663   1188   1035    363       O
ATOM    454  O5'  DT B 220     -29.149 -13.231  43.391  1.00 20.51           O
ANISOU  454  O5'  DT B 220     2703   2812   2278    545    616    287       O
ATOM    455  C5'  DT B 220     -29.767 -14.423  43.010  1.00 20.95           C
ANISOU  455  C5'  DT B 220     2260   3288   2409    428    280    -27       C
ATOM    456  C4'  DT B 220     -29.607 -15.382  44.113  1.00 17.77           C
ANISOU  456  C4'  DT B 220     2022   2731   1996    299    424    120       C
ATOM    457  O4'  DT B 220     -28.252 -15.754  44.207  1.00 17.43           O
ANISOU  457  O4'  DT B 220     2212   2466   1944    452     24   -255       O
ATOM    458  C3'  DT B 220     -30.058 -14.941  45.497  1.00 18.85           C
ANISOU  458  C3'  DT B 220     2617   2324   2218    530    215    251       C
ATOM    459  O3'  DT B 220     -31.138 -15.833  45.836  1.00 20.41           O
ANISOU  459  O3'  DT B 220     2175   3281   2296    248    526    460       O
ATOM    460  C2'  DT B 220     -28.807 -15.138  46.366  1.00 17.66           C
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ANISOU  460  C2′  DT B 220     2543   2273   1893    353    402   -229       C
ATOM    461  C1′  DT B 220     -27.992 -16.112  45.578  1.00 17.13           C
ANISOU  461  C1′  DT B 220     2384   2426   1697    370   -117   -211       C
ATOM    462  N1   DT B 220     -26.521 -16.056  45.719  1.00 15.76           N
ANISOU  462  N1   DT B 220     2330   2037   1620    351    -67   -362       N
ATOM    463  C2   DT B 220     -25.867 -17.207  46.051  1.00 14.47           C
ANISOU  463  C2   DT B 220     2047   1828   1623    163   -163   -468       C
ATOM    464  O2   DT B 220     -26.439 -18.207  46.343  1.00 15.08           O
ANISOU  464  O2   DT B 220     2100   1840   1788    207    -36   -371       O
ATOM    465  N3   DT B 220     -24.529 -17.137  46.025  1.00 14.38           N
ANISOU  465  N3   DT B 220     2014   1939   1508    202    -56   -448       N
ATOM    466  C4   DT B 220     -23.763 -16.044  45.683  1.00 16.04           C
ANISOU  466  C4   DT B 220     2365   2194   1536    190    -89   -675       C
ATOM    467  O4   DT B 220     -22.536 -16.127  45.630  1.00 16.50           O
ANISOU  467  O4   DT B 220     2333   2193   1741    133   -138   -623       O
ATOM    468  C5   DT B 220     -24.485 -14.806  45.394  1.00 16.27           C
ANISOU  468  C5   DT B 220     2787   1771   1623    222     -5   -593       C
ATOM    469  C7   DT B 220     -23.738 -13.523  45.046  1.00 19.31           C
ANISOU  469  C7   DT B 220     3006   2366   1964    316     55   -695       C
ATOM    470  C6   DT B 220     -25.812 -14.896  45.382  1.00 17.07           C
ANISOU  470  C6   DT B 220     2703   2028   1754    160     -7   -430       C
ATOM    471  P    DC B 221     -32.013 -15.721  47.113  1.00 21.67           P
ANISOU  471  P    DC B 221     2349   3329   2552    147     86    509       P
ATOM    472  OP1  DC B 221     -33.264 -16.430  46.817  1.00 26.94           O
ANISOU  472  OP1  DC B 221     2787   4347   3102   -735   -117   1152       O
ATOM    473  OP2  DC B 221     -31.991 -14.315  47.521  1.00 24.40           O
ANISOU  473  OP2  DC B 221     3285   3745   2239     97    587    369       O
ATOM    474  O5′  DC B 221     -31.216 -16.499  48.256  1.00 19.22           O
ANISOU  474  O5′  DC B 221     2302   2832   2168    355    437    338       O
ATOM    475  C5′  DC B 221     -31.061 -17.812  48.102  1.00 19.01           C
ANISOU  475  C5′  DC B 221     2149   2770   2305    214   -272    394       C
ATOM    476  C4′  DC B 221     -30.069 -18.302  49.064  1.00 15.80           C
ANISOU  476  C4′  DC B 221     1694   2241   2066   -120   -135     10       C
ATOM    477  O4′  DC B 221     -28.761 -17.837  48.745  1.00 16.58           O
ANISOU  477  O4′  DC B 221     1704   2466   2129     -1    -46   -180       O
ATOM    478  C3′  DC B 221     -30.274 -17.878  50.498  1.00 16.90           C
ANISOU  478  C3′  DC B 221     1971   2487   1963   -222   -232    226       C
ATOM    479  O3′  DC B 221     -30.946 -18.915  51.160  1.00 18.16           O
ANISOU  479  O3′  DC B 221     1834   2925   2140   -299   -295    321       O
ATOM    480  C2′  DC B 221     -28.854 -17.616  51.099  1.00 16.61           C
ANISOU  480  C2′  DC B 221     1923   2464   1922   -109   -122    -22       C
ATOM    481  C1′  DC B 221     -27.986 -18.029  49.932  1.00 15.68           C
ANISOU  481  C1′  DC B 221     1721   2296   1937     60   -267    -77       C
ATOM    482  N1   DC B 221     -26.739 -17.262  49.740  1.00 15.64           N
ANISOU  482  N1   DC B 221     1601   2421   1917    -59    -35   -209       N
ATOM    483  C2   DC B 221     -25.515 -17.878  49.888  1.00 14.45           C
ANISOU  483  C2   DC B 221     1725   2065   1699     67   -106   -316       C
ATOM    484  O2   DC B 221     -25.481 -19.034  50.272  1.00 16.15           O
ANISOU  484  O2   DC B 221     1452   2490   2194   -111   -267     39       O
ATOM    485  N3   DC B 221     -24.380 -17.174  49.596  1.00 14.05           N
ANISOU  485  N3   DC B 221     1561   2118   1659   -134   -135   -298       N
ATOM    486  C4   DC B 221     -24.441 -15.938  49.192  1.00 13.90           C
ANISOU  486  C4   DC B 221     1817   2009   1456    -69     -7   -417       C
ATOM    487  N4   DC B 221     -23.301 -15.332  48.862  1.00 14.98           N
ANISOU  487  N4   DC B 221     1888   2301   1500   -102     -7   -502       N
ATOM    488  C5   DC B 221     -25.687 -15.248  49.104  1.00 15.48           C
ANISOU  488  C5   DC B 221     2015   2255   1612    -36    -86   -415       C
ATOM    489  C6   DC B 221     -26.796 -15.961  49.370  1.00 16.27           C
ANISOU  489  C6   DC B 221     2026   2169   1985    -22    111   -411       C
ATOM    490  P    DG B 222     -31.526 -18.740  52.661  1.00 20.08           P
ANISOU  490  P    DG B 222     1772   3487   2370   -204   -108    561       P
ATOM    491  OP1  DG B 222     -32.549 -19.772  52.866  1.00 24.79           O
ANISOU  491  OP1  DG B 222     1927   4748   2743   -577   -561    529       O
ATOM    492  OP2  DG B 222     -31.825 -17.355  52.936  1.00 21.72           O
ANISOU  492  OP2  DG B 222     2180   4117   1955   -489    216    118       O
ATOM    493  O5′  DG B 222     -30.322 -19.023  53.587  1.00 18.81           O
ANISOU  493  O5′  DG B 222     1592   3062   2490     24   -511    292       O
ATOM    494  C5′  DG B 222     -29.755 -20.291  53.655  1.00 19.01           C
ANISOU  494  C5′  DG B 222     1955   2522   2744   -503   -440    134       C
ATOM    495  C4′  DG B 222     -28.501 -20.240  54.553  1.00 17.19           C
ANISOU  495  C4′  DG B 222     1701   2554   2274    -79   -475     73       C
ATOM    496  O4′  DG B 222     -27.458 -19.485  53.886  1.00 15.46           O
ANISOU  496  O4′  DG B 222     1713   2097   2063   -251   -318     26       O
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ATOM    497  C3′  DG B 222     -28.728 -19.560  55.905  1.00 16.75           C
ANISOU  497  C3′  DG B 222     1743   2446   2174     27   -385    283       C
ATOM    498  O3′  DG B 222     -27.966 -20.315  56.887  1.00 15.43           O
ANISOU  498  O3′  DG B 222     1599   2236   2028     27   -224    174       O
ATOM    499  C2′  DG B 222     -28.084 -18.192  55.714  1.00 15.01           C
ANISOU  499  C2′  DG B 222     1429   2081   2190     59   -285    112       C
ATOM    500  C1′  DG B 222     -26.906 -18.592  54.824  1.00 14.88           C
ANISOU  500  C1′  DG B 222     1681   2042   1927     94   -432   -107       C
ATOM    501  N9   DG B 222     -26.278 -17.512  54.122  1.00 13.82           N
ANISOU  501  N9   DG B 222     1737   1770   1742     95   -135     31       N
ATOM    502  C8   DG B 222     -26.826 -16.338  53.681  1.00 14.46           C
ANISOU  502  C8   DG B 222     1760   1765   1967     66   -264   -116       C
ATOM    503  N7   DG B 222     -25.948 -15.583  53.061  1.00 14.04           N
ANISOU  503  N7   DG B 222     1630   1921   1782    166   -163    -94       N
ATOM    504  C5   DG B 222     -24.760 -16.301  53.100  1.00 12.93           C
ANISOU  504  C5   DG B 222     1620   1669   1624    237   -311   -157       C
ATOM    505  C6   DG B 222     -23.478 -15.983  52.607  1.00 12.31           C
ANISOU  505  C6   DG B 222     1542   1720   1412     -6   -107   -270       C
ATOM    506  O6   DG B 222     -23.132 -14.984  52.004  1.00 13.05           O
ANISOU  506  O6   DG B 222     1626   1705   1627    100   -224   -192       O
ATOM    507  N1   DG B 222     -22.547 -16.999  52.904  1.00 12.11           N
ANISOU  507  N1   DG B 222     1650   1503   1446    160   -213   -212       N
ATOM    508  C2   DG B 222     -22.829 -18.145  53.553  1.00 12.04           C
ANISOU  508  C2   DG B 222     1465   1675   1433     67   -207   -199       C
ATOM    509  N2   DG B 222     -21.828 -19.024  53.779  1.00 13.40           N
ANISOU  509  N2   DG B 222     1718   1854   1518    205   -203   -238       N
ATOM    510  N3   DG B 222     -24.036 -18.452  53.981  1.00 12.96           N
ANISOU  510  N3   DG B 222     1647   1741   1533     36   -225   -165       N
ATOM    511  C4   DG B 222     -24.945 -17.483  53.726  1.00 12.63           C
ANISOU  511  C4   DG B 222     1365   1777   1656    -34   -259   -156       C
ATOM    512  P    DC B 223     -28.469 -20.407  58.402  1.00 15.99           P
ANISOU  512  P    DC B 223     1574   2183   2315    -50   -174    285       P
ATOM    513  OP1  DC B 223     -29.574 -21.336  58.463  1.00 18.53           O
ANISOU  513  OP1  DC B 223     1480   2808   2750   -252    -82    425       O
ATOM    514  OP2  DC B 223     -28.672 -19.076  58.933  1.00 17.48           O
ANISOU  514  OP2  DC B 223     1764   2560   2317    164   -150    343       O
ATOM    515  O5′  DC B 223     -27.172 -20.986  59.061  1.00 14.87           O
ANISOU  515  O5′  DC B 223     1495   1992   2159     57   -226    198       O
ATOM    516  C5′  DC B 223     -26.660 -22.236  58.704  1.00 15.33           C
ANISOU  516  C5′  DC B 223     1568   2118   2138   -139   -285     80       C
ATOM    517  C4′  DC B 223     -25.165 -22.164  58.471  1.00 14.04           C
ANISOU  517  C4′  DC B 223     1587   1795   1949    -89   -269      0       C
ATOM    518  O4′  DC B 223     -24.883 -21.310  57.376  1.00 13.67           O
ANISOU  518  O4′  DC B 223     1586   1679   1926   -262   -249     16       O
ATOM    519  C3′  DC B 223     -24.310 -21.634  59.599  1.00 13.68           C
ANISOU  519  C3′  DC B 223     1727   1611   1856   -127   -327    268       C
ATOM    520  O3′  DC B 223     -24.101 -22.662  60.568  1.00 15.09           O
ANISOU  520  O3′  DC B 223     1842   1714   2177   -244   -402    258       O
ATOM    521  C2′  DC B 223     -23.045 -21.246  58.852  1.00 13.49           C
ANISOU  521  C2′  DC B 223     1657   1717   1748   -114   -235    115       C
ATOM    522  C1′  DC B 223     -23.620 -20.694  57.625  1.00 13.40           C
ANISOU  522  C1′  DC B 223     1420   1841   1830    -97   -293      1       C
ATOM    523  N1   DC B 223     -23.794 -19.228  57.556  1.00 11.94           N
ANISOU  523  N1   DC B 223     1441   1452   1640     16   -170     20       N
ATOM    524  C2   DC B 223     -22.732 -18.453  57.138  1.00 11.21           C
ANISOU  524  C2   DC B 223     1226   1498   1534    127   -130    -10       C
ATOM    525  O2   DC B 223     -21.605 -19.004  57.030  1.00 12.00           O
ANISOU  525  O2   DC B 223     1393   1473   1691     66   -136    -22       O
ATOM    526  N3   DC B 223     -22.932 -17.154  56.878  1.00 10.94           N
ANISOU  526  N3   DC B 223     1260   1495   1401     65   -187    -70       N
ATOM    527  C4   DC B 223     -24.142 -16.640  57.072  1.00 10.86           C
ANISOU  527  C4   DC B 223     1193   1484   1447     14   -104     30       C
ATOM    528  N4   DC B 223     -24.334 -15.368  56.732  1.00 12.16           N
ANISOU  528  N4   DC B 223     1306   1611   1702     23    -65     54       N
ATOM    529  C5   DC B 223     -25.184 -17.382  57.608  1.00 12.52           C
ANISOU  529  C5   DC B 223     1306   1684   1767    132      4    177       C
ATOM    530  C6   DC B 223     -24.982 -18.646  57.840  1.00 12.54           C
ANISOU  530  C6   DC B 223     1385   1585   1793    -21   -143    -57       C
ATOM    531  P    DG B 224     -23.673 -22.293  62.083  1.00 14.70           P
ANISOU  531  P    DG B 224     1838   1764   1982   -214   -254    295       P
ATOM    532  OP1  DG B 224     -23.779 -23.572  62.823  1.00 17.09           O
ANISOU  532  OP1  DG B 224     2059   2029   2402   -224   -285    574       O
ATOM    533  OP2  DG B 224     -24.452 -21.118  62.539  1.00 15.80           O
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ANISOU  533  OP2  DG B 224     1807   2314   1881   -157   -181    241       O
ATOM    534  O5′  DG B 224     -22.163 -21.793  62.001  1.00 13.37           O
ANISOU  534  O5′  DG B 224     1621   1522   1936   -130   -303     86       O
ATOM    535  C5′  DG B 224     -21.120 -22.673  61.644  1.00 13.85           C
ANISOU  535  C5′  DG B 224     1824   1542   1896    -97   -420    150       C
ATOM    536  C4′  DG B 224     -19.837 -21.907  61.421  1.00 12.33           C
ANISOU  536  C4′  DG B 224     1635   1343   1704   -135   -342     90       C
ATOM    537  O4′  DG B 224     -20.012 -21.030  60.294  1.00 12.38           O
ANISOU  537  O4′  DG B 224     1692   1332   1678    -78   -254     -7       O
ATOM    538  C3′  DG B 224     -19.380 -21.012  62.549  1.00 13.07           C
ANISOU  538  C3′  DG B 224     1818   1408   1737    110   -418    128       C
ATOM    539  O3′  DG B 224     -18.632 -21.790  63.489  1.00 13.60           O
ANISOU  539  O3′  DG B 224     1929   1424   1814     72   -370    128       O
ATOM    540  C2′  DG B 224     -18.520 -19.971  61.801  1.00 12.94           C
ANISOU  540  C2′  DG B 224     1733   1380   1803     -1   -405     70       C
ATOM    541  C1′  DG B 224     -19.308 -19.795  60.537  1.00 12.19           C
ANISOU  541  C1′  DG B 224     1593   1298   1738     21   -200     -5       C
ATOM    542  N9   DG B 224     -20.293 -18.723  60.521  1.00 11.44           N
ANISOU  542  N9   DG B 224     1357   1437   1551    112   -246     21       N
ATOM    543  C8   DG B 224     -21.590 -18.813  60.929  1.00 12.22           C
ANISOU  543  C8   DG B 224     1483   1462   1698    -48   -145    -60       C
ATOM    544  N7   DG B 224     -22.294 -17.721  60.692  1.00 11.74           N
ANISOU  544  N7   DG B 224     1351   1518   1589     81   -191     -9       N
ATOM    545  C5   DG B 224     -21.368 -16.880  60.084  1.00 10.97           C
ANISOU  545  C5   DG B 224     1313   1329   1526    -11   -144    -35       C
ATOM    546  C6   DG B 224     -21.551 -15.594  59.544  1.00 10.72           C
ANISOU  546  C6   DG B 224     1326   1310   1433    221   -161    -45       C
ATOM    547  O6   DG B 224     -22.575 -14.906  59.515  1.00 11.94           O
ANISOU  547  O6   DG B 224     1383   1551   1603    166    -73     13       O
ATOM    548  N1   DG B 224     -20.385 -15.082  59.020  1.00 11.22           N
ANISOU  548  N1   DG B 224     1416   1433   1415     56    -60     19       N
ATOM    549  C2   DG B 224     -19.164 -15.696  59.022  1.00 10.35           C
ANISOU  549  C2   DG B 224     1322   1247   1361     63   -172     -4       C
ATOM    550  N2   DG B 224     -18.139 -15.042  58.512  1.00 11.63           N
ANISOU  550  N2   DG B 224     1403   1413   1603     42   -147     29       N
ATOM    551  N3   DG B 224     -19.002 -16.947  59.487  1.00 10.97           N
ANISOU  551  N3   DG B 224     1370   1326   1469     43   -142     -3       N
ATOM    552  C4   DG B 224     -20.146 -17.479  59.977  1.00 10.78           C
ANISOU  552  C4   DG B 224     1367   1262   1465    106   -198     31       C
TER     553        DG B 224
HETATM  554 MG    MG A 301     -27.540 -30.955  46.173  1.00 12.50          MG
ANISOU  554 MG    MG A 301     1523   1581   1643   -203   -159    -27       MG
HETATM  555 NA    NA A 400     -28.527 -17.902  41.651  1.00 16.02          NA
ANISOU  555 NA    NA A 400     1841   2032   2214    -68    118     40       NA
HETATM  556 NA    NA A 401     -31.349 -28.975  47.038  1.00 19.11          NA
ANISOU  556 NA    NA A 401     2360   2445   2456   -120    304     71       NA
HETATM  557 NA    NA A 402     -21.293 -22.888  52.187  1.00 25.53          NA
ANISOU  557 NA    NA A 402     3062   3512   3125    120   -596   -626       NA
HETATM  558 NA    NA B 403     -18.410 -31.423  26.719  1.00 23.23          NA
ANISOU  558 NA    NA B 403     3087   2836   2903    726    185     20       NA
HETATM  559  O   HOH A 404     -28.370 -26.667  41.716  1.00 15.77           O
ANISOU  559  O   HOH A 404     2017   1819   2153   -491    362   -263       O
HETATM  560  O   HOH A 406     -23.827 -12.210  54.204  1.00 12.76           O
ANISOU  560  O   HOH A 406     1472   1617   1758    264   -177     57       O
HETATM  561  O   HOH A 407     -27.544 -29.365  44.814  1.00 13.11           O
ANISOU  561  O   HOH A 407     1519   1636   1823   -271   -212      7       O
HETATM  562  O   HOH A 408     -25.457 -30.907  46.090  1.00 14.26           O
ANISOU  562  O   HOH A 408     1664   1791   1961   -211   -253   -160       O
HETATM  563  O   HOH A 409     -21.650 -10.776  52.774  1.00 14.12           O
ANISOU  563  O   HOH A 409     1589   1910   1866    277    -99    211       O
HETATM  564  O   HOH A 410     -27.554 -29.689  47.823  1.00 14.23           O
ANISOU  564  O   HOH A 410     1821   1833   1750   -222   -149   -130       O
HETATM  565  O   HOH A 411     -28.843 -24.034  34.572  1.00 17.01           O
ANISOU  565  O   HOH A 411     2259   1934   2268   -560   -127    215       O
HETATM  566  O   HOH A 413     -28.156 -20.350  45.776  1.00 16.90           O
ANISOU  566  O   HOH A 413     1870   2282   2266     52    405     17       O
HETATM  567  O   HOH A 418     -29.761 -18.455  26.444  1.00 18.88           O
ANISOU  567  O   HOH A 418     1808   2548   2816    196   -255     17       O
HETATM  568  O   HOH A 419     -17.468  -9.954  51.690  1.00 17.02           O
ANISOU  568  O   HOH A 419     2002   2177   2285    231    345    119       O
HETATM  569  O   HOH A 420     -25.452 -11.828  56.404  1.00 18.52           O
ANISOU  569  O   HOH A 420     2026   2689   2319    431     79     66       O
HETATM  570  O   HOH A 422     -19.793 -22.473  42.599  1.00 24.42           O
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ANISOU  570  O   HOH A 422     2577   3274   3428    547    521   -201       O
HETATM  571  O   HOH A 424     -31.090 -20.642  31.411  1.00 22.08           O
ANISOU  571  O   HOH A 424     2556   3117   2716   -447   -199    -45       O
HETATM  572  O   HOH A 426     -23.463 -16.727  30.006  1.00 16.62           O
ANISOU  572  O   HOH A 426     2298   1917   2099    -58    330    268       O
HETATM  573  O   HOH A 427     -25.540 -16.648  22.366  1.00 24.78           O
ANISOU  573  O   HOH A 427     2749   3126   3537   1330     -6    761       O
HETATM  574  O   HOH A 430     -12.730  -6.656  56.166  0.50 18.69           O
ANISOU  574  O   HOH A 430     2189   2079   2832   -159   -167   -170       O
HETATM  575  O   HOH A 431     -26.793 -11.861  34.893  1.00 26.67           O
ANISOU  575  O   HOH A 431     4052   1503   4578    857   -844   -309       O
HETATM  576  O   HOH A 432     -25.837 -23.222  48.914  1.00 59.65           O
ANISOU  576  O   HOH A 432     9752   7293   5618    521   1841    239       O
HETATM  577  O   HOH A 433     -24.396 -25.455  37.491  1.00 20.33           O
ANISOU  577  O   HOH A 433     3454   1970   2299    230    381     69       O
HETATM  578  O   HOH A 434     -19.548 -12.662  48.981  1.00 25.48           O
ANISOU  578  O   HOH A 434     3113   3404   3162    337    831    861       O
HETATM  579  O   HOH A 438     -24.092 -15.761  34.221  1.00 13.61           O
ANISOU  579  O   HOH A 438     1988   1375   1807    -74    289    -72       O
HETATM  580  O   HOH A 440     -29.875 -26.644  39.358  1.00 18.58           O
ANISOU  580  O   HOH A 440     2565   2106   2386   -940    190     57       O
HETATM  581  O   HOH A 442     -25.809 -14.206  35.836  1.00 16.21           O
ANISOU  581  O   HOH A 442     2402   1503   2254   -124    372      5       O
HETATM  582  O   HOH A 443     -29.684 -28.835  49.199  1.00 18.41           O
ANISOU  582  O   HOH A 443     2277   2664   2053    161    104    -94       O
HETATM  583  O   HOH A 444     -23.013 -14.857  31.813  1.00 22.48           O
ANISOU  583  O   HOH A 444     3448   2351   2739   -823    192    530       O
HETATM  584  O   HOH A 447     -26.743 -28.406  40.511  0.50 15.47           O
ANISOU  584  O   HOH A 447     2133   1708   2035   -168    500   -190       O
HETATM  585  O   HOH A 449     -21.427 -24.403  40.623  1.00 23.19           O
ANISOU  585  O   HOH A 449     2339   2895   3577    607    327    346       O
HETATM  586  O   HOH A 451     -28.732 -22.056  47.917  1.00 28.29           O
ANISOU  586  O   HOH A 451     4142   3517   3089   -340    504    501       O
HETATM  587  O   HOH A 452     -31.073 -23.166  36.031  1.00 23.48           O
ANISOU  587  O   HOH A 452     3122   2442   3355    101     51   -384       O
HETATM  588  O   HOH A 453     -24.528 -10.748  29.688  1.00 27.99           O
ANISOU  588  O   HOH A 453     4423   2349   3861    351   -271   -410       O
HETATM  589  O   HOH A 456     -25.754 -29.065  42.751  1.00 22.66           O
ANISOU  589  O   HOH A 456     2973   3243   2392  -1219    342   -129       O
HETATM  590  O   HOH A 457     -17.113 -11.382  49.400  1.00 26.01           O
ANISOU  590  O   HOH A 457     3469   3660   2753    -21    207      9       O
HETATM  591  O   HOH A 459     -29.550 -23.306  32.119  1.00 23.42           O
ANISOU  591  O   HOH A 459     2835   3314   2749   -762    -47    138       O
HETATM  592  O   HOH A 460     -18.226 -18.463  45.076  1.00 30.21           O
ANISOU  592  O   HOH A 460     3575   4144   3756    250    -69    -11       O
HETATM  593  O   HOH A 461     -21.184 -15.362  21.628  1.00 24.87           O
ANISOU  593  O   HOH A 461     3381   2339   3728    137    337    -88       O
HETATM  594  O   HOH A 462     -15.334 -16.651  22.696  0.50 17.95           O
ANISOU  594  O   HOH A 462     2212   2020   2587    -16    122   -108       O
HETATM  595  O   HOH A 463     -17.791 -20.993  45.564  1.00 30.84           O
ANISOU  595  O   HOH A 463     3939   3805   3973    455    772   -346       O
HETATM  596  O   HOH A 465     -23.770 -27.752  44.241  1.00 27.84           O
ANISOU  596  O   HOH A 465     3632   2987   3959   -201    223   -147       O
HETATM  597  O   HOH A 468     -17.724  -4.920  53.793  1.00 22.23           O
ANISOU  597  O   HOH A 468     2708   2506   3229     93   -109    126       O
HETATM  598  O   HOH A 471     -31.459 -24.613  38.449  1.00 27.37           O
ANISOU  598  O   HOH A 471     2624   4874   2901    487    435     54       O
HETATM  599  O   HOH A 474     -31.475 -25.273  48.292  1.00 24.92           O
ANISOU  599  O   HOH A 474     3763   3180   2525     83    557   -269       O
HETATM  600  O   HOH A 475     -10.268 -13.392  54.048  0.50 22.30           O
ANISOU  600  O   HOH A 475     1959   3429   3083    696    282   -398       O
HETATM  601  O   HOH A 478     -25.594 -27.646  38.278  1.00 26.90           O
ANISOU  601  O   HOH A 478     4627   2109   3481   -297    523   -121       O
HETATM  602  O   HOH A 479     -23.050 -12.212  31.305  1.00 25.89           O
ANISOU  602  O   HOH A 479     3561   2287   3986   -399   -150    328       O
HETATM  603  O   HOH A 483     -29.385 -26.205  50.183  1.00 26.87           O
ANISOU  603  O   HOH A 483     4124   3214   2869   -128    -89   -368       O
HETATM  604  O   HOH A 484     -19.669 -25.109  53.002  0.50 18.78           O
ANISOU  604  O   HOH A 484     2917   1736   2483     98   -165   -545       O
HETATM  605  O   HOH A 486      -8.934 -16.211  51.071  0.50 25.64           O
ANISOU  605  O   HOH A 486     2377   3645   3719   1099   1031    -80       O
HETATM  606  O   HOH A 488     -28.208 -27.538  37.374  1.00 25.48           O
ANISOU  606  O   HOH A 488     3627   2517   3537    190    473   -295       O
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HETATM  607  O   HOH A 490     -19.223 -14.914  47.644  1.00 23.30           O
ANISOU  607  O   HOH A 490     2612   3575   2663   -492     44   -149       O
HETATM  608  O   HOH A 491     -11.392  -9.469  53.049  0.50 22.62           O
ANISOU  608  O   HOH A 491     2306   3185   3103    -68    589   -250       O
HETATM  609  O   HOH A 493     -34.386 -20.484  43.763  1.00 33.28           O
ANISOU  609  O   HOH A 493     2238   5490   4914    299    875   -696       O
HETATM  610  O   HOH A 495     -27.370 -15.155  23.927  1.00 29.39           O
ANISOU  610  O   HOH A 495     4156   3102   3906    979   -288    582       O
HETATM  611  O   HOH A 496     -25.615 -28.110  51.609  1.00 32.44           O
ANISOU  611  O   HOH A 496     4966   4906   2454  -1373    -13    512       O
HETATM  612  O   HOH A 498     -28.615  -9.577  30.683  0.50 19.27           O
ANISOU  612  O   HOH A 498     2695   1791   2833    909    272    311       O
HETATM  613  O   HOH A 499     -31.832 -18.808  33.040  1.00 35.69           O
ANISOU  613  O   HOH A 499     3786   3745   6027    -16    299  -1138       O
HETATM  614  O   HOH A 505     -33.198 -14.649  38.478  1.00 47.77           O
ANISOU  614  O   HOH A 505     5548   6672   5930   -741  -1455    -75       O
HETATM  615  O   HOH A 508     -31.881 -15.989  30.122  1.00 58.81           O
ANISOU  615  O   HOH A 508     5657   8832   7853   1516    813  -3793       O
HETATM  616  O   HOH A 509     -33.616 -13.837  34.753  1.00 41.21           O
ANISOU  616  O   HOH A 509     4640   4972   6043   1395     99   1877       O
HETATM  617  O   HOH A 510     -21.443 -30.463  47.448  1.00 44.52           O
ANISOU  617  O   HOH A 510     4738   4338   7839   -984     -1   -851       O
HETATM  618  O   HOH A 511     -17.165 -16.659  47.470  1.00 31.78           O
ANISOU  618  O   HOH A 511     4111   4508   3453    619    335   -493       O
HETATM  619  O   HOH A 514     -14.284  -4.581  55.730  1.00 52.38           O
ANISOU  619  O   HOH A 514     4951   7160   7789   1282   -387    254       O
HETATM  620  O   HOH A 515     -15.682  -5.842  52.180  1.00 30.24           O
ANISOU  620  O   HOH A 515     3318   3167   5002    240    882    743       O
HETATM  621  O   HOH A 518     -33.771 -26.388  49.515  1.00 42.84           O
ANISOU  621  O   HOH A 518     4895   6374   5008  -1051   1532  -1841       O
HETATM  622  O   HOH A 519     -23.908 -24.169  51.382  1.00 35.86           O
ANISOU  622  O   HOH A 519     3783   4546   5296   -521   -528    662       O
HETATM  623  O   HOH A 527     -21.655 -29.254  51.617  1.00 37.47           O
ANISOU  623  O   HOH A 527     3927   5682   4629  -1151   -554   -274       O
HETATM  624  O   HOH A 528     -15.067 -21.300  46.876  1.00 59.93           O
ANISOU  624  O   HOH A 528     4960   9475   8335   -747   -954   2520       O
HETATM  625  O   HOH A 529     -24.760 -12.491  23.314  1.00 38.02           O
ANISOU  625  O   HOH A 529     5280   5184   3979   -743    528   1852       O
HETATM  626  O   HOH A 531     -32.284 -21.321  28.902  1.00 30.09           O
ANISOU  626  O   HOH A 531     3855   4454   3123  -1153   -527   -378       O
HETATM  627  O   HOH A 532     -33.958 -22.418  45.616  1.00 34.30           O
ANISOU  627  O   HOH A 532     4689   3031   5309    891    890   -759       O
HETATM  628  O   HOH A 535     -29.506 -16.004  25.061  1.00 36.14           O
ANISOU  628  O   HOH A 535     4520   4412   4798    -57  -1104   1213       O
HETATM  629  O   HOH B 405     -23.794 -12.410  51.398  1.00 14.56           O
ANISOU  629  O   HOH B 405     1946   1873   1712    205   -140    -40       O
HETATM  630  O   HOH B 412     -26.645 -16.033  37.775  1.00 13.50           O
ANISOU  630  O   HOH B 412     1912   1433   1781    -63    189   -145       O
HETATM  631  O   HOH B 414     -26.946 -13.125  52.113  1.00 16.39           O
ANISOU  631  O   HOH B 414     1645   2085   2496    111   -321   -116       O
HETATM  632  O   HOH B 415     -23.611 -12.455  48.625  1.00 17.92           O
ANISOU  632  O   HOH B 415     2404   2382   2021     16     92   -361       O
HETATM  633  O   HOH B 416     -24.829 -18.470  61.786  1.00 16.62           O
ANISOU  633  O   HOH B 416     1911   2180   2224   -200     10    -41       O
HETATM  634  O   HOH B 417     -18.849 -17.687  42.315  1.00 23.27           O
ANISOU  634  O   HOH B 417     2350   3253   3238   -105   -118    195       O
HETATM  635  O   HOH B 421     -27.211 -17.480  60.636  1.00 20.23           O
ANISOU  635  O   HOH B 421     2287   2686   2713    199    337   -136       O
HETATM  636  O   HOH B 423     -22.780 -11.496  42.115  1.00 22.93           O
ANISOU  636  O   HOH B 423     3460   2191   3060   -737    154   -416       O
HETATM  637  O   HOH B 425     -24.189 -25.401  34.849  1.00 19.12           O
ANISOU  637  O   HOH B 425     3072   1848   2343    -36    197    411       O
HETATM  638  O   HOH B 428     -24.596 -21.219  54.232  1.00 19.36           O
ANISOU  638  O   HOH B 428     2339   2080   2935    104   -409   -190       O
HETATM  639  O   HOH B 429     -18.049 -24.578  63.191  0.50 14.69           O
ANISOU  639  O   HOH B 429     1948   1342   2290    263     88    176       O
HETATM  640  O   HOH B 435     -25.049 -14.950  60.707  1.00 27.87           O
ANISOU  640  O   HOH B 435     2293   4944   3350   1212    732    464       O
HETATM  641  O   HOH B 436     -31.069 -22.119  24.406  1.00 21.22           O
ANISOU  641  O   HOH B 436     1919   3008   3135    255    280   -320       O
HETATM  642  O   HOH B 437     -27.114 -14.361  57.033  1.00 21.12           O
ANISOU  642  O   HOH B 437     2183   2707   3132    759    471    169       O
HETATM  643  O   HOH B 439     -20.597 -23.979  37.799  1.00 27.29           O
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ANISOU  643  O   HOH B 439     3072   3142   4153    251    428    983       O
HETATM  644  O   HOH B 441     -28.807 -16.054  39.575  1.00 17.79           O
ANISOU  644  O   HOH B 441     2220   2167   2371    214    313     30       O
HETATM  645  O   HOH B 445     -26.157 -11.578  47.987  0.50 20.95           O
ANISOU  645  O   HOH B 445     2486   3025   2446    211   -788    -34       O
HETATM  646  O   HOH B 446     -21.470 -10.976  48.023  1.00 25.41           O
ANISOU  646  O   HOH B 446     3141   3288   3223      2     -8    299       O
HETATM  647  O   HOH B 448     -25.838 -21.186  64.823  0.50 18.79           O
ANISOU  647  O   HOH B 448     1564   3270   2305   -129   -195    544       O
HETATM  648  O   HOH B 450     -29.866 -19.187  43.850  1.00 19.75           O
ANISOU  648  O   HOH B 450     2463   2455   2585    -20    310     46       O
HETATM  649  O   HOH B 454     -20.416 -14.567  45.370  1.00 28.32           O
ANISOU  649  O   HOH B 454     3306   3383   4069   -763   -201    134       O
HETATM  650  O   HOH B 455     -24.819 -10.149  43.511  1.00 30.47           O
ANISOU  650  O   HOH B 455     4424   3516   3637   -485    649  -1057       O
HETATM  651  O   HOH B 458     -19.004 -20.553  40.425  1.00 29.12           O
ANISOU  651  O   HOH B 458     2518   3864   4682   -122   -258   1118       O
HETATM  652  O   HOH B 464     -17.087 -10.582  31.961  0.50 20.76           O
ANISOU  652  O   HOH B 464     2734   2479   2674  -1416    552   -346       O
HETATM  653  O   HOH B 466     -28.837 -25.759  28.739  1.00 27.26           O
ANISOU  653  O   HOH B 466     2516   3734   4105   -145    615   -115       O
HETATM  654  O   HOH B 467     -26.682 -26.680  33.071  1.00 73.19           O
ANISOU  654  O   HOH B 467     8395   7640  11773   1992  -2392   1951       O
HETATM  655  O   HOH B 469     -30.475 -17.015  58.393  1.00 25.97           O
ANISOU  655  O   HOH B 469     2864   3522   3482    332   -241    556       O
HETATM  656  O   HOH B 470     -26.479 -21.159  51.577  1.00 22.81           O
ANISOU  656  O   HOH B 470     2694   2624   3347   -115    512   -712       O
HETATM  657  O   HOH B 472     -22.218 -25.682  63.755  0.50 18.58           O
ANISOU  657  O   HOH B 472     2527   1933   2598   -379   -672    298       O
HETATM  658  O   HOH B 473     -26.193  -8.559  39.900  1.00 30.77           O
ANISOU  658  O   HOH B 473     5083   2155   4452    260    717    -24       O
HETATM  659  O   HOH B 476     -29.948 -15.476  53.880  1.00 25.24           O
ANISOU  659  O   HOH B 476     2312   3933   3343    707    279    211       O
HETATM  660  O   HOH B 477     -19.659 -11.003  39.436  1.00 30.82           O
ANISOU  660  O   HOH B 477     3714   4733   3260   -473    434   -887       O
HETATM  661  O   HOH B 480     -18.623 -22.161  37.515  1.00 25.33           O
ANISOU  661  O   HOH B 480     3014   2903   3707    240     91    891       O
HETATM  662  O   HOH B 481     -29.396 -23.457  28.337  1.00 31.97           O
ANISOU  662  O   HOH B 481     3228   4833   4086    -96   1146   -641       O
HETATM  663  O   HOH B 482     -21.447 -28.618  32.733  1.00 29.42           O
ANISOU  663  O   HOH B 482     4774   3065   3336    639    907    138       O
HETATM  664  O   HOH B 485     -16.799 -18.356  37.760  1.00 28.43           O
ANISOU  664  O   HOH B 485     3397   4147   3255   -119    266   -118       O
HETATM  665  O   HOH B 487     -30.604 -14.029  39.163  1.00 27.29           O
ANISOU  665  O   HOH B 487     3515   3247   3608   1084   -286   -403       O
HETATM  666  O   HOH B 489     -29.981 -23.481  60.106  1.00 29.95           O
ANISOU  666  O   HOH B 489     4014   3431   3933   -362    769    699       O
HETATM  667  O   HOH B 492     -32.479 -18.600  44.228  1.00 26.45           O
ANISOU  667  O   HOH B 492     2364   3843   3839     33    462   -216       O
HETATM  668  O   HOH B 494     -29.640 -15.129  56.533  1.00 26.35           O
ANISOU  668  O   HOH B 494     2279   3799   3931    403     94    567       O
HETATM  669  O   HOH B 497     -28.617 -15.628  62.280  1.00 41.56           O
ANISOU  669  O   HOH B 497     4741   4463   6587   -708   1445  -1687       O
HETATM  670  O   HOH B 500     -30.958 -24.065  22.291  1.00 26.64           O
ANISOU  670  O   HOH B 500     2240   4208   3674    215   -443   -686       O
HETATM  671  O   HOH B 501     -26.808 -11.712  45.471  1.00 27.29           O
ANISOU  671  O   HOH B 501     4219   2449   3700    768   -375   -583       O
HETATM  672  O   HOH B 502     -20.552 -11.849  43.807  1.00 32.82           O
ANISOU  672  O   HOH B 502     4499   4061   3907   -231      8  -1485       O
HETATM  673  O   HOH B 503     -17.387 -15.819  41.111  1.00 31.62           O
ANISOU  673  O   HOH B 503     2672   4666   4673   -736   -215   -170       O
HETATM  674  O   HOH B 504     -15.526 -27.929  28.146  0.50 20.03           O
ANISOU  674  O   HOH B 504     2565   2567   2476    349    -51    307       O
HETATM  675  O   HOH B 506     -28.410 -24.004  21.346  0.50 18.51           O
ANISOU  675  O   HOH B 506     1762   2924   2346   -166    -44    102       O
HETATM  676  O   HOH B 507     -29.297 -12.216  37.289  1.00 29.27           O
ANISOU  676  O   HOH B 507     4104   3431   3584    784   -168    195       O
HETATM  677  O   HOH B 512     -28.439 -26.692  35.144  1.00 30.77           O
ANISOU  677  O   HOH B 512     4358   3310   4023     64    636   -896       O
HETATM  678  O   HOH B 513     -13.125 -25.545  30.455  1.00 25.64           O
ANISOU  678  O   HOH B 513     2756   3724   3261   -113    170   -183       O
HETATM  679  O   HOH B 516     -30.541 -22.619  56.340  1.00 36.10           O
ANISOU  679  O   HOH B 516     5118   4616   3981  -1893   -235   -385       O
```

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HETATM  680  O   HOH B 517     -17.072 -25.265  36.040  1.00 60.10           O
ANISOU  680  O   HOH B 517     8179  11039   3616   2568   1977    850       O
HETATM  681  O   HOH B 520     -27.410 -23.070  52.990  1.00 34.04           O
ANISOU  681  O   HOH B 520     5599   4394   2939   -695   -353    602       O
HETATM  682  O   HOH B 521     -32.470 -20.853  46.716  1.00 38.52           O
ANISOU  682  O   HOH B 521     4070   4597   5968   -425   1328  -1005       O
HETATM  683  O   HOH B 522     -21.100  -9.880  45.611  1.00 31.94           O
ANISOU  683  O   HOH B 522     5284   4022   2828    502    344    582       O
HETATM  684  O   HOH B 523     -19.457  -9.262  34.799  0.50 23.50           O
ANISOU  684  O   HOH B 523     3307   1745   3876   -366   1024    -22       O
HETATM  685  O   HOH B 524     -31.552 -22.225  51.367  1.00 39.15           O
ANISOU  685  O   HOH B 524     4540   6755   3580   -564      8  -1047       O
HETATM  686  O   HOH B 525     -14.157 -15.302  34.801  1.00 35.15           O
ANISOU  686  O   HOH B 525     2950   4019   6385  -1005    870   -882       O
HETATM  687  O   HOH B 526     -28.960 -20.152  62.532  1.00 54.17           O
ANISOU  687  O   HOH B 526    10279   5288   5014  -1442   1660   1521       O
HETATM  688  O   HOH B 530     -18.506 -28.781  33.391  1.00 33.34           O
ANISOU  688  O   HOH B 530     4641   4256   3767    818   -219    697       O
HETATM  689  O   HOH B 533     -15.829 -30.438  27.042  0.50 16.87           O
ANISOU  689  O   HOH B 533     2247   1933   2229    162   -275    192       O
HETATM  690  O   HOH B 534     -26.267 -29.632  29.396  1.00 31.19           O
ANISOU  690  O   HOH B 534     4096   3052   4702    -33   1659    806       O
HETATM  691  O   HOH B 536     -31.020 -26.749  26.610  1.00 38.34           O
ANISOU  691  O   HOH B 536     3055   6119   5390  -1612    838  -1482       O
CONECT  119  145
CONECT  120  146
CONECT  145  119  147  149  151
CONECT  146  120  148  150  152
CONECT  147  145
CONECT  148  146
CONECT  149  145
CONECT  150  146
CONECT  151  145  175
CONECT  152  146  176
CONECT  153  155  171  181
CONECT  154  156  172  182
CONECT  155  153  157  167
CONECT  156  154  158  168
CONECT  157  155  159
CONECT  158  156  160
CONECT  159  157  161
CONECT  160  158  162
CONECT  161  159  163
CONECT  162  160  164
CONECT  163  161  165  167
CONECT  164  162  166  168
CONECT  165  163
CONECT  166  164
CONECT  167  155  163  169
CONECT  168  156  164  170
CONECT  169  167  171
CONECT  170  168  172
CONECT  171  153  169
CONECT  172  154  170
CONECT  173  181  183
CONECT  174  182  184
CONECT  175  151  177
CONECT  176  152  178
CONECT  177  175  179  183
CONECT  178  176  180  184
CONECT  179  177  181
CONECT  180  178  182
CONECT  181  153  173  179
CONECT  182  154  174  180
CONECT  183  173  177  185
CONECT  184  174  178  186
CONECT  185  183  187
CONECT  186  184  187
CONECT  187  185  186
CONECT  188  556
CONECT  200  555
CONECT  349  558
CONECT  397  410
```

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CONECT  410  397  411  412  413
CONECT  411  410
CONECT  412  410
CONECT  413  410  425
CONECT  414  415  423  428
CONECT  415  414  416  421
CONECT  416  415  417
CONECT  417  416  418
CONECT  418  417  419
CONECT  419  418  420  421
CONECT  420  419
CONECT  421  415  419  422
CONECT  422  421  423
CONECT  423  414  422
CONECT  424  428  429
CONECT  425  413  426
CONECT  426  425  427  429
CONECT  427  426  428
CONECT  428  414  424  427
CONECT  429  424  426  430
CONECT  430  429  431
CONECT  431  430
CONECT  444  555
CONECT  554  561  562  564
CONECT  555  200  444  644  648
CONECT  556  188  582
CONECT  557  604  622
CONECT  558  349  689
CONECT  561  554
CONECT  562  554
CONECT  564  554
CONECT  582  556
CONECT  604  557
CONECT  622  557
CONECT  644  555
CONECT  648  555
CONECT  689  558
MASTER      375    0    7    0    0    0    9    6  624    2   86    2
END
```

File A-2: NMR solution structure of perimidinone-derived synthetic nucleoside paired with guanine in DNA duplex. (PDB code 2M11).

```
HEADER    DNA                                     09-NOV-12   2M11
TITLE     STRUCTURE OF PERIMIDINONE-DERIVED SYNTHETIC NUCLEOSIDE PAIRED WITH
TITLE    2 GUANINE IN DNA DUPLEX
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: DNA (5'-D(*CP*GP*CP*GP*AP*AP*TP*TP*(D3N)P*GP*CP*G)-3');
COMPND   3 CHAIN: A, B;
COMPND   4 ENGINEERED: YES
SOURCE    MOL_ID: 1;
SOURCE   2 SYNTHETIC: YES
KEYWDS    B-FORM DNA, DPER, PERIMIDINONE-DERIVED NUCLEOSIDE, DICKERSON-DREW
KEYWDS   2 DODECAMER, DNA
EXPDTA    SOLUTION NMR
AUTHOR    E.A.KOWAL,R.LAD,P.S.PALLAN,E.MUFFLY,Z.WAWRZAK,M.EGLI,S.J.STURLA,
AUTHOR   2 M.P.STONE
JRNL        AUTH   E.A.KOWAL,R.LAD,P.S.PALLAN,E.MUFFLY,Z.WAWRZAK,M.EGLI,
JRNL        AUTH 2 S.J.STURLA,M.P.STONE
JRNL        TITL   RECOGNITION OF O6-BENZYL-2'-DEOXYGUANOSINE BY A
JRNL        TITL 2 PERIMIDINONE-DERIVED SYNTHETIC NUCLEOSIDE: A UNIQUE
JRNL        TITL 3 INTERSTRAND STACKING INTERACTION
JRNL        REF    TO BE PUBLISHED
JRNL        REFN
REMARK   2
REMARK   2 RESOLUTION. NOT APPLICABLE.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : AMBER
REMARK   3   AUTHORS     : CASE, DARDEN, CHEATHAM, III, SIMMERLING, WANG,
REMARK   3                 DUKE, LUO, ... AND KOLLMAN
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: NULL
REMARK   4
REMARK   4 2M11 COMPLIES WITH FORMAT V. 3.30, 13-JUL-11
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 12-NOV-12.
REMARK 100 THE RCSB ID CODE IS RCSB103073.
REMARK 210
REMARK 210 EXPERIMENTAL DETAILS
REMARK 210  EXPERIMENT TYPE                : NMR
REMARK 210  TEMPERATURE           (KELVIN) : 283; 278
REMARK 210  PH                             : 7.0; 7.0
REMARK 210  IONIC STRENGTH                 : 100; 100
REMARK 210  PRESSURE                       : AMBIENT; AMBIENT
REMARK 210  SAMPLE CONTENTS                : 0.53 MM 5'-D(*CP*GP*CP*GP*AP*AP*
REMARK 210  TP*TP)[D3N]P-D(*GP*CP*GP)-3', 100 MM SODIUM CHLORIDE, 50 UM EDTA,
REMARK 210  10 MM SODIUM PHOSPHATE, 100% D2O; 0.53 MM 5'-D(*CP*GP*CP*GP*AP*
REMARK 210  AP*TP*TP)[D3N]P-D(*GP*CP*GP)-3', 10 MM SODIUM PHOSPHATE, 50 UM
REMARK 210  EDTA, 100 MM SODIUM CHLORIDE, 90% H2O/10% D2O
REMARK 210
REMARK 210  NMR EXPERIMENTS CONDUCTED      : 2D 1H-1H NOESY; 2D 1H-1H COSY
REMARK 210  SPECTROMETER FIELD STRENGTH    : 800 MHZ; 600 MHZ
REMARK 210  SPECTROMETER MODEL             : AVANCE
REMARK 210  SPECTROMETER MANUFACTURER      : BRUKER
REMARK 210
REMARK 210  STRUCTURE DETERMINATION.
REMARK 210   SOFTWARE USED                 : TOPSPIN, CORMA, CURVES 5.3,
REMARK 210                                   MARDIGRAS, SPARKY
REMARK 210   METHOD USED                   : SIMULATED ANNEALING
REMARK 210
REMARK 210 CONFORMERS, NUMBER CALCULATED   : 10
REMARK 210 CONFORMERS, NUMBER SUBMITTED    : 1
REMARK 210 CONFORMERS, SELECTION CRITERIA  : BACK CALCULATED DATA AGREE WITH
REMARK 210                                   EXPERIMENTAL NOESY SPECTRUM
REMARK 210
REMARK 210 BEST REPRESENTATIVE CONFORMER IN THIS ENSEMBLE : 1
REMARK 210
REMARK 210 REMARK: NULL
REMARK 215
REMARK 215 NMR STUDY
```

```
REMARK 215 THE COORDINATES IN THIS ENTRY WERE GENERATED FROM SOLUTION
REMARK 215 NMR DATA.  PROTEIN DATA BANK CONVENTIONS REQUIRE THAT
REMARK 215 CRYST1 AND SCALE RECORDS BE INCLUDED, BUT THE VALUES ON
REMARK 215 THESE RECORDS ARE MEANINGLESS.
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 SEE REMARK 350 FOR THE AUTHOR PROVIDED AND/OR PROGRAM
REMARK 300 GENERATED ASSEMBLY INFORMATION FOR THE STRUCTURE IN
REMARK 300 THIS ENTRY. THE REMARK MAY ALSO PROVIDE INFORMATION ON
REMARK 300 BURIED SURFACE AREA.
REMARK 350
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW.  BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: DIMERIC
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, B
REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT3   1  0.000000  0.000000  1.000000        0.00000
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,2(A3,1X,A1,I4,A1,1X,A4,3X),1X,F6.3)
REMARK 500
REMARK 500 EXPECTED VALUES PROTEIN: ENGH AND HUBER, 1999
REMARK 500 EXPECTED VALUES NUCLEIC ACID: CLOWNEY ET AL 1996
REMARK 500
REMARK 500  M RES CSSEQI ATM1   RES CSSEQI ATM2   DEVIATION
REMARK 500     DC A   1   O5'    DC A   1   C5'    -0.417
REMARK 500     DC A   1   C5'    DC A   1   C4'    -0.135
REMARK 500     DC A   1   C4'    DC A   1   C3'    -0.167
REMARK 500     DC A   1   C2'    DC A   1   C1'    -0.063
REMARK 500     DC A   1   O4'    DC A   1   C1'    -0.095
REMARK 500     DC A   1   O3'    DC A   1   C3'    -0.092
REMARK 500     DC A   1   N1     DC A   1   C6     -0.039
REMARK 500     DC A   1   N3     DC A   1   C4     -0.048
REMARK 500     DG A   2   P      DG A   2   OP1    -0.157
REMARK 500     DG A   2   P      DG A   2   OP2    -0.139
REMARK 500     DG A   2   O5'    DG A   2   C5'    -0.528
REMARK 500     DC A   1   O3'    DG A   2   P      -0.127
REMARK 500     DC B  13   O5'    DC B  13   C5'    -0.556
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,3(1X,A4,2X),12X,F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES PROTEIN: ENGH AND HUBER, 1999
REMARK 500 EXPECTED VALUES NUCLEIC ACID: CLOWNEY ET AL 1996
REMARK 500
REMARK 500  M RES CSSEQI ATM1   ATM2   ATM3
REMARK 500     DC A   1   O4' -  C1' -  N1  ANGL. DEV. =   5.0 DEGREES
REMARK 500     DC A   1   N3  -  C2  -  O2  ANGL. DEV. =  -5.2 DEGREES
REMARK 500     DG A   2   O5' -  C5' -  C4' ANGL. DEV. =  26.2 DEGREES
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REMARK 500      DG A   2   P    -  O5' -  C5' ANGL. DEV. =  22.5 DEGREES
REMARK 500      DC A   3   O4' -  C1' -  N1  ANGL. DEV. =   5.1 DEGREES
REMARK 500      DC A   3   N3  -  C2  -  O2  ANGL. DEV. =  -5.2 DEGREES
REMARK 500      DG A   4   O4' -  C1' -  N9  ANGL. DEV. =   1.9 DEGREES
REMARK 500      DA A   5   O4' -  C1' -  N9  ANGL. DEV. =   1.9 DEGREES
REMARK 500      DA A   5   C4  -  C5  -  C6  ANGL. DEV. =  -3.1 DEGREES
REMARK 500      DA A   5   C5  -  C6  -  N1  ANGL. DEV. =   3.5 DEGREES
REMARK 500      DA A   5   N1  -  C6  -  N6  ANGL. DEV. =  -4.7 DEGREES
REMARK 500      DA A   6   C5  -  C6  -  N1  ANGL. DEV. =   3.3 DEGREES
REMARK 500      DA A   6   N1  -  C6  -  N6  ANGL. DEV. =  -4.9 DEGREES
REMARK 500      DT A   7   O4' -  C1' -  N1  ANGL. DEV. =   2.1 DEGREES
REMARK 500      DT A   7   N3  -  C2  -  O2  ANGL. DEV. =  -3.9 DEGREES
REMARK 500      DT A   8   O4' -  C1' -  N1  ANGL. DEV. =   2.4 DEGREES
REMARK 500      DT A   8   N3  -  C2  -  O2  ANGL. DEV. =  -4.0 DEGREES
REMARK 500      DT A   8   C6  -  C5  -  C7  ANGL. DEV. =  -3.6 DEGREES
REMARK 500      DG A  10   O4' -  C1' -  N9  ANGL. DEV. =   2.9 DEGREES
REMARK 500      DC A  11   N1  -  C2  -  O2  ANGL. DEV. =   3.8 DEGREES
REMARK 500      DC A  11   N3  -  C2  -  O2  ANGL. DEV. =  -5.4 DEGREES
REMARK 500      DG A  12   O4' -  C1' -  N9  ANGL. DEV. =   3.6 DEGREES
REMARK 500      DC B  13   O4' -  C1' -  N1  ANGL. DEV. =   2.8 DEGREES
REMARK 500      DC B  13   N3  -  C2  -  O2  ANGL. DEV. =  -5.1 DEGREES
REMARK 500      DC B  15   O4' -  C1' -  N1  ANGL. DEV. =   4.9 DEGREES
REMARK 500      DC B  15   N1  -  C2  -  O2  ANGL. DEV. =   3.9 DEGREES
REMARK 500      DC B  15   N3  -  C2  -  O2  ANGL. DEV. =  -5.2 DEGREES
REMARK 500      DG B  16   O4' -  C1' -  N9  ANGL. DEV. =   1.9 DEGREES
REMARK 500      DA B  17   O4' -  C1' -  N9  ANGL. DEV. =   2.0 DEGREES
REMARK 500      DA B  17   C4  -  C5  -  C6  ANGL. DEV. =  -3.3 DEGREES
REMARK 500      DA B  17   C5  -  C6  -  N1  ANGL. DEV. =   3.3 DEGREES
REMARK 500      DA B  17   N1  -  C6  -  N6  ANGL. DEV. =  -4.6 DEGREES
REMARK 500      DA B  18   C4  -  C5  -  C6  ANGL. DEV. =  -3.2 DEGREES
REMARK 500      DA B  18   C5  -  C6  -  N1  ANGL. DEV. =   3.5 DEGREES
REMARK 500      DA B  18   N1  -  C6  -  N6  ANGL. DEV. =  -4.6 DEGREES
REMARK 500      DT B  19   O4' -  C1' -  N1  ANGL. DEV. =   2.4 DEGREES
REMARK 500      DT B  19   N3  -  C2  -  O2  ANGL. DEV. =  -4.1 DEGREES
REMARK 500      DT B  20   O4' -  C1' -  N1  ANGL. DEV. =   2.4 DEGREES
REMARK 500      DT B  20   N3  -  C2  -  O2  ANGL. DEV. =  -4.2 DEGREES
REMARK 500      DG B  22   O4' -  C1' -  N9  ANGL. DEV. =   2.5 DEGREES
REMARK 500      DC B  23   N3  -  C2  -  O2  ANGL. DEV. =  -5.1 DEGREES
REMARK 500      DG B  24   O4' -  C1' -  N9  ANGL. DEV. =   4.2 DEGREES
REMARK 500
REMARK 500 REMARK: NULL
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 18835   RELATED DB: BMRB
DBREF  2M11 A    1    12  PDB    2M11     2M11             1     12
DBREF  2M11 B   13    24  PDB    2M11     2M11            13     24
SEQRES   1 A   12   DC  DG  DC  DG  DA  DA  DT  DT D3N  DG  DC  DG
SEQRES   1 B   12   DC  DG  DC  DG  DA  DA  DT  DT D3N  DG  DC  DG
HET    D3N  A   9      39
HET    D3N  B  21      39
HETNAM     D3N 1-(2-DEOXY-5-O-PHOSPHONO-BETA-D-ERYTHRO-
HETNAM   2 D3N  PENTOFURANOSYL)-1H-PERIMIDIN-2(3H)-ONE
FORMUL   1  D3N    2(C16 H17 N2 O7 P)
LINK         O3'  DT A   8                 P   D3N A   9     1555   1555  1.62
LINK         O3'  DT B  20                 P   D3N B  21     1555   1555  1.62
CRYST1    1.000    1.000    1.000  90.00  90.00  90.00 P 1           1
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      1.000000  0.000000  0.000000        0.00000
SCALE2      0.000000  1.000000  0.000000        0.00000
SCALE3      0.000000  0.000000  1.000000        0.00000
ATOM      1  O5'  DC A   1       5.516 -17.607  25.163  1.00  0.00           O
ATOM      2  C5'  DC A   1       5.501 -16.607  25.196  1.00  0.00           C
ATOM      3  C4'  DC A   1       6.260 -16.093  24.173  1.00  0.00           C
ATOM      4  O4'  DC A   1       5.768 -16.411  22.900  1.00  0.00           O
ATOM      5  C3'  DC A   1       6.288 -14.740  24.228  1.00  0.00           C
ATOM      6  O3'  DC A   1       7.222 -14.282  25.052  1.00  0.00           O
ATOM      7  C2'  DC A   1       6.228 -14.296  22.786  1.00  0.00           C
ATOM      8  C1'  DC A   1       6.172 -15.523  22.006  1.00  0.00           C
ATOM      9  N1   DC A   1       5.330 -15.486  20.804  1.00  0.00           N
ATOM     10  C2   DC A   1       5.923 -15.484  19.550  1.00  0.00           C
ATOM     11  O2   DC A   1       7.119 -15.504  19.415  1.00  0.00           O
```

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ATOM     12  N3   DC A   1       5.188 -15.478  18.423  1.00  0.00           N
ATOM     13  C4   DC A   1       3.907 -15.433  18.533  1.00  0.00           C
ATOM     14  N4   DC A   1       3.241 -15.458  17.416  1.00  0.00           N
ATOM     15  C5   DC A   1       3.260 -15.422  19.776  1.00  0.00           C
ATOM     16  C6   DC A   1       4.006 -15.445  20.901  1.00  0.00           C
ATOM     17  H5'  DC A   1       5.738 -16.380  26.037  1.00  0.00           H
ATOM     18 H5''  DC A   1       4.688 -16.401  25.139  1.00  0.00           H
ATOM     19  H4'  DC A   1       7.145 -16.428  24.302  1.00  0.00           H
ATOM     20  H3'  DC A   1       5.460 -14.469  24.603  1.00  0.00           H
ATOM     21  H2'  DC A   1       5.366 -13.728  22.605  1.00  0.00           H
ATOM     22 H2''  DC A   1       7.050 -13.745  22.534  1.00  0.00           H
ATOM     23  H1'  DC A   1       7.100 -15.763  21.728  1.00  0.00           H
ATOM     24  H41  DC A   1       2.256 -15.422  17.430  1.00  0.00           H
ATOM     25  H42  DC A   1       3.749 -15.463  16.560  1.00  0.00           H
ATOM     26  H5   DC A   1       2.216 -15.394  19.854  1.00  0.00           H
ATOM     27  H6   DC A   1       3.564 -15.459  21.870  1.00  0.00           H
ATOM     28 HO5'  DC A   1       5.110 -18.014  25.137  1.00  0.00           H
ATOM     29  P    DG A   2       8.684 -14.442  24.883  1.00  0.00           P
ATOM     30  OP1  DG A   2       8.934 -15.712  24.585  1.00  0.00           O
ATOM     31  OP2  DG A   2       9.198 -13.975  26.036  1.00  0.00           O
ATOM     32  O5'  DG A   2       9.173 -13.528  23.669  1.00  0.00           O
ATOM     33  C5'  DG A   2       9.500 -12.726  23.465  1.00  0.00           C
ATOM     34  C4'  DG A   2       9.971 -12.008  22.233  1.00  0.00           C
ATOM     35  O4'  DG A   2       9.197 -12.394  21.129  1.00  0.00           O
ATOM     36  C3'  DG A   2       9.892 -10.478  22.341  1.00  0.00           C
ATOM     37  O3'  DG A   2      11.190  -9.958  22.085  1.00  0.00           O
ATOM     38  C2'  DG A   2       8.850 -10.094  21.287  1.00  0.00           C
ATOM     39  C1'  DG A   2       8.874 -11.276  20.340  1.00  0.00           C
ATOM     40  N9   DG A   2       7.606 -11.540  19.620  1.00  0.00           N
ATOM     41  C8   DG A   2       6.353 -11.747  20.135  1.00  0.00           C
ATOM     42  N7   DG A   2       5.453 -12.073  19.242  1.00  0.00           N
ATOM     43  C5   DG A   2       6.152 -12.024  18.030  1.00  0.00           C
ATOM     44  C6   DG A   2       5.734 -12.249  16.672  1.00  0.00           C
ATOM     45  O6   DG A   2       4.644 -12.607  16.229  1.00  0.00           O
ATOM     46  N1   DG A   2       6.739 -12.031  15.749  1.00  0.00           N
ATOM     47  C2   DG A   2       8.007 -11.684  16.080  1.00  0.00           C
ATOM     48  N2   DG A   2       8.857 -11.494  15.110  1.00  0.00           N
ATOM     49  N3   DG A   2       8.447 -11.503  17.320  1.00  0.00           N
ATOM     50  C4   DG A   2       7.468 -11.675  18.256  1.00  0.00           C
ATOM     51  H5'  DG A   2       9.811 -12.880  23.973  1.00  0.00           H
ATOM     52 H5''  DG A   2       9.134 -12.467  23.689  1.00  0.00           H
ATOM     53  H4'  DG A   2      10.988 -12.280  22.060  1.00  0.00           H
ATOM     54  H3'  DG A   2       9.549 -10.180  23.329  1.00  0.00           H
ATOM     55  H2'  DG A   2       7.874  -9.966  21.747  1.00  0.00           H
ATOM     56 H2''  DG A   2       9.099  -9.184  20.748  1.00  0.00           H
ATOM     57  H1'  DG A   2       9.659 -11.099  19.614  1.00  0.00           H
ATOM     58  H8   DG A   2       6.153 -11.672  21.191  1.00  0.00           H
ATOM     59  H1   DG A   2       6.498 -12.138  14.776  1.00  0.00           H
ATOM     60  H21  DG A   2       9.796 -11.227  15.360  1.00  0.00           H
ATOM     61  H22  DG A   2       8.564 -11.577  14.149  1.00  0.00           H
ATOM     62  P    DC A   3      11.568  -8.405  22.259  1.00  0.00           P
ATOM     63  OP1  DC A   3      13.039  -8.307  22.390  1.00  0.00           O
ATOM     64  OP2  DC A   3      10.715  -7.819  23.316  1.00  0.00           O
ATOM     65  O5'  DC A   3      11.144  -7.777  20.842  1.00  0.00           O
ATOM     66  C5'  DC A   3      11.802  -8.148  19.642  1.00  0.00           C
ATOM     67  C4'  DC A   3      11.060  -7.666  18.387  1.00  0.00           C
ATOM     68  O4'  DC A   3       9.865  -8.424  18.203  1.00  0.00           O
ATOM     69  C3'  DC A   3      10.657  -6.185  18.472  1.00  0.00           C
ATOM     70  O3'  DC A   3      10.990  -5.541  17.247  1.00  0.00           O
ATOM     71  C2'  DC A   3       9.154  -6.291  18.662  1.00  0.00           C
ATOM     72  C1'  DC A   3       8.855  -7.520  17.814  1.00  0.00           C
ATOM     73  N1   DC A   3       7.483  -8.065  17.975  1.00  0.00           N
ATOM     74  C2   DC A   3       6.793  -8.451  16.824  1.00  0.00           C
ATOM     75  O2   DC A   3       7.304  -8.414  15.707  1.00  0.00           O
ATOM     76  N3   DC A   3       5.516  -8.889  16.893  1.00  0.00           N
ATOM     77  C4   DC A   3       4.931  -8.911  18.072  1.00  0.00           C
ATOM     78  N4   DC A   3       3.699  -9.331  18.083  1.00  0.00           N
ATOM     79  C5   DC A   3       5.580  -8.552  19.277  1.00  0.00           C
ATOM     80  C6   DC A   3       6.863  -8.136  19.195  1.00  0.00           C
ATOM     81  H5'  DC A   3      11.886  -9.231  19.591  1.00  0.00           H
ATOM     82 H5''  DC A   3      12.806  -7.730  19.640  1.00  0.00           H
ATOM     83  H4'  DC A   3      11.711  -7.803  17.527  1.00  0.00           H
ATOM     84  H3'  DC A   3      11.126  -5.690  19.320  1.00  0.00           H
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ATOM     85  H2'  DC A   3       8.959  -6.472  19.716  1.00  0.00           H
ATOM     86 H2''  DC A   3       8.602  -5.419  18.320  1.00  0.00           H
ATOM     87  H1'  DC A   3       9.019  -7.249  16.773  1.00  0.00           H
ATOM     88  H41  DC A   3       3.220  -9.403  18.966  1.00  0.00           H
ATOM     89  H42  DC A   3       3.280  -9.619  17.213  1.00  0.00           H
ATOM     90  H5   DC A   3       5.092  -8.608  20.236  1.00  0.00           H
ATOM     91  H6   DC A   3       7.401  -7.865  20.090  1.00  0.00           H
ATOM     92  P    DG A   4      11.040  -3.942  17.073  1.00  0.00           P
ATOM     93  OP1  DG A   4      12.451  -3.543  16.950  1.00  0.00           O
ATOM     94  OP2  DG A   4      10.207  -3.303  18.112  1.00  0.00           O
ATOM     95  O5'  DG A   4      10.301  -3.725  15.663  1.00  0.00           O
ATOM     96  C5'  DG A   4      10.902  -4.143  14.457  1.00  0.00           C
ATOM     97  C4'  DG A   4      10.035  -3.892  13.220  1.00  0.00           C
ATOM     98  O4'  DG A   4       8.916  -4.768  13.228  1.00  0.00           O
ATOM     99  C3'  DG A   4       9.512  -2.452  13.117  1.00  0.00           C
ATOM    100  O3'  DG A   4       9.569  -2.023  11.760  1.00  0.00           O
ATOM    101  C2'  DG A   4       8.083  -2.590  13.640  1.00  0.00           C
ATOM    102  C1'  DG A   4       7.721  -4.000  13.172  1.00  0.00           C
ATOM    103  N9   DG A   4       6.671  -4.624  14.011  1.00  0.00           N
ATOM    104  C8   DG A   4       6.659  -4.796  15.374  1.00  0.00           C
ATOM    105  N7   DG A   4       5.578  -5.359  15.837  1.00  0.00           N
ATOM    106  C5   DG A   4       4.797  -5.560  14.682  1.00  0.00           C
ATOM    107  C6   DG A   4       3.477  -6.102  14.493  1.00  0.00           C
ATOM    108  O6   DG A   4       2.697  -6.573  15.317  1.00  0.00           O
ATOM    109  N1   DG A   4       3.050  -6.084  13.181  1.00  0.00           N
ATOM    110  C2   DG A   4       3.800  -5.632  12.148  1.00  0.00           C
ATOM    111  N2   DG A   4       3.259  -5.692  10.960  1.00  0.00           N
ATOM    112  N3   DG A   4       5.025  -5.129  12.265  1.00  0.00           N
ATOM    113  C4   DG A   4       5.469  -5.115  13.558  1.00  0.00           C
ATOM    114  H5'  DG A   4      11.121  -5.206  14.518  1.00  0.00           H
ATOM    115 H5''  DG A   4      11.839  -3.617  14.315  1.00  0.00           H
ATOM    116  H4'  DG A   4      10.635  -4.101  12.339  1.00  0.00           H
ATOM    117  H3'  DG A   4      10.093  -1.789  13.752  1.00  0.00           H
ATOM    118  H2'  DG A   4       8.097  -2.520  14.725  1.00  0.00           H
ATOM    119 H2''  DG A   4       7.400  -1.851  13.229  1.00  0.00           H
ATOM    120  H1'  DG A   4       7.379  -3.937  12.142  1.00  0.00           H
ATOM    121  H8   DG A   4       7.484  -4.475  15.991  1.00  0.00           H
ATOM    122  H1   DG A   4       2.112  -6.401  12.987  1.00  0.00           H
ATOM    123  H21  DG A   4       3.800  -5.350  10.180  1.00  0.00           H
ATOM    124  H22  DG A   4       2.342  -6.090  10.827  1.00  0.00           H
ATOM    125  P    DA A   5       9.197  -0.536  11.283  1.00  0.00           P
ATOM    126  OP1  DA A   5       9.864  -0.296   9.980  1.00  0.00           O
ATOM    127  OP2  DA A   5       9.461   0.406  12.401  1.00  0.00           O
ATOM    128  O5'  DA A   5       7.609  -0.594  11.024  1.00  0.00           O
ATOM    129  C5'  DA A   5       7.056  -1.345   9.950  1.00  0.00           C
ATOM    130  C4'  DA A   5       5.524  -1.354   9.950  1.00  0.00           C
ATOM    131  O4'  DA A   5       5.009  -2.130  11.018  1.00  0.00           O
ATOM    132  C3'  DA A   5       4.887   0.043  10.023  1.00  0.00           C
ATOM    133  O3'  DA A   5       4.232   0.350   8.806  1.00  0.00           O
ATOM    134  C2'  DA A   5       3.930  -0.082  11.212  1.00  0.00           C
ATOM    135  C1'  DA A   5       3.756  -1.581  11.376  1.00  0.00           C
ATOM    136  N9   DA A   5       3.401  -1.974  12.755  1.00  0.00           N
ATOM    137  C8   DA A   5       4.149  -1.842  13.898  1.00  0.00           C
ATOM    138  N7   DA A   5       3.593  -2.336  14.973  1.00  0.00           N
ATOM    139  C5   DA A   5       2.362  -2.812  14.491  1.00  0.00           C
ATOM    140  C6   DA A   5       1.251  -3.473  15.069  1.00  0.00           C
ATOM    141  N6   DA A   5       1.160  -3.828  16.332  1.00  0.00           N
ATOM    142  N1   DA A   5       0.187  -3.795  14.342  1.00  0.00           N
ATOM    143  C2   DA A   5       0.203  -3.508  13.045  1.00  0.00           C
ATOM    144  N3   DA A   5       1.171  -2.914  12.357  1.00  0.00           N
ATOM    145  C4   DA A   5       2.231  -2.578  13.146  1.00  0.00           C
ATOM    146  H5'  DA A   5       7.412  -2.372  10.009  1.00  0.00           H
ATOM    147 H5''  DA A   5       7.394  -0.928   9.004  1.00  0.00           H
ATOM    148  H4'  DA A   5       5.208  -1.821   9.018  1.00  0.00           H
ATOM    149  H3'  DA A   5       5.643   0.794  10.227  1.00  0.00           H
ATOM    150  H2'  DA A   5       4.391   0.332  12.101  1.00  0.00           H
ATOM    151 H2''  DA A   5       2.973   0.390  11.019  1.00  0.00           H
ATOM    152  H1'  DA A   5       2.986  -1.908  10.683  1.00  0.00           H
ATOM    153  H8   DA A   5       5.125  -1.382  13.892  1.00  0.00           H
ATOM    154  H61  DA A   5       0.357  -4.360  16.632  1.00  0.00           H
ATOM    155  H62  DA A   5       1.928  -3.634  16.955  1.00  0.00           H
ATOM    156  H2   DA A   5      -0.677  -3.795  12.492  1.00  0.00           H
ATOM    157  P    DA A   6       3.580   1.795   8.496  1.00  0.00           P
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ATOM    158  OP1  DA A   6       3.605   2.012   7.037  1.00  0.00           O
ATOM    159  OP2  DA A   6       4.213   2.803   9.367  1.00  0.00           O
ATOM    160  O5'  DA A   6       2.054   1.616   8.956  1.00  0.00           O
ATOM    161  C5'  DA A   6       1.178   0.758   8.244  1.00  0.00           C
ATOM    162  C4'  DA A   6      -0.220   0.684   8.865  1.00  0.00           C
ATOM    163  O4'  DA A   6      -0.185   0.015  10.113  1.00  0.00           O
ATOM    164  C3'  DA A   6      -0.866   2.063   9.074  1.00  0.00           C
ATOM    165  O3'  DA A   6      -2.097   2.093   8.363  1.00  0.00           O
ATOM    166  C2'  DA A   6      -1.011   2.145  10.590  1.00  0.00           C
ATOM    167  C1'  DA A   6      -1.049   0.681  11.017  1.00  0.00           C
ATOM    168  N9   DA A   6      -0.565   0.454  12.397  1.00  0.00           N
ATOM    169  C8   DA A   6       0.648   0.808  12.927  1.00  0.00           C
ATOM    170  N7   DA A   6       0.819   0.445  14.174  1.00  0.00           N
ATOM    171  C5   DA A   6      -0.394  -0.187  14.485  1.00  0.00           C
ATOM    172  C6   DA A   6      -0.924  -0.811  15.641  1.00  0.00           C
ATOM    173  N6   DA A   6      -0.304  -0.921  16.799  1.00  0.00           N
ATOM    174  N1   DA A   6      -2.142  -1.342  15.634  1.00  0.00           N
ATOM    175  C2   DA A   6      -2.846  -1.274  14.513  1.00  0.00           C
ATOM    176  N3   DA A   6      -2.498  -0.715  13.362  1.00  0.00           N
ATOM    177  C4   DA A   6      -1.237  -0.195  13.409  1.00  0.00           C
ATOM    178  H5'  DA A   6       1.595  -0.246   8.227  1.00  0.00           H
ATOM    179 H5''  DA A   6       1.072   1.105   7.221  1.00  0.00           H
ATOM    180  H4'  DA A   6      -0.841   0.102   8.192  1.00  0.00           H
ATOM    181  H3'  DA A   6      -0.205   2.851   8.719  1.00  0.00           H
ATOM    182  H2'  DA A   6      -0.135   2.645  10.998  1.00  0.00           H
ATOM    183 H2''  DA A   6      -1.909   2.680  10.897  1.00  0.00           H
ATOM    184  H1'  DA A   6      -2.067   0.310  10.908  1.00  0.00           H
ATOM    185  H8   DA A   6       1.398   1.337  12.359  1.00  0.00           H
ATOM    186  H61  DA A   6      -0.743  -1.447  17.539  1.00  0.00           H
ATOM    187  H62  DA A   6       0.617  -0.527  16.906  1.00  0.00           H
ATOM    188  H2   DA A   6      -3.838  -1.697  14.543  1.00  0.00           H
ATOM    189  P    DT A   7      -3.046   3.392   8.284  1.00  0.00           P
ATOM    190  OP1  DT A   7      -3.837   3.317   7.032  1.00  0.00           O
ATOM    191  OP2  DT A   7      -2.236   4.601   8.549  1.00  0.00           O
ATOM    192  O5'  DT A   7      -4.035   3.167   9.529  1.00  0.00           O
ATOM    193  C5'  DT A   7      -4.933   2.061   9.543  1.00  0.00           C
ATOM    194  C4'  DT A   7      -5.674   1.941  10.878  1.00  0.00           C
ATOM    195  O4'  DT A   7      -4.771   1.620  11.923  1.00  0.00           O
ATOM    196  C3'  DT A   7      -6.442   3.207  11.293  1.00  0.00           C
ATOM    197  O3'  DT A   7      -7.841   2.936  11.297  1.00  0.00           O
ATOM    198  C2'  DT A   7      -5.863   3.520  12.680  1.00  0.00           C
ATOM    199  C1'  DT A   7      -5.284   2.176  13.121  1.00  0.00           C
ATOM    200  N1   DT A   7      -4.212   2.285  14.143  1.00  0.00           N
ATOM    201  C2   DT A   7      -4.429   1.668  15.378  1.00  0.00           C
ATOM    202  O2   DT A   7      -5.454   1.078  15.710  1.00  0.00           O
ATOM    203  N3   DT A   7      -3.402   1.754  16.286  1.00  0.00           N
ATOM    204  C4   DT A   7      -2.195   2.381  16.093  1.00  0.00           C
ATOM    205  O4   DT A   7      -1.355   2.327  16.989  1.00  0.00           O
ATOM    206  C5   DT A   7      -2.046   3.041  14.796  1.00  0.00           C
ATOM    207  C7   DT A   7      -0.776   3.806  14.472  1.00  0.00           C
ATOM    208  C6   DT A   7      -3.047   2.970  13.879  1.00  0.00           C
ATOM    209  H5'  DT A   7      -4.389   1.133   9.374  1.00  0.00           H
ATOM    210 H5''  DT A   7      -5.661   2.174   8.743  1.00  0.00           H
ATOM    211  H4'  DT A   7      -6.386   1.125  10.775  1.00  0.00           H
ATOM    212  H3'  DT A   7      -6.198   4.018  10.609  1.00  0.00           H
ATOM    213  H2'  DT A   7      -5.083   4.273  12.577  1.00  0.00           H
ATOM    214 H2''  DT A   7      -6.623   3.881  13.373  1.00  0.00           H
ATOM    215  H1'  DT A   7      -6.100   1.549  13.480  1.00  0.00           H
ATOM    216  H3   DT A   7      -3.546   1.295  17.172  1.00  0.00           H
ATOM    217  H71  DT A   7      -0.457   3.967  14.256  1.00  0.00           H
ATOM    218  H72  DT A   7      -0.525   4.109  14.466  1.00  0.00           H
ATOM    219  H73  DT A   7      -0.383   3.898  14.503  1.00  0.00           H
ATOM    220  H6   DT A   7      -2.946   3.439  12.915  1.00  0.00           H
ATOM    221  P    DT A   8      -8.966   4.063  11.575  1.00  0.00           P
ATOM    222  OP1  DT A   8     -10.224   3.618  10.925  1.00  0.00           O
ATOM    223  OP2  DT A   8      -8.415   5.394  11.222  1.00  0.00           O
ATOM    224  O5'  DT A   8      -9.173   4.016  13.169  1.00  0.00           O
ATOM    225  C5'  DT A   8      -9.690   2.847  13.792  1.00  0.00           C
ATOM    226  C4'  DT A   8      -9.608   2.909  15.315  1.00  0.00           C
ATOM    227  O4'  DT A   8      -8.255   2.910  15.736  1.00  0.00           O
ATOM    228  C3'  DT A   8     -10.301   4.144  15.928  1.00  0.00           C
ATOM    229  O3'  DT A   8     -11.328   3.708  16.815  1.00  0.00           O
ATOM    230  C2'  DT A   8      -9.141   4.840  16.642  1.00  0.00           C
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ATOM    231  C1'  DT A   8      -8.184   3.679  16.915  1.00  0.00           C
ATOM    232  N1   DT A   8      -6.779   4.083  17.195  1.00  0.00           N
ATOM    233  C2   DT A   8      -6.182   3.564  18.353  1.00  0.00           C
ATOM    234  O2   DT A   8      -6.712   2.785  19.140  1.00  0.00           O
ATOM    235  N3   DT A   8      -4.888   3.956  18.597  1.00  0.00           N
ATOM    236  C4   DT A   8      -4.123   4.780  17.802  1.00  0.00           C
ATOM    237  O4   DT A   8      -2.964   5.025  18.147  1.00  0.00           O
ATOM    238  C5   DT A   8      -4.791   5.262  16.593  1.00  0.00           C
ATOM    239  C7   DT A   8      -4.052   6.148  15.606  1.00  0.00           C
ATOM    240  C6   DT A   8      -6.082   4.914  16.338  1.00  0.00           C
ATOM    241  H5'  DT A   8      -9.121   1.983  13.452  1.00  0.00           H
ATOM    242 H5''  DT A   8     -10.729   2.710  13.498  1.00  0.00           H
ATOM    243  H4'  DT A   8     -10.091   2.014  15.703  1.00  0.00           H
ATOM    244  H3'  DT A   8     -10.709   4.776  15.142  1.00  0.00           H
ATOM    245  H2'  DT A   8      -8.683   5.577  15.984  1.00  0.00           H
ATOM    246 H2''  DT A   8      -9.437   5.330  17.568  1.00  0.00           H
ATOM    247  H1'  DT A   8      -8.579   3.099  17.747  1.00  0.00           H
ATOM    248  H3   DT A   8      -4.474   3.621  19.454  1.00  0.00           H
ATOM    249  H71  DT A   8      -3.993   6.310  15.227  1.00  0.00           H
ATOM    250  H72  DT A   8      -3.900   6.521  15.490  1.00  0.00           H
ATOM    251  H73  DT A   8      -3.684   6.265  15.407  1.00  0.00           H
ATOM    252  H6   DT A   8      -6.570   5.262  15.440  1.00  0.00           H
HETATM  253  O1P D3N A   9     -12.542   5.914  16.713  1.00  0.00           O
HETATM  254  P   D3N A   9     -12.332   4.723  17.571  1.00  0.00           P
HETATM  255  O2P D3N A   9     -13.514   3.948  18.014  1.00  0.00           O
HETATM  256  O5' D3N A   9     -11.504   5.179  18.886  1.00  0.00           O
HETATM  257  C5' D3N A   9     -11.033   4.226  19.833  1.00  0.00           C
HETATM  258  C4' D3N A   9      -9.976   4.790  20.783  1.00  0.00           C
HETATM  259  O4' D3N A   9      -8.767   5.122  20.116  1.00  0.00           O
HETATM  260  C3' D3N A   9     -10.399   6.048  21.545  1.00  0.00           C
HETATM  261  O3' D3N A   9     -11.094   5.706  22.739  1.00  0.00           O
HETATM  262  C2' D3N A   9      -9.050   6.732  21.800  1.00  0.00           C
HETATM  263  C1' D3N A   9      -8.033   5.849  21.068  1.00  0.00           C
HETATM  264  N1   D3N A   9      -6.895   6.608  20.483  1.00  0.00           N
HETATM  265  C2   D3N A   9      -5.710   6.467  21.171  1.00  0.00           C
HETATM  266  O2   D3N A   9      -5.609   5.989  22.292  1.00  0.00           O
HETATM  267  N3   D3N A   9      -4.586   6.925  20.559  1.00  0.00           N
HETATM  268  C4   D3N A   9      -4.596   7.704  19.434  1.00  0.00           C
HETATM  269  C5   D3N A   9      -5.822   8.007  18.833  1.00  0.00           C
HETATM  270  C6   D3N A   9      -7.001   7.427  19.354  1.00  0.00           C
HETATM  271  C7   D3N A   9      -8.231   7.777  18.747  1.00  0.00           C
HETATM  272  C8   D3N A   9      -8.268   8.749  17.733  1.00  0.00           C
HETATM  273  C9   D3N A   9      -7.085   9.259  17.195  1.00  0.00           C
HETATM  274  C10  D3N A   9      -5.854   8.897  17.746  1.00  0.00           C
HETATM  275  C11  D3N A   9      -4.668   9.489  17.278  1.00  0.00           C
HETATM  276  C12  D3N A   9      -3.448   9.179  17.899  1.00  0.00           C
HETATM  277  C13  D3N A   9      -3.399   8.258  18.950  1.00  0.00           C
HETATM  278  H3   D3N A   9     -10.602   3.367  19.321  1.00  0.00           H
HETATM  279  H4   D3N A   9     -11.871   3.869  20.428  1.00  0.00           H
HETATM  280  H5   D3N A   9      -9.750   4.016  21.515  1.00  0.00           H
HETATM  281  H6   D3N A   9     -11.007   6.678  20.899  1.00  0.00           H
HETATM  282  H8   D3N A   9      -8.810   6.752  22.862  1.00  0.00           H
HETATM  283  H9   D3N A   9      -9.068   7.739  21.386  1.00  0.00           H
HETATM  284  H10  D3N A   9      -7.665   5.127  21.796  1.00  0.00           H
HETATM  285  H11  D3N A   9      -3.725   6.788  21.065  1.00  0.00           H
HETATM  286  H12  D3N A   9      -9.144   7.263  18.997  1.00  0.00           H
HETATM  287  H13  D3N A   9      -9.212   9.084  17.334  1.00  0.00           H
HETATM  288  H14  D3N A   9      -7.133   9.974  16.390  1.00  0.00           H
HETATM  289  H15  D3N A   9      -4.690  10.158  16.437  1.00  0.00           H
HETATM  290  H16  D3N A   9      -2.536   9.623  17.533  1.00  0.00           H
HETATM  291  H17  D3N A   9      -2.452   7.968  19.374  1.00  0.00           H
ATOM    292  P    DG A  10     -11.748   6.831  23.675  1.00  0.00           P
ATOM    293  OP1  DG A  10     -12.720   6.166  24.573  1.00  0.00           O
ATOM    294  OP2  DG A  10     -12.209   7.955  22.825  1.00  0.00           O
ATOM    295  O5'  DG A  10     -10.507   7.346  24.560  1.00  0.00           O
ATOM    296  C5'  DG A  10      -9.882   6.496  25.516  1.00  0.00           C
ATOM    297  C4'  DG A  10      -8.703   7.172  26.222  1.00  0.00           C
ATOM    298  O4'  DG A  10      -7.602   7.314  25.326  1.00  0.00           O
ATOM    299  C3'  DG A  10      -9.040   8.559  26.790  1.00  0.00           C
ATOM    300  O3'  DG A  10      -8.597   8.633  28.141  1.00  0.00           O
ATOM    301  C2'  DG A  10      -8.272   9.472  25.841  1.00  0.00           C
ATOM    302  C1'  DG A  10      -7.062   8.614  25.498  1.00  0.00           C
ATOM    303  N9   DG A  10      -6.334   9.057  24.285  1.00  0.00           N
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ATOM    304  C8   DG A  10      -6.828   9.400  23.055  1.00  0.00           C
ATOM    305  N7   DG A  10      -5.913   9.746  22.185  1.00  0.00           N
ATOM    306  C5   DG A  10      -4.718   9.638  22.909  1.00  0.00           C
ATOM    307  C6   DG A  10      -3.345   9.878  22.545  1.00  0.00           C
ATOM    308  O6   DG A  10      -2.879  10.213  21.460  1.00  0.00           O
ATOM    309  N1   DG A  10      -2.458   9.709  23.586  1.00  0.00           N
ATOM    310  C2   DG A  10      -2.829   9.350  24.831  1.00  0.00           C
ATOM    311  N2   DG A  10      -1.883   9.195  25.716  1.00  0.00           N
ATOM    312  N3   DG A  10      -4.072   9.080  25.211  1.00  0.00           N
ATOM    313  C4   DG A  10      -4.975   9.243  24.203  1.00  0.00           C
ATOM    314  H5'  DG A  10      -9.523   5.588  25.037  1.00  0.00           H
ATOM    315 H5''  DG A  10     -10.613   6.233  26.277  1.00  0.00           H
ATOM    316  H4'  DG A  10      -8.400   6.523  27.040  1.00  0.00           H
ATOM    317  H3'  DG A  10     -10.108   8.754  26.728  1.00  0.00           H
ATOM    318  H2'  DG A  10      -8.881   9.669  24.962  1.00  0.00           H
ATOM    319 H2''  DG A  10      -7.972  10.405  26.314  1.00  0.00           H
ATOM    320  H1'  DG A  10      -6.379   8.627  26.344  1.00  0.00           H
ATOM    321  H8   DG A  10      -7.883   9.380  22.837  1.00  0.00           H
ATOM    322  H1   DG A  10      -1.478   9.832  23.380  1.00  0.00           H
ATOM    323  H21  DG A  10      -2.145   8.897  26.640  1.00  0.00           H
ATOM    324  H22  DG A  10      -0.924   9.388  25.474  1.00  0.00           H
ATOM    325  P    DC A  11      -8.889   9.896  29.099  1.00  0.00           P
ATOM    326  OP1  DC A  11      -9.395   9.382  30.392  1.00  0.00           O
ATOM    327  OP2  DC A  11      -9.695  10.895  28.362  1.00  0.00           O
ATOM    328  O5'  DC A  11      -7.419  10.504  29.323  1.00  0.00           O
ATOM    329  C5'  DC A  11      -6.436   9.795  30.064  1.00  0.00           C
ATOM    330  C4'  DC A  11      -5.100  10.536  30.172  1.00  0.00           C
ATOM    331  O4'  DC A  11      -4.491  10.610  28.892  1.00  0.00           O
ATOM    332  C3'  DC A  11      -5.229  11.958  30.739  1.00  0.00           C
ATOM    333  O3'  DC A  11      -4.228  12.156  31.725  1.00  0.00           O
ATOM    334  C2'  DC A  11      -5.028  12.813  29.496  1.00  0.00           C
ATOM    335  C1'  DC A  11      -4.102  11.945  28.648  1.00  0.00           C
ATOM    336  N1   DC A  11      -4.210  12.226  27.196  1.00  0.00           N
ATOM    337  C2   DC A  11      -3.041  12.494  26.482  1.00  0.00           C
ATOM    338  O2   DC A  11      -1.931  12.531  27.014  1.00  0.00           O
ATOM    339  N3   DC A  11      -3.083  12.744  25.156  1.00  0.00           N
ATOM    340  C4   DC A  11      -4.253  12.744  24.560  1.00  0.00           C
ATOM    341  N4   DC A  11      -4.234  12.958  23.283  1.00  0.00           N
ATOM    342  C5   DC A  11      -5.476  12.471  25.222  1.00  0.00           C
ATOM    343  C6   DC A  11      -5.415  12.208  26.547  1.00  0.00           C
ATOM    344  H5'  DC A  11      -6.270   8.834  29.590  1.00  0.00           H
ATOM    345 H5''  DC A  11      -6.804   9.617  31.066  1.00  0.00           H
ATOM    346  H4'  DC A  11      -4.450   9.959  30.826  1.00  0.00           H
ATOM    347  H3'  DC A  11      -6.219  12.119  31.159  1.00  0.00           H
ATOM    348  H2'  DC A  11      -5.993  12.968  29.018  1.00  0.00           H
ATOM    349 H2''  DC A  11      -4.568  13.779  29.699  1.00  0.00           H
ATOM    350  H1'  DC A  11      -3.084  12.097  29.001  1.00  0.00           H
ATOM    351  H41  DC A  11      -5.090  12.940  22.752  1.00  0.00           H
ATOM    352  H42  DC A  11      -3.334  13.103  22.852  1.00  0.00           H
ATOM    353  H5   DC A  11      -6.430  12.458  24.720  1.00  0.00           H
ATOM    354  H6   DC A  11      -6.306  11.980  27.109  1.00  0.00           H
ATOM    355  P    DG A  12      -4.158  13.483  32.630  1.00  0.00           P
ATOM    356  OP1  DG A  12      -3.466  13.145  33.895  1.00  0.00           O
ATOM    357  OP2  DG A  12      -5.514  14.081  32.701  1.00  0.00           O
ATOM    358  O5'  DG A  12      -3.212  14.466  31.786  1.00  0.00           O
ATOM    359  C5'  DG A  12      -1.823  14.200  31.640  1.00  0.00           C
ATOM    360  C4'  DG A  12      -1.132  15.180  30.681  1.00  0.00           C
ATOM    361  O4'  DG A  12      -1.520  14.911  29.345  1.00  0.00           O
ATOM    362  C3'  DG A  12      -1.453  16.656  30.969  1.00  0.00           C
ATOM    363  O3'  DG A  12      -0.265  17.434  31.100  1.00  0.00           O
ATOM    364  C2'  DG A  12      -2.207  17.083  29.718  1.00  0.00           C
ATOM    365  C1'  DG A  12      -1.598  16.150  28.686  1.00  0.00           C
ATOM    366  N9   DG A  12      -2.354  16.053  27.418  1.00  0.00           N
ATOM    367  C8   DG A  12      -3.704  15.929  27.218  1.00  0.00           C
ATOM    368  N7   DG A  12      -4.070  15.935  25.961  1.00  0.00           N
ATOM    369  C5   DG A  12      -2.857  16.075  25.268  1.00  0.00           C
ATOM    370  C6   DG A  12      -2.558  16.165  23.863  1.00  0.00           C
ATOM    371  O6   DG A  12      -3.313  16.142  22.889  1.00  0.00           O
ATOM    372  N1   DG A  12      -1.216  16.330  23.602  1.00  0.00           N
ATOM    373  C2   DG A  12      -0.260  16.396  24.556  1.00  0.00           C
ATOM    374  N2   DG A  12       0.971  16.578  24.160  1.00  0.00           N
ATOM    375  N3   DG A  12      -0.486  16.319  25.861  1.00  0.00           N
ATOM    376  C4   DG A  12      -1.808  16.151  26.159  1.00  0.00           C
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ATOM    377  H5'  DG A  12      -1.671  13.193  31.264  1.00  0.00           H
ATOM    378 H5''  DG A  12      -1.336  14.269  32.608  1.00  0.00           H
ATOM    379  H4'  DG A  12      -0.056  15.041  30.755  1.00  0.00           H
ATOM    380  H3'  DG A  12      -2.088  16.769  31.843  1.00  0.00           H
ATOM    381 HO3'  DG A  12      -0.218  17.856  31.635  1.00  0.00           H
ATOM    382  H2'  DG A  12      -3.267  16.872  29.842  1.00  0.00           H
ATOM    383 H2''  DG A  12      -2.041  18.127  29.467  1.00  0.00           H
ATOM    384  H1'  DG A  12      -0.594  16.501  28.457  1.00  0.00           H
ATOM    385  H8   DG A  12      -4.396  15.832  28.038  1.00  0.00           H
ATOM    386  H1   DG A  12      -0.943  16.408  22.636  1.00  0.00           H
ATOM    387  H21  DG A  12       1.687  16.633  24.866  1.00  0.00           H
ATOM    388  H22  DG A  12       1.189  16.705  23.185  1.00  0.00           H
TER     389       DG A  12
ATOM    390  O5'  DC B  13       3.611  18.919  15.413  1.00  0.00           O
ATOM    391  C5'  DC B  13       4.048  18.258  15.752  1.00  0.00           C
ATOM    392  C4'  DC B  13       3.964  17.818  17.215  1.00  0.00           C
ATOM    393  O4'  DC B  13       2.633  17.851  17.694  1.00  0.00           O
ATOM    394  C3'  DC B  13       4.441  16.384  17.436  1.00  0.00           C
ATOM    395  O3'  DC B  13       5.827  16.370  17.757  1.00  0.00           O
ATOM    396  C2'  DC B  13       3.554  15.894  18.577  1.00  0.00           C
ATOM    397  C1'  DC B  13       2.596  17.052  18.855  1.00  0.00           C
ATOM    398  N1   DC B  13       1.216  16.582  19.138  1.00  0.00           N
ATOM    399  C2   DC B  13       0.767  16.618  20.455  1.00  0.00           C
ATOM    400  O2   DC B  13       1.486  16.980  21.384  1.00  0.00           O
ATOM    401  N3   DC B  13      -0.499  16.258  20.767  1.00  0.00           N
ATOM    402  C4   DC B  13      -1.273  15.819  19.801  1.00  0.00           C
ATOM    403  N4   DC B  13      -2.495  15.519  20.142  1.00  0.00           N
ATOM    404  C5   DC B  13      -0.868  15.734  18.444  1.00  0.00           C
ATOM    405  C6   DC B  13       0.390  16.124  18.145  1.00  0.00           C
ATOM    406  H5'  DC B  13       4.613  18.469  15.439  1.00  0.00           H
ATOM    407 H5''  DC B  13       3.910  17.859  15.259  1.00  0.00           H
ATOM    408  H4'  DC B  13       4.583  18.482  17.811  1.00  0.00           H
ATOM    409  H3'  DC B  13       4.246  15.803  16.541  1.00  0.00           H
ATOM    410  H2'  DC B  13       3.018  15.005  18.249  1.00  0.00           H
ATOM    411 H2''  DC B  13       4.129  15.667  19.472  1.00  0.00           H
ATOM    412  H1'  DC B  13       2.974  17.636  19.688  1.00  0.00           H
ATOM    413  H41  DC B  13      -3.135  15.184  19.439  1.00  0.00           H
ATOM    414  H42  DC B  13      -2.763  15.602  21.108  1.00  0.00           H
ATOM    415  H5   DC B  13      -1.520  15.388  17.661  1.00  0.00           H
ATOM    416  H6   DC B  13       0.744  16.104  17.128  1.00  0.00           H
ATOM    417 HO5'  DC B  13       3.347  19.157  15.184  1.00  0.00           H
ATOM    418  P    DG B  14       6.685  15.019  17.835  1.00  0.00           P
ATOM    419  OP1  DG B  14       8.120  15.388  17.757  1.00  0.00           O
ATOM    420  OP2  DG B  14       6.140  14.052  16.857  1.00  0.00           O
ATOM    421  O5'  DG B  14       6.382  14.455  19.306  1.00  0.00           O
ATOM    422  C5'  DG B  14       6.834  15.134  20.465  1.00  0.00           C
ATOM    423  C4'  DG B  14       6.381  14.461  21.760  1.00  0.00           C
ATOM    424  O4'  DG B  14       4.977  14.590  21.933  1.00  0.00           O
ATOM    425  C3'  DG B  14       6.736  12.975  21.838  1.00  0.00           C
ATOM    426  O3'  DG B  14       7.548  12.766  22.990  1.00  0.00           O
ATOM    427  C2'  DG B  14       5.371  12.287  21.907  1.00  0.00           C
ATOM    428  C1'  DG B  14       4.458  13.378  22.441  1.00  0.00           C
ATOM    429  N9   DG B  14       3.043  13.242  22.022  1.00  0.00           N
ATOM    430  C8   DG B  14       2.530  13.207  20.757  1.00  0.00           C
ATOM    431  N7   DG B  14       1.220  13.190  20.699  1.00  0.00           N
ATOM    432  C5   DG B  14       0.846  13.173  22.049  1.00  0.00           C
ATOM    433  C6   DG B  14      -0.444  13.126  22.689  1.00  0.00           C
ATOM    434  O6   DG B  14      -1.569  13.142  22.191  1.00  0.00           O
ATOM    435  N1   DG B  14      -0.371  13.057  24.063  1.00  0.00           N
ATOM    436  C2   DG B  14       0.789  13.076  24.763  1.00  0.00           C
ATOM    437  N2   DG B  14       0.709  12.988  26.063  1.00  0.00           N
ATOM    438  N3   DG B  14       1.997  13.154  24.222  1.00  0.00           N
ATOM    439  C4   DG B  14       1.963  13.188  22.856  1.00  0.00           C
ATOM    440  H5'  DG B  14       6.461  16.154  20.465  1.00  0.00           H
ATOM    441 H5''  DG B  14       7.919  15.176  20.456  1.00  0.00           H
ATOM    442  H4'  DG B  14       6.864  14.976  22.586  1.00  0.00           H
ATOM    443  H3'  DG B  14       7.255  12.666  20.935  1.00  0.00           H
ATOM    444  H2'  DG B  14       5.068  11.963  20.916  1.00  0.00           H
ATOM    445 H2''  DG B  14       5.372  11.429  22.571  1.00  0.00           H
ATOM    446  H1'  DG B  14       4.521  13.361  23.525  1.00  0.00           H
ATOM    447  H8   DG B  14       3.168  13.219  19.892  1.00  0.00           H
ATOM    448  H1   DG B  14      -1.237  12.966  24.568  1.00  0.00           H
ATOM    449  H21  DG B  14       1.564  12.994  26.595  1.00  0.00           H
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ATOM    450  H22  DG B  14      -0.191  12.878  26.504  1.00  0.00           H
ATOM    451  P    DC B  15       8.271  11.372  23.317  1.00  0.00           P
ATOM    452  OP1  DC B  15       9.370  11.648  24.269  1.00  0.00           O
ATOM    453  OP2  DC B  15       8.588  10.688  22.042  1.00  0.00           O
ATOM    454  O5'  DC B  15       7.141  10.524  24.074  1.00  0.00           O
ATOM    455  C5'  DC B  15       6.651  10.933  25.340  1.00  0.00           C
ATOM    456  C4'  DC B  15       5.381  10.167  25.738  1.00  0.00           C
ATOM    457  O4'  DC B  15       4.281  10.613  24.946  1.00  0.00           O
ATOM    458  C3'  DC B  15       5.514   8.645  25.552  1.00  0.00           C
ATOM    459  O3'  DC B  15       5.043   7.993  26.721  1.00  0.00           O
ATOM    460  C2'  DC B  15       4.604   8.415  24.355  1.00  0.00           C
ATOM    461  C1'  DC B  15       3.530   9.463  24.608  1.00  0.00           C
ATOM    462  N1   DC B  15       2.602   9.683  23.473  1.00  0.00           N
ATOM    463  C2   DC B  15       1.233   9.752  23.749  1.00  0.00           C
ATOM    464  O2   DC B  15       0.783   9.729  24.891  1.00  0.00           O
ATOM    465  N3   DC B  15       0.334   9.858  22.742  1.00  0.00           N
ATOM    466  C4   DC B  15       0.767   9.868  21.506  1.00  0.00           C
ATOM    467  N4   DC B  15      -0.145   9.950  20.586  1.00  0.00           N
ATOM    468  C5   DC B  15       2.143   9.816  21.164  1.00  0.00           C
ATOM    469  C6   DC B  15       3.033   9.728  22.177  1.00  0.00           C
ATOM    470  H5'  DC B  15       6.412  11.991  25.320  1.00  0.00           H
ATOM    471 H5''  DC B  15       7.414  10.768  26.095  1.00  0.00           H
ATOM    472  H4'  DC B  15       5.172  10.383  26.782  1.00  0.00           H
ATOM    473  H3'  DC B  15       6.541   8.368  25.325  1.00  0.00           H
ATOM    474  H2'  DC B  15       5.170   8.623  23.452  1.00  0.00           H
ATOM    475 H2''  DC B  15       4.187   7.413  24.299  1.00  0.00           H
ATOM    476  H1'  DC B  15       2.967   9.147  25.483  1.00  0.00           H
ATOM    477  H41  DC B  15       0.120  10.023  19.624  1.00  0.00           H
ATOM    478  H42  DC B  15      -1.105  10.029  20.877  1.00  0.00           H
ATOM    479  H5   DC B  15       2.490   9.862  20.147  1.00  0.00           H
ATOM    480  H6   DC B  15       4.092   9.700  21.975  1.00  0.00           H
ATOM    481  P    DG B  16       5.315   6.434  27.030  1.00  0.00           P
ATOM    482  OP1  DG B  16       6.252   6.336  28.158  1.00  0.00           O
ATOM    483  OP2  DG B  16       5.647   5.731  25.775  1.00  0.00           O
ATOM    484  O5'  DG B  16       3.874   5.920  27.501  1.00  0.00           O
ATOM    485  C5'  DG B  16       3.320   6.340  28.731  1.00  0.00           C
ATOM    486  C4'  DG B  16       1.919   5.768  28.992  1.00  0.00           C
ATOM    487  O4'  DG B  16       0.986   6.352  28.097  1.00  0.00           O
ATOM    488  C3'  DG B  16       1.844   4.237  28.840  1.00  0.00           C
ATOM    489  O3'  DG B  16       1.033   3.693  29.875  1.00  0.00           O
ATOM    490  C2'  DG B  16       1.228   4.098  27.454  1.00  0.00           C
ATOM    491  C1'  DG B  16       0.318   5.323  27.388  1.00  0.00           C
ATOM    492  N9   DG B  16       0.065   5.744  25.997  1.00  0.00           N
ATOM    493  C8   DG B  16       0.986   6.065  25.032  1.00  0.00           C
ATOM    494  N7   DG B  16       0.465   6.380  23.878  1.00  0.00           N
ATOM    495  C5   DG B  16      -0.912   6.244  24.097  1.00  0.00           C
ATOM    496  C6   DG B  16      -2.042   6.421  23.220  1.00  0.00           C
ATOM    497  O6   DG B  16      -2.082   6.765  22.042  1.00  0.00           O
ATOM    498  N1   DG B  16      -3.248   6.134  23.818  1.00  0.00           N
ATOM    499  C2   DG B  16      -3.391   5.774  25.110  1.00  0.00           C
ATOM    500  N2   DG B  16      -4.608   5.560  25.532  1.00  0.00           N
ATOM    501  N3   DG B  16      -2.387   5.615  25.962  1.00  0.00           N
ATOM    502  C4   DG B  16      -1.163   5.852  25.392  1.00  0.00           C
ATOM    503  H5'  DG B  16       3.265   7.426  28.755  1.00  0.00           H
ATOM    504 H5''  DG B  16       3.967   6.009  29.534  1.00  0.00           H
ATOM    505  H4'  DG B  16       1.655   6.016  30.011  1.00  0.00           H
ATOM    506  H3'  DG B  16       2.841   3.800  28.865  1.00  0.00           H
ATOM    507  H2'  DG B  16       2.012   4.153  26.702  1.00  0.00           H
ATOM    508 H2''  DG B  16       0.664   3.176  27.323  1.00  0.00           H
ATOM    509  H1'  DG B  16      -0.622   5.075  27.877  1.00  0.00           H
ATOM    510  H8   DG B  16       2.045   6.035  25.234  1.00  0.00           H
ATOM    511  H1   DG B  16      -4.076   6.169  23.241  1.00  0.00           H
ATOM    512  H21  DG B  16      -4.722   5.293  26.497  1.00  0.00           H
ATOM    513  H22  DG B  16      -5.398   5.679  24.921  1.00  0.00           H
ATOM    514  P    DA B  17       0.856   2.102  30.095  1.00  0.00           P
ATOM    515  OP1  DA B  17       0.415   1.876  31.492  1.00  0.00           O
ATOM    516  OP2  DA B  17       2.070   1.412  29.602  1.00  0.00           O
ATOM    517  O5'  DA B  17      -0.366   1.717  29.124  1.00  0.00           O
ATOM    518  C5'  DA B  17      -1.687   2.177  29.398  1.00  0.00           C
ATOM    519  C4'  DA B  17      -2.681   1.828  28.283  1.00  0.00           C
ATOM    520  O4'  DA B  17      -2.421   2.562  27.096  1.00  0.00           O
ATOM    521  C3'  DA B  17      -2.711   0.335  27.918  1.00  0.00           C
ATOM    522  O3'  DA B  17      -3.935  -0.243  28.364  1.00  0.00           O
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ATOM    523  C2'  DA B  17      -2.564   0.354  26.395  1.00  0.00           C
ATOM    524  C1'  DA B  17      -2.887   1.787  26.011  1.00  0.00           C
ATOM    525  N9   DA B  17      -2.243   2.225  24.753  1.00  0.00           N
ATOM    526  C8   DA B  17      -0.902   2.394  24.496  1.00  0.00           C
ATOM    527  N7   DA B  17      -0.636   2.858  23.301  1.00  0.00           N
ATOM    528  C5   DA B  17      -1.909   2.971  22.720  1.00  0.00           C
ATOM    529  C6   DA B  17      -2.401   3.408  21.466  1.00  0.00           C
ATOM    530  N6   DA B  17      -1.656   3.875  20.481  1.00  0.00           N
ATOM    531  N1   DA B  17      -3.703   3.384  21.194  1.00  0.00           N
ATOM    532  C2   DA B  17      -4.542   2.959  22.127  1.00  0.00           C
ATOM    533  N3   DA B  17      -4.232   2.534  23.354  1.00  0.00           N
ATOM    534  C4   DA B  17      -2.892   2.570  23.590  1.00  0.00           C
ATOM    535  H5'  DA B  17      -1.673   3.259  29.526  1.00  0.00           H
ATOM    536 H5''  DA B  17      -2.045   1.736  30.327  1.00  0.00           H
ATOM    537  H4'  DA B  17      -3.673   2.111  28.631  1.00  0.00           H
ATOM    538  H3'  DA B  17      -1.865  -0.181  28.368  1.00  0.00           H
ATOM    539  H2'  DA B  17      -1.541   0.113  26.115  1.00  0.00           H
ATOM    540 H2''  DA B  17      -3.251  -0.336  25.909  1.00  0.00           H
ATOM    541  H1'  DA B  17      -3.970   1.867  25.924  1.00  0.00           H
ATOM    542  H8   DA B  17      -0.146   2.198  25.240  1.00  0.00           H
ATOM    543  H61  DA B  17      -2.114   4.220  19.651  1.00  0.00           H
ATOM    544  H62  DA B  17      -0.656   3.951  20.593  1.00  0.00           H
ATOM    545  H2   DA B  17      -5.590   2.972  21.871  1.00  0.00           H
ATOM    546  P    DA B  18      -4.229  -1.824  28.290  1.00  0.00           P
ATOM    547  OP1  DA B  18      -5.186  -2.162  29.370  1.00  0.00           O
ATOM    548  OP2  DA B  18      -2.941  -2.556  28.234  1.00  0.00           O
ATOM    549  O5'  DA B  18      -4.971  -2.005  26.876  1.00  0.00           O
ATOM    550  C5'  DA B  18      -6.264  -1.451  26.648  1.00  0.00           C
ATOM    551  C4'  DA B  18      -6.759  -1.670  25.218  1.00  0.00           C
ATOM    552  O4'  DA B  18      -6.018  -0.886  24.299  1.00  0.00           O
ATOM    553  C3'  DA B  18      -6.690  -3.135  24.762  1.00  0.00           C
ATOM    554  O3'  DA B  18      -8.003  -3.545  24.388  1.00  0.00           O
ATOM    555  C2'  DA B  18      -5.692  -3.090  23.601  1.00  0.00           C
ATOM    556  C1'  DA B  18      -5.784  -1.643  23.122  1.00  0.00           C
ATOM    557  N9   DA B  18      -4.542  -1.147  22.481  1.00  0.00           N
ATOM    558  C8   DA B  18      -3.265  -1.136  22.984  1.00  0.00           C
ATOM    559  N7   DA B  18      -2.367  -0.606  22.193  1.00  0.00           N
ATOM    560  C5   DA B  18      -3.128  -0.251  21.068  1.00  0.00           C
ATOM    561  C6   DA B  18      -2.841   0.348  19.820  1.00  0.00           C
ATOM    562  N6   DA B  18      -1.643   0.747  19.433  1.00  0.00           N
ATOM    563  N1   DA B  18      -3.799   0.554  18.915  1.00  0.00           N
ATOM    564  C2   DA B  18      -5.033   0.177  19.214  1.00  0.00           C
ATOM    565  N3   DA B  18      -5.455  -0.401  20.331  1.00  0.00           N
ATOM    566  C4   DA B  18      -4.449  -0.578  21.235  1.00  0.00           C
ATOM    567  H5'  DA B  18      -6.245  -0.382  26.853  1.00  0.00           H
ATOM    568 H5''  DA B  18      -6.973  -1.915  27.331  1.00  0.00           H
ATOM    569  H4'  DA B  18      -7.798  -1.347  25.178  1.00  0.00           H
ATOM    570  H3'  DA B  18      -6.311  -3.769  25.563  1.00  0.00           H
ATOM    571  H2'  DA B  18      -4.698  -3.299  23.993  1.00  0.00           H
ATOM    572 H2''  DA B  18      -5.932  -3.786  22.798  1.00  0.00           H
ATOM    573  H1'  DA B  18      -6.624  -1.561  22.434  1.00  0.00           H
ATOM    574  H8   DA B  18      -3.039  -1.536  23.960  1.00  0.00           H
ATOM    575  H61  DA B  18      -1.535   1.197  18.536  1.00  0.00           H
ATOM    576  H62  DA B  18      -0.862   0.629  20.060  1.00  0.00           H
ATOM    577  H2   DA B  18      -5.776   0.355  18.453  1.00  0.00           H
ATOM    578  P    DT B  19      -8.354  -5.053  23.923  1.00  0.00           P
ATOM    579  OP1  DT B  19      -9.773  -5.320  24.256  1.00  0.00           O
ATOM    580  OP2  DT B  19      -7.315  -5.975  24.432  1.00  0.00           O
ATOM    581  O5'  DT B  19      -8.214  -4.960  22.328  1.00  0.00           O
ATOM    582  C5'  DT B  19      -9.076  -4.124  21.568  1.00  0.00           C
ATOM    583  C4'  DT B  19      -8.662  -4.049  20.095  1.00  0.00           C
ATOM    584  O4'  DT B  19      -7.418  -3.384  19.955  1.00  0.00           O
ATOM    585  C3'  DT B  19      -8.553  -5.427  19.414  1.00  0.00           C
ATOM    586  O3'  DT B  19      -9.551  -5.532  18.406  1.00  0.00           O
ATOM    587  C2'  DT B  19      -7.125  -5.415  18.869  1.00  0.00           C
ATOM    588  C1'  DT B  19      -6.780  -3.924  18.819  1.00  0.00           C
ATOM    589  N1   DT B  19      -5.316  -3.657  18.861  1.00  0.00           N
ATOM    590  C2   DT B  19      -4.751  -2.964  17.789  1.00  0.00           C
ATOM    591  O2   DT B  19      -5.356  -2.602  16.782  1.00  0.00           O
ATOM    592  N3   DT B  19      -3.398  -2.695  17.871  1.00  0.00           N
ATOM    593  C4   DT B  19      -2.576  -3.023  18.920  1.00  0.00           C
ATOM    594  O4   DT B  19      -1.402  -2.668  18.882  1.00  0.00           O
ATOM    595  C5   DT B  19      -3.230  -3.771  20.001  1.00  0.00           C
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ATOM    596  C7   DT B  19      -2.420  -4.232  21.206  1.00  0.00           C
ATOM    597  C6   DT B  19      -4.556  -4.055  19.940  1.00  0.00           C
ATOM    598  H5'  DT B  19      -9.071  -3.115  21.974  1.00  0.00           H
ATOM    599 H5''  DT B  19     -10.091  -4.511  21.621  1.00  0.00           H
ATOM    600  H4'  DT B  19      -9.415  -3.464  19.570  1.00  0.00           H
ATOM    601  H3'  DT B  19      -8.655  -6.226  20.145  1.00  0.00           H
ATOM    602  H2'  DT B  19      -6.477  -5.953  19.560  1.00  0.00           H
ATOM    603 H2''  DT B  19      -7.048  -5.870  17.883  1.00  0.00           H
ATOM    604  H1'  DT B  19      -7.218  -3.490  17.922  1.00  0.00           H
ATOM    605  H3   DT B  19      -2.984  -2.198  17.096  1.00  0.00           H
ATOM    606  H71  DT B  19      -2.066  -4.182  21.475  1.00  0.00           H
ATOM    607  H72  DT B  19      -2.373  -4.331  21.627  1.00  0.00           H
ATOM    608  H73  DT B  19      -2.161  -4.525  21.380  1.00  0.00           H
ATOM    609  H6   DT B  19      -5.040  -4.593  20.741  1.00  0.00           H
ATOM    610  P    DT B  20      -9.808  -6.872  17.553  1.00  0.00           P
ATOM    611  OP1  DT B  20     -11.219  -6.860  17.097  1.00  0.00           O
ATOM    612  OP2  DT B  20      -9.308  -8.032  18.328  1.00  0.00           O
ATOM    613  O5'  DT B  20      -8.856  -6.681  16.268  1.00  0.00           O
ATOM    614  C5'  DT B  20      -9.090  -5.629  15.333  1.00  0.00           C
ATOM    615  C4'  DT B  20      -7.972  -5.502  14.294  1.00  0.00           C
ATOM    616  O4'  DT B  20      -6.760  -5.085  14.919  1.00  0.00           O
ATOM    617  C3'  DT B  20      -7.686  -6.800  13.515  1.00  0.00           C
ATOM    618  O3'  DT B  20      -7.856  -6.546  12.126  1.00  0.00           O
ATOM    619  C2'  DT B  20      -6.238  -7.105  13.905  1.00  0.00           C
ATOM    620  C1'  DT B  20      -5.691  -5.717  14.238  1.00  0.00           C
ATOM    621  N1   DT B  20      -4.462  -5.716  15.074  1.00  0.00           N
ATOM    622  C2   DT B  20      -3.390  -4.931  14.630  1.00  0.00           C
ATOM    623  O2   DT B  20      -3.382  -4.232  13.620  1.00  0.00           O
ATOM    624  N3   DT B  20      -2.267  -4.938  15.420  1.00  0.00           N
ATOM    625  C4   DT B  20      -2.119  -5.605  16.609  1.00  0.00           C
ATOM    626  O4   DT B  20      -1.057  -5.484  17.216  1.00  0.00           O
ATOM    627  C5   DT B  20      -3.278  -6.381  17.033  1.00  0.00           C
ATOM    628  C7   DT B  20      -3.238  -7.156  18.335  1.00  0.00           C
ATOM    629  C6   DT B  20      -4.397  -6.418  16.261  1.00  0.00           C
ATOM    630  H5'  DT B  20      -9.165  -4.686  15.871  1.00  0.00           H
ATOM    631 H5''  DT B  20     -10.026  -5.811  14.808  1.00  0.00           H
ATOM    632  H4'  DT B  20      -8.266  -4.729  13.586  1.00  0.00           H
ATOM    633  H3'  DT B  20      -8.343  -7.601  13.850  1.00  0.00           H
ATOM    634  H2'  DT B  20      -6.237  -7.762  14.773  1.00  0.00           H
ATOM    635 H2''  DT B  20      -5.669  -7.572  13.103  1.00  0.00           H
ATOM    636  H1'  DT B  20      -5.499  -5.203  13.297  1.00  0.00           H
ATOM    637  H3   DT B  20      -1.471  -4.417  15.083  1.00  0.00           H
ATOM    638  H71  DT B  20      -3.111  -7.223  18.738  1.00  0.00           H
ATOM    639  H72  DT B  20      -3.396  -7.332  18.667  1.00  0.00           H
ATOM    640  H73  DT B  20      -3.133  -7.482  18.576  1.00  0.00           H
ATOM    641  H6   DT B  20      -5.250  -6.997  16.579  1.00  0.00           H
HETATM  642  O1P D3N B  21      -8.163  -8.990  11.593  1.00  0.00           O
HETATM  643  P   D3N B  21      -7.730  -7.699  11.000  1.00  0.00           P
HETATM  644  O2P D3N B  21      -8.397  -7.210   9.771  1.00  0.00           O
HETATM  645  O5' D3N B  21      -6.143  -7.785  10.704  1.00  0.00           O
HETATM  646  C5' D3N B  21      -5.412  -6.665  10.230  1.00  0.00           C
HETATM  647  C4' D3N B  21      -3.894  -6.811  10.374  1.00  0.00           C
HETATM  648  O4' D3N B  21      -3.481  -6.888  11.732  1.00  0.00           O
HETATM  649  C3' D3N B  21      -3.298  -8.041   9.685  1.00  0.00           C
HETATM  650  O3' D3N B  21      -3.023  -7.777   8.321  1.00  0.00           O
HETATM  651  C2' D3N B  21      -2.050  -8.300  10.530  1.00  0.00           C
HETATM  652  C1' D3N B  21      -2.133  -7.283  11.663  1.00  0.00           C
HETATM  653  N1   D3N B  21      -1.620  -7.790  12.965  1.00  0.00           N
HETATM  654  C2   D3N B  21      -0.377  -7.300  13.310  1.00  0.00           C
HETATM  655  O2   D3N B  21       0.364  -6.701  12.545  1.00  0.00           O
HETATM  656  N3   D3N B  21       0.039  -7.515  14.588  1.00  0.00           N
HETATM  657  C4   D3N B  21      -0.572  -8.387  15.451  1.00  0.00           C
HETATM  658  C5   D3N B  21      -1.724  -9.062  15.017  1.00  0.00           C
HETATM  659  C6   D3N B  21      -2.276  -8.745  13.757  1.00  0.00           C
HETATM  660  C7   D3N B  21      -3.414  -9.464  13.334  1.00  0.00           C
HETATM  661  C8   D3N B  21      -3.903 -10.529  14.107  1.00  0.00           C
HETATM  662  C9   D3N B  21      -3.370 -10.814  15.361  1.00  0.00           C
HETATM  663  C10  D3N B  21      -2.290 -10.057  15.835  1.00  0.00           C
HETATM  664  C11  D3N B  21      -1.694 -10.389  17.060  1.00  0.00           C
HETATM  665  C12  D3N B  21      -0.547  -9.712  17.480  1.00  0.00           C
HETATM  666  C13  D3N B  21      -0.008  -8.680  16.704  1.00  0.00           C
HETATM  667  H3   D3N B  21      -5.697  -5.775  10.789  1.00  0.00           H
HETATM  668  H4   D3N B  21      -5.651  -6.497   9.183  1.00  0.00           H
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HETATM  669  H5  D3N B  21      -3.436  -5.934   9.920  1.00  0.00           H
HETATM  670  H6  D3N B  21      -3.990  -8.872   9.791  1.00  0.00           H
HETATM  671  H8  D3N B  21      -1.135  -8.128   9.968  1.00  0.00           H
HETATM  672  H9  D3N B  21      -2.074  -9.321  10.904  1.00  0.00           H
HETATM  673  H10 D3N B  21      -1.565  -6.406  11.357  1.00  0.00           H
HETATM  674  H11 D3N B  21       0.923  -7.093  14.836  1.00  0.00           H
HETATM  675  H12 D3N B  21      -3.995  -9.130  12.491  1.00  0.00           H
HETATM  676  H13 D3N B  21      -4.707 -11.140  13.728  1.00  0.00           H
HETATM  677  H14 D3N B  21      -3.756 -11.632  15.947  1.00  0.00           H
HETATM  678  H15 D3N B  21      -2.132 -11.154  17.680  1.00  0.00           H
HETATM  679  H16 D3N B  21      -0.088  -9.976  18.420  1.00  0.00           H
HETATM  680  H17 D3N B  21       0.867  -8.155  17.054  1.00  0.00           H
ATOM    681  P    DG B  22      -2.504  -8.926   7.332  1.00  0.00           P
ATOM    682  OP1  DG B  22      -2.666  -8.452   5.937  1.00  0.00           O
ATOM    683  OP2  DG B  22      -3.137 -10.206   7.722  1.00  0.00           O
ATOM    684  O5'  DG B  22      -0.935  -9.027   7.659  1.00  0.00           O
ATOM    685  C5'  DG B  22      -0.040  -7.983   7.316  1.00  0.00           C
ATOM    686  C4'  DG B  22       1.399  -8.267   7.766  1.00  0.00           C
ATOM    687  O4'  DG B  22       1.510  -8.213   9.182  1.00  0.00           O
ATOM    688  C3'  DG B  22       1.907  -9.640   7.288  1.00  0.00           C
ATOM    689  O3'  DG B  22       3.173  -9.481   6.664  1.00  0.00           O
ATOM    690  C2'  DG B  22       1.965 -10.420   8.600  1.00  0.00           C
ATOM    691  C1'  DG B  22       2.305  -9.314   9.590  1.00  0.00           C
ATOM    692  N9   DG B  22       2.030  -9.667  10.998  1.00  0.00           N
ATOM    693  C8   DG B  22       0.906 -10.231  11.551  1.00  0.00           C
ATOM    694  N7   DG B  22       0.974 -10.424  12.837  1.00  0.00           N
ATOM    695  C5   DG B  22       2.253  -9.955  13.175  1.00  0.00           C
ATOM    696  C6   DG B  22       2.947  -9.885  14.434  1.00  0.00           C
ATOM    697  O6   DG B  22       2.560 -10.204  15.560  1.00  0.00           O
ATOM    698  N1   DG B  22       4.236  -9.382  14.323  1.00  0.00           N
ATOM    699  C2   DG B  22       4.796  -8.995  13.156  1.00  0.00           C
ATOM    700  N2   DG B  22       6.017  -8.554  13.192  1.00  0.00           N
ATOM    701  N3   DG B  22       4.188  -9.020  11.977  1.00  0.00           N
ATOM    702  C4   DG B  22       2.910  -9.509  12.047  1.00  0.00           C
ATOM    703  H5'  DG B  22      -0.368  -7.047   7.759  1.00  0.00           H
ATOM    704 H5'' DG B  22      -0.033  -7.858   6.237  1.00  0.00           H
ATOM    705  H4'  DG B  22       2.035  -7.503   7.326  1.00  0.00           H
ATOM    706  H3'  DG B  22       1.198 -10.101   6.603  1.00  0.00           H
ATOM    707  H2'  DG B  22       0.989 -10.849   8.817  1.00  0.00           H
ATOM    708 H2'' DG B  22       2.722 -11.202   8.585  1.00  0.00           H
ATOM    709  H1'  DG B  22       3.360  -9.065   9.485  1.00  0.00           H
ATOM    710  H8   DG B  22       0.043 -10.491  10.960  1.00  0.00           H
ATOM    711  H1   DG B  22       4.754  -9.272  15.181  1.00  0.00           H
ATOM    712  H21  DG B  22       6.442  -8.261  12.327  1.00  0.00           H
ATOM    713  H22  DG B  22       6.531  -8.515  14.060  1.00  0.00           H
ATOM    714  P    DC B  23       3.965 -10.682   5.929  1.00  0.00           P
ATOM    715  OP1  DC B  23       4.414 -10.190   4.607  1.00  0.00           O
ATOM    716  OP2  DC B  23       3.149 -11.917   5.999  1.00  0.00           O
ATOM    717  O5'  DC B  23       5.259 -10.879   6.862  1.00  0.00           O
ATOM    718  C5'  DC B  23       6.271  -9.875   6.923  1.00  0.00           C
ATOM    719  C4'  DC B  23       7.425 -10.234   7.872  1.00  0.00           C
ATOM    720  O4'  DC B  23       6.957 -10.278   9.216  1.00  0.00           O
ATOM    721  C3'  DC B  23       8.087 -11.590   7.555  1.00  0.00           C
ATOM    722  O3'  DC B  23       9.502 -11.449   7.586  1.00  0.00           O
ATOM    723  C2'  DC B  23       7.539 -12.488   8.655  1.00  0.00           C
ATOM    724  C1'  DC B  23       7.328 -11.505   9.805  1.00  0.00           C
ATOM    725  N1   DC B  23       6.276 -11.934  10.767  1.00  0.00           N
ATOM    726  C2   DC B  23       6.585 -11.953  12.124  1.00  0.00           C
ATOM    727  O2   DC B  23       7.697 -11.648  12.549  1.00  0.00           O
ATOM    728  N3   DC B  23       5.658 -12.318  13.045  1.00  0.00           N
ATOM    729  C4   DC B  23       4.461 -12.674  12.619  1.00  0.00           C
ATOM    730  N4   DC B  23       3.602 -12.979  13.543  1.00  0.00           N
ATOM    731  C5   DC B  23       4.084 -12.670  11.249  1.00  0.00           C
ATOM    732  C6   DC B  23       5.020 -12.295  10.344  1.00  0.00           C
ATOM    733  H5'  DC B  23       5.824  -8.946   7.269  1.00  0.00           H
ATOM    734 H5'' DC B  23       6.684  -9.712   5.931  1.00  0.00           H
ATOM    735  H4'  DC B  23       8.175  -9.451   7.790  1.00  0.00           H
ATOM    736  H3'  DC B  23       7.755 -11.951   6.584  1.00  0.00           H
ATOM    737  H2'  DC B  23       6.600 -12.919   8.313  1.00  0.00           H
ATOM    738 H2'' DC B  23       8.209 -13.295   8.948  1.00  0.00           H
ATOM    739  H1'  DC B  23       8.282 -11.376  10.313  1.00  0.00           H
ATOM    740  H41  DC B  23       2.670 -13.273  13.296  1.00  0.00           H
ATOM    741  H42  DC B  23       3.911 -12.937  14.503  1.00  0.00           H
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ATOM    742  H5   DC B  23       3.096 -12.940  10.912  1.00  0.00           H
ATOM    743  H6   DC B  23       4.782 -12.248   9.294  1.00  0.00           H
ATOM    744  P    DG B  24      10.511 -12.622   7.147  1.00  0.00           P
ATOM    745  OP1  DG B  24      11.806 -12.014   6.755  1.00  0.00           O
ATOM    746  OP2  DG B  24       9.827 -13.506   6.177  1.00  0.00           O
ATOM    747  O5'  DG B  24      10.728 -13.443   8.502  1.00  0.00           O
ATOM    748  C5'  DG B  24      11.474 -12.893   9.571  1.00  0.00           C
ATOM    749  C4'  DG B  24      11.445 -13.773  10.818  1.00  0.00           C
ATOM    750  O4'  DG B  24      10.176 -13.695  11.454  1.00  0.00           O
ATOM    751  C3'  DG B  24      11.726 -15.258  10.544  1.00  0.00           C
ATOM    752  O3'  DG B  24      12.773 -15.757  11.358  1.00  0.00           O
ATOM    753  C2'  DG B  24      10.412 -15.925  10.931  1.00  0.00           C
ATOM    754  C1'  DG B  24       9.912 -14.966  12.000  1.00  0.00           C
ATOM    755  N9   DG B  24       8.489 -15.143  12.363  1.00  0.00           N
ATOM    756  C8   DG B  24       7.402 -15.380  11.560  1.00  0.00           C
ATOM    757  N7   DG B  24       6.288 -15.580  12.205  1.00  0.00           N
ATOM    758  C5   DG B  24       6.667 -15.470  13.557  1.00  0.00           C
ATOM    759  C6   DG B  24       5.915 -15.603  14.776  1.00  0.00           C
ATOM    760  O6   DG B  24       4.720 -15.836  14.948  1.00  0.00           O
ATOM    761  N1   DG B  24       6.688 -15.460  15.906  1.00  0.00           N
ATOM    762  C2   DG B  24       8.017 -15.208  15.892  1.00  0.00           C
ATOM    763  N2   DG B  24       8.621 -15.090  17.039  1.00  0.00           N
ATOM    764  N3   DG B  24       8.750 -15.071  14.797  1.00  0.00           N
ATOM    765  C4   DG B  24       8.018 -15.217  13.652  1.00  0.00           C
ATOM    766  H5'  DG B  24      11.076 -11.919   9.831  1.00  0.00           H
ATOM    767 H5''  DG B  24      12.508 -12.765   9.261  1.00  0.00           H
ATOM    768  H4'  DG B  24      12.199 -13.404  11.503  1.00  0.00           H
ATOM    769  H3'  DG B  24      11.949 -15.434   9.497  1.00  0.00           H
ATOM    770 HO3'  DG B  24      13.255 -16.130  11.060  1.00  0.00           H
ATOM    771  H2'  DG B  24       9.746 -15.932  10.076  1.00  0.00           H
ATOM    772 H2''  DG B  24      10.563 -16.927  11.320  1.00  0.00           H
ATOM    773  H1'  DG B  24      10.518 -15.105  12.887  1.00  0.00           H
ATOM    774  H8   DG B  24       7.471 -15.396  10.485  1.00  0.00           H
ATOM    775  H1   DG B  24       6.215 -15.521  16.791  1.00  0.00           H
ATOM    776  H21  DG B  24       9.611 -14.903  17.029  1.00  0.00           H
ATOM    777  H22  DG B  24       8.117 -15.220  17.895  1.00  0.00           H
TER     778       DG B  24
CONECT  229  254
CONECT  253  254
CONECT  254  229  253  255  256
CONECT  255  254
CONECT  256  254  257
CONECT  257  256  258  278  279
CONECT  258  257  259  260  280
CONECT  259  258  263
CONECT  260  258  261  262  281
CONECT  261  260
CONECT  262  260  263  282  283
CONECT  263  259  262  264  284
CONECT  264  263  265  270
CONECT  265  264  266  267
CONECT  266  265
CONECT  267  265  268  285
CONECT  268  267  269  277
CONECT  269  268  270  274
CONECT  270  264  269  271
CONECT  271  270  272  286
CONECT  272  271  273  287
CONECT  273  272  274  288
CONECT  274  269  273  275
CONECT  275  274  276  289
CONECT  276  275  277  290
CONECT  277  268  276  291
CONECT  278  257
CONECT  279  257
CONECT  280  258
CONECT  281  260
CONECT  282  262
CONECT  283  262
CONECT  284  263
CONECT  285  267
CONECT  286  271
CONECT  287  272
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CONECT  288  273
CONECT  289  275
CONECT  290  276
CONECT  291  277
CONECT  618  643
CONECT  642  643
CONECT  643  618  642  644  645
CONECT  644  643
CONECT  645  643  646
CONECT  646  645  647  667  668
CONECT  647  646  648  649  669
CONECT  648  647  652
CONECT  649  647  650  651  670
CONECT  650  649
CONECT  651  649  652  671  672
CONECT  652  648  651  653  673
CONECT  653  652  654  659
CONECT  654  653  655  656
CONECT  655  654
CONECT  656  654  657  674
CONECT  657  656  658  666
CONECT  658  657  659  663
CONECT  659  653  658  660
CONECT  660  659  661  675
CONECT  661  660  662  676
CONECT  662  661  663  677
CONECT  663  658  662  664
CONECT  664  663  665  678
CONECT  665  664  666  679
CONECT  666  657  665  680
CONECT  667  646
CONECT  668  646
CONECT  669  647
CONECT  670  649
CONECT  671  651
CONECT  672  651
CONECT  673  652
CONECT  674  656
CONECT  675  660
CONECT  676  661
CONECT  677  662
CONECT  678  664
CONECT  679  665
CONECT  680  666
MASTER      164    0    2    0    0    0    0    6  498    2   80    2
END
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File A-3: Crystal structure of O^6-benzyl-2'-deoxyguanosine opposite perimidinone-derived synthetic nucleoside in DNA duplex. (PDB code 4HQI).

```
HEADER    DNA                                     25-OCT-12   4HQI
TITLE     STRUCTURE OF O6-BENZYL-2'-DEOXYGUANOSINE OPPOSITE PERIMIDINONE-DERIVED
TITLE    2 SYNTHETIC NUCLEOSIDE IN DNA DUPLEX
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: SHORT MODIFIED NUCLEIC ACIDS;
COMPND   3 CHAIN: A, B;
COMPND   4 ENGINEERED: YES
SOURCE    MOL_ID: 1;
SOURCE   2 SYNTHETIC: YES;
SOURCE   3 ORGANISM_SCIENTIFIC: SYNTHETIC CONSTRUCT;
SOURCE   4 ORGANISM_TAXID: 32630;
SOURCE   5 OTHER_DETAILS: CHEMICALLY SYNTHESIZED MODIFIED OLIGONUCLEOTIDES
KEYWDS    B-FORM DNA, O6-BENZYL-2'-DEOXYGUANOSINE, DPER, PERIMIDINONE-DERIVED
KEYWDS   2 NUCLEOSIDE, DICKERSON-DREW DODECAMER, DNA
EXPDTA    X-RAY DIFFRACTION
AUTHOR    E.A.KOWAL,R.LAD,P.S.PALLAN,E.MUFFLY,Z.WAWRZAK,M.EGLI,S.J.STURLA,
AUTHOR   2 M.P.STONE
JRNL        AUTH   E.A.KOWAL,R.LAD,P.S.PALLAN,E.MUFFLY,Z.WAWRZAK,M.EGLI,
JRNL        AUTH 2 S.J.STURLA,M.P.STONE
JRNL        TITL   RECOGNITION OF O6-BENZYL-2'-DEOXYGUANOSINE BY A
JRNL        TITL 2 PERIMIDINONE-DERIVED SYNTHETIC NUCLEOSIDE: A UNIQUE
JRNL        TITL 3 INTERSTRAND STACKING INTERACTION
JRNL        REF    TO BE PUBLISHED
JRNL        REFN
REMARK   2
REMARK   2 RESOLUTION.    1.70 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC 5.7.0029
REMARK   3   AUTHORS     : MURSHUDOV,VAGIN,DODSON
REMARK   3
REMARK   3    REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 1.70
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 20.67
REMARK   3   DATA CUTOFF            (SIGMA(F)) : NULL
REMARK   3   COMPLETENESS FOR RANGE        (%) : 93.4
REMARK   3   NUMBER OF REFLECTIONS             : 7486
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD          : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION  : RANDOM
REMARK   3   R VALUE     (WORKING + TEST SET) : 0.262
REMARK   3   R VALUE            (WORKING SET) : 0.259
REMARK   3   FREE R VALUE                     : 0.298
REMARK   3   FREE R VALUE TEST SET SIZE   (%) : 8.900
REMARK   3   FREE R VALUE TEST SET COUNT      : 734
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           : 20
REMARK   3   BIN RESOLUTION RANGE HIGH       (A) : 1.70
REMARK   3   BIN RESOLUTION RANGE LOW        (A) : 1.75
REMARK   3   REFLECTION IN BIN     (WORKING SET) : 338
REMARK   3   BIN COMPLETENESS (WORKING+TEST) (%) : 57.01
REMARK   3   BIN R VALUE           (WORKING SET) : 0.3360
REMARK   3   BIN FREE R VALUE SET COUNT          : 36
REMARK   3   BIN FREE R VALUE                    : 0.3360
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS            : 0
REMARK   3   NUCLEIC ACID ATOMS       : 481
REMARK   3   HETEROGEN ATOMS          : 15
REMARK   3   SOLVENT ATOMS            : 49
REMARK   3
REMARK   3  B VALUES.
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REMARK   3   FROM WILSON PLOT           (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : 44.14
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) : 3.33000
REMARK   3    B22 (A**2) : 1.38000
REMARK   3    B33 (A**2) : -4.71000
REMARK   3    B12 (A**2) : -0.00000
REMARK   3    B13 (A**2) : -0.00000
REMARK   3    B23 (A**2) : 0.00000
REMARK   3
REMARK   3  ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3   ESU BASED ON R VALUE                            (A): 0.149
REMARK   3   ESU BASED ON FREE R VALUE                       (A): 0.144
REMARK   3   ESU BASED ON MAXIMUM LIKELIHOOD                 (A): 0.130
REMARK   3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): 4.224
REMARK   3
REMARK   3 CORRELATION COEFFICIENTS.
REMARK   3   CORRELATION COEFFICIENT FO-FC      : 0.954
REMARK   3   CORRELATION COEFFICIENT FO-FC FREE : 0.940
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES        COUNT    RMS    WEIGHT
REMARK   3   BOND LENGTHS REFINED ATOMS        (A):   554 ; 0.011 ; 0.013
REMARK   3   BOND LENGTHS OTHERS               (A):  NULL ;  NULL ;  NULL
REMARK   3   BOND ANGLES REFINED ATOMS   (DEGREES):   833 ; 1.652 ; 1.578
REMARK   3   BOND ANGLES OTHERS          (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   TORSION ANGLES, PERIOD 1    (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   TORSION ANGLES, PERIOD 2    (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   TORSION ANGLES, PERIOD 3    (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   TORSION ANGLES, PERIOD 4    (DEGREES):  NULL ;  NULL ;  NULL
REMARK   3   CHIRAL-CENTER RESTRAINTS       (A**3):    66 ; 0.125 ; 0.200
REMARK   3   GENERAL PLANES REFINED ATOMS      (A):   260 ; 0.023 ; 0.020
REMARK   3   GENERAL PLANES OTHERS             (A):  NULL ;  NULL ;  NULL
REMARK   3   NON-BONDED CONTACTS REFINED ATOMS (A):  NULL ;  NULL ;  NULL
REMARK   3   NON-BONDED CONTACTS OTHERS        (A):  NULL ;  NULL ;  NULL
REMARK   3   NON-BONDED TORSION REFINED ATOMS  (A):  NULL ;  NULL ;  NULL
REMARK   3   NON-BONDED TORSION OTHERS         (A):  NULL ;  NULL ;  NULL
REMARK   3   H-BOND (X...Y) REFINED ATOMS      (A):  NULL ;  NULL ;  NULL
REMARK   3   H-BOND (X...Y) OTHERS             (A):  NULL ;  NULL ;  NULL
REMARK   3   POTENTIAL METAL-ION REFINED ATOMS (A):  NULL ;  NULL ;  NULL
REMARK   3   POTENTIAL METAL-ION OTHERS        (A):  NULL ;  NULL ;  NULL
REMARK   3   SYMMETRY VDW REFINED ATOMS        (A):  NULL ;  NULL ;  NULL
REMARK   3   SYMMETRY VDW OTHERS               (A):  NULL ;  NULL ;  NULL
REMARK   3   SYMMETRY H-BOND REFINED ATOMS     (A):  NULL ;  NULL ;  NULL
REMARK   3   SYMMETRY H-BOND OTHERS            (A):  NULL ;  NULL ;  NULL
REMARK   3   SYMMETRY METAL-ION REFINED ATOMS  (A):  NULL ;  NULL ;  NULL
REMARK   3   SYMMETRY METAL-ION OTHERS         (A):  NULL ;  NULL ;  NULL
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.     COUNT   RMS    WEIGHT
REMARK   3   MAIN-CHAIN BOND REFINED ATOMS  (A**2):  NULL ;  NULL ;  NULL
REMARK   3   MAIN-CHAIN BOND OTHER ATOMS    (A**2):  NULL ;  NULL ;  NULL
REMARK   3   MAIN-CHAIN ANGLE REFINED ATOMS (A**2):  NULL ;  NULL ;  NULL
REMARK   3   SIDE-CHAIN BOND REFINED ATOMS  (A**2):  NULL ;  NULL ;  NULL
REMARK   3   SIDE-CHAIN ANGLE REFINED ATOMS (A**2):  NULL ;  NULL ;  NULL
REMARK   3
REMARK   3 ANISOTROPIC THERMAL FACTOR RESTRAINTS.    COUNT   RMS   WEIGHT
REMARK   3   RIGID-BOND RESTRAINTS          (A**2):  NULL ;  NULL ;  NULL
REMARK   3   SPHERICITY; FREE ATOMS         (A**2):  NULL ;  NULL ;  NULL
REMARK   3   SPHERICITY; BONDED ATOMS       (A**2):  NULL ;  NULL ;  NULL
REMARK   3
REMARK   3  NCS RESTRAINTS STATISTICS
REMARK   3   NUMBER OF DIFFERENT NCS GROUPS : NULL
REMARK   3
REMARK   3  TLS DETAILS
REMARK   3   NUMBER OF TLS GROUPS  : NULL
REMARK   3
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3   METHOD USED : MASK
REMARK   3   PARAMETERS FOR MASK CALCULATION
REMARK   3   VDW PROBE RADIUS   : 1.20
REMARK   3   ION PROBE RADIUS   : 0.80
REMARK   3   SHRINKAGE RADIUS   : 0.80
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: NULL
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REMARK   4
REMARK   4 4HQI COMPLIES WITH FORMAT V. 3.30, 13-JUL-11
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 02-NOV-12.
REMARK 100 THE RCSB ID CODE IS RCSB075793.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        : 17-JUL-09; 18-JUL-08
REMARK 200  TEMPERATURE           (KELVIN) : 100; 100
REMARK 200  PH                             : 7.0; 7.0
REMARK 200  NUMBER OF CRYSTALS USED        : 2
REMARK 200
REMARK 200  SYNCHROTRON              (Y/N) : Y; Y
REMARK 200  RADIATION SOURCE               : APS; APS
REMARK 200  BEAMLINE                       : 21-ID-D; 21-ID-G
REMARK 200  X-RAY GENERATOR MODEL          : NULL; NULL
REMARK 200  MONOCHROMATIC OR LAUE    (M/L) : M; M
REMARK 200  WAVELENGTH OR RANGE        (A) : 1.60499; 0.97857
REMARK 200  MONOCHROMATOR                  : SI(111); C(111)
REMARK 200  OPTICS                         : SI(111); C(111)
REMARK 200
REMARK 200  DETECTOR TYPE                  : CCD; CCD
REMARK 200  DETECTOR MANUFACTURER          : MARMOSAIC 300 MM CCD; MARMOSAIC
REMARK 200                                   300 MM CCD
REMARK 200  INTENSITY-INTEGRATION SOFTWARE : HKL2000
REMARK 200  DATA SCALING SOFTWARE          : HKL2000
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : 8236
REMARK 200  RESOLUTION RANGE HIGH      (A) : 1.700
REMARK 200  RESOLUTION RANGE LOW       (A) : 30.000
REMARK 200  REJECTION CRITERIA  (SIGMA(I)) : 5.000
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE     (%) : 93.4
REMARK 200  DATA REDUNDANCY                : 6.400
REMARK 200  R MERGE                    (I) : 0.04400
REMARK 200  R SYM                      (I) : NULL
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET  : 52.3300
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 1.70
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 1.76
REMARK 200  COMPLETENESS FOR SHELL     (%) : NULL
REMARK 200  DATA REDUNDANCY IN SHELL       : 4.00
REMARK 200  R MERGE FOR SHELL          (I) : 0.22800
REMARK 200  R SYM FOR SHELL            (I) : NULL
REMARK 200  <I/SIGMA(I)> FOR SHELL         : 5.650
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH; SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: SAD
REMARK 200 SOFTWARE USED: PHENIX
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS   (%): 50.02
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 2.46
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 20 MM SODIUM CACODYLATE (PH 7.0), 6 MM
REMARK 280  SPERMINE TETRA-HCL, 20 MM LICL, 40 MM SRCL2 AND 5% V/V 2-METHYL-
REMARK 280  2,4-PENTANEDIOL (MPD), VAPOR DIFFUSION, HANGING DROP, TEMPERATURE
REMARK 280  291K. 20 MM SODIUM CACODYLATE (PH 7.0), 6 MM SPERMINE TETRA-HCL,
REMARK 280  40 MM KCL, 10 MM BACL2 AND 5% V/V 2-METHYL-2,4-PENTANEDIOL (MPD),
REMARK 280  VAPOR DIFFUSION, HANGING DROP, TEMPERATURE 291K
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 21 21 21
REMARK 290
REMARK 290      SYMOP   SYMMETRY
REMARK 290     NNNMMM   OPERATOR
REMARK 290       1555   X,Y,Z
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REMARK 290       2555   -X+1/2,-Y,Z+1/2
REMARK 290       3555   -X,Y+1/2,-Z+1/2
REMARK 290       4555   X+1/2,-Y+1/2,-Z
REMARK 290
REMARK 290     WHERE NNN -> OPERATOR NUMBER
REMARK 290           MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290   SMTRY1   1  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   1  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   1  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   2 -1.000000  0.000000  0.000000       13.19200
REMARK 290   SMTRY2   2  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   2  0.000000  0.000000  1.000000       38.82650
REMARK 290   SMTRY1   3 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   3  0.000000  1.000000  0.000000       18.38700
REMARK 290   SMTRY3   3  0.000000  0.000000 -1.000000       38.82650
REMARK 290   SMTRY1   4  1.000000  0.000000  0.000000       13.19200
REMARK 290   SMTRY2   4  0.000000 -1.000000  0.000000       18.38700
REMARK 290   SMTRY3   4  0.000000  0.000000 -1.000000        0.00000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 SEE REMARK 350 FOR THE AUTHOR PROVIDED AND/OR PROGRAM
REMARK 300 GENERATED ASSEMBLY INFORMATION FOR THE STRUCTURE IN
REMARK 300 THIS ENTRY. THE REMARK MAY ALSO PROVIDE INFORMATION ON
REMARK 300 BURIED SURFACE AREA.
REMARK 350
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW.  BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: DIMERIC
REMARK 350 SOFTWARE DETERMINED QUATERNARY STRUCTURE: DIMERIC
REMARK 350 SOFTWARE USED: PISA
REMARK 350 TOTAL BURIED SURFACE AREA: 1890 ANGSTROM**2
REMARK 350 SURFACE AREA OF THE COMPLEX: 4860 ANGSTROM**2
REMARK 350 CHANGE IN SOLVENT FREE ENERGY: -24.0 KCAL/MOL
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, B
REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT3   1  0.000000  0.000000  1.000000        0.00000
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465   M RES C SSSEQI
REMARK 465      DC A     1
REMARK 470
REMARK 470 MISSING ATOM
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470   M RES CSSEQI  ATOMS
REMARK 470      DC B  13    O5'  C5'  C4'  O4'  C3'  C2'  C1'
REMARK 470      DC B  13    N1   C2   O2   N3   C4   N4   C5
REMARK 470      DC B  13    C6
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
REMARK 500  ATM1  RES C  SSEQI   ATM2  RES C  SSEQI          DISTANCE
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REMARK 500   O    HOH A   225     O    HOH A   226              2.09
REMARK 500   O    HOH B   103     O    HOH B   104              2.19
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,3(1X,A4,2X),12X,F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES PROTEIN: ENGH AND HUBER, 1999
REMARK 500 EXPECTED VALUES NUCLEIC ACID: CLOWNEY ET AL 1996
REMARK 500
REMARK 500  M RES CSSEQI ATM1   ATM2   ATM3
REMARK 500     DC A   3   C1' -  O4' -  C4' ANGL. DEV. =  -6.2 DEGREES
REMARK 500
REMARK 500 REMARK: NULL
REMARK 525
REMARK 525 SOLVENT
REMARK 525
REMARK 525 THE SOLVENT MOLECULES HAVE CHAIN IDENTIFIERS THAT
REMARK 525 INDICATE THE POLYMER CHAIN WITH WHICH THEY ARE MOST
REMARK 525 CLOSELY ASSOCIATED. THE REMARK LISTS ALL THE SOLVENT
REMARK 525 MOLECULES WHICH ARE MORE THAN 5A AWAY FROM THE
REMARK 525 NEAREST POLYMER CHAIN (M = MODEL NUMBER;
REMARK 525 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 525 NUMBER; I=INSERTION CODE):
REMARK 525
REMARK 525  M RES CSSEQI
REMARK 525    HOH B 105        DISTANCE =  5.49 ANGSTROMS
REMARK 525    HOH B 121        DISTANCE =  5.08 ANGSTROMS
REMARK 800
REMARK 800 SITE
REMARK 800 SITE_IDENTIFIER: AC1
REMARK 800 EVIDENCE_CODE: SOFTWARE
REMARK 800 SITE_DESCRIPTION: BINDING SITE FOR RESIDUE SPM A 101
REMARK 800
REMARK 800 SITE_IDENTIFIER: AC2
REMARK 800 EVIDENCE_CODE: SOFTWARE
REMARK 800 SITE_DESCRIPTION: BINDING SITE FOR RESIDUE SR A 102
DBREF  4HQI A    1    12  PDB    4HQI     4HQI             1     12
DBREF  4HQI B   13    24  PDB    4HQI     4HQI            13     24
SEQRES   1 A   12   DC  DG  DC BZG  DA  DA  DT  DT D3N  DG  DC  DG
SEQRES   1 B   12   DC  DG  DC BZG  DA  DA  DT  DT D3N  DG  DC  DG
HET    BZG  A   4      29
HET    D3N  A   9      25
HET    BZG  B  16      29
HET    D3N  B  21      25
HET    SPM  A 101      14
HET     SR  A 102       1
HETNAM     BZG 6-(BENZYLOXY)-9-(2-DEOXY-5-O-PHOSPHONO-BETA-D-ERYTHRO-
HETNAM   2 BZG  PENTOFURANOSYL)-9H-PURIN-2-AMINE
HETNAM     D3N 1-(2-DEOXY-5-O-PHOSPHONO-BETA-D-ERYTHRO-
HETNAM   2 D3N  PENTOFURANOSYL)-1H-PERIMIDIN-2(3H)-ONE
HETNAM     SPM SPERMINE
HETNAM      SR STRONTIUM ION
HETSYN     BZG O6-BENZYL-2'-DEOXYGUANOSINE-5'-MONOPHOSPHATE
FORMUL   1  BZG    2(C17 H20 N5 O7 P)
FORMUL   1  D3N    2(C16 H17 N2 O7 P)
FORMUL   3  SPM    C10 H26 N4
FORMUL   4   SR    SR 2+
FORMUL   5  HOH   *49(H2 O)
LINK         O6   DG A  12                SR    SR A 102     1555   1555  2.69
LINK         O3'  DT A   8                 P   D3N A   9     1555   1555  1.58
LINK         O3'  DT B  20                 P   D3N B  21     1555   1555  1.59
LINK         O3'  DC A   3                 P   BZG A   4     1555   1555  1.59
LINK         O3'  DC B  15                 P   BZG B  16     1555   1555  1.60
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SITE     1 AC1  5  DG A   2  D3N A   9   DG A  10   DG B  14
SITE     2 AC1  5  DG B  22
SITE     1 AC2  1  DG A  12
CRYST1   26.384   36.774   77.653  90.00  90.00  90.00 P 21 21 21    8
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.037902  0.000000  0.000000        0.00000
SCALE2      0.000000  0.027193  0.000000        0.00000
SCALE3      0.000000  0.000000  0.012878        0.00000
ATOM      1  P    DG A   2       9.239 -10.993  30.734  0.60 64.21           P
ATOM      2  OP1  DG A   2       9.072 -10.756  32.190  0.60 60.29           O
ATOM      3  OP2  DG A   2       9.385 -12.395  30.228  0.60 53.30           O
ATOM      4  O5'  DG A   2       8.014 -10.291  29.981  1.00 66.68           O
ATOM      5  C5'  DG A   2       6.825  -9.899  30.702  1.00 55.81           C
ATOM      6  C4'  DG A   2       5.949  -8.961  29.894  1.00 52.59           C
ATOM      7  O4'  DG A   2       6.194  -7.574  30.229  1.00 47.03           O
ATOM      8  C3'  DG A   2       6.021  -9.044  28.371  1.00 47.01           C
ATOM      9  O3'  DG A   2       4.664  -8.805  27.971  1.00 43.95           O
ATOM     10  C2'  DG A   2       6.953  -7.905  28.004  1.00 43.36           C
ATOM     11  C1'  DG A   2       6.723  -6.873  29.101  1.00 38.71           C
ATOM     12  N9   DG A   2       7.941  -6.215  29.539  1.00 38.13           N
ATOM     13  C8   DG A   2       9.159  -6.806  29.783  1.00 40.71           C
ATOM     14  N7   DG A   2      10.037  -5.980  30.285  1.00 37.92           N
ATOM     15  C5   DG A   2       9.326  -4.799  30.471  1.00 34.44           C
ATOM     16  C6   DG A   2       9.751  -3.550  30.963  1.00 33.16           C
ATOM     17  O6   DG A   2      10.873  -3.233  31.386  1.00 39.27           O
ATOM     18  N1   DG A   2       8.717  -2.611  30.947  1.00 31.66           N
ATOM     19  C2   DG A   2       7.432  -2.858  30.522  1.00 26.82           C
ATOM     20  N2   DG A   2       6.580  -1.803  30.529  1.00 29.37           N
ATOM     21  N3   DG A   2       7.035  -4.016  30.020  1.00 32.27           N
ATOM     22  C4   DG A   2       8.029  -4.933  30.021  1.00 32.15           C
ATOM     23  P    DC A   3       4.239  -8.657  26.447  1.00 46.97           P
ATOM     24  OP1  DC A   3       2.751  -8.762  26.393  1.00 49.89           O
ATOM     25  OP2  DC A   3       5.133  -9.515  25.605  1.00 53.26           O
ATOM     26  O5'  DC A   3       4.520  -7.119  26.124  1.00 43.44           O
ATOM     27  C5'  DC A   3       3.632  -6.106  26.576  1.00 38.31           C
ATOM     28  C4'  DC A   3       4.287  -4.774  26.306  1.00 36.86           C
ATOM     29  O4'  DC A   3       5.592  -4.779  26.930  1.00 42.11           O
ATOM     30  C3'  DC A   3       4.561  -4.493  24.826  1.00 34.95           C
ATOM     31  O3'  DC A   3       3.753  -3.403  24.382  1.00 46.76           O
ATOM     32  C2'  DC A   3       6.019  -4.016  24.799  1.00 40.64           C
ATOM     33  C1'  DC A   3       6.290  -3.756  26.261  1.00 38.02           C
ATOM     34  N1   DC A   3       7.686  -3.832  26.664  1.00 41.53           N
ATOM     35  C2   DC A   3       8.245  -2.738  27.324  1.00 33.63           C
ATOM     36  O2   DC A   3       7.552  -1.720  27.493  1.00 33.20           O
ATOM     37  N3   DC A   3       9.537  -2.790  27.708  1.00 34.36           N
ATOM     38  C4   DC A   3      10.247  -3.901  27.511  1.00 35.83           C
ATOM     39  N4   DC A   3      11.529  -3.895  27.888  1.00 38.69           N
ATOM     40  C5   DC A   3       9.691  -5.046  26.867  1.00 36.91           C
ATOM     41  C6   DC A   3       8.397  -4.990  26.524  1.00 35.23           C
HETATM   42  P   BZG A   4       2.649  -3.637  23.267  1.00 46.63           P
HETATM   43  O1P BZG A   4       3.306  -3.955  21.993  1.00 44.93           O
HETATM   44  O2P BZG A   4       1.836  -4.638  23.969  1.00 55.23           O
HETATM   45  O5' BZG A   4       1.933  -2.246  23.191  1.00 39.01           O
HETATM   46  CZ1 BZG A   4      11.175   0.290  21.777  1.00 37.59           C
HETATM   47  CT1 BZG A   4      12.294  -0.517  21.686  1.00 39.06           C
HETATM   48  CI  BZG A   4      13.507   0.035  22.067  1.00 33.85           C
HETATM   49  CT2 BZG A   4      13.624   1.374  22.446  1.00 36.75           C
HETATM   50  CZ2 BZG A   4      12.497   2.161  22.581  1.00 36.31           C
HETATM   51  CE  BZG A   4      11.293   1.609  22.203  1.00 36.33           C
HETATM   52  CW  BZG A   4      10.069   2.471  22.307  1.00 34.89           C
HETATM   53  OL  BZG A   4       8.937   1.590  22.071  1.00 37.78           O
HETATM   54  CK  BZG A   4       7.707   2.091  22.327  1.00 35.01           C
HETATM   55  NJ  BZG A   4       7.570   3.379  22.668  1.00 36.53           N
HETATM   56  CH  BZG A   4       6.358   3.899  22.966  1.00 39.60           C
HETATM   57  NI  BZG A   4       6.258   5.215  23.214  1.00 42.29           N
HETATM   58  NG  BZG A   4       5.249   3.116  22.978  1.00 37.80           N
HETATM   59  CF  BZG A   4       5.361   1.799  22.674  1.00 35.38           C
HETATM   60  CM  BZG A   4       6.607   1.239  22.361  1.00 37.85           C
HETATM   61  NN  BZG A   4       6.455  -0.083  22.118  1.00 39.19           N
HETATM   62  CO  BZG A   4       5.137  -0.349  22.296  1.00 39.06           C
HETATM   63  NE  BZG A   4       4.484   0.814  22.580  1.00 38.14           N
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HETATM   64  CT' BZG A   4       3.049   1.004  22.890  1.00 40.97           C
HETATM   65  OS' BZG A   4       2.752   0.367  24.126  1.00 41.96           O
HETATM   66  CP' BZG A   4       2.139   0.420  21.818  1.00 42.75           C
HETATM   67  C5' BZG A   4       1.432  -1.656  24.357  1.00 40.60           C
HETATM   68  C4' BZG A   4       1.409  -0.173  24.040  1.00 46.89           C
HETATM   69  C3' BZG A   4       0.883   0.134  22.623  1.00 46.88           C
HETATM   70  O3' BZG A   4       0.164   1.363  22.838  1.00 55.09           O
ATOM     71  P     DA A   5      -0.648   2.070  21.637  1.00 58.27           P
ATOM     72  OP1   DA A   5      -1.834   2.738  22.239  1.00 59.14           O
ATOM     73  OP2   DA A   5      -0.808   1.074  20.536  1.00 59.17           O
ATOM     74  O5'   DA A   5       0.307   3.265  21.217  1.00 49.03           O
ATOM     75  C5'   DA A   5       0.681   4.240  22.198  1.00 48.58           C
ATOM     76  C4'   DA A   5       1.593   5.267  21.581  1.00 56.65           C
ATOM     77  O4'   DA A   5       2.908   4.711  21.358  1.00 53.36           O
ATOM     78  C3'   DA A   5       1.123   5.797  20.227  1.00 59.46           C
ATOM     79  O3'   DA A   5       1.300   7.208  20.242  1.00 60.34           O
ATOM     80  C2'   DA A   5       2.038   5.114  19.223  1.00 55.75           C
ATOM     81  C1'   DA A   5       3.316   4.936  20.017  1.00 51.87           C
ATOM     82  N9    DA A   5       4.126   3.793  19.610  1.00 46.83           N
ATOM     83  C8    DA A   5       3.701   2.511  19.368  1.00 43.90           C
ATOM     84  N7    DA A   5       4.669   1.681  19.062  1.00 44.68           N
ATOM     85  C5    DA A   5       5.813   2.463  19.135  1.00 42.49           C
ATOM     86  C6    DA A   5       7.172   2.158  18.979  1.00 36.19           C
ATOM     87  N6    DA A   5       7.619   0.949  18.637  1.00 36.49           N
ATOM     88  N1    DA A   5       8.060   3.168  19.099  1.00 36.14           N
ATOM     89  C2    DA A   5       7.610   4.377  19.460  1.00 36.19           C
ATOM     90  N3    DA A   5       6.358   4.781  19.670  1.00 42.40           N
ATOM     91  C4    DA A   5       5.498   3.760  19.499  1.00 35.08           C
ATOM     92  P     DA A   6       0.679   8.066  19.071  1.00 66.25           P
ATOM     93  OP1   DA A   6      -0.038   9.214  19.677  1.00 73.87           O
ATOM     94  OP2   DA A   6      -0.026   7.124  18.154  1.00 62.28           O
ATOM     95  O5'   DA A   6       1.965   8.619  18.327  1.00 55.29           O
ATOM     96  C5'   DA A   6       3.074   9.156  19.054  1.00 56.56           C
ATOM     97  C4'   DA A   6       4.288   9.061  18.166  1.00 53.18           C
ATOM     98  O4'   DA A   6       4.605   7.667  17.970  1.00 48.57           O
ATOM     99  C3'   DA A   6       4.033   9.623  16.761  1.00 59.75           C
ATOM    100  O3'   DA A   6       4.671  10.904  16.635  1.00 59.83           O
ATOM    101  C2'   DA A   6       4.466   8.501  15.815  1.00 57.57           C
ATOM    102  C1'   DA A   6       5.241   7.571  16.732  1.00 43.65           C
ATOM    103  N9    DA A   6       5.326   6.159  16.375  1.00 38.41           N
ATOM    104  C8    DA A   6       4.358   5.195  16.240  1.00 32.72           C
ATOM    105  N7    DA A   6       4.833   4.013  15.917  1.00 34.57           N
ATOM    106  C5    DA A   6       6.209   4.200  15.909  1.00 39.39           C
ATOM    107  C6    DA A   6       7.281   3.323  15.681  1.00 36.78           C
ATOM    108  N6    DA A   6       7.130   2.029  15.402  1.00 36.24           N
ATOM    109  N1    DA A   6       8.529   3.843  15.685  1.00 40.20           N
ATOM    110  C2    DA A   6       8.683   5.138  15.979  1.00 42.40           C
ATOM    111  N3    DA A   6       7.757   6.057  16.242  1.00 44.66           N
ATOM    112  C4    DA A   6       6.526   5.514  16.198  1.00 39.31           C
ATOM    113  P     DT A   7       4.489  11.764  15.293  1.00 63.69           P
ATOM    114  OP1   DT A   7       4.824  13.180  15.604  1.00 69.37           O
ATOM    115  OP2   DT A   7       3.191  11.401  14.662  1.00 58.46           O
ATOM    116  O5'   DT A   7       5.636  11.175  14.367  1.00 46.43           O
ATOM    117  C5'   DT A   7       7.007  11.417  14.718  1.00 51.47           C
ATOM    118  C4'   DT A   7       7.866  10.655  13.748  1.00 46.90           C
ATOM    119  O4'   DT A   7       7.578   9.255  13.892  1.00 48.09           O
ATOM    120  C3'   DT A   7       7.495  10.983  12.306  1.00 43.45           C
ATOM    121  O3'   DT A   7       8.490  11.822  11.752  1.00 52.70           O
ATOM    122  C2'   DT A   7       7.380   9.628  11.617  1.00 50.70           C
ATOM    123  C1'   DT A   7       7.913   8.677  12.663  1.00 47.48           C
ATOM    124  N1    DT A   7       7.376   7.317  12.639  1.00 41.31           N
ATOM    125  C2    DT A   7       8.289   6.297  12.506  1.00 41.88           C
ATOM    126  O2    DT A   7       9.493   6.487  12.429  1.00 42.96           O
ATOM    127  N3    DT A   7       7.745   5.043  12.494  1.00 38.18           N
ATOM    128  C4    DT A   7       6.413   4.714  12.593  1.00 39.17           C
ATOM    129  O4    DT A   7       6.074   3.542  12.534  1.00 42.62           O
ATOM    130  C5    DT A   7       5.502   5.840  12.688  1.00 39.25           C
ATOM    131  C7    DT A   7       4.033   5.582  12.805  1.00 37.23           C
ATOM    132  C6    DT A   7       6.024   7.068  12.690  1.00 36.63           C
ATOM    133  P     DT A   8       8.228  12.450  10.338  1.00 52.32           P
ATOM    134  OP1   DT A   8       8.908  13.746  10.289  1.00 52.05           O
ATOM    135  OP2   DT A   8       6.757  12.374  10.063  1.00 55.19           O
ATOM    136  O5'   DT A   8       8.910  11.384   9.375  1.00 46.41           O
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ATOM    137  C5'  DT A   8      10.246  10.929   9.583  1.00 44.52           C
ATOM    138  C4'  DT A   8      10.482   9.804   8.610  1.00 43.89           C
ATOM    139  O4'  DT A   8       9.790   8.651   9.114  1.00 42.41           O
ATOM    140  C3'  DT A   8       9.850  10.104   7.249  1.00 48.97           C
ATOM    141  O3'  DT A   8      10.867  10.316   6.277  1.00 53.05           O
ATOM    142  C2'  DT A   8       8.964   8.904   6.950  1.00 40.46           C
ATOM    143  C1'  DT A   8       9.334   7.892   8.018  1.00 41.47           C
ATOM    144  N1   DT A   8       8.211   7.065   8.474  1.00 38.36           N
ATOM    145  C2   DT A   8       8.433   5.721   8.676  1.00 39.71           C
ATOM    146  O2   DT A   8       9.530   5.206   8.573  1.00 42.69           O
ATOM    147  N3   DT A   8       7.323   5.008   9.045  1.00 37.19           N
ATOM    148  C4   DT A   8       6.055   5.502   9.280  1.00 42.23           C
ATOM    149  O4   DT A   8       5.156   4.739   9.627  1.00 44.03           O
ATOM    150  C5   DT A   8       5.887   6.917   9.020  1.00 38.33           C
ATOM    151  C7   DT A   8       4.544   7.541   9.235  1.00 43.91           C
ATOM    152  C6   DT A   8       6.956   7.612   8.618  1.00 36.11           C
HETATM  153  O1P D3N A   9       9.151  11.502   5.034  1.00 57.06           O
HETATM  154  P   D3N A   9      10.467  10.803   4.830  1.00 59.57           P
HETATM  155  O2P D3N A   9      11.529  11.563   4.178  1.00 57.35           O
HETATM  156  O5' D3N A   9      10.132   9.407   4.099  1.00 45.73           O
HETATM  157  C5' D3N A   9       9.339   9.445   2.962  1.00 56.53           C
HETATM  158  C4' D3N A   9       9.661   8.312   2.011  1.00 49.95           C
HETATM  159  O4' D3N A   9       8.863   7.224   2.387  1.00 46.67           O
HETATM  160  C3' D3N A   9       9.320   8.677   0.601  1.00 47.42           C
HETATM  161  O3' D3N A   9      10.640   8.976  -0.003  1.00 54.09           O
HETATM  162  C2' D3N A   9       8.658   7.422   0.042  1.00 44.59           C
HETATM  163  C1' D3N A   9       8.417   6.534   1.230  1.00 46.91           C
HETATM  164  N1   D3N A   9       7.078   6.124   1.580  1.00 36.46           N
HETATM  165  C2   D3N A   9       6.110   7.057   1.685  1.00 38.72           C
HETATM  166  O2   D3N A   9       6.297   8.251   1.417  1.00 48.10           O
HETATM  167  N3   D3N A   9       4.887   6.635   2.099  1.00 41.54           N
HETATM  168  C4   D3N A   9       4.594   5.301   2.451  1.00 36.92           C
HETATM  169  C5   D3N A   9       5.607   4.371   2.331  1.00 36.17           C
HETATM  170  C6   D3N A   9       6.891   4.763   1.888  1.00 36.76           C
HETATM  171  C7   D3N A   9       7.850   3.823   1.781  1.00 37.28           C
HETATM  172  C8   D3N A   9       7.548   2.482   2.091  1.00 38.67           C
HETATM  173  C9   D3N A   9       6.313   2.075   2.503  1.00 34.82           C
HETATM  174  C10 D3N A   9       5.329   3.022   2.649  1.00 36.15           C
HETATM  175  C11 D3N A   9       4.040   2.682   3.115  1.00 39.57           C
HETATM  176  C12 D3N A   9       3.039   3.617   3.226  1.00 43.64           C
HETATM  177  C13 D3N A   9       3.306   4.953   2.885  1.00 37.78           C
ATOM    178  P     DG A  10      10.766   9.455  -1.541  1.00 52.40           P
ATOM    179  OP1   DG A  10      11.926  10.387  -1.619  1.00 52.96           O
ATOM    180  OP2   DG A  10       9.429   9.942  -2.020  1.00 49.83           O
ATOM    181  O5'   DG A  10      11.122   8.085  -2.299  1.00 46.54           O
ATOM    182  C5'   DG A  10      12.098   7.130  -1.833  1.00 40.41           C
ATOM    183  C4'   DG A  10      11.817   5.781  -2.467  1.00 46.19           C
ATOM    184  O4'   DG A  10      10.495   5.337  -2.050  1.00 41.89           O
ATOM    185  C3'   DG A  10      11.772   5.751  -3.999  1.00 42.11           C
ATOM    186  O3'   DG A  10      11.986   4.386  -4.405  1.00 43.10           O
ATOM    187  C2'   DG A  10      10.312   6.041  -4.278  1.00 37.56           C
ATOM    188  C1'   DG A  10       9.649   5.223  -3.182  1.00 39.74           C
ATOM    189  N9    DG A  10       8.318   5.670  -2.791  1.00 36.64           N
ATOM    190  C8    DG A  10       7.813   6.946  -2.904  1.00 38.12           C
ATOM    191  N7    DG A  10       6.596   7.058  -2.443  1.00 33.59           N
ATOM    192  C5    DG A  10       6.277   5.778  -1.999  1.00 32.82           C
ATOM    193  C6    DG A  10       5.098   5.289  -1.387  1.00 33.36           C
ATOM    194  O6    DG A  10       4.056   5.900  -1.124  1.00 33.85           O
ATOM    195  N1    DG A  10       5.178   3.921  -1.139  1.00 32.10           N
ATOM    196  C2    DG A  10       6.298   3.154  -1.316  1.00 32.80           C
ATOM    197  N2    DG A  10       6.170   1.847  -1.011  1.00 30.07           N
ATOM    198  N3    DG A  10       7.410   3.596  -1.892  1.00 30.93           N
ATOM    199  C4    DG A  10       7.337   4.916  -2.184  1.00 36.17           C
ATOM    200  P     DC A  11      12.576   3.993  -5.867  1.00 45.72           P
ATOM    201  OP1   DC A  11      14.013   3.708  -5.707  1.00 55.46           O
ATOM    202  OP2   DC A  11      12.140   4.979  -6.893  1.00 40.18           O
ATOM    203  O5'   DC A  11      11.897   2.569  -6.086  1.00 42.94           O
ATOM    204  C5'   DC A  11      12.323   1.462  -5.304  1.00 35.76           C
ATOM    205  C4'   DC A  11      11.244   0.407  -5.260  1.00 38.62           C
ATOM    206  O4'   DC A  11      10.071   0.969  -4.638  1.00 38.55           O
ATOM    207  C3'   DC A  11      10.785  -0.117  -6.624  1.00 41.61           C
ATOM    208  O3'   DC A  11      10.597  -1.537  -6.580  1.00 36.55           O
ATOM    209  C2'   DC A  11       9.399   0.483  -6.801  1.00 35.59           C
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ATOM    210  C1'  DC A  11       8.928   0.621  -5.361  1.00 32.15           C
ATOM    211  N1   DC A  11       7.930   1.697  -5.184  1.00 32.78           N
ATOM    212  C2   DC A  11       6.724   1.419  -4.517  1.00 33.71           C
ATOM    213  O2   DC A  11       6.588   0.324  -3.936  1.00 35.86           O
ATOM    214  N3   DC A  11       5.767   2.369  -4.474  1.00 30.73           N
ATOM    215  C4   DC A  11       5.992   3.574  -5.013  1.00 31.53           C
ATOM    216  N4   DC A  11       5.017   4.482  -4.943  1.00 29.21           N
ATOM    217  C5   DC A  11       7.212   3.886  -5.677  1.00 29.13           C
ATOM    218  C6   DC A  11       8.141   2.926  -5.747  1.00 34.19           C
ATOM    219  P    DG A  12      11.039  -2.438  -7.862  1.00 43.78           P
ATOM    220  OP1  DG A  12      10.876  -3.861  -7.477  1.00 44.28           O
ATOM    221  OP2  DG A  12      12.357  -1.933  -8.370  1.00 40.00           O
ATOM    222  O5'  DG A  12       9.983  -2.054  -8.975  1.00 40.27           O
ATOM    223  C5'  DG A  12       8.619  -2.501  -8.874  1.00 43.08           C
ATOM    224  C4'  DG A  12       7.882  -2.053 -10.106  1.00 39.93           C
ATOM    225  O4'  DG A  12       7.921  -0.607 -10.134  1.00 36.76           O
ATOM    226  C3'  DG A  12       8.562  -2.505 -11.397  1.00 40.02           C
ATOM    227  O3'  DG A  12       7.910  -3.662 -11.897  1.00 39.85           O
ATOM    228  C2'  DG A  12       8.360  -1.335 -12.320  1.00 38.74           C
ATOM    229  C1'  DG A  12       8.439  -0.157 -11.368  1.00 39.35           C
ATOM    230  N9   DG A  12       9.781   0.359 -11.119  1.00 37.62           N
ATOM    231  C8   DG A  12      10.976  -0.269 -11.381  1.00 44.00           C
ATOM    232  N7   DG A  12      12.012   0.429 -11.001  1.00 42.04           N
ATOM    233  C5   DG A  12      11.465   1.537 -10.366  1.00 41.36           C
ATOM    234  C6   DG A  12      12.096   2.635  -9.733  1.00 46.68           C
ATOM    235  O6   DG A  12      13.304   2.848  -9.585  1.00 44.90           O
ATOM    236  N1   DG A  12      11.166   3.555  -9.257  1.00 37.19           N
ATOM    237  C2   DG A  12       9.805   3.432  -9.369  1.00 37.43           C
ATOM    238  N2   DG A  12       9.081   4.437  -8.858  1.00 34.27           N
ATOM    239  N3   DG A  12       9.202   2.383  -9.905  1.00 34.44           N
ATOM    240  C4   DG A  12      10.088   1.495 -10.408  1.00 38.94           C
TER     241       DG A  12
ATOM    242  O3'  DC B  13      -6.095   1.968  -3.008  1.00104.56           O
ATOM    243  P    DG B  14      -4.822   1.409  -3.812  1.00105.65           P
ATOM    244  OP1  DG B  14      -3.885   2.550  -4.035  1.00 96.18           O
ATOM    245  OP2  DG B  14      -5.315   0.603  -4.976  1.00 78.96           O
ATOM    246  O5'  DG B  14      -4.185   0.364  -2.794  1.00 74.48           O
ATOM    247  C5'  DG B  14      -3.928  -0.984  -3.220  1.00 57.72           C
ATOM    248  C4'  DG B  14      -2.876  -1.621  -2.345  1.00 54.83           C
ATOM    249  O4'  DG B  14      -1.555  -1.129  -2.675  1.00 52.37           O
ATOM    250  C3'  DG B  14      -3.040  -1.398  -0.847  1.00 47.69           C
ATOM    251  O3'  DG B  14      -2.610  -2.634  -0.294  1.00 47.75           O
ATOM    252  C2'  DG B  14      -2.064  -0.272  -0.550  1.00 44.50           C
ATOM    253  C1'  DG B  14      -0.942  -0.523  -1.550  1.00 46.21           C
ATOM    254  N9   DG B  14      -0.301   0.694  -2.022  1.00 32.96           N
ATOM    255  C8   DG B  14      -0.949   1.860  -2.348  1.00 38.11           C
ATOM    256  N7   DG B  14      -0.162   2.749  -2.890  1.00 34.89           N
ATOM    257  C5   DG B  14       1.083   2.136  -2.918  1.00 35.32           C
ATOM    258  C6   DG B  14       2.324   2.613  -3.403  1.00 32.74           C
ATOM    259  O6   DG B  14       2.594   3.731  -3.859  1.00 38.67           O
ATOM    260  N1   DG B  14       3.340   1.683  -3.204  1.00 33.06           N
ATOM    261  C2   DG B  14       3.155   0.400  -2.738  1.00 30.22           C
ATOM    262  N2   DG B  14       4.259  -0.379  -2.677  1.00 32.78           N
ATOM    263  N3   DG B  14       1.989  -0.073  -2.324  1.00 33.84           N
ATOM    264  C4   DG B  14       1.002   0.844  -2.441  1.00 34.05           C
ATOM    265  P    DC B  15      -2.707  -2.910   1.247  1.00 52.14           P
ATOM    266  OP1  DC B  15      -2.794  -4.367   1.421  1.00 52.06           O
ATOM    267  OP2  DC B  15      -3.707  -1.995   1.828  1.00 47.13           O
ATOM    268  O5'  DC B  15      -1.258  -2.522   1.759  1.00 45.23           O
ATOM    269  C5'  DC B  15      -0.153  -3.310   1.307  1.00 46.29           C
ATOM    270  C4'  DC B  15       1.130  -2.589   1.622  1.00 42.32           C
ATOM    271  O4'  DC B  15       1.192  -1.371   0.856  1.00 45.55           O
ATOM    272  C3'  DC B  15       1.296  -2.166   3.088  1.00 47.96           C
ATOM    273  O3'  DC B  15       2.440  -2.809   3.642  1.00 56.55           O
ATOM    274  C2'  DC B  15       1.637  -0.684   3.018  1.00 42.57           C
ATOM    275  C1'  DC B  15       2.050  -0.520   1.577  1.00 36.84           C
ATOM    276  N1   DC B  15       1.874   0.836   1.061  1.00 37.49           N
ATOM    277  C2   DC B  15       2.964   1.476   0.473  1.00 35.12           C
ATOM    278  O2   DC B  15       4.049   0.859   0.377  1.00 30.92           O
ATOM    279  N3   DC B  15       2.818   2.739   0.015  1.00 30.96           N
ATOM    280  C4   DC B  15       1.651   3.370   0.160  1.00 35.63           C
ATOM    281  N4   DC B  15       1.553   4.608  -0.306  1.00 31.76           N
ATOM    282  C5   DC B  15       0.510   2.724   0.715  1.00 31.16           C
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ATOM    283  C6    DC B  15       0.664   1.466   1.147  1.00 30.61           C
HETATM  284  P    BZG B  16       2.251  -3.983   4.705  1.00 59.25           P
HETATM  285  O1P  BZG B  16       1.758  -3.334   5.965  1.00 59.84           O
HETATM  286  O2P  BZG B  16       1.431  -4.994   3.984  1.00 58.44           O
HETATM  287  O5'  BZG B  16       3.716  -4.525   4.868  1.00 53.19           O
HETATM  288  CZ1  BZG B  16       6.738   6.622   5.264  1.00 37.15           C
HETATM  289  CT1  BZG B  16       5.819   7.656   5.321  1.00 40.05           C
HETATM  290  CI   BZG B  16       4.485   7.425   5.686  1.00 46.13           C
HETATM  291  CT2  BZG B  16       4.042   6.151   6.055  1.00 42.60           C
HETATM  292  CZ2  BZG B  16       4.968   5.094   6.004  1.00 41.87           C
HETATM  293  CE   BZG B  16       6.295   5.331   5.627  1.00 36.41           C
HETATM  294  CW   BZG B  16       7.263   4.189   5.618  1.00 39.93           C
HETATM  295  OL   BZG B  16       6.564   2.941   5.856  1.00 43.12           O
HETATM  296  CK   BZG B  16       7.211   1.733   5.634  1.00 40.04           C
HETATM  297  NJ   BZG B  16       8.525   1.744   5.314  1.00 43.22           N
HETATM  298  CH   BZG B  16       9.182   0.577   5.068  1.00 43.83           C
HETATM  299  NI   BZG B  16      10.491   0.578   4.779  1.00 45.60           N
HETATM  300  NG   BZG B  16       8.549  -0.623   5.114  1.00 42.53           N
HETATM  301  CF   BZG B  16       7.252  -0.663   5.426  1.00 39.41           C
HETATM  302  CM   BZG B  16       6.539   0.509   5.663  1.00 37.34           C
HETATM  303  NN   BZG B  16       5.264   0.119   5.947  1.00 45.16           N
HETATM  304  CO   BZG B  16       5.213  -1.240   5.844  1.00 37.18           C
HETATM  305  NE   BZG B  16       6.447  -1.687   5.551  1.00 41.81           N
HETATM  306  CT'  BZG B  16       6.866  -3.092   5.296  1.00 48.18           C
HETATM  307  OS'  BZG B  16       6.296  -3.544   4.063  1.00 50.49           O
HETATM  308  CP'  BZG B  16       6.358  -4.070   6.336  1.00 51.14           C
HETATM  309  C5'  BZG B  16       4.448  -5.049   3.759  1.00 55.03           C
HETATM  310  C4'  BZG B  16       5.918  -4.932   4.128  1.00 54.38           C
HETATM  311  C3'  BZG B  16       6.225  -5.365   5.557  1.00 49.35           C
HETATM  312  O3'  BZG B  16       7.520  -5.968   5.495  1.00 53.57           O
ATOM    313  P     DA B  17       8.189  -6.628   6.814  1.00 57.46           P
ATOM    314  OP1   DA B  17       9.109  -7.704   6.368  1.00 58.86           O
ATOM    315  OP2   DA B  17       7.101  -6.947   7.780  1.00 55.69           O
ATOM    316  O5'   DA B  17       9.148  -5.476   7.354  1.00 51.31           O
ATOM    317  C5'   DA B  17      10.239  -4.994   6.552  1.00 51.08           C
ATOM    318  C4'   DA B  17      10.920  -3.871   7.294  1.00 53.59           C
ATOM    319  O4'   DA B  17      10.038  -2.714   7.363  1.00 48.85           O
ATOM    320  C3'   DA B  17      11.227  -4.235   8.747  1.00 51.37           C
ATOM    321  O3'   DA B  17      12.439  -3.577   9.077  1.00 65.84           O
ATOM    322  C2'   DA B  17      10.084  -3.589   9.514  1.00 43.01           C
ATOM    323  C1'   DA B  17       9.935  -2.310   8.712  1.00 45.18           C
ATOM    324  N9    DA B  17       8.669  -1.606   8.891  1.00 38.03           N
ATOM    325  C8    DA B  17       7.432  -2.107   9.213  1.00 42.14           C
ATOM    326  N7    DA B  17       6.518  -1.183   9.394  1.00 44.19           N
ATOM    327  C5    DA B  17       7.198   0.006   9.158  1.00 37.91           C
ATOM    328  C6    DA B  17       6.787   1.346   9.175  1.00 34.62           C
ATOM    329  N6    DA B  17       5.538   1.734   9.450  1.00 40.59           N
ATOM    330  N1    DA B  17       7.719   2.290   8.930  1.00 38.79           N
ATOM    331  C2    DA B  17       8.969   1.901   8.648  1.00 40.00           C
ATOM    332  N3    DA B  17       9.474   0.671   8.592  1.00 45.23           N
ATOM    333  C4    DA B  17       8.526  -0.240   8.865  1.00 35.76           C
ATOM    334  P     DA B  18      13.626  -4.397   9.688  1.00 60.35           P
ATOM    335  OP1   DA B  18      14.221  -5.214   8.602  1.00 63.82           O
ATOM    336  OP2   DA B  18      13.144  -5.035  10.931  1.00 49.85           O
ATOM    337  O5'   DA B  18      14.622  -3.248  10.144  1.00 59.82           O
ATOM    338  C5'   DA B  18      15.222  -2.375   9.182  1.00 53.72           C
ATOM    339  C4'   DA B  18      15.373  -1.007   9.798  1.00 52.59           C
ATOM    340  O4'   DA B  18      14.075  -0.384   9.913  1.00 55.38           O
ATOM    341  C3'   DA B  18      15.965  -1.026  11.205  1.00 44.97           C
ATOM    342  O3'   DA B  18      17.114  -0.188  11.173  1.00 59.93           O
ATOM    343  C2'   DA B  18      14.828  -0.567  12.111  1.00 50.88           C
ATOM    344  C1'   DA B  18      13.928   0.218  11.180  1.00 45.59           C
ATOM    345  N9    DA B  18      12.502   0.193  11.505  1.00 41.89           N
ATOM    346  C8    DA B  18      11.681  -0.902  11.603  1.00 35.00           C
ATOM    347  N7    DA B  18      10.436  -0.601  11.890  1.00 40.93           N
ATOM    348  C5    DA B  18      10.425   0.789  11.911  1.00 39.79           C
ATOM    349  C6    DA B  18       9.393   1.726  12.103  1.00 41.31           C
ATOM    350  N6    DA B  18       8.115   1.390  12.303  1.00 35.05           N
ATOM    351  N1    DA B  18       9.715   3.037  12.035  1.00 37.78           N
ATOM    352  C2    DA B  18      10.985   3.371  11.805  1.00 39.76           C
ATOM    353  N3    DA B  18      12.041   2.585  11.605  1.00 44.05           N
ATOM    354  C4    DA B  18      11.682   1.290  11.641  1.00 39.60           C
ATOM    355  P     DT B  19      18.150  -0.225  12.366  1.00 66.24           P
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ATOM    356  OP1  DT B  19      19.404   0.414  11.889  1.00 73.70           O
ATOM    357  OP2  DT B  19      18.168  -1.604  12.915  1.00 73.00           O
ATOM    358  O5'  DT B  19      17.480   0.772  13.403  1.00 63.34           O
ATOM    359  C5'  DT B  19      17.286   2.131  12.994  1.00 59.35           C
ATOM    360  C4'  DT B  19      16.414   2.851  13.989  1.00 52.77           C
ATOM    361  O4'  DT B  19      15.043   2.464  13.823  1.00 43.01           O
ATOM    362  C3'  DT B  19      16.741   2.544  15.448  1.00 50.15           C
ATOM    363  O3'  DT B  19      17.589   3.588  15.904  1.00 57.13           O
ATOM    364  C2'  DT B  19      15.385   2.585  16.142  1.00 47.40           C
ATOM    365  C1'  DT B  19      14.405   2.874  15.005  1.00 44.86           C
ATOM    366  N1   DT B  19      13.128   2.183  15.087  1.00 41.99           N
ATOM    367  C2   DT B  19      11.999   2.961  15.192  1.00 40.74           C
ATOM    368  O2   DT B  19      12.029   4.180  15.200  1.00 45.09           O
ATOM    369  N3   DT B  19      10.821   2.257  15.242  1.00 38.44           N
ATOM    370  C4   DT B  19      10.670   0.889  15.267  1.00 39.65           C
ATOM    371  O4   DT B  19       9.546   0.403  15.355  1.00 40.87           O
ATOM    372  C5   DT B  19      11.901   0.129  15.196  1.00 37.60           C
ATOM    373  C7   DT B  19      11.834  -1.365  15.237  1.00 38.18           C
ATOM    374  C6   DT B  19      13.055   0.806  15.109  1.00 40.86           C
ATOM    375  P    DT B  20      18.294   3.480  17.302  1.00 61.96           P
ATOM    376  OP1  DT B  20      19.496   4.353  17.267  1.00 72.95           O
ATOM    377  OP2  DT B  20      18.438   2.030  17.625  1.00 58.29           O
ATOM    378  O5'  DT B  20      17.227   4.175  18.257  1.00 52.32           O
ATOM    379  C5'  DT B  20      16.699   5.464  17.926  1.00 47.16           C
ATOM    380  C4'  DT B  20      15.636   5.844  18.927  1.00 54.14           C
ATOM    381  O4'  DT B  20      14.406   5.175  18.571  1.00 51.72           O
ATOM    382  C3'  DT B  20      15.945   5.420  20.366  1.00 55.66           C
ATOM    383  O3'  DT B  20      15.647   6.479  21.276  1.00 62.72           O
ATOM    384  C2'  DT B  20      15.020   4.243  20.607  1.00 48.82           C
ATOM    385  C1'  DT B  20      13.848   4.604  19.724  1.00 48.53           C
ATOM    386  N1   DT B  20      13.035   3.471  19.303  1.00 41.47           N
ATOM    387  C2   DT B  20      11.693   3.702  19.147  1.00 42.38           C
ATOM    388  O2   DT B  20      11.182   4.786  19.358  1.00 40.94           O
ATOM    389  N3   DT B  20      10.961   2.597  18.790  1.00 39.48           N
ATOM    390  C4   DT B  20      11.440   1.329  18.529  1.00 43.13           C
ATOM    391  O4   DT B  20      10.665   0.442  18.187  1.00 43.85           O
ATOM    392  C5   DT B  20      12.874   1.170  18.676  1.00 36.61           C
ATOM    393  C7   DT B  20      13.491  -0.170  18.421  1.00 41.24           C
ATOM    394  C6   DT B  20      13.588   2.240  19.037  1.00 31.95           C
HETATM  395  O1P D3N B  21      17.527   5.577  22.677  1.00 57.63           O
HETATM  396  P   D3N B  21      16.324   6.477  22.716  1.00 73.10           P
HETATM  397  O2P D3N B  21      16.449   7.907  23.055  1.00 71.06           O
HETATM  398  O5' D3N B  21      15.191   5.843  23.617  1.00 65.54           O
HETATM  399  C5' D3N B  21      15.589   5.167  24.785  1.00 68.44           C
HETATM  400  C4' D3N B  21      14.459   5.106  25.773  1.00 63.43           C
HETATM  401  O4' D3N B  21      13.681   4.031  25.359  1.00 56.75           O
HETATM  402  C3' D3N B  21      14.935   4.721  27.123  1.00 63.88           C
HETATM  403  O3' D3N B  21      15.133   5.944  27.827  1.00 67.07           O
HETATM  404  C2' D3N B  21      13.814   3.859  27.696  1.00 56.92           C
HETATM  405  C1' D3N B  21      12.920   3.605  26.492  1.00 52.83           C
HETATM  406  N1  D3N B  21      12.484   2.276  26.132  1.00 47.27           N
HETATM  407  C2  D3N B  21      13.435   1.323  25.912  1.00 47.67           C
HETATM  408  O2  D3N B  21      14.627   1.553  26.095  1.00 53.65           O
HETATM  409  N3  D3N B  21      13.009   0.096  25.555  1.00 43.83           N
HETATM  410  C4  D3N B  21      11.663  -0.223  25.295  1.00 39.23           C
HETATM  411  C5  D3N B  21      10.696   0.762  25.488  1.00 44.29           C
HETATM  412  C6  D3N B  21      11.081   2.040  25.924  1.00 42.62           C
HETATM  413  C7  D3N B  21      10.111   2.990  26.145  1.00 52.13           C
HETATM  414  C8  D3N B  21       8.771   2.646  25.913  1.00 39.74           C
HETATM  415  C9  D3N B  21       8.378   1.426  25.500  1.00 47.35           C
HETATM  416  C10 D3N B  21       9.330   0.451  25.258  1.00 41.01           C
HETATM  417  C11 D3N B  21       8.992  -0.837  24.848  1.00 43.98           C
HETATM  418  C12 D3N B  21       9.952  -1.768  24.635  1.00 45.05           C
HETATM  419  C13 D3N B  21      11.312  -1.482  24.872  1.00 47.17           C
ATOM    420  P    DG B  22      15.736   5.916  29.307  1.00 60.70           P
ATOM    421  OP1  DG B  22      16.433   7.208  29.532  1.00 63.59           O
ATOM    422  OP2  DG B  22      16.495   4.640  29.465  1.00 51.49           O
ATOM    423  O5'  DG B  22      14.420   5.963  30.208  1.00 56.71           O
ATOM    424  C5'  DG B  22      13.283   6.789  29.854  1.00 44.99           C
ATOM    425  C4'  DG B  22      12.025   6.262  30.509  1.00 50.00           C
ATOM    426  O4'  DG B  22      11.708   4.952  29.984  1.00 42.89           O
ATOM    427  C3'  DG B  22      12.105   6.068  32.024  1.00 48.07           C
ATOM    428  O3'  DG B  22      10.760   6.110  32.488  1.00 50.84           O
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ATOM    429  C2'  DG B  22      12.570   4.634  32.149  1.00 41.22           C
ATOM    430  C1'  DG B  22      11.752   3.990  31.034  1.00 41.10           C
ATOM    431  N9   DG B  22      12.282   2.747  30.485  1.00 35.88           N
ATOM    432  C8   DG B  22      13.594   2.339  30.459  1.00 41.27           C
ATOM    433  N7   DG B  22      13.753   1.160  29.926  1.00 35.66           N
ATOM    434  C5   DG B  22      12.468   0.765  29.576  1.00 38.68           C
ATOM    435  C6   DG B  22      12.009  -0.426  28.970  1.00 36.57           C
ATOM    436  O6   DG B  22      12.660  -1.408  28.615  1.00 38.62           O
ATOM    437  N1   DG B  22      10.636  -0.396  28.759  1.00 32.06           N
ATOM    438  C2   DG B  22       9.801   0.614  29.146  1.00 37.35           C
ATOM    439  N2   DG B  22       8.497   0.408  28.941  1.00 33.23           N
ATOM    440  N3   DG B  22      10.210   1.716  29.751  1.00 37.31           N
ATOM    441  C4   DG B  22      11.553   1.741  29.897  1.00 35.81           C
ATOM    442  P    DC B  23      10.442   6.622  33.947  1.00 54.63           P
ATOM    443  OP1  DC B  23      10.081   8.062  33.835  1.00 72.54           O
ATOM    444  OP2  DC B  23      11.572   6.234  34.816  1.00 46.04           O
ATOM    445  O5'  DC B  23       9.071   5.874  34.286  1.00 50.89           O
ATOM    446  C5'  DC B  23       7.872   6.214  33.569  1.00 44.12           C
ATOM    447  C4'  DC B  23       6.937   5.029  33.482  1.00 43.81           C
ATOM    448  O4'  DC B  23       7.576   3.958  32.740  1.00 42.06           O
ATOM    449  C3'  DC B  23       6.528   4.432  34.832  1.00 38.81           C
ATOM    450  O3'  DC B  23       5.132   4.149  34.847  1.00 45.37           O
ATOM    451  C2'  DC B  23       7.300   3.124  34.901  1.00 40.79           C
ATOM    452  C1'  DC B  23       7.379   2.736  33.434  1.00 33.88           C
ATOM    453  N1   DC B  23       8.504   1.846  33.120  1.00 36.40           N
ATOM    454  C2   DC B  23       8.272   0.685  32.369  1.00 32.79           C
ATOM    455  O2   DC B  23       7.131   0.479  31.908  1.00 36.07           O
ATOM    456  N3   DC B  23       9.293  -0.184  32.167  1.00 30.32           N
ATOM    457  C4   DC B  23      10.503   0.081  32.671  1.00 32.96           C
ATOM    458  N4   DC B  23      11.472  -0.815  32.470  1.00 32.29           N
ATOM    459  C5   DC B  23      10.777   1.286  33.385  1.00 32.52           C
ATOM    460  C6   DC B  23       9.753   2.117  33.606  1.00 37.44           C
ATOM    461  P    DG B  24       4.277   4.492  36.173  1.00 52.39           P
ATOM    462  OP1  DG B  24       2.829   4.210  35.898  1.00 51.58           O
ATOM    463  OP2  DG B  24       4.739   5.811  36.678  1.00 48.36           O
ATOM    464  O5'  DG B  24       4.756   3.384  37.209  1.00 46.27           O
ATOM    465  C5'  DG B  24       4.451   2.002  36.974  1.00 44.58           C
ATOM    466  C4'  DG B  24       5.053   1.193  38.090  1.00 39.93           C
ATOM    467  O4'  DG B  24       6.494   1.319  38.004  1.00 36.23           O
ATOM    468  C3'  DG B  24       4.673   1.705  39.476  1.00 41.18           C
ATOM    469  O3'  DG B  24       3.540   0.965  39.948  1.00 45.43           O
ATOM    470  C2'  DG B  24       5.937   1.493  40.281  1.00 44.61           C
ATOM    471  C1'  DG B  24       7.030   1.711  39.250  1.00 39.64           C
ATOM    472  N9   DG B  24       7.442   3.094  39.113  1.00 44.84           N
ATOM    473  C8   DG B  24       6.712   4.200  39.471  1.00 50.34           C
ATOM    474  N7   DG B  24       7.292   5.323  39.143  1.00 46.30           N
ATOM    475  C5   DG B  24       8.422   4.933  38.443  1.00 46.08           C
ATOM    476  C6   DG B  24       9.446   5.712  37.846  1.00 53.78           C
ATOM    477  O6   DG B  24       9.530   6.948  37.769  1.00 50.57           O
ATOM    478  N1   DG B  24      10.419   4.908  37.254  1.00 42.62           N
ATOM    479  C2   DG B  24      10.434   3.531  37.278  1.00 42.89           C
ATOM    480  N2   DG B  24      11.496   2.933  36.700  1.00 37.64           N
ATOM    481  N3   DG B  24       9.495   2.796  37.851  1.00 42.44           N
ATOM    482  C4   DG B  24       8.524   3.556  38.405  1.00 45.36           C
TER     483       DG B  24
HETATM  484  N1  SPM A 101      15.307  -2.224  30.707  0.50 45.16           N
HETATM  485  C2  SPM A 101      14.648  -3.505  30.906  1.00 50.52           C
HETATM  486  C3  SPM A 101      14.177  -3.681  32.355  1.00 49.96           C
HETATM  487  C4  SPM A 101      13.198  -4.830  32.413  1.00 46.18           C
HETATM  488  N5  SPM A 101      12.876  -5.334  33.745  1.00 49.66           N
HETATM  489  C6  SPM A 101      11.836  -6.363  33.800  1.00 40.82           C
HETATM  490  C7  SPM A 101      11.700  -6.958  35.173  1.00 44.69           C
HETATM  491  C8  SPM A 101      10.292  -7.489  35.304  1.00 45.41           C
HETATM  492  C9  SPM A 101      10.370  -8.593  36.328  1.00 39.65           C
HETATM  493  N10 SPM A 101       9.328  -8.480  37.308  1.00 48.73           N
HETATM  494  C11 SPM A 101       8.275  -9.514  37.339  1.00 42.36           C
HETATM  495  C12 SPM A 101       8.417 -10.350  38.617  1.00 40.48           C
HETATM  496  C13 SPM A 101       7.395 -11.529  38.711  1.00 36.10           C
HETATM  497  N14 SPM A 101       7.319 -12.113  37.413  1.00 26.41           N
HETATM  498 SR    SR A 102      15.511   4.253 -10.211  1.00 80.43          SR
HETATM  499  O   HOH A 201       5.745  10.707   7.973  1.00 50.57           O
HETATM  500  O   HOH A 202       3.981   2.092  12.526  1.00 55.74           O
HETATM  501  O   HOH A 203       5.535   7.189  -5.997  1.00 37.30           O
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HETATM  502  O   HOH A 204       5.857  10.607   2.957  1.00 39.96           O
HETATM  503  O   HOH A 205      16.122  -0.073  -7.306  1.00 76.18           O
HETATM  504  O   HOH A 206      12.456  -9.842  29.587  0.50 39.91           O
HETATM  505  O   HOH A 207      15.126   0.991 -11.310  1.00 64.27           O
HETATM  506  O   HOH A 208      11.936  -2.931 -12.948  1.00 43.14           O
HETATM  507  O   HOH A 209      16.727  -3.172  -8.920  1.00 68.21           O
HETATM  508  O   HOH A 210      13.771  10.608  -3.551  0.50 32.95           O
HETATM  509  O   HOH A 211       9.441   1.770  -2.007  1.00 36.92           O
HETATM  510  O   HOH A 212       9.916  -4.279 -14.180  1.00 39.00           O
HETATM  511  O   HOH A 213       5.425  -5.959 -10.092  1.00 56.75           O
HETATM  512  O   HOH A 214       6.736  11.394   5.248  0.50 34.77           O
HETATM  513  O   HOH A 215      11.867 -15.768  30.801  1.00 47.55           O
HETATM  514  O   HOH A 216      14.392  -5.303  36.717  0.50 36.19           O
HETATM  515  O   HOH A 217       3.012 -10.254  22.862  1.00 67.16           O
HETATM  516  O   HOH A 218      13.213   9.047  -5.011  0.50 43.01           O
HETATM  517  O   HOH A 219      -2.568  -2.294  17.282  0.50 44.49           O
HETATM  518  O   HOH A 220      10.725 -14.748  28.779  0.50 39.46           O
HETATM  519  O   HOH A 221      15.703   9.836  -2.496  0.50 31.11           O
HETATM  520  O   HOH A 222       9.346   8.423  16.634  1.00 52.47           O
HETATM  521  O   HOH A 223      11.510   1.193  -0.164  0.50 40.92           O
HETATM  522  O   HOH A 224      12.332  12.804  -0.232  1.00 59.02           O
HETATM  523  O   HOH A 225      14.811 -18.153  31.387  1.00 54.50           O
HETATM  524  O   HOH A 226      12.781 -17.856  31.806  1.00 47.82           O
HETATM  525  O   HOH A 227       1.224   6.114  15.685  1.00 60.25           O
HETATM  526  O   HOH A 228      10.603   6.919  -7.970  1.00 37.70           O
HETATM  527  O   HOH B 101      -0.922   0.065  -5.369  1.00 42.62           O
HETATM  528  O   HOH B 102       8.026   9.832  35.707  1.00 68.74           O
HETATM  529  O   HOH B 103      15.975  -1.008  15.507  1.00 52.27           O
HETATM  530  O   HOH B 104      14.793  -2.822  15.169  1.00 58.11           O
HETATM  531  O   HOH B 105      -0.287   5.138   4.841  1.00 62.89           O
HETATM  532  O   HOH B 106       2.869   1.485   6.566  1.00 45.01           O
HETATM  533  O   HOH B 107       2.751   0.192   9.510  0.50 39.34           O
HETATM  534  O   HOH B 108      17.774   2.975  22.558  1.00 57.77           O
HETATM  535  O   HOH B 109      16.850   0.536  28.081  1.00 66.55           O
HETATM  536  O   HOH B 110       8.401  -1.858  12.571  0.50 37.14           O
HETATM  537  O   HOH B 111       5.873  -5.073   9.869  1.00 47.64           O
HETATM  538  O   HOH B 112       6.830   8.002  40.323  1.00 55.54           O
HETATM  539  O   HOH B 113      12.523  -2.219   4.994  1.00 56.73           O
HETATM  540  O   HOH B 114       8.144   3.642  30.083  1.00 38.91           O
HETATM  541  O   HOH B 115      10.239  -1.894  19.211  1.00 41.32           O
HETATM  542  O   HOH B 116      11.394   6.208  23.097  1.00 61.62           O
HETATM  543  O   HOH B 117      -8.777   1.487  -2.112  1.00 70.13           O
HETATM  544  O   HOH B 118      -1.820   0.663   3.075  1.00 52.05           O
HETATM  545  O   HOH B 119      21.214   2.225  19.730  1.00 65.35           O
HETATM  546  O   HOH B 120      16.869   1.303  20.043  1.00 54.01           O
HETATM  547  O   HOH B 121      -2.810  -4.632   7.767  1.00 63.68           O
CONECT   31   42
CONECT   42   31   43   44   45
CONECT   43   42
CONECT   44   42
CONECT   45   42   67
CONECT   46   47   51
CONECT   47   46   48
CONECT   48   47   49
CONECT   49   48   50
CONECT   50   49   51
CONECT   51   46   50   52
CONECT   52   51   53
CONECT   53   52   54
CONECT   54   53   55   60
CONECT   55   54   56
CONECT   56   55   57   58
CONECT   57   56
CONECT   58   56   59
CONECT   59   58   60   63
CONECT   60   54   59   61
CONECT   61   60   62
CONECT   62   61   63
CONECT   63   59   62   64
CONECT   64   63   65   66
CONECT   65   64   68
CONECT   66   64   69
CONECT   67   45   68
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CONECT   68   65   67   69
CONECT   69   66   68   70
CONECT   70   69
CONECT  141  154
CONECT  153  154
CONECT  154  141  153  155  156
CONECT  155  154
CONECT  156  154  157
CONECT  157  156  158
CONECT  158  157  159  160
CONECT  159  158  163
CONECT  160  158  161  162
CONECT  161  160
CONECT  162  160  163
CONECT  163  159  162  164
CONECT  164  163  165  170
CONECT  165  164  166  167
CONECT  166  165
CONECT  167  165  168
CONECT  168  167  169  177
CONECT  169  168  170  174
CONECT  170  164  169  171
CONECT  171  170  172
CONECT  172  171  173
CONECT  173  172  174
CONECT  174  169  173  175
CONECT  175  174  176
CONECT  176  175  177
CONECT  177  168  176
CONECT  235  498
CONECT  273  284
CONECT  284  273  285  286  287
CONECT  285  284
CONECT  286  284
CONECT  287  284  309
CONECT  288  289  293
CONECT  289  288  290
CONECT  290  289  291
CONECT  291  290  292
CONECT  292  291  293
CONECT  293  288  292  294
CONECT  294  293  295
CONECT  295  294  296
CONECT  296  295  297  302
CONECT  297  296  298
CONECT  298  297  299  300
CONECT  299  298
CONECT  300  298  301
CONECT  301  300  302  305
CONECT  302  296  301  303
CONECT  303  302  304
CONECT  304  303  305
CONECT  305  301  304  306
CONECT  306  305  307  308
CONECT  307  306  310
CONECT  308  306  311
CONECT  309  287  310
CONECT  310  307  309  311
CONECT  311  308  310  312
CONECT  312  311
CONECT  383  396
CONECT  395  396
CONECT  396  383  395  397  398
CONECT  397  396
CONECT  398  396  399
CONECT  399  398  400
CONECT  400  399  401  402
CONECT  401  400  405
CONECT  402  400  403  404
CONECT  403  402
CONECT  404  402  405
CONECT  405  401  404  406
CONECT  406  405  407  412
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CONECT  407  406  408  409
CONECT  408  407
CONECT  409  407  410
CONECT  410  409  411  419
CONECT  411  410  412  416
CONECT  412  406  411  413
CONECT  413  412  414
CONECT  414  413  415
CONECT  415  414  416
CONECT  416  411  415  417
CONECT  417  416  418
CONECT  418  417  419
CONECT  419  410  418
CONECT  484  485
CONECT  485  484  486
CONECT  486  485  487
CONECT  487  486  488
CONECT  488  487  489
CONECT  489  488  490
CONECT  490  489  491
CONECT  491  490  492
CONECT  492  491  493
CONECT  493  492  494
CONECT  494  493  495
CONECT  495  494  496
CONECT  496  495  497
CONECT  497  496
CONECT  498  235
MASTER      307    0    6    0    0    0    3    6  545    2  128    2
END
```

APPENDIX B

NMR RESONANCE ASSIGNMENTS

Table B-1. NMR resonance assignments for DDD–GY duplex.

Group	Atom	Nuc	Shift	SDev	Assignments
C1	H1'	1H	5.547	0.002	10
C1	H2''	1H	2.220	0.005	11
C1	H2'	1H	1.813	0.000	10
C1	H3'	1H	4.513	0.003	9
C1	H4'	1H	3.782	0.003	4
C1	H5	1H	5.645	0.002	5
C1	H5''	1H	3.866	0.002	6
C1	H5'	1H	3.560	0.126	9
C1	H6	1H	7.421	0.002	8
G2	H1'	1H	5.745	0.002	10
G2	H2''	1H	2.572	0.048	14
G2	H2'	1H	2.422	0.147	13
G2	H3'	1H	4.799	0.004	10
G2	H4'	1H	4.052	0.000	1
G2	H5''	1H	4.044	0.140	5
G2	H5'	1H	4.102	0.094	3
G2	H8	1H	7.757	0.001	14
C3	H1'	1H	5.503	0.003	13
C3	H2''	1H	2.246	0.003	10
C3	H2'	1H	1.946	0.001	10
C3	H3'	1H	4.652	0.002	12
C3	H4'	1H	4.166	0.002	3
C3	H5	1H	5.299	0.002	11
C3	H5''	1H	4.050	0.002	3
C3	H5'	1H	3.953	0.004	8
C3	H6	1H	7.189	0.001	14
G4	H1'	1H	5.583	0.004	9
G4	H2''	1H	2.607	0.006	6
G4	H2'	1H	2.407	0.002	6
G4	H3'	1H	4.830	0.002	5
G4	H4'	1H	4.095	0.071	3
G4	H5''	1H	4.040	0.158	2
G4	H5'	1H	4.103	0.111	5
G4	H8	1H	7.628	0.002	13
A5	H1'	1H	5.723	0.003	8
A5	H2	1H	7.092	0.003	4
A5	H2''	1H	2.706	0.004	7
A5	H2'	1H	2.391	0.004	5
A5	H3'	1H	4.841	0.001	3
A5	H5''	1H	4.232	0.012	6
A5	H5'	1H	4.039	0.002	3
A5	H8	1H	7.828	0.002	12

A6	H1'	1H	5.937	0.003	14
A6	H2	1H	7.391	0.000	4
A6	H2''	1H	2.693	0.002	6
A6	H2'	1H	2.385	0.008	5
A6	H3'	1H	4.825	0.002	8
A6	H4'	1H	3.933	0.000	3
A6	H5''	1H	4.266	0.002	8
A6	H5'	1H	4.035	0.000	3
A6	H8	1H	7.982	0.002	13
T7	H1'	1H	5.596	0.004	12
T7	H2''	1H	2.088	0.002	9
T7	H2'	1H	1.557	0.002	8
T7	H3'	1H	4.548	0.003	11
T7	H4'	1H	3.955	0.109	3
T7	H5''	1H	3.957	0.053	8
T7	H5'	1H	4.043	0.078	3
T7	H6	1H	6.807	0.002	14
T7	M7	1H	1.056	0.004	16
T8	H1'	1H	5.762	0.003	14
T8	H2''	1H	2.008	0.003	10
T8	H2'	1H	1.212	0.328	7
T8	H3'	1H	4.493	0.003	11
T8	H4'	1H	3.798	0.000	1
T8	H5''	1H	3.801	0.003	4
T8	H5'	1H	3.904	0.006	4
T8	H6	1H	6.409	0.003	15
T8	M7	1H	0.784	0.001	15
Y9	H6	1H	6.936	0.000	1
Y9	H1'	1H	6.013	0.004	11
Y9	H2''	1H	2.403	0.003	8
Y9	H2'	1H	1.654	0.001	6
Y9	H3'	1H	4.885	0.002	11
Y9	H4'	1H	4.097	0.000	5
Y9	H5''	1H	3.739	0.005	7
Y9	H5'	1H	3.930	0.003	4
Y9	H9	1H	6.477	0.002	16
Y9	H8	1H	7.121	0.001	9
Y9	H7	1H	7.081	0.001	3
Y9	H6	1H	6.936	0.003	4
Y9	H5	1H	6.860	0.008	3
Y9	H6	1H	6.005	0.000	2
G10	H1'	1H	5.579	0.003	7
G10	H2''	1H	2.569	0.001	5
G10	H2'	1H	2.413	0.010	7
G10	H3'	1H	4.741	0.070	8
G10	H4'	1H	3.801	0.000	1
G10	H5''	1H	3.796	0.000	1
G10	H5'	1H	4.060	0.128	3
G10	H8	1H	7.739	0.001	13
C11	H1'	1H	5.612	0.003	8
C11	H2''	1H	2.186	0.081	9
C11	H2'	1H	1.709	0.001	7
C11	H3'	1H	4.654	0.063	10
C11	H4'	1H	3.870	0.000	1
C11	H5	1H	5.218	0.002	12

C11	H5''	1H	3.914	0.002	3
C11	H5'	1H	3.984	0.005	6
C11	H6	1H	7.146	0.001	13
G12	H1'	1H	5.941	0.002	7
G12	H2''	1H	2.437	0.018	4
G12	H2'	1H	2.147	0.007	3
G12	H3'	1H	4.476	0.003	6
G12	H5''	1H	3.833	0.037	2
G12	H5'	1H	4.030	0.155	3
G12	H8	1H	7.746	0.004	11

APPENDIX C

NMR RESTRAINTS FOR DDD–GY DUPLEX

Table C-1. NMR cross peaks intensities for DDD-GY duplex

```
#####################################################################
#       Chemical Shift Ambiguity Index Value Definitions            #
#                                                                   #
# The values other than 1 are used for those atoms with different #
# chemical shifts that cannot be assigned to stereospecific atoms #
# or to specific residues or chains.                                #
#                                                                   #
#   Index Value            Definition                               #
#                                                                   #
#      1             Unique (including isolated meDT l protons,   #
#                         geminal atoms, and geminal meDT l         #
#                         groups with identical chemical shifts)    #
#                         (e.g. ILE HD11, HD12, HD13 protons)       #
#      2             Ambiguity of geminal atoms or geminal meDT l #
#                         proton groups (e.g. ASP HB2 and HB3       #
#                         protons, LEU CD1 and CD2 carbons, or      #
#                         LEU HD11, HD12, HD13 and HD21, HD22,      #
#                         HD23 meDT l protons)                      #
#      3             Aromatic atoms on opposite sides of          #
#                         symmetrical rings (e.g. TYR HE1 and HE2 #
#                         protons)                                  #
#      4             Intraresidue ambiguities (e.g. LYS HG and    #
#                         HD protons or TRP HZ2 and HZ3 protons)    #
#      5             Interresidue ambiguities (LYS 12 vs. LYS 27) #
#      6             Intermolecular ambiguities (e.g. ASP 31 CA   #
#                         in monomer 1 and ASP 31 CA in monomer 2 #
#                         of an asymmetrical homodimer, duplex      #
#                         DNA assignments, or other assignments     #
#                         that may apply to atoms in one or more    #
#                         molecule in the molecular assembly)       #
#      9             Ambiguous, specific ambiguity not defined    #
#                                                                   #
#####################################################################
loop_
    _Homonucl_NOE.Atom_ID_1
    _Homonucl_NOE.Comp_ID_1
    _Homonucl_NOE.Comp_index_ID_1
    _Homonucl_NOE.Atom_ID_2
    _Homonucl_NOE.Comp_ID_2
    _Homonucl_NOE.Comp_index_ID_2
    _Homonucl_NOE.Val
    _Homonucl_NOE.Val_err

H1'     DC5     1      H6     DC5      1      1.8500e+07     30
H2''    DC5     1      H6     DC5      1      2.7280e+07     20
H2''    DC5     1      H3'    DG       2      2.2345e+06     10
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H2''	DC5	1	H8	DG	2	2.8264e+07	50
H2'	DC5	1	H1'	DC5	1	2.7478e+07	10
H2'	DC5	1	H5	DC5	1	9.9835e+06	20
H2'	DC5	1	H8	DG	2	1.8965e+07	20
H3'	DC5	1	H1'	DC5	1	1.1729e+07	10
H3'	DC5	1	H5	DC5	1	3.1184e+06	10
H3'	DC5	1	H6	DC5	1	1.6842e+07	10
H6	DC5	1	H8	DG	2	2.5979e+06	10
H1'	DG	2	H8	DG	2	1.4521e+07	20
H1'	DG	2	H6	DC	3	1.7044e+07	10
H2''	DG	2	H1'	DG	2	5.259e+07	50
H2''	DG	2	H3'	DC	3	2.7748e+06	20
H2''	DG	2	H5	DC	3	1.1931e+07	20
H2''	DG	2	H6	DC	3	2.6255e+07	30
H2'	DG	2	H1'	DG	2	4.1266e+07	40
H2'	DG	2	H5	DC	3	1.3024e+07	20
H2'	DG	2	H6	DC	3	2.4689e+07	30
H3'	DG	2	H5	DC	3	2.1857e+06	10
H3'	DG	2	H6	DC	3	4.7725e+06	10
H1'	DC	3	H1'	DG	2	5.5637e+06	40
H1'	DC	3	H6	DC	3	8.3959e+06	30
H1'	DC	3	H8	DG	4	9.033e+06	30
H2''	DC	3	H1'	DC	3	4.1730e+07	50
H2''	DC	3	H5	DC	3	7.2183e+06	20
H2''	DC	3	H6	DC	3	3.1138e+07	20
H2'	DC	3	H2''	DG	2	9.6576e+06	20
H2'	DC	3	H1'	DC	3	2.9638e+07	20
H2'	DC	3	H6	DC	3	5.2993e+07	30
H2'	DC	3	H8	DG	4	1.5373e+07	20
H3'	DC	3	H1'	DC	3	8.8871e+06	10
H3'	DC	3	H6	DC	3	1.4571e+07	30
H3'	DC	3	H8	DG	4	4.0192e+06	10
H5	DC	3	H1'	DG	2	8.2349e+06	10
H5	DC	3	H8	DG	2	8.3938e+06	10
H6	DC	3	H8	DG	4	3.3767e+06	10
H1'	DG	4	H8	DG	4	8.9004e+06	30
H1'	DG	4	H8	DA	5	8.0315e+06	10
H2''	DG	4	H8	DG	4	3.0329e+07	40
H2''	DG	4	H8	DA	5	2.5773e+07	50
H2'	DG	4	H8	DG	4	5.5189e+07	50
H3'	DG	4	H8	DG	4	1.103e+07	10
H8	DG	4	H8	DA	5	6.8863e+06	10
H1'	DA	5	H8	DA	5	1.0548e+07	10
H1'	DA	5	H8	DA	6	1.6193e+07	20
H2''	DA	5	H1'	DA	5	5.8752e+07	40
H2''	DA	5	H8	DA	5	3.0333e+07	40
H2'	DA	5	H1'	DA	5	4.0086e+07	50
H3'	DA	5	H8	DA	6	1.3360e+07	50
H8	DA	5	H8	DA	6	4.5120e+06	20
H1'	DA	6	H8	DA	6	1.0829e+07	20
H1'	DA	6	H6	DT	7	1.178e+07	30
H2''	DA	6	H6	DT	7	1.682e+07	10
H2'	DA	6	H6	DT	7	1.3715e+07	10
H3'	DA	6	H1'	DA	6	1.2222e+07	10
H3'	DA	6	H8	DA	6	1.5840e+07	20

H3'	DA	6	H6	DT	7	4.2424e+06	10
H1'	DT	7	H1'	DA	6	9.0064e+06	10
H1'	DT	7	H6	DT	7	7.3137e+06	10
H1'	DT	7	H6	DT	8	3.2437e+06	10
H2''	DT	7	H6	DT	7	1.4262e+07	10
H2''	DT	7	H6	DT	8	1.8998e+07	30
H2'	DT	7	H1'	DT	7	2.1848e+07	30
H2'	DT	7	H3'	DT	7	3.3618e+07	30
H2'	DT	7	H6	DT	7	2.3621e+07	30
H2'	DT	7	H6	DT	8	9.8526e+06	10
H3'	DT	7	H1'	DA	6	1.9241e+06	10
H3'	DT	7	H1'	DT	7	1.3879e+07	40
H3'	DT	7	H6	DT	7	9.3188e+06	10
H3'	DT	7	H6	DT	8	1.9528e+07	40
H6	DT	7	H8	DA	6	2.8226e+06	10
H7	DT	7	H1'	DA	6	1.1042e+07	10
H7	DT	7	H2''	DA	6	4.0887e+07	30
H7	DT	7	H2'	DA	6	4.3215e+07	20
H7	DT	7	H3'	DA	6	1.3697e+07	10
H7	DT	7	H8	DA	6	3.955e+07	30
H7	DT	7	H1'	DT	7	3.8837e+06	10
H7	DT	7	H2''	DT	7	1.6815e+07	10
H7	DT	7	H2'	DT	7	1.5449e+07	10
H7	DT	7	H3'	DT	7	9.2721e+06	10
H7	DT	7	H6	DT	7	5.0478e+07	40
H1'	DT	8	H6	DT	8	6.4454e+06	10
H1'	DT	8	H9	D3N	9	6.0477e+06	10
H2''	DT	8	H1'	DT	8	2.9243e+07	50
H2''	DT	8	H6	DT	8	1.6861e+07	30
H2''	DT	8	H9	D3N	9	1.3137e+07	30
H2''	DT	8	H8	D3N	9	1.0204e+07	20
H2''	DT	8	H7	D3N	9	4.0523e+06	20
H2'	DT	8	H1'	DT	8	1.4809e+07	20
H2'	DT	8	H3'	DT	8	2.2218e+07	20
H2'	DT	8	H9	D3N	9	7.108e+06	10
H2'	DT	8	H8	D3N	9	4.9097e+06	10
H3'	DT	8	H1'	DT	8	1.048e+07	10
H3'	DT	8	H6	DT	8	1.9528e+07	40
H3'	DT	8	H9	D3N	9	3.0617e+06	10
H3'	DT	8	H8	D3N	9	1.5892e+06	10
H6	DT	8	H8	D3N	9	1.8126e+06	30
H7	DT	8	H1'	DT	7	7.4343e+06	10
H7	DT	8	H2''	DT	7	2.4374e+07	10
H7	DT	8	H2'	DT	7	2.6337e+07	20
H7	DT	8	H3'	DT	7	1.2479e+07	10
H7	DT	8	H6	DT	7	2.5216e+07	40
H7	DT	8	H7	DT	7	2.4146e+07	50
H7	DT	8	H3'	DT	8	3.2143e+06	10
H7	DT	8	H6	DT	8	2.403e+07	20
H7	DT	8	H1'	D3N	9	2.9721e+06	10
H7	DT	8	H6	D3N	9	9.4389e+06	30
H7	DT	8	H5	D3N	9	1.8345e+07	40
H2''	DG	10	H5	DC	11	1.5044e+07	20
H2''	DG	10	H6	DC	11	1.3644e+07	30
H2'	DG	10	H5	DC	11	1.7122e+07	20

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H2'     DG      10     H6     DC       11     1.4172e+07     50
H3'     DG      10     H5     DC       11     2.1493e+06     10
H3'     DG      10     H6     DC       11     1.3973e+06     10
H2''    DC      11     H5     DC       11     6.5443e+06     10
H2''    DC      11     H6     DC       11     3.8247e+07     30
H2'     DC      11     H1'    DC       11     3.9816e+07     40
H2'     DC      11     H5     DC       11     1.7942e+07     20
H2'     DC      11     H8     DG3      12     2.1152e+07     50
H3'     DC      11     H5     DC       11     2.2216e+06     10
H3'     DC      11     H6     DC       11     1.8525e+07     30
H3'     DC      11     H8     DG3      12     6.9485e+06     10
H5      DC      11     H1'    DG       10     1.6703e+07     30
H5      DC      11     H8     DG       10     8.674e+06      10
H1'     DG3     12     H8     DG3      12     1.6640e+07     30
H2''    DG3     12     H3'    DG3      12     5.5826e+07     30
H3'     DG3     12     H1'    DG3      12     1.6763e+07     10
H1'     D3N     9      H8     DG       10     4.2233e+06     30
H1'     D3N     9      H9     D3N      9      1.1813e+07     20
H2''    D3N     9      H1'    D3N      9      2.618e+07      40
H2''    D3N     9      H9     D3N      9      2.3525e+07     20
H2''    D3N     9      H8     D3N      9      8.7712e+06     50
H2'     D3N     9      H8     DG       10     9.1596e+06     50
H2'     D3N     9      H1'    D3N      9      2.685e+07      20
H2'     D3N     9      H2''   D3N      9      5.3028e+07     40
H2'     D3N     9      H9     D3N      9      1.2836e+07     20
H3'     D3N     9      H8     DG       10     5.7155e+06     10
H3'     D3N     9      H1'    D3N      9      9.3039e+06     10
H3'     D3N     9      H9     D3N      9      3.017e+07      20
H3'     D3N     9      H8     D3N      9      6.121e+06      10
H9      D3N     9      H8     DG       10     2.6102e+06     10
H2'     DG      10     H3'    DG       10     5.11098e+07    50
H3'     DG      10     H1'    DG       10     1.35213e+07    50
H1'     DG      10     H8     DG       10     1.7400e+07     50
H1'     DG      10     H2''   DG       10     4.1550e+07     50
H2''    DG      10     H3'    DG       10     5.1100e+07     50
H1'     DT      8      H6     DT       8      6.4454e+06     10
H2'     DG      10     H3'    DG       10     5.11098e+07    50
H2''    DG      10     H3'    DG       10     7.8800e+07     50
H1'     DG      10     H2'    DG       10     4.1450e+07     50
H3'     DC      11     H8     DG3      12     6.9485e+06     10

stop_
```

Table C-2. NOE distance restraints generated from intensity file.

1	DC5	H2'1	1	DC5	H1'	2.250	3.410
1	DC5	H3'	1	DC5	H1'	2.910	4.740
1	DC5	H6	1	DC5	H1'	2.220	3.890
1	DC5	H6	1	DC5	H2'2	2.530	5.010
1	DC5	H5	1	DC5	H2'1	2.930	5.950
1	DC5	H5	1	DC5	H3'	3.350	6.070
1	DC5	H6	1	DC5	H3'	3.000	5.000
2	DG	H2'1	2	DG	H1'	2.070	3.400
2	DG	H2'2	2	DG	H1'	1.780	3.040
2	DG	H3'	1	DC5	H2'2	5.380	5.560
2	DG	H8	1	DC5	H2'1	2.650	3.670
2	DG	H8	1	DC5	H2'2	2.390	3.810
2	DG	H8	1	DC5	H6	4.680	5.410
2	DG	H8	2	DG	H1'	3.170	4.440
3	DC	H1'	2	DG	H1'	2.720	5.020
3	DC	H2'1	2	DG	H2'2	2.860	5.750
3	DC	H2'1	3	DC	H1'	2.220	3.120
3	DC	H2'2	3	DC	H1'	1.880	3.100
3	DC	H3'	2	DG	H2'2	3.940	5.900
3	DC	H3'	3	DC	H1'	3.610	5.380
3	DC	H6	2	DG	H1'	2.820	3.980
3	DC	H6	2	DG	H2'1	2.170	4.100
3	DC	H6	2	DG	H2'2	2.480	3.230
3	DC	H6	2	DG	H3'	4.280	6.580
3	DC	H6	3	DC	H1'	3.010	4.580
3	DC	H6	3	DC	H2'1	2.090	3.300
3	DC	H6	3	DC	H2'2	2.070	3.340
3	DC	H6	3	DC	H3'	3.330	4.830
3	DC	H5	2	DG	H1'	3.450	5.250
3	DC	H5	2	DG	H2'1	3.200	4.080
3	DC	H5	2	DG	H2'2	3.180	4.740
3	DC	H5	2	DG	H3'	5.080	6.810
3	DC	H5	2	DG	H8	3.280	4.110
3	DC	H5	3	DC	H2'1	3.270	5.130
3	DC	H5	3	DC	H2'2	3.620	4.760
4	DG	H8	3	DC	H1'	3.100	4.090
4	DG	H8	3	DC	H2'1	2.740	3.900
4	DG	H8	3	DC	H3'	4.590	6.660
4	DG	H8	3	DC	H6	4.530	6.100
4	DG	H8	4	DG	H1'	3.500	5.320
4	DG	H8	4	DG	H2'1	1.850	3.870
4	DG	H8	4	DG	H2'2	2.370	4.770
4	DG	H8	4	DG	H3'	3.490	5.890
5	DA	H2'1	5	DA	H1'	2.180	3.290
5	DA	H2'2	5	DA	H1'	1.740	3.070
5	DA	H8	4	DG	H1'	3.680	4.170

```
5 DA  H8    4 DG   H2'2  2.210   5.080
5 DA  H8    4 DG   H8    4.070   6.460
5 DA  H8    5 DA   H1'   3.230   4.110
5 DA  H8    5 DA   H2'2  2.420   3.790
6 DA  H3'   6 DA   H1'   3.210   5.090
6 DA  H8    5 DA   H1'   2.400   3.970
6 DA  H8    5 DA   H3'   2.640   5.260
6 DA  H8    5 DA   H8    3.490   5.190
6 DA  H8    6 DA   H1'   3.200   4.440
6 DA  H8    6 DA   H3'   2.640   4.810
7 DT  H1'   6 DA   H1'   2.690   5.000
7 DT  H2'1  7 DT   H1'   2.390   3.460
7 DT  H3'   7 DT   H1'   2.940   4.740
7 DT  H3'   6 DA   H1'   4.000   5.600
7 DT  H3'   7 DT   H2'1  2.440   2.990
7 DT  H6    6 DA   H1'   3.080   4.030
7 DT  H6    6 DA   H2'1  2.220   5.100
7 DT  H6    6 DA   H2'2  2.750   3.530
7 DT  H6    6 DA   H3'   4.290   6.760
7 DT  H6    6 DA   H8    4.700   6.050
7 DT  H6    7 DT   H1'   3.360   4.430
7 DT  H6    7 DT   H2'1  2.220   3.860
7 DT  H6    7 DT   H2'2  2.450   3.750
7 DT  H6    7 DT   H3'   3.500   4.680
7 DT  H7    6 DA   H1'   3.130   5.340
7 DT  H7    6 DA   H2'1  2.290   3.680
7 DT  H7    6 DA   H2'2  2.270   3.680
7 DT  H7    6 DA   H3'   3.900   5.420
7 DT  H7    6 DA   H8    2.040   3.430
7 DT  H7    7 DT   H1'   3.300   5.340
7 DT  H7    7 DT   H2'1  3.140   5.250
7 DT  H7    7 DT   H2'2  2.800   4.180
7 DT  H7    7 DT   H3'   3.870   6.480
7 DT  H7    7 DT   H6    2.760   3.890
8 DT  H2'1  8 DT   H1'   2.390   3.370
8 DT  H2'2  8 DT   H1'   2.330   3.390
8 DT  H3'   8 DT   H1'   3.400   4.720
8 DT  H3'   8 DT   H2'1  2.710   3.340
8 DT  H6    7 DT   H1'   2.300   4.250
8 DT  H6    7 DT   H2'1  2.400   4.500
8 DT  H6    7 DT   H2'2  2.820   3.940
8 DT  H6    7 DT   H3'   3.300   4.900
8 DT  H6    7 DT   H6    4.440   6.000
8 DT  H6    8 DT   H1'   3.560   3.880
8 DT  H6    8 DT   H2'2  2.200   3.820
8 DT  H6    8 DT   H3'   3.200   4.400
8 DT  H7    7 DT   H1'   3.390   4.800
8 DT  H7    7 DT   H2'1  2.830   4.590
```

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 8 DT  H7    7 DT   H2'2  3.170   4.270
 8 DT  H7    7 DT   H3'   3.770   5.480
 8 DT  H7    7 DT   H6    2.560   3.760
 8 DT  H7    7 DT   H7    2.450   5.760
 8 DT  H7    8 DT   H3'   4.480   6.670
 8 DT  H7    8 DT   H6    2.630   4.650
 9 D3N H5    8 DT   H7    3.260   4.070
 9 D3N H9    8 DT   H1'   2.540   4.640
 9 D3N H9    8 DT   H2'1  2.250   3.920
 9 D3N H9    8 DT   H2'2  2.210   3.600
 9 D3N H9    8 DT   H3'   3.790   6.490
 9 D3N H8    8 DT   H2'1  3.680   5.280
 9 D3N H8    8 DT   H2'2  3.130   4.030
 9 D3N H8    8 DT   H3'   5.030   6.900
 9 D3N H8    8 DT   H6    4.270   5.350
 9 D3N H7    8 DT   H2'2  4.010   6.170
 9 D3N H6    8 DT   H7    3.490   4.660
 9 D3N H1'   8 DT   H7    3.710   6.370
 9 D3N H1'   9 D3N  H9    1.790   3.820
 9 D3N H2'1  9 D3N  H9    2.000   3.970
 9 D3N H2'1  9 D3N  H1'   2.200   3.180
 9 D3N H2'2  9 D3N  H9    2.320   3.510
 9 D3N H2'2  9 D3N  H8    2.370   4.330
 9 D3N H2'2  9 D3N  H1'   1.830   3.100
 9 D3N H2'2  9 D3N  H2'1  1.690   2.860
 9 D3N H3'   9 D3N  H9    1.880   3.150
 9 D3N H3'   9 D3N  H8    3.910   6.460
 9 D3N H3'   9 D3N  H1'   3.050   5.540
 9 D3N H3'   9 D3N  H2'1  2.560   3.840
 9 D3N H3'   9 D3N  H2'2  1.970   3.050
10 DG  H8    9 D3N  H9    3.350   4.830
10 DG  H8    9 D3N  H1'   3.550   4.570
10 DG  H8    9 D3N  H2'1  2.760   4.440
10 DG  H8    9 D3N  H3'   3.510   5.000
10 DG  H3'  10 DG   H2'1  2.290   4.120
10 DG  H3'  10 DG   H2'2  1.890   2.730
10 DG  H8   10 DG   H1'   2.620   4.260
10 DG  H3'  10 DG   H1'   2.940   5.000
10 DG  H1'  10 DG   H2'1  2.110   3.140
10 DG  H1'  10 DG   H2'2  1.960   3.300
11 DC  H2'1 11 DC   H1'   2.320   3.640
11 DC  H6   10 DG   H2'1  2.650   4.750
11 DC  H6   10 DG   H2'2  2.140   4.090
11 DC  H6   10 DG   H3'   3.910   6.690
11 DC  H6   11 DC   H2'2  2.000   3.430
11 DC  H6   11 DC   H3'   3.110   4.530
11 DC  H5   10 DG   H1'   2.800   4.200
11 DC  H5   10 DG   H2'1  2.890   3.360
```

```
11 DC   H5    10 DG    H2'2   2.940    5.320
11 DC   H5    10 DG    H3'    3.790    6.310
11 DC   H5    10 DG    H8     3.430    4.070
11 DC   H5    11 DC    H2'1   2.630    5.450
11 DC   H5    11 DC    H2'2   3.440    6.080
11 DC   H5    11 DC    H3'    4.130    6.580
12 DG3  H3'   12 DG3   H1'    3.250    5.840
12 DG3  H3'   12 DG3   H2'2   2.250    2.880
12 DG3  H8    11 DC    H2'1   2.480    3.880
12 DG3  H8    11 DC    H3'    3.740    5.900
12 DG3  H8    12 DG3   H1'    2.800    4.860
```

Table C-3. Backbone restraints file

```
  2 DG   ALPHA     -90.0  -30.0
  3 DC   ALPHA     -90.0  -30.0
  4 DG   ALPHA     -90.0  -30.0
  5 DA   ALPHA     -90.0  -30.0
  6 DA   ALPHA     -90.0  -30.0
  7 DT   ALPHA     -90.0  -30.0
  8 DT   ALPHA     -90.0  -30.0
  9 D3N  ALPHA    -120.0    0.0
 10 DG   ALPHA     -90.0  -30.0
 11 DC   ALPHA     -90.0  -30.0
 14 DG   ALPHA     -90.0  -30.0
 15 DC   ALPHA     -90.0  -30.0
 16 DG   ALPHA     -90.0  -30.0
 17 DA   ALPHA     -90.0  -30.0
 18 DA   ALPHA     -90.0  -30.0
 19 DT   ALPHA     -90.0  -30.0
 20 DT   ALPHA     -90.0  -30.0
 21 D3N  ALPHA    -120.0    0.0
 22 DG   ALPHA     -90.0  -30.0
 23 DC   ALPHA     -90.0  -30.0
  2 DG   BETA      150.0  210.0
  3 DC   BETA      150.0  210.0
  4 DG   BETA      150.0  210.0
  5 DA   BETA      150.0  210.0
  6 DA   BETA      150.0  210.0
  7 DT   BETA      150.0  210.0
  8 DT   BETA      150.0  210.0
  9 D3N  BETA      120.0  240.0
 10 DG   BETA      150.0  210.0
 11 DC   BETA      150.0  210.0
 14 DG   BETA      150.0  210.0
 15 DC   BETA      150.0  210.0
 16 DG   BETA      150.0  210.0
 17 DA   BETA      150.0  210.0
 18 DA   BETA      150.0  210.0
 19 DT   BETA      150.0  210.0
 20 DT   BETA      150.0  210.0
 21 D3N  BETA      120.0  240.0
 22 DG   BETA      150.0  210.0
 23 DC   BETA      150.0  210.0
  2 DG   GAMMA      30.0   90.0
  3 DC   GAMMA      30.0   90.0
  4 DG   GAMMA      30.0   90.0
  5 DA   GAMMA      30.0   90.0
  6 DA   GAMMA      30.0   90.0
  7 DT   GAMMA      30.0   90.0
```

8	DT	GAMMA	30.0	90.0
9	D3N	GAMMA	0.0	120.0
10	DG	GAMMA	30.0	90.0
11	DC	GAMMA	30.0	90.0
14	DG	GAMMA	30.0	90.0
15	DC	GAMMA	30.0	90.0
16	DG	GAMMA	30.0	90.0
17	DA	GAMMA	30.0	90.0
18	DA	GAMMA	30.0	90.0
19	DT	GAMMA	30.0	90.0
20	DT	GAMMA	30.0	90.0
21	D3N	GAMMA	0.0	120.0
22	DG	GAMMA	30.0	90.0
23	DC	GAMMA	30.0	90.0
2	DG	EPSILN	165.0	225.0
3	DC	EPSILN	165.0	225.0
4	DG	EPSILN	165.0	225.0
5	DA	EPSILN	165.0	225.0
6	DA	EPSILN	165.0	225.0
7	DT	EPSILN	165.0	225.0
8	DT	EPSILN	165.0	225.0
9	D3N	EPSILN	135.0	255.0
10	DG	EPSILN	165.0	225.0
11	DC	EPSILN	165.0	225.0
14	DG	EPSILN	165.0	225.0
15	DC	EPSILN	165.0	225.0
16	DG	EPSILN	165.0	225.0
17	DA	EPSILN	165.0	225.0
18	DA	EPSILN	165.0	225.0
19	DT	EPSILN	165.0	225.0
20	DT	EPSILN	165.0	225.0
21	D3N	EPSILN	135.0	255.0
22	DG	EPSILN	165.0	225.0
23	DC	EPSILN	165.0	225.0
2	DG	ZETA	-135.0	-75.0
3	DC	ZETA	-135.0	-75.0
4	DG	ZETA	-135.0	-75.0
5	DA	ZETA	-135.0	-75.0
6	DA	ZETA	-135.0	-75.0
7	DT	ZETA	-135.0	-75.0
8	DT	ZETA	-135.0	-75.0
9	D3N	ZETA	-165.0	-45.0
10	DG	ZETA	-135.0	-75.0
11	DC	ZETA	-135.0	-75.0
14	DG	ZETA	-135.0	-75.0
15	DC	ZETA	-135.0	-75.0
16	DG	ZETA	-135.0	-75.0
17	DA	ZETA	-135.0	-75.0

```
18 DA   ZETA      -135.0   -75.0
19 DT   ZETA      -135.0   -75.0
20 DT   ZETA      -135.0   -75.0
21 D3N  ZETA      -165.0   -45.0
22 DG   ZETA      -135.0   -75.0
23 DC   ZETA      -135.0   -75.0
```

Table C-4. Sugar restraints file

```
  2 DG   PPA       100.0   165.0
  3 DC   PPA        90.0   130.0
  4 DG   PPA       125.0   165.0
  5 DA   PPA       125.0   165.0
  6 DA   PPA       125.0   165.0
  7 DT   PPA        90.0   130.0
  8 DT   PPA        90.0   130.0
 10 DG   PPA       125.0   165.0
 11 DC   PPA       100.0   165.0
 14 DG   PPA       100.0   165.0
 15 DC   PPA        90.0   130.0
 16 DG   PPA       125.0   165.0
 17 DA   PPA       125.0   165.0
 18 DA   PPA       125.0   165.0
 19 DT   PPA        90.0   130.0
 20 DT   PPA        90.0   130.0
 22 DG   PPA       125.0   165.0
 23 DC   PPA       100.0   165.0
```

Table C-5. Base pairing restraints file.

1	DC5	H42	24	DG3	O6	1.80	2.00
1	DC5	N3	24	DG3	H1	1.84	2.04
1	DC5	N3	24	DG3	N1	2.85	3.05
1	DC5	N4	24	DG3	O6	2.81	3.01
1	DC5	O2	24	DG3	H22	1.75	1.95
2	DG	H1	23	DC	N3	1.84	2.04
2	DG	H22	23	DC	O2	1.75	1.95
2	DG	N1	23	DC	N3	2.85	3.05
2	DG	O6	23	DC	H42	1.80	2.00
2	DG	O6	23	DC	N4	2.81	3.01
3	DC	H42	22	DG	O6	1.80	2.00
3	DC	N3	22	DG	H1	1.84	2.04
3	DC	N3	22	DG	N1	2.85	3.05
3	DC	N4	22	DG	O6	2.81	3.01
3	DC	O2	22	DG	H22	1.75	1.95
4	DG	O6	21	D3N	HN	1.70	2.10
4	DG	H1	21	D3N	O2	1.70	2.10
4	DG	O6	21	D3N	N3	2.80	3.10
4	DG	N1	21	D3N	O2	2.80	3.10
5	DA	N1	20	DT	H3	1.71	1.91
5	DA	N1	20	DT	N3	2.72	2.92
5	DA	H61	20	DT	O4	1.84	2.04
6	DA	N1	19	DT	H3	1.71	1.91
6	DA	N1	19	DT	N3	2.72	2.92
6	DA	H61	19	DT	O4	1.84	2.04
7	DT	H3	18	DA	N1	1.71	1.91
7	DT	N3	18	DA	N1	2.72	2.92
7	DT	O4	18	DA	H61	1.84	2.04
8	DT	H3	17	DA	N1	1.71	1.91
8	DT	N3	17	DA	N1	2.72	2.92
8	DT	O4	17	DA	H61	1.84	2.04
9	D3N	HN	16	DG	O6	1.80	2.00
9	D3N	O2	16	DG	H1	1.84	2.04
9	D3N	N3	16	DG	O6	2.80	3.00
9	D3N	O2	16	DG	N1	2.80	3.00
10	DG	H1	15	DC	N3	1.84	2.04
10	DG	H22	15	DC	O2	1.75	1.95
10	DG	N1	15	DC	N3	2.85	3.05
10	DG	O6	15	DC	H42	1.80	2.00
10	DG	O6	15	DC	N4	2.81	3.01
11	DC	H42	14	DG	O6	1.80	2.00
11	DC	N3	14	DG	H1	1.84	2.04
11	DC	N3	14	DG	N1	2.85	3.05
11	DC	N4	14	DG	O6	2.81	3.01
11	DC	O2	14	DG	H22	1.75	1.95
12	DG3	H1	13	DC5	N3	1.84	2.04

12	DG3	H22	13	DC5	O2	1.75	1.95
12	DG3	N1	13	DC5	N3	2.85	3.05
12	DG3	O6	13	DC5	H42	1.80	2.00
12	DG3	O6	13	DC5	N4	2.81	3.01

Table C-6. PREP file used to generate topology, input files for AMBER calculations. It defines parameters for modified base.

```
    0    0    2

 5'.dPer base
 dPer.prep
 DNP   INT     1
 CORRECT OMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00      0.00      0.00       0.000
   2   DUMM  DU    M    1   0  -1    1.00      0.00      0.00       0.000
   3   DUMM  DU    M    2   1   0    1.00     90.00      0.00       0.000
   4   P     P     M    3   2   1    1.60    119.04    200.00       1.098
   5   O1P   O2    E    4   3   2    1.48    109.61    150.00      -0.704
   6   O2P   O2    E    4   3   2    1.48    109.58     20.00      -0.704
   7   O5'   OS    M    4   3   2    1.60    101.43    -98.89      -0.413
   8   C5'   CT    M    7   4   3    1.44    119.00    -39.22      -0.111
   9   H5'1  H1    E    8   7   4    1.09    109.50     60.00       0.089
  10   H5'2  H1    E    8   7   4    1.09    109.50    -60.00       0.089
  11   C4'   CT    M    8   7   4    1.52    110.00    180.00       0.089
  12   H4'   H1    E   11   8   7    1.09    109.50   -200.00       0.089
  13   O4'   OS    S   11   8   7    1.46    108.86    -86.31      -0.551
  14   C1'   CT    B   13  11   8    1.42    110.04    105.60       0.051
  15   H1'   H2    E   14  13  11    1.09    109.50   -240.00       0.164
  16   N1    N*    S   14  13  11    1.46    113.87   -127.70      -0.608
  17   C2    C     B   16  14  13    1.38    126.07     -3.46       0.771
  18   O2    O     E   17  16  14    1.23    122.92      5.83      -0.537
  19   N3    NA    B   17  16  14    1.38    115.44   -173.37      -0.778
  20   HN    H     E   19  17  16    1.01    113.92    179.68       0.344
  21   C4    CA    S   19  17  16    1.40    126.07     -1.65       0.378
  22   C13   CD    B   21  19  17    1.38    122.34    177.97      -0.198
  23   H4    HA    E   22  21  19    1.09    120.23     -1.46       0.126
  24   C12   CD    B   22  21  19    1.41    119.31    178.13      -0.135
  25   H5    HA    E   24  22  21    1.09    118.80    179.99       0.133
  26   C11   CD    B   24  22  21    1.38    121.27     -0.46      -0.203
  27   H6    HA    E   26  24  22    1.09    120.59   -179.25       0.129
  28   C10   CA    S   26  24  22    1.42    120.54      0.30       0.129
  29   C9    CD    B   28  26  24    1.42    123.19   -178.81      -0.202
  30   H7    HA    E   29  28  26    1.09    119.10     -0.73       0.120
  31   C8    CD    B   29  28  26    1.38    120.13    178.24      -0.136
  32   H8    HA    E   31  29  28    1.09    119.83   -178.40       0.134
  33   C7    CD    B   31  29  28    1.41    121.76      1.29      -0.203
  34   H9    HA    E   33  31  29    1.08    119.55   -177.12       0.161
  35   C6    CA    S   33  31  29    1.39    119.68      0.82       0.360
  36   C5    CA    E   35  33  31    1.43    119.53     -2.90       0.003
  37   C3'   CT    M   11   8   7    1.53    115.78   -329.11       0.215
  38   H3'   H1    E   37  11   8    1.09    109.50     30.00       0.089
  39   C2'   CT    B   37  11   8    1.53    102.80    -86.30      -0.006
  40   H2'1  H1    E   39  37  11    1.09    109.50    120.00       0.089
  41   H2'2  H1    E   39  37  11    1.09    109.50    240.00       0.089
  42   O3'   OS    M   37  11   8    1.42    116.52   -203.47      -0.450



IMPROPER
 C4   H4   C13  C12
 N1   C5   C6   C7
```

```
 C6   C4   C5   C10
 N3   C5   C4   C13
 C13  C11  C12  H5
 C12  C10  C11  H6
 C11  C9   C10  C5
 C10  C8   C9   H7
 C9   C7   C8   H8
 C8   C4   C7   H9
 C4   HN   N3   C2
 N3   O2   C2   N1

LOOP CLOSING EXPLICIT
 C1'  C2'
 C6   N1
 C10  C5
 C4   C5


DONE
STOP
```

Table C-7. dPer.frcmod file used to generate topology, input files for AMBER calculations. It defines angles for modified base.

```
remark goes here
MASS

BOND
CD-CA  469.0    1.400
CA-CD  469.0    1.400
N*-CA  424.0    1.383
CD-CA  469.0    1.400

ANGLE
HA-CD-CA    50.0       120.00
CD-CA-CA    50.0       120.00
CD-CD-CA    50.0       120.00
CD-CD-CD    50.0       120.00
CA-CD-HA    50.0       120.00
CA-CD-CD    50.0       120.00
CD-CA-CD    50.0       120.00
NA-CA-CD    50.0       120.00
NA-CA-CA    50.0       120.00
N*-CA-CA    50.0       120.00
N*-CA-CD    50.0       120.00
C-N*-CA     70.0       125.20
N*-C-O      50.0       122.34
CT-N*-CA    50.0       120.00


DIHE
HA-CD-CA-CA    4   14.50        180.0
CD-CD-CA-CA    4   14.50        180.0
HA-CD-CA-CD    4   14.50        180.0
CD-CA-CD-HA    4   14.50        180.0
CD-CA-CD-CD    4   14.50        180.0
 H-NA-CA-CD    6    1.80        180.0
CD-CA-CD-CD    4   14.50        180.0
 H-NA-CA-CA    4   14.50        180.0
NA- C-N*-CA    6    1.10        180.0
NA-CA-CD-HA    4    0.00        180.0
N*-CA-CD-HA    4    0.00        180.0
NA-CA-CD-CD    4    4.00        180.0
N*-CA-CD-CD    4    4.00        180.0
 C-N*-CA-CD    4   14.50        180.0
 C-N*-CA-CA    6    1.80        180.0
CT-N*- C- O    1    1.10        180.0
CT-N*- C-NT    1    0.00        180.0
```

```
CT-N*-CA-CA     4    14.50          180.0
CT-N*-CA-CD     4    14.50          180.0
NA-CA-CD-HA     4     0.00          180.0
N*-CA-CD-HA     4     0.00          180.0
CD-CD-CA-CD     4    14.50          180.0

DIHE

IMPROPER

NONBON
```

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