SEQUENCE DEPENDENCE OF STRUCTURAL PERTURBATIONS TO DNA INDUCED BY AFLATOXIN B_1 FORMAMIDOPYRIMIDINE LESIONS

By

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CHAPTER I

Introduction

Deoxyribonucleic acid (DNA)

Deoxyribonucleic acids (DNA) are one of the most important biological macromolecules. DNA encodes the genetic instructions used in the development and functioning of all known living organisms, ranging from single–celled to multicellular organisms. The function of DNA is to replicate itself during cell division, and to direct transcription of ribonucleic acid (RNA). DNA was first identified and isolated by the Swiss physician Friedrich Miescher.[1] Following his work, in 1944, Oswald Avery, along with his coworkers, identified DNA as the transforming principle.[2] Nine years later, a famous paper published in *Nature* by James Watson and Francis Crick reported what is now accepted as the first double-helix model of DNA structure,[3] which is essential to store and replicate genetic information safely.

Duplex DNA molecules are comprised of two biopolymer strands coiled around each other to form a double helix. Both strands are known as polynucleotides since they are made up of repeating units known as nucleotides. Each nucleotide is composed of three components: a nitrogen-containing nucleobase: guanine (G), adenine (A), thymine (T), or cytosine (C), as well as a pentose (five-carbon) sugar, and a phosphate group[4] (Figure 1). In each helix, the phosphate group and the sugar of each nucleotide bond with each other to form the backbone of the nucleic acid.

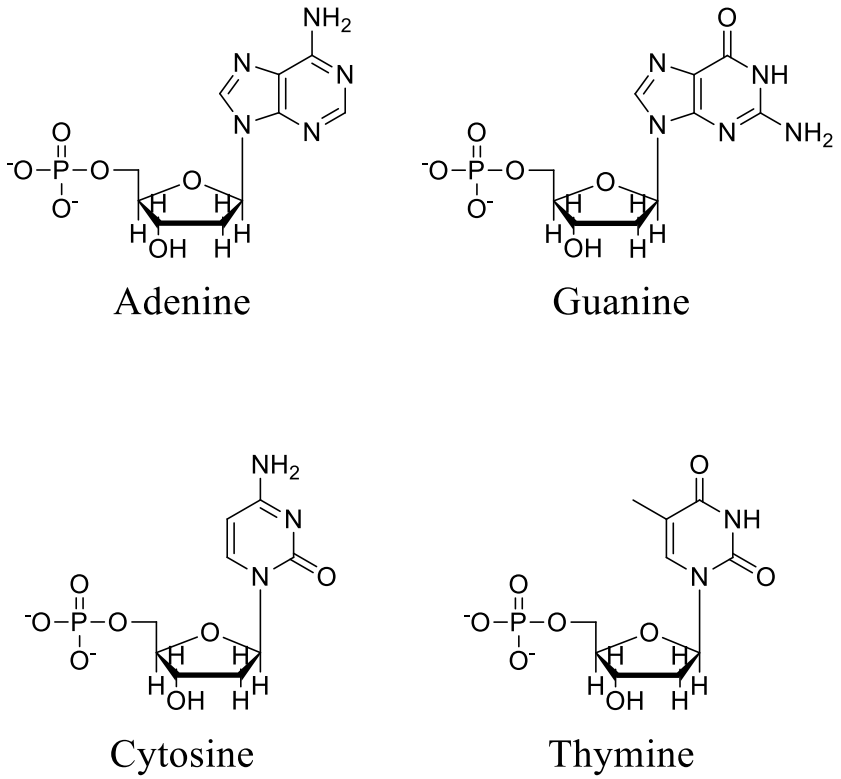


Figure 1-1: The chemical structures of DNA nucleotides.

In a double helix DNA, the two strands are antiparallel, which means the 5′ → 3′ direction of the nucleotides in one strand is opposite to their direction in the other strand. Each strand has two asymmetric ends, the 5′ end and the 3′ end. Each base in a single strand is separated by a distance of 3.4 Å and the strand turns every 10 residues due to a 36 °angle between residues. DNA contains two grooves, the major groove and the minor groove. The major groove is 10 Å wide and the minor groove is 12 Å wide and many sequence specific proteins interact in the major groove. A molecule model of DNA and its components is shown in Figure 1-2.

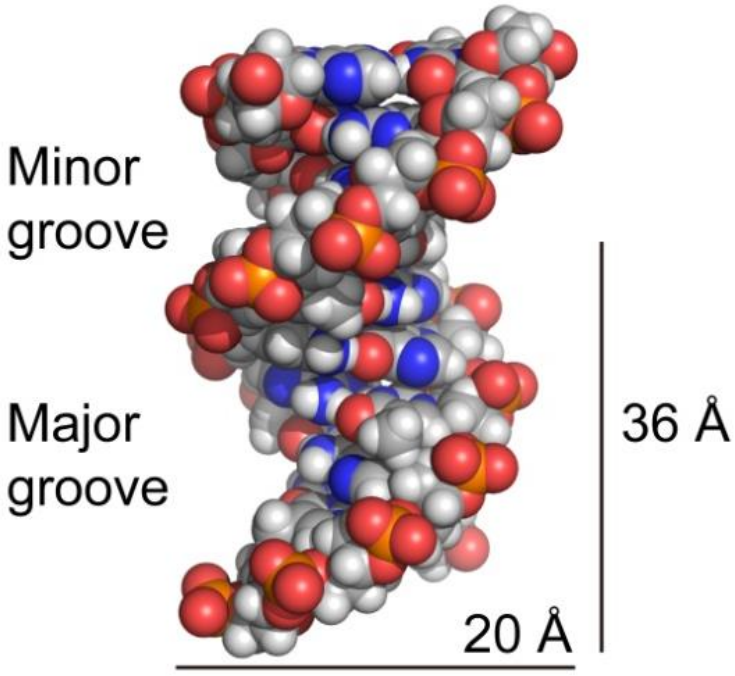


Figure 1-2: Chemical structure and components of B-DNA.

There are many possible conformations of DNA in nature. The factors affecting the conformation that adopts include DNA sequence, chemical modifications of the bases, and the type and concentration of metal ions. The most common conformations of DNA is B-DNA, which is present at neutral pH and physiological salt concentrations.[5] B-DNA is a right-handed helix, each residue in a single strand is separated by a distance of 3.4 Å and the strand turns every 10 residues due to a 36 ° angle between residues. A-DNA, although also adopting the right-handed helix, is shorter than B-DNA in rise/turn. The more shallow, wider minor groove and narrower major groove are also observable in A-DNA. This form usually occurs under non-physiological conditions in partially dehydrated samples of DNA.[6,7] Z-DNA, unlike B-DNA, forms as the left-handed helix and has a structure that repeats every 2 base pairs.[8] Z-DNA occurs in conditions, such as alternating purine-

pyrimidine sequences (especially poly(dGC)$_2$), negative DNA supercoiling, or high salt concentration and in the presence of specific cations.[9] Methylated DNA may also undergo a large change in conformation and may adopt the Z form.[10] These unusual structures can be recognized by specific Z-DNA binding proteins and may be involved in the regulation of transcription.[11] The chemical structures of A-, B-, and Z- DNA are shown in Figure 1-3.

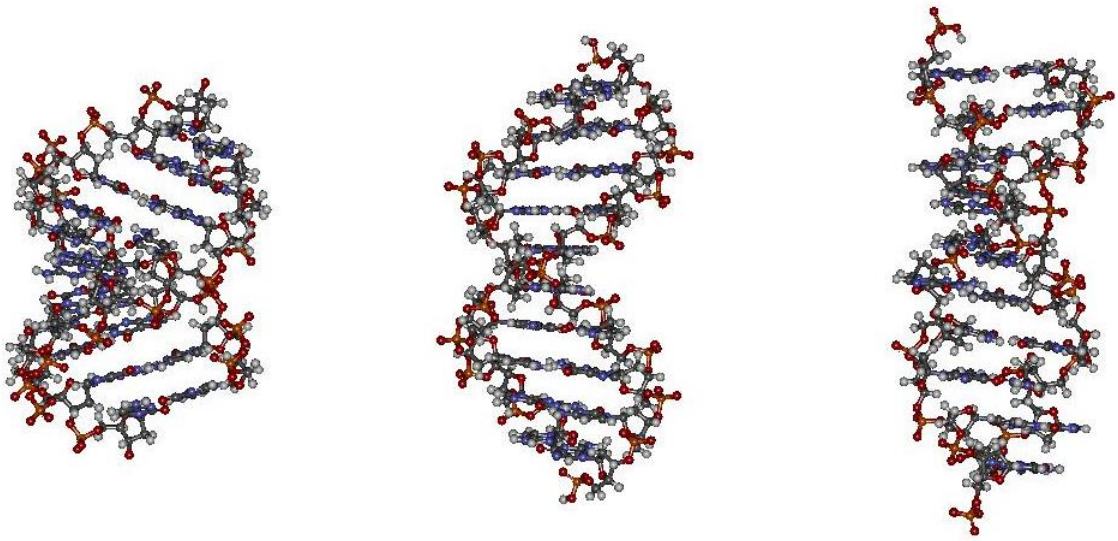
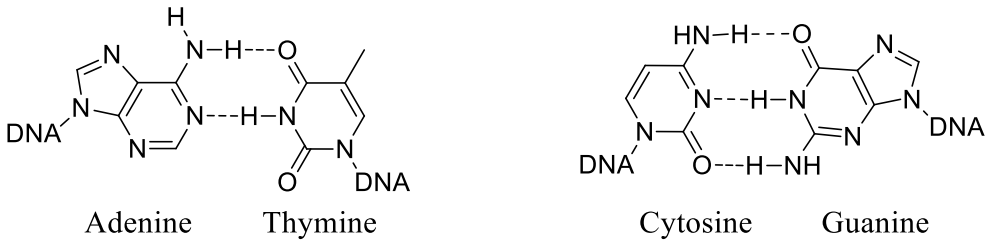


Figure 1-3. Chemical structures of A-form, B-form, and Z-form DNA.

In double helix DNA, each nucleobase is hydrogen bonded to another nucleobase in the complementary strand. This arrangement of two nucleotides binding together across the double helix is called a base pair. In the canonical Watson-Crick base pairing model, there are two types of base pairs: A-T and G-C (Scheme 1-1). Hydrogen bonding between nucleobases is an important factor for the stability of DNA double helices. In addition to hydrogen bonding, base stacking between adjacent bases is also a major stabilizing factor for DNA duplexes.[10]



Scheme 1-1. Watson-Crick base pairing: A to T and G to C.

DNA damage

DNA damage is a problem for living organisims because DNA is the repository of genetic information and its integrity and stability are essential. As a chemical entity, DNA is assaulted by many types of mutagens. There are two main types of DNA damage, endogenous and exogenous damage. Endogenous damage occurs when the DNA is attacked by oxidizing and alkylating agents produced during cellular metabolism, while exogenous damage is caused by external souces, such as high-energy electromagnetic radiation or environmental or dietary exposures to toxic chemicals. The rate of DNA damage varies from 1,000 to 1,000,000 lesions per cell per day.[12-14]

Once damaged, genetic information stored in DNA might be compromised and cellular metabolism might be altered, ultimately leading to mutations and genomic instability. This could result in the development of a variety of cancers. Multiple DNA repair mechanisms have evolved in cells to detect and repair damage that occurs in DNA. Mechanisms of DNA repair include direct chemical reversal, base excision repair, nucleotide excision repair, mismatch repair, double-strand break repair, and translesion synthesis.[15] If not properly repaired, the damaged DNA could result in blockage of

replication, leading to the death of a cell. Alternatively, the wrong bases could also be incorporated opposite the damaged lesion during replication, which is known as mutation.

Aflatoxin B_1 Formamidopyrimidine Adducts

Aflatoxins are a group of toxic and carcinogenic fungal metabolites which are isolated from *Aspergillus flavus* and *Aspergillus parasiticus*, and related fungi that contaminate peanuts, corn, and other agricultural products.[16-20] The name of aflatoxin was first created after the discovery that the cause of the death of more than 100,000 turkeys was *Aspergillus flavus toxins*, in 1960.[21,22] These toxins are human liver carcinogens, especially in combination with chronic infection with hepatitis B virus, and some of them have been designated as human liver carcinogens by the International Agency for Research on Cancer (IARC) in 1987. Exposure to aflatoxins occurs most commonly in developing areas, such as Africa and China.[23-25]

So far, at least 14 different aflatoxins have been discovered in nature[26] and there are four major aflatoxins: B_1, B_2, G_1 and G_2[27] (Figure 1-4). The designation of B and G comes from their blue or yellow-green fluorescence. Aflatoxin M_1 and M_2, where the M designates that these aflatoxins were isolated from milk of lactating animals fed aflatoxins, are two additional metabolic products.[28,29]

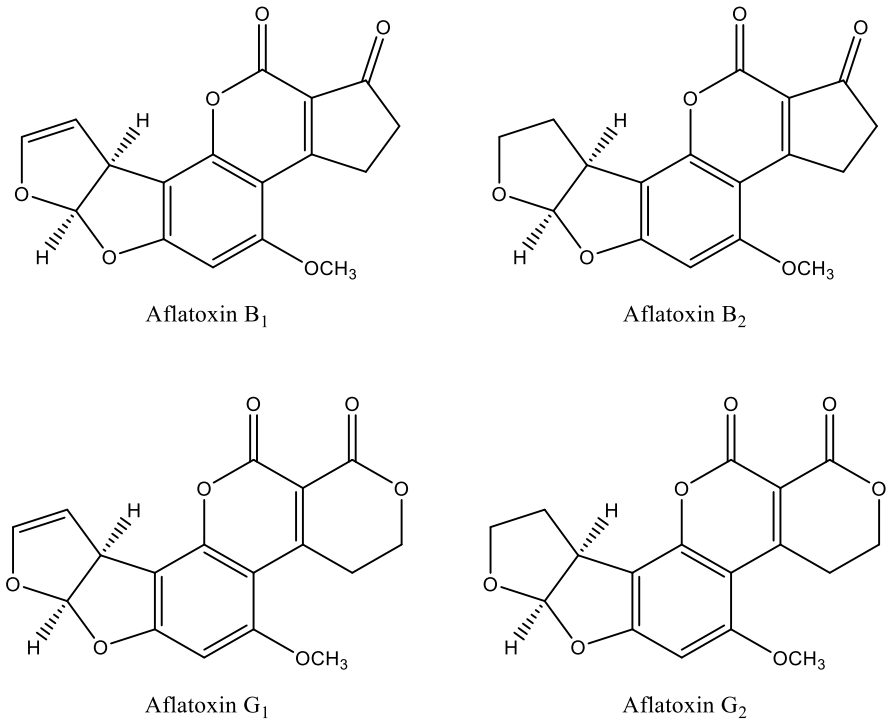


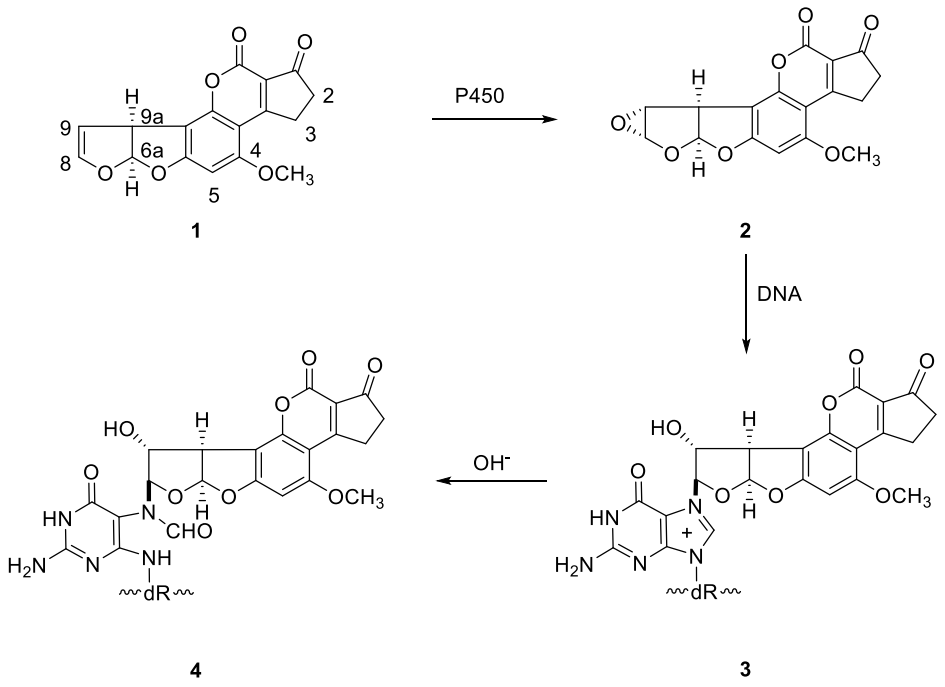
Figure 1-4. Four major aflatoxins.

Among the many different aflatoxins that have been discovered, aflatoxin B_1 (AFB_1) is the most toxic and potent,[19] and consequently, the most extensively studied. AFB_1 is a mutagen in bacteria,[30] and is a carcinogen in fish[31] and rodents.[32] Epidemiological studies suggest that AFB_1 causes cancer in humans.[33]

The main disease correlated to consumption of AFB_1 contaminated food is hepatocellular carcinoma (HCC), *[18, 24]* the most common form of primary liver cancer and the third leading cause of cancer death worldwide due to its poor prognosis.[34,35] Every year approximately 0.5–1 million new cases of HCC are diagnosed, causing 600,000 deaths globally per year.[36-38] Although chronic hepatitis B Virus (HBV) infection is a major factor for HCC, aflatoxins have been shown to increase risk.[39] In the regions with high aflatoxin exposure, such as China, India, Southern Africa, Gambia, Senegal, and Mozambique,

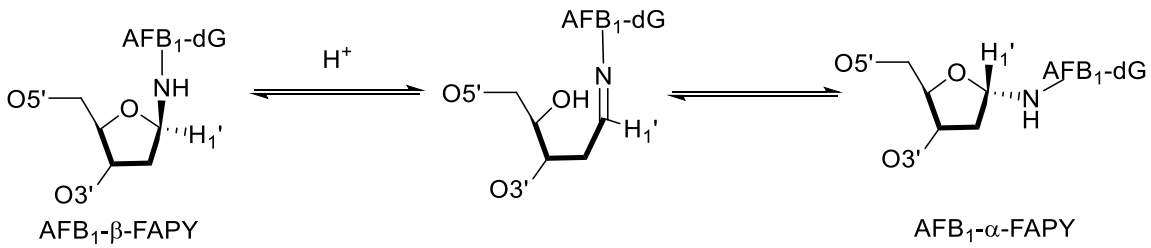
assessing liver tumor tissues revealed specific G to T mutations at the third base of codon 249 in the human cancer suppressor gene *p53,* which leads to a substitution of arginine for serine (R249S).[40] In comparison, in countries that do not consume aflatoxins-contaminated food, the rate of *p53* mutation in HCC is low.

Once digested, AFB_1 (**1**, Scheme 1-2) is primarily metabolized in humans by the liver enzyme cytochrome P450 3A4[41-43] to yield the genotoxic form, AFB_1-*exo*-8,9-epoxide (**2,** Scheme 1-2).[44] AFB_1-*exo*-8,9-epoxide is highly reactive with a $t_{1/2}$ of 1 s in water[45] and is the electrophilic species that covalently modifies DNA with high affinity.[41,43] Its regioselectivity of DNA adduction is attributed to intercalation above the 5′-face of guanine,[46] which places the epoxide in proximity and in the proper orientation to the N7 atom of guanine, facilitating a S_N2 reaction[47] to yield the cationic adduct **3** (Scheme 1-2), trans-8,9-dihydro-8-(N^7-guanyl)-9-hydroxyaflatoxin B_1.[44,46-50] The isomeric AFB_1 *endo*-8, 9-epoxide[51] does not react with DNA because the stereochemistry of this species prevents the S_N2 reaction from occuring.[49,52,53] While regioselectivity favors the adduct formed at the N7 position of guanine, low level other AFB_1-DNA adducts have been reported at other sites of guanine, adenine, or cytosine.[48,52,54-56] The cationic adduct is chemically labile and can depurinate to yield an apurinic site and AFB_1-guanine. Alternatively, it can undergo a base-catalyzed reaction resulting in the imidazole ring opening and the formation of AFB_1 formamidopyrimidine (AFB_1-FAPY) adduct (**4,**Scheme 1-2).[19,57-60] The FAPY adduct, which has a greater biological half-life in DNA, is more mutagenic, compared with the cationic adduct, and induces G → T transversions.[61]



Scheme 1-2: AFB_1 induced DNA damage *in vivo.*

The chemistry of the AFB_1-FAPY adduct has been characterized.[58,62,63] Chromatographically, there are a pair of separable isomers originally designated as the "major" and "minor" isomer[64,65] based on their equilibrium populations. Brown et al. demonstrated that those isomers correspond to the β and α anomers of AFB_1-FAPY adduct.[62] The β anomer stabilizes DNA and is mutagenic.[66] The α anomer destabilizes DNA and blocks replication (Scheme 1-3).



Scheme 1-3: Equilibrium between β and α anomers of AFB_1-FAPY adduct.

In addition to the α and β anomers, there are two possible geometrical isomers that are determined by the orientation of the formyl group of AFB_1-FAPY adduct. The isomer in which the oxygen of the formyl group and the adjacent H8 proton are on the same side is the *E* geometrical isomer, in contrast to the *Z* geometrical isomer that occurs when the oxygen and H8 are on the opposite side (Figure 1-5). [58,62,63] In previous reports,[58,62,63] a hydrogen-bond between the formyl group of FAPY and the exocyclic amino group of the 3′-neighboring adenine (X^5 CHO→A^6 H62) was predicted to stabilize the *E* geometrical isomer as opposed to the *Z* isomer (Figure 1-6). Hence, by changing the 3′-neighboring base to the guanine containg AFB_1 FAPY lesion, the ability to form this hydrogen bond would change. Consequently, the *E* geometrical isomer might not be the predominant species, due to the absence of hydrogen bond stabilization. When the 3′-neighboring base of the FAPY is thymine, in which the exocyclic amino group does not exist, a corresponding hydrogen bond with 3'-thymine is not possible. Thus, different rotameric forms are predicted according to loss of the stability provided by this hydrogen bond. For the same reason, when guanine is placed at the 3′-neighboring base of the FAPY, this hydrogen bond is also not possible. In the XC sequence, cytosine also has the exocyclic amino group, but the position of this group is different than in adenine. The strength of the potential hydrogen bond might be different as well. It is uncertain whether the *E* geometrical isomer still remains as the predominant species. Hydrogen bond stabilization has been also considered as one of the factors contributing to the abnormal thermal stability of AFB_1-β-FAPY modified DNA duplex, in addition to the base stacking. Hence, a lower melting temperature is predicted when placing a thymine at the 3′-neighbor of the damaged guanine, as well as guanine.

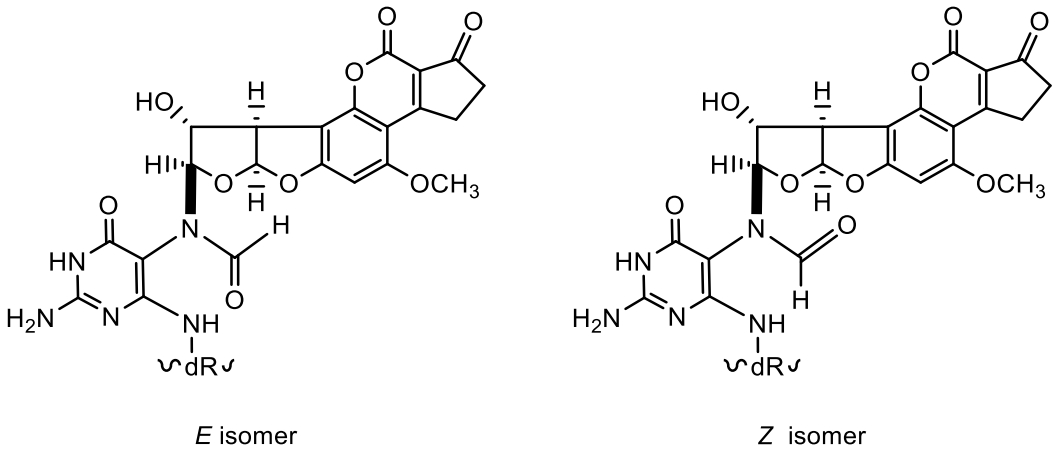


Figure 1-5. *E* and *Z* geometrical isomers of the AFB_1-FAPY adduct.

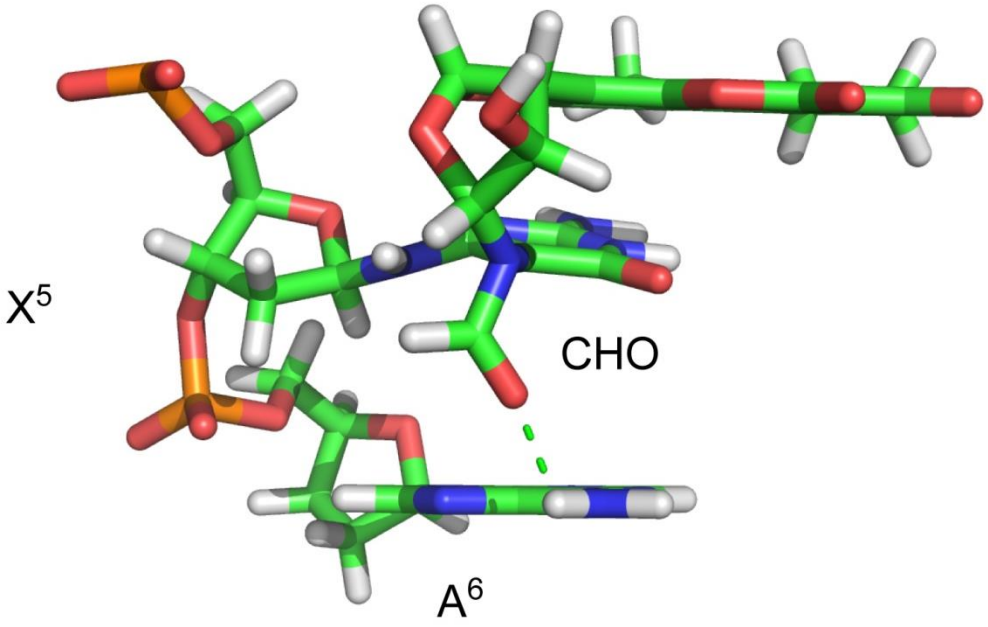


Figure 1-6. *E* geometrical isomer of AFB_1-β-FAPY adduct. The green dot line represents the potential hydrogen bond between the formyl group and 3′-adenine (PDB: 1HM1).

The primary focus of this dissertation is the elucidation of structures of specific oligonucleotides in which different bases are placed as the 3′ neighbor to the AFB_1 FAPY

adduct. Will the *E* geometrical isomer stabilized by a hydrogen bond in 5′-XA-3′ context still exist in other sequence contexts? How does the presence or absence of this hydrogen bond affect the overall structures and the thermal stabilities?

Structural Studies of Biological Macromolecules

The determination of the three-dimensional (3D) structures of biological macromolecules, such as proteins, DNA, and polysaccharides, is important and can help to understand their biological function during cellular processes. X-ray crystallography has been widely used as a crucial approach to biomolecular structural elucidation. The advantage of this technique is that there is almost no molecular weight restriction for solving high resolution structures, which makes X-ray crystallography an extremely important method for the structural determination of large biomolecules. To date, almost 90,000 crystal structures have been solved and deposited in the Protein Data Bank (PDB). Nuclear magnetic resonance (NMR) spectroscopy, another well proven tool for solving 3D structures, is usually used to analyze smaller molecules. One beneficial supplement of NMR to X-ray crystallography is that almost all biological macromolecules can be dissolved in aqueous solution easily. Moreover, many biological macromolecules are difficult to crystallize.

Structural Studies of Oligonucleotides Using NMR Spectroscopy

Structure determination by NMR is routinely used to determine 3D structures of smaller molecules, such as oligonucleotides. Compared to X-ray crystallography, NMR does not directly produce an image of a biomolecule but rather gives indirect structural

information, e.g. peak intensity and chemical shifts of individual nuclei. Analysis of this information, combined with computer calculations and refinements, can reveal the overall structure of a biomolecule.

To detertime a structure from NMR data, each individual proton needs to be assigned. Even oligonucleotides, however, still have many protons and the resonances for each proton may be severely overlapped in 1-D NMR spectra. 2-D NMR techniques, therefore, are widely used to alleviate this problem. Two most widely used NMR experiments exploit are through-bond interactions and through-space interactions, respectively. These are Correlated spectroscopy (COSY) and nuclear Overhauser effect spectroscopy (NOESY). COSY spectroscopy correlates the chemical shift of ^{1}H nuclei that are J-coupled to one another.[67] In the investigation of DNA duplexes, COSY spectroscopy gives important information about the H5 and H6 protons on cytosine, as well as the methyl group and H6 proton on thymine.

NOESY spectroscopy, on the other hand, exploits the dipolar interactions of nuclear spins for correlation of protons located within approximately 5 Å of each other, thus, providing distance information between protons.[68] Because there are in DNA mino and amino protons, which are solvent-exchangeable, the NOESY experiment must be performed within H_2O.[69-71] For non-exchangeable protons, D_2O is usually used to avoid excessive solvent signals. A typical NOESY spectrum for the non-exchangeable protons in a DNA duplex is shown in Figure 1-7. The spectrum can be divided into several areas according to the distinctive chemical shifts of different groups in DNA.

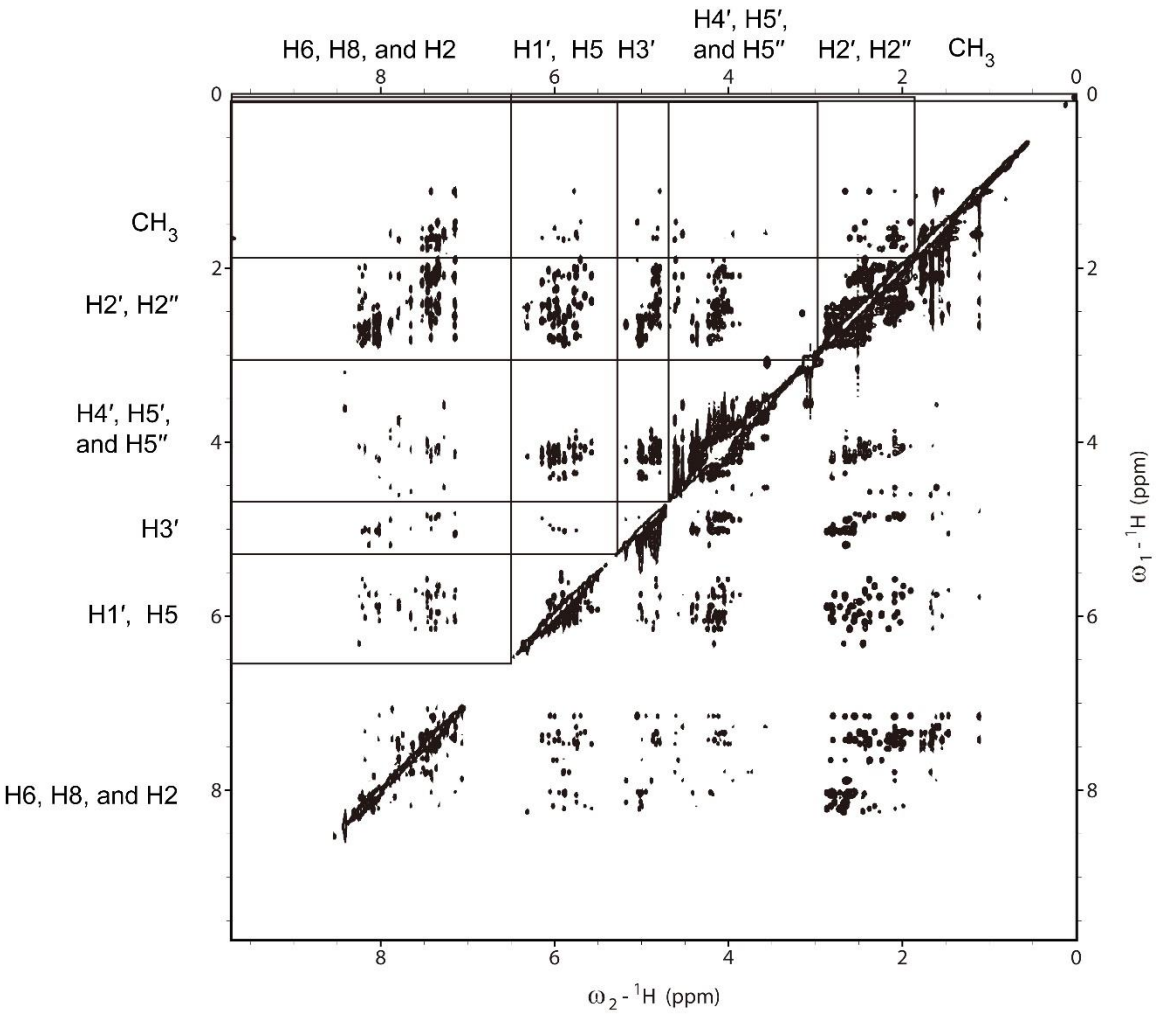


Figure 1-7. Typical chemical shift regions for non-exchangeable oligonucleotide protons in a typical two-dimensional NOESY spectrum.

The key to the assignment for a NOESY spectrum of the non-exchangeable protons of a DNA duplex is to follow the distance restriction (<5Å) between adjacent bases through the DNA strand.[72] Starting from the 5′ end of the DNA strand, an intra-base cross peak can be observed between the aromatic proton (H6 or H8) on the base (purine or pyrimidine, and its own H1' proton on the sugar ring. Next, another inter-base cross peak of this H1' proton to the aromatic proton (H6 or H8) on the 3'-neighboring base can be also observed. The connectivity between the aromatic proton and H1' proton can proceed through the entire strand, as well as

between the aromatic proton and other deoxyribose protons, such as H2', H2", and H3'. This sequential assignment method is known as a "NOESY walk" (Figure 1-7). A COSY experiment can be used to complete the assignment by providing information for the H6 proton on cytosine. For the exchangeable protons, the NOESY walk method can also be used to assign the cross peaks between the amino protons of guanine and the imino protons of thymine in an H_2O NOESY spectrum.

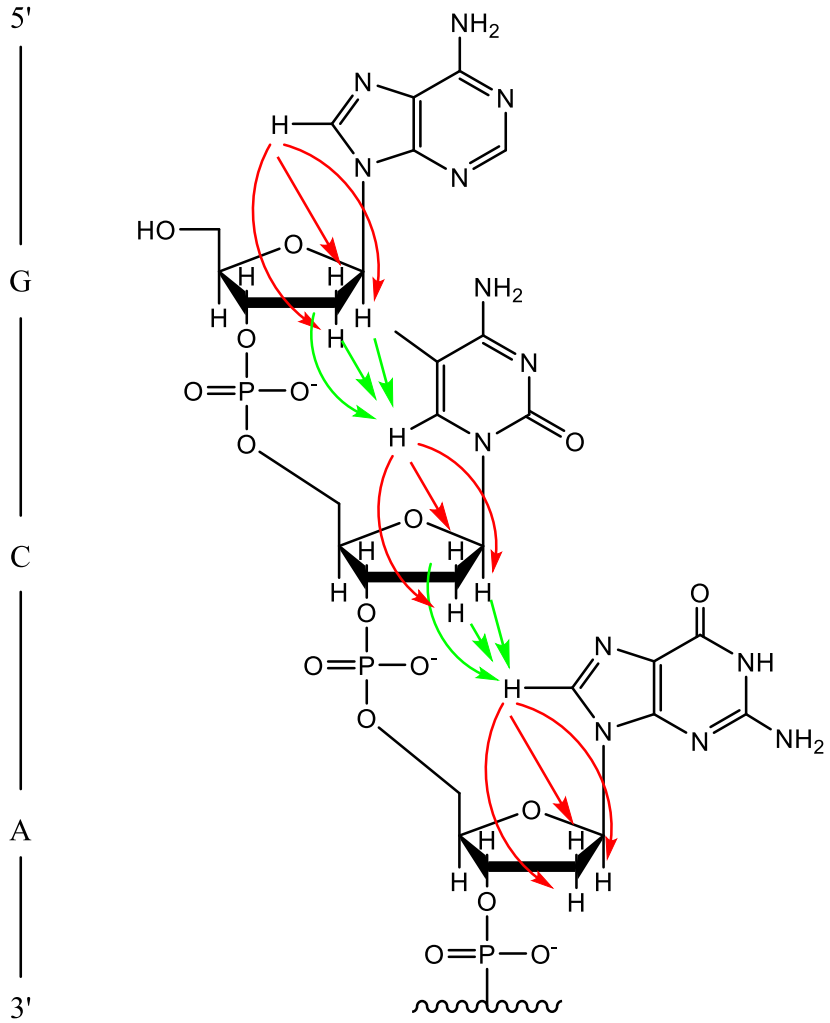


Figure 1-8. Sequential assignment (NOESY walk) of an oligonucleotide using NOESY spectroscopy.

After the assignment of a NOESY spectrum is completed, the cross-peak volumes are measured using a Gaussian function and converted into inter-proton distance restraints using the Matrix Analysis of Relaxation for Discerning Geometry of an Aqueous Solution (MARDIGRAS)[73-76] program. Complete relaxation matrix analysis (CORMA) is implemented to derive inter-proton distances. The algorithm can also correct for the spin diffusion effect at long NOE mixing times.[77] Combined with other restraints, e.g. backbone torsion angle and base pairing restrains, a complete restraints file is formed for the restrained molecular dynamics (rMD) calculation. To begin the rMD calculation, an initial starting structure, along with molecular topology and parameter information, is necessary as a reference. This starting structure, which can be an available PDB structure, or can be built using computer software, is refined by potential energy minimizations (PEM) to relax the bonds and remove any unnecessary stress on the molecule in order to reach the local energy minimum point without making drastic changes in the structures. This relaxed molecule is then refined by rMD calculations using a simulated annealing protocol and appropriate force field.

During the simulated annealing method, the system is heated to a high temperature, such as 600 K, allowing the molecule to overcome the conformational energy barriers. When the system is cooled slowly, the molecule seeks the lowest energy state with the complete restraints file applied. The rMD calculation can be run multiple times to find the structure that best agrees the experimental data. The root mean square deviation (rmsd) of the emerging structures is used to evaluate the convergence of the rMD calculations. The accuracy of the solution structure obtained from the rMD calculations is evaluated by comparing the calculated NOE intensities of the structure coordinate files to actual

intensity files from NMR data, using the program complete relaxation matrix analysis (CORMA).[77-79] Finally, helicoidal analysis is performed using the programs, 3DNA[80] and CURVES (Figure 1-9).[81,82]

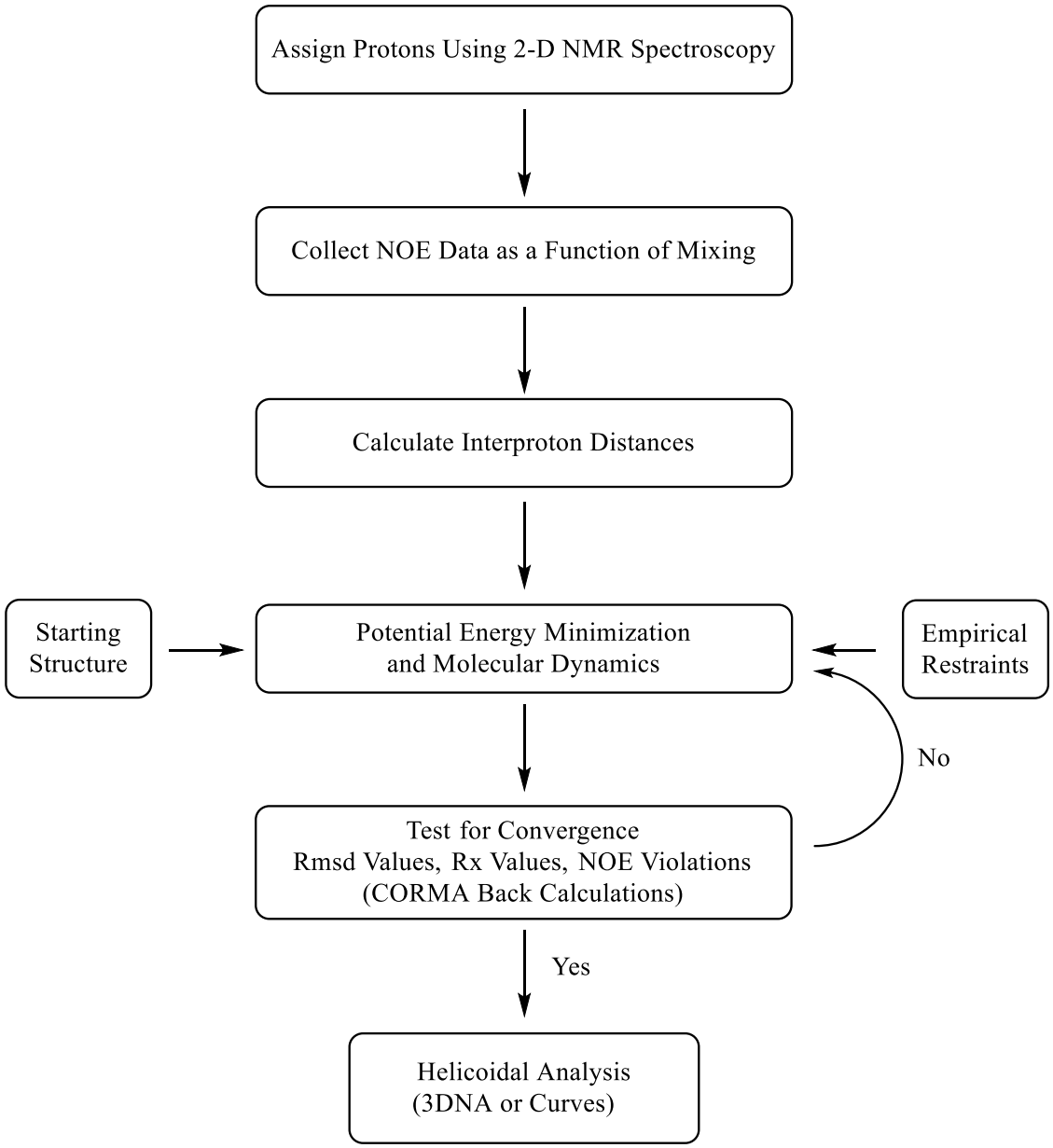


Figure 1-9. Strategy for the NMR-generated structural refinement of the oligodeoxynucleotide.

CHAPTER II

Materials and methods

Biological Hazards

Aflatoxin and its epoxides are highly toxic and potently carcinogenic because of their electrostatic nature. Appropriate experimental conditions, e.g. well-ventilated hood and respiratory mask, and suitable containment procedures should be used to prevent inhalation. NaOCl can be used to destroy aflatoxin.

Materials

The unmodified oligodeoxynucleotides were synthesized and purified by anion-exchange high performance liquid chromatography (HPLC) from the Midland Certified Reagent Co. (Midland, TX). Samples were repurified by reverse-phase HPLC and analyzed by mass spectrometry after receiving. The concentrations of single-stranded oligodeoxynucleotide were determined by UV absorbance at 260 nm on the basis of the extinction coefficient of each strand. AFB_1 was purchased from Sigma-Aldrich Chemicals (Milwaukee, WI).

Dimethyldioxirane Synthesis

Dimethyldioxirane was synthesized from oxidization of acetone following the general protocol.[83] Reagent grade H_2O (15mL), $NaHCO_3$ (16 g, 190 mmol), and acetone (15 mL) were added to a stirred reaction vessel after the cold finger was chilled. Water

aspiration was used to apply a slight vacuum as nitrogen was flowed through the system. Then, H_2O (10 mL) and acetone (10 mL) were dripped into the reaction vessel via a liquid addition funnel, while OXANE® (monopersulfate compound, CAS 70693-62-8) (30 g, 49 mmol) was added in approximately 1 g increments via a solid addition funnel. The collection for the dimethyldioxirane solution in aceteone was approximately 45 min. A polypropylene container containing anhydrous $MgSO_4$ was used to store the yellowish dimethyldioxirane solution at -20 ℃. The concentration for this dimethyldioxirane solution was determined as 50 mM by ^{1}H NMR (solvent = acetone). The height of the ^{13}C satellite peak to the right of the acetone signal[83] was used to compare the height of the dimethyldioxirane methyl proton peak (δ 1.65 ppm). Successful drying of the dimethyldioxirane was established by the magnitude of the residual water peak (δ 2.8 ppm).

Aflatoxin B_1 Adduct Synthesis

Aflatoxin B1 epoxide was synthesized from oxidization of acetone following the general protocol.[44] AFB_1 (1 mg, 3.2 μmol) was dissolved in anhydrous CH_2Cl_2 (0.5 mL, 3.2 mM) in an amber glass reaction vial in order to block ambient light and avoid potential photo products. Dimethyldioxirane solution (0.3 mL, 6.4 μmol) was then added to the AFB_1 solution. After approximately 15 minutes, the reaction solution was dried by gently blowing nitrogen to give the resulting AFB_1 epoxide. ^{1}H NMR was used to determine the completeness of the reaction and possible presence of dihydrodiol.[44] To synthesize the AFB_1 modified sample, the unmodified oligonucleotide, 5'-d(CTAAGATTCA)-3' containing the targeted N7-dG alkylation site (underlined), was annealed with 5'-

d(AATCTTA)-3' to form a partially double-stranded scaffold strand in 200 μL of 100 mM sodium phosphate buffer (pH 6.5, 100 mM NaCl). AFB_1 epoxide was dissovled in 200 μL of anhydrous CH_2Cl_2 (< 0.003% H2O), and was then added into the oligonucleotide solution. The biphasic mixture was stirred at 5 ℃ for 30 min. The aqueous phase was extracted from the resulting mixture and then directly dissolved in Na_2CO_3 solution (5 mL, 100 mM, pH 10) for 2 hours at room temperature to form the AFB_1 formamidopyrimidine (FAPY) adduct. The reaction was monitored and the the AFB_1-FAPY modified oligonucleotide was purified by using semi preparative reverse-phase HPLC (Gemini C-18 250 × 10 mm column, Phenomenix, Inc., Torrance, CA) at a flow rate of 2 mL/min, with a linear 30 minutes gradient of 5-30% CH_3CN in 0.1 M ammonium formate (pH 6.5). The diode array detector was configured to monitor both 254 and 360 nm wavelengths for the eluent. The adducted oligodeoxynucleotide was lyophilized and characterized by MALDI-TOF mass spectrometry. MALDI-TOF mass spectra were obtained on a Voyager-DE (PerSeptive Biosystems, Inc., Inc., Foster City, CA) instrument in negative reflector mode. The matrix used in each of these studies contained 0.5 M 4-hydroxypicolinic acid and 0.1 M ammonium citrate. The oligodeoxynucleotides 5'-d(CTAAGCTTCA)-3', 5'-d(CTAAGTTTCA)-3', 5'-d(CTAAGYTTCA)-3' (Y=7-deazaG) were synthesized and characterized using the same procedures.

NMR sample preparation

The unmodified and modified oligodeoxynucleotide and their complementary strands were annealed in a 10 mM sodium phosphate buffer containg 0.1 M NaCl and 50 μM Na_2EDTA at pH 7.0. In each study, the annealed duplex oligodeoxynucleotide was

eluted from a column containing DNA Grade Biogel hydroxylapatite (Bio-Rad Laboratories, Richmond, CA) with a gradient from 10 to 200 mM NaH_2PO_4 at pH 7.0 to remove excess single DNA strand. The eluent was then lyophilized, resuspended in H_2O (0.5 mL), and desalted using Sephadex G-25 (Bio-Rad Laboratories, Richmond, CA).

Thermal Melting Experiments

The melting temperature (T_m value) experiments were carried in 10 mM sodium phosphate buffer containing 0.1 M NaCl, and 50 μM Na_2EDTA at pH 7.0. The concentration of AFB_1-FAPY modified duplex was approximately 2 μM for each sample. The temperature was increased at a rate of 1 ℃ from 10 to 80 °C. Absorbance was measured at 260 nm on a Varian Cary 4E spectrometer. The T_m of the unmodified and modified oligodeoxynucleotides were obtained by determining the inflection points of the absorbance vs. temperature curves from the first derivatives.

NMR Spectroscopy

The modified duplex samples were prepared in 10 mM sodium phosphate buffer containing 0.1 M NaCl, and 50 μM Na_2EDTA at pH 7.0 to reach the final concentration of 2 mM. For observation of non-exchangeable protons, the samples were exchanged three times with 99.9% D_2O and dissolved in 99.99% D_2O (180 μL). To observe exchangeable protons, the samples were dissolved in 9:1 H_2O/D_2O (180 μL). For each of the studies, ^1H NMR spectra for unmodified and modified oligodeoxynucleotides were collected at 800 MHz and 900 MHz on Bruker spectrometers. Chemical shifts were referenced to water. Data were processed using TOPSPIN software (Bruker Biospin Inc., Billerica, MA). The

Nuclear Overhauser Effect Spectroscopy (NOESY) and Correlated Spectroscopy (COSY) spectra of the unmodified and modified samples in D_2O were collected at 283 K at 800 MHz and 900 MHz respectively. The Heteronuclear Multiple Quantum Correlation Spectroscopy (HMQC) spectra of the modified samples in D_2O were collected at 283 K at 600 MHz. The NOESY and 1D spectra of the modified and unmodified samples in H_2O were collected at 278 K at 800 MHz.

NOESY spectra of the non-exchangeable protons were recorded using TPPI phase cycling with mixing times of 60, 150, 200, and 250 ms at 900 MHz. Spectra for the exchangeable protons were recorded using a 250 ms mixing time. These experiments were recorded with 1024 real data points in the d1 dimension and 2048 real data points in the d2 dimension. A relaxation delay of 1.5 s was used. Water suppression was performed using the WATERGATE sequence[84].

COSY spectra were obtained in magnitude modes, using 512 data points in the d1 dimension and 2048 data points in the d2 dimension at 800 MHz. The indirect dimension was zero-filled achieving a 2048 x 2048 overall matrix. The skewed sine-bell squared apodization was utilized with a 180 ° phase shift. States-TPPI quadrature detection was used. A relaxation delay of 1.5 s was used and the sweep width was set to 10 ppm.

HMQC spectra were recorded at 600 MHz for modified DNA samples. Spectra were recorded with a ^{1}H sweep width of 10 ppm and a ^{13}C sweep width of 80 (125-205) ppm. A relaxation delay of 1.4 s was used. Echo-Antiecho quadrature detection was used. An 80 μs pulse was used for garp proton decoupling. Pulses were optimized for ^{1}J CH coupling constants (190 Hz). Experiments were recorded with 1024 real data points in d2 and 96 real data points in d1. The indirect dimension was zero filled and linear predicted

to obtain an overall matrix size of 2048 x 1024 real points. A skewed sinebell-squared apodization function with a 90 ^{o}phase shift was applied in both dimensions.

Experimental Restraints

The chemical shift values of the oligonucleotide protons were assigned in the NOESY spectra using the program SPARKY.[85] Footprints were drawn around the NOE cross-peaks obtained at a mixing time of 150, 200 and 250 ms using SPARKY software. Cross-peak intensities were determined by volume integration. A hybrid intensity matrix was generated by combining the intensities of the cross-peaks and the intensities generated from complete relaxation matrix analysis of a starting DNA structure.[86-88] The program MARDIGRAS,[73-76] using the RANDMARDI algorithm, was used to refine the hybrid matrix by iteration for better agreement between the calculated and experimental NOE intensities. The calculations were initiated using isotropic correlation times of 2, 3 and 4 ns, and with site-specific modified B-form starting structure and the three mixing times to convert the intensities to distances. Analysis of this resulting data allowed creation of upper and lower bound distance restraints used in subsequent restrained molecular dynamics (rMD) calculations, and the corresponding standard deviations for the distance restraints. 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.

Starting Structures

An unmodified classical B type DNA was used to create the starting structures for the refinement.[89] The AFB_1-FAPY modified guanine was constructed using the BUILDER module of INSIGHT II (Accelrys, Inc., San Diego, CA). The atomic partial charges of FAPY modified lesion were calculated by using GAUSSIAN 03.[90] Geometry optimization and frequency calculations were performed using the B3LYP density functional (DFT) method with the 6-31G* basis set. Potential points were written out with a density of 6 points per unit area in the electrostatic potential (ESP) fit. Gaussian ESP output was converted to restrained electrostatic potential (RESP) charges using the program ANTECHAMBER.[91] The AFB_1-FAPY residue is not directly tractable to quantum calculations due to its comparatively large size (35 heavy atoms). Therefore, RESP charges were calculated for AFB_1 and the modified base + sugar separately. For this reason, unique library input files for AMBER were prepared for the AFB_1 adduct and modified base-deoxyribose. The resultant optimized structures and charges were used as parameters for rMD calculations. Frequency analysis was used to test for convergence. Diagonalization of the Hessian matrix will produce positive eigenvalues when a structure is at a minimum.[92-95]

Restrained Molecular Dynamics (rMD) Calculations

Restrained molecular dynamics were conducted using the AMBER 12 suite.[96] Coordinate and topology files were generated with xLEaP[97] using ff10 force field. The restraint energy function was comprised of terms describing distance and dihedral restraints as square-well potentials.[98] The generalized Born solvent model was used with a salt

concentration of 0.2 mM.[99,100] The temperature was controlled by coupling the molecule to a temperature bath during the 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. The During steps 1001-2000, the system was kept at 600 K with a coupling of 0.5 ps. 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.

Ten 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 and energy-minimized for 200 iterations using the conjugate gradient algorithm. Complete relaxation matrix analysis (CORMA)[77-79] was used to performed back-caculation on the intensities calculated from these emergent structures with the distance restraints. Helicodial analysis of the backbone was carried out using 3DNA[80] and Curves.[81,82]

Neutralizing sodium ions was added into a representative structure from simulated annealing calculations to counterize the charge on DNA chain. The DNA chain was immersed by a truncated octahedral TIP3P water box with a periodic boundaries at a distance of 8 Å from the edge of the water box. The solvated system was then equilibrated

using standard protocols. Briefly, in the first stage, the the positions of the water and ions was minimized for 1000 steps (500 steps of steepest descent minimization followed by 500 steps of conjugate gradient minimization) at constant volume periodic boundaries using fixed position after the initial minimization, thus allowing the solvent and counter ions to equilibrate. In the second stage, the entire system was minimized for 2500 steps with no positional restraints at a constant volume allowing the solute to equilibrate to its solvent. Next, the system was allowed to heated from 0 K to 300 K over 20 ps at constant volume with weak restraints on the DNA, followed by a 1 ns rMD production; NMR restraints and empirical restraints were slowly applied to the DNA duplex during the calculation period. The Langevin thermostat[101,102] with a collision frequency of 1 ps^{-1} was used to control the temperature and electrostatic interactions were treated with the particle mesh Ewald (PME) method[103] throughout the equilibration and production periods. A 10 Å cutoff for non-bonded interactions was used and bond lengths involving hydrogen were held fixed using the SHAKE algorithm.[104] Assessment of the accuracy of calculated MD structures was achieved by complete relaxation matrix analysis (CORMA). SUPPOSE was used to compare the RMSD values of heavy atoms between each final structure. PTRAJ was used to extract hydrogen bonding occupancies, ring puckers, average structures, and other dynamic properties from molecular dynamics trajectories. Both SUPPOSE and PTRAJ are distributed with AMBER.[96]

CHAPTER III

Solution structure of AFB_1-β-FAPY modified AXA duplex

Introduction

This chapter addresses the solution structure of AFB_1-β-FAPY in the oligonucleotide 5'-CTAAXATTCA-3'•5'-TGAATCTTAG-3'. The solution structure of AFB_1-β-FAPY in the AXA sequence context agrees with the FAPY structure in previous data, indicating that the FAPY structure is independent of the 5'-neighbor.

Results

Sample Properties

The double strand AFB_1-β-FAPY modified oligonucleotide, 5′-d($C^1T^2A^3A^4X^5A^6T^7T^8C^9A^{10}$)-3′•5′-d($T^{11}G^{12}A^{13}A^{14}T^{15}C^{16}T^{17}T^{18}A^{19}G^{20}$)-3′, was purified using HPLC. The identity of the duplex was verified using MALDI-TOF mass spectroscopy: for 5′-d($C^1T^2A^3A^4X^5A^6T^7T^8C^9A^{10}$)-3′, calc'd 3357.1, found 3356.5; for the complementary strand 5′-d($T^{11}G^{12}A^{13}A^{14}T^{15}C^{16}T^{17}T^{18}A^{19}G^{20}$)-3′, calc'd 3042.0, found 3042.8 (Figure 3-1). The ratio of two strands was determined to be 1:1 after correction for the respective absorbance coefficients by using capillary gel electrophoresis. The melting temperature of the AFB_1-FAPY modified duplex was 41 ℃ (Figure 3-2), higher than the 31 ℃ melting temperature of the unmodified duplex.

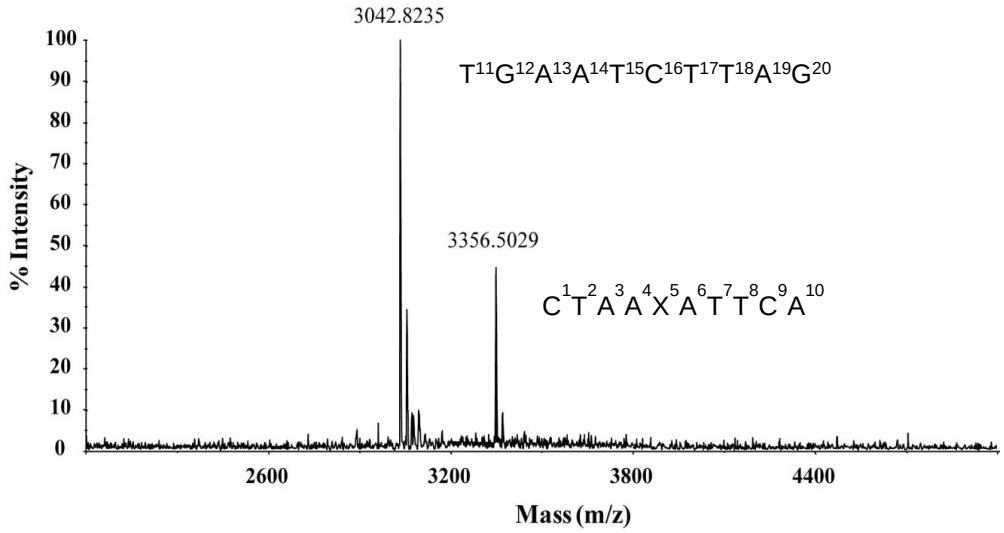


Figure 3-1. MALDI mass spectrum of AFB_1-β-FAPY modified AGA duplex.

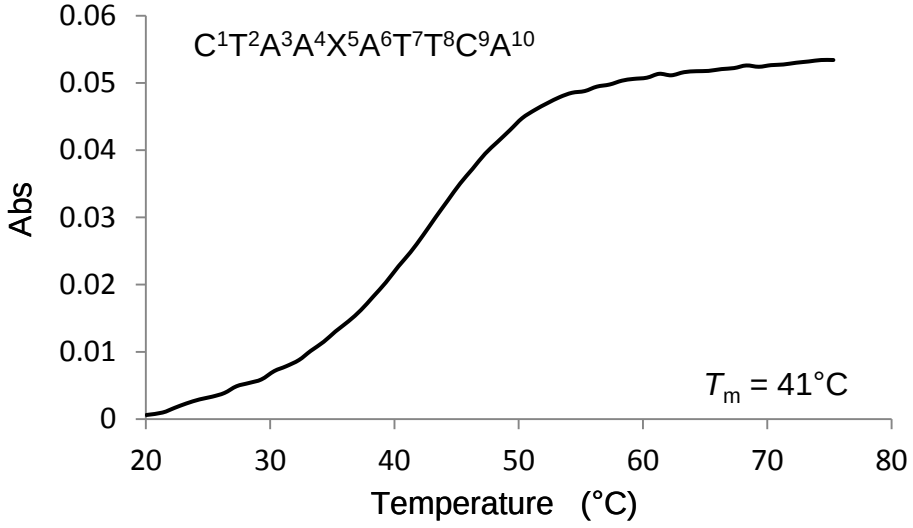


Figure 3-2. UV-melting curves of AFB_1-β-FAPY modified AGA duplex.

DNA ^1H Resonance Assignments

Nonexchangeable DNA Protons

The resonances of the non-exchangeable protons of the AFB_1-β-FAPY modified AGA duplex were assigned using the sequential NOE connectivity of the base proton H6

or H8 dipolar couplings with H1′ deoxyribose protons.[105,106] For the modified strand, the NOE connectivity started from C^1 to A^4 Then an interruption was observed between A^4 H1′ and X^5 NOE connectivity, due to the loss of the guanine H8 proton because of the opening of the guanine imidazole ring in the FAPY formation. The connectivity was then observed from the formyl proton of the FAPY base and the 3′-neighbor, continuing to the 3′-terminus. For the complementary strand, the interruption of the sequential NOE connectivity was also observed between C^{16} H1′ and T^{17} H8. Expanded plots of the NOESY spectrum for the AFB_1-β-FAPY modified AGA duplex are shown in Figure 3-3. The purine and pyrimidine aromatic protons, the thymine methyl protons and the deoxyribose H1′, H2′, H2″, and H3′ protons were successfully assigned. The H4′, H5′, and H5″ protons were only partially assigned due to heavy overlapping peaks and the effects of spin diffusion at higher mixing times.

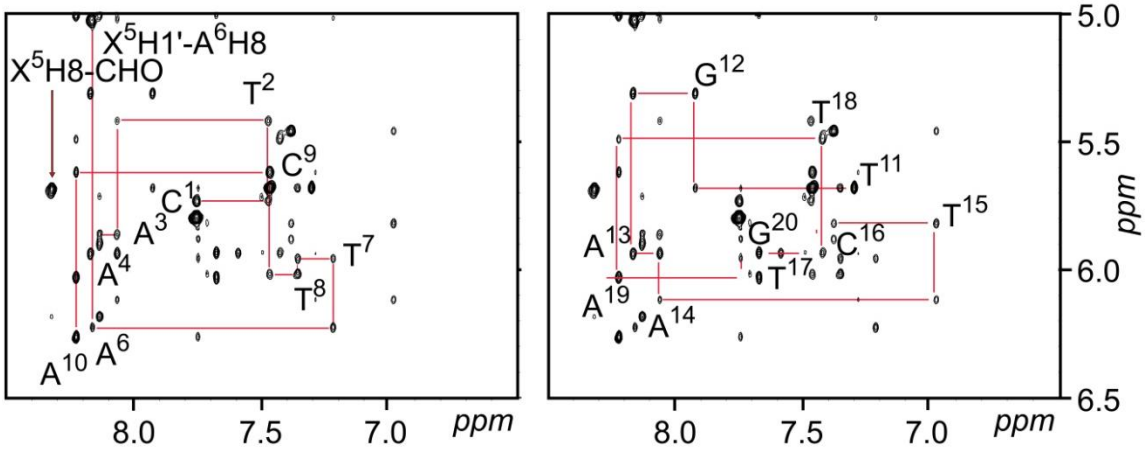


Figure 3-3. NOE connectivity of base H8/H6 protons with deoxyribose H1′ protons of the AFB_1-β-FAPY modified AXA duplex. (A) The modified strand. (B) The complementary strand. X = AFB_1-β-FAPY. The experiment was carried out at 250 ms mixing time and 900 MHz. The temperature was 283 K.

Anomeric Configuration

The assignment of the H2′ and H2″ resonances were based on their relative cross peak intensities to H3′ at NOE mixing time of 60 ms. The configuration at C1′ at X^5 was determined by unequivocally identifying the H2′ and H2″ to H1′ (Figure 3-4). The intensity of the X^5 H1′ to X^5 H2′ NOE was less than the X^5 H1′ to X^5 H2″ NOE, indicating the β configuration.

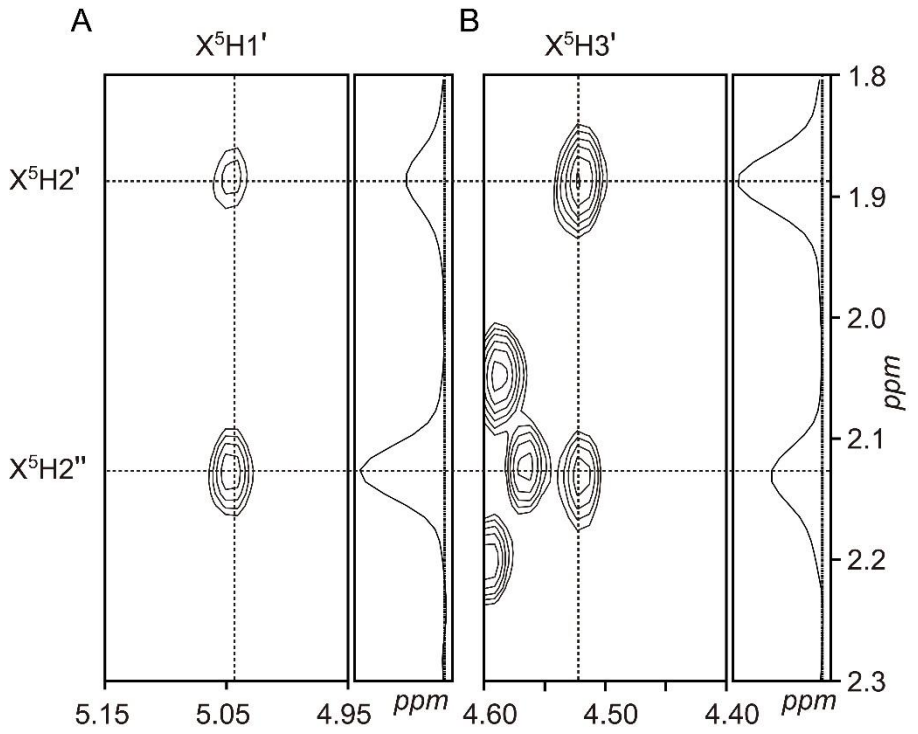


Figure 3-4. Analysis of NOE intensities for the deoxyribose protons of the AFB_1-β-FAPY modified AXA duplex. (A) The NOE peaks from H1′ to H2′, H2″. (B) The NOE peaks from H3′ to H2′, H2″. X = AFB_1-β-FAPY. The experiment was carried out at 250 ms mixing time and 800 MHz. The temperature was 283 K.

Exchangeable DNA Protons

The resonances of the base imino protons were assigned on the basis of sequential connectivity between adjacent base pairs in the NOESY spectra, and the assignments were supported by NOEs to the amino protons of Watson-Crick base pairs.[107] There was an interruption of the sequential imino-to-imino proton NOEs of adjacent base pairs between X^5 N1H and T^{17} N3H imino resonances. The strong cross peaks from X^5 N1H to C^{16} N4H1 and C^{16} N4H2 amino protons indicated that Watson-Crick hydrogen bonding between X^5 and C^{16} was intact. Compared to unmodified duplex, the A^6 N6H2 non hydrogen bonded exocyclic amine proton shifted downfield 0.72 ppm at 278 K, suggesting involved in a hydrogen bond(Figure 3-5).

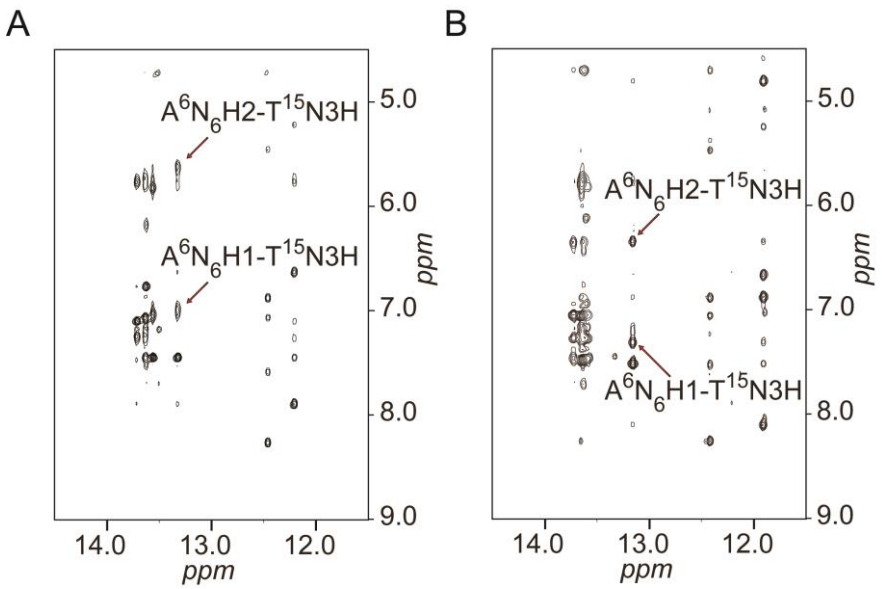


Figure 3-5**.** Comparison between the A^6 H61 and H62 imino protons. (A) Unmodified duplex. (B) AFB_1-β-FAPY modified AGA duplex. The experiment was carried out at 250 ms mixing time and 800 MHz. The temperature was 278 K.

NMR Spectroscopy of Formyl Proton Resonance (CHO)

A single peak was observed for the AFB_1-β-FAPY modified AXA duplex in an HMQC experiment acquired at 283 K. This peak revealed the presence of carbonyl resonance at 168.35 ppm, coupled to proton resonance at 8.4 ppm, confirming the assignment of the formyl proton (Figure 3-9).

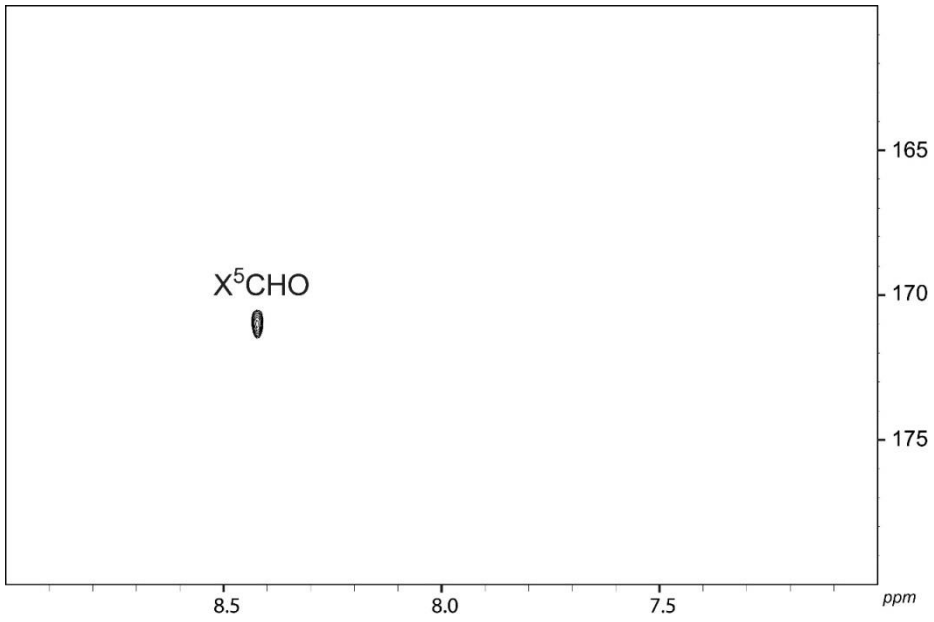


Figure 3-6. NMR analysis of ^{1}H-^{13}C HMQC of AFB_1- β-FAPY modified AXA duplex. The experiment was carried out at 600 MHz and the temperature was 283 K.

Aflatoxin FAPY Protons

The AFB_1 H5, H6a, H8, H9, H9a, and $–OCH_3$ resonances were assigned from a combination of NOE connectivities and chemical shift data (Figure 3-6). AFB_1 H6a and H9a were identified from both COSY and NOESY experiments. AFB_1 H8 and H9 were assigned based on NOEs between H6a or H9a, and between themselves. A strong NOE was observed between AFB_1 H5 and AFB_1 $–OCH_3$, revealing that the latter resonance was

at δ 3.52 ppm, while AFB_1 H5 was at δ 5.74 ppm. The observation of a strong NOE peak between X^5 CHO to H8 established the X^5 CHO resonance at δ 8.30 ppm, confirming the assignment of X^5 CHO in the HMQC experiment. The assignment of X^5 CHO resonance was supported by NOEs to AFB_1 H6a, H9a and H9. The cyclopentenone ring protons AFB_1 $H2_\alpha$, $H2_\beta$, $H3_\alpha$, and $H3_\beta$ were identified from a combination of COSY and NOESY experiments.

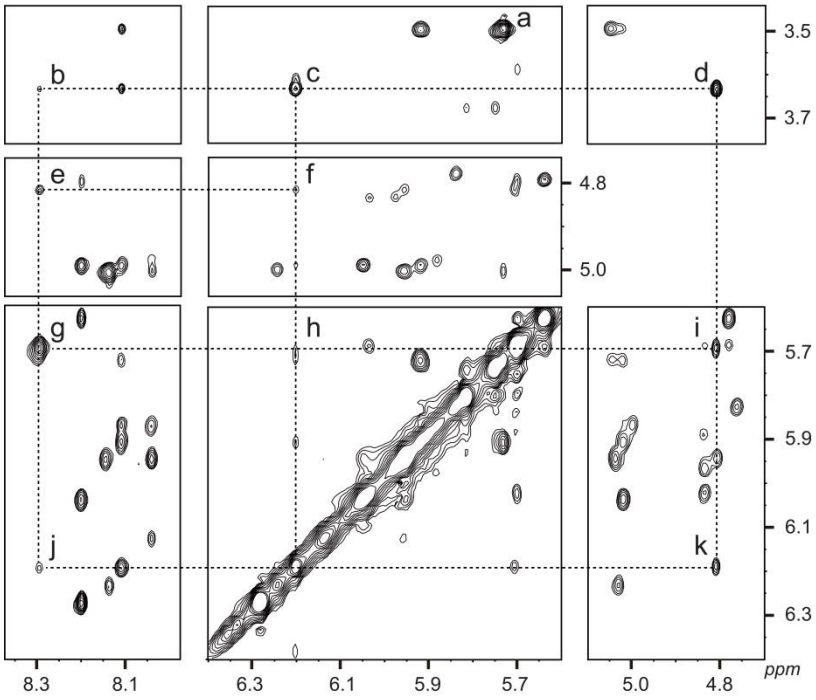


Figure 3-7. NOE assignments of the FAPY protons of the AFB_1-β-FAPY modified AXA duplex. The cross peaks are assigned as: (a) $X^5OCH_3 \rightarrow X^5H5$; (b) $X^5H9a \rightarrow X^5CHO$; (c) $X^5H9a \rightarrow X^5H6a$; (d) $X^5H9a \rightarrow X^5H9$; (e) $X^5H9 \rightarrow X^5CHO$; (f) $X^5H9 \rightarrow X^5H6a$; (g) $X^5H8 \rightarrow X^5CHO$; (h) $X^5H8 \rightarrow X^5H6a$; (i) $X^5H8 \rightarrow X^5H9$; (j) $X^5H6a \rightarrow X^5CHO$. The experiment was carried out at 250 ms mixing time and 900 MHz. The temperature was 283 K.

Aflatoxin FAPY to DNA NOEs

A total of 34 NOEs from AFB_1 protons to DNA protons were observed. The protons of the two AFB_1-fused furan rings showed NOEs to major groove and imino protons of the DNA; most of which were to the 5′ neighboring base-pair A^4•T^{17}. Thus, H6a and H9a, which are located on the same face of the AFB_1 moiety, both exhibited NOEs to A^4H8. A weaker NOE was observed for AFB_1 H9. The AFB_1 H5 and $–OCH_3$ protons exhibited NOEs with minor groove and imino DNA protons. These were primarily to base A^4•T^{17}, in the 5′ direction, and to the modified nucleotide X^5 (Figure 3-7). These included NOEs between AFB_1 $–OCH_3$ and A^4 H1′, A^4 H2′, A^4 H2″, A^4 H2, T^{17} N3H, X^5 H1′, and X^5 N1H. The cyclopentenone ring H2α and H2β produced NOEs with H1′, H2′, and H2″ of C^{16}, and H1′, and H3′ of T17, in the complementary strand.

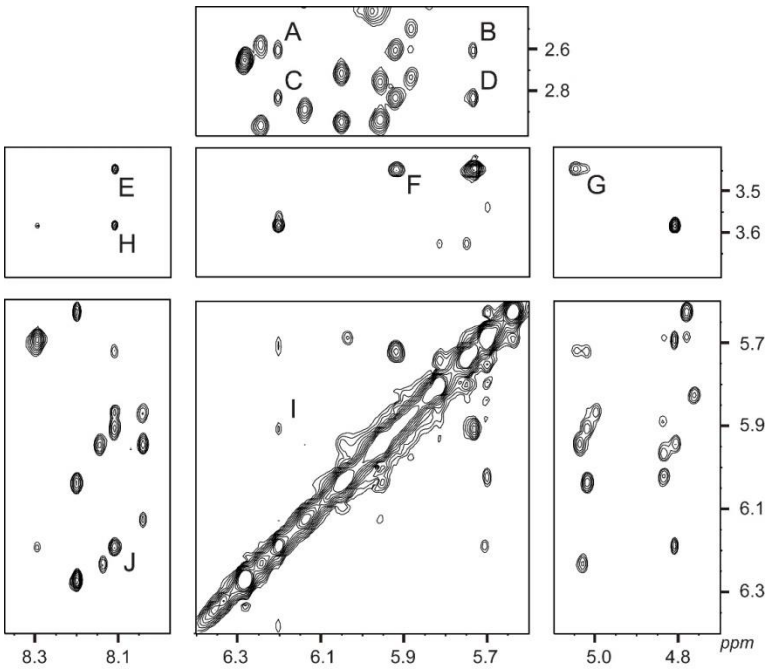


Figure 3-8. NOE assignments of the FAPY to DNA protons of the AFB_1- β-FAPY modified AXA duplex. The cross peaks are assigned as: (A) $X^5H2' \rightarrow X^5H6a$; (B) X^5 $H2' \rightarrow X^5H5$; (C) $X^5H2'' \rightarrow X^5H6a$; (D) X^5 $H2'' \rightarrow X^5H5$; (E) $X^5OCH_3 \rightarrow A^4H8$; (F) $X^5OCH_3 \rightarrow A^4H1'$; (G) $X^5OCH_3 \rightarrow A^4H3'$; (H) $X^5H9a \rightarrow A^4H8$; (I) $A^4H1' \rightarrow X^5H6a$; (M) $X^5H6a \rightarrow A^4H8$. The experiment was carried out at 250 ms mixing time and 900 MHz. The temperature was 283 K.

NMR Melting Experiments

The thermal melting of the AFB_1-β-FAPY modified AXA duplex was compared to the corresponding unmodified AGA duplex by monitoring spectra of the imino protons as a function of temperature. For the X^5 N1H imino proton, a single resonance was observed at 10 ℃ and a shoulder peak was observed at 40 ℃. A second peak at 40 ℃ was also observed for $T^{15}N3H$, 3'-neighbor base pair of X^5 (Figure 3-9).

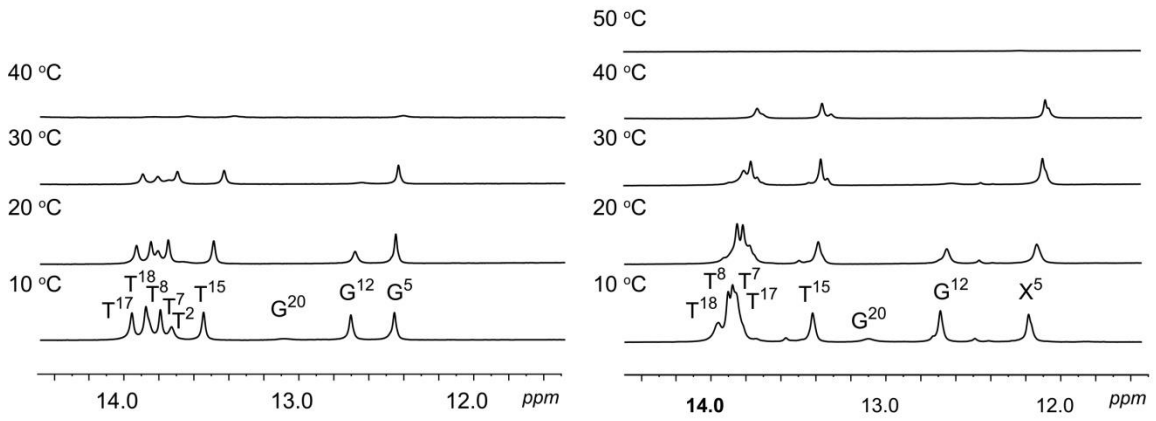
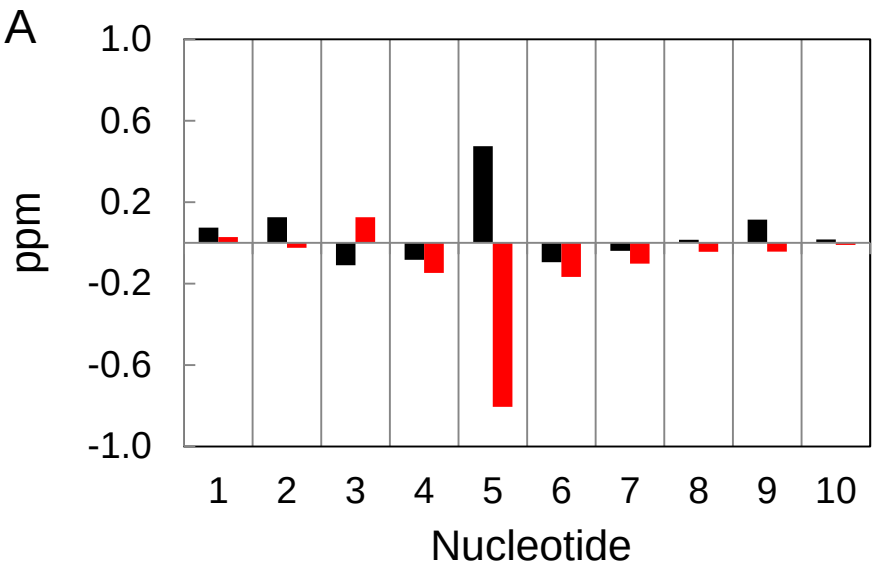


Figure 3-9. Expanded 1D spectra of AFB$_1$-β-FAPY Modified AXA Duplex compared with the corresponding unmodified duplex at different temperature. (A) The unmodified duplex. (B) The modified duplex. X = AFB$_1$-β-FAPY. The experiment was carried out at 800 MHz.

Chemical Shift Effects

The ^{1}H spectrum of the AFB$_1$-β-FAPY modified AXA duplex exhibited significant chemical shift differences around the modified base X^5 compared to that of the unmodified oligodeoxynucleotide (Figure 3-10). In the major groove, at the 3′-side of X^5, a downfield shift of 0.17 ppm was observed for A^6 H8, as well as a downfield shift of 0.15 ppm for A^4 H8 and a downfield shift of 0.21 ppm for T^{17} H6 at the 5′-side of X^5. In the minor groove, an upfield chemical shift of 0.48 ppm was observed for X^5 H1', whereas a downfield shift of 0.10 ppm was observed for A^6 H1' and a downfield shift of 0.08 ppm for A^4 H1'. Examination of the exchangeable protons revealed that T^{17} N3H at the 5′-side of X^5 shifted 0.09 ppm downfield. The greater shift of 0.3 ppm upfield and 0.2 ppm downfield were observed for X^5 N1H and T^{15} N3H, respectively.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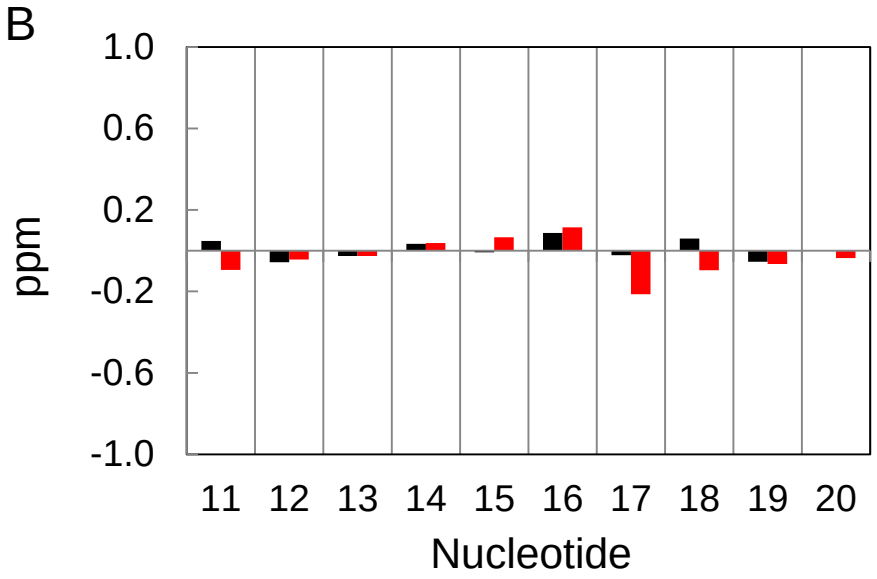
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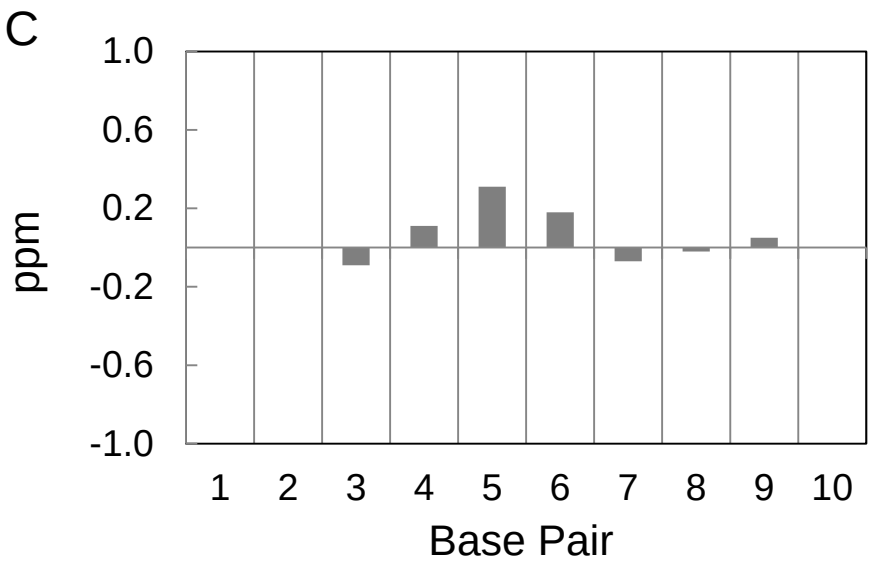


Figure 3-10. Chemical shift differences of protons of the AFB_1-β-FAPY Modified AXA Duplex, relative to the unmodified onligodeoxynucleotide. **A**. Nucleotides $C^1 \rightarrow A^{10}$ of the AFB_1-β-FAPY Modified AXA duplex. **B**. Nucleotides $T^{11} \rightarrow G^{20}$ of the AFB_1-β-FAPY Modified AXA duplex. **C**. Base pairs 1→10 of AFB_1-β-FAPY Modified AXA duplex. Black bars represents the deoxyribose H1' protons; red bars represent the purine H8 or pyrimidine H6 protons, respectively; gray bars represent the imino guanine N1H or thymine N3H protons.

Structural Refinement

A total of 256 distance restraints, including 160 intranucleotide and 96 internucleotide restraints, were calculated from the intensities of NOE cross-peaks using MARDIGRAS.[73-76] A total of 34 restrains were either intranucleotide or internucleotide AFB_1-FAPY to DNA NOEs. In addition to those experimental restraints, a total of 36 empirical distance restraints arising from Watson-Crick base pairing interactions were used, but not at the AFB_1-FAPY adduct. A totoal of 84 backbone torsion restraints were also applied; however, at the AFB_1-FAPY adduct, the backbone torsion angles were not restrained.

The rMD calculations for the AFB_1-β-FAPY modified AXA duplex were performed from the initial B- form DNA staring structures. The final ten structures with lowest energies were obtained. All structures converged as indicated by pairwise rmsd comparison (Table 3-1). The accuracies of the emergent structures were evaluated by comparison of theoretical NOE intensities calculated by CORMA[77-79] for the refined structure to the experimental NOE intensities to yield sixth root residuals (R_1^x). The R_1^x values for overall residuals, as well as the residuals for intra- or internucleotide NOEs, were consistently less than 0.1, and for each nucleotide were less than 0.15, suggesting that the refined structures were in good agreement with the NOESY data (Figure 3-11).

Table 3-1. Distribution of restraints applied to structural refinement and statistical analysis for the AFB_1-β-FAPY modified AXA duplex.

	restrains
Experimental NOE Distance Restraints	256
Intra-residue NOE Restraints	160
Inter-residue NOE Restraints	96
NOEs of FAPY	34
Empirical Base Pairing Restraints	36
Empirical Backbone Torsion Restraints	42
Empirical Deoxyribose Torsion Restraints	42
Total Restraints for rMD Caculation	376
Structure Statistics	
NMR R-factor (R^*) ($\times 10^{-2}$)	8.09
Intra-residue NOEs	8.48
Inter-residue NOEs	7.35
rmsd Deviation of Refined Structures	0.483

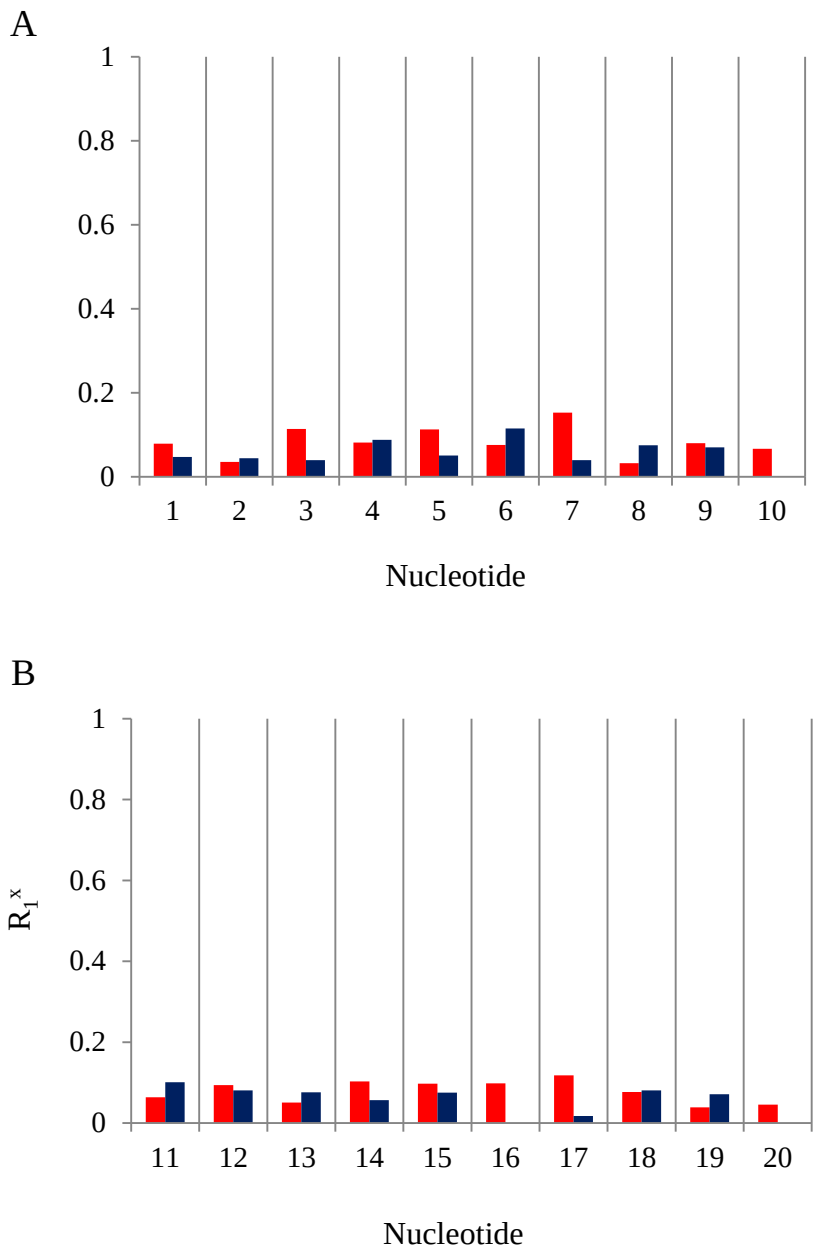


Figure 3-11. Sixth root residuals between calculated NOE intensities and experimental NOE intensities (R_1^x values) as a function of position in the AFB_1-β-FAPY modified AXA duplex. (A) Nucleotides C^1-A^{10} of the modified oligonucleotide containing AFB_1-β-FAPY. (B) Nucleotides T^{11}-G^{20} of the complementary strand. The red bars represent intranuclear sixth root residuals and the black bars represent internuclear sixth root residuals.

Molecular Dynamics Calculations in Explicit Solvent

The 1 ns of equilibrium rMD calculation was performed in explicit water at constant pressure at 300K, to examine the dynamics of the refined structure and to analyze hydrogen bond occupancies involving the formamido group of the FAPY moiety. The 1 ns rMD trajectory was analyzed for occupancies of hydrogen bonding motifs. Hydrogen bond occupancies were calculated using a distance cutoff of 3.5 Å and an angle cutoff of 120 °. On the basis, The A^6 H61 non Watson-Crick hydrogen bonded exocyclic amine proton was within hydrogen bonding distance of the X^5 formyl oxygen; this positioned the formamide in the *E* conformation. This hydrogen bond was satisfied for 95% of the trajectory of 1 ns of equilibrium rMD calculation performed in explicit water.

Structure of the AFB$_1$-β-FAPY Modified AXA Duplex

Stereo view of 10 rMD refined solution structures for the AFB$_1$-β-FAPY modified AXA duplex DNA is depicted in Figure 3-12. The root mean squared deviation (RMSD) between the 10 structures is 0.62 Å. The overall structure maintains Watson-Crick base pairing. The AFB$_1$ adduct is intercalated between A^4●T^{17} and X^5●C^{16}. The formyl group has an *E* geometrical configuration.

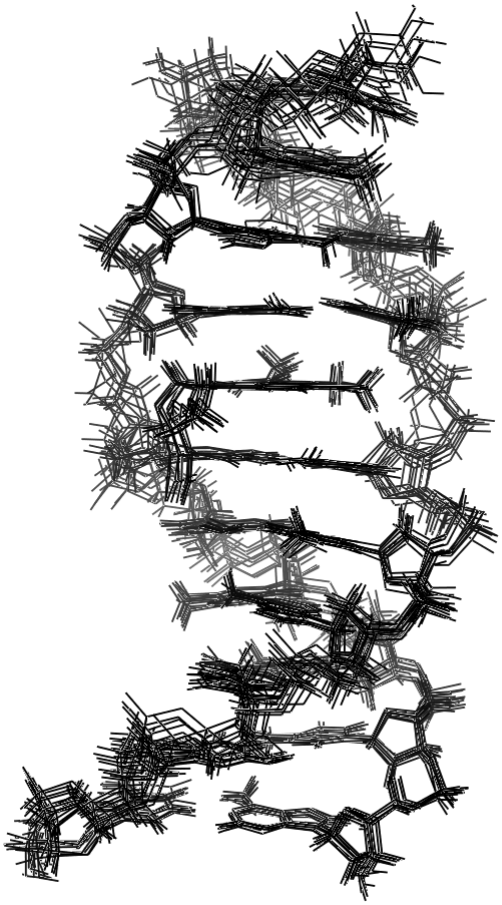


Figure 3-12: Stereo view of 10 superimposed structures of AFB_1-β-FAPY modified AXA duplex resulting from the simulated annealing rMD protocol. (X= AFB_1-β-FAPY).

Expanded views of the structure are shown in Figure 3-13. The AFB_1 moiety is intercalated above the 5′-face of the modified nucleotide X^5 and between base pairs A^4•T^{17} and X^5•C^{16}, causing the rise between these base pairs to increase to 5 Å. The adduct-induced unwinding is localized to the adducted base pair X^5•C^{16}, and its 5′- and 3′-neighbor base pairs A^4•T^{17} and A^6•T^{15}. The modified duplex is unwound approximately 15 ° at the adducted site. The X^5 N9H exocyclic amine proton is within hydrogen bonding distance of

the X^5 formyl oxygen and positioned the formamide in the *E* conformation. Figure 3-14 shows the damaged site from 3′ -neighbor base, confirming the *E* conformation.

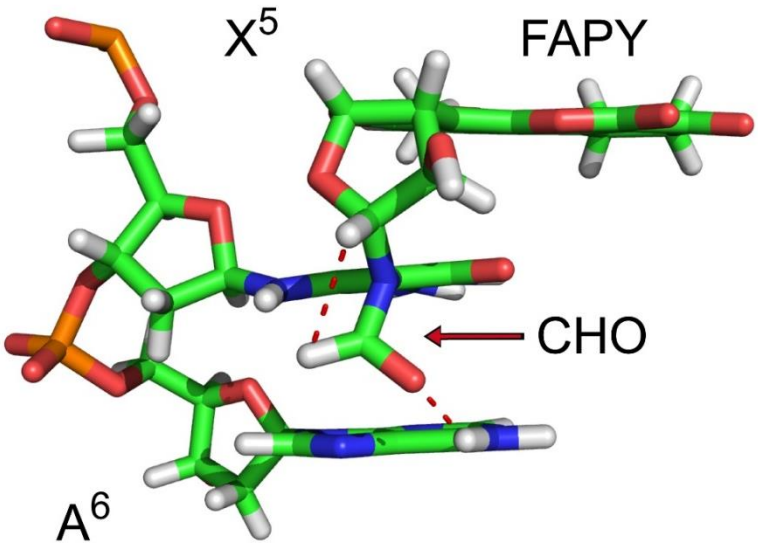


Figure 3-13. Expanded view of the refined structure of the AFB_1-β-FAPY modified AXA duplex at the lesion site. X = AFB_1-β-FAPY.

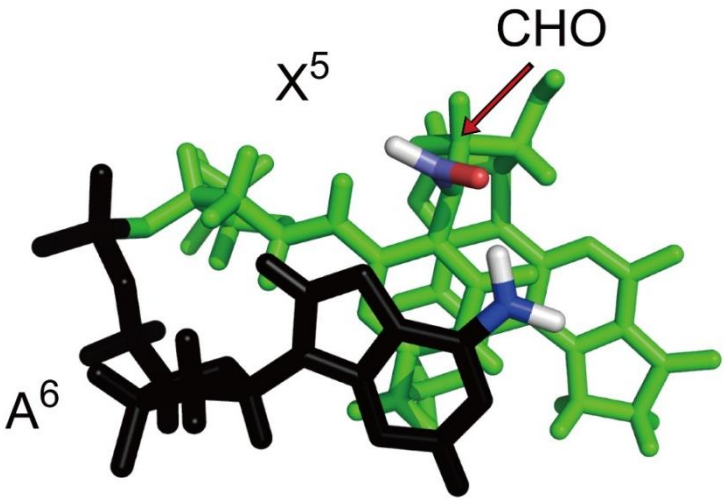


Figure 3-14. Expanded view of the refined structure of the AFB_1-β-FAPY modified AXA duplex at the lesion site from the 3′-neighbor base. X = AFB_1-β-FAPY.

Helicoidal Analysis

A helicoidal analysis of the average solution structure was performed using CURVES*, following rMD calculations. As a result of the modification at X^5, a bend is present in the structure. The base pair parameters are normal for both the X- axis and Y-axis at the lesion site (Figure 3-15). The parameters for base-base interactions show that the modification causes more than a 10 °opening at the lesion site. Disruptions also occurr in the shear, the stretch, and the stagger, primarily at the lesion site (Figure 3-16). As is predicted by NOESY data, a 5 Å increase in rise was observed between X^5 and A^6 (Figure 3-17).

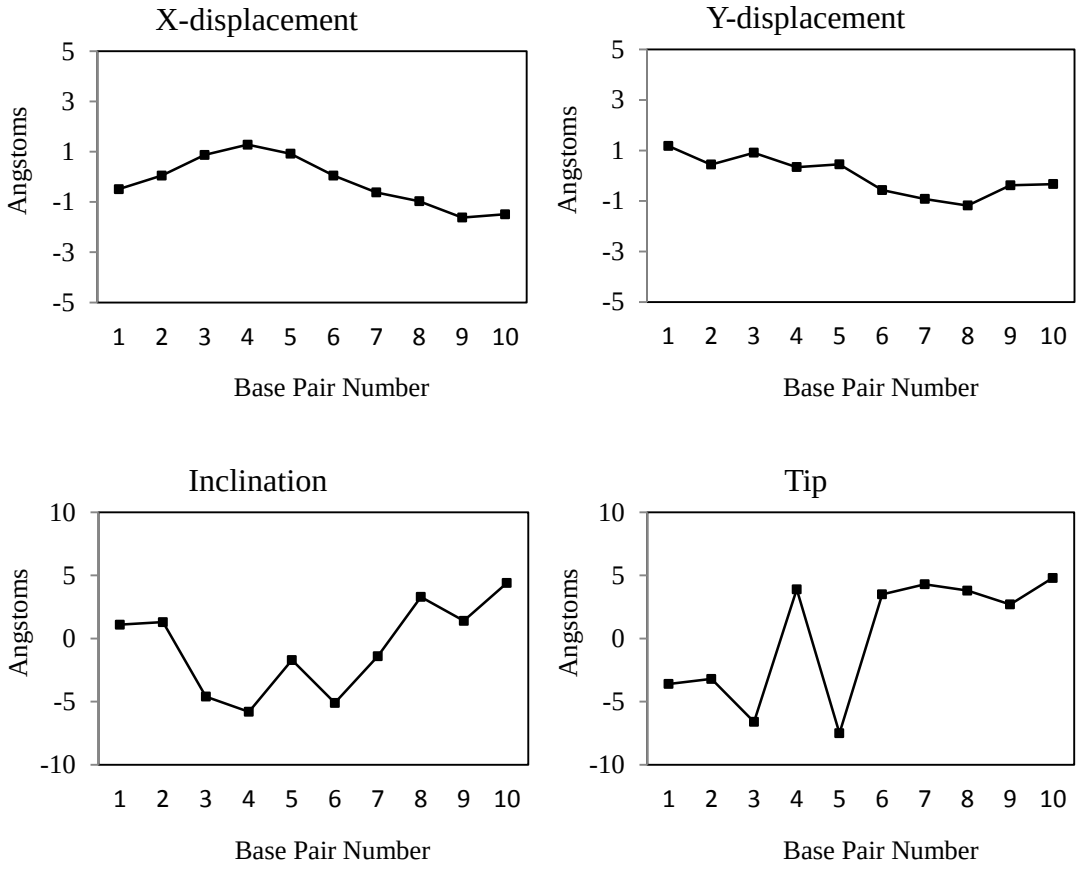


Figure 3-15: Global base pair helicoidal parameters. Helicoidal parameters for the AFB_1-FAPY modified AXA oligonucleotide 5′-$C^1T^2A^3A^4X^5A^6T^7T^8C^9A^{10}$-3′·5′-$T^{11}G^{12}A^{13}A^{14}T^{15}C^{16}T^{17}T^{18}$ A^{19} G^{20}-3′.

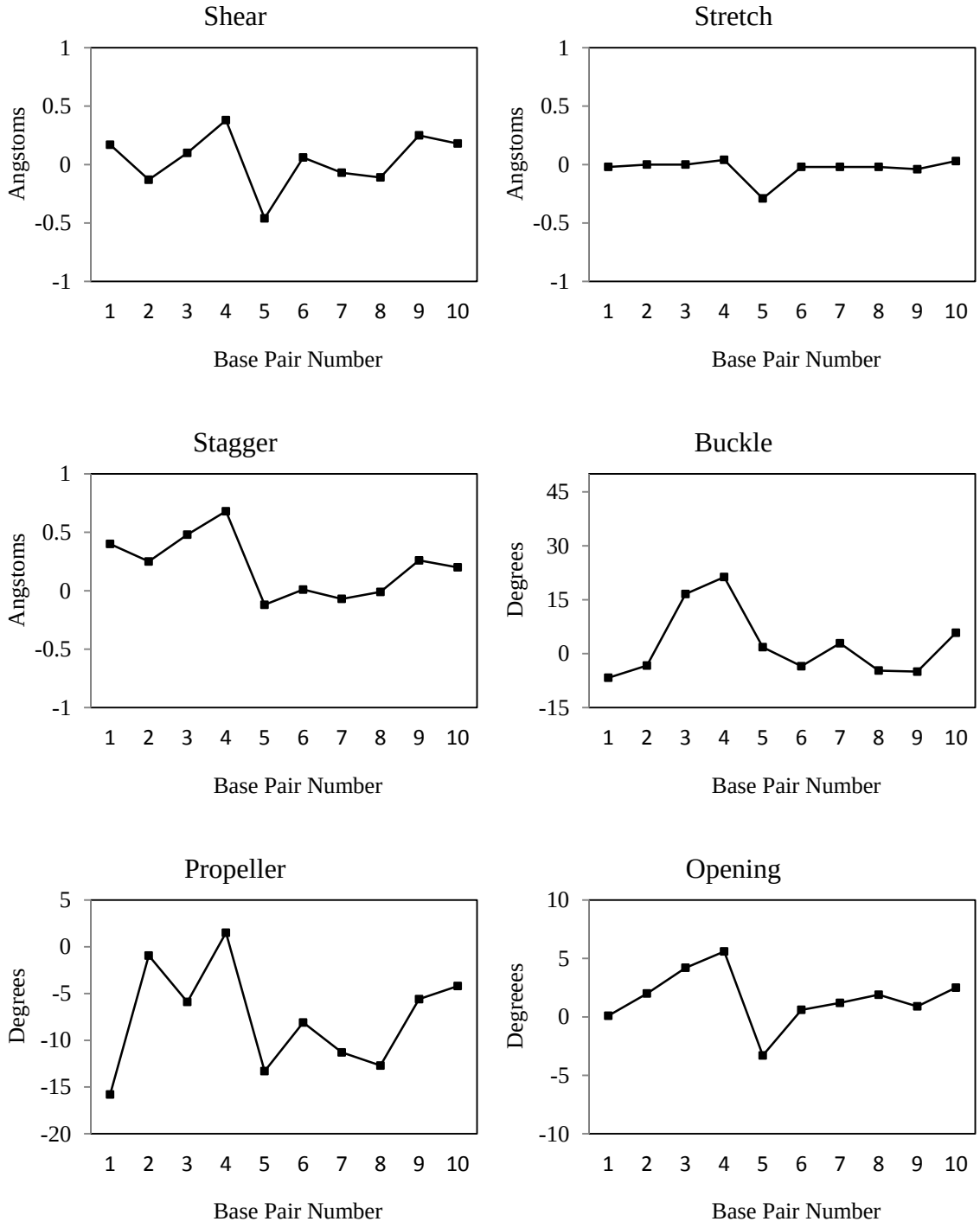


Figure 3-16: Global Intra-base pair helicoidal parameters. Helicoidal parameters for the AFB_1-FAPY modified AXA oligonucleotide 5′-$C^1T^2A^3A^4X^5A^6T^7T^8C^9A^{10}$-3′·5′-$T^{11}G^{12}A^{13}A^{14}T^{15}C^{16}T^{17}T^{18}$ A^{19} G^{20}-3′.

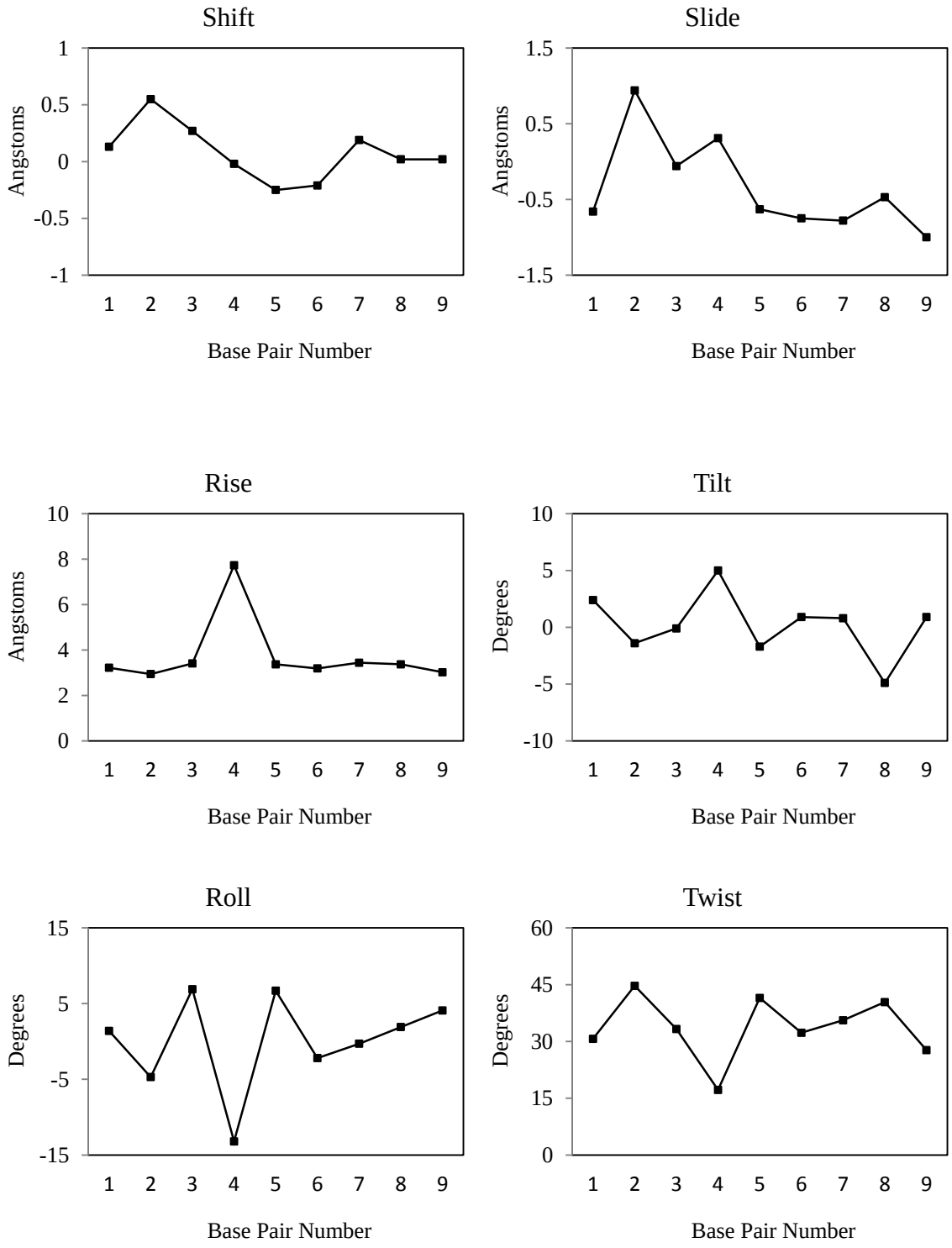


Figure 3-17: Global Inter-base pair helicoidal parameters. Helicoidal parameters for the AFB_1-FAPY modified AXA oligonucleotide 5′-$C^1T^2A^3A^4X^5A^6T^7T^8C^9A^{10}$-3′·5′-$T^{11}G^{12}A^{13}A^{14}T^{15}C^{16}T^{17}T^{18}$ A^{19} G^{20}-3′.

Discussion

NMR analysis of the AFB_1-β-FAPY modified AXA duplex reveals that the formamide moiety of the AFB_1-β-FAPY adduct is held in the *E* configuration by the hydrogen bond between the formyl oxygen and the N^6 non Watson-Crick hydrogen bonded exocyclic amino proton of the 3′-neighbor A^6. The result is consistent with the previous data reported by Mao et al[58] and further corroborated by Brown et al[62,63]. The hydrogen bonding is also supported by the deshielding of the A^6 non-Watson-Crick exocyclic amino proton chemical shift relative to unmodified DNA duplex, since a consequence of hydrogen bonding is electron withdrawing, causing the proton deshielding. A second resonance of X^5 N1H and the T^{15} N3H, the 3′- neighbor base pair, imino protons appears at 40 ℃, suggesting the appearance of the *Z* configuration of the formamide moiety with extra energy at higher temperature.

CHAPTER IV

Solution structure of AFB_1-β-FAPY modified AXT duplex

Introduction

The solution structure of a double strand AFB_1-β-FAPY modified sample, 5′-d($C^1T^2A^3A^4X^5T^6T^7T^8C^9A^{10}$)-3′•5′-d($T^{11}G^{12}A^{13}A^{14}A^{15}C^{16}T^{17}T^{18}A^{19}G^{20}$)-3′ has been investigated. The refined structure reveals that, in contrast to the *E* isomer in the AXA sequence context, the formyl group adopts the *Z* configuration in AXT sequence context.

Results

Sample purity

The double strand AFB_1-β-FAPY modified oligonucleotide, 5′-d($C^1T^2A^3A^4X^5T^6T^7T^8C^9A^{10}$)-3′•5′-d($T^{11}G^{12}A^{13}A^{14}A^{15}C^{16}T^{17}T^{18}A^{19}G^{20}$)-3′, was purified using HPLC. The identity of the duplex was verified using MALDI-TOF mass spectroscopy for 5′-d($C^1T^2A^3A^4X^5T^6T^7T^8C^9A^{10}$)-3′, calc'd 3348.1, found 3348.0; for the complementary strand 5′-d($T^{11}G^{12}A^{13}A^{14}A^{15}C^{16}T^{17}T^{18}A^{19}G^{20}$)-3′, calc'd 3051.1, found 3051.4 (Figure 4-1). The molar ratio of two strands was determined to be 1:1 after correction for the respective absorbance coefficients by using capillary gel electrophoresis. The melting temperature of the AFB_1-FAPY modified duplex was 41 ℃ (Figure 4-2), 10 ℃ higher than the 31 ℃ melting temperature of the unmodified duplex.

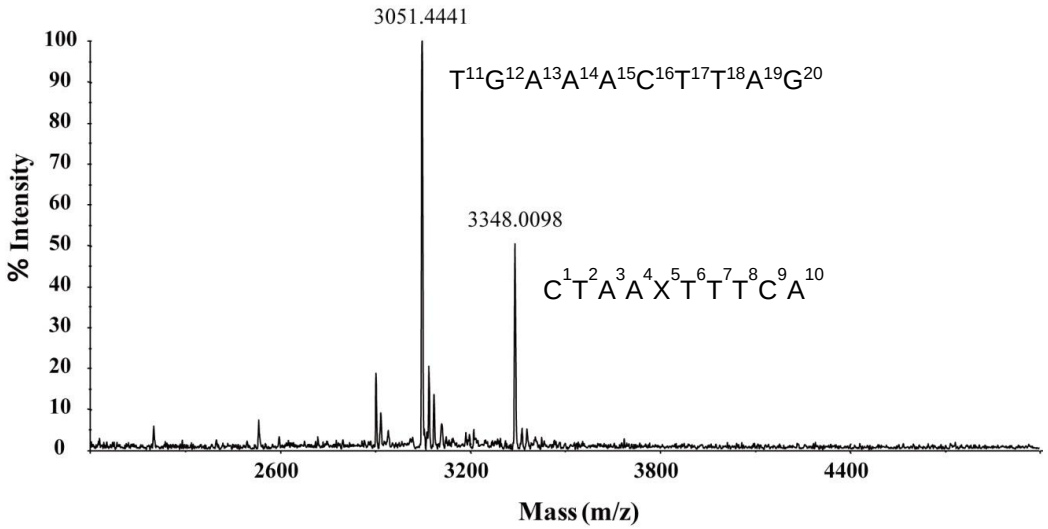


Figure 4-1. MALDI mass spectrum of AFB_1-β-FAPY modified AXT duplex sample.

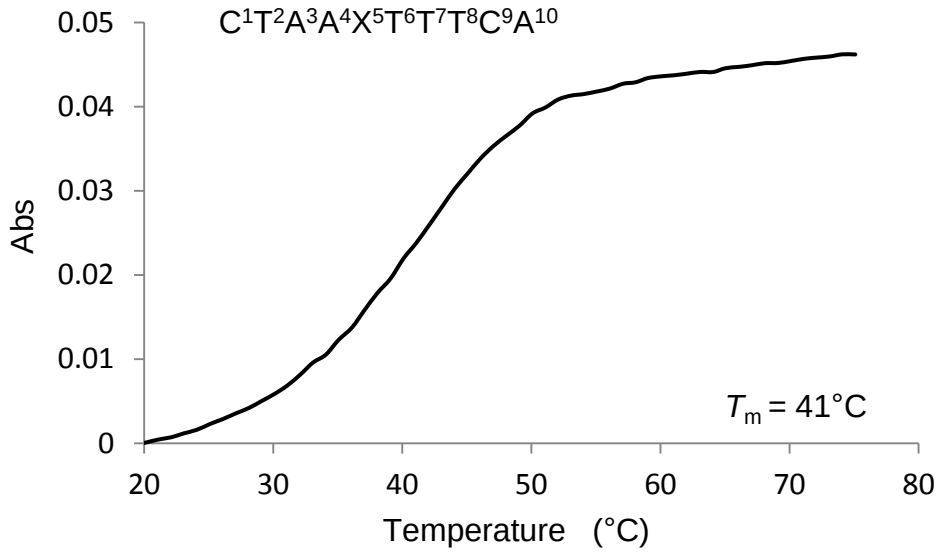


Figure 4-2. UV-melting curves of AFB_1-β-FAPY modified AXT duplex sample.

DNA ^1H Resonance Assignments

Nonexchangeable DNA Protons

The resonances of the non-exchangeable protons of the AFB_1-β-FAPY modified AGA duplex were assigned using the sequential NOE connectivity of the base proton H6

or H8 dipolar couplings with H1′ deoxyribose protons.[105,106] For the modified strand, the NOE connectivity started from C^1 to A^4. Then an interruption was observed between A^4 H1′ and X^5 NOE connectivity, due to the loss of the guanine H8 proton because of the opening of the guanine imidazole ring in the FAPY formation. The connectivity was then observed from the formyl proton of the FAPY base and the 3′-neighbor, continuing to the 3′-terminus. For the complementary strand, the interruption of the sequential NOE connectivity was also observed between C^{16} H1′ and T^{17} H8. Expanded plots of the NOESY spectrum for the AFB_1-β-FAPY modified AGA duplex are shown in Figure 3-3. The purine and pyrimidine aromatic protons, the thymine methyl protons and the deoxyribose H1′, H2′, H2″, and H3′ protons were successfully assigned. The H4′, H5′, and H5″ protons were only partially assigned due to heavy overlapping peaks and the effects of spin diffusion at higher mixing times.

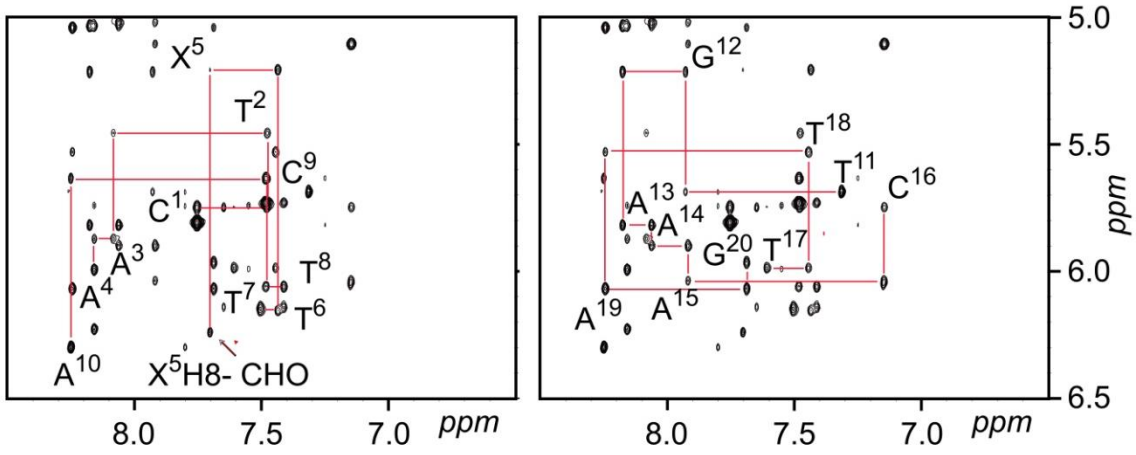


Figure 4-3. NOE connectivity of base H8/H6 protons with deoxyribose H1′ protons of the AFB_1-β-FAPY modified AXT duplex. (A) The modified strand. (B) The complementary strand. X = AFB_1-β-FAPY. The experiment was carried out at 250 ms mixing time and 900 MHz. The temperature was 283 K.

Anomeric Configuration

The assignment of the H2′ and H2″ resonances were based on their relative cross peak intensities to H3′ at NOE mixing time of 60 ms. The configuration at C1′ at X5 was determined by unequivocally identifying the H2′ and H2″ to H1′ (Figure 3). The intensity of the X^5 H1′ to X^5 H2′ NOE was less than the X^5 H1′ to X^5 H2″ NOE, suggesting the β configuration.

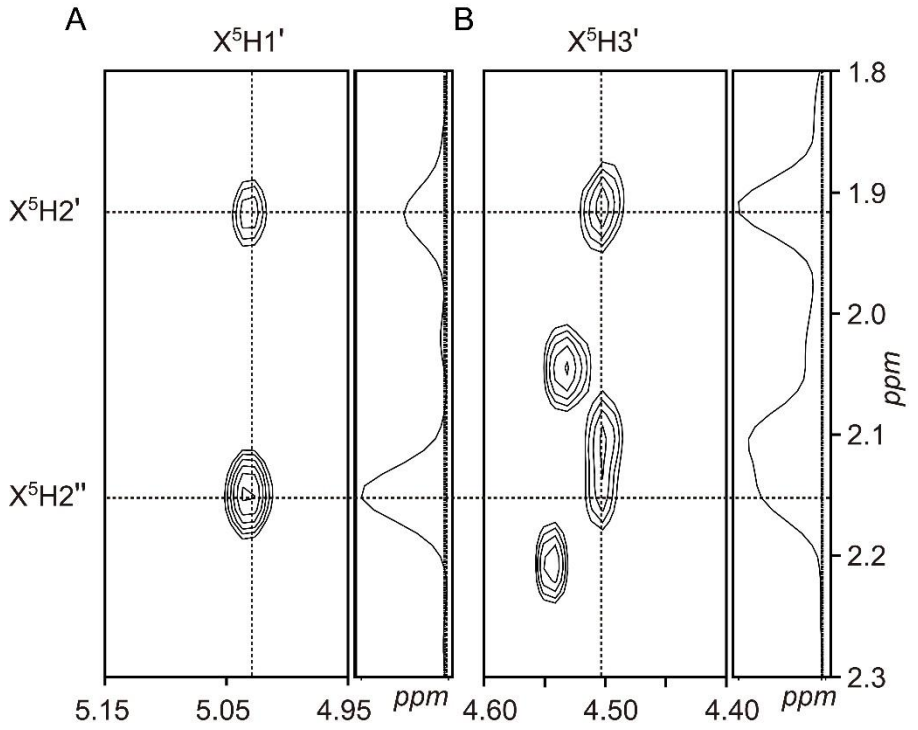


Figure 4-4. Analysis of NOE intensities for the deoxyribose protons. (A) The NOE peaks from H1′ to H2′, H2″. (B) The NOE peaks from H3′ to H2′, H2″. X = AFB_1-β-FAPY. The experiment was carried out at 250 ms mixing time and 800 MHz. The temperature was 283 K.

Exchangeable DNA Protons

The resonances of the base imino protons were assigned on the basis of sequential connectivity between adjacent base pairs in NOESY spectra, and the assignments were supported by NOEs to the amino protons of Watson-Crick base pairs.[107] Between X^5 N1H and T^{17} N3H imino resonances, there was an interruption of the sequential imino-to-imino proton NOEs of adjacent base pairs. The strong cross peaks from X^5 N1H to C^{16} N4H1 and C^{16} N4H2 amino protons indicated that Watson-Crick hydrogen bonding between X^5 and C^{16} was intact.

NMR Spectroscopy of Formyl Proton Resonance (CHO)

A single peak was observed for the AFB_1-β-FAPY modified AXT duplex in HMQC experiment acquired at 283 K. This peak revealed the presence of carbonyl resonance at 168.35 ppm, coupled to a proton resonance at 7.71 ppm (Figure 4-5).

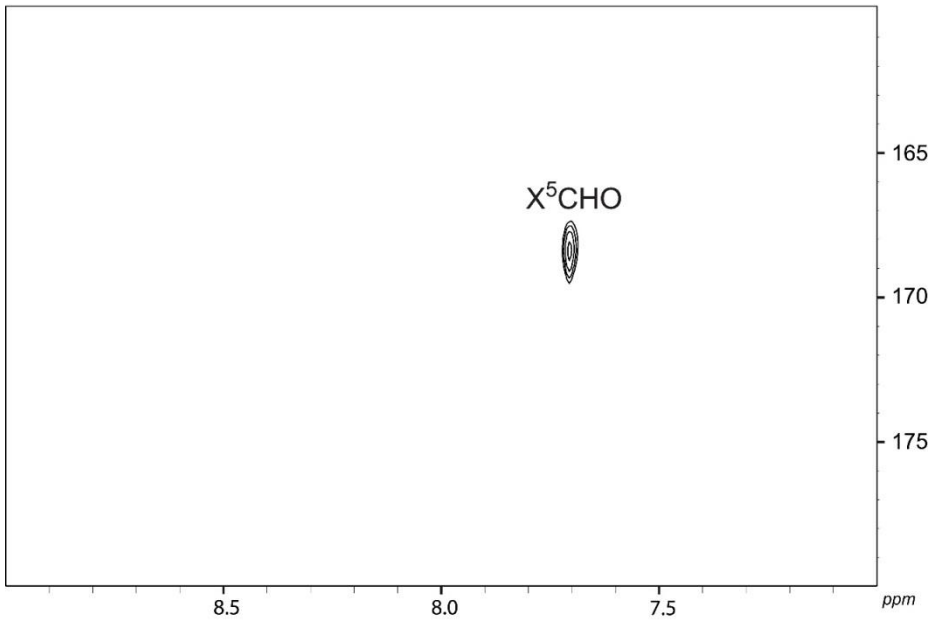


Figure 4-5. NMR analysis of ^{1}H-^{13}C HMQC of AFB_1- β-FAPY modified AXT duplex. The experiment was carried out at 600 MHz and the temperature was 283 K.

Aflatoxin FAPY Protons

The AFB_1 H5, H6a, H8, H9, H9a, and $–OCH_3$ resonances were assigned from a combination of NOE connectivities and chemical shift data (Figure 3-6). AFB_1 H6a and H9a were identified from both COSY and NOESY experiments. AFB_1 H8 and H9 were assigned based on NOEs between H6a or H9a, and between themselves. A strong NOE was observed between AFB_1 H5 and AFB_1 $–OCH_3$, revealing that the latter resonance was at δ 3.52 ppm, while AFB_1 H5 was at δ 5.74 ppm. In contrast to AXA sequence, a weak NOE peak was observed between AFB_1 H8 and CHO (Figure 4-6). The X^5 CHO resonance was observed at δ 7.73 ppm, confirming the assignment of the carbonyl resonance in the HMQC experiment. The assignment of X^5 CHO resonance was also supported by NOEs

to AFB_1 H6a. The cyclopentenone ring protons AFB_1 $H2_\alpha$, $H2_\beta$, $H3_\alpha$, and $H3_\beta$ were identified from a combination of COSY and NOESY experiments.

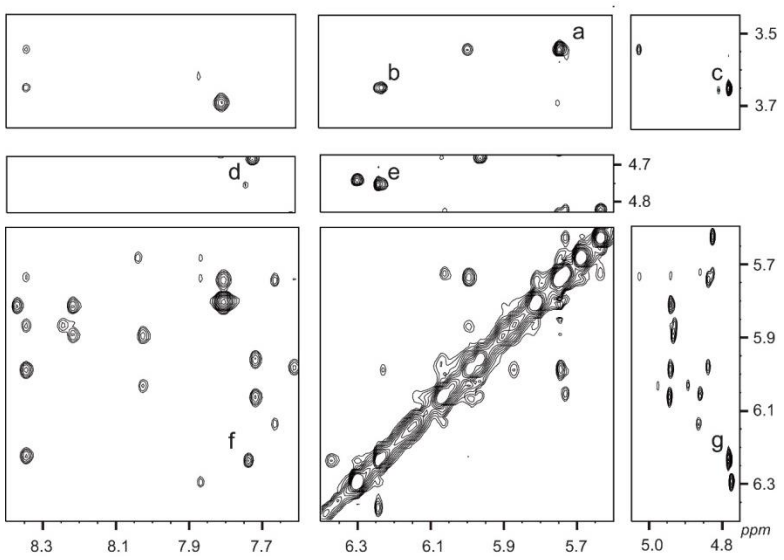


Figure 4-6. Select NOE assignments of the FAPY protons of the β-AFB_1-FAPY modified AXT duplex. The cross peaks are assigned as: (a) X^5OCH_3 → X^5H5; (b) X^5H9a → X^5H6a; (c) X^5H9a →X^5H9; (d) X^5H9 →X^5CHO; (e) X^5H9 →X^5H6a; (f) X^5H6a →X^5CHO; (g) X^5H6a →X^5H9a. The experiment was carried out at 250 ms mixing time and 900 MHz. The temperature was 283 K.

Aflatoxin FAPY to DNA NOEs

A total of 41 NOEs from AFB_1 protons to DNA protons were observed. The protons of the two AFB_1-fused furan rings showed NOEs to major groove and imino protons of the DNA; most of these were to the 5′ neighboring base-pair A^4•T^{17}. Thus, H6a and H9a, which are located on the same face of the AFB_1 moiety, both exhibited NOEs to A^4 H8. A weaker NOE was observed for AFB_1 H9. The AFB_1 H5 and $–OCH_3$ protons exhibited NOEs with minor groove and imino DNA protons. These were primarily to base A^4•T^{17}, in the 5′ direction, and to the modified nucleotide X^5 (Figure 4-7). These included

NOEs between the AFB_1 $-OCH_3$ and A^4 H1′, A^4 H2′, A^4 H2″, A^4 H2, T^{17} N3H, X^5 H1′, and X^5 N1H protons. The cyclopentenone ring H2α and H2β produced NOEs with H1′, H2′, and H2″ of C^{16}, and H1′, and H3′ of T17, in the complementary strand.

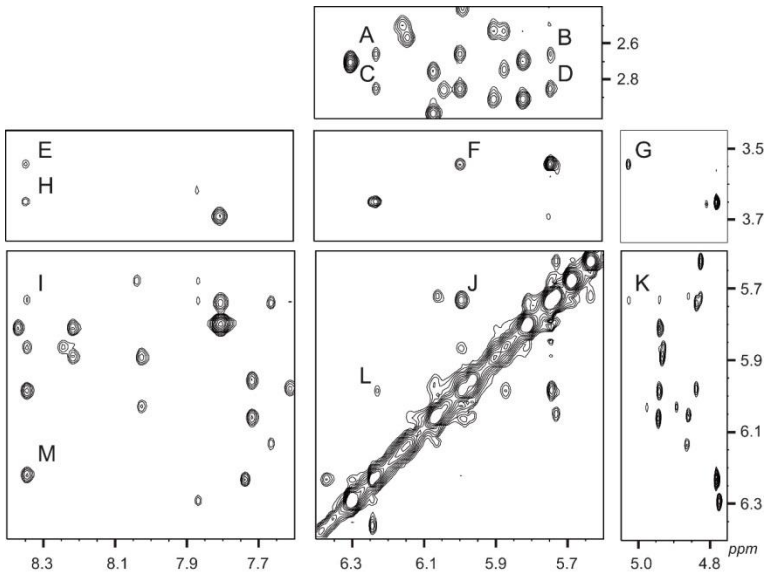


Figure 4-7. Select NOE assignments of the FAPY to DNA protons of the AFB_1- β-FAPY modified AXT duplex. The cross peaks are assigned as: (A) X^5H2′ → X^5H6a; (B) X^5 H2′ → X^5H5; (C) X^5H2″ → X^5H6a; (D) X^5 H2″ → X^5H5; (E) X^5OCH_3 → A^4H8; (F) X^5OCH_3 → A^4H1′; (G) X^5OCH_3 → A^4H3′; (H) X^5H9a → A^4H8; (I) X^5H5 → A^4H8; (J) X^5H5 → A^4H1′; (K) X^5H5 → A^4H3′; (L) A^4H1′ →X^5H6a; (M) X^5H6a → A^4H8. The experiment was carried out at 250 ms mixing time and 900 MHz. The temperature was 283 K.

NMR Melting Experiments

The thermal melting of the AFB_1-β-FAPY modified AXT duplex was compared to the corresponding unmodified AGT duplex by monitoring spectra of the imino protons

as a function of temperature. For the X^5 N1H imino proton, a single resonance was observed at both 10 and 40 ℃ (Figure 4-8).

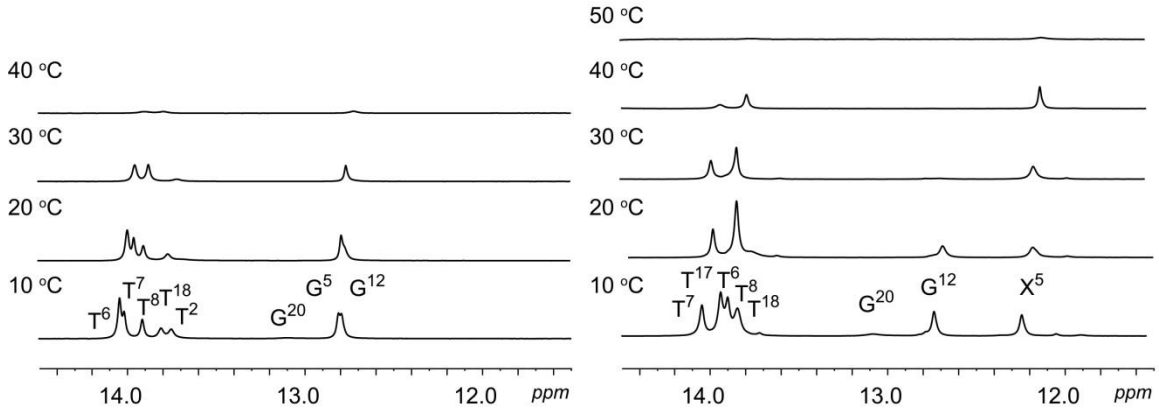
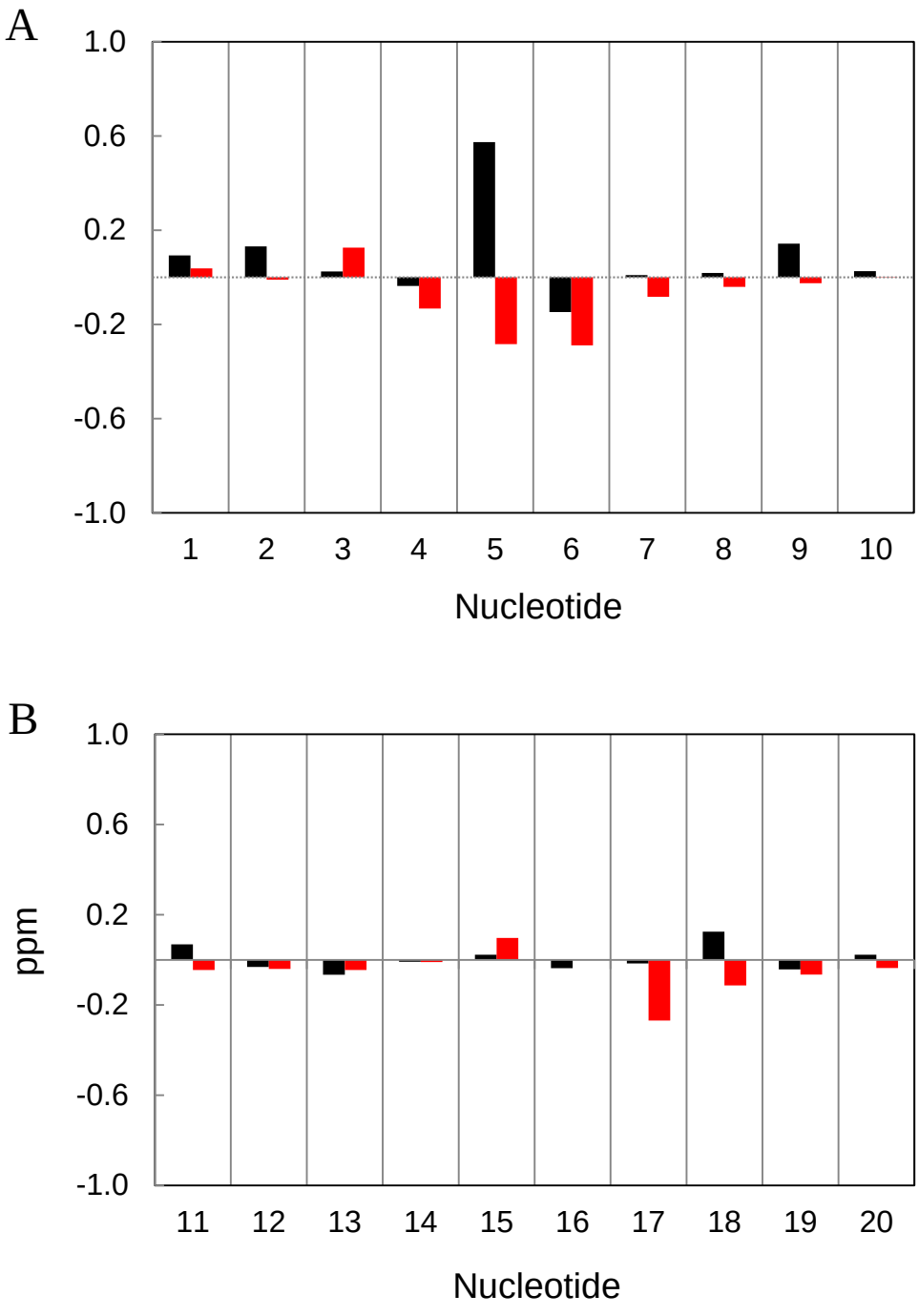


Figure 4-8. Expanded 1D spectra of AFB_1-β-FAPY modified AXT duplex compared with the corresponding unmodified duplex at different temperature. (A) The unmodified duplex. (B) The modified duplex. X = AFB_1-β-FAPY. The experiment was carried out at 800 MHz.

Chemical Shift Effects

The ^1H spectrum of the AFB_1-β-FAPY modified AXT duplex exhibited significant chemical shift differences around the modified base X^5 compared to that of the unmodified oligodeoxynucleotide (Figure 4-9). In the major groove, at the 3′-side of X^5, a downfield shift of 0.29 ppm was observed for T^6 H6, as well as a downfield shift of 0.13 ppm for A^4 H8 and a downfield shift of 0.27 ppm for T^{17} H6 at the 5′-side of X^5. In the minor groove, an upfield chemical shift of 0.57 ppm was observed for X^5 H1', whereas a downfield shift of 0.15 ppm was observed for T^6 H1'. Examination of the exchangeable protons revealed that T^{17} N3H at the 5′-side of X^5 shifted 0.07 ppm downfield. The greater

shift of 0.6 ppm upfield and 0.2 ppm downfield were observed for X^5 N1H and T^6 N3H, respectively.



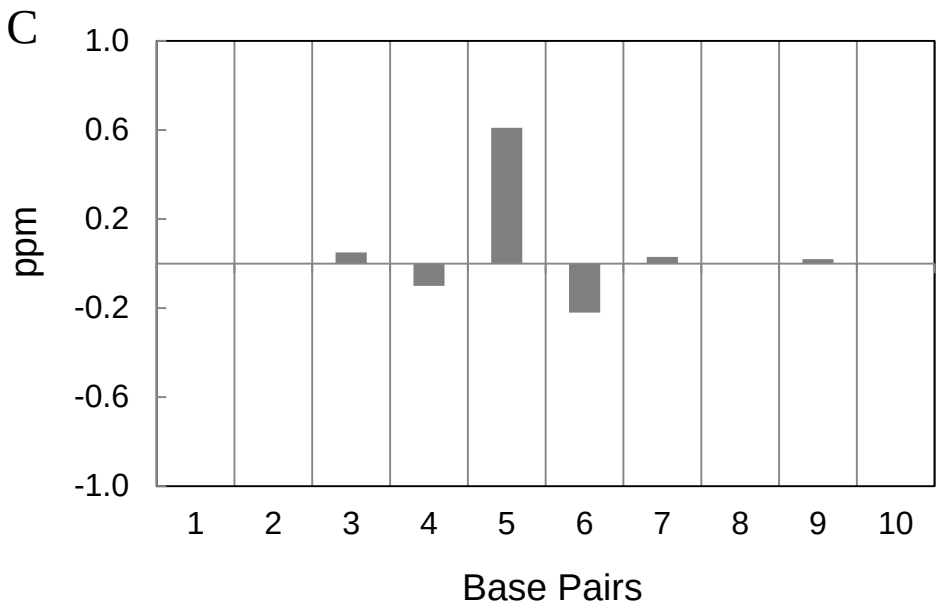


Figure 4-9. Chemical shift differences of protons of the AFB_1-β-FAPY modified AXT duplex, relative to the unmodified onligodeoxynucleotide. **A**. Nucleotides $C^1 \rightarrow A^{10}$ of the AFB_1-β-FAPY Modified AXT duplex. **B**. Nucleotides $T^{11} \rightarrow G^{20}$ of the AFB_1-β-FAPY Modified AXT duplex. **C**. Base pairs 1→10 of AFB_1-β-FAPY Modified AXT duplex. Black bars represents the deoxyribose H1' protons; red bars represent the purine H8 or pyrimidine H6 protons, respectively; grey bars represent the imino guanine N1H or thymine N3H protons.

Structural Refinement

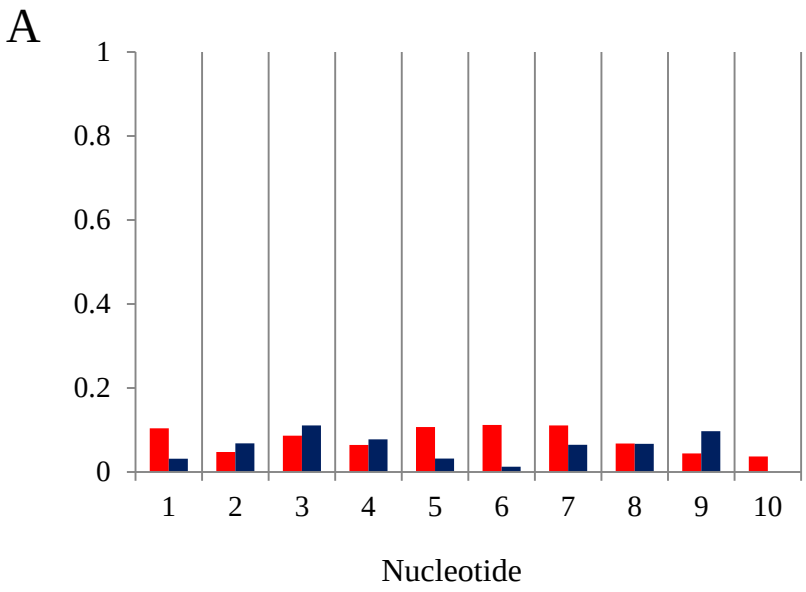
A total of 244 distance restraints, including 152 intranucleotide and 92 internucleotide restraints, were calculated from the intensities of NOE cross-peaks using MARDIGRAS.[73-76] A total of 41 restrains were either intranucleotide or internucleotide AFB_1-FAPY to DNA NOEs. In addition to those experimental restraints, a total of 36 empirical distance restraints arising from Watson-Crick base pairing interactions were used, but not at the AFB_1-FAPY adduct. A total of 84 backbone torsion restraints were also

applied; however, at the AFB_1-FAPY adduct, the backbone torsion angles were not restrained.

The rMD calculations for the AFB_1-β-FAPY modified AXT duplex were performed from the initial B- form DNA staring structures. The final ten structures with lowest energies were obtained. All structures converged as indicated by pairwise rmsd comparison (Table 4-1). The accuracies of the emergent structures were evaluated by comparison of theoretical NOE intensities calculated by CORMA[77-79] for the refined structure to the experimental NOE intensities to yield sixth root residuals (R_1^x). The R_1^x values for overall residuals, as well as the residuals for intra- or internucleotide NOEs, were consistently less than 0.1 (Figure 4-10), and for each nucleotide were less than 0.15, suggesting that the refined structures were in good agreement with the NOESY data.

Table 4-1. Distribution of Restraints Applied to Structural Refinement and Statistical Analysis for the AFB_1-β-FAPY modified AXT duplex.

	restrains
Experimental NOE Distance Restraints	244
Intra-residue NOE Restraints	152
Inter-residue NOE Restraints	92
NOEs of FAPY	41
Empirical Base Pairing Restraints	36
Empirical Backbone Torsion Restraints	42
Empirical Deoxyribose Torsion Restraints	42
Total Restraints for rMD Caculation	364
Structure Statistics	
NMR R-factor (*R**) ($\times 10^{-2}$)	6.88
Intra-residue NOEs	7.03
Inter-residue NOEs	6.60
rmsd Deviation of Refined Structures	0.483



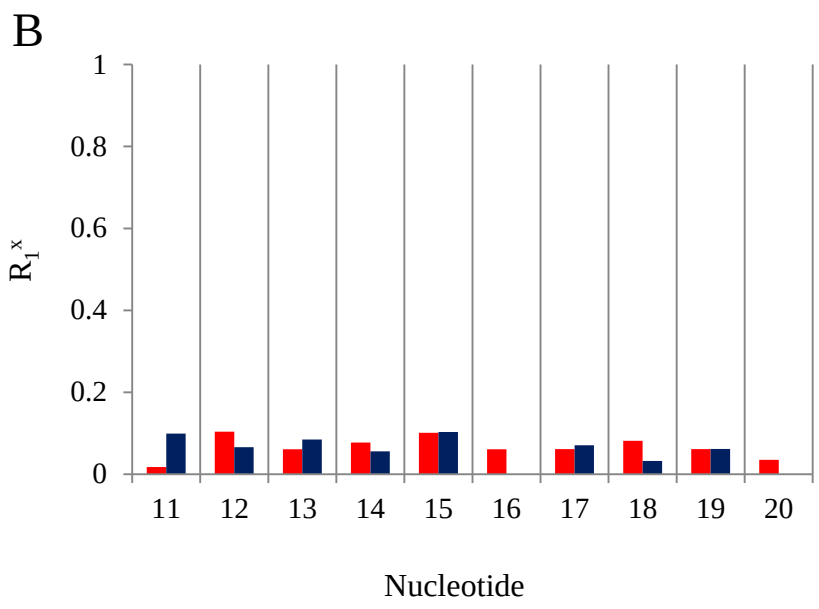


Figure 4-10. Sixth root residuals between calculated NOE intensities and experimental NOE intensities (R_1^x values) as a function of position in the AFB_1-β-FAPY modified AXT duplex. (A) Nucleotides C^1-A^{10} of the modified oligonucleotide containing AFB_1-β-FAPY. (B) Nucleotides T^{11}-G^{20} of the complementary strand. The red bars represent intranuclear sixth root residuals and the black bars represent internuclear sixth root residuals.

Molecular Dynamics Calculations in Explicit Solvent.

The 1 ns of equilibrium rMD calculation was performed in explicit water at constant pressure at 300K, to examine the dynamics of the refined structure and to analyze hydrogen bond occupancies involving the formamido group of the FAPY moiety. The 1 ns rMD trajectory was analyzed for occupancies of hydrogen bonding motifs. Hydrogen bond occupancies were calculated using a distance cutoff of 3.5 Å and an angle cutoff of 120 °. On the basis, the X^5 N9H exocyclic amine proton was within hydrogen bonding distance of the X^5 formyl oxygen; this positioned the formamide in the *Z* conformation. This

hydrogen bond was satisfied for 76% of the trajectory of 1 ns of equilibrium rMD calculation performed in explicit water.

Structure of the AFB$_1$-β-FAPY Modified AXT Duplex.

Stereo views of 10 rMD refined solution structures for the AFB$_1$-β-FAPY modified AXT duplex DNA are depicted in Figure 4-11. The root mean squared deviation (RMSD) between the 10 structures is 0.58 Å. The overall structure maintains Watson-Crick base pairing. The AFB$_1$ adduct is intercalated between A^4●T^{17} and X^5●C^{16}. The formyl group has a *Z* geometrical configuration.

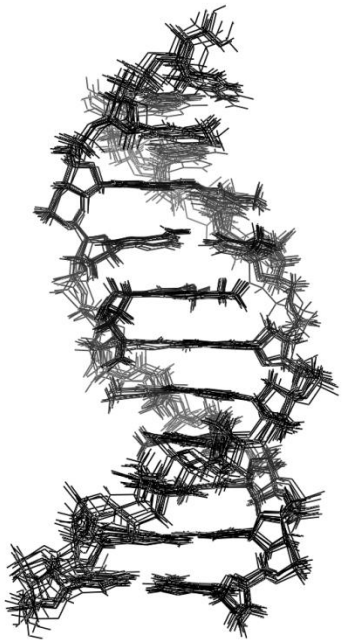


Figure 4-11: Stereo view of 10 superimposed structures of AFB$_1$-β-FAPY modified AXT (X= AFB$_1$-β-FAPY) resulting from the simulated annealing rMD protocol.

Expanded views of the structure are shown in Figure 4-12. The AFB_1 moiety intercalats above the 5′- face of the modified nucleotide X^5 and between base pairs A^4•T^{17} and X^5•C^{16}, causing the rise between these base pairs to increase to 5 Å. The adduct-induced unwinding is localized to the adducted base pair X^5•C^{16}, and its 5′- and 3′- neighbor base pairs A^4•T^{17} and A^6•T^{15}. The modified duplex is unwound approximately 15 ° at the adducted site. The X^5 N9H exocyclic amine proton is within hydrogen bonding distance of the X^5 formyl oxygen and positions the formamide in the *Z* conformation. Figure 4-13 shows the bottom view from 3′- neighbor base of the damaged site, confirming the *Z* conformation.

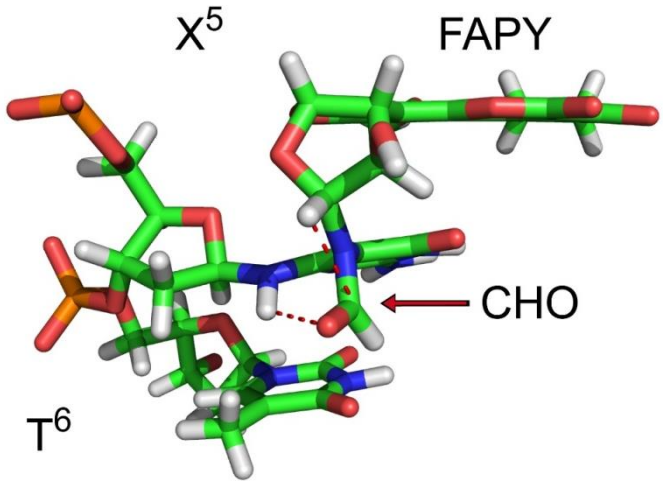


Figure 4-12. Expanded view of the refined structure of the AFB_1-β-FAPY modified AXT duplex at the lesion site. X = AFB_1-β-FAPY.

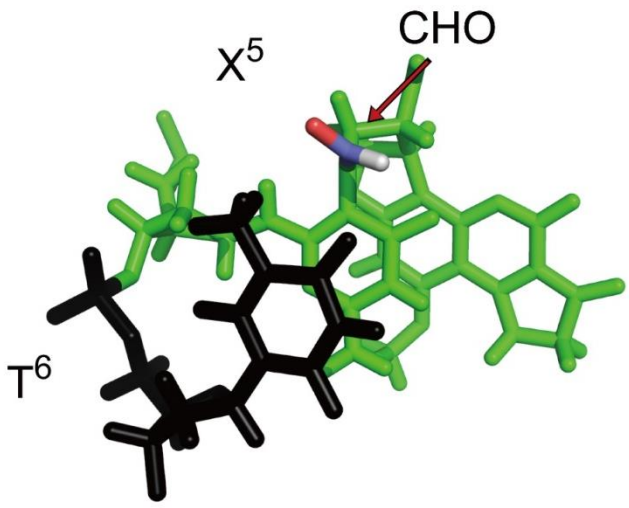


Figure 4-13. Expanded view of the refined structure of the AFB_1-β-FAPY modified AXT duplex at the lesion site from the 3′ - neighbor base. X = AFB_1-β-FAPY.

Helicoidal Analysis

A helicoidal analysis of the average solution structure was performed using CURVES*, following rMD calculations. As a result of the modification at X^5, a bend was present in the structure. The base pair parameters were normal for both the X- axis and Y-axis at the lesion site (Figure 4-14). The parameters for base-base interactions showed that the modification causes more than a 15 ° opening at the lesion site. Disruptions also occurred in the shear, the stretch, and the stagger, primarily at the lesion site (Figure 4-15). As was predicted by NOESY data, a 5 Å increase in rise was observed between X^5 and T^6 (Figure 4-16).

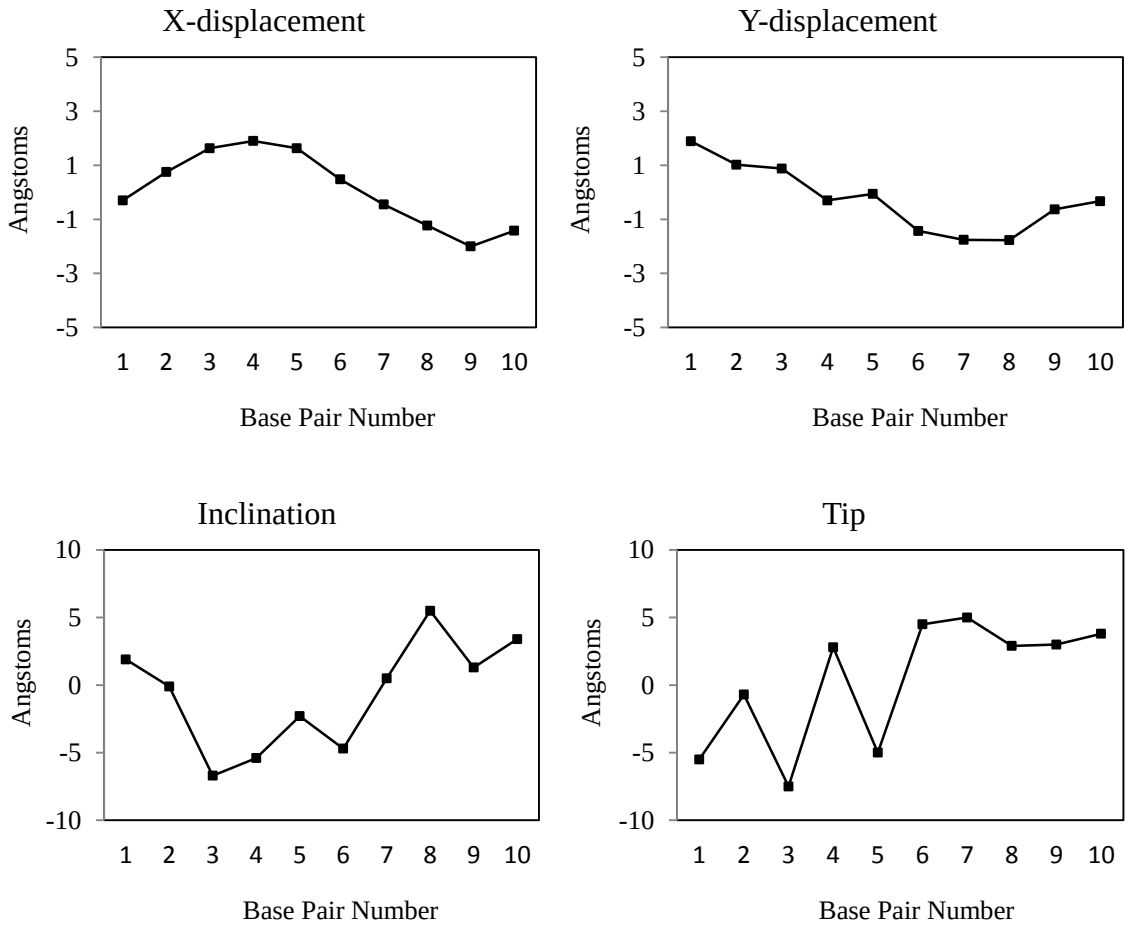


Figure 4-14: Global base pair helicoidal parameters. Helicoidal parameters for the AFB_1-β-FAPY modified AXT oligonucleotide 5′-$C^1T^2A^3A^4X^5T^6T^7T^8C^9A^{10}$-3′·5′-$T^{11}G^{12}A^{13}A^{14}A^{15}C^{16}T^{17}T^{18}$ A^{19} G^{20}-3′.

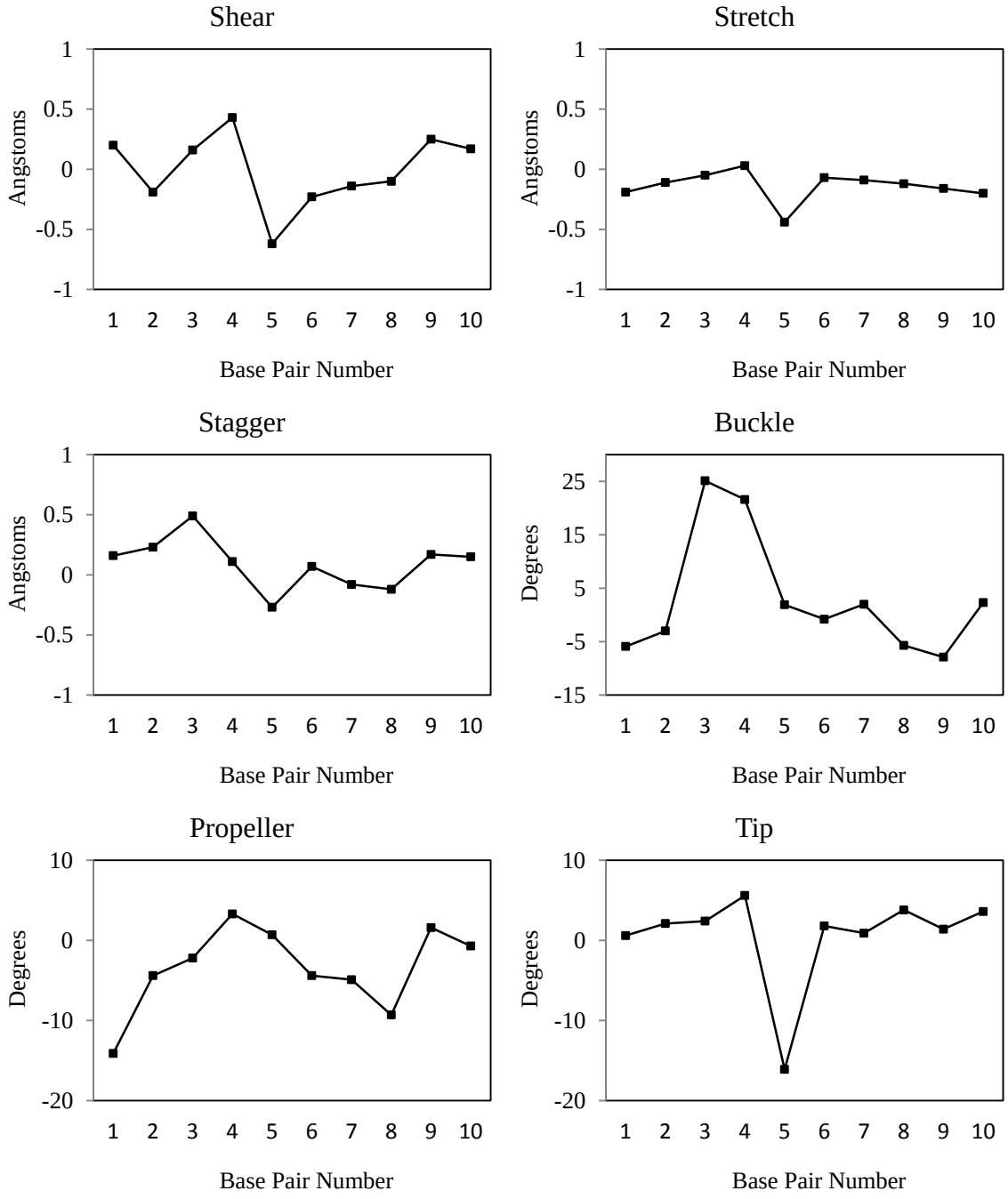


Figure 4-15: Global Intra-base pair helicoidal parameters. Helicoidal parameters for the AFB_1-β-FAPY modified AXT oligonucleotide 5′-$C^1T^2A^3A^4X^5T^6T^7T^8C^9A^{10}$-3′·5′-$T^{11}G^{12}A^{13}A^{14}A^{15}C^{16}T^{17}T^{18}$ A^{19} G^{20}-3′.

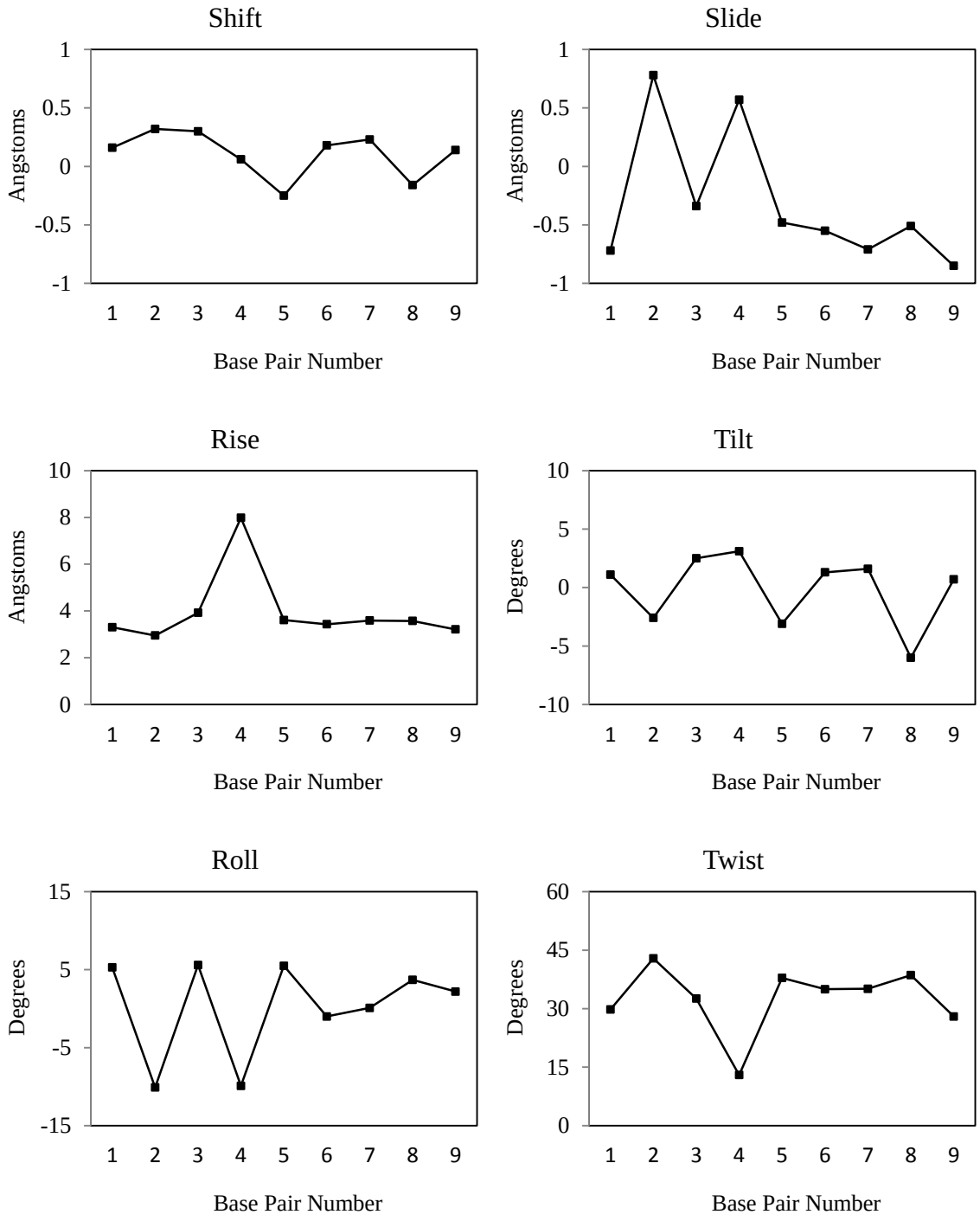


Figure 4-16: Global Inter-base pair helicoidal parameters. Helicoidal parameters for the AFB_1-β-FAPY modified AXT oligonucleotide 5′-$C^1T^2A^3A^4X^5T^6T^7T^8C^9A^{10}$-3′·5′-$T^{11}G^{12}A^{13}A^{14}A^{15}C^{16}T^{17}T^{18}$ A^{19} G^{20}-3′.

Discussion

Without the exocyclic amino proton on the 3′- neighbor thymine of the AFB_1-β-FAPY modified AXT duplex, the hydrogen bond that holds the formamide moiety in AXA context at *E* configuration does not exist. Thus, the formamide moiety of the AFB_1-β-FAPY adduct adopts the *Z* configuration. The evidence supporting the *Z* configuration includes the observation of a weaker NOE between the formyl proton and AFB_1 H8 proton, than the corresponding strong NOE in AXA duplex, indicating a longer distance between the two protons in AXT duplex. Moreover, the 0.7 ppm upfield shift for the formyl proton, compared to the correspondence in AXA sample, also suggests that the formyl proton is in a better stacked area. This is consistent with the *Z* configuration, since the formyl proton is orientated between the X^5 and T^6 bases. An additional potential force for the *Z* configuration could be attributed to a hydrogen bond between the formyl oxygen of the AFB_1-β-FAPY adduct and the X^5 N9H exocyclic amine proton. In the AXT duplex, the distance between the formyl oxygen and X^5 N9H is 3.1 Å, and the calculated angle O···H—N is 138°, which are in the range forming hydrogen bond. Analysis of rMD trajectories in explicit solvent indicates 76% occupancies for this hydrogen bond. Again, only one resonance of X^5 N1H is observed at both 10 ℃ and 40 ℃ in AXT duplex, suggesting the formamide moiety of the AFB_1-β-FAPY adduct is restrained as *Z* configuration, regardless of the temperature. The single resonance is also observed for the 3′- neighbor base T^6 N3H imino proton at both 10 ℃ and 40 ℃.

CHAPTER V

Solution structure of AFB_1-β-FAPY modified AX(7-deazaG) duplex

Introduction

In this chapter, the oligonucleotide 5′-d($C^1T^2A^3A^4G^5Y^6T^7T^8C^9A^{10}$)-3′•5′-d($T^{11}G^{12}A^{13}A^{14}A^{15}C^{16}C^{17}T^{18}A^{19}G^{20}$)-3′ (Y=7-deazaG) has been used to study the structure of AFB_1-β-FAPY in AXG context. Changing guanine to 7-deazaG makes the site-specific modification on X^5 possible since the potential reaction 7-nitrogen in guanine is replaced by a CH group in 7-deazaG. NMR analysis shows that, similar to the AXT context, the formyl group in AFB_1-β-FAPY is also held at the *Z* configuration.

Results

Sample Properties

The double strand AFB_1-β-FAPY modified oligonucleotide, 5′-d($C^1T^2A^3A^4G^5Y^6T^7T^8C^9A^{10}$)-3′•5′-d($T^{11}G^{12}A^{13}A^{14}A^{15}C^{16}C^{17}T^{18}A^{19}G^{20}$)-3′, was purified using HPLC. The identity of the duplex was verified using MALDI-TOF mass spectroscopy: for 5′-d($C^1T^2A^3A^4X^5Y^6T^7T^8C^9A^{10}$)-3′, calc'd 3372.1, found 3372.8; for the complementary strand 5′-d($T^{11}G^{12}A^{13}A^{14}C^{15}C^{16}T^{17}T^{18}A^{19}G^{20}$)-3′, calc'd 3027.0, found 3027.4 (Figure 5-1). The ratio of two strands was determined to be 1:1 after correction for the respective absorbance coefficients by using capillary gel electrophoresis. The melting temperature of the AFB_1-FAPY modified duplex was 46 ℃ (Figure 5-2), which is higher than the 37 ℃ melting temperature of the unmodified duplex.

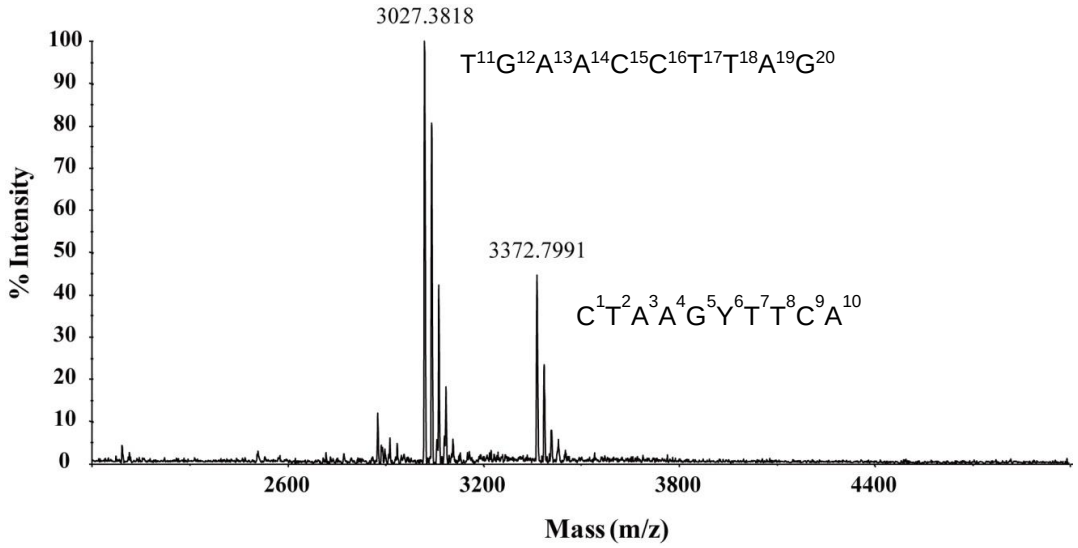


Figure 5-1. MALDI mass spectrum of AFB_1-β-FAPY modified AXY duplex sample. X = AFB_1-β-FAPY, Y= 7-deazaG.

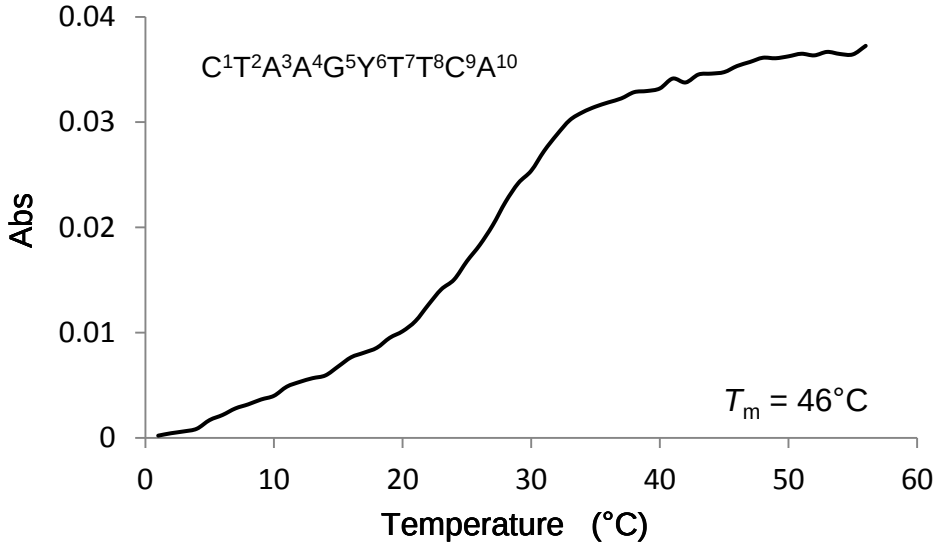


Figure 5-2. UV-melting curves of AFB_1-β-FAPY modified AXY duplex sample. X = AFB_1-β-FAPY, Y=7-deazaG.

DNA ^{1}H Resonance Assignment

Nonexchangeable DNA Protons

The resonances of the non-exchangeable protons of the AFB_1-β-FAPY modified AGA duplex were assigned using the sequential NOE connectivity of the base proton H6 or H8 dipolar couplings with H1′ deoxyribose protons.[105,106] For the modified strand, the NOE connectivity started from C^1 to A^4. Then an interruption was observed between A^4 H1′ and X^5 NOE connectivity, due to the loss of the guanine H8 proton because of the opening of the guanine imidazole ring in the FAPY formation. The connectivity was then observed from the formyl proton of the FAPY base and the 3′-neighbor, continuing to the 3′-terminus. For the complementary strand, the interruption of the sequential NOE connectivity was also observed between C^{16} H1′ and T^{17} H8. Expanded plots of the NOESY spectrum for the AFB_1-β-FAPY modified AGA duplex are shown in Figure 3-3. The purine and pyrimidine aromatic protons, the thymine methyl protons and the deoxyribose H1′, H2′, H2″, and H3′ protons were successfully assigned. The H4′, H5′, and H5″ protons were only partially assigned due to heavy overlapping peaks and the effects of spin diffusion at higher mixing times.

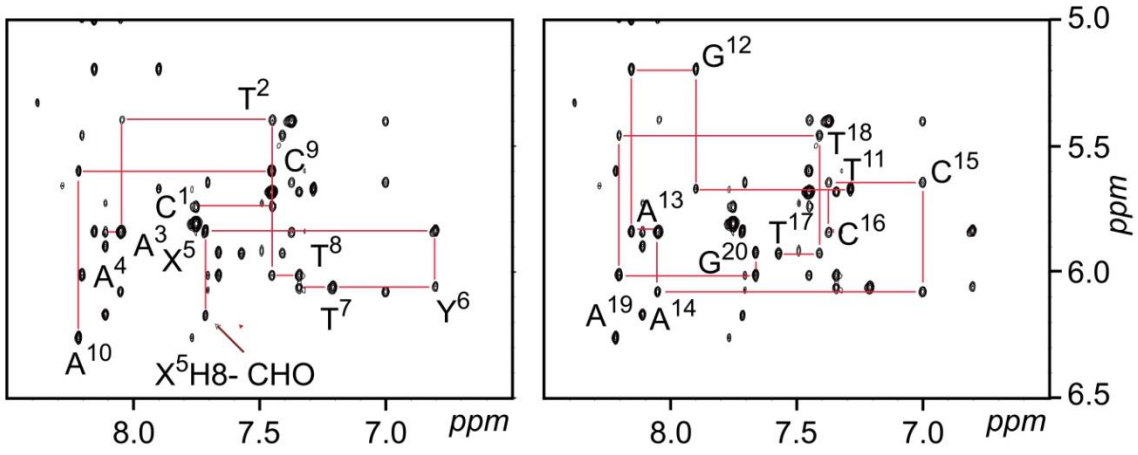


Figure 5-3. NOE connectivity of base H8/H6 protons with deoxyribose H1′ protons of the AFB$_1$-β-FAPY modified AXY duplex. (A) The modified strand. (B) The complementary strand. X = AFB$_1$-β-FAPY, Y=7-deazaG. The experiment was carried out at 250 ms mixing time and 900 MHz. The temperature was 283 K.

Anomeric Configuration

Due to the heavy overlap of the peaks of the deoxyribose H1′, H2′, H2″, and H3′ protons, the determination of the anomeric configuration of the AFB$_1$-β-FAPY modified AGY duplex was implausible.

Exchangeable DNA Protons

The resonances of the base imino protons were assigned on the basis of sequential connectivity between adjacent base pairs in NOESY spectra, and the assignments were supported by NOEs to the amino protons of Watson-Crick base pairs.[107] Between X^5 N1H and T^{17} N3H imino resonances, there is an interruption of the sequential imino-to-imino proton NOEs of adjacent base pairs. The strong cross peaks from X^5 N1H to C^{16} N4H1 and

C^{16} N4H2 amino protons indicated that Watson-Crick hydrogen bonding between X^5 and C^{16} was intact.

NMR Spectroscopy of Formyl Proton Resonance (CHO)

A single peak was observed for the AFB_1-β-FAPY modified AXY duplex in HMQC experiment acquired at 283 K. This peak revealed the presence of carbonyl resonance at 168.66 ppm, coupled to proton resonance at 7.71 ppm (Figure 5-4).

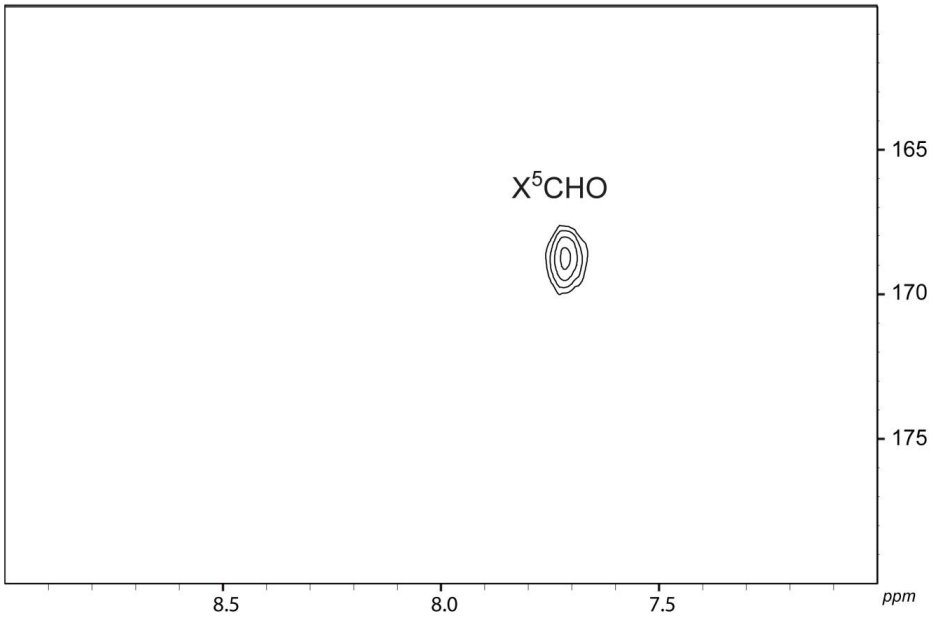


Figure 5-4. NMR analysis of ^{1}H-^{13}C HMQC of AFB_1- β-FAPY modified AXY duplex. The experiment was carried out at 600 MHz and the temperature was 283 K.

Aflatoxin FAPY Protons

The AFB_1 H5, H6a, H8, H9, H9a, and $–OCH_3$ resonances were assigned from a combination of NOE connectivities and chemical shift data (Figure 3-6). AFB_1 H6a and H9a were identified from both COSY and NOESY experiments. AFB_1 H8 and H9 were

assigned based on NOEs between H6a or H9a, and between themselves. A strong NOE was observed between AFB_1 H5 and AFB_1 –OCH_3, revealing that the latter resonance was at δ 3.62 ppm, while AFB_1 H5 was at δ 5.74 ppm. Similar to AXT sequence, a weak NOE peak was observed between AFB_1 H8 and CHO (Figure 5-5). The X^5 CHO resonance was observed at δ 7.73 ppm, confirming the assignment of the carbonyl resonance in the HMQC experiment. The assignment of X^5 CHO resonance was also supported by NOEs to AFB_1 H6a and H9. The cyclopentenone ring protons AFB_1 H2$_\alpha$, H2$_\beta$, H3$_\alpha$, and H3$_\beta$ were identified from a combination of COSY and NOESY experiments.

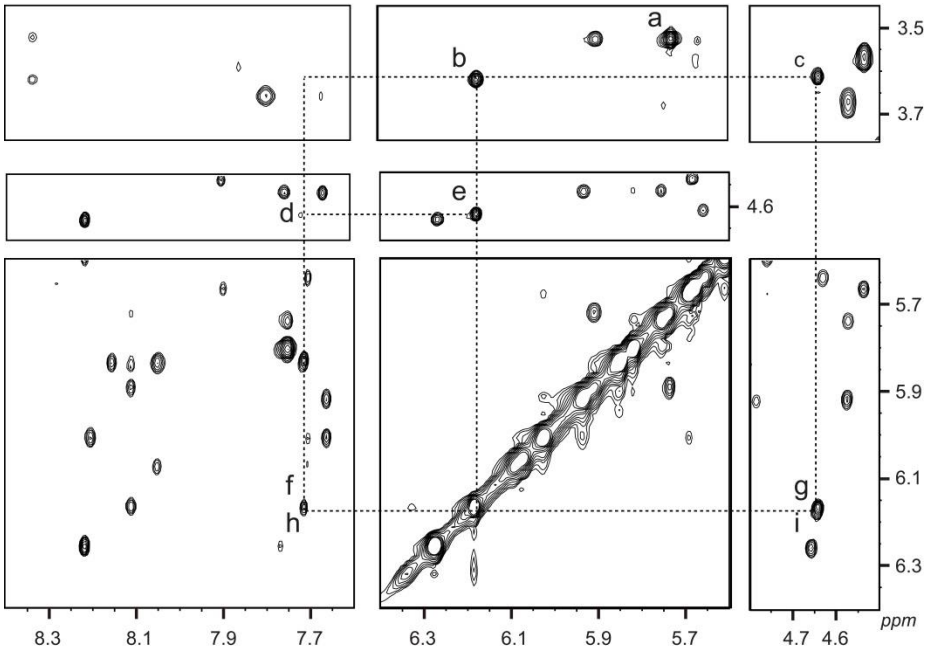


Figure 5-5. NOE assignments of the FAPY protons of the AFB_1-β-FAPY modified AXY duplex. The cross peaks are assigned as: (a) X^5OCH_3 → X^5H5; (b) X^5H9a → X^5H6a; (c) X^5H9a →X^5H9; (d) X^5H9 →X^5CHO; (e) X^5H9 →X^5H6a; (f) X^5H6a →X^5CHO; (g) X^5H6a →X^5H9. The experiment was carried out at 250 ms mixing time and 900 MHz. The temperature was 283 K. X = AFB_1-β-FAPY, Y=7-deazaG.

Aflatoxin FAPY to DNA NOEs

A total of 39 NOEs from AFB_1 protons to DNA protons were observed. The protons of the two AFB_1-fused furan rings showed NOEs to major groove and imino protons of the DNA; most of these were to the 5′ neighboring base-pair A^4•T^{17}. Thus, H6a and H9a, which are located on the same face of the AFB_1 moiety, both exhibited NOEs to A^4H8. A weaker NOE was observed for AFB_1 H9. The AFB_1 H5 and $–OCH_3$ protons exhibited NOEs with minor groove and imino DNA protons. These were primarily to base A^4•T^{17}, in the 5′ direction, and to the modified nucleotide X^5 (Figure 5-6). These included NOEs between AFB_1 $–OCH_3$ and A^4 H1′, A^4 H2′, A^4 H2″, A^4 H2, T^{17} N3H, X^5 H1′, and X^5 N1H. The cyclopentenone ring H2α and H2β produced NOEs with H1′, H2′, and H2″ of C^{16}, and H1′, and H3′ of T17 of the complementary strand.

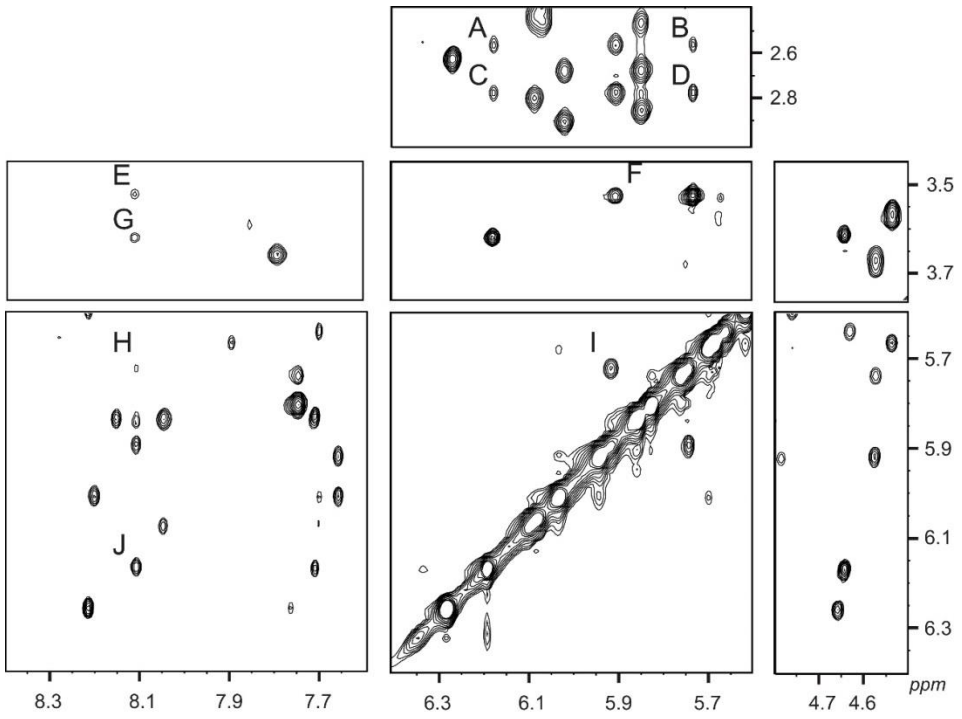


Figure 5-6. NOE assignments of the FAPY to DNA protons of the AFB_1- β-FAPY modified AXY duplex. The cross peaks are assigned as: (A) $X^5H2' \rightarrow X^5H6a$; (B) X^5 $H2' \rightarrow X^5H5$; (C) $X^5H2'' \rightarrow X^5H6a$; (D) X^5 $H2'' \rightarrow X^5H5$; (E) $X^5OCH_3 \rightarrow A^4H8$; (F) $X^5OCH_3 \rightarrow A^4H1'$; (G) $X^5H9a \rightarrow A^4H8$; (H) $X^5H5 \rightarrow A^4H8$; (I) $X^5H5 \rightarrow A^4H1'$; (J) $X^5H6a \rightarrow A^4H8$. The experiment was carried out at 250 ms mixing time and 900 MHz. The temperature was 283 K. X = AFB_1-β-FAPY, Y=7-deazaG.

NMR Melting Experiments

The thermal melting of the AFB_1-β-FAPY modified AXY duplex was compared to the corresponding unmodified AGY duplex by monitoring spectra of the imino protons as a function of temperature. A single resonance was also observed at both 10 and 40 ℃ for the X^5 N1H imino proton (Figure 5-7).

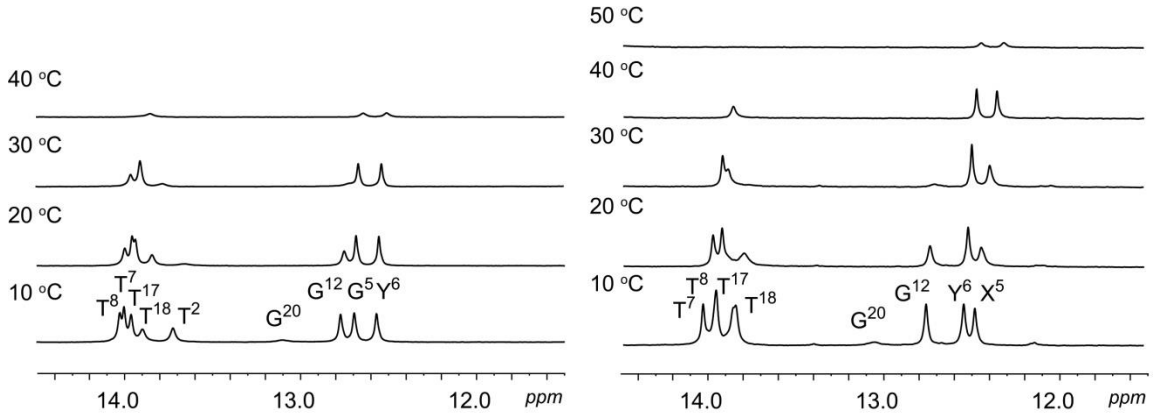
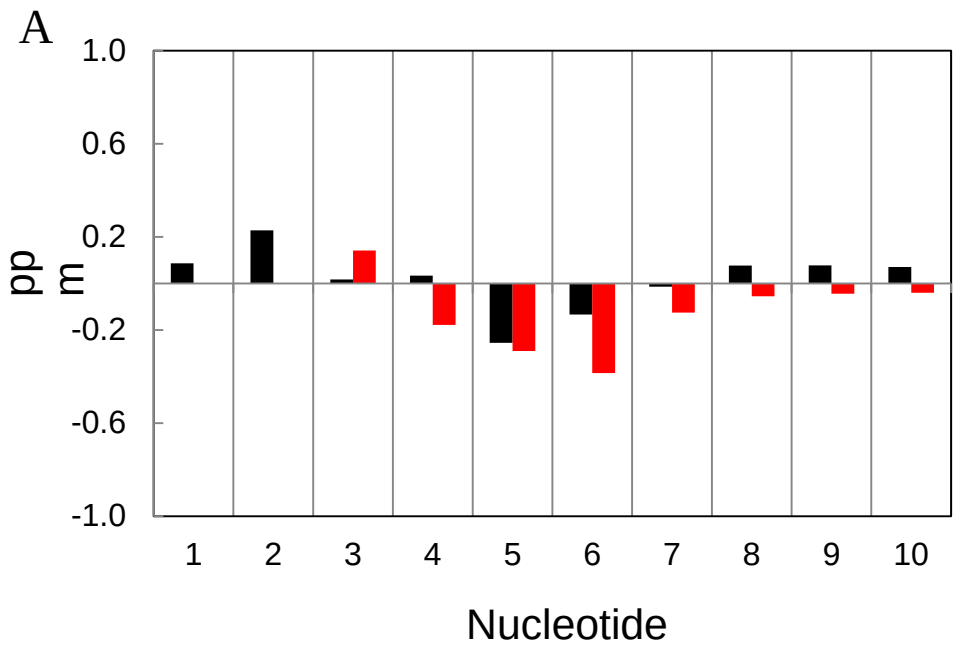


Figure 5-7. Expanded spectra of AFB$_1$-β-FAPY modified AXY duplex compared with the corresponding unmodified duplex at different temperature. (A) The unmodified duplex. (B) The modified duplex. X = AFB$_1$-β-FAPY. The experiment was carried out at 800 MHz. X = AFB$_1$-β-FAPY, Y=7-deazaG.

Chemical Shift Effects

The ^{1}H spectrum of the AFB$_1$-β-FAPY modified AXY duplex exhibited significant chemical shift differences around the modified base X^5 compared to that of the unmodified oligodeoxynucleotide (Figure 5-8). In the major groove, at the 3′-side of X^5, a downfield shift of 0.39 ppm was observed for Y6 H8, as well as a downfield shift of 0.18 ppm for A^4 H8 and a downfield shift of 0.22 ppm for T^{17} H6 at the 5′-side of X^5. In the minor groove, A downfield chemical shift of 0.26 ppm was observed for X^5 H1', whereas a downfield shift of 0.13 ppm was observed for T^6 H1'. For the imino protons, an upfield shift of 0.19 ppm was observed for X^5 H1H. T^7 N3H, two base pairs from the adducted site, also experienced a 0.1 ppm downfield shift.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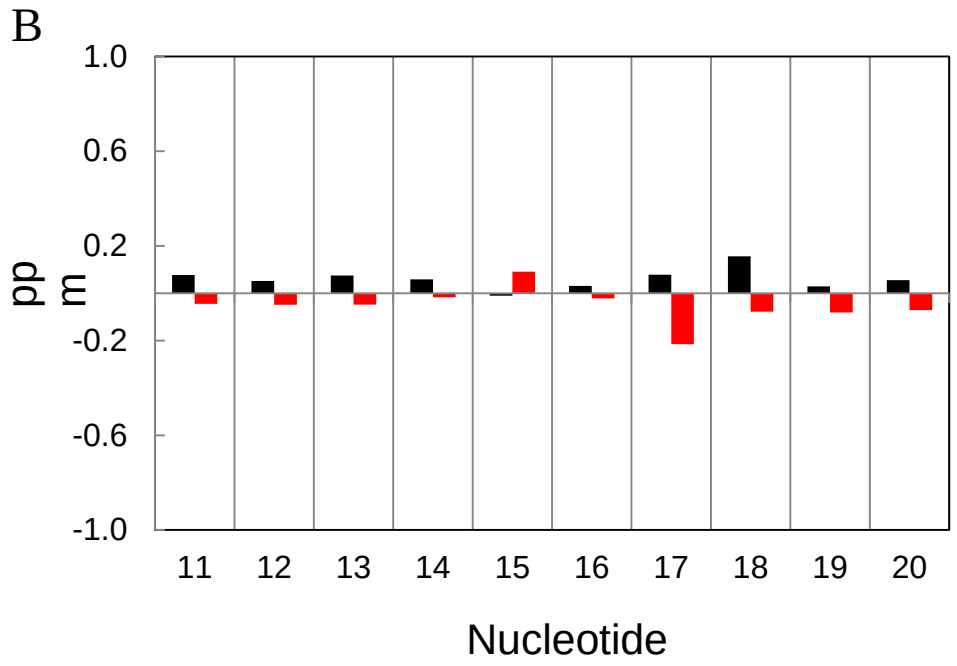
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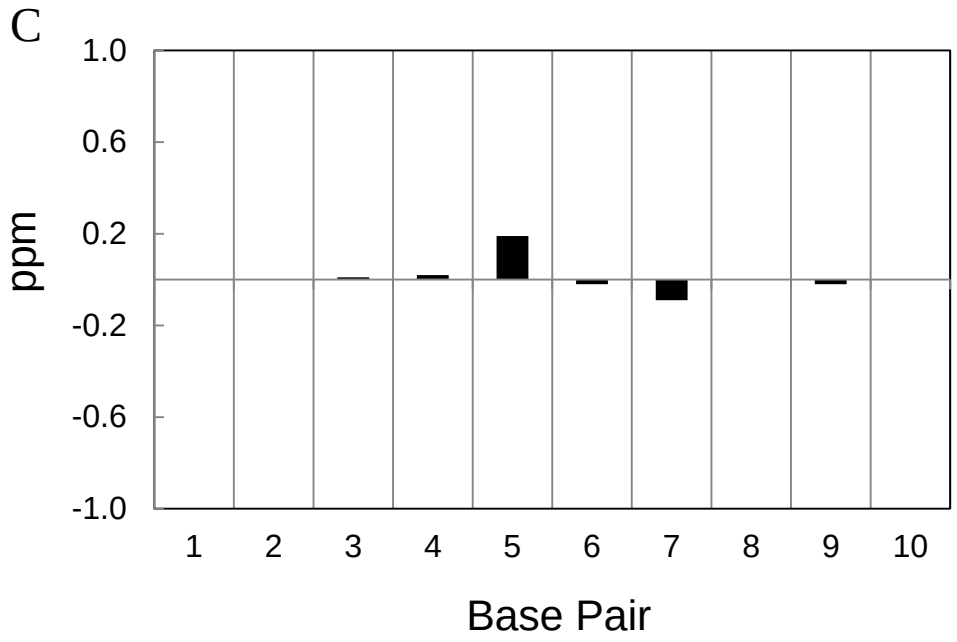


Figure 5-8. Chemical shift differences of protons of the AFB_1-β-FAPY Modified AXY Duplex, relative to the unmodified onligodeoxynucleotide. **A**. Nucleotides $C^1 \rightarrow A^{10}$ of the AFB_1-β-FAPY Modified AXT duplex. **B**. Nucleotides $T^{11} \rightarrow G^{20}$ of the AFB_1-β-FAPY Modified AXY duplex. **C**. Base pairs 1→10 of AFB_1-β-FAPY Modified AXY duplex. Black bars represents the deoxyribose H1' protons; red bars represent the purine H8 or pyrimidine H6 protons, respectively; grey bars represent the imino guanine N1H or thymine N3H protons. X = AFB_1-β-FAPY, Y=7-deazaG.

Structural Refinement

A total of 264 distance restraints, including 161 intranucleotide and 103 internucleotide restraints, were calculated from the intensities of NOE cross-peaks using MARDIGRAS[73-76]. A total of 39 restrains were either intranucleotide or internucleotide AFB_1-FAPY to DNA NOEs. In addition to those experimental restraints, a total of 36 empirical distance restraints arising from Watson-Crick base pairing interactions were used, but not at the AFB_1-FAPY adduct. A total of 84 backbone torsion restraints were also

applied; however, at the AFB_1-FAPY adduct, the backbone torsion angles were not restrained.

The rMD calculations for the AFB_1-β-FAPY modified AXT duplex were performed from the initial B- form DNA staring structures. The final ten structures with lowest energies were obtained. All structures converged as indicated by pairwise rmsd comparison (Table 5-1). The accuracies of the emergent structures were evaluated by comparison of theoretical NOE intersities calculated by CORMA[77-79] for the refined structure to the experimental NOE intensities to yield sixth root residuals (R_1^x). The R_1^x values for overall residuals, as well as the residuals for intra- or inter-nucleotide NOEs, were consistently less than 0.1 (Figure 5-9), and for each nucleotide were less than 0.15, suggesting that the refined structures were in good agreement with the NOESY data.

Table 5-1. Distribution of restrainss applied to structural refinement and statistical analysis for the AFB_1-β-FAPY modified AXY duplex.

	restrains
Experimental NOE Distance Restraints	264
Intra-residue NOE Restraints	161
Inter-residue NOE Restraints	103
NOEs of FAPY	39
Empirical Base Pairing Restraints	36
Empirical Backbone Torsion Restraints	42
Empirical Deoxyribose Torsion Restraints	42
Total Restraints for rMD Caculation	384
Structure Statistics	
NMR R-factor (R^*) ($\times 10^{-2}$)	8.28
Intra-residue NOEs	7.64
Inter-residue NOEs	9.40
rmsd Deviation of Refined Structures	0.628

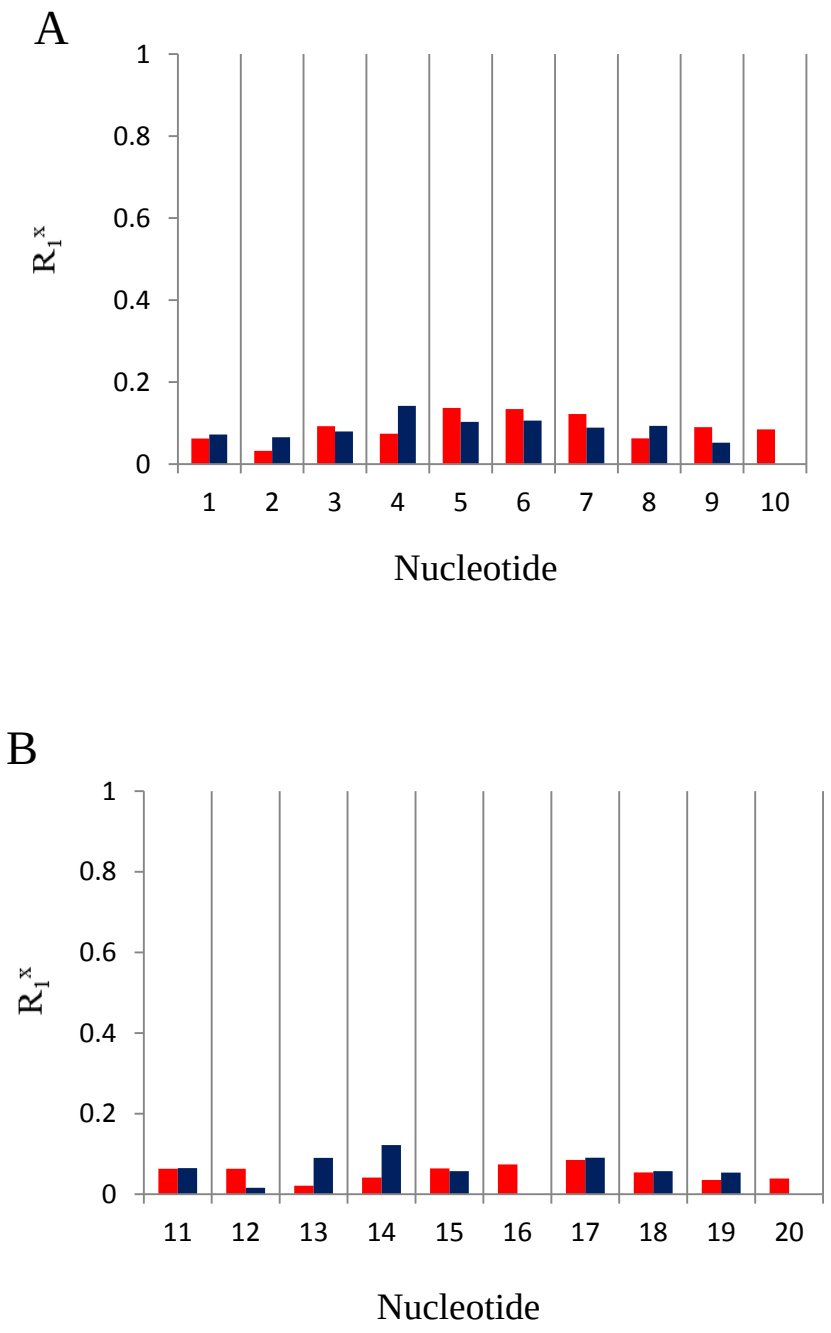


Figure 5-9. Sixth root residuals between calculated NOE intensities and experimental NOE intensities (R_1^x values) as a function of position in the AFB_1-β-FAPY modified AXY duplex. (A) Nucleotides C^1-A^{10} of the modified oligonucleotide containing AFB_1-β-FAPY. (B) Nucleotides T^{11}-G^{20} of the complementary strand. The red bars represent intranuclear sixth root residuals and the black bars represent internuclear sixth root residuals. X = AFB_1-β-FAPY, Y=7-deazaG.

Molecular Dynamics Calculations in Explicit Solvent.

The 1 ns of equilibrium rMD calculation was performed in explicit water at constant pressure at 300K to examine the dynamics of the refined structure and to analyze hydrogen bond occupancies involving the formamido group of the FAPY moiety. The 1 ns rMD trajectory was analyzed for occupancies of hydrogen bonding motifs. Hydrogen bond occupancies were calculated using a distance cutoff of 3.5 Å and an angle cutoff of 120 °. On the basis, the X^5 N9H exocyclic amine proton was within hydrogen bonding distance of the X^5 formyl oxygen; this positioned the formamide in the Z conformation. This hydrogen bond was satisfied for 81% of the trajectory of 1 ns of equilibrium rMD calculation performed in explicit water.

Structure of the AFB_1-β-FAPY Modified AXY Duplex

Stereo views of 10 rMD refined solution structures for the AFB_1-β-FAPY modified AXY duplex DNA are depicted in Figure 5-10. The root mean squared deviation (RMSD) between the 10 structures was 0.63 Å. The overall structure maintained Watson-Crick base pairing. The AFB_1 adduct is intercalated between A^4●T^{17} and X^5●C^{16}. The formyl group has a *Z* geometrical configuration.

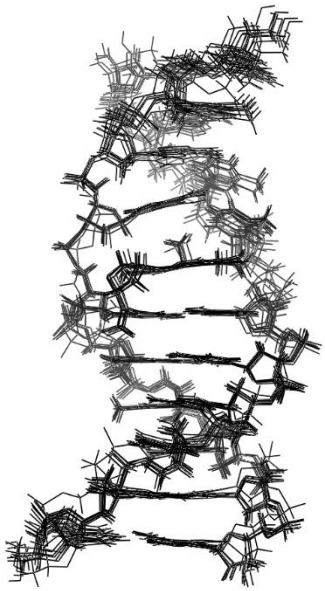


Figure 5-10: Stereo view of 10 superimposed structures of AFB_1-β-FAPY modified AXY (X= AFB_1-β-FAPY) resulting from the simulated annealing rMD protocol. X = AFB_1-β-FAPY, Y=7-deazaG.

Expanded views of the structure are shown in Figure 5-11. The AFB_1 moiety intercalated above the 5′- face of the modified nucleotide X^5 and between base pairs A^4•T^{17} and X^5•C^{16}, causing the rise between these base pairs to increase to 7 Å. The adduct-induced unwinding was localized to the adducted base pair X^5•C^{16}, and its 5′ - and 3′ - neighbor base pairs A^4•T^{17} and Y^6•C^{15}. The modified duplex was unwound approximately 15 °at the adducted site. The X^5 N9H exocyclic amine proton was within hydrogen bonding distance of the X^5 formyl oxygen and positioned the formamide in the *Z* conformation. Figure 5-12 shows the damaged site from 3′ - neighbor base, confirming the *Z* conformation.

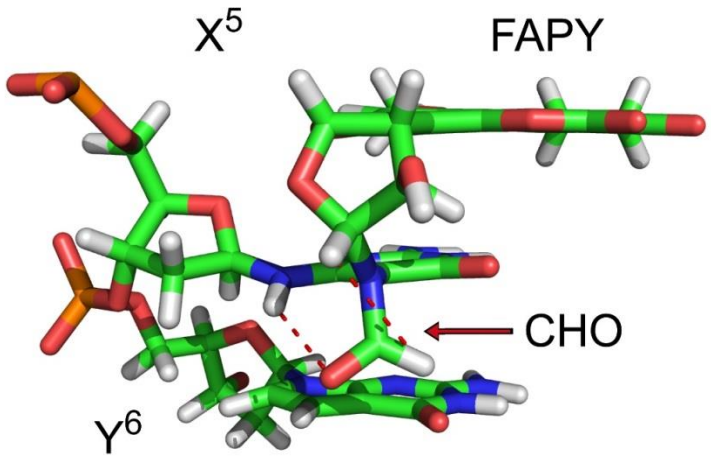


Figure 5-11. Expanded view of the refined structure of the AFB_1-β-FAPY modified AXy duplex at the lesion site X = AFB_1-β-FAPY, Y=7-deazaG.

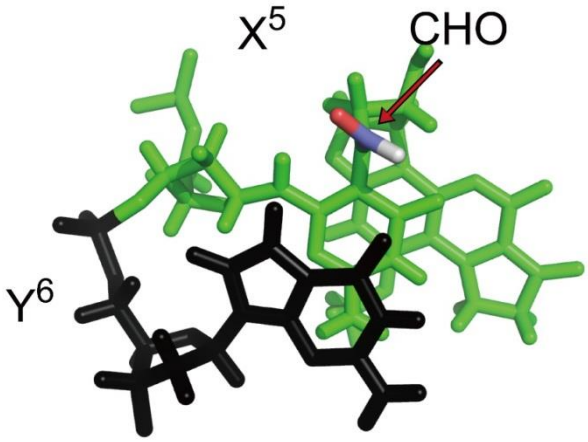


Figure 5-12. Expanded view of the refined structure of the AFB_1-β-FAPY modified AXY duplex at the lesion site from the 3′ - neighbor base. X = AFB_1-β-FAPY, Y=7-deazaG.

Helicoidal Analysis

A helicoidal analysis of the average solution structure was performed using CURVES*, following rMD calculations. A bend was present in the structure as a result of the modification at X^5,. The base pair parameters were normal for both the X- axis and Y-

axis at the lesion site (Figure 5-13). The parameters for base-base interactions showed that the modification caused more than a 10 ° opening at the lesion site. Disruptions also occurred in the shear, the stretch, and the stagger, primarily at the lesion site (Figure 5-14). As was predicted by NOESY data, a 5 Å increase in rise was observed between X^5 and Y^6 (Figure 5-15).

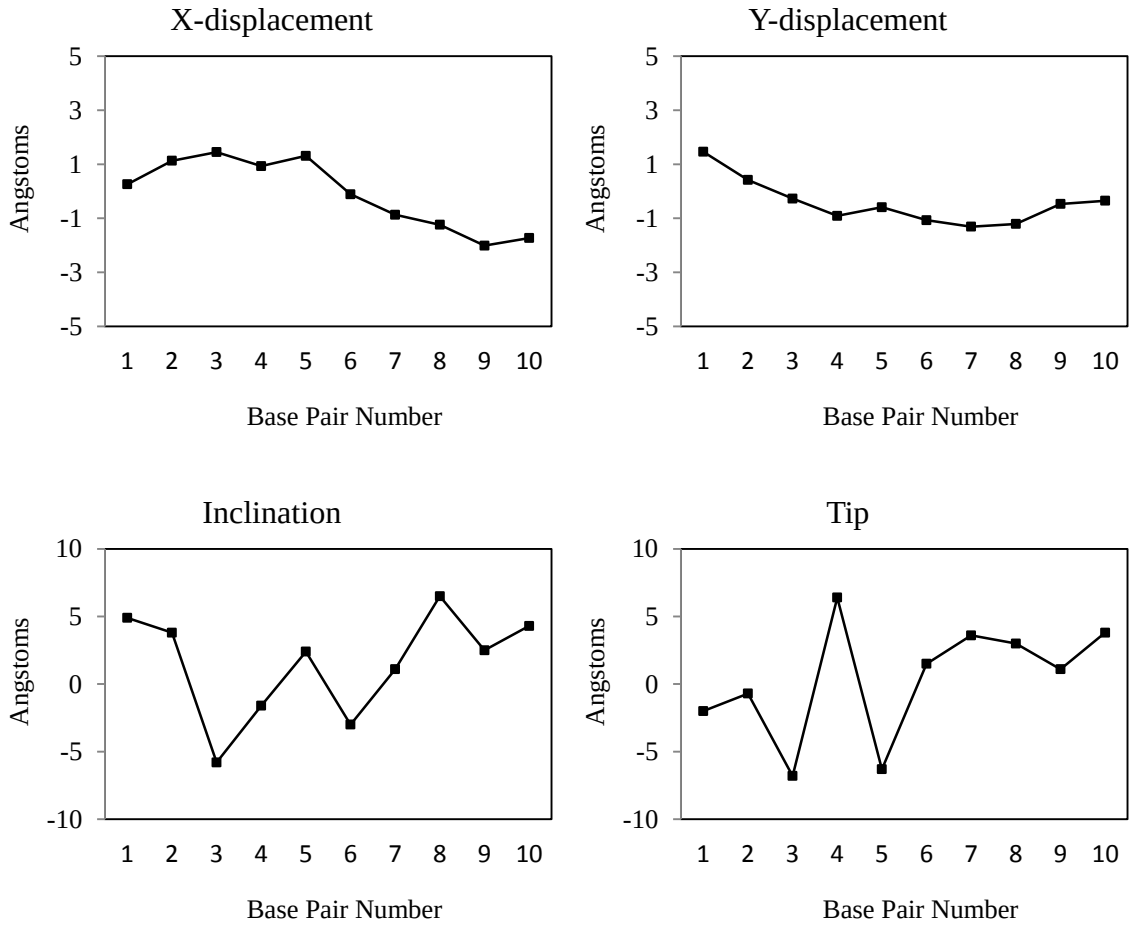


Figure 5-13: Global base pair helicoidal parameters. Helicoidal parameters for the AFB_1-FAPY modified AXY oligonucleotide 5′-$C^1T^2A^3A^4X^5Y^6T^7T^8C^9A^{10}$-3′·5′-$T^{11}G^{12}A^{13}A^{14}C^{15}C^{16}T^{17}T^{18}$ A^{19} G^{20}-3′.

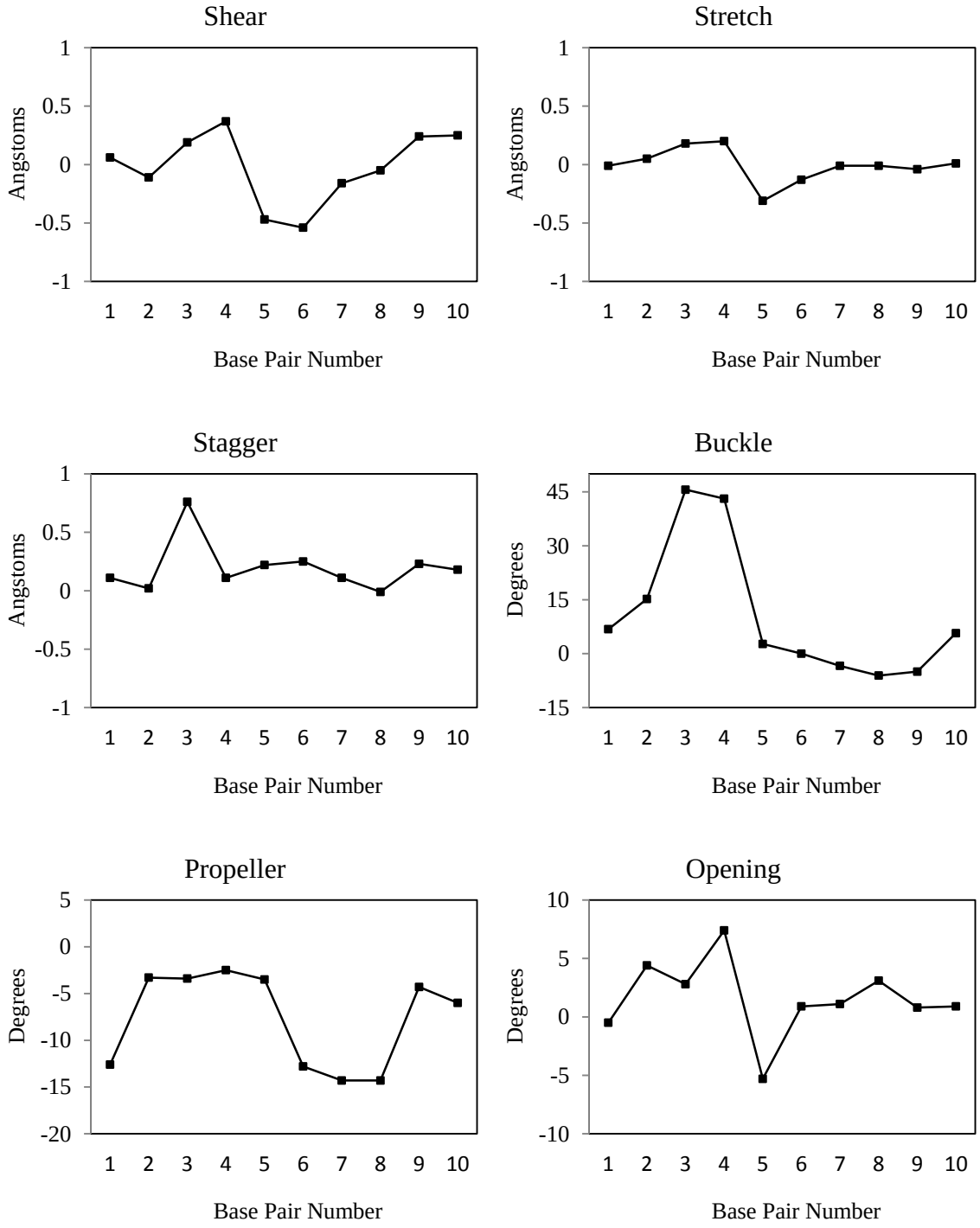


Figure 5-14: Global Intra-base pair helicoidal parameters. Helicoidal parameters for the AFB_1-FAPY modified AXY oligonucleotide 5′-$C^1T^2A^3A^4X^5Y^6T^7T^8C^9A^{10}$-3′·5′-$T^{11}G^{12}A^{13}A^{14}C^{15}C^{16}T^{17}T^{18}$ A^{19} G^{20}-3′.

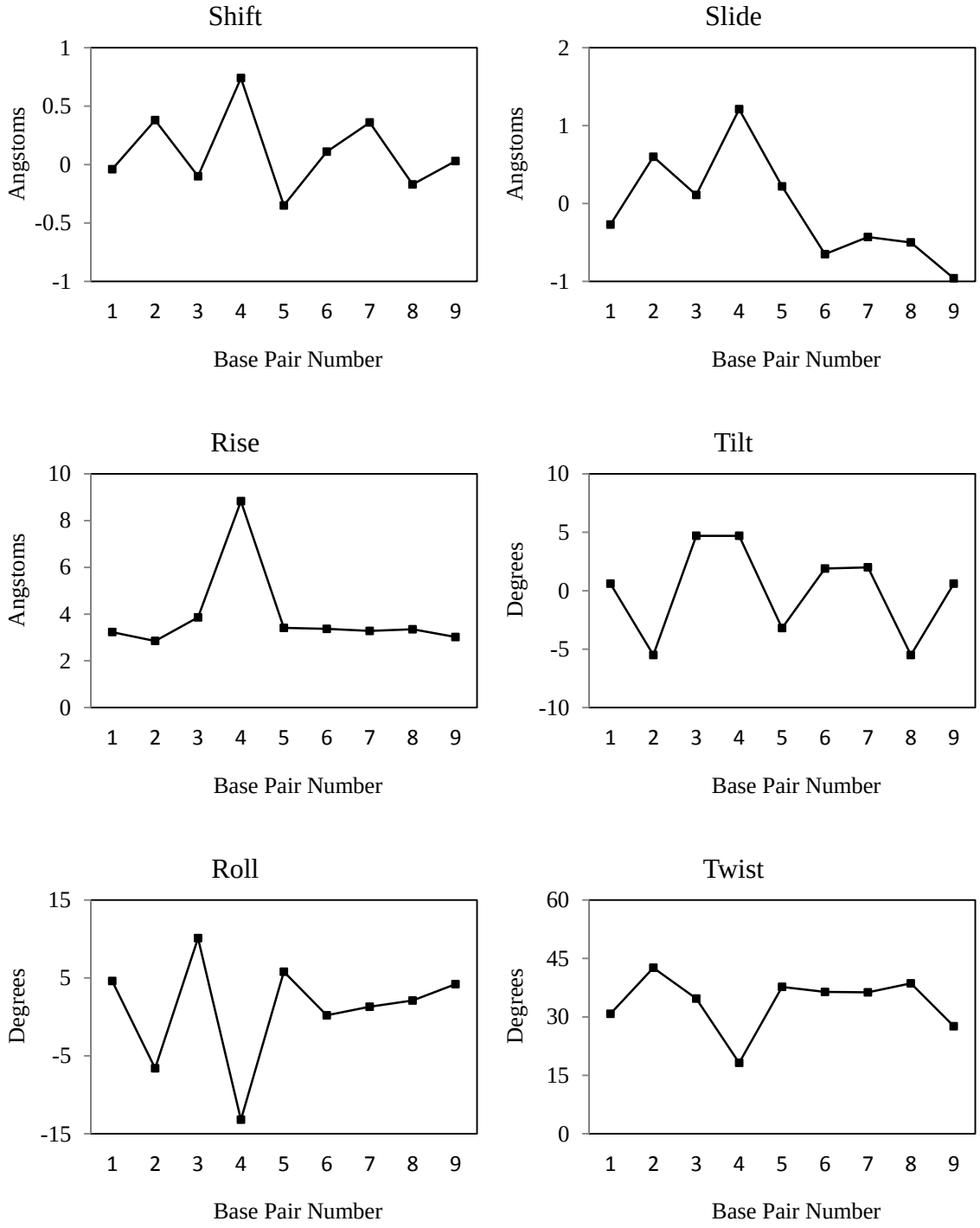


Figure 5-15: Global Inter-base pair helicoidal parameters. Helicoidal parameters for the AFB_1-FAPY modified AXY oligonucleotide 5′-$C^1T^2A^3A^4X^5Y^6T^7T^8C^9A^{10}$-3′·5′-$T^{11}G^{12}A^{13}A^{14}C^{15}C^{16}T^{17}T^{18}$ A^{19} G^{20}-3′.

Discussion

In the AFB_1-β-FAPY modified AXY duplex, without the exocyclic amino proton on the 3′- neighbor thymine, the hydrogen bond that holds the formamide moiety in AXA context at *E* configuration does not exist. Thus, the formamide moiety of the AFB_1-β-FAPY adduct is held in the *Z* configuration. The evidence supporting the *Z* configuration includes the observation of a weaker NOE between the formyl proton and AFB_1 H8 proton, than the corresponding strong NOE in AXA duplex, indicating a longer distance between the two protons in AXY duplex. Moreover, the 0.7 ppm upfield shift for the formyl proton, compared to the correspondence in AXA sample, also suggests that the formyl proton in a better stacked area, which is consistent with the *Z* configuration, in which the formyl proton is orientated between the X^5 and Y^6 bases. An additional potential force for the *Z* configuration could be also attributed by a hydrogen bond between the formyl oxygen of the AFB_1-β-FAPY adduct and the X^5 N9H exocyclic amine proton. In AXY duplex, the distance between the formyl oxygen and X^5 N9H is 3.1 Å, and the calculated angle O···H—N is 138°, which are in the range forming hydrogen bond. Analysis of rMD trajectories in explicit solvent indicates 76% occupancies for this hydrogen bond. Again, only one resonance of X^5 N1H is observed at both 10 ℃ and 40 ℃ in AXY duplex, suggesting the formamide moiety of the AFB_1-β-FAPY adduct is restrained as *Z* configuration, regardless of the temperature. The single resonance is also observed for the imino proton of the 3′- neighbor base, Y^6 N3H, at both 10 ℃ and 40 ℃.

CHAPTER VI

Solution structure of AFB_1-β-FAPY modified AXC duplex

Introduction

This chapter addresses the solution structure of AFB_1-β-FAPY modified sample, 5′-d($C^1T^2A^3A^4X^5C^6T^7T^8C^9A^{10}$)-3′•5′-d($T^{11}G^{12}A^{13}A^{14}G^{15}C^{16}T^{17}T^{18}A^{19}G^{20}$)-3′. In the AXC sequence context, two species are observed. Both species are β anomers. The "major" isomer is characterized as *E* geometrical isomer and the "minor" isomer is identified as *Z* geometrical isomer.

Results

Sample Properties

The double strand AFB_1-β-FAPY modified oligonucleotide, 5′-d($C^1T^2A^3A^4G^5C^6T^7T^8C^9A^{10}$)-3′•5′-d($T^{11}G^{12}A^{13}A^{14}G^{15}C^{16}T^{17}T^{18}A^{19}G^{20}$)-3′, was purified using HPLC. The identity of the duplex was verified using MALDI-TOF mass spectroscopy: for 5′-d($C^1T^2A^3A^4X^5C^6T^7T^8C^9A^{10}$)-3′, calc'd 3333.1, found 3333.2; for the complementary strand 5′-d($T^{11}G^{12}A^{13}A^{14}G^{15}C^{16}T^{17}T^{18}A^{19}G^{20}$)-3′, calc'd 3067.1, found 3067.2 (Figure 6-1). The molar ratio of two strands was determined to be 1:1 after correction for the respective absorbance coefficients by using capillary gel electrophoresis. The melting temperature of the AFB_1-FAPY modified duplex was 46 ℃ (Figure 6-2), higher than the 36 ℃ melting temperature of the unmodified duplex.

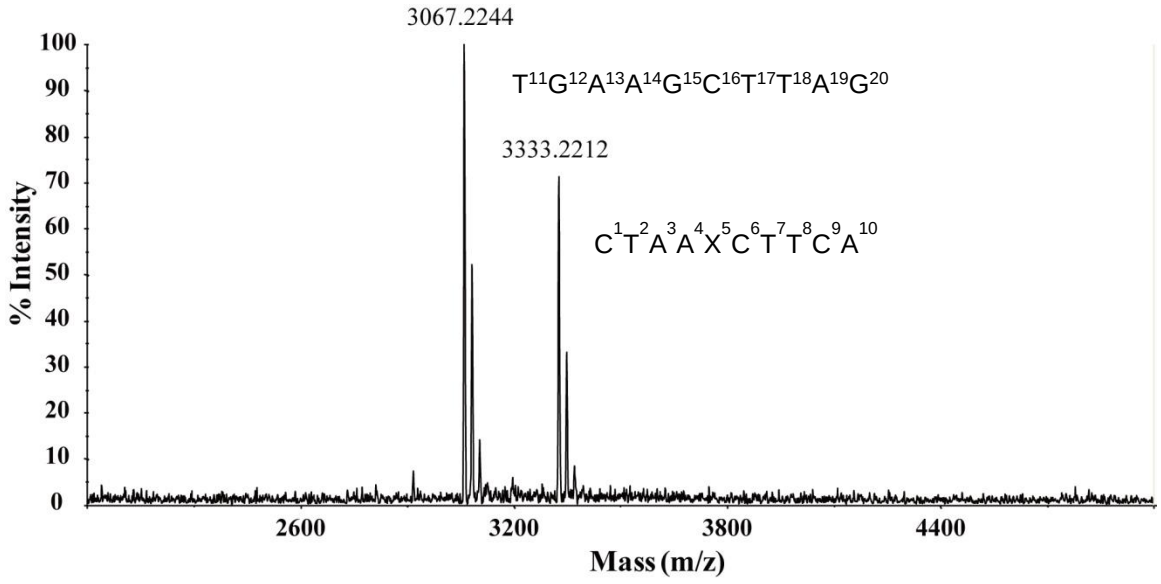


Figure 6-1. MALDI mass spectrum of AFB_1-β-FAPY modified AXC duplex sample. X = AFB_1-β-FAPY.

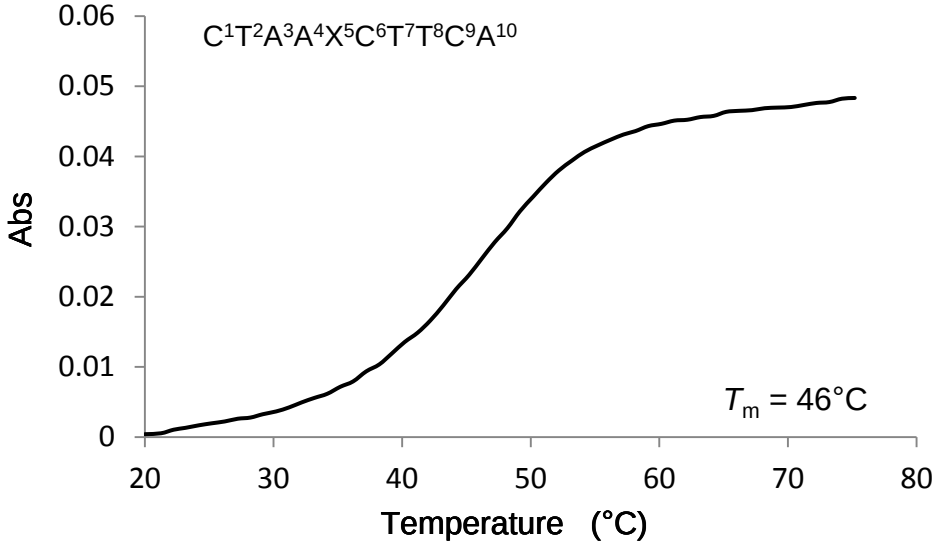


Figure 6-2. UV-melting curves of AFB_1-β-FAPY modified AXC duplex sample. X = AFB_1-β-FAPY.

DNA ^{1}H Resonance Assignments

Nonexchangeable DNA Protons

The resonances of the non-exchangeable protons of the AFB_1-β-FAPY modified AGA duplex were assigned using the sequential NOE connectivity of the base proton H6 or H8 dipolar couplings with H1′ deoxyribose protons.[105,106] For the modified strand, the NOE connectivity started from C^1 to A^4. Then an interruption was observed between A^4 H1′ and X^5 NOE connectivity, due to the loss of the guanine H8 proton because of the opening of the guanine imidazole ring in the FAPY formation. The connectivity was then observed from the formyl proton of the FAPY base and the 3′-neighbor, continuing to the 3′-terminus. For the complementary strand, the interruption of the sequential NOE connectivity was also observed between C^{16} H1′ and T^{17} H8. Two sets of resonances for several protons were observed for the base pairs X^5•C^{16}, C^6•G^{15}, and T^7•A^{14}, in both COSY and NOESY experiments, suggesting the existence of two isomers. The ratio between the two isomers was established as 2.2: 1, based on the comparison of intensities of two H5-H6 cross peaks on C^{16}. However, only 1 set of resonance of AFB_1 moiety in X^5 was observed. Expanded plots of the NOESY spectrum for the major isomer of AFB_1-β-FAPY modified AGC duplex are shown in Figure 6-3. Assignments of the purine and pyrimidine aromatic protons, the thymine methyl protons and the deoxyribose H1′, H2′, H2″, and H3′ protons were successfully completed. The H4′, H5′, and H5″ protons were only partially assigned due to heavy overlapping peaks and the effects of spin diffusion at higher mixing times.

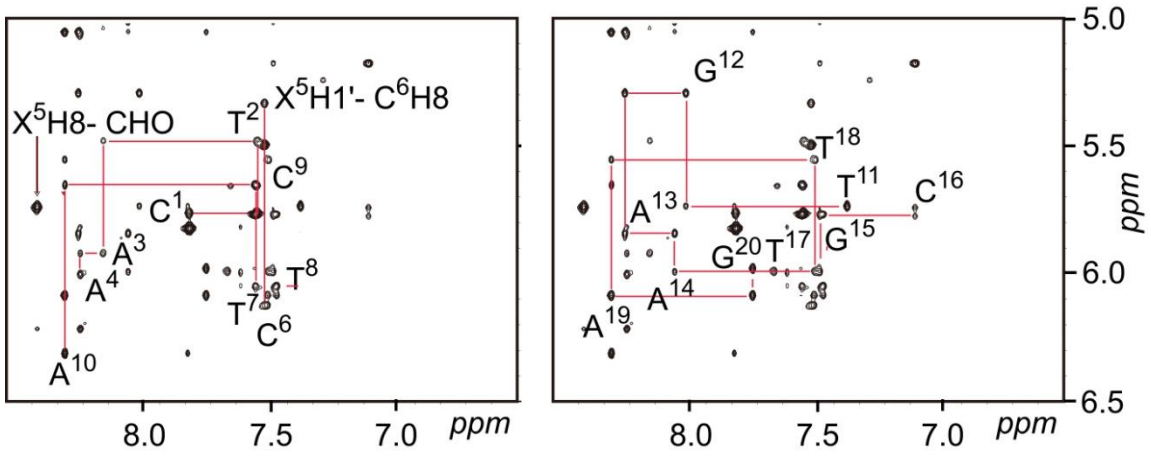


Figure 6-3. NOE connectivity of base H8/H6 protons with deoxyribose H1′ protons of the AFB_1-β-FAPY modified AXC duplex. (A) The modified strand. (B) The complementary strand. X = AFB_1-β-FAPY. The experiment was carried out at 250 ms mixing time and 900 MHz. The temperature was 283 K.

Anomeric Configuration

For both isomers, the β configuration was established by the fact that the intensity of the X^5 H1′ to X^5 H2′ NOEs were less than the X^5 H1′ to X^5 H2″ NOEs. The assignment of the H2′ and H2″ resonances were based on their relative cross peak intensities to H3′ at NOE mixing time of 60 ms. The configuration at C1′ at X5 was determined by unequivocally identifying the H2′ and H2″ to H1′ (Figure 6-4). The intensity of the X^5 H1′ to X^5 H2′ NOE was less than the X^5 H1′ to X^5 H2″ NOE, suggesting the β configuration in both isomers.

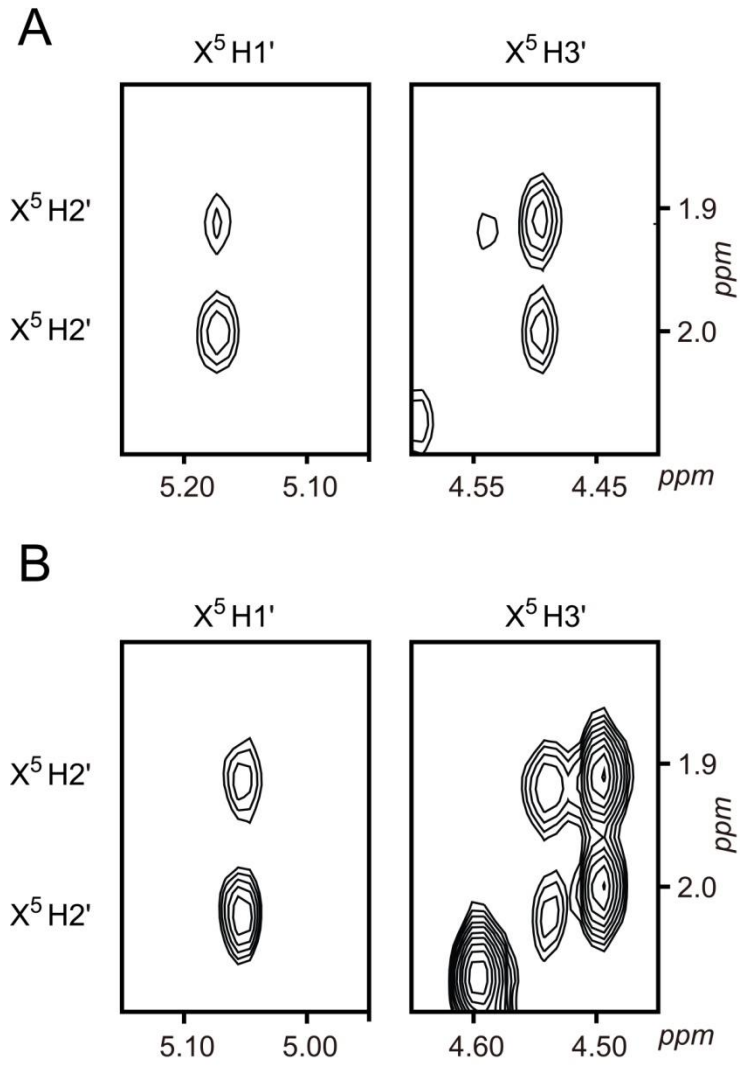


Figure 6-4. Analysis of NOE intensities for the deoxyribose protons of the major and minor isomers of AFB_1-β-FAPY modified AXC duplex. (A) The NOE peaks from H1′ and H3′ to H2′, H2″ of the major isomer. (B) The NOE peaks from H1′ and H3′ to H2′, H2″ of the minor isomer. X = AFB_1-β-FAPY. The experiment was carried out at 250 ms mixing time and 800 MHz. The temperature was 283 K.

Exchangeable DNA protons for the Major Isomer

The resonances of the base imino protons were assigned on the basis of sequential connectivity between adjacent base pairs in NOESY spectra, and the assignments were supported by NOEs to the amino protons of Watson-Crick base pairs.[107] Between X^5 N1H

and T^{17} N3H imino resonances, there is an interruption of the sequential imino-to-imino proton NOEs of adjacent base pairs. The strong cross peaks from X^5 N1H to C^{16} N4H1 and C^{16} N4H2 amino protons indicated that Watson-Crick hydrogen bonding between X^5 and C^{16} was intact. Compared to unmodified duplex, the C^6 H42 non hydrogen bonded exocyclic amine proton shifted downfield 0.21 ppm, significantly higher than 0.72 ppm shift perturbation of the A^6 H62 hydrogen bonded exocyclic amine proton in AXA context, suggesting that the C^6 H42 is involved a weaker hydrogen bond. (Figure 6-5).

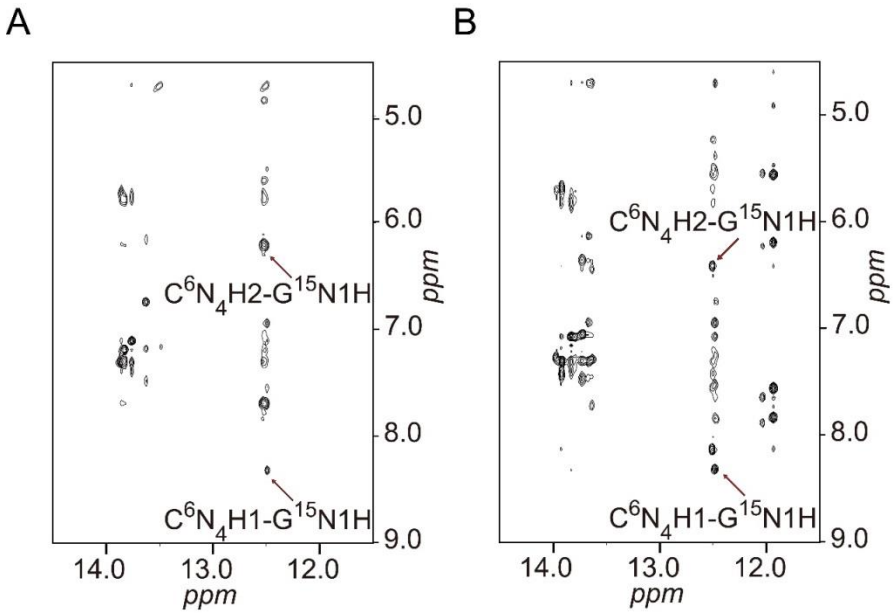


Figure 6-5. Comparison between the C^6 H41 and H42 imino protons. (A) Unmodified duplex. (B) AFB_1-β-FAPY modified AGC duplex. The experiment was carried out at 250 ms mixing time and 800 MHz. The temperature was 283 K.

NMR Spectroscopy of Formyl Proton Resonance (CHO)

Two peaks were observed for the AFB_1-β-FAPY modified AXC duplex in the formyl group region of HMQC experiment acquired at 283 K, indicating the existence of

2 isomers. One peak was coupled between the carbonyl resonance at 167.05 ppm and proton resonance at 8.33 ppm, which is consistent with the *E* geometrical isomer. Another peak had a carbonyl resonance at 168.19 ppm and a proton resonance at 7.47 ppm, indicating the *Z* geometrical isomer (Figure 6-6).

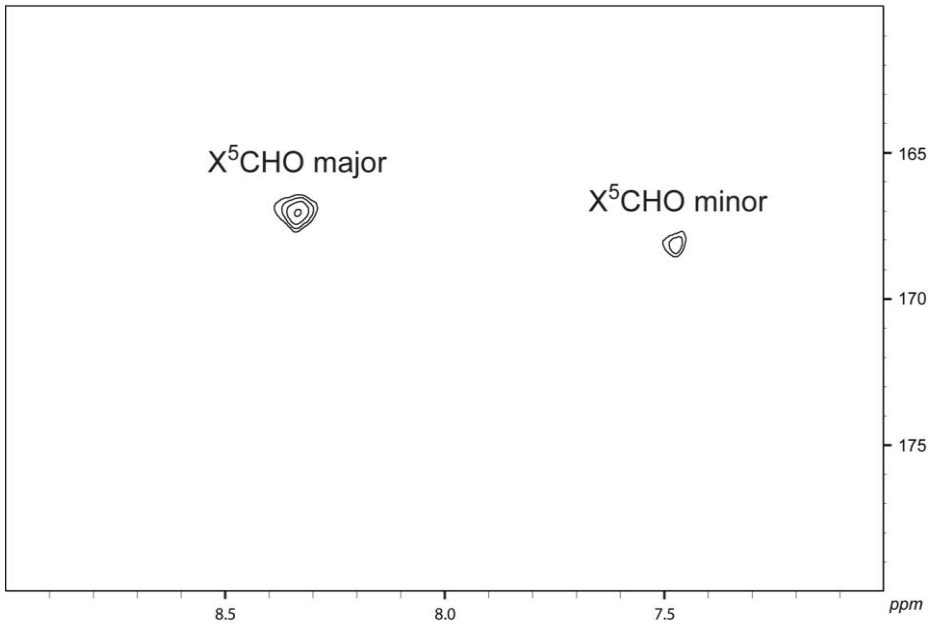


Figure 6-6. NMR analysis of ^{1}H-^{13}C HMQC of AFB_1- β-FAPY modified AXC duplex. The experiment was carried out at 600 MHz and the temperature was 283 K.

Aflatoxin FAPY Protons for the Major Isomer

The AFB_1 H5, H6a, H8, H9, H9a, and $–OCH_3$ resonances were assigned from a combination of NOE connectivities and chemical shift data. AFB_1 H6a and H9a were identified from both COSY and NOESY experiments. AFB_1 H8 and H9 were assigned based on NOEs between H6a and H9a, and between themselves. A strong NOE from AFB_1 H5 to AFB_1 $–OCH_3$ revealed that the latter resonance was at δ 3.52 ppm, while AFB_1 was

at δ 5.74 ppm. Similar to AXA sequence, the observation of a strong NOE peak between X^5 CHO to H8 established the X^5 CHO resonance at δ 8.20 ppm, confirming the assignment of X^5 CHO in the HMQC experiment. The assignment of X^5 CHO resonance was also supported by NOEs to AFB_1 H6a, H9 and H9a protons (Figure 6-7). The cyclopentenone ring protons AFB_1 $H2_\alpha$, $H2_\beta$, $H3_\alpha$, and $H3_\beta$ were identified from a combination of COSY and NOESY experiments.

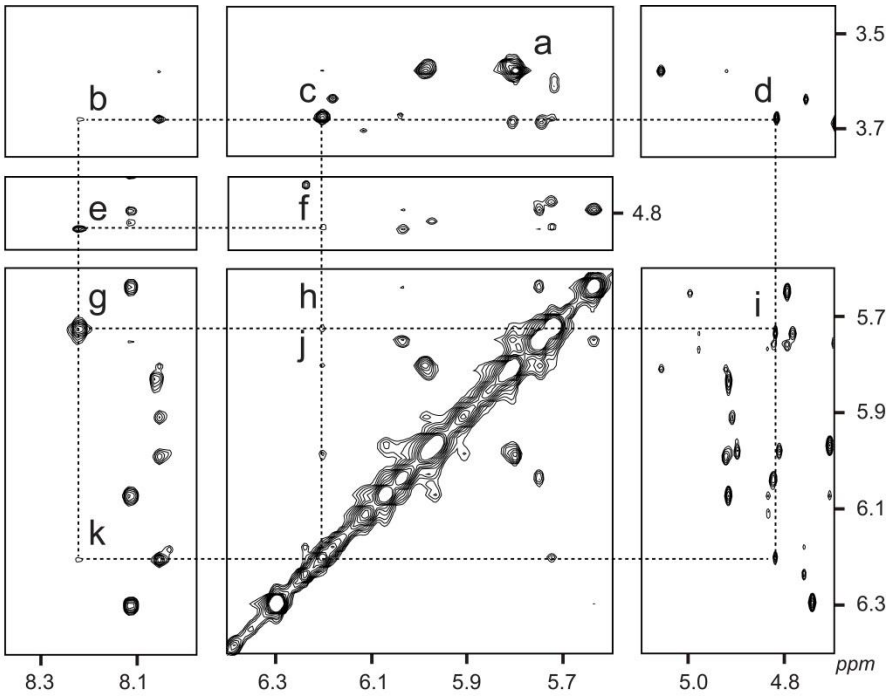


Figure 6-7. NOE assignments of the FAPY protons of the β-AFB_1-FAPY modified AXT duplex. The cross peaks are assigned as: (a) X^5OCH_3 → X^5H5; (b) X^5H9a → X^5CHO; (c) X^5H9a →X^5H6a9; (d) X^5H9a →X^5H9; (e) X^5H9 →X^5CHO; (f) X^5H9 →X^5H6a; (g) X^5H8 →X^5CHO, (h) X^5H8 →X^5H6a, (i) X^5H8 →X^5H9, (j) X^5H5 →X^5H6a, (k) X^5H6a →X^5CHO. The experiment was carried out at 250 ms mixing time and 900 MHz. The temperature was 283 K.

Aflatoxin FAPY to DNA NOEs for the Major Isomer.

A total of 26 NOEs from AFB_1 protons to DNA protons were observed. The protons of the two AFB_1-fused furan rings showed NOEs to major groove and imino protons of the DNA; most of these were to the 5′ neighboring base-pair A^4•T^{17}. Thus, H6a and H9a, which are located on the same face of the AFB_1 moiety, both exhibited NOEs to A^4H8. Weaker NOE was observed for AFB_1 H9. The AFB_1 H5 and $–OCH_3$ protons exhibited NOEs with minor groove and imino DNA protons. These were primarily to base A^4•T^{17}, in the 5′ direction, and to the modified nucleotide X^5 (Figure 6-8). These included NOEs between AFB_1 $–OCH_3$ and A^4 H1′, A^4 H2′, A^4 H2″, A^4 H2, T^{17} N3H, X^5 H1′, and X^5 N1H. The cyclopentenone ring H2α and H2β produced NOEs with H1′, H2′, and H2″ of C^{16}, and H1′, and H3′ of T17, in the complementary strand.

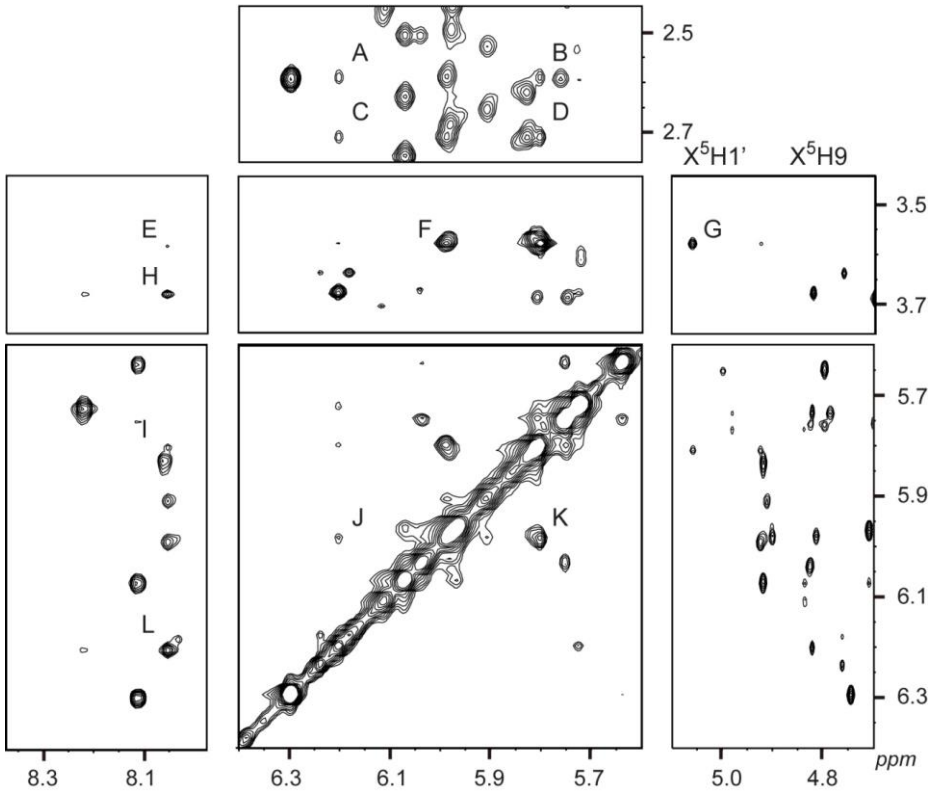


Figure 6-8. NOE assignments of the FAPY to DNA protons of the AFB_1- β-FAPY modified AXT duplex. The cross peaks are assigned as: (A) $X^5H2' \rightarrow X^5H6a$; (B) X^5 $H2' \rightarrow X^5H5$; (C) $X^5H2'' \rightarrow X^5H6a$; (D) X^5 $H2'' \rightarrow X^5H5$; (E) $X^5OCH_3 \rightarrow A^4H8$; (F) $X^5OCH_3 \rightarrow A^4H1'$; (G) $X^5OCH_3 \rightarrow A^4H3'$; (H) $X^5H9a \rightarrow A^4H8$; (I) $X^5H5 \rightarrow A^4H8$; (J) $X^5H5 \rightarrow A^4H1'$; (K) $X^5H5 \rightarrow A^4H3'$; (L) $A^4H1' \rightarrow X^5H6a$; (M) $X^5H6a \rightarrow A^4H8$. The experiment was carried out at 250 ms mixing time and 900 MHz. The temperature was 283 K.

NMR Melting Experiments

The thermal melting of the AFB_1-β-FAPY modified AXC duplex was compared to the corresponding unmodified AGC duplex by monitoring spectra of the imino protons as a function of temperature. For the X^5 N1H imino proton, two sets of resonance were observed at 10 ℃ and the molar ratio between them was 1:2.8. The ratio is consistent with ratio in NOESY and HMQC experiment. The ratio between the two isomers changed to

1:2.2 at 40 ℃ (Figure 6-9), suggesting the ratio was temperature dependent. The additional imino resonances at 40 ℃ were also observed for the G^{15} N1H (Figure 6-9).

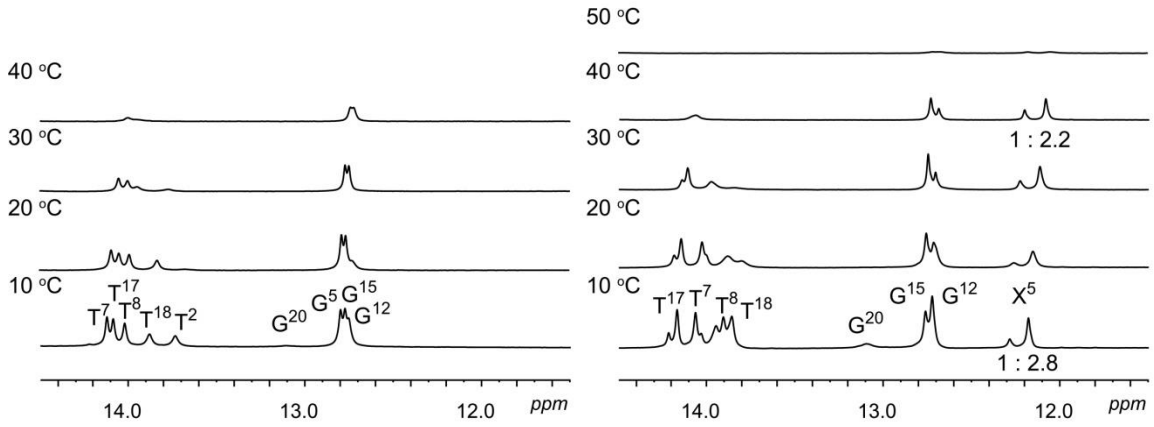
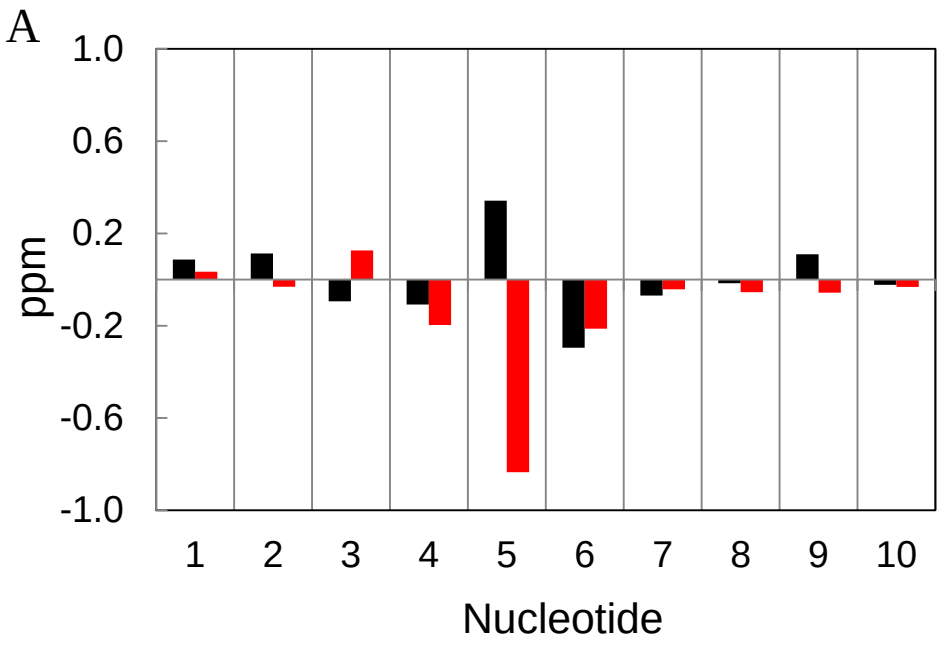


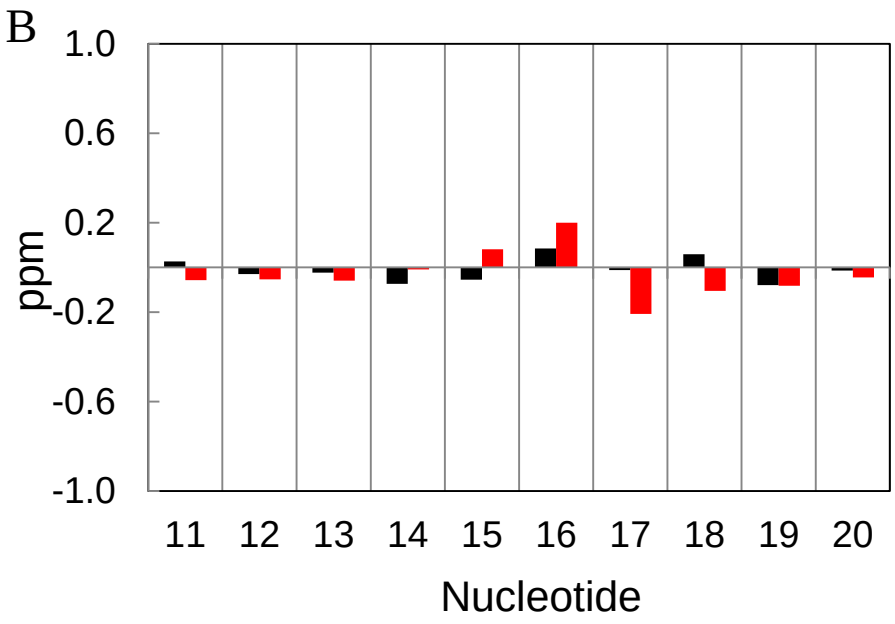
Figure 6-9. Expanded spectra of AFB_1-β-FAPY modified AXC duplex compared with the corresponding unmodified duplex at different temperature. (A) The unmodified duplex. (B) The modified duplex. X = AFB_1-β-FAPY. The experiment was carried out at 800 MHz.

Chemical Shift Effects for the Major Isomer

The ^{1}H spectrum of the AFB_1-β-FAPY modified AXC duplex exhibited significant chemical shift differences around the modified base X^5 compared to that of the unmodified oligodeoxynucleotide (Figure 6-10). In the major groove, at the 3′-side of X^5, a downfield shift of 0.2 ppm was observed for C^6 H6, as well as a downfield shift of 0.20 ppm for A^4 H8 and a downfield shift of 0.21 ppm for T^{17} H6 at the 5′-side of X^5. In the minor groove, an upfield chemical shift of 0.34 ppm was observed for X^5 H1', whereas a downfield shift of 0.30 ppm was observed for c^6 H1' and a downfield shift of 0.11 ppm for A^4 H1'. Examination of the exchangeable protons revealed that T^{17} N1H at the 5′-side of

X^5 shifted 0.13 ppm downfield. The greater shift of 0.59 ppm upfield and 0.04 ppm downfield were observed for X^5 N1H and G^{15} N3H, respectively.





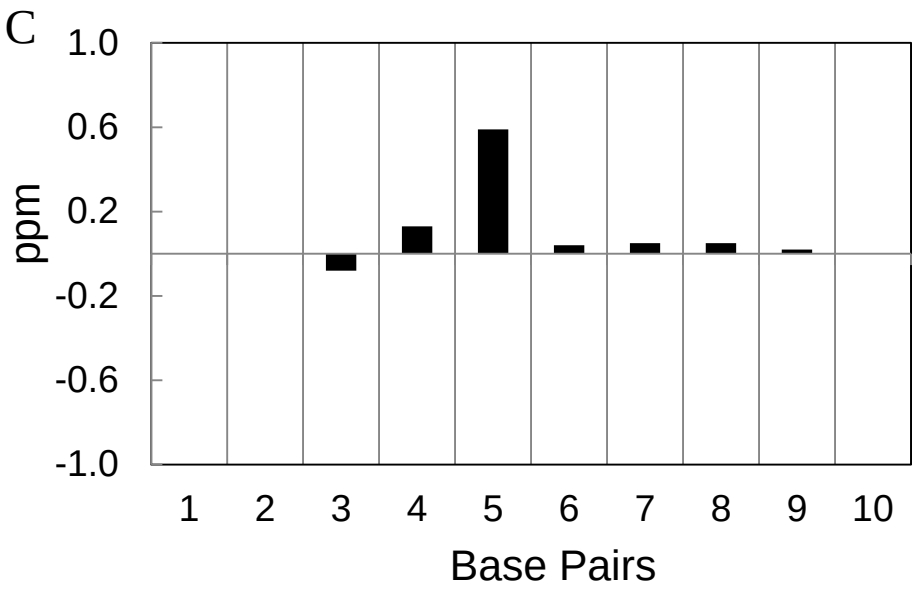


Figure 6-10. Chemical shift differences of protons of the AFB_1-β-FAPY modified AXC duplex, relative to the unmodified onligodeoxynucleotide. **A**. Nucleotides $C^1 \rightarrow A^{10}$ of the AFB_1-β-FAPY Modified AXT duplex. **B**. Nucleotides $T^{11} \rightarrow G^{20}$ of the AFB_1-β-FAPY Modified AXY duplex. **C**. Base pairs 1→10 of AFB_1-β-FAPY Modified AXC duplex. Black bars represents the deoxyribose H1' protons; red bars represent the purine H8 or pyrimidine H6 protons, respectively; grey bars represent the imino guanine N1H or thymine N3H protons. X = AFB_1-β-FAPY.

Structural Refinement

The structure of the major isomer has been refined. A total of 250 distance restraints, including 159 intranucleotide and 91 internucleotide restraints, were calculated from the intensities of NOE cross-peaks using MARDIGRAS[73-76]. A total of 34 restrains were either intranucleotide or internucleotide AFB_1-FAPY to DNA NOEs. In addition to those experimental restraints, a total of 36 empirical distance restraints arising from Watson-Crick base pairing interactions were used, but not at the AFB_1-FAPY adduct. 84

backbone torsion restraints were also applied; however, at the AFB_1-FAPY adduct, the backbone torsion angles were not restrained.

The rMD calculations for the AFB_1-β-FAPY modified AXC duplex were performed from the initial B- form DNA staring structures. The final ten structures with lowest energies were obtained. All structures converged as indicated by pairwise rmsd comparison (Table 6-1). The accuracies of the emergent structures were evaluated by comparison of theoretical NOE intersities calculated by CORMA[77-79] for the refined structure to the experimental NOE intensities to yield sixth root residuals (R_1^x). The R_1^x values for overall residuals, as well as the residuals for intra- or internucleotide NOEs, were consistently less than 0.1 (Figure 6-11), and for each nucleotide were less than 0.15, suggesting that the refined structures were in good agreement with the NOESY data.

Table 6-1. Distribution of restraints applied to structural refinement and statistical analysis for the major isomer of the AFB_1-β-FAPY modified AXC duplex.

	restrains
Experimental NOE Distance Restraints	250
Intra-residue NOE Restraints	159
Inter-residue NOE Restraints	91
NOEs of FAPY	34
Empirical Base Pairing Restraints	36
Empirical Backbone Torsion Restraints	42
Empirical Deoxyribose Torsion Restraints	42
Total Restraints for rMD Caculation	370
Structure Statistics	
NMR R-factor (R^*) ($\times 10^{-2}$)	7.47
Intra-residue NOEs	6.68
Inter-residue NOEs	8.82
rmsd Deviation of Refined Structures	0.503

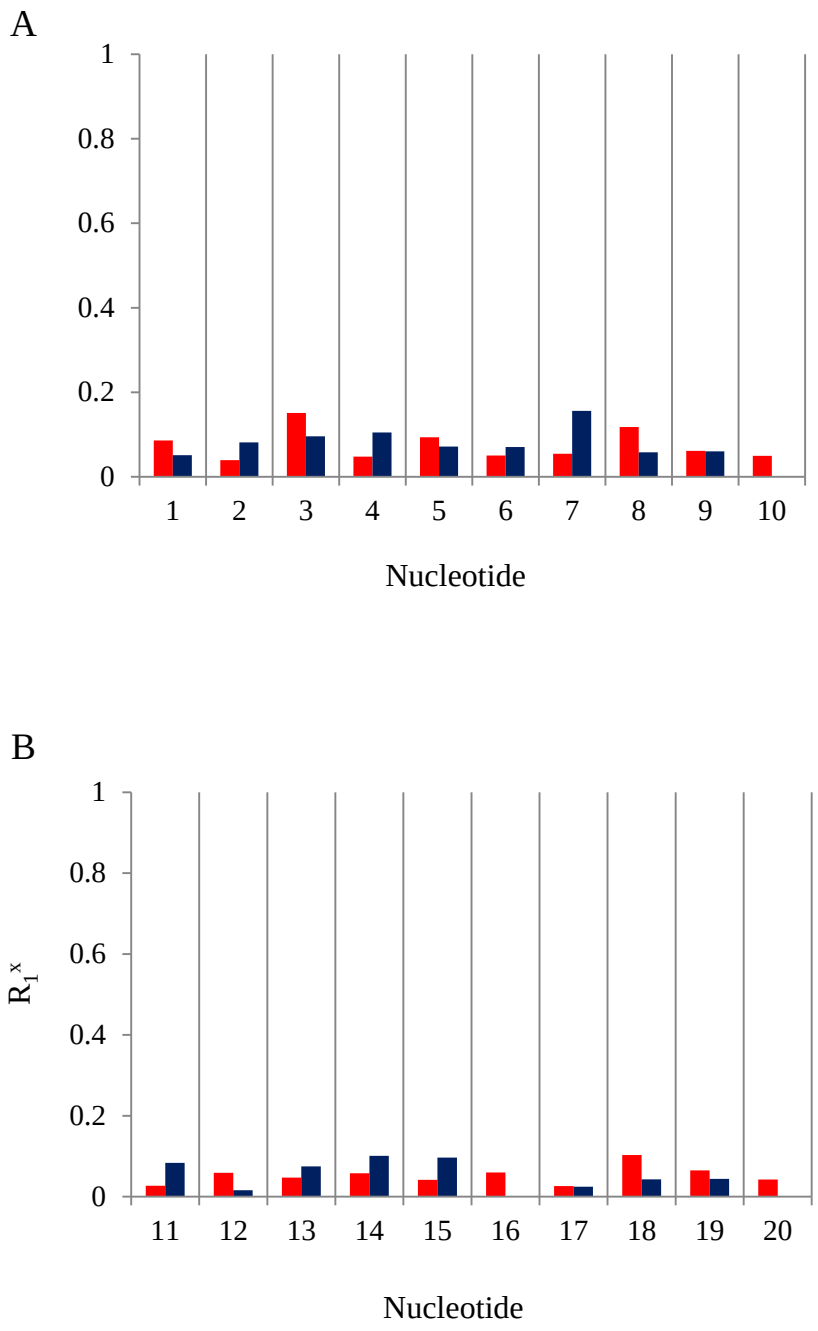


Figure 6-11. Sixth root residuals between calculated NOE intensities and experimental NOE intensities (R_1^x values) as a function of position in the AFB_1-β-FAPY modified AXC duplex. (A) Nucleotides C^1-A^{10} of the modified oligonucleotide containing AFB_1-β-FAPY. (B) Nucleotides T^{11}-G^{20} of the complementary strand. The red bars represent intranuclear sixth root residuals and the black bars represent internuclear sixth root residuals. X = AFB_1-β-FAPY.

Molecular Dynamics Calculations in Explicit Solvent.

The 1 ns of equilibrium rMD calculation was performed in explicit water at constant pressure at 300K to examine the dynamics of the refined structure and to analyze hydrogen bond occupancies involving the formamido group of the FAPY moiety. The 1 ns rMD trajectory was analyzed for occupancies of hydrogen bonding motifs. Hydrogen bond occupancies were calculated using a distance cutoff of 3.5 Å and an angle cutoff of 120 °. On the basis, the C^6 H41 non Watson-Crick hydrogen bonded exocyclic amine proton was within hydrogen bonding distance of the X^5 formyl oxygen; this positioned the formamide in the *E* conformation. This hydrogen bond was satisfied for 93% of the trajectory of 1 ns of equilibrium rMD calculation performed in explicit water.

Structure of the Major Isomer of the AFB$_1$-β-FAPY Modified AXC Duplex.

Stereo views of 10 rMD refined solution structures for the AFB$_1$-β-FAPY modified AXC duplex DNA are depicted in Figure 6-12. The root mean squared deviation (RMSD) between the 10 structures was 0.52 Å. The overall structure maintained Watson-Crick base pairing. The AFB$_1$ adduct is intercalated between A^4●T^{17} and X^5●C^{16}. The formyl group has a *Z* geometrical configuration.

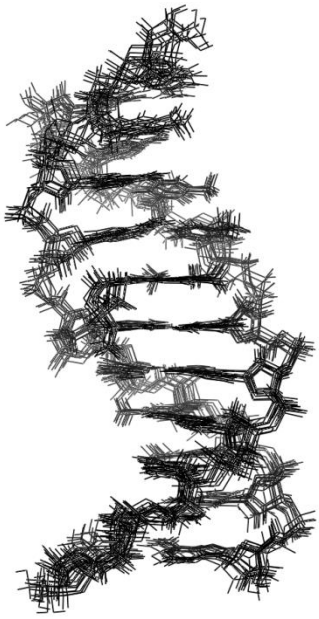


Figure 6-12: Stereo view of 10 superimposed structures of AFB_1-β-FAPY modified AXC duplex resulting from the simulated annealing rMD protocol. X = AFB_1-β-FAPY.

Expanded views of the structure are shown in Figure 6-13. The AFB_1 moiety is intercalated above the 5′- face of the modified nucleotide X^5 and between base pairs A^4•T^{17} and X^5•C^{16}, causing the rise between these base pairs to increase to 5 Å. The adduct-induced unwinding is localized to the adducted base pair X^5•C^{16}, and its 5′- and 3′- neighbor base pairs A^4•T^{17} and C^6•G^{15}. The modified duplex is unwound approximately 15 ° at the adducted site. The X^5 N9H exocyclic amine proton is within hydrogen bonding distance of the X^5 formyl oxygen and positioned the formamide in the *E* conformation. Figure 6-14 shows the damaged site from 3′ - neighbor base, confirming the *E* conformation.

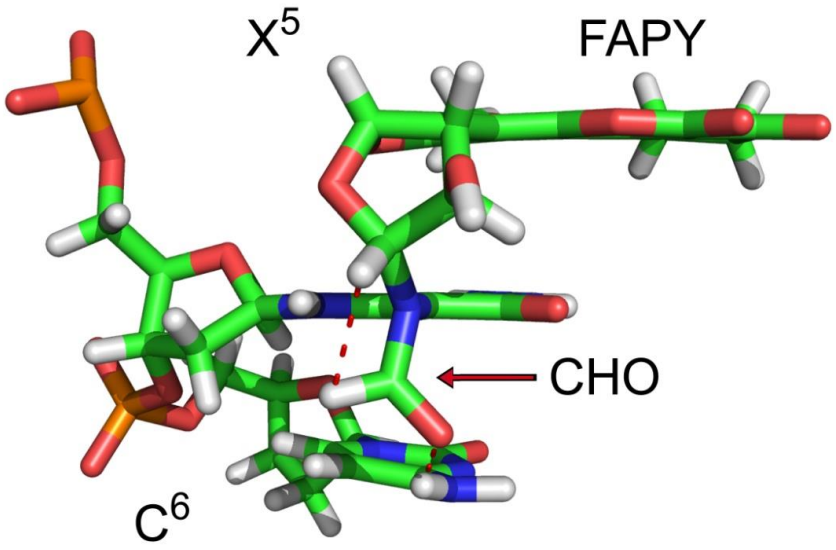


Figure 6-13. Expanded view of the refined structure of the major isomer of the AFB_1-β-FAPY modified AXC duplex at the lesion site. X = AFB_1-β-FAPY.

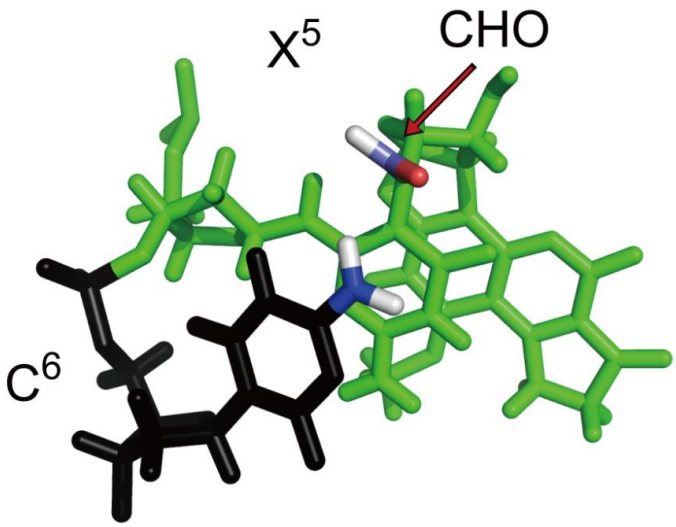


Figure 6-14. Expanded view of the refined structure of the major isomer of the AFB_1-β-FAPY modified AXC duplex at the lesion site from the 3′ - neighbor base. X = AFB_1-β-FAPY.

Helicoidal Analysis for the Major Isomer

A helicoidal analysis of the average solution structure was performed using CURVES*, following rMD calculations. As a result of the modification at X^5, a bend was

present in the structure. The base pair parameters were normal for both the X- axis and Y-axis at the lesion site (Figure 6-15). The parameters for base-base interactions showed that at the lesion site, the modification causes more than a 10 ° opening. Disruptions also occurred in the shear, the stretch, and the stagger, primarily at the lesion site (Figure 6-16). As was predicted by NOESY data, a 5 Å increase in rise was observed between X^5 and C^6 (Figure 6-17).

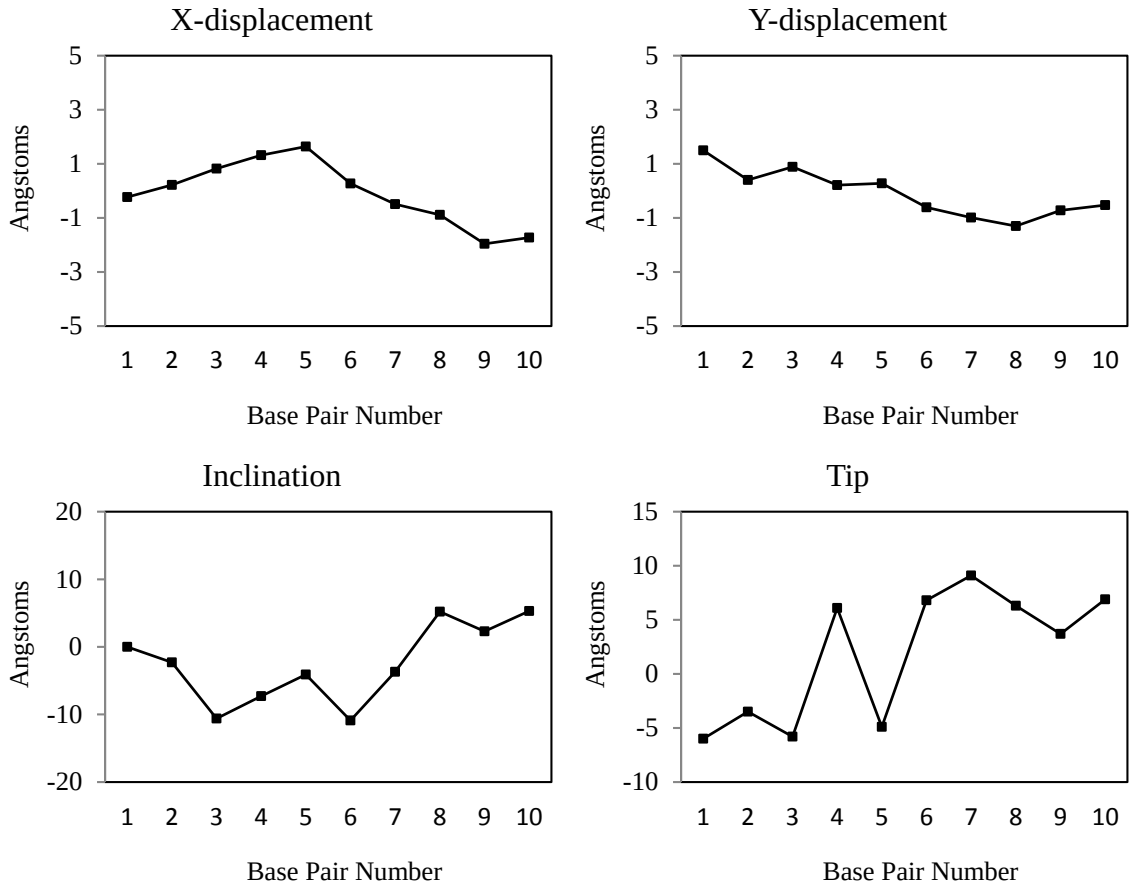


Figure 6-15: Global base pair helicoidal parameters. Helicoidal parameters for the AFB_1-FAPY modified AXC oligonucleotide 5′-$C^1T^2A^3A^4X^5C^6T^7T^8C^9A^{10}$-3′·5′-$T^{11}G^{12}A^{13}A^{14}G^{15}C^{16}T^{17}T^{18}$ A^{19} G^{20}-3′.

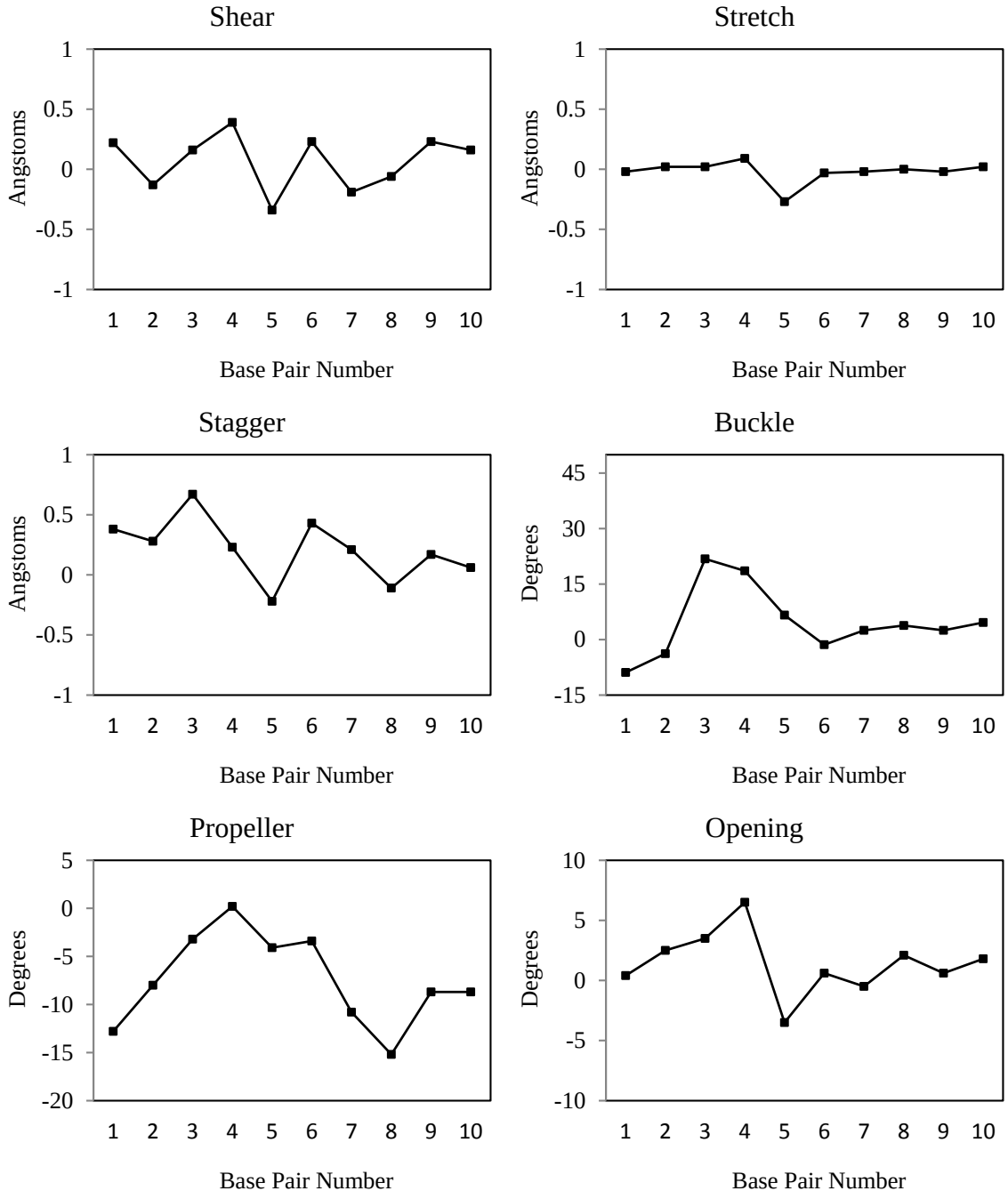


Figure 6-16: Global Intra-base pair helicoidal parameters. Helicoidal parameters for the AFB_1-FAPY modified AXC oligonucleotide 5′-$C^1T^2A^3A^4X^5C^6T^7T^8C^9A^{10}$-3′·5′-$T^{11}G^{12}A^{13}A^{14}G^{15}C^{16}T^{17}T^{18}$ A^{19} G^{20}-3′.

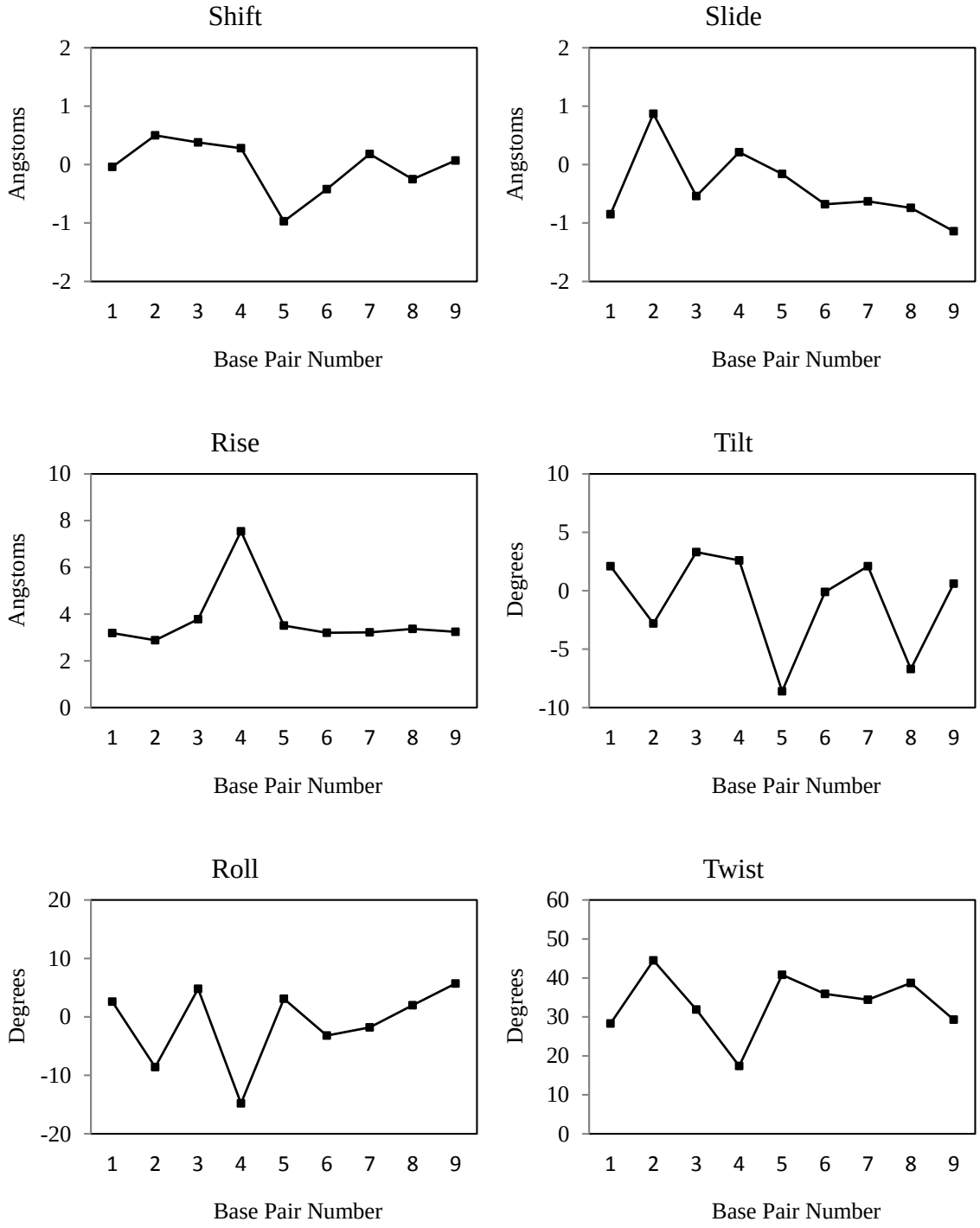


Figure 6-17: Global Inter-base pair helicoidal parameters. Helicoidal parameters for the AFB_1-FAPY modified AXC oligonucleotide 5′-$C^1T^2A^3A^4X^5C^6T^7T^8C^9A^{10}$-3′·5′-$T^{11}G^{12}A^{13}A^{14}G^{15}C^{16}T^{17}T^{18}$ A^{19} G^{20}-3′.

Discussion

When a cytosine is the 3′- neighboring base, two isomers are observed. In both COSY and NOESY spectra, two cross peaks of H5 and H6 on C^{16}, the opposite base of damaged X^5, are observed and the ratio between them is determined by the comparison of the intensities of both cross peaks, as 2.8 to 1 at 283 K. In the 1D experiment, two sets of resonance are also observed for the imino protons of X^5 and the ratio between them is consistent with the ratio of cross peaks of H5 and H6 on C^{16}. The ratio appears to be temperature dependent, changing from 1:2.8 at 10 ℃, to 1:2.2 at 40 ℃. In the NOESY spectrum, the major difference between the 2 isomers focuses on the base pairs X^5•C^{16}, C^6•G^{15}, and T^7•A^{14}, and two set of resonance are observed for those bases. The difference becomes smaller when the base pair goes further from the modified base. The possibility of co-existence of α and β anomers is ruled out by comparison of the NOEs intensities between the X^5 H1′ to H2′ and H2″ in both isomers. A strong NOE cross peak between the formamide proton and H8 proton establishes the major isomer as *E* geometrical isomer. Less deshielding of C^6H41 exocyclic non-Watson-Crick amino proton (0.2 ppm upfield) in NMR data might indicate a weaker hydrogen bond between this proton and the formyl oxygen. In the refined structure, the distance between the formyl oxygen and C^6 H41 is 2.7 Å, and the calculated angle O···H—N is 110°. Analysis of rMD trajectories indicates 92% occupancy for this hydrogen bond. For the minor isomer, the HMQC experiment shows a second resonance of the aldehyde proton at 7.5 ppm, which is consistent with the chemical shift of formyl proton of *Z* geographic isomer in AXT and AXY context. In addition to the formyl proton, there is no observation for the second set of resonance of AFB_1-FAPY

protons, suggesting that the rotation of formyl group has very little effect on the AFB_1-FAPY structure.

CHAPTER VII

Summary and future directions

SUMMARY

Structures and Role of Hydrogen Bond

Solution structures of the aflatoxin formamidopyrimidine adduct site-specifically incorporated into decamer oligonucleotides with dA, dT, 7-deazadG, and dC as the 3′-neighbouring bases have been elucidated using NMR spectroscopy and rMD calculations. NMR data reveals that, when adenine is the ′-neighboring base to the damaged guanine, *E* configuration of the formmamido is held by the hydrogen bond between formyl oxygen and the exocyclic amino proton of 3′-neighboring adenine. Such a hydrogen bond does not exist, when thymine or 7-deaza guanine is the 3′ neighboring base to the damaged guanine. Therefore, the formyl group adopts *Z* conformation predominantly in these sequences. Two isomers co-exist when the cytosine is placed in the 3′-neighbor position. The ratio between the two isomers is ~3: 1 at 10 ℃ and the ratio is temperature dependent. The major isomer has been identified as *E* geometric isomer. The chemical shift of the formyl proton of the minor isomer is found at 7.5 ppm in the HMQC experiment, suggesting the *Z* configuration.

Thermodynamic Considerations

A previous report suggested that the hydrogen bond between the formyl group of the AFB_1 moiety and the N^6 non Watson-Crick hydrogen bonded exocyclic amino proton

of the 3′- neighboring A^6 might provide an additional potential source of thermal stability.[57] However, the thermal analysis revealed a different result. Although in the AFB_1-β-FAPY modified AXA and AXT duplex, the formamide moiety of the AFB_1-β-FAPY adduct is held in the *E* and *Z* configurations, respectively, and the intercalation of AFB_1 moiety stabilizes both modified AXA and AXT duplexes by a similar 10 ℃ increase in melting temperature relative to the unadducted AGA and AGT duplexes. The same T_m 10 ℃ increasing is also observed in the AFB_1-β-FAPY modified AX(7-deaza)G and AXC duplexes relative to the undamaged AG(7-deaza)G and AGC duplexes (Figure 7-1). Those results indicate that the role of the hydrogen bond between the formyl group of the AFB_1 moiety and 3′-neighbor base is not related to the increased stability of the AFB_1-β-FAPY modified oligonucleotide. One possible reason might be that such a hydrogen bond is only an intrastrand hydrogen bond between the modified base and 3′- neighbor, thus having little effect on improving duplex stability.

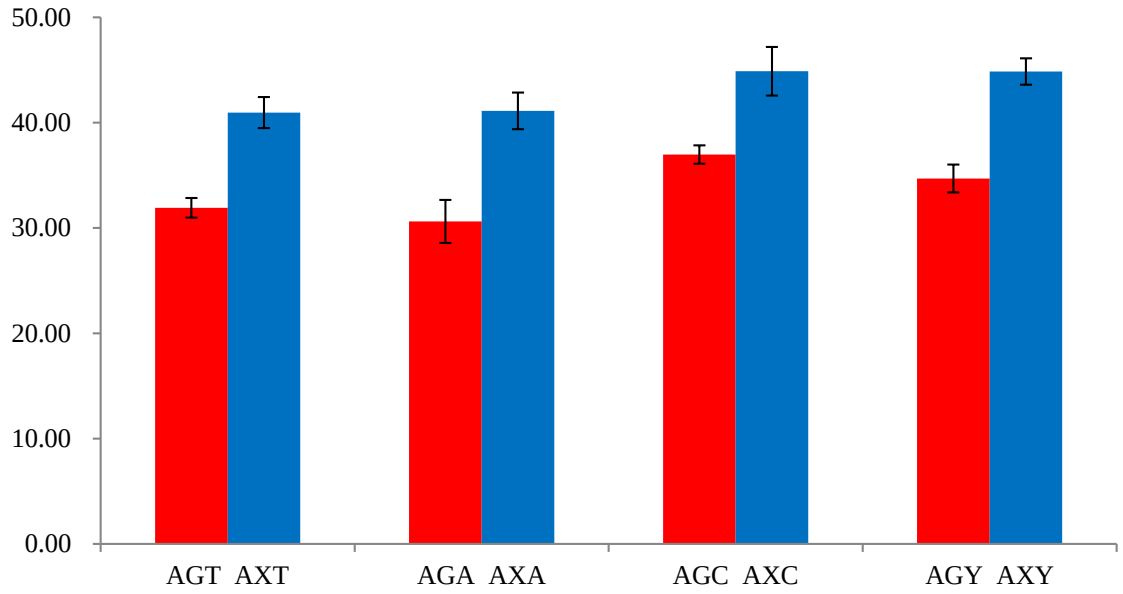


Figure 7-1. Comparison of the *T*m between 4 unmodified duplexes and AFB_1-β-FAPY Modified Duplexes. X = AFB_1-β-FAPY, Y = (7-deaza)G. The concentration of oligonucleotides is 1.6 μM. The salt concentration is 100 mM.

FUTURE DIRECTIONS

Extension of primer in Dpo4-DNA complex and pol ζ-DNA complex

The *Sulfolobus solfataricus* P2 DNA polymerase IV (Dpo4)[108] and translesion synthesis polymerase zeta (pol ζ)[109,110] have been shown to be able to bypass AFB_1–FAPY adduct in an error-prone manner, including misinsertion of dATP, consistent with the G→T mutations observed in *E. coli*. In both studies, the XA sequence context was used in the AFB_1-FAPY modified template. Thus, the extension study on other sequence context, such as XC, XG and XT, will be of interest. The result might be useful to answer the question why the third base of codon 249 in p53 has the highest G to T mutation frequency.

APPENDIX A

MOLECULAR DYNAMICS TOPOLOGY OF NON-STANDARD BASES

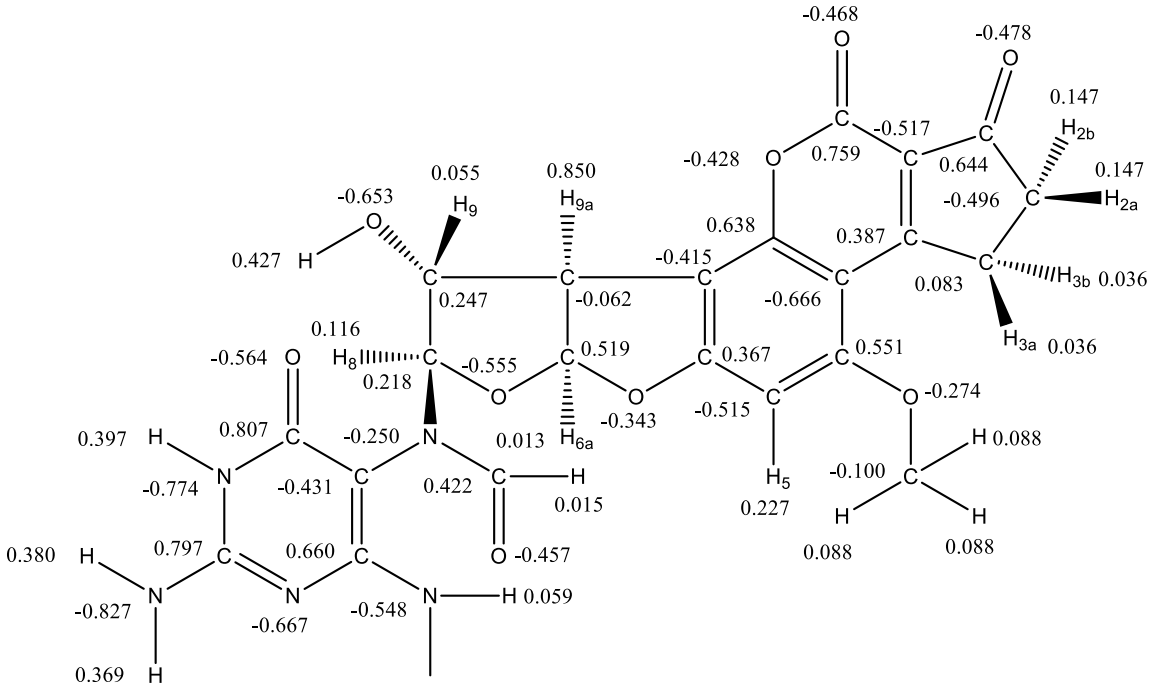


Figure A-1: Atomic charges for the aflatoxin B_1 adduct calculated by Gaussian 03 and used in rMD simulations.

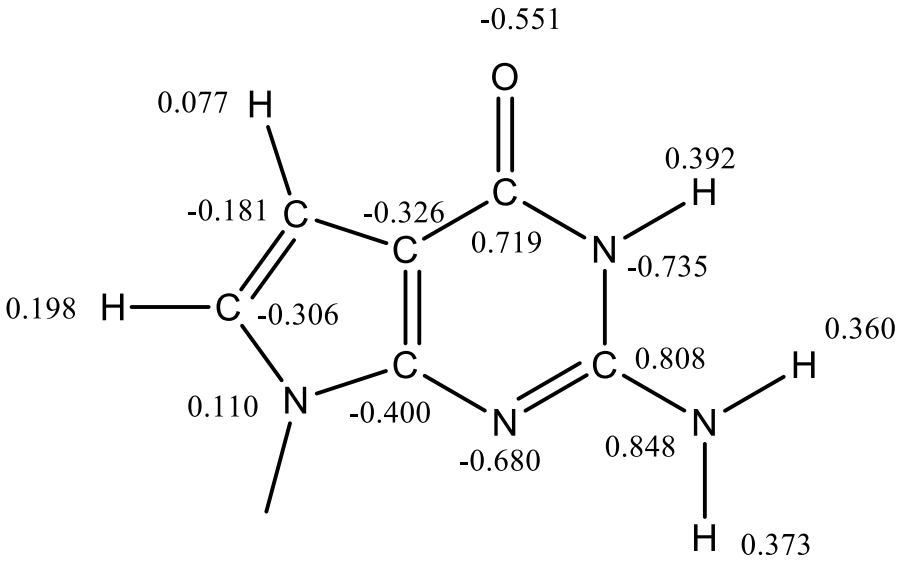


Figure A-2: Atomic charges for the 7-deaza guanine adduct calculated by Gaussian 03 and used in rMD simulations.

APPENDIX B

CHEMICAL SHIFT ASSIGNMENTS

Table B-1: Chemical shift assignments of the AFB_1-β-FAPY modified AXA duplex.

Group	Atom	Nuc	Shift	Group	Atom	Nuc	Shift
C1	H1'	1H	5.746	T11	CH3	1H	1.556
C1	H2'	1H	2.061	T11	H1'	1H	5.694
C1	H2''	1H	2.448	T11	H2'	1H	1.697
C1	H3'	1H	4.574	T11	H2'	1H	2.137
C1	H4'	1H	3.995	T11	H3'	1H	4.560
C1	H5	1H	5.814	T11	H4'	1H	3.961
C1	H5'	1H	3.697	T11	H5'	1H	3.574
C1	H5''	1H	3.697	T11	H5'	1H	3.587
C1	H6	1H	7.753	T11	H6	1H	7.303
T2	CH3	1H	1.622	G12	H1'	1H	5.323
T2	H1'	1H	5.430	G12	H2'	1H	2.678
T2	H2'	1H	2.021	G12	H2'	1H	2.733
T2	H2''	1H	2.254	G12	H3'	1H	4.931
T2	H3'	1H	4.780	G12	H4'	1H	4.249
T2	H6	1H	7.470	G12	H5'	1H	3.972
A3	H1'	1H	5.875	G12	H5'	1H	3.884
A3	H2'	1H	2.569	G12	H8	1H	7.925
A3	H2''	1H	2.725	A13	H1'	1H	5.951
A3	H3'	1H	5.000	A13	H2'	1H	2.733
A3	H4'	1H	4.326	A13	H2'	1H	2.851
A3	H8	1H	8.066	A13	H4'	1H	4.415
A4	H1'	1H	5.914	A13	H8	1H	8.168
A4	H2'	1H	2.634	A14	H1'	1H	6.135
A4	H2''	1H	2.784	A14	H2'	1H	2.474
A4	H3'	1H	5.022	A14	H2'	1H	2.822
A4	H4'	1H	4.351	A14	H4'	1H	4.407
A4	H8	1H	8.133	A14	H5'	1H	4.219
G5	H1'	1H	5.045	A14	H5'	1H	4.081
G5	H2'	1H	1.900	A14	H8	1H	8.065
G5	H2''	1H	2.143	T15	CH3	1H	1.137
G5	H2A	1H	1.673	T15	H1'	1H	5.833
G5	H2B	1H	1.790	T15	H2'	1H	1.889
G5	H3'	1H	4.516	T15	H2'	1H	2.472
G5	H3A	1H	2.520	T15	H3'	1H	4.756
G5	H3B	1H	2.766	T15	H6	1H	6.979
G5	H4'	1H	4.018	C16	H1'	1H	5.895
G5	H5	1H	5.726	C16	H2'	1H	2.239
G5	H5'	1H	3.974	C16	H2'	1H	2.245
G5	H5''	1H	3.822	C16	H3'	1H	4.838
G5	H6a	1H	6.197	C16	H5	1H	5.471
G5	H8	1H	8.321	C16	H6	1H	7.384
G5	H8a	1H	5.703	T17	CH3	1H	1.782

G5	H9	1H	4.801	T17	H1'	1H	5.950
G5	H9a	1H	3.643	T17	H2'	1H	2.370
G5	OCH3	1H	3.471	T17	H2'	1H	2.478
A6	H1'	1H	6.221	T17	H3'	1H	4.798
A6	H2'	1H	2.622	T17	H6	1H	7.589
A6	H2''	1H	2.872	T18	CH3	1H	1.665
A6	H3'	1H	5.025	T18	H1'	1H	5.501
A6	H4'	1H	4.417	T18	H2'	1H	2.045
A6	H5'	1H	4.233	T18	H2'	1H	2.317
A6	H5''	1H	4.122	T18	H3'	1H	4.809
A6	H8	1H	8.163	T18	H6	1H	7.427
T7	CH3	1H	1.263	A19	H1'	1H	6.045
T7	H1'	1H	5.972	A19	H2'	1H	2.707
T7	H2'	1H	2.010	A19	H2'	1H	2.861
T7	H2''	1H	2.519	A19	H3'	1H	5.011
T7	H3'	1H	4.827	A19	H4'	1H	4.386
T7	H6	1H	7.217	A19	H5'	1H	4.214
T8	CH3	1H	1.557	A19	H8	1H	8.225
T8	H1'	1H	6.032	G20	H1'	1H	5.949
T8	H2'	1H	1.994	G20	H2'	1H	2.355
T8	H2''	1H	2.384	G20	H2'	1H	2.213
T8	H3'	1H	4.825	G20	H3'	1H	4.590
T8	H6	1H	7.358	G20	H4'	1H	4.220
C9	H1'	1H	5.630	G20	H5'	1H	4.127
C9	H2'	1H	1.978	G20	H5'	1H	4.084
C9	H2''	1H	2.243	G20	H8	1H	7.675
C9	H3'	1H	4.779				
C9	H5	1H	5.693				
C9	H6	1H	7.466				
A10	H1'	1H	6.281				
A10	H2'	1H	2.666				
A10	H2''	1H	2.412				
A10	H3'	1H	4.669				
A10	H4'	1H	4.152				
A10	H5'	1H	4.039				
A10	H8	1H	8.224				

Table B-2: Chemical shift assignments of the AFB_1-β-FAPY modified AXT duplex.

Group	Atom	Nuc	Shift	Group	Atom	Nuc	Shift
C1	H1'	1H	5.746	T11	CH3	1H	1.592
C1	H2'	1H	2.457	T11	H1'	1H	5.686
C1	H2''	1H	2.071	T11	H2'	1H	1.670
C1	H3'	1H	4.583	T11	H2''	1H	2.133
C1	H5	1H	5.808	T11	H3'	1H	4.567
C1	H6	1H	7.754	T11	H6	1H	7.313
T2	CH3	1H	1.632	G12	H1'	1H	5.210
T2	H1'	1H	5.454	G12	H2'	1H	2.687
T2	H2'	1H	2.024	G12	H2''	1H	2.735
T2	H2''	1H	2.256	G12	H3'	1H	4.927
T2	H3'	1H	4.798	G12	H8	1H	7.929
T2	H6	1H	7.476	A13	H1'	1H	5.817
A3	H1'	1H	5.871	A13	H2	1H	7.248
A3	H2	1H	7.276	A13	H2'	1H	2.696
A3	H2'	1H	2.589	A13	H2''	1H	2.830
A3	H2''	1H	2.722	A13	H3'	1H	5.027
A3	H3'	1H	5.008	A13	H8	1H	8.174
A3	H8	1H	8.084	A14	H1'	1H	5.898
A4	H1'	1H	5.993	A14	H2	1H	7.150
A4	H2	1H	7.551	A14	H2'	1H	2.586
A4	H2'	1H	2.670	A14	H2''	1H	2.830
A4	H2''	1H	2.793	A14	H3'	1H	5.015
A4	H3'	1H	5.028	A14	H8	1H	8.064
A4	H8	1H	8.158	A15	H1'	1H	6.035
G5	H1'	1H	5.205	A15	H2	1H	7.647
G5	H2'	1H	1.946	A15	H2'	1H	2.417
G5	H2''	1H	2.184	A15	H2''	1H	2.800
G5	H2A	1H	1.684	A15	H3'	1H	4.936
G5	H2B	1H	1.764	A15	H8	1H	7.916
G5	H3'	1H	4.571	C16	H1'	1H	5.748
G5	H3A	1H	2.561	C16	H2'	1H	2.097
G5	H3B	1H	2.974	C16	H2''	1H	2.154
G5	H5	1H	5.740	C16	H3'	1H	4.813
G5	H6a	1H	6.229	C16	H5	1H	5.095
G5	H8	1H	7.703	C16	H6	1H	7.147
G5	H8a	1H	6.239	T17	CH3	1H	1.766
G5	H9	1H	4.705	T17	H1'	1H	5.987
G5	H9a	1H	3.660	T17	H2'	1H	2.384
G5	OCH3	1H	3.525	T17	H2''	1H	2.507
T6	CH3	1H	1.615	T17	H3'	1H	4.820
T6	H1'	1H	6.153	T17	H6	1H	7.607
T6	H2'	1H	2.303	T18	CH3	1H	1.679
T6	H2''	1H	2.568	T18	H1'	1H	5.528
T6	H6	1H	7.435	T18	H2'	1H	2.073
T7	CH3	1H	1.622	T18	H2''	1H	2.340
T7	H1'	1H	6.140	T18	H3'	1H	4.827
T7	H2'	1H	2.185	T18	H6	1H	7.444
T7	H2''	1H	2.613	A19	H1'	1H	6.067
T7	H3'	1H	4.878	A19	H2	1H	7.512
T7	H6	1H	7.503	A19	H2'	1H	2.731
T8	CH3	1H	1.665	A19	H2''	1H	2.883
T8	H1'	1H	6.058	A19	H3'	1H	5.036

T8	H2'	1H	2.041	A19	H8	1H	8.244
T8	H2''	1H	2.435	G20	H1'	1H	5.962
T8	H3'	1H	4.866	G20	H2'	1H	2.415
T8	H6	1H	7.413	G20	H2''	1H	2.239
C9	H1'	1H	5.631	G20	H3'	1H	4.611
C9	H2'	1H	1.983	G20	H8	1H	7.688
C9	H2''	1H	2.253				
C9	H3'	1H	4.797				
C9	H5	1H	5.727				
C9	H6	1H	7.481				
A10	H1'	1H	6.297				
A10	H2	1H	7.801				
A10	H2'	1H	2.700				
A10	H2''	1H	2.434				
A10	H3'	1H	4.692				
A10	H8	1H	8.251				

Table B-3: Chemical shift assignments of the AFB_1-β-FAPY modified AXY duplex.

Group	Atom	Nuc	Shift	Group	Atom	Nuc	Shift
C1	H1'	1H	5.749	T11	CH3	1H	1.550
C1	H2'	1H	2.039	T11	H1'	1H	5.677
C1	H2''	1H	2.427	T11	H2'	1H	1.642
C1	H3'	1H	4.562	T11	H2''	1H	2.094
C1	H5	1H	5.819	T11	H3'	1H	4.527
C1	H6	1H	7.751	T11	H6	1H	7.286
T2	CH3	1H	1.605	G12	H1'	1H	5.202
T2	H1'	1H	5.406	G12	H2'	1H	2.646
T2	H2'	1H	2.000	G12	H2''	1H	2.659
T2	H2''	1H	2.220	G12	H8	1H	7.900
T2	H3'	1H	4.762	A13	H1'	1H	5.847
T2	H6	1H	7.449	A13	H2'	1H	2.676
A3	H1'	1H	5.850	A13	H2''	1H	2.798
A3	H2'	1H	2.549	A13	H3'	1H	4.997
A3	H2''	1H	2.683	A13	H8	1H	8.154
A3	H3'	1H	4.978	A14	H1'	1H	6.086
A3	H8	1H	8.047	A14	H2'	1H	2.529
A4	H1'	1H	5.908	A14	H2''	1H	2.762
A4	H2'	1H	2.610	A14	H3'	1H	4.917
A4	H2''	1H	2.746	A14	H8	1H	8.051
A4	H3'	1H	4.976	C15	H1'	1H	5.652
A4	H8	1H	8.111	C15	H2'	1H	1.821
G5	H1'	1H	5.844	C15	H2''	1H	2.347
G5	H2'	1H	1.847	C15	H3'	1H	4.619
G5	H2''	1H	2.093	C15	H5	1H	4.923
G5	H3'	1H	4.488	C15	H6	1H	7.000
G5	H5	1H	5.732	C16	H1'	1H	5.853
G5	H6a	1H	6.183	C16	H2'	1H	2.193
G5	H8	1H	7.714	C16	H2''	1H	2.260
G5	H8a	1H	6.181	C16	H3'	1H	4.794
G5	H9	1H	4.630	C16	H5	1H	5.407
G5	H9a	1H	3.609	C16	H6	1H	7.372
G5	OCH3	1H	3.486	T17	CH3	1H	1.748
G6	H1'	1H	6.072	T17	H1'	1H	5.935
G6	H2'	1H	2.463	T17	H2'	1H	2.346
G6	H2''	1H	2.547	T17	H2''	1H	2.444
G6	H8	1H	6.802	T17	H3'	1H	4.774
G6	H9	1H	4.910	T17	H6	1H	7.571
T7	CH3	1H	1.182	T18	CH3	1H	1.641
T7	H1'	1H	6.071	T18	H1'	1H	5.465
T7	H2'	1H	2.120	T18	H2'	1H	2.021
T7	H2''	1H	2.508	T18	H2''	1H	2.278
T7	H3'	1H	4.829	T18	H3'	1H	4.776
T7	H6	1H	7.210	T18	H6	1H	7.409
T8	CH3	1H	1.556	A19	H1'	1H	6.020
T8	H1'	1H	6.023	A19	H2'	1H	2.683
T8	H2'	1H	1.988	A19	H2''	1H	2.830
T8	H2''	1H	2.381	A19	H3'	1H	4.988
T8	H3'	1H	4.805	A19	H8	1H	8.204
T8	H6	1H	7.343	G20	H1'	1H	5.932

C9	H1'	1H	5.607	G20	H2'	1H	2.367
C9	H2'	1H	1.950	G20	H2''	1H	2.189
C9	H2''	1H	2.212	G20	H3'	1H	4.566
C9	H3'	1H	4.749	G20	H8	1H	7.662
C9	H5	1H	5.691				
C9	H6	1H	7.451				
A10	H1'	1H	6.272				
A10	H2'	1H	2.651				
A10	H2''	1H	2.388				
A10	H3'	1H	4.648				
A10	H8	1H	8.218				

Table B-4: Chemical shift assignments of the major isomer of AFB_1-β-FAPY modified AXC duplex.

Group	Atom	Nuc	Shift	Group	Atom	Nuc	Shift
C1	H1'	1H	5.747	T11	CH3	1H	1.572
C1	H2'	1H	2.080	T11	H1'	1H	5.719
C1	H2''	1H	2.463	T11	H2'	1H	1.708
C1	H3'	1H	4.586	T11	H2''	1H	2.148
C1	H5	1H	5.808	T11	H3'	1H	4.575
C1	H6	1H	7.754	T11	H6	1H	7.318
T2	CH3	1H	1.638	G12	H1'	1H	5.276
T2	H1'	1H	5.465	G12	H2'	1H	2.696
T2	H2'	1H	2.043	G12	H2''	1H	2.732
T2	H2''	1H	2.282	G12	H8	1H	7.949
T2	H3'	1H	4.805	A13	H1'	1H	5.827
T2	H6	1H	7.486	A13	H2	1H	7.320
A3	H1'	1H	5.906	A13	H2'	1H	2.721
A3	H2	1H	7.275	A13	H2''	1H	2.838
A3	H2'	1H	2.602	A13	H3'	1H	5.037
A3	H2''	1H	2.765	A13	H8	1H	8.189
A3	H8	1H	8.092	A14	H1'	1H	5.976
A4	H1'	1H	5.986	A14	H2	1H	7.553
A4	H2	1H	7.554	A14	H2'	1H	2.559
A4	H2'	1H	2.681	A14	H2''	1H	2.801
A4	H2''	1H	2.837	A14	H3'	1H	5.001
A4	H3'	1H	5.042	A14	H8	1H	7.993
A4	H8	1H	8.181	G15	H1'	1H	5.759
G5	H1'	1H	5.318	G15	H2'	1H	2.323
G5	H2'	1H	1.916	G15	H2''	1H	2.688
G5	H2''	1H	2.009	G15	H8	1H	7.425
G5	H2A	1H	1.771	C16	H1'	1H	5.726
G5	H2B	1H	1.880	C16	H2'	1H	2.118
G5	H3'	1H	4.488	C16	H2''	1H	2.202
G5	H3A	1H	2.579	C16	H3'	1H	4.768
G5	H3B	1H	2.873	C16	H5	1H	5.160
G5	H5	1H	5.802	C16	H6	1H	7.052
G5	H6A	1H	6.200	T17	CH3	1H	1.772
G5	H8	1H	8.350	T17	H1'	1H	5.975
G5	H8A	1H	5.723	T17	H2'	1H	2.405
G5	H9	1H	4.841	T17	H2''	1H	2.498
G5	H9A	1H	3.700	T17	H3'	1H	4.824
G5	OCH3	1H	3.572	T17	H6	1H	7.604
C6	H1'	1H	6.108	T18	CH3	1H	1.681
C6	H2'	1H	2.183	T18	H1'	1H	5.539
C6	H2''	1H	2.506	T18	H2'	1H	2.077
C6	H5	1H	5.480	T18	H2''	1H	2.345
C6	H6	1H	7.458	T18	H3'	1H	4.822
T7	CH3	1H	1.568	T18	H6	1H	7.443
T7	H1'	1H	6.068	A19	H1'	1H	6.068
T7	H2'	1H	2.181	A19	H2	1H	7.499
T7	H2''	1H	2.574	A19	H2'	1H	2.731
T7	H6	1H	7.446	A19	H2''	1H	2.886

T8	CH3	1H	1.679	A19	H3'	1H	5.037
T8	H1'	1H	6.035	A19	H8	1H	8.242
T8	H2'	1H	2.025	G20	H1'	1H	5.964
T8	H2''	1H	2.407	G20	H2'	1H	2.414
T8	H3'	1H	4.846	G20	H2''	1H	2.242
T8	H6	1H	7.413	G20	H3'	1H	4.614
C9	H1'	1H	5.635	G20	H8	1H	7.687
C9	H2'	1H	2.020				
C9	H2''	1H	2.263				
C9	H3'	1H	4.790				
C9	H5	1H	5.750				
C9	H6	1H	7.493				
A10	H1'	1H	6.296				
A10	H2	1H	7.759				
A10	H2'	1H	2.687				
A10	H2''	1H	2.439				
A10	H3'	1H	4.686				
A10	H8	1H	8.241				

APPENDIX C

NMR RESTRAINTS FILE

Table C-1. PREP file used to generate topology for aflatoxin B_1 adduct, input files for AMBER calculations. It defines parameters for aflatoxin B_1 modified base.

```
   0     0     2

AFB1 link to DG5
AFB1.prep
 FAG    INT      0
 CORRECT OMIT DU   BEG
   0.0
   1    DUMM  DU    M     0  -1  -2     0.00       0.00       0.00         0.0000
   2    DUMM  DU    M     1   0  -1     1.00       0.00       0.00         0.0000
   3    DUMM  DU    M     2   1   0     1.00      90.00       0.00         0.0000
   4    P     P     M     3   2   1     1.60     119.04     200.00         1.1659
   5    O1P   O2    E     4   3   2     1.48     109.61     150.00        -0.7761
   6    O2P   O2    E     4   3   2     1.48     109.58      20.00        -0.7761
   7    O5'   OS    M     4   3   2     1.60     101.43     -98.89        -0.4954
   8    C5'   CT    M     7   4   3     1.44     119.00     -39.22        -0.0069
   9    H5'1  H1    E     8   7   4     1.09     109.50      60.00         0.0754
  10    H5'2  H1    E     8   7   4     1.09     109.50     -60.00         0.0754
  11    C4'   CT    M     8   7   4     1.52     110.00     180.00         0.1629
  12    H4'   H1    E    11   8   7     1.09     109.50    -200.00         0.1176
  13    O4'   OS    S    11   8   7     1.46     108.86     -86.31        -0.4691
  14    C1'   CT    B    13  11   8     1.42     110.04     105.60         0.0358
  15    H1'   H2    E    14  13  11     1.09     109.50    -240.00         0.1368
  16    N9    N2    B    14  13  11     1.45     112.31     147.92        -0.5480
  17    HN9   H     E    16  14  13     1.01     116.95      -6.91         0.0590
```

18	C4	CM	S	16	14	13	1.35	123.46	-175.42	0.6600
19	N3	NC	S	18	16	14	1.37	121.22	-9.43	-0.6670
20	C2	CA	B	19	18	16	1.31	117.33	-179.18	0.7970
21	N2	N2	B	20	19	18	1.38	118.77	-177.82	-0.8270
22	HN21	H	E	21	20	19	1.01	112.07	-16.96	0.3690
23	HN22	H	E	21	20	19	1.01	116.81	-150.12	0.3800
24	N1	NA	B	20	19	18	1.36	123.59	-1.01	-0.7740
25	H1	H	E	24	20	19	1.01	122.07	-175.99	0.3970
26	C6	C	B	24	20	19	1.43	123.35	1.56	0.8070
27	O6	O	E	26	24	20	1.23	118.31	-179.53	-0.5640
28	C5	CM	S	26	24	20	1.43	112.70	-0.99	-0.4310
29	N7	N2	B	28	26	24	1.43	120.49	172.42	-0.2500
30	C8	C	B	29	28	26	1.39	118.41	-86.00	0.4220
31	H8	HA	E	30	29	28	1.11	111.97	179.89	0.0150
32	O8	O	E	30	29	28	1.21	125.09	-0.43	-0.4570
33	C8A	CT	B	29	28	26	1.44	121.95	92.67	0.2180
34	H8A	HC	E	33	29	28	1.09	107.46	-179.59	0.1160
35	C9	CT	3	33	29	28	1.55	122.10	-94.00	0.2470
36	O9	OH	S	35	33	29	1.42	106.59	-126.23	-0.6530
37	HO9	HO	E	36	35	33	0.97	107.31	163.35	0.4270
38	H9	H1	E	35	33	29	1.09	109.83	-5.96	0.0550
39	C9A	CT	B	35	33	29	1.56	89.60	90.60	-0.0620
40	H9A	HC	E	39	35	33	1.09	108.78	123.39	0.8500
41	C9B	CB	S	39	35	33	1.46	121.80	-86.20	-0.4150
42	CAA	CA	S	41	39	35	1.38	131.44	-67.75	0.6380
43	O10	OS	S	42	41	39	1.36	116.55	-3.58	-0.4280
44	C11	C	B	43	42	41	1.42	123.58	-179.88	0.7590
45	O11	O	E	44	43	42	1.20	116.68	-179.61	-0.4680
46	CBA	CB	S	44	43	42	1.45	113.79	0.61	-0.5170
47	C1	C	B	46	44	43	1.48	125.39	179.19	0.6440
48	O1	O	E	47	46	44	1.21	128.27	-0.09	-0.4780
49	C2A	CT	3	47	46	44	1.54	106.42	-179.92	-0.4960
50	H2A	HC	E	49	47	46	1.10	109.05	-122.23	0.1470

51	H2B	HC	E	49	47	46	1.10	108.99	121.58	0.1470
52	C3	CT	3	49	47	46	1.54	106.15	-0.25	0.0830
53	H3A	HC	E	52	49	47	1.09	112.96	-119.71	0.0360
54	H3B	HC	E	52	49	47	1.09	113.06	120.41	0.0360
55	C3A	CB	S	52	49	47	1.52	104.92	0.33	0.3870
56	C4A	CA	S	55	52	49	1.43	127.94	179.50	-0.6660
57	C4B	CA	B	56	55	52	1.43	126.26	1.18	0.5510
58	O4	OS	S	57	56	55	1.36	115.47	0.26	-0.2740
59	CM	CT	3	58	57	56	1.43	118.89	-170.20	-0.1000
60	HA1	H1	E	59	58	57	1.10	110.89	-61.22	0.0880
61	HA2	H1	E	59	58	57	1.10	111.28	61.52	0.0880
62	HA3	H1	E	59	58	57	1.10	105.50	-179.97	0.0880
63	C5B	CA	B	57	56	55	1.40	121.69	-179.72	-0.5150
64	H5	HA	E	63	57	56	1.08	122.64	-179.32	0.2270
65	C5M	CB	S	63	57	56	1.40	117.23	-0.24	0.3670
66	O6A	OS	S	65	63	57	1.38	122.71	-179.67	-0.3430
67	C6A	CT	B	66	65	63	1.37	105.10	-177.90	0.5190
68	H6A	HC	E	67	66	65	1.09	105.28	121.77	0.0130
69	O7	OS	E	67	66	65	1.25	120.50	-117.20	-0.5550
70	C3’	CT	M	11	8	7	1.53	115.78	-329.11	0.0713
71	H3’	H1	E	30	11	8	1.09	109.50	30.00	0.0985
72	C2’	CT	B	30	11	8	1.53	102.80	-86.30	-0.0854
73	H2’1	H1	E	32	30	11	1.09	109.50	120.00	0.0718
74	H2’2	H1	E	32	30	11	1.09	109.50	240.00	0.0718
75	O3’	OS	M	30	11	8	1.42	116.52	-203.47	-0.6232

IMPROPER

N2 N1 C2 N3

C2 C6 N1 H1

N1 C5 C6 O6

O10 O11 C11 CBA

CBA O1 C1 C2A

C4A O4 C4B C5B

C4B H5 C5B C5M

LOOP

C1’ C2’

C4 C5

C9A C6A

C9B C5M

CAA C4A

CBA C3A

C8A O7

DONE

STOP

Table C-2. frcmod file used to generate topology for aflatoxin B_1 adduct, input files for AMBER calculations. It defines angles for aflatoxin B_1 modified base.

```
remark goes here
MASS

BOND
CA - H1   367.0  1.080
CD - C    410.0  1.444
C - H1    367.0  1.080
C - HA    367.0  1.080
CM - N2   490.0  1.335
NT - CM   490.0  1.370
NC - CM   490.0  1.335
CB - OS   490.0  1.335
CA - OS   490.0  1.335
CT - CB   410.0  1.444
C - N2    490.0  1.380

ANGLE
HC - CT - CB    50.0      109.50
HC - CT - OS    50.0      109.50
HC - CT - OS    50.0      110.60
CB - OS - CT    50.0      105.10
CA - CB - OS    50.0      122.70
CA - CA - OS    50.0      121.90
CB - CA - OS    50.0      118.80
CB - CB - OS    50.0      113.80
CA - OS - CT    50.0      122.40
CB - CT - CT    50.0      121.80
CB - C - CT     50.0      105.90
CB - CB - CT    50.0      103.80
CB - CB - CB    50.0      123.80
OS - C - CB     50.0      115.70
C - OS - CB     50.0      121.30
```

```
HA - C - O      50.0      121.20
N2 - C - O      50.0      120.60
N2 - C - HA     50.0      118.20
CM - N2 - C     50.0      109.20
N2 - CM - C     50.0      115.00
NC - CM - CM    50.0      126.70
CM - NC - CA    50.0      113.10
H - N2 - CM     50.0      117.70
N2 - CM - CM    50.0      125.70
N2 - CT - H2    50.0      108.60
CT - N2 - CM    50.0      134.20
CT - NT - CM    50.0      123.50
N2 - CT - OS    50.0      136.00
HC - CT - N2    50.0      109.10
C - CB - C      50.0      126.50
CT - N2 - C     50.0      134.20
CT - N2 - C     50.0      134.20
NT - CM - CM    50.0      107.90
N2 - CM - NC    50.0      122.90
OS - CT - NT    50.0      111.00
CT - CB - CA    50.0      133.10
CA - OS - C     50.0      123.10

DIHE
X -CB-CT-X      4   0.00    0.0     4.
X -OS-CA-X      4   0.00    0.0     4.
X -OS-CB-X      4   0.00    0.0     4.
X -CM-NC-X      4   0.00    0.0     4.
X-CM-N2-X       4   0.00    0.0     4.
X-C-N2-X        4   0.00    0.0     4.
X-CM-NT-X       4   0.00    0.0     4.

IMPROPER

NONBON
```

Table C-3. PREP file used to generate topology for 7-deaza adduct, input files for AMBER calculations. It defines parameters for aflatoxin B_1 modified base.

```
    0    0    2

7dG link to DG6
7dG.prep
 7dG   INT     0
 CORRECT OMIT DU   BEG
   0.0
1    DUMM  DU    M    0  -1  -2    0.00      0.00      0.00      0.0000
2    DUMM  DU    M    1   0  -1    1.00      0.00      0.00      0.0000
3    DUMM  DU    M    2   1   0    1.00     90.00      0.00      0.0000
4    P     P     M    3   2   1    1.60    119.04    200.00      1.1659
5    O1P   O2    E    4   3   2    1.48    109.61    150.00     -0.7761
6    O2P   O2    E    4   3   2    1.48    109.58     20.00     -0.7761
7    O5'   OS    M    4   3   2    1.60    101.43    -98.89     -0.4954
8    C5'   CT    M    7   4   3    1.44    119.00    -39.22     -0.0069
9    H5'1  H1    E    8   7   4    1.09    109.50     60.00      0.0754
10   H5'2  H1    E    8   7   4    1.09    109.50    -60.00      0.0754
11   C4'   CT    M    8   7   4    1.52    110.00    180.00      0.1629
12   H4'   H1    E   11   8   7    1.09    109.50   -200.00      0.1176
13   O4'   OS    S   11   8   7    1.46    108.86    -86.31     -0.4691
14   C1'   CT    B   13  11   8    1.42    110.04    105.60      0.0358
15   H1'   H2    E   14  13  11    1.09    109.50   -240.00      0.1368
16   N9    N*    S   14  13  11    1.45    109.50    179.79       0.110
17   C8    CD    B   16  14  13    1.39    127.30    112.31      -0.306
18   H8    HA    E   17  16  14    1.08    123.00      0.50       0.198
19   C7    CD    B   17  16  14    1.37    114.00    179.50      -0.181
20   H7    HA    E   19  17  16    1.08    128.20    179.50       0.177
21   C5    CM    S   19  17  16    1.43    103.70    -0.600      -0.326
22   C6    C     B   21  19  17    1.44    130.00    179.16       0.719
23   O6    O     E   22  21  19    1.22    129.20     0.045      -0.551
24   N1    NA    B   22  21  19    1.31    111.40   -179.40      -0.735
25   H1    H     E   24  22  21    1.01    117.40    179.90       0.392
26   C2    CA    B   24  22  21    1.37    125.20     -0.10       0.808
27   N2    N2    B   26  24  22    1.37    116.50    180.00      -0.848
28   HN21  H     E   27  26  24    1.01    120.00     -0.10       0.360
29   HN22  H     E   27  26  24    1.01    120.00   -180.00       0.373
```

```
30   N3    NC    S   27  26  24    1.31    123.30      0.20      -0.680
31   C4    CM    E   30  27  26    1.36    112.00     -0.30       0.400
32   C3'   CT    M   11   8   7    1.53    115.78   -329.11       0.0713
33   H3'   H1    E   32  11   8    1.09    109.50     30.00       0.0985
34   C2'   CT    B   11   8   7    1.53    102.80    -86.30      -0.0854
35   H2'1  H1    E   34  32  11    1.09    109.50    120.00       0.0718
36   H2'2  H1    E   34  32  11    1.09    109.50    240.00       0.0718
37   O3'   OS    M   11   8   7    1.42    116.52   -203.47      -0.6232

IMPROPER
 N2  N1  C2  N3
 C2  C6  N1  H1
 N1  C5  C6  O6


LOOP
 C1'  C2'
 C4   C5
 C4   N9

DONE
STOP
```

Table C-4. frcmod file used to generate topology for 7-deaza adduct, input files for AMBER calculations. It defines angles for aflatoxin B1 modified base.

```
remark goes here
MASS

BOND
CA - H1   367.0  1.080
CD - C    410.0  1.444
C - H1    367.0  1.080
C - HA    367.0  1.080
CM - N2   490.0  1.335
N* - CD   490.0  1.370
NC - CM   490.0  1.335
CB - OS   490.0  1.335
CA - OS   490.0  1.335
CT - CB   410.0  1.444
C - N2    490.0  1.380

ANGLE
HC - CT - CB    50.0      109.50
HC - CT - OS    50.0      109.50
HC - CT - OS    50.0      110.60
CB - OS - CT    50.0      105.10
CA - CB - OS    50.0      122.70
CA - CA - OS    50.0      121.90
CB - CA - OS    50.0      118.80
CB - CB - OS    50.0      113.80
CA - OS - CT    50.0      122.40
CB - CT - CT    50.0      121.80
CB - C - CT     50.0      105.90
CB - CB - CT    50.0      103.80
CB - CB - CB    50.0      123.80
OS - C - CB     50.0      115.70
C - OS - CB     50.0      121.30
```

```
HA - C - O      50.0      121.20
N2 - C - O      50.0      120.60
N2 - C - HA     50.0      118.20
CM - N2 - C     50.0      109.20
N2 - CM - C     50.0      115.00
NC - CM - CM    50.0      126.70
CM - NC - CA    50.0      113.10
H - N2 - CM     50.0      117.70
N2 - CM - CM    50.0      125.70
N2 - CT - H2    50.0      108.60
CT - N2 - CM    50.0      134.20
CT - NT - CM    50.0      123.50
N2 - CT - OS    50.0      136.00
HC - CT - N2    50.0      109.10
C - CB - C      50.0      126.50
CT - N2 - C     50.0      134.20
CT - N2 - C     50.0      134.20
NT - CM - CM    50.0      107.90
N* - CM - NC    50.0      122.90
OS - CT - NT    50.0      111.00
CT - CB - CA    50.0      133.10
CA - OS - C     50.0      123.10
CD - CM - C     50.0      130.92
CD - CM - CM    50.0      110.50
N* - CD - HA    50.0      123.92
N* - CD - CD    50.0      114.92
CT - N* - CD    50.0      127.92
CM - N* - CD    50.0      127.92


DIHE
X -CD-N*-X      4   0.00    0.0     4.


IMPROPER

NONBON
```

Table C-5. Experimental distance and torsion angle restraints used in the rMD calculations of the AFB1-β-FAPY modified AXA adduct.

```
#
#   1 DC5   H2'1  1 DC5 H3'     1.660   2.380
 &rst
  ixpk= 0, nxpk= 0, iat=  26,  24, r1= 1.16, r2= 1.66, r3= 2.38, r4= 2.88,
     rk2=32.0, rk3=32.0, ir6=1, ialtd=0,
 &end
#
#   1 DC5   H2'2  1 DC5 H3'     2.090   2.850
 &rst
  ixpk= 0, nxpk= 0, iat=  27,  24, r1= 1.59, r2= 2.09, r3= 2.85, r4= 3.35,  &end
#
#   1 DC5   H1'   1 DC5 H3'     2.990   3.870
 &rst
  ixpk= 0, nxpk= 0, iat=  10,  24, r1= 2.49, r2= 2.99, r3= 3.87, r4= 4.37,  &end
#
#   1 DC5   H1'   1 DC5 H2'1    2.440   3.030
 &rst
  ixpk= 0, nxpk= 0, iat=  10,  26, r1= 1.94, r2= 2.44, r3= 3.03, r4= 3.53,  &end
#
#   1 DC5   H5    1 DC5 H3'     6.190   6.590
 &rst
  ixpk= 0, nxpk= 0, iat=  15,  24, r1= 5.69, r2= 6.19, r3= 6.59, r4= 7.09,  &end
#
#   1 DC5   H5    1 DC5 H2'1    4.060   4.500
 &rst
  ixpk= 0, nxpk= 0, iat=  15,  26, r1= 3.56, r2= 4.06, r3= 4.50, r4= 5.00,  &end
#
#   1 DC5   H5    1 DC5 H2'2    5.260   5.700
 &rst
  ixpk= 0, nxpk= 0, iat=  15,  27, r1= 4.76, r2= 5.26, r3= 5.70, r4= 6.20,  &end
#
#   1 DC5   H6    1 DC5 H3'     3.440   4.280
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  24, r1= 2.94, r2= 3.44, r3= 4.28, r4= 4.78,  &end
#
#   1 DC5   H6    1 DC5 H2'1    1.670   2.340
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  26, r1= 1.17, r2= 1.67, r3= 2.34, r4= 2.84,  &end
#
#   1 DC5   H6    1 DC5 H2'2    3.160   3.820
 &rst
```

```
  ixpk= 0, nxpk= 0, iat=  13,  27, r1= 2.66, r2= 3.16, r3= 3.82, r4= 4.32,  &end
#
#   1 DC5   H6    1 DC5 H1'     3.160   3.790
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  10, r1= 2.66, r2= 3.16, r3= 3.79, r4= 4.29,  &end
#
#   2 DT    H3   20 DG3 H1      3.100   3.510
 &rst
  ixpk= 0, nxpk= 0, iat=  52, 661, r1= 2.60, r2= 3.10, r3= 3.51, r4= 4.01,  &end
#
#   2 DT    Q5    1 DC5 H2'1    2.500   3.510
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  26, r1= 2.00, r2= 2.50, r3= 4.22, r4= 4.72,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H2'2    2.610   3.590
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  27, r1= 2.11, r2= 2.61, r3= 4.31, r4= 4.81,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H1'     2.960   4.530
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  10, r1= 2.46, r2= 2.96, r3= 5.44, r4= 5.94,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H5      1.570   2.930
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  15, r1= 1.07, r2= 1.57, r3= 3.52, r4= 4.02,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H6      2.010   3.060
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  13, r1= 1.51, r2= 2.01, r3= 3.67, r4= 4.17,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    H6    1 DC5 H1'     3.980   4.180
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  10, r1= 3.48, r2= 3.98, r3= 4.18, r4= 4.68,  &end
#
#   2 DT    H6    1 DC5 H2'2    2.500   2.710
 &rst
```

```
  ixpk= 0, nxpk= 0, iat=  43,  27, r1= 2.00, r2= 2.50, r3= 2.71, r4= 3.21,  &end
#
#   2 DT    H6    1 DC5 H2'1    3.810   4.290
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  26, r1= 3.31, r2= 3.81, r3= 4.29, r4= 4.79,  &end
#
#   2 DT    H6    1 DC5 H3'     4.980   5.280
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  24, r1= 4.48, r2= 4.98, r3= 5.28, r4= 5.78,  &end
#
#   2 DT    H6    1 DC5 H6      5.000   5.320
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  13, r1= 4.50, r2= 5.00, r3= 5.32, r4= 5.82,  &end
#
#   2 DT    Q5    2 DT  H3'     3.250   6.510
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  56, r1= 2.75, r2= 3.25, r3= 7.82, r4= 8.32,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    2 DT  H1'     3.800   5.670
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  40, r1= 3.30, r2= 3.80, r3= 6.81, r4= 7.31,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    H2'2  2 DT  H3'     2.290   2.950
 &rst
  ixpk= 0, nxpk= 0, iat=  59,  56, r1= 1.79, r2= 2.29, r3= 2.95, r4= 3.45,  &end
#
#   2 DT    H1'   2 DT  H3'     3.590   4.010
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  56, r1= 3.09, r2= 3.59, r3= 4.01, r4= 4.51,  &end
#
#   2 DT    H1'   2 DT  H2'1    2.510   3.080
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  58, r1= 2.01, r2= 2.51, r3= 3.08, r4= 3.58,  &end
#
#   2 DT    H1'   2 DT  H2'2    1.870   2.490
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  59, r1= 1.37, r2= 1.87, r3= 2.49, r4= 2.99,  &end
#
#   2 DT    H6    2 DT  H1'     3.540   3.960
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  40, r1= 3.04, r2= 3.54, r3= 3.96, r4= 4.46,  &end
#
```

```
#   3 DA    H61   2 DT  H3      3.570   3.720
 &rst
  ixpk= 0, nxpk= 0, iat=  80,  52, r1= 3.07, r2= 3.57, r3= 3.72, r4= 4.22,  &end
#
#   3 DA    H62   2 DT  H3      4.270   4.520
 &rst
  ixpk= 0, nxpk= 0, iat=  81,  52, r1= 3.77, r2= 4.27, r3= 4.52, r4= 5.02,  &end
#
#   3 DA    H2    2 DT  H3      3.770   4.220
 &rst
  ixpk= 0, nxpk= 0, iat=  84,  52, r1= 3.27, r2= 3.77, r3= 4.22, r4= 4.72,  &end
#
#   3 DA    H61  18 DT  H3      2.370   2.620
 &rst
  ixpk= 0, nxpk= 0, iat=  80, 600, r1= 1.87, r2= 2.37, r3= 2.62, r4= 3.12,  &end
#
#   3 DA    H62  18 DT  H3      3.770   4.120
 &rst
  ixpk= 0, nxpk= 0, iat=  81, 600, r1= 3.27, r2= 3.77, r3= 4.12, r4= 4.62,  &end
#
#   3 DA    H2   19 DA  H2      2.570   3.020
 &rst
  ixpk= 0, nxpk= 0, iat=  84, 632, r1= 2.07, r2= 2.57, r3= 3.02, r4= 3.52,  &end
#
#   3 DA    H8    2 DT  H3'     4.970   5.220
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  56, r1= 4.47, r2= 4.97, r3= 5.22, r4= 5.72,  &end
#
#   3 DA    H8    2 DT  H2'1    4.400   4.660
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  58, r1= 3.90, r2= 4.40, r3= 4.66, r4= 5.16,  &end
#
#   3 DA    H8    2 DT  H2'2    2.650   3.060
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  59, r1= 2.15, r2= 2.65, r3= 3.06, r4= 3.56,  &end
#
#   3 DA    H8    2 DT  H1'     3.640   3.950
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  40, r1= 3.14, r2= 3.64, r3= 3.95, r4= 4.45,  &end
#
#   3 DA    H1'   3 DA  H2'2    2.260   2.960
 &rst
  ixpk= 0, nxpk= 0, iat=  72,  91, r1= 1.76, r2= 2.26, r3= 2.96, r4= 3.46,  &end
#
#   3 DA    H1'   3 DA  H2'1    3.070   3.850
 &rst
```

```
  ixpk= 0, nxpk= 0, iat=  72,  90, r1= 2.57, r2= 3.07, r3= 3.85, r4= 4.35,  &end
#
#   3 DA    H8    3 DA  H1'     3.710   4.120
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  72, r1= 3.21, r2= 3.71, r3= 4.12, r4= 4.62,  &end
#
#   3 DA    H8    3 DA  H2'2    3.310   4.320
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  91, r1= 2.81, r2= 3.31, r3= 4.32, r4= 4.82,  &end
#
#   4 DA    H2    3 DA  H2      4.470   4.820
 &rst
  ixpk= 0, nxpk= 0, iat= 116,  84, r1= 3.97, r2= 4.47, r3= 4.82, r4= 5.32,  &end
#
#   4 DA    H2   18 DT  H3      4.270   4.420
 &rst
  ixpk= 0, nxpk= 0, iat= 116, 600, r1= 3.77, r2= 4.27, r3= 4.42, r4= 4.92,  &end
#
#   4 DA    H61  18 DT  H3      4.870   5.120
 &rst
  ixpk= 0, nxpk= 0, iat= 112, 600, r1= 4.37, r2= 4.87, r3= 5.12, r4= 5.62,  &end
#
#   4 DA    H62  18 DT  H3      5.770   6.120
 &rst
  ixpk= 0, nxpk= 0, iat= 113, 600, r1= 5.27, r2= 5.77, r3= 6.12, r4= 6.62,  &end
#
#   4 DA    H2   17 DT  H3      2.370   2.620
 &rst
  ixpk= 0, nxpk= 0, iat= 116, 568, r1= 1.87, r2= 2.37, r3= 2.62, r4= 3.12,  &end
#
#   4 DA    H61  17 DT  H3      2.770   3.020
 &rst
  ixpk= 0, nxpk= 0, iat= 112, 568, r1= 2.27, r2= 2.77, r3= 3.02, r4= 3.52,  &end
#
#   4 DA    H62  17 DT  H3      4.170   4.620
 &rst
  ixpk= 0, nxpk= 0, iat= 113, 568, r1= 3.67, r2= 4.17, r3= 4.62, r4= 5.12,  &end
#
#   4 DA    H1'   3 DA  H1'     5.410   5.610
 &rst
  ixpk= 0, nxpk= 0, iat= 104,  72, r1= 4.91, r2= 5.41, r3= 5.61, r4= 6.11,  &end
#
#   4 DA    H8    3 DA  H2'1    3.820   4.010
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  90, r1= 3.32, r2= 3.82, r3= 4.01, r4= 4.51,  &end
#
```

```
#   4 DA    H8    3 DA  H2'2    2.420   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  91, r1= 1.92, r2= 2.42, r3= 2.61, r4= 3.11,  &end
#
#   4 DA    H8    3 DA  H1'     3.860   4.060
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  72, r1= 3.36, r2= 3.86, r3= 4.06, r4= 4.56,  &end
#
#   4 DA    H8    3 DA  H8      4.670   4.980
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  75, r1= 4.17, r2= 4.67, r3= 4.98, r4= 5.48,  &end
#
#   4 DA    H1'   4 DA  H3'     3.580   4.240
 &rst
  ixpk= 0, nxpk= 0, iat= 104, 120, r1= 3.08, r2= 3.58, r3= 4.24, r4= 4.74,  &end
#
#   4 DA    H1'   4 DA  H2'1    2.700   3.090
 &rst
  ixpk= 0, nxpk= 0, iat= 104, 122, r1= 2.20, r2= 2.70, r3= 3.09, r4= 3.59,  &end
#
#   4 DA    H1'   4 DA  H2'2    2.040   2.500
 &rst
  ixpk= 0, nxpk= 0, iat= 104, 123, r1= 1.54, r2= 2.04, r3= 2.50, r4= 3.00,  &end
#
#   4 DA    H8    4 DA  H2'1    1.800   2.290
 &rst
  ixpk= 0, nxpk= 0, iat= 107, 122, r1= 1.30, r2= 1.80, r3= 2.29, r4= 2.79,  &end
#
#   4 DA    H8    4 DA  H2'2    3.340   3.500
 &rst
  ixpk= 0, nxpk= 0, iat= 107, 123, r1= 2.84, r2= 3.34, r3= 3.50, r4= 4.00,  &end
#
#   4 DA    H8    4 DA  H1'     3.160   3.740
 &rst
  ixpk= 0, nxpk= 0, iat= 107, 104, r1= 2.66, r2= 3.16, r3= 3.74, r4= 4.24,  &end
#
#   5 FAG   H9A   4 DA  H8      3.150   3.670
 &rst
  ixpk= 0, nxpk= 0, iat= 161, 107, r1= 2.65, r2= 3.15, r3= 3.67, r4= 4.17,  &end
#
#   5 FAG   H6A   4 DA  H3'     4.070   4.620
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 120, r1= 3.57, r2= 4.07, r3= 4.62, r4= 5.12,  &end
#
#   5 FAG   H6A   4 DA  H2'1    2.370   3.840
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 189, 122, r1= 1.87, r2= 2.37, r3= 3.84, r4= 4.34,  &end
#
#   5 FAG   H6A   4 DA  H2'2    1.870   2.240
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 123, r1= 1.37, r2= 1.87, r3= 2.24, r4= 2.74,  &end
#
#   5 FAG   H6A   4 DA  H1'     2.340   3.160
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 104, r1= 1.84, r2= 2.34, r3= 3.16, r4= 3.66,  &end
#
#   5 FAG   H6A   4 DA  H8      2.310   2.890
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 107, r1= 1.81, r2= 2.31, r3= 2.89, r4= 3.39,  &end
#
#   5 FAG   H5    4 DA  H2'1    5.450   5.860
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 122, r1= 4.95, r2= 5.45, r3= 5.86, r4= 6.36,  &end
#
#   5 FAG   H5    4 DA  H2'2    4.420   4.830
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 123, r1= 3.92, r2= 4.42, r3= 4.83, r4= 5.33,  &end
#
#   5 FAG   H5    4 DA  H1'     3.070   3.480
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 104, r1= 2.57, r2= 3.07, r3= 3.48, r4= 3.98,  &end
#
#   5 FAG   H5    4 DA  H8      5.070   6.200
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 107, r1= 4.57, r2= 5.07, r3= 6.20, r4= 6.70,  &end
#
#   5 FAG   MA   17 DT  H3      2.500   5.500
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 568, r1= 2.00, r2= 2.50, r3= 6.61, r4= 7.11,
 igr1= 181, 182, 183,
 &end
#
#   5 FAG   MA          4 DA  H2      2.000   3.000
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 116, r1= 1.50, r2= 2.00, r3= 3.60, r4= 4.10,
 igr1= 181, 182, 183,
 &end
#
#   5 FAG  H2'1         5 FAG H1'    3.000   3.500
 &rst
  ixpk= 0, nxpk= 0, iat= 194, 136, r1= 2.50, r2= 3.00, r3= 3.50, r4= 4.00,  &end
#
```

```
#   5 FAG  H2'2         5 FAG H1'    2.400   2.800
 &rst
  ixpk= 0, nxpk= 0, iat= 195, 136, r1= 1.90, r2= 2.40, r3= 2.80, r4= 3.30,  &end
#
#   5 FAG  H3'5 FAG H1'    3.700   4.100
 &rst
  ixpk= 0, nxpk= 0, iat= 192, 136, r1= 3.20, r2= 3.70, r3= 4.10, r4= 4.60,  &end
#
#   5 FAG  H3'5 FAG H2'1   2.500   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 192, 194, r1= 2.00, r2= 2.50, r3= 2.90, r4= 3.40,  &end
#
#   5 FAG  H3'5 FAG H2'2   2.700   3.100
 &rst
  ixpk= 0, nxpk= 0, iat= 192, 195, r1= 2.20, r2= 2.70, r3= 3.10, r4= 3.60,  &end
#
#   5 FAG  H8 5 FAG H8A    1.800   2.400
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 155, r1= 1.30, r2= 1.80, r3= 2.40, r4= 2.90,  &end
#
#   5 FAG  H9A         5 FAG H8A    3.600   4.000
 &rst
  ixpk= 0, nxpk= 0, iat= 161, 155, r1= 3.10, r2= 3.60, r3= 4.00, r4= 4.50,  &end
#
#   5 FAG  H9A         5 FAG H8     5.200   6.800
 &rst
  ixpk= 0, nxpk= 0, iat= 161, 152, r1= 4.70, r2= 5.20, r3= 6.80, r4= 7.30,  &end
#
#   5 FAG  H9A         5 FAG H9     2.500   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 161, 159, r1= 2.00, r2= 2.50, r3= 2.90, r4= 3.40,  &end
#
#   5 FAG  H6A         5 FAG H8A    3.400   3.900
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 155, r1= 2.90, r2= 3.40, r3= 3.90, r4= 4.40,  &end
#
#   5 FAG  H6A         5 FAG H9     3.800   4.200
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 159, r1= 3.30, r2= 3.80, r3= 4.20, r4= 4.70,  &end
#
#   5 FAG  H6A         5 FAG H9A    2.300   2.600
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 161, r1= 1.80, r2= 2.30, r3= 2.60, r4= 3.10,  &end
#
#   5 FAG  H6A         5 FAG H8     5.000   5.700
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 189, 152, r1= 4.50, r2= 5.00, r3= 5.70, r4= 6.20,  &end
#
#   5 FAG  H5 5 FAG H1'    4.680   5.530
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 136, r1= 4.18, r2= 4.68, r3= 5.53, r4= 6.03,  &end
#
#   5 FAG  H8 5 FAG HN9    3.050   5.720
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 138, r1= 2.55, r2= 3.05, r3= 5.72, r4= 6.22,  &end
#
#   5 FAG  H2'1          5 FAG HN9    2.040   3.780
 &rst
  ixpk= 0, nxpk= 0, iat= 194, 138, r1= 1.54, r2= 2.04, r3= 3.78, r4= 4.28,  &end
#
#   5 FAG  H2'2          5 FAG HN9    1.900   3.460
 &rst
  ixpk= 0, nxpk= 0, iat= 195, 138, r1= 1.40, r2= 1.90, r3= 3.46, r4= 3.96,  &end
#
#   5 FAG  H8 6 DA   H8     3.170   5.230
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 211, r1= 2.67, r2= 3.17, r3= 5.23, r4= 5.73,  &end
#
#   5 FAG  O8 6 DA   H61    2.100   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 153, 216, r1= 1.60, r2= 2.10, r3= 2.90, r4= 3.40,  &end
#
#   6 DA   H8   5 FAG H1'    2.900   3.500
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 136, r1= 2.40, r2= 2.90, r3= 3.50, r4= 4.00,  &end
#
#   6 DA   H8   5 FAG H2'1   4.600   5.000
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 194, r1= 4.10, r2= 4.60, r3= 5.00, r4= 5.50,  &end
#
#   6 DA   H8   5 FAG H2'2   2.900   3.500
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 195, r1= 2.40, r2= 2.90, r3= 3.50, r4= 4.00,  &end
#
#   6 DA   H8   5 FAG H3'    5.200   5.900
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 192, r1= 4.70, r2= 5.20, r3= 5.90, r4= 6.40,  &end
#
#   6 DA   H1'  6 DA   H3'    3.700   4.100
 &rst
  ixpk= 0, nxpk= 0, iat= 208, 224, r1= 3.20, r2= 3.70, r3= 4.10, r4= 4.60,  &end
#
```

```
#   6 DA   H1'  6 DA   H2'1   2.800   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 208, 226, r1= 2.30, r2= 2.80, r3= 3.20, r4= 3.70,  &end
#
#   6 DA   H1'  6 DA   H2'2   2.100   2.500
 &rst
  ixpk= 0, nxpk= 0, iat= 208, 227, r1= 1.60, r2= 2.10, r3= 2.50, r4= 3.00,  &end
#
#   6 DA   H8   6 DA   H1'    3.700   4.100
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 208, r1= 3.20, r2= 3.70, r3= 4.10, r4= 4.60,  &end
#
#   7 DT    H2'1  7 DT  H3'     2.200   2.820
 &rst
  ixpk= 0, nxpk= 0, iat= 258, 256, r1= 1.70, r2= 2.20, r3= 2.82, r4= 3.32,  &end
#
#   7 DT    H2'2  7 DT  H3'     2.470   3.090
 &rst
  ixpk= 0, nxpk= 0, iat= 259, 256, r1= 1.97, r2= 2.47, r3= 3.09, r4= 3.59,  &end
#
#   7 DT    H1'   7 DT  H2'1    2.780   3.220
 &rst
  ixpk= 0, nxpk= 0, iat= 240, 258, r1= 2.28, r2= 2.78, r3= 3.22, r4= 3.72,  &end
#
#   7 DT    H1'   7 DT  H2'2    2.020   2.520
 &rst
  ixpk= 0, nxpk= 0, iat= 240, 259, r1= 1.52, r2= 2.02, r3= 2.52, r4= 3.02,  &end
#
#   7 DT    H6    7 DT  H2'1    1.710   2.250
 &rst
  ixpk= 0, nxpk= 0, iat= 243, 258, r1= 1.21, r2= 1.71, r3= 2.25, r4= 2.75,  &end
#
#   7 DT    H6    7 DT  H2'2    3.220   3.730
 &rst
  ixpk= 0, nxpk= 0, iat= 243, 259, r1= 2.72, r2= 3.22, r3= 3.73, r4= 4.23,  &end
#
#   8 DT    H6    7 DT  H2'1    3.650   4.120
 &rst
  ixpk= 0, nxpk= 0, iat= 275, 258, r1= 3.15, r2= 3.65, r3= 4.12, r4= 4.62,  &end
#
#   8 DT    H6    7 DT  H2'2    2.180   2.660
 &rst
  ixpk= 0, nxpk= 0, iat= 275, 259, r1= 1.68, r2= 2.18, r3= 2.66, r4= 3.16,  &end
#
#   8 DT    H6    7 DT  H1'     2.800   3.290
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 275, 240, r1= 2.30, r2= 2.80, r3= 3.29, r4= 3.79,  &end
#
#   8 DT    H6    7 DT  H6      4.810   5.390
 &rst
  ixpk= 0, nxpk= 0, iat= 275, 243, r1= 4.31, r2= 4.81, r3= 5.39, r4= 5.89,  &end
#
#   8 DT    Q5  7 DT  H3'     2.380   4.510
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 256, r1= 1.88, r2= 2.38, r3= 5.42, r4= 5.92,
 igr1= 278, 279, 280,
 &end
#
#   8 DT    Q5  7 DT  H2'1    2.170   3.000
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 258, r1= 1.67, r2= 2.17, r3= 3.60, r4= 4.10,
 igr1= 278, 279, 280,
 &end
#
#   8 DT    Q5  7 DT  H2'2    2.130   3.040
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 259, r1= 1.63, r2= 2.13, r3= 3.65, r4= 4.15,
 igr1= 278, 279, 280,
 &end
#
#   8 DT    Q5  7 DT  H1'     2.910   4.410
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 240, r1= 2.41, r2= 2.91, r3= 5.30, r4= 5.80,
 igr1= 278, 279, 280,
 &end
#
#   8 DT    Q5  7 DT  H6      2.520   3.470
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 243, r1= 2.02, r2= 2.52, r3= 4.17, r4= 4.67,
 igr1= 278, 279, 280,
 &end
#
#   8 DT    H3'   7 DT  H1'     4.610   5.490
 &rst
  ixpk= 0, nxpk= 0, iat= 288, 240, r1= 4.11, r2= 4.61, r3= 5.49, r4= 5.99,  &end
#
#   8 DT    H2'1  8 DT  H3'     2.500   3.230
 &rst
  ixpk= 0, nxpk= 0, iat= 290, 288, r1= 2.00, r2= 2.50, r3= 3.23, r4= 3.73,  &end
#
#   8 DT    H2'2  8 DT  H3'     2.400   3.060
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 291, 288, r1= 1.90, r2= 2.40, r3= 3.06, r4= 3.56,  &end
#
#   8 DT    H1'   8 DT  H3'     3.500   5.100
 &rst
  ixpk= 0, nxpk= 0, iat= 272, 288, r1= 3.00, r2= 3.50, r3= 5.10, r4= 5.60,  &end
#
#   8 DT    H1'   8 DT  H2'1    2.720   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 272, 290, r1= 2.22, r2= 2.72, r3= 3.20, r4= 3.70,  &end
#
#   8 DT    Q5    8 DT  H3'     3.050   5.940
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 288, r1= 2.55, r2= 3.05, r3= 7.13, r4= 7.63,
 igr1= 278, 279, 280,
 &end
#
#   8 DT    Q5    8 DT  H1'     3.190   5.960
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 272, r1= 2.69, r2= 3.19, r3= 7.16, r4= 7.66,
 igr1= 278, 279, 280,
 &end
#
#   8 DT    H6    8 DT  H2'1    2.000   2.880
 &rst
  ixpk= 0, nxpk= 0, iat= 275, 290, r1= 1.50, r2= 2.00, r3= 2.88, r4= 3.38,  &end
#
#   8 DT    H6    8 DT  H2'2    3.770   4.280
 &rst
  ixpk= 0, nxpk= 0, iat= 275, 291, r1= 3.27, r2= 3.77, r3= 4.28, r4= 4.78,  &end
#
#   8 DT    H6    8 DT  H1'     3.530   4.220
 &rst
  ixpk= 0, nxpk= 0, iat= 275, 272, r1= 3.03, r2= 3.53, r3= 4.22, r4= 4.72,  &end
#
#   9 DC    H6  8 DT  H2'1    3.600   4.310
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 290, r1= 3.10, r2= 3.60, r3= 4.31, r4= 4.81,  &end
#
#   9 DC    H6  8 DT  H2'2    2.200   2.840
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 291, r1= 1.70, r2= 2.20, r3= 2.84, r4= 3.34,  &end
#
#   9 DC    H6  8 DT  H1'     2.830   3.390
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 272, r1= 2.33, r2= 2.83, r3= 3.39, r4= 3.89,  &end
#
```

```
#   9 DC    H6  8 DT  H6      4.900   5.300
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 275, r1= 4.40, r2= 4.90, r3= 5.30, r4= 5.80,  &end
#
#   9 DC    H5  8 DT  H3'     5.000   5.500
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 288, r1= 4.50, r2= 5.00, r3= 5.50, r4= 6.00,  &end
#
#   9 DC    H5  8 DT  H2'2    2.410   3.360
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 291, r1= 1.91, r2= 2.41, r3= 3.36, r4= 3.86,  &end
#
#   9 DC    H5  8 DT  H1'     3.320   4.050
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 272, r1= 2.82, r2= 3.32, r3= 4.05, r4= 4.55,  &end
#
#   9 DC    H5  8 DT  Q5      2.810   3.900
 &rst
  ixpk= 0, nxpk= 0, iat= 309,  -1, r1= 2.31, r2= 2.81, r3= 4.68, r4= 5.18,
 igr2= 278, 279, 280,
 &end
#
#   9 DC    H5  8 DT  H6      3.590   4.080
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 275, r1= 3.09, r2= 3.59, r3= 4.08, r4= 4.58,  &end
#
#   9 DC    H1'   9 DC  H3'     3.730   4.290
 &rst
  ixpk= 0, nxpk= 0, iat= 304, 318, r1= 3.23, r2= 3.73, r3= 4.29, r4= 4.79,  &end
#
#   9 DC    H1'   9 DC  H2'1    2.780   3.270
 &rst
  ixpk= 0, nxpk= 0, iat= 304, 320, r1= 2.28, r2= 2.78, r3= 3.27, r4= 3.77,  &end
#
#   9 DC    H1'   9 DC  H2'2    2.120   2.660
 &rst
  ixpk= 0, nxpk= 0, iat= 304, 321, r1= 1.62, r2= 2.12, r3= 2.66, r4= 3.16,  &end
#
#   9 DC    H5    9 DC  H2'1    4.100   4.680
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 320, r1= 3.60, r2= 4.10, r3= 4.68, r4= 5.18,  &end
#
#   9 DC    H5    9 DC  H2'2    5.300   5.740
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 321, r1= 4.80, r2= 5.30, r3= 5.74, r4= 6.24,  &end
#
```

```
#   9 DC    H6    9 DC  H2'1    1.700   2.160
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 320, r1= 1.20, r2= 1.70, r3= 2.16, r4= 2.66,  &end
#
#   9 DC    H6    9 DC  H2'2    3.220   3.730
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 321, r1= 2.72, r2= 3.22, r3= 3.73, r4= 4.23,  &end
#
#   9 DC    H6    9 DC  H1'     3.500   4.210
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 304, r1= 3.00, r2= 3.50, r3= 4.21, r4= 4.71,  &end
#
#  10 DA3   H8    9 DC  H2'1    3.690   4.290
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 320, r1= 3.19, r2= 3.69, r3= 4.29, r4= 4.79,  &end
#
#  10 DA3   H8    9 DC  H2'2    2.480   2.980
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 321, r1= 1.98, r2= 2.48, r3= 2.98, r4= 3.48,  &end
#
#  10 DA3   H8    9 DC  H6      4.430   5.240
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 307, r1= 3.93, r2= 4.43, r3= 5.24, r4= 5.74,  &end
#
#  10 DA3   H8    9 DC  H1'     3.590   4.290
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 304, r1= 3.09, r2= 3.59, r3= 4.29, r4= 4.79,  &end
#
#  10 DA3   H2'1 10 DA3 H3'     2.270   2.770
 &rst
  ixpk= 0, nxpk= 0, iat= 352, 350, r1= 1.77, r2= 2.27, r3= 2.77, r4= 3.27,  &end
#
#  10 DA3   H2'2 10 DA3 H3'     2.510   3.070
 &rst
  ixpk= 0, nxpk= 0, iat= 353, 350, r1= 2.01, r2= 2.51, r3= 3.07, r4= 3.57,  &end
#
#  10 DA3   H1'  10 DA3 H3'     3.550   4.060
 &rst
  ixpk= 0, nxpk= 0, iat= 334, 350, r1= 3.05, r2= 3.55, r3= 4.06, r4= 4.56,  &end
#
#  10 DA3   H1'  10 DA3 H2'1    2.710   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 334, 352, r1= 2.21, r2= 2.71, r3= 3.20, r4= 3.70,  &end
#
#  10 DA3   H1'  10 DA3 H2'2    1.980   2.550
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 334, 353, r1= 1.48, r2= 1.98, r3= 2.55, r4= 3.05,  &end
#
#  10 DA3   H8   10 DA3 H3'     4.150   4.730
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 350, r1= 3.65, r2= 4.15, r3= 4.73, r4= 5.23,  &end
#
#  10 DA3   H8   10 DA3 H2'2    3.460   3.960
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 353, r1= 2.96, r2= 3.46, r3= 3.96, r4= 4.46,  &end
#
#  10 DA3   H8   10 DA3 H1'     3.570   4.070
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 334, r1= 3.07, r2= 3.57, r3= 4.07, r4= 4.57,  &end
#
#  11 DT5   H1'  11 DT5 H3'     3.740   4.280
 &rst
  ixpk= 0, nxpk= 0, iat= 365, 381, r1= 3.24, r2= 3.74, r3= 4.28, r4= 4.78,  &end
#
#  11 DT5   H1'  11 DT5 H2'1    2.720   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 365, 383, r1= 2.22, r2= 2.72, r3= 3.20, r4= 3.70,  &end
#
#  11 DT5   H1'  11 DT5 H2'2    2.120   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 365, 384, r1= 1.62, r2= 2.12, r3= 2.61, r4= 3.11,  &end
#
#  11 DT5   Q5   11 DT5 H1'     3.410   5.850
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 365, r1= 2.91, r2= 3.41, r3= 7.03, r4= 7.53,
 igr1= 371, 372, 373,
 &end
#
#  11 DT5   H6   11 DT5 H3'     3.820   4.280
 &rst
  ixpk= 0, nxpk= 0, iat= 368, 381, r1= 3.32, r2= 3.82, r3= 4.28, r4= 4.78,  &end
#
#  11 DT5   H6   11 DT5 H2'1    1.730   2.340
 &rst
  ixpk= 0, nxpk= 0, iat= 368, 383, r1= 1.23, r2= 1.73, r3= 2.34, r4= 2.84,  &end
#
#  11 DT5   H6   11 DT5 H2'2    3.110   3.810
 &rst
  ixpk= 0, nxpk= 0, iat= 368, 384, r1= 2.61, r2= 3.11, r3= 3.81, r4= 4.31,  &end
#
#  11 DT5   H6   11 DT5 H1'     2.730   4.390
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 368, 365, r1= 2.23, r2= 2.73, r3= 4.39, r4= 4.89,  &end
#
#  11 DT5   H6   11 DT5 Q5      2.020   2.850
 &rst
  ixpk= 0, nxpk= 0, iat= 368,  -1, r1= 1.52, r2= 2.02, r3= 3.42, r4= 3.92,
 igr2= 371, 372, 373,
 &end
#
#  12 DG    H8   11 DT5 H3'     4.990   5.480
 &rst
  ixpk= 0, nxpk= 0, iat= 400, 381, r1= 4.49, r2= 4.99, r3= 5.48, r4= 5.98,  &end
#
#  12 DG    H8   11 DT5 H2'1    3.590   4.680
 &rst
  ixpk= 0, nxpk= 0, iat= 400, 383, r1= 3.09, r2= 3.59, r3= 4.68, r4= 5.18,  &end
#
#  12 DG    H8   11 DT5 H2'2    2.570   3.640
 &rst
  ixpk= 0, nxpk= 0, iat= 400, 384, r1= 2.07, r2= 2.57, r3= 3.64, r4= 4.14,  &end
#
#  12 DG    H8   11 DT5 H1'     3.550   4.020
 &rst
  ixpk= 0, nxpk= 0, iat= 400, 365, r1= 3.05, r2= 3.55, r3= 4.02, r4= 4.52,  &end
#
#  12 DG    H8   11 DT5 H6      4.660   5.240
 &rst
  ixpk= 0, nxpk= 0, iat= 400, 368, r1= 4.16, r2= 4.66, r3= 5.24, r4= 5.74,  &end
#
#  12 DG    H8   12 DG  H1'     3.700   5.260
 &rst
  ixpk= 0, nxpk= 0, iat= 400, 397, r1= 3.20, r2= 3.70, r3= 5.26, r4= 5.76,  &end
#
#  13 DA    H8   12 DG  H1'     3.440   4.080
 &rst
  ixpk= 0, nxpk= 0, iat= 433, 397, r1= 2.94, r2= 3.44, r3= 4.08, r4= 4.58,  &end
#
#  13 DA    H8   12 DG  H8      5.080   5.690
 &rst
  ixpk= 0, nxpk= 0, iat= 433, 400, r1= 4.58, r2= 5.08, r3= 5.69, r4= 6.19,  &end
#
#  13 DA    H8   12 DG  H2'1    4.500   5.000
 &rst
  ixpk= 0, nxpk= 0, iat= 433, 416, r1= 4.00, r2= 4.50, r3= 5.00, r4= 5.50,  &end
#
#  13 DA    H8   12 DG  H2'2    2.800   3.400
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 433, 417, r1= 2.30, r2= 2.80, r3= 3.40, r4= 3.90,  &end
#
#  13 DA    H1'  13 DA  H3'     3.630   4.150
 &rst
  ixpk= 0, nxpk= 0, iat= 430, 446, r1= 3.13, r2= 3.63, r3= 4.15, r4= 4.65,  &end
#
#  13 DA    H1'  13 DA  H2'1    2.750   3.230
 &rst
  ixpk= 0, nxpk= 0, iat= 430, 448, r1= 2.25, r2= 2.75, r3= 3.23, r4= 3.73,  &end
#
#  13 DA    H1'  13 DA  H2'2    2.120   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 430, 449, r1= 1.62, r2= 2.12, r3= 2.61, r4= 3.11,  &end
#
#  13 DA    H8   13 DA  H1'     3.680   4.180
 &rst
  ixpk= 0, nxpk= 0, iat= 433, 430, r1= 3.18, r2= 3.68, r3= 4.18, r4= 4.68,  &end
#
#  13 DA    H8   13 DA  H2'2    3.480   3.980
 &rst
  ixpk= 0, nxpk= 0, iat= 433, 449, r1= 2.98, r2= 3.48, r3= 3.98, r4= 4.48,  &end
#
#  14 DA    H8   13 DA  H1'     2.410   3.190
 &rst
  ixpk= 0, nxpk= 0, iat= 465, 430, r1= 1.91, r2= 2.41, r3= 3.19, r4= 3.69,  &end
#
#  14 DA    H8   13 DA  H8      4.490   4.990
 &rst
  ixpk= 0, nxpk= 0, iat= 465, 433, r1= 3.99, r2= 4.49, r3= 4.99, r4= 5.49,  &end
#
#  14 DA    H8   13 DA  H2'1    3.800   4.300
 &rst
  ixpk= 0, nxpk= 0, iat= 465, 448, r1= 3.30, r2= 3.80, r3= 4.30, r4= 4.80,  &end
#
#  14 DA    H8   13 DA  H2'2    2.400   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 465, 449, r1= 1.90, r2= 2.40, r3= 2.90, r4= 3.40,  &end
#
#  14 DA    H1'  14 DA  H2'1    2.800   3.310
 &rst
  ixpk= 0, nxpk= 0, iat= 462, 480, r1= 2.30, r2= 2.80, r3= 3.31, r4= 3.81,  &end
#
#  14 DA    H1'  14 DA  H2'2    2.120   2.630
 &rst
  ixpk= 0, nxpk= 0, iat= 462, 481, r1= 1.62, r2= 2.12, r3= 2.63, r4= 3.13,  &end
#
```

```
#  14 DA    H8   14 DA  H2'1    2.030   2.510
 &rst
  ixpk= 0, nxpk= 0, iat= 465, 480, r1= 1.53, r2= 2.03, r3= 2.51, r4= 3.01,  &end
#
#  14 DA    H8   14 DA  H1'     3.650   4.130
 &rst
  ixpk= 0, nxpk= 0, iat= 465, 462, r1= 3.15, r2= 3.65, r3= 4.13, r4= 4.63,  &end
#
#    15 DT   H2'1  15 DT    H3'           2.100   2.700
 &rst
  ixpk= 0, nxpk= 0, iat= 512, 510, r1= 1.60, r2= 2.10, r3= 2.70, r4= 3.20,  &end
#
#    15 DT   H2'2  15 DT    H3'           2.500   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 513, 510, r1= 2.00, r2= 2.50, r3= 2.90, r4= 3.40,  &end
#
#    15 DT   H1'   15 DT    H3' 3.700   4.100
 &rst
  ixpk= 0, nxpk= 0, iat= 494, 510, r1= 3.20, r2= 3.70, r3= 4.10, r4= 4.60,  &end
#
#    15 DT   H1'   15 DT    H2'1   2.800   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 494, 512, r1= 2.30, r2= 2.80, r3= 3.20, r4= 3.70,  &end
#
#    15 DT   H1'   15 DT    H2'2   2.100   2.500
 &rst
  ixpk= 0, nxpk= 0, iat= 494, 513, r1= 1.60, r2= 2.10, r3= 2.50, r4= 3.00,  &end
#
#    15 DT   Q5    14 DA    H1'           3.790   5.190
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 462, r1= 3.29, r2= 3.79, r3= 6.23, r4= 6.73,
 igr1= 500, 501, 502,
 &end
#
#    15 DT   Q5    14 DA    H8 2.630   3.810
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 465, r1= 2.13, r2= 2.63, r3= 4.58, r4= 5.08,
 igr1= 500, 501, 502,
 &end
#
#    15 DT   H6    14 DA    H2'2   1.900   2.300
 &rst
  ixpk= 0, nxpk= 0, iat= 497, 481, r1= 1.40, r2= 1.90, r3= 2.30, r4= 2.80,  &end
#
#    15 DT   H6    14 DA    H1'           3.200   3.800
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 497, 462, r1= 2.70, r2= 3.20, r3= 3.80, r4= 4.30,  &end
#
#    15 DT   H6    14 DA    H8 4.700   5.200
 &rst
  ixpk= 0, nxpk= 0, iat= 497, 465, r1= 4.20, r2= 4.70, r3= 5.20, r4= 5.70,  &end
#
#    15 DT   H6    15 DT    H3'            4.000   4.600
 &rst
  ixpk= 0, nxpk= 0, iat= 497, 510, r1= 3.50, r2= 4.00, r3= 4.60, r4= 5.10,  &end
#
#    15 DT   H6    15 DT    H1'            3.500   3.900
 &rst
  ixpk= 0, nxpk= 0, iat= 497, 494, r1= 3.00, r2= 3.50, r3= 3.90, r4= 4.40,  &end
#
#    15 DT   H6    15 DT    Q5  2.240   3.710
 &rst
  ixpk= 0, nxpk= 0, iat= 497,  -1, r1= 1.74, r2= 2.24, r3= 4.46, r4= 4.96,
 igr2= 500, 501, 502,
 &end
#
#    16 DC   H2'2   5 FAG   H2B    3.500        4.000
 &rst
  ixpk= 0, nxpk= 0, iat= 543, 172, r1= 3.00, r2= 3.50, r3= 4.00, r4= 4.50,  &end
#
#    16 DC   H1'    5 FAG   H2B          4.100   4.600
 &rst
  ixpk= 0, nxpk= 0, iat= 526, 172, r1= 3.60, r2= 4.10, r3= 4.60, r4= 5.10,  &end
#
#    16 DC   H2'2  16 DC    H3'            2.500   3.000
 &rst
  ixpk= 0, nxpk= 0, iat= 543, 540, r1= 2.00, r2= 2.50, r3= 3.00, r4= 3.50,  &end
#
#    16 DC   H1'   16 DC    H3'            3.700   4.100
 &rst
  ixpk= 0, nxpk= 0, iat= 526, 540, r1= 3.20, r2= 3.70, r3= 4.10, r4= 4.60,  &end
#
#    16 DC   H5    15 DT    H3'            5.200   5.600
 &rst
  ixpk= 0, nxpk= 0, iat= 531, 510, r1= 4.70, r2= 5.20, r3= 5.60, r4= 6.10,  &end
#
#    16 DC   H5    15 DT    H2'1   3.000   3.400
 &rst
  ixpk= 0, nxpk= 0, iat= 531, 512, r1= 2.50, r2= 3.00, r3= 3.40, r4= 3.90,  &end
#
#    16 DC   H5    15 DT    H2'2   2.700   3.300
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 531, 513, r1= 2.20, r2= 2.70, r3= 3.30, r4= 3.80,  &end
#
#    16 DC   H5    15 DT    Q5  2.630   4.110
 &rst
  ixpk= 0, nxpk= 0, iat= 531,  -1, r1= 2.13, r2= 2.63, r3= 4.94, r4= 5.44,
 igr2= 500, 501, 502,
 &end
#
#    16 DC   H5    15 DT    H6  3.500   3.900
 &rst
  ixpk= 0, nxpk= 0, iat= 531, 497, r1= 3.00, r2= 3.50, r3= 3.90, r4= 4.40,  &end
#
#    16 DC   H6    15 DT    H3'             4.600   5.200
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 510, r1= 4.10, r2= 4.60, r3= 5.20, r4= 5.70,  &end
#
#    16 DC   H6    15 DT    H2'1   3.400   3.800
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 512, r1= 2.90, r2= 3.40, r3= 3.80, r4= 4.30,  &end
#
#    16 DC   H6    15 DT    H2'2   2.200   2.600
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 513, r1= 1.70, r2= 2.20, r3= 2.60, r4= 3.10,  &end
#
#    16 DC   H6    15 DT    H1'             3.700   4.200
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 494, r1= 3.20, r2= 3.70, r3= 4.20, r4= 4.70,  &end
#
#    16 DC   H6    15 DT    H6  4.700   5.100
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 497, r1= 4.20, r2= 4.70, r3= 5.10, r4= 5.60,  &end
#
#    16 DC   H6    16 DC    H1'             3.500   3.900
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 526, r1= 3.00, r2= 3.50, r3= 3.90, r4= 4.40,  &end
#
#    17 DT   H2'1  17 DT     H3'             2.300   2.700
 &rst
  ixpk= 0, nxpk= 0, iat= 574, 572, r1= 1.80, r2= 2.30, r3= 2.70, r4= 3.20,  &end
#
#    17 DT   H2'2  17 DT     H3'             2.500   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 575, 572, r1= 2.00, r2= 2.50, r3= 2.90, r4= 3.40,  &end
#
#    17 DT   H1'   17 DT    H3' 3.700   4.100
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 556, 572, r1= 3.20, r2= 3.70, r3= 4.10, r4= 4.60,  &end
#
#    17 DT   H1'   17 DT    H2'2   2.100   2.500
 &rst
  ixpk= 0, nxpk= 0, iat= 556, 575, r1= 1.60, r2= 2.10, r3= 2.50, r4= 3.00,  &end
#
#    17 DT   H6    17 DT    H3'            3.800   4.200
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 572, r1= 3.30, r2= 3.80, r3= 4.20, r4= 4.70,  &end
#
#    17 DT   H6    17 DT    H2'1   1.700   2.300
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 574, r1= 1.20, r2= 1.70, r3= 2.30, r4= 2.80,  &end
#
#    17 DT   H6    17 DT    H2'2   3.200   3.700
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 575, r1= 2.70, r2= 3.20, r3= 3.70, r4= 4.20,  &end
#
#    17 DT   H6    17 DT    H1'            3.500   3.900
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 556, r1= 3.00, r2= 3.50, r3= 3.90, r4= 4.40,  &end
#
#    17 DT   Q5    17 DT    H2'1   2.160   4.620
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 574, r1= 1.66, r2= 2.16, r3= 5.55, r4= 6.05,
 igr1= 562, 563, 564,
 &end
#
#    17 DT   Q5    17 DT    H6  2.000   3.550
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 559, r1= 1.50, r2= 2.00, r3= 4.26, r4= 4.76,
 igr1= 562, 563, 564,
 &end
#
#    18 DT   Q5    17 DT    H2'1   2.570   3.270
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 574, r1= 2.07, r2= 2.57, r3= 3.93, r4= 4.43,
 igr1= 594, 595, 596,
 &end
#
#    18 DT   Q5    17 DT    H2'2   2.550   3.330
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 575, r1= 2.05, r2= 2.55, r3= 4.00, r4= 4.50,
 igr1= 594, 595, 596,
 &end
#
```

```
#    18 DT   Q5    17 DT    H1'           3.400   4.750
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 556, r1= 2.90, r2= 3.40, r3= 5.70, r4= 6.20,
 igr1= 594, 595, 596,
 &end
#
#    18 DT   Q5    17 DT    H6  2.200   3.340
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 559, r1= 1.70, r2= 2.20, r3= 4.01, r4= 4.51,
 igr1= 594, 595, 596,
 &end
#
#    18 DT   Q5    17 DT    Q5  2.750   3.330
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  -1, r1= 2.25, r2= 2.75, r3= 4.80, r4= 5.30,
 igr1= 594, 595, 596,
 igr2= 562, 563, 564,
 &end
#
#    18 DT   Q5    17 DT    H3'           3.750   4.330
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 572, r1= 3.25, r2= 3.75, r3= 5.20, r4= 5.70,
 igr1= 594, 595, 596,
 &end
#
#    18 DT   Q5    18 DT    H2'1   2.640   4.570
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 606, r1= 2.14, r2= 2.64, r3= 5.49, r4= 5.99,
 igr1= 594, 595, 596,
 &end
#
#    18 DT   H6    17 DT    H1'    2.900   3.300
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 556, r1= 2.40, r2= 2.90, r3= 3.30, r4= 3.80,  &end
#
#    18 DT   H6    17 DT    H2'1   4.000   4.500
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 574, r1= 3.50, r2= 4.00, r3= 4.50, r4= 5.00,  &end
#
#    18 DT   H6    17 DT    H2'2   2.500   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 575, r1= 2.00, r2= 2.50, r3= 2.90, r4= 3.40,  &end
#
#    18 DT   H6    17 DT    H6  5.000   5.500
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 559, r1= 4.50, r2= 5.00, r3= 5.50, r4= 6.00,  &end
```

```
#
#    18 DT   H2'2  18 DT    H3'           2.500   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 607, 604, r1= 2.00, r2= 2.50, r3= 2.90, r4= 3.40,  &end
#
#    18 DT   H1'   18 DT    H3' 3.700   4.100
 &rst
  ixpk= 0, nxpk= 0, iat= 588, 604, r1= 3.20, r2= 3.70, r3= 4.10, r4= 4.60,  &end
#
#    18 DT   H1'   18 DT    H2'1   2.800   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 588, 606, r1= 2.30, r2= 2.80, r3= 3.20, r4= 3.70,  &end
#
#    18 DT   H1'   18 DT    H2'2   2.100   2.500
 &rst
  ixpk= 0, nxpk= 0, iat= 588, 607, r1= 1.60, r2= 2.10, r3= 2.50, r4= 3.00,  &end
#
#    18 DT   Q5    17 DT    H3'           2.810   4.960
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 572, r1= 2.31, r2= 2.81, r3= 5.96, r4= 6.46,
 igr1= 594, 595, 596,
 &end
#
#    18 DT   H6    18 DT    H2'1   2.000   2.400
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 606, r1= 1.50, r2= 2.00, r3= 2.40, r4= 2.90,  &end
#
#    18 DT   H6    18 DT    H2'2   3.100   3.600
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 607, r1= 2.60, r2= 3.10, r3= 3.60, r4= 4.10,  &end
#
#    18 DT   H6    18 DT    H1'           3.500   3.900
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 588, r1= 3.00, r2= 3.50, r3= 3.90, r4= 4.40,  &end
#
#    18 DT   H6    18 DT    Q5  2.210   3.270
 &rst
  ixpk= 0, nxpk= 0, iat= 591,  -1, r1= 1.71, r2= 2.21, r3= 3.93, r4= 4.43,
 igr2= 594, 595, 596,
 &end
#
#    19 DA   H1'   19 DA    H2'1   2.800   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 620, 638, r1= 2.30, r2= 2.80, r3= 3.20, r4= 3.70,  &end
#
#    19 DA   H1'   19 DA    H2'2   2.100   2.500
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 620, 639, r1= 1.60, r2= 2.10, r3= 2.50, r4= 3.00,  &end
#
#    19 DA   H8    18 DT    H2'1   4.800   5.200
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 606, r1= 4.30, r2= 4.80, r3= 5.20, r4= 5.70,  &end
#
#    19 DA   H8    18 DT    H2'2   3.000   3.400
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 607, r1= 2.50, r2= 3.00, r3= 3.40, r4= 3.90,  &end
#
#    19 DA   H8    18 DT    H1'            3.800   4.200
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 588, r1= 3.30, r2= 3.80, r3= 4.20, r4= 4.70,  &end
#
#    19 DA   H8    18 DT    H6 6.000   6.600
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 591, r1= 5.50, r2= 6.00, r3= 6.60, r4= 7.10,  &end
#
#    19 DA   H8    19 DA    H3'            4.200   4.600
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 636, r1= 3.70, r2= 4.20, r3= 4.60, r4= 5.10,  &end
#
#    19 DA   H8    19 DA    H2'2   3.500   4.000
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 639, r1= 3.00, r2= 3.50, r3= 4.00, r4= 4.50,  &end
#
#    19 DA   H8    19 DA    H1'            3.700   4.100
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 620, r1= 3.20, r2= 3.70, r3= 4.10, r4= 4.60,  &end
#
#    20 DG3  H2'1  20 DG3   H3'          2.300   2.700
 &rst
  ixpk= 0, nxpk= 0, iat= 671, 669, r1= 1.80, r2= 2.30, r3= 2.70, r4= 3.20,  &end
#
#    20 DG3  H2'2  20 DG3   H3'          2.500   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 672, 669, r1= 2.00, r2= 2.50, r3= 2.90, r4= 3.40,  &end
#
#    20 DG3  H1'   20 DG3   H3'          3.700   4.100
 &rst
  ixpk= 0, nxpk= 0, iat= 652, 669, r1= 3.20, r2= 3.70, r3= 4.10, r4= 4.60,  &end
#
#    20 DG3  H1'   20 DG3   H2'1   2.800   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 652, 671, r1= 2.30, r2= 2.80, r3= 3.20, r4= 3.70,  &end
```

```
#
#    20 DG3  H1'   20 DG3   H2'2   2.100   2.600
 &rst
  ixpk= 0, nxpk= 0, iat= 652, 672, r1= 1.60, r2= 2.10, r3= 2.60, r4= 3.10,  &end
#
#    20 DG3  H8    19 DA    H3'          4.700   5.200
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 636, r1= 4.20, r2= 4.70, r3= 5.20, r4= 5.70,  &end
#
#    20 DG3  H8    19 DA    H2'1   3.500   4.100
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 638, r1= 3.00, r2= 3.50, r3= 4.10, r4= 4.60,  &end
#
#    20 DG3  H8    19 DA    H2'2   2.100   2.500
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 639, r1= 1.60, r2= 2.10, r3= 2.50, r4= 3.00,  &end
#
#    20 DG3  H8    19 DA    H1'          3.000   3.600
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 620, r1= 2.50, r2= 3.00, r3= 3.60, r4= 4.10,  &end
#
#    20 DG3  H8    19 DA    H8           4.800   5.200
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 623, r1= 4.30, r2= 4.80, r3= 5.20, r4= 5.70,  &end
#
#    20 DG3  H8    20 DG3   H3'          4.200   4.600
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 669, r1= 3.70, r2= 4.20, r3= 4.60, r4= 5.10,  &end
#
#    20 DG3  H8    20 DG3   H2'1   2.000   2.500
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 671, r1= 1.50, r2= 2.00, r3= 2.50, r4= 3.00,  &end
# 674 atoms read from pdb file AGA_mod_amber.pdb.
# 2 DT ALPHA:  (1 DC5 O3')-(2 DT P)-(2 DT O5')-(2 DT C5') -90.0 -30.0
 &rst     iat =    28,    29,    32,    33,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
           rk2 =   2.0, rk3 =   2.0,                                    &end

# 3 DA ALPHA:  (2 DT O3')-(3 DA P)-(3 DA O5')-(3 DA C5') -90.0 -30.0
 &rst     iat =    60,    61,    64,    65,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 4 DA ALPHA:  (3 DA O3')-(4 DA P)-(4 DA O5')-(4 DA C5') -90.0 -30.0
 &rst     iat =    92,    93,    96,    97,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
```

```
        &end

# 6 DA ALPHA:  (5 FAG O3')-(6 DA P)-(6 DA O5')-(6 DA C5') -90.0 -30.0
 &rst    iat =   196,   197,   200,   201,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 7 DT ALPHA:  (6 DA O3')-(7 DT P)-(7 DT O5')-(7 DT C5') -90.0 -30.0
 &rst    iat =   228,   229,   232,   233,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 8 DT ALPHA:  (7 DT O3')-(8 DT P)-(8 DT O5')-(8 DT C5') -90.0 -30.0
 &rst    iat =   260,   261,   264,   265,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 9 DC ALPHA:  (8 DT O3')-(9 DC P)-(9 DC O5')-(9 DC C5') -90.0 -30.0
 &rst    iat =   292,   293,   296,   297,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 12 DG ALPHA:  (11 DT5 O3')-(12 DG P)-(12 DG O5')-(12 DG C5') -90.0 -30.0
 &rst    iat =   385,   386,   389,   390,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 13 DA ALPHA:  (12 DG O3')-(13 DA P)-(13 DA O5')-(13 DA C5') -90.0 -30.0
 &rst    iat =   418,   419,   422,   423,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 14 DA ALPHA:  (13 DA O3')-(14 DA P)-(14 DA O5')-(14 DA C5') -90.0 -30.0
 &rst    iat =   450,   451,   454,   455,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 15 DT ALPHA:  (14 DA O3')-(15 DT P)-(15 DT O5')-(15 DT C5') -90.0 -30.0
 &rst    iat =   482,   483,   486,   487,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 17 DT ALPHA:  (16 DC O3')-(17 DT P)-(17 DT O5')-(17 DT C5') -90.0 -30.0
 &rst    iat =   544,   545,   548,   549,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end
```

```
# 18 DT ALPHA:  (17 DT O3')-(18 DT P)-(18 DT O5')-(18 DT C5') -90.0 -30.0
 &rst     iat =   576,   577,   580,   581,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 19 DA ALPHA:  (18 DT O3')-(19 DA P)-(19 DA O5')-(19 DA C5') -90.0 -30.0
 &rst     iat =   608,   609,   612,   613,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 2 DT BETA:  (2 DT P)-(2 DT O5')-(2 DT C5')-(2 DT C4') 150.0 210.0
 &rst     iat =    29,    32,    33,    36,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 3 DA BETA:  (3 DA P)-(3 DA O5')-(3 DA C5')-(3 DA C4') 150.0 210.0
 &rst     iat =    61,    64,    65,    68,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 4 DA BETA:  (4 DA P)-(4 DA O5')-(4 DA C5')-(4 DA C4') 150.0 210.0
 &rst     iat =    93,    96,    97,   100,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 6 DA BETA:  (6 DA P)-(6 DA O5')-(6 DA C5')-(6 DA C4') 150.0 210.0
 &rst     iat =   197,   200,   201,   204,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 7 DT BETA:  (7 DT P)-(7 DT O5')-(7 DT C5')-(7 DT C4') 150.0 210.0
 &rst     iat =   229,   232,   233,   236,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 8 DT BETA:  (8 DT P)-(8 DT O5')-(8 DT C5')-(8 DT C4') 150.0 210.0
 &rst     iat =   261,   264,   265,   268,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 9 DC BETA:  (9 DC P)-(9 DC O5')-(9 DC C5')-(9 DC C4') 150.0 210.0
 &rst     iat =   293,   296,   297,   300,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end
```

```
# 12 DG BETA:  (12 DG P)-(12 DG O5')-(12 DG C5')-(12 DG C4') 150.0 210.0
 &rst     iat =   386,   389,   390,   393,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 13 DA BETA:  (13 DA P)-(13 DA O5')-(13 DA C5')-(13 DA C4') 150.0 210.0
 &rst     iat =   419,   422,   423,   426,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 14 DA BETA:  (14 DA P)-(14 DA O5')-(14 DA C5')-(14 DA C4') 150.0 210.0
 &rst     iat =   451,   454,   455,   458,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 15 DT BETA:  (15 DT P)-(15 DT O5')-(15 DT C5')-(15 DT C4') 150.0 210.0
 &rst     iat =   483,   486,   487,   490,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 17 DT BETA:  (17 DT P)-(17 DT O5')-(17 DT C5')-(17 DT C4') 150.0 210.0
 &rst     iat =   545,   548,   549,   552,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 18 DT BETA:  (18 DT P)-(18 DT O5')-(18 DT C5')-(18 DT C4') 150.0 210.0
 &rst     iat =   577,   580,   581,   584,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 19 DA BETA:  (19 DA P)-(19 DA O5')-(19 DA C5')-(19 DA C4') 150.0 210.0
 &rst     iat =   609,   612,   613,   616,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 2 DT GAMMA:  (2 DT O5')-(2 DT C5')-(2 DT C4')-(2 DT C3')  30.0  90.0
 &rst     iat =    32,    33,    36,    55,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 3 DA GAMMA:  (3 DA O5')-(3 DA C5')-(3 DA C4')-(3 DA C3')  30.0  90.0
 &rst     iat =    64,    65,    68,    87,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 4 DA GAMMA:  (4 DA O5')-(4 DA C5')-(4 DA C4')-(4 DA C3')  30.0  90.0
```

```
 &rst     iat =    96,    97,   100,   119,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 6 DA GAMMA:  (6 DA O5')-(6 DA C5')-(6 DA C4')-(6 DA C3')  30.0  90.0
 &rst     iat =   200,   201,   204,   223,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 7 DT GAMMA:  (7 DT O5')-(7 DT C5')-(7 DT C4')-(7 DT C3')  30.0  90.0
 &rst     iat =   232,   233,   236,   255,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 8 DT GAMMA:  (8 DT O5')-(8 DT C5')-(8 DT C4')-(8 DT C3')  30.0  90.0
 &rst     iat =   264,   265,   268,   287,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 9 DC GAMMA:  (9 DC O5')-(9 DC C5')-(9 DC C4')-(9 DC C3')  30.0  90.0
 &rst     iat =   296,   297,   300,   317,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 12 DG GAMMA:  (12 DG O5')-(12 DG C5')-(12 DG C4')-(12 DG C3')  30.0  90.0
 &rst     iat =   389,   390,   393,   413,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 13 DA GAMMA:  (13 DA O5')-(13 DA C5')-(13 DA C4')-(13 DA C3')  30.0  90.0
 &rst     iat =   422,   423,   426,   445,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 14 DA GAMMA:  (14 DA O5')-(14 DA C5')-(14 DA C4')-(14 DA C3')  30.0  90.0
 &rst     iat =   454,   455,   458,   477,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 15 DT GAMMA:  (15 DT O5')-(15 DT C5')-(15 DT C4')-(15 DT C3')  30.0  90.0
 &rst     iat =   486,   487,   490,   509,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 17 DT GAMMA:  (17 DT O5')-(17 DT C5')-(17 DT C4')-(17 DT C3')  30.0  90.0
 &rst     iat =   548,   549,   552,   571,
```

```
  r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
 &end

# 18 DT GAMMA:  (18 DT O5')-(18 DT C5')-(18 DT C4')-(18 DT C3')  30.0  90.0
 &rst    iat =   580,   581,   584,   603,
  r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
 &end

# 19 DA GAMMA:  (19 DA O5')-(19 DA C5')-(19 DA C4')-(19 DA C3')  30.0  90.0
 &rst    iat =   612,   613,   616,   635,
  r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
 &end

# 2 DT EPSILN:  (2 DT C4')-(2 DT C3')-(2 DT O3')-(3 DA P) 165.0 225.0
 &rst    iat =    36,    55,    60,    61,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 3 DA EPSILN:  (3 DA C4')-(3 DA C3')-(3 DA O3')-(4 DA P) 165.0 225.0
 &rst    iat =    68,    87,    92,    93,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 4 DA EPSILN:  (4 DA C4')-(4 DA C3')-(4 DA O3')-(5 FAG P) 165.0 225.0
 &rst    iat =   100,   119,   124,   125,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 6 DA EPSILN:  (6 DA C4')-(6 DA C3')-(6 DA O3')-(7 DT P) 165.0 225.0
 &rst    iat =   204,   223,   228,   229,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 7 DT EPSILN:  (7 DT C4')-(7 DT C3')-(7 DT O3')-(8 DT P) 165.0 225.0
 &rst    iat =   236,   255,   260,   261,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 8 DT EPSILN:  (8 DT C4')-(8 DT C3')-(8 DT O3')-(9 DC P) 165.0 225.0
 &rst    iat =   268,   287,   292,   293,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 9 DC EPSILN:  (9 DC C4')-(9 DC C3')-(9 DC O3')-(10 DA3 P) 165.0 225.0
 &rst    iat =   300,   317,   322,   323,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
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```
        &end

# 12 DG EPSILN:  (12 DG C4')-(12 DG C3')-(12 DG O3')-(13 DA P) 165.0 225.0
 &rst    iat =   393,   413,   418,   419,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
        &end

# 13 DA EPSILN:  (13 DA C4')-(13 DA C3')-(13 DA O3')-(14 DA P) 165.0 225.0
 &rst    iat =   426,   445,   450,   451,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
        &end

# 14 DA EPSILN:  (14 DA C4')-(14 DA C3')-(14 DA O3')-(15 DT P) 165.0 225.0
 &rst    iat =   458,   477,   482,   483,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
        &end

# 15 DT EPSILN:  (15 DT C4')-(15 DT C3')-(15 DT O3')-(16 DC P) 165.0 225.0
 &rst    iat =   490,   509,   514,   515,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
        &end

# 17 DT EPSILN:  (17 DT C4')-(17 DT C3')-(17 DT O3')-(18 DT P) 165.0 225.0
 &rst    iat =   552,   571,   576,   577,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
        &end

# 18 DT EPSILN:  (18 DT C4')-(18 DT C3')-(18 DT O3')-(19 DA P) 165.0 225.0
 &rst    iat =   584,   603,   608,   609,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
        &end

# 19 DA EPSILN:  (19 DA C4')-(19 DA C3')-(19 DA O3')-(20 DG3 P) 165.0 225.0
 &rst    iat =   616,   635,   640,   641,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
        &end

# 2 DT ZETA:  (2 DT C3')-(2 DT O3')-(3 DA P)-(3 DA O5') -135.0 -75.0
 &rst    iat =    55,    60,    61,    64,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end

# 3 DA ZETA:  (3 DA C3')-(3 DA O3')-(4 DA P)-(4 DA O5') -135.0 -75.0
 &rst    iat =    87,    92,    93,    96,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end
```

```
# 4 DA ZETA:  (4 DA C3')-(4 DA O3')-(5 FAG P)-(5 FAG O5') -135.0 -75.0
 &rst    iat =   119,   124,   125,   128,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 6 DA ZETA:  (6 DA C3')-(6 DA O3')-(7 DT P)-(7 DT O5') -135.0 -75.0
 &rst    iat =   223,   228,   229,   232,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 7 DT ZETA:  (7 DT C3')-(7 DT O3')-(8 DT P)-(8 DT O5') -135.0 -75.0
 &rst    iat =   255,   260,   261,   264,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 8 DT ZETA:  (8 DT C3')-(8 DT O3')-(9 DC P)-(9 DC O5') -135.0 -75.0
 &rst    iat =   287,   292,   293,   296,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 9 DC ZETA:  (9 DC C3')-(9 DC O3')-(10 DA3 P)-(10 DA3 O5') -135.0 -75.0
 &rst    iat =   317,   322,   323,   326,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 12 DG ZETA:  (12 DG C3')-(12 DG O3')-(13 DA P)-(13 DA O5') -135.0 -75.0
 &rst    iat =   413,   418,   419,   422,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 13 DA ZETA:  (13 DA C3')-(13 DA O3')-(14 DA P)-(14 DA O5') -135.0 -75.0
 &rst    iat =   445,   450,   451,   454,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 14 DA ZETA:  (14 DA C3')-(14 DA O3')-(15 DT P)-(15 DT O5') -135.0 -75.0
 &rst    iat =   477,   482,   483,   486,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 15 DT ZETA:  (15 DT C3')-(15 DT O3')-(16 DC P)-(16 DC O5') -135.0 -75.0
 &rst    iat =   509,   514,   515,   518,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end
```

```
# 17 DT ZETA:  (17 DT C3')-(17 DT O3')-(18 DT P)-(18 DT O5') -135.0 -75.0
 &rst     iat =   571,   576,   577,   580,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
          &end

# 18 DT ZETA:  (18 DT C3')-(18 DT O3')-(19 DA P)-(19 DA O5') -135.0 -75.0
 &rst     iat =   603,   608,   609,   612,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
          &end

# 19 DA ZETA:  (19 DA C3')-(19 DA O3')-(20 DG3 P)-(20 DG3 O5') -135.0 -75.0
 &rst     iat =   635,   640,   641,   644,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
          &end

#
# 1  DC5  H42          20  DG3  O6    1.80    2.00
 &rst
  ixpk= 0, nxpk= 0, iat=  19, 659, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,
     rk2=20.0, rk3=20.0, ir6=1, ialtd=0,
 &end
#
# 1  DC5  N3 20  DG3  H1    1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  20, 661, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 1  DC5  N3 20  DG3  N1    2.85    3.05
 &rst
  ixpk= 0, nxpk= 0, iat=  20, 660, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
# 1  DC5  N4 20  DG3  O6    2.81    3.01
 &rst
  ixpk= 0, nxpk= 0, iat=  17, 659, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
# 1  DC5  O2 20  DG3  H22   1.75    1.95
 &rst
  ixpk= 0, nxpk= 0, iat=  22, 665, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
# 2  DT   H3   19  DA   N1     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat=  52, 630, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 2  DT   N3   19  DA   N1     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat=  51, 630, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
```

```
# 2 DT   O4   19 DA   H61   1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  50, 628, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 3 DA   H61 18 DT   O4     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  80, 598, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 3 DA   N1   18 DT   H3     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat=  82, 600, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 3 DA   N1   18 DT   N3     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat=  82, 599, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 4 DA   H61 17 DT   O4     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 112, 566, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 4 DA   N1   17 DT   H3     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 114, 568, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 4 DA   N1   17 DT   N3     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 114, 567, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 5 FAG  H1 16 DC   N3     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 146, 536, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 5 FAG  H22          16 DC   O2     1.75    1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 144, 538, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
# 5 FAG  N1 16 DC   N3     2.85    3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 145, 536, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
# 5 FAG  O6 16 DC   H42    1.80    2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 148, 535, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
# 5 FAG  O6 16 DC   N4     2.81    3.01
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 148, 533, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
# 7 DT   H3   14 DA   N1     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 252, 472, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 7 DT   N3   14 DA   N1     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 251, 472, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 7 DT   O4   14 DA   H61    1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 250, 470, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 8 DT   H3   13 DA   N1     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 284, 440, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 8 DT   N3   13 DA   N1     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 283, 440, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 8 DT   O4   13 DA   H61    1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 282, 438, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 9 DC   H42 12 DG   O6     1.80    2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 313, 404, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
# 9 DC   N3   12 DG   H1     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 314, 406, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 9 DC   N3   12 DG   N1     2.85    3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 314, 405, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
# 9 DC   N4   12 DG   O6     2.81    3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 311, 404, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
# 9 DC   O2   12 DG   H22    1.75    1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 316, 410, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
```

```
#  10 DA3  H61          11  DT5  O4     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 342, 375, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#  10 DA3  N1 11  DT5  H3     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 344, 377, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
#  10 DA3  N1 11  DT5  N3     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 344, 376, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
# 674 atoms read from pdb file AGA_mod_amber.pdb.
# 2 DT NU0:  (2 DT C4')-(2 DT O4')-(2 DT C1')-(2 DT C2') -52.1 -22.1
 &rst     iat =    36,    38,    39,    57,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
           rk2 =   2.0, rk3 =   2.0,                                  &end

# 2 DT NU1:  (2 DT O4')-(2 DT C1')-(2 DT C2')-(2 DT C3')  15.0  45.0
 &rst     iat =    38,    39,    57,    55,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
          &end

# 2 DT NU2:  (2 DT C1')-(2 DT C2')-(2 DT C3')-(2 DT C4') -27.4   2.6
 &rst     iat =    39,    57,    55,    36,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
          &end

# 2 DT NU3:  (2 DT C2')-(2 DT C3')-(2 DT C4')-(2 DT O4') -25.0   5.0
 &rst     iat =    57,    55,    36,    38,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
          &end

# 2 DT NU4:  (2 DT C3')-(2 DT C4')-(2 DT O4')-(2 DT C1')  13.5  43.5
 &rst     iat =    55,    36,    38,    39,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
          &end

# 3 DA NU0:  (3 DA C4')-(3 DA O4')-(3 DA C1')-(3 DA C2') -43.9 -13.9
 &rst     iat =    68,    70,    71,    89,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
          &end

# 3 DA NU1:  (3 DA O4')-(3 DA C1')-(3 DA C2')-(3 DA C3')  22.2  52.2
 &rst     iat =    70,    71,    89,    87,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
          &end
```

```
# 3 DA NU2:  (3 DA C1')-(3 DA C2')-(3 DA C3')-(3 DA C4') -44.6 -14.6
 &rst     iat =    71,    89,    87,    68,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
         &end

# 3 DA NU3:  (3 DA C2')-(3 DA C3')-(3 DA C4')-(3 DA O4')  -3.2  26.8
 &rst     iat =    89,    87,    68,    70,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
         &end

# 3 DA NU4:  (3 DA C3')-(3 DA C4')-(3 DA O4')-(3 DA C1')  -4.4  25.6
 &rst     iat =    87,    68,    70,    71,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
         &end

# 4 DA NU0:  (4 DA C4')-(4 DA O4')-(4 DA C1')-(4 DA C2') -43.9 -13.9
 &rst     iat =   100,   102,   103,   121,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
         &end

# 4 DA NU1:  (4 DA O4')-(4 DA C1')-(4 DA C2')-(4 DA C3')  22.2  52.2
 &rst     iat =   102,   103,   121,   119,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
         &end

# 4 DA NU2:  (4 DA C1')-(4 DA C2')-(4 DA C3')-(4 DA C4') -44.6 -14.6
 &rst     iat =   103,   121,   119,   100,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
         &end

# 4 DA NU3:  (4 DA C2')-(4 DA C3')-(4 DA C4')-(4 DA O4')  -3.2  26.8
 &rst     iat =   121,   119,   100,   102,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
         &end

# 4 DA NU4:  (4 DA C3')-(4 DA C4')-(4 DA O4')-(4 DA C1')  -4.4  25.6
 &rst     iat =   119,   100,   102,   103,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
         &end

# 6 DA NU0:  (6 DA C4')-(6 DA O4')-(6 DA C1')-(6 DA C2') -43.9 -13.9
 &rst     iat =   204,   206,   207,   225,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
         &end
```

```
# 6 DA NU1:  (6 DA O4')-(6 DA C1')-(6 DA C2')-(6 DA C3')  22.2  52.2
 &rst     iat =   206,   207,   225,   223,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
         &end

# 6 DA NU2:  (6 DA C1')-(6 DA C2')-(6 DA C3')-(6 DA C4') -44.6 -14.6
 &rst     iat =   207,   225,   223,   204,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
         &end

# 6 DA NU3:  (6 DA C2')-(6 DA C3')-(6 DA C4')-(6 DA O4')  -3.2  26.8
 &rst     iat =   225,   223,   204,   206,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
         &end

# 6 DA NU4:  (6 DA C3')-(6 DA C4')-(6 DA O4')-(6 DA C1')  -4.4  25.6
 &rst     iat =   223,   204,   206,   207,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
         &end

# 7 DT NU0:  (7 DT C4')-(7 DT O4')-(7 DT C1')-(7 DT C2') -52.1 -22.1
 &rst     iat =   236,   238,   239,   257,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
         &end

# 7 DT NU1:  (7 DT O4')-(7 DT C1')-(7 DT C2')-(7 DT C3')  15.0  45.0
 &rst     iat =   238,   239,   257,   255,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 7 DT NU2:  (7 DT C1')-(7 DT C2')-(7 DT C3')-(7 DT C4') -27.4   2.6
 &rst     iat =   239,   257,   255,   236,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 7 DT NU3:  (7 DT C2')-(7 DT C3')-(7 DT C4')-(7 DT O4') -25.0   5.0
 &rst     iat =   257,   255,   236,   238,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 7 DT NU4:  (7 DT C3')-(7 DT C4')-(7 DT O4')-(7 DT C1')  13.5  43.5
 &rst     iat =   255,   236,   238,   239,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end

# 8 DT NU0:  (8 DT C4')-(8 DT O4')-(8 DT C1')-(8 DT C2') -52.1 -22.1
```

```
 &rst     iat =   268,   270,   271,   289,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
          &end

# 8 DT NU1:  (8 DT O4')-(8 DT C1')-(8 DT C2')-(8 DT C3')  15.0  45.0
 &rst     iat =   270,   271,   289,   287,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
          &end

# 8 DT NU2:  (8 DT C1')-(8 DT C2')-(8 DT C3')-(8 DT C4') -27.4   2.6
 &rst     iat =   271,   289,   287,   268,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
          &end

# 8 DT NU3:  (8 DT C2')-(8 DT C3')-(8 DT C4')-(8 DT O4') -25.0   5.0
 &rst     iat =   289,   287,   268,   270,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
          &end

# 8 DT NU4:  (8 DT C3')-(8 DT C4')-(8 DT O4')-(8 DT C1')  13.5  43.5
 &rst     iat =   287,   268,   270,   271,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
          &end

# 9 DC NU0:  (9 DC C4')-(9 DC O4')-(9 DC C1')-(9 DC C2') -44.7 -14.7
 &rst     iat =   300,   302,   303,   319,
           r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
          &end

# 9 DC NU1:  (9 DC O4')-(9 DC C1')-(9 DC C2')-(9 DC C3')  18.1  48.1
 &rst     iat =   302,   303,   319,   317,
           r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
          &end

# 9 DC NU2:  (9 DC C1')-(9 DC C2')-(9 DC C3')-(9 DC C4') -37.2  -6.7
 &rst     iat =   303,   319,   317,   300,
           r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
          &end

# 9 DC NU3:  (9 DC C2')-(9 DC C3')-(9 DC C4')-(9 DC O4') -16.9  24.2
 &rst     iat =   319,   317,   300,   302,
           r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
          &end

# 9 DC NU4:  (9 DC C3')-(9 DC C4')-(9 DC O4')-(9 DC C1')  -1.9  34.0
 &rst     iat =   317,   300,   302,   303,
```

```
  r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
 &end

# 12 DG NU0:  (12 DG C4')-(12 DG O4')-(12 DG C1')-(12 DG C2') -44.7 -14.7
 &rst    iat =   393,   395,   396,   415,
  r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
 &end

# 12 DG NU1:  (12 DG O4')-(12 DG C1')-(12 DG C2')-(12 DG C3')  18.1  48.1
 &rst    iat =   395,   396,   415,   413,
  r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
 &end

# 12 DG NU2:  (12 DG C1')-(12 DG C2')-(12 DG C3')-(12 DG C4') -37.2  -6.7
 &rst    iat =   396,   415,   413,   393,
  r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
 &end

# 12 DG NU3:  (12 DG C2')-(12 DG C3')-(12 DG C4')-(12 DG O4') -16.9  24.2
 &rst    iat =   415,   413,   393,   395,
  r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
 &end

# 12 DG NU4:  (12 DG C3')-(12 DG C4')-(12 DG O4')-(12 DG C1')  -1.9  34.0
 &rst    iat =   413,   393,   395,   396,
  r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
 &end

# 13 DA NU0:  (13 DA C4')-(13 DA O4')-(13 DA C1')-(13 DA C2') -43.9 -13.9
 &rst    iat =   426,   428,   429,   447,
  r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
 &end

# 13 DA NU1:  (13 DA O4')-(13 DA C1')-(13 DA C2')-(13 DA C3')  22.2  52.2
 &rst    iat =   428,   429,   447,   445,
  r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
 &end

# 13 DA NU2:  (13 DA C1')-(13 DA C2')-(13 DA C3')-(13 DA C4') -44.6 -14.6
 &rst    iat =   429,   447,   445,   426,
  r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
 &end

# 13 DA NU3:  (13 DA C2')-(13 DA C3')-(13 DA C4')-(13 DA O4')  -3.2  26.8
 &rst    iat =   447,   445,   426,   428,
  r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
```

```
        &end

# 13 DA NU4:  (13 DA C3')-(13 DA C4')-(13 DA O4')-(13 DA C1')  -4.4  25.6
 &rst    iat =   445,   426,   428,   429,
          r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
        &end

# 14 DA NU0:  (14 DA C4')-(14 DA O4')-(14 DA C1')-(14 DA C2') -43.9 -13.9
 &rst    iat =   458,   460,   461,   479,
          r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
        &end

# 14 DA NU1:  (14 DA O4')-(14 DA C1')-(14 DA C2')-(14 DA C3')  22.2  52.2
 &rst    iat =   460,   461,   479,   477,
          r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
        &end

# 14 DA NU2:  (14 DA C1')-(14 DA C2')-(14 DA C3')-(14 DA C4') -44.6 -14.6
 &rst    iat =   461,   479,   477,   458,
          r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
        &end

# 14 DA NU3:  (14 DA C2')-(14 DA C3')-(14 DA C4')-(14 DA O4')  -3.2  26.8
 &rst    iat =   479,   477,   458,   460,
          r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
        &end

# 14 DA NU4:  (14 DA C3')-(14 DA C4')-(14 DA O4')-(14 DA C1')  -4.4  25.6
 &rst    iat =   477,   458,   460,   461,
          r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
        &end

# 15 DT NU0:  (15 DT C4')-(15 DT O4')-(15 DT C1')-(15 DT C2') -52.1 -22.1
 &rst    iat =   490,   492,   493,   511,
          r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
        &end

# 15 DT NU1:  (15 DT O4')-(15 DT C1')-(15 DT C2')-(15 DT C3')  15.0  45.0
 &rst    iat =   492,   493,   511,   509,
          r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
        &end

# 15 DT NU2:  (15 DT C1')-(15 DT C2')-(15 DT C3')-(15 DT C4') -27.4   2.6
 &rst    iat =   493,   511,   509,   490,
          r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
        &end
```

```
# 15 DT NU3:  (15 DT C2')-(15 DT C3')-(15 DT C4')-(15 DT O4') -25.0   5.0
 &rst     iat =   511,   509,   490,   492,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 15 DT NU4:  (15 DT C3')-(15 DT C4')-(15 DT O4')-(15 DT C1')  13.5  43.5
 &rst     iat =   509,   490,   492,   493,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end

# 17 DT NU0:  (17 DT C4')-(17 DT O4')-(17 DT C1')-(17 DT C2') -52.1 -22.1
 &rst     iat =   552,   554,   555,   573,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
         &end

# 17 DT NU1:  (17 DT O4')-(17 DT C1')-(17 DT C2')-(17 DT C3')  15.0  45.0
 &rst     iat =   554,   555,   573,   571,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 17 DT NU2:  (17 DT C1')-(17 DT C2')-(17 DT C3')-(17 DT C4') -27.4   2.6
 &rst     iat =   555,   573,   571,   552,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 17 DT NU3:  (17 DT C2')-(17 DT C3')-(17 DT C4')-(17 DT O4') -25.0   5.0
 &rst     iat =   573,   571,   552,   554,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 17 DT NU4:  (17 DT C3')-(17 DT C4')-(17 DT O4')-(17 DT C1')  13.5  43.5
 &rst     iat =   571,   552,   554,   555,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end

# 18 DT NU0:  (18 DT C4')-(18 DT O4')-(18 DT C1')-(18 DT C2') -52.1 -22.1
 &rst     iat =   584,   586,   587,   605,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
         &end

# 18 DT NU1:  (18 DT O4')-(18 DT C1')-(18 DT C2')-(18 DT C3')  15.0  45.0
 &rst     iat =   586,   587,   605,   603,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end
```

```
# 18 DT NU2:  (18 DT C1')-(18 DT C2')-(18 DT C3')-(18 DT C4') -27.4   2.6
 &rst     iat =   587,   605,   603,   584,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 18 DT NU3:  (18 DT C2')-(18 DT C3')-(18 DT C4')-(18 DT O4') -25.0   5.0
 &rst     iat =   605,   603,   584,   586,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 18 DT NU4:  (18 DT C3')-(18 DT C4')-(18 DT O4')-(18 DT C1')  13.5  43.5
 &rst     iat =   603,   584,   586,   587,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end

# 19 DA NU0:  (19 DA C4')-(19 DA O4')-(19 DA C1')-(19 DA C2') -43.9 -13.9
 &rst     iat =   616,   618,   619,   637,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
         &end

# 19 DA NU1:  (19 DA O4')-(19 DA C1')-(19 DA C2')-(19 DA C3')  22.2  52.2
 &rst     iat =   618,   619,   637,   635,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
         &end

# 19 DA NU2:  (19 DA C1')-(19 DA C2')-(19 DA C3')-(19 DA C4') -44.6 -14.6
 &rst     iat =   619,   637,   635,   616,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
         &end

# 19 DA NU3:  (19 DA C2')-(19 DA C3')-(19 DA C4')-(19 DA O4')  -3.2  26.8
 &rst     iat =   637,   635,   616,   618,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
         &end

# 19 DA NU4:  (19 DA C3')-(19 DA C4')-(19 DA O4')-(19 DA C1')  -4.4  25.6
 &rst     iat =   635,   616,   618,   619,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
         &end
```

Table C-6. Experimental distance and torsion angle restraints used in the rMD calculations of the AFB1-β-FAPY modified AXT adduct.

```
#
#   1 DC5   H2'1  1 DC5 H3'     1.660   2.380
 &rst
  ixpk= 0, nxpk= 0, iat=  26,  24, r1= 1.16, r2= 1.66, r3= 2.38, r4= 2.88,
     rk2=32.0, rk3=32.0, ir6=1, ialtd=0,
 &end
#
#   1 DC5   H2'2  1 DC5 H3'     2.090   2.850
 &rst
  ixpk= 0, nxpk= 0, iat=  27,  24, r1= 1.59, r2= 2.09, r3= 2.85, r4= 3.35,  &end
#
#   1 DC5   H1'   1 DC5 H3'     2.990   3.870
 &rst
  ixpk= 0, nxpk= 0, iat=  10,  24, r1= 2.49, r2= 2.99, r3= 3.87, r4= 4.37,  &end
#
#   1 DC5   H1'   1 DC5 H2'1    2.440   3.030
 &rst
  ixpk= 0, nxpk= 0, iat=  10,  26, r1= 1.94, r2= 2.44, r3= 3.03, r4= 3.53,  &end
#
#   1 DC5   H5    1 DC5 H3'     6.190   6.590
 &rst
  ixpk= 0, nxpk= 0, iat=  15,  24, r1= 5.69, r2= 6.19, r3= 6.59, r4= 7.09,  &end
#
#   1 DC5   H5    1 DC5 H2'1    4.060   4.500
 &rst
  ixpk= 0, nxpk= 0, iat=  15,  26, r1= 3.56, r2= 4.06, r3= 4.50, r4= 5.00,  &end
#
#   1 DC5   H5    1 DC5 H2'2    5.260   5.700
 &rst
  ixpk= 0, nxpk= 0, iat=  15,  27, r1= 4.76, r2= 5.26, r3= 5.70, r4= 6.20,  &end
#
#   1 DC5   H6    1 DC5 H3'     3.440   4.280
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  24, r1= 2.94, r2= 3.44, r3= 4.28, r4= 4.78,  &end
#
#   1 DC5   H6    1 DC5 H2'1    1.670   2.340
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  26, r1= 1.17, r2= 1.67, r3= 2.34, r4= 2.84,  &end
#
#   1 DC5   H6    1 DC5 H2'2    3.160   3.820
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  27, r1= 2.66, r2= 3.16, r3= 3.82, r4= 4.32,  &end
#
#   1 DC5   H6    1 DC5 H1'     3.160   3.790
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  10, r1= 2.66, r2= 3.16, r3= 3.79, r4= 4.29,  &end
#
#   2 DT    H3   20 DG3 H1      3.100   3.510
 &rst
  ixpk= 0, nxpk= 0, iat=  52, 661, r1= 2.60, r2= 3.10, r3= 3.51, r4= 4.01,  &end
#
#   2 DT    Q5    1 DC5 H2'1    2.500   3.510
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  26, r1= 2.00, r2= 2.50, r3= 4.22, r4= 4.72,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H2'2    2.610   3.590
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  27, r1= 2.11, r2= 2.61, r3= 4.31, r4= 4.81,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H1'     2.960   4.530
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  10, r1= 2.46, r2= 2.96, r3= 5.44, r4= 5.94,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H5      1.570   2.930
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  15, r1= 1.07, r2= 1.57, r3= 3.52, r4= 4.02,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H6      2.010   3.060
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  13, r1= 1.51, r2= 2.01, r3= 3.67, r4= 4.17,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    H6    1 DC5 H1'     3.980   4.180
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  10, r1= 3.48, r2= 3.98, r3= 4.18, r4= 4.68,  &end
#
#   2 DT    H6    1 DC5 H2'2    2.500   2.710
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  27, r1= 2.00, r2= 2.50, r3= 2.71, r4= 3.21,  &end
#
#   2 DT    H6    1 DC5 H2'1    3.810   4.290
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  26, r1= 3.31, r2= 3.81, r3= 4.29, r4= 4.79,  &end
#
#   2 DT    H6    1 DC5 H3'     4.980   5.280
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  24, r1= 4.48, r2= 4.98, r3= 5.28, r4= 5.78,  &end
#
#   2 DT    H6    1 DC5 H6      5.000   5.320
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  13, r1= 4.50, r2= 5.00, r3= 5.32, r4= 5.82,  &end
#
#   2 DT    Q5    2 DT  H3'     3.250   6.510
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  56, r1= 2.75, r2= 3.25, r3= 7.82, r4= 8.32,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    2 DT  H1'     3.800   5.670
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  40, r1= 3.30, r2= 3.80, r3= 6.81, r4= 7.31,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    H2'2  2 DT  H3'     2.290   2.950
 &rst
  ixpk= 0, nxpk= 0, iat=  59,  56, r1= 1.79, r2= 2.29, r3= 2.95, r4= 3.45,  &end
#
#   2 DT    H1'   2 DT  H3'     3.590   4.010
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  56, r1= 3.09, r2= 3.59, r3= 4.01, r4= 4.51,  &end
#
#   2 DT    H1'   2 DT  H2'1    2.510   3.080
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  58, r1= 2.01, r2= 2.51, r3= 3.08, r4= 3.58,  &end
#
#   2 DT    H1'   2 DT  H2'2    1.870   2.490
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  59, r1= 1.37, r2= 1.87, r3= 2.49, r4= 2.99,  &end
#
#   2 DT    H6    2 DT  H1'     3.540   3.960
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  40, r1= 3.04, r2= 3.54, r3= 3.96, r4= 4.46,  &end
```

```
#
#   3 DA    H61   2 DT  H3      3.570   3.720
 &rst
  ixpk= 0, nxpk= 0, iat=  80,  52, r1= 3.07, r2= 3.57, r3= 3.72, r4= 4.22,  &end
#
#   3 DA    H62   2 DT  H3      4.270   4.520
 &rst
  ixpk= 0, nxpk= 0, iat=  81,  52, r1= 3.77, r2= 4.27, r3= 4.52, r4= 5.02,  &end
#
#   3 DA    H2    2 DT  H3      3.770   4.220
 &rst
  ixpk= 0, nxpk= 0, iat=  84,  52, r1= 3.27, r2= 3.77, r3= 4.22, r4= 4.72,  &end
#
#   3 DA    H61  18 DT  H3      2.370   2.620
 &rst
  ixpk= 0, nxpk= 0, iat=  80, 600, r1= 1.87, r2= 2.37, r3= 2.62, r4= 3.12,  &end
#
#   3 DA    H62  18 DT  H3      3.770   4.120
 &rst
  ixpk= 0, nxpk= 0, iat=  81, 600, r1= 3.27, r2= 3.77, r3= 4.12, r4= 4.62,  &end
#
#   3 DA    H2   19 DA  H2      2.570   3.020
 &rst
  ixpk= 0, nxpk= 0, iat=  84, 632, r1= 2.07, r2= 2.57, r3= 3.02, r4= 3.52,  &end
#
#   3 DA    H8    2 DT  H3'     4.970   5.220
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  56, r1= 4.47, r2= 4.97, r3= 5.22, r4= 5.72,  &end
#
#   3 DA    H8    2 DT  H2'1    4.400   4.660
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  58, r1= 3.90, r2= 4.40, r3= 4.66, r4= 5.16,  &end
#
#   3 DA    H8    2 DT  H2'2    2.650   3.060
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  59, r1= 2.15, r2= 2.65, r3= 3.06, r4= 3.56,  &end
#
#   3 DA    H8    2 DT  H1'     3.640   3.950
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  40, r1= 3.14, r2= 3.64, r3= 3.95, r4= 4.45,  &end
#
#   3 DA    H1'   3 DA  H2'2    2.260   2.960
 &rst
  ixpk= 0, nxpk= 0, iat=  72,  91, r1= 1.76, r2= 2.26, r3= 2.96, r4= 3.46,  &end
#
#   3 DA    H1'   3 DA  H2'1    3.070   3.850
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  72,  90, r1= 2.57, r2= 3.07, r3= 3.85, r4= 4.35,  &end
#
#   3 DA    H8    3 DA  H1'     3.710   4.120
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  72, r1= 3.21, r2= 3.71, r3= 4.12, r4= 4.62,  &end
#
#   3 DA    H8    3 DA  H2'2    3.310   4.320
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  91, r1= 2.81, r2= 3.31, r3= 4.32, r4= 4.82,  &end
#
#   4 DA    H2    3 DA  H2      4.470   4.820
 &rst
  ixpk= 0, nxpk= 0, iat= 116,  84, r1= 3.97, r2= 4.47, r3= 4.82, r4= 5.32,  &end
#
#   4 DA    H2   18 DT  H3      4.270   4.420
 &rst
  ixpk= 0, nxpk= 0, iat= 116, 600, r1= 3.77, r2= 4.27, r3= 4.42, r4= 4.92,  &end
#
#   4 DA    H61  18 DT  H3      4.870   5.120
 &rst
  ixpk= 0, nxpk= 0, iat= 112, 600, r1= 4.37, r2= 4.87, r3= 5.12, r4= 5.62,  &end
#
#   4 DA    H62  18 DT  H3      5.770   6.120
 &rst
  ixpk= 0, nxpk= 0, iat= 113, 600, r1= 5.27, r2= 5.77, r3= 6.12, r4= 6.62,  &end
#
#   4 DA    H2   17 DT  H3      2.370   2.620
 &rst
  ixpk= 0, nxpk= 0, iat= 116, 568, r1= 1.87, r2= 2.37, r3= 2.62, r4= 3.12,  &end
#
#   4 DA    H61  17 DT  H3      2.770   3.020
 &rst
  ixpk= 0, nxpk= 0, iat= 112, 568, r1= 2.27, r2= 2.77, r3= 3.02, r4= 3.52,  &end
#
#   4 DA    H62  17 DT  H3      4.170   4.620
 &rst
  ixpk= 0, nxpk= 0, iat= 113, 568, r1= 3.67, r2= 4.17, r3= 4.62, r4= 5.12,  &end
#
#   4 DA    H1'   3 DA  H1'     5.410   5.610
 &rst
  ixpk= 0, nxpk= 0, iat= 104,  72, r1= 4.91, r2= 5.41, r3= 5.61, r4= 6.11,  &end
#
#   4 DA    H8    3 DA  H2'1    3.820   4.010
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  90, r1= 3.32, r2= 3.82, r3= 4.01, r4= 4.51,  &end
```

```
#
#   4 DA    H8    3 DA  H2'2    2.420   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  91, r1= 1.92, r2= 2.42, r3= 2.61, r4= 3.11,  &end
#
#   4 DA    H8    3 DA  H1'     3.860   4.060
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  72, r1= 3.36, r2= 3.86, r3= 4.06, r4= 4.56,  &end
#
#   4 DA    H8    3 DA  H8      4.670   4.980
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  75, r1= 4.17, r2= 4.67, r3= 4.98, r4= 5.48,  &end
#
#   4 DA    H1'   4 DA  H3'     3.580   4.240
 &rst
  ixpk= 0, nxpk= 0, iat= 104, 120, r1= 3.08, r2= 3.58, r3= 4.24, r4= 4.74,  &end
#
#   4 DA    H1'   4 DA  H2'1    2.700   3.090
 &rst
  ixpk= 0, nxpk= 0, iat= 104, 122, r1= 2.20, r2= 2.70, r3= 3.09, r4= 3.59,  &end
#
#   4 DA    H1'   4 DA  H2'2    2.040   2.500
 &rst
  ixpk= 0, nxpk= 0, iat= 104, 123, r1= 1.54, r2= 2.04, r3= 2.50, r4= 3.00,  &end
#
#   4 DA    H8    4 DA  H2'1    1.800   2.290
 &rst
  ixpk= 0, nxpk= 0, iat= 107, 122, r1= 1.30, r2= 1.80, r3= 2.29, r4= 2.79,  &end
#
#   4 DA    H8    4 DA  H2'2    3.340   3.500
 &rst
  ixpk= 0, nxpk= 0, iat= 107, 123, r1= 2.84, r2= 3.34, r3= 3.50, r4= 4.00,  &end
#
#   4 DA    H8    4 DA  H1'     3.160   3.740
 &rst
  ixpk= 0, nxpk= 0, iat= 107, 104, r1= 2.66, r2= 3.16, r3= 3.74, r4= 4.24,  &end
#
#   5 FAG   H9A   4 DA  H8      3.150   3.670
 &rst
  ixpk= 0, nxpk= 0, iat= 161, 107, r1= 2.65, r2= 3.15, r3= 3.67, r4= 4.17,  &end
#
#   5 FAG   H6A   4 DA  H3'     4.070   4.620
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 120, r1= 3.57, r2= 4.07, r3= 4.62, r4= 5.12,  &end
#
#   5 FAG   H6A   4 DA  H2'1    2.370   3.840
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 122, r1= 1.87, r2= 2.37, r3= 3.84, r4= 4.34,  &end
#
#   5 FAG   H6A   4 DA  H2'2    1.870   2.240
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 123, r1= 1.37, r2= 1.87, r3= 2.24, r4= 2.74,  &end
#
#   5 FAG   H6A   4 DA  H1'     2.340   3.160
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 104, r1= 1.84, r2= 2.34, r3= 3.16, r4= 3.66,  &end
#
#   5 FAG   H6A   4 DA  H8      2.310   2.890
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 107, r1= 1.81, r2= 2.31, r3= 2.89, r4= 3.39,  &end
#
#   5 FAG   H5    4 DA  H2'1    5.450   5.860
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 122, r1= 4.95, r2= 5.45, r3= 5.86, r4= 6.36,  &end
#
#   5 FAG   H5    4 DA  H2'2    4.420   4.830
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 123, r1= 3.92, r2= 4.42, r3= 4.83, r4= 5.33,  &end
#
#   5 FAG   H5    4 DA  H1'     3.070   3.480
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 104, r1= 2.57, r2= 3.07, r3= 3.48, r4= 3.98,  &end
#
#   5 FAG   H5    4 DA  H8      5.070   6.200
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 107, r1= 4.57, r2= 5.07, r3= 6.20, r4= 6.70,  &end
#
#   5 FAG   MA   17 DT  H3      2.500   5.500
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 568, r1= 2.00, r2= 2.50, r3= 6.61, r4= 7.11,
 igr1= 181, 182, 183,
 &end
#
#   5 FAG   MA          4 DA  H2      2.000   3.000
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 116, r1= 1.50, r2= 2.00, r3= 3.60, r4= 4.10,
 igr1= 181, 182, 183,
 &end
#
#   5 FAG   H2A   5 FAG H3A     2.190   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 171, 174, r1= 1.69, r2= 2.19, r3= 2.61, r4= 3.11,  &end
```

```
#
#   5 FAG   H2B   5 FAG H3A     2.970   3.440
 &rst
  ixpk= 0, nxpk= 0, iat= 172, 174, r1= 2.47, r2= 2.97, r3= 3.44, r4= 3.94,  &end
#
#   5 FAG   H2'1  5 FAG H1'     2.690   3.230
 &rst
  ixpk= 0, nxpk= 0, iat= 194, 136, r1= 2.19, r2= 2.69, r3= 3.23, r4= 3.73,  &end
#
#   5 FAG   H2'2  5 FAG H1'     2.080   2.600
 &rst
  ixpk= 0, nxpk= 0, iat= 195, 136, r1= 1.58, r2= 2.08, r3= 2.60, r4= 3.10,  &end
#
#   5 FAG   H3'   5 FAG H1'     3.630   4.150
 &rst
  ixpk= 0, nxpk= 0, iat= 192, 136, r1= 3.13, r2= 3.63, r3= 4.15, r4= 4.65,  &end
#
#   5 FAG   H3'   5 FAG H2'1    2.430   3.070
 &rst
  ixpk= 0, nxpk= 0, iat= 192, 194, r1= 1.93, r2= 2.43, r3= 3.07, r4= 3.57,  &end
#
#   5 FAG   H8    5 FAG H1'     5.230   5.990
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 136, r1= 4.73, r2= 5.23, r3= 5.99, r4= 6.49,  &end
#
#   5 FAG   H8    5 FAG H8A     3.440   4.200
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 155, r1= 2.94, r2= 3.44, r3= 4.20, r4= 4.70,  &end
#
#   5 FAG   H9    5 FAG H8A     2.420   2.950
 &rst
  ixpk= 0, nxpk= 0, iat= 159, 155, r1= 1.92, r2= 2.42, r3= 2.95, r4= 3.45,  &end
#
#   5 FAG   H9    5 FAG H8      2.540   3.690
 &rst
  ixpk= 0, nxpk= 0, iat= 159, 152, r1= 2.04, r2= 2.54, r3= 3.69, r4= 4.19,  &end
#
#   5 FAG   H9A   5 FAG H9      2.490   2.960
 &rst
  ixpk= 0, nxpk= 0, iat= 161, 159, r1= 1.99, r2= 2.49, r3= 2.96, r4= 3.46,  &end
#
#   5 FAG   H6A   5 FAG H9A     1.600   2.420
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 161, r1= 1.10, r2= 1.60, r3= 2.42, r4= 2.92,  &end
#
#   5 FAG   H5    5 FAG H3A     4.710   5.360
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 174, r1= 4.21, r2= 4.71, r3= 5.36, r4= 5.86,  &end
#
#   5 FAG   H5    5 FAG H3B     4.710   5.260
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 175, r1= 4.21, r2= 4.71, r3= 5.26, r4= 5.76,  &end
#
#   5 FAG   H5    5 FAG H1'     5.030   5.500
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 136, r1= 4.53, r2= 5.03, r3= 5.50, r4= 6.00,  &end
#
#   5 FAG   H5    5 FAG H6A     4.100   4.590
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 189, r1= 3.60, r2= 4.10, r3= 4.59, r4= 5.09,  &end
#
#   5 FAG   H8    5 FAG HN9     1.990   2.710
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 138, r1= 1.49, r2= 1.99, r3= 2.71, r4= 3.21,  &end
#
#   5 FAG   H2'1  5 FAG HN9     2.050   3.370
 &rst
  ixpk= 0, nxpk= 0, iat= 194, 138, r1= 1.55, r2= 2.05, r3= 3.37, r4= 3.87,  &end
#
#   5 FAG   H2'2  5 FAG HN9     2.130   3.810
 &rst
  ixpk= 0, nxpk= 0, iat= 195, 138, r1= 1.63, r2= 2.13, r3= 3.81, r4= 4.31,  &end
#
#   6 DT    H6    5 FAG HN9     2.660   4.670
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 138, r1= 2.16, r2= 2.66, r3= 4.67, r4= 5.17,  &end
#
#   6 DT    H6    5 FAG H1'     3.020   3.530
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 136, r1= 2.52, r2= 3.02, r3= 3.53, r4= 4.03,  &end
#
#   6 DT    H6    5 FAG H2'2    3.000   3.690
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 195, r1= 2.50, r2= 3.00, r3= 3.69, r4= 4.19,  &end
#
#   6 DT    H6    5 FAG H3'     5.340   5.940
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 192, r1= 4.84, r2= 5.34, r3= 5.94, r4= 6.44,  &end
#
#   6 DT    H6    5 FAG H8      6.580   7.340
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 152, r1= 6.08, r2= 6.58, r3= 7.34, r4= 7.84,  &end
```

```
#
#   6 DT    Q5    5 FAG H1'     2.510   3.560
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 136, r1= 2.01, r2= 2.51, r3= 4.28, r4= 4.78,
 igr1= 214, 215, 216,
 &end
#
#   6 DT    Q5    5 FAG H2'1    2.900   4.470
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 194, r1= 2.40, r2= 2.90, r3= 5.37, r4= 5.87,
 igr1= 214, 215, 216,
 &end
#
#   6 DT    Q5    5 FAG H2'2    2.590   3.500
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 195, r1= 2.09, r2= 2.59, r3= 4.20, r4= 4.70,
 igr1= 214, 215, 216,
 &end
#
#   6 DT    Q5    5 FAG H8      2.790   4.990
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 152, r1= 2.29, r2= 2.79, r3= 5.99, r4= 6.49,
 igr1= 214, 215, 216,
 &end
#
#   6 DT    H1'   6 DT  H2'1    2.570   3.220
 &rst
  ixpk= 0, nxpk= 0, iat= 208, 226, r1= 2.07, r2= 2.57, r3= 3.22, r4= 3.72,  &end
#
#   6 DT    H1'   6 DT  H2'2    2.140   2.690
 &rst
  ixpk= 0, nxpk= 0, iat= 208, 227, r1= 1.64, r2= 2.14, r3= 2.69, r4= 3.19,  &end
#
#   6 DT    H6    6 DT  H1'     3.470   3.930
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 208, r1= 2.97, r2= 3.47, r3= 3.93, r4= 4.43,  &end
#
#   6 DT    H6    6 DT  H2'2    3.240   3.690
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 227, r1= 2.74, r2= 3.24, r3= 3.69, r4= 4.19,  &end
#
#   7 DT    Q5    6 DT  H2'1    2.840   4.850
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 226, r1= 2.34, r2= 2.84, r3= 5.82, r4= 6.32,
 igr1= 246, 247, 248,
 &end
```

```
#
#   7 DT    Q5    6 DT  H2'2    3.010   4.500
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 227, r1= 2.51, r2= 3.01, r3= 5.40, r4= 5.90,
 igr1= 246, 247, 248,
 &end
#
#   7 DT    Q5  6 DT  H3'     3.180   4.690
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 224, r1= 2.68, r2= 3.18, r3= 5.63, r4= 6.13,
 igr1= 246, 247, 248,
 &end
#
#   7 DT    Q5    6 DT  H1'     3.100   4.140
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 208, r1= 2.60, r2= 3.10, r3= 4.97, r4= 5.47,
 igr1= 246, 247, 248,
 &end
#
#   7 DT    Q5  6 DT  H6      2.460   3.640
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 211, r1= 1.96, r2= 2.46, r3= 4.37, r4= 4.87,
 igr1= 246, 247, 248,
 &end
#
#   7 DT    H6    6 DT  H2'1    3.320   3.870
 &rst
  ixpk= 0, nxpk= 0, iat= 243, 226, r1= 2.82, r2= 3.32, r3= 3.87, r4= 4.37,  &end
#
#   7 DT    H6  6 DT  H2'2    1.900   2.400
 &rst
  ixpk= 0, nxpk= 0, iat= 243, 227, r1= 1.40, r2= 1.90, r3= 2.40, r4= 2.90,  &end
#
#   7 DT    H6  6 DT  H1'     2.900   3.800
 &rst
  ixpk= 0, nxpk= 0, iat= 243, 208, r1= 2.40, r2= 2.90, r3= 3.80, r4= 4.30,  &end
#
#   7 DT    H6  6 DT  H3'     4.600   5.000
 &rst
  ixpk= 0, nxpk= 0, iat= 243, 224, r1= 4.10, r2= 4.60, r3= 5.00, r4= 5.50,  &end
#
#   7 DT    H6  6 DT  H6      4.800   5.300
 &rst
  ixpk= 0, nxpk= 0, iat= 243, 211, r1= 4.30, r2= 4.80, r3= 5.30, r4= 5.80,  &end
#
#   7 DT    H2'1  7 DT  H3'     2.200   2.820
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 258, 256, r1= 1.70, r2= 2.20, r3= 2.82, r4= 3.32,  &end
#
#   7 DT    H2'2  7 DT  H3'     2.470   3.090
 &rst
  ixpk= 0, nxpk= 0, iat= 259, 256, r1= 1.97, r2= 2.47, r3= 3.09, r4= 3.59,  &end
#
#   7 DT    H1'   7 DT  H2'1    2.780   3.220
 &rst
  ixpk= 0, nxpk= 0, iat= 240, 258, r1= 2.28, r2= 2.78, r3= 3.22, r4= 3.72,  &end
#
#   7 DT    H1'   7 DT  H2'2    2.020   2.520
 &rst
  ixpk= 0, nxpk= 0, iat= 240, 259, r1= 1.52, r2= 2.02, r3= 2.52, r4= 3.02,  &end
#
#   7 DT    H6    7 DT  H2'1    1.710   2.250
 &rst
  ixpk= 0, nxpk= 0, iat= 243, 258, r1= 1.21, r2= 1.71, r3= 2.25, r4= 2.75,  &end
#
#   7 DT    H6    7 DT  H2'2    3.220   3.730
 &rst
  ixpk= 0, nxpk= 0, iat= 243, 259, r1= 2.72, r2= 3.22, r3= 3.73, r4= 4.23,  &end
#
#   8 DT    H6    7 DT  H2'1    3.650   4.120
 &rst
  ixpk= 0, nxpk= 0, iat= 275, 258, r1= 3.15, r2= 3.65, r3= 4.12, r4= 4.62,  &end
#
#   8 DT    H6    7 DT  H2'2    2.180   2.660
 &rst
  ixpk= 0, nxpk= 0, iat= 275, 259, r1= 1.68, r2= 2.18, r3= 2.66, r4= 3.16,  &end
#
#   8 DT    H6    7 DT  H1'     2.800   3.590
 &rst
  ixpk= 0, nxpk= 0, iat= 275, 240, r1= 2.30, r2= 2.80, r3= 3.59, r4= 4.09,  &end
#
#   8 DT    H6    7 DT  H6      4.710   5.390
 &rst
  ixpk= 0, nxpk= 0, iat= 275, 243, r1= 4.21, r2= 4.71, r3= 5.39, r4= 5.89,  &end
#
#   8 DT    Q5  7 DT  H3'     2.380   4.510
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 256, r1= 1.88, r2= 2.38, r3= 5.42, r4= 5.92,
 igr1= 278, 279, 280,
 &end
#
#   8 DT    Q5  7 DT  H2'1    2.170   3.000
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 258, r1= 1.67, r2= 2.17, r3= 3.60, r4= 4.10,
 igr1= 278, 279, 280,
 &end
#
#   8 DT    Q5  7 DT  H2'2    2.130   3.040
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 259, r1= 1.63, r2= 2.13, r3= 3.65, r4= 4.15,
 igr1= 278, 279, 280,
 &end
#
#   8 DT    Q5  7 DT  H1'     2.910   4.410
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 240, r1= 2.41, r2= 2.91, r3= 5.30, r4= 5.80,
 igr1= 278, 279, 280,
 &end
#
#   8 DT    Q5  7 DT  H6      2.520   3.470
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 243, r1= 2.02, r2= 2.52, r3= 4.17, r4= 4.67,
 igr1= 278, 279, 280,
 &end
#
#   8 DT    H3'   7 DT  H1'     4.610   5.490
 &rst
  ixpk= 0, nxpk= 0, iat= 288, 240, r1= 4.11, r2= 4.61, r3= 5.49, r4= 5.99,  &end
#
#   8 DT    H2'1  8 DT  H3'     2.300   3.230
 &rst
  ixpk= 0, nxpk= 0, iat= 290, 288, r1= 1.80, r2= 2.30, r3= 3.23, r4= 3.73,  &end
#
#   8 DT    H2'2  8 DT  H3'     2.400   3.060
 &rst
  ixpk= 0, nxpk= 0, iat= 291, 288, r1= 1.90, r2= 2.40, r3= 3.06, r4= 3.56,  &end
#
#   8 DT    H1'   8 DT  H3'     3.500   5.100
 &rst
  ixpk= 0, nxpk= 0, iat= 272, 288, r1= 3.00, r2= 3.50, r3= 5.10, r4= 5.60,  &end
#
#   8 DT    H1'   8 DT  H2'1    2.720   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 272, 290, r1= 2.22, r2= 2.72, r3= 3.20, r4= 3.70,  &end
#
#   8 DT    Q5    8 DT  H3'     3.050   5.940
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 288, r1= 2.55, r2= 3.05, r3= 7.13, r4= 7.63,
```

```
 igr1= 278, 279, 280,
 &end
#
#   8 DT    Q5    8 DT  H1'     3.190   5.960
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 272, r1= 2.69, r2= 3.19, r3= 7.16, r4= 7.66,
 igr1= 278, 279, 280,
 &end
#
#   8 DT    H6    8 DT  H2'1    2.000   2.880
 &rst
  ixpk= 0, nxpk= 0, iat= 275, 290, r1= 1.50, r2= 2.00, r3= 2.88, r4= 3.38,  &end
#
#   8 DT    H6    8 DT  H2'2    3.770   4.280
 &rst
  ixpk= 0, nxpk= 0, iat= 275, 291, r1= 3.27, r2= 3.77, r3= 4.28, r4= 4.78,  &end
#
#   8 DT    H6    8 DT  H1'     3.530   4.220
 &rst
  ixpk= 0, nxpk= 0, iat= 275, 272, r1= 3.03, r2= 3.53, r3= 4.22, r4= 4.72,  &end
#
#   9 DC    H6  8 DT  H2'1    3.600   4.310
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 290, r1= 3.10, r2= 3.60, r3= 4.31, r4= 4.81,  &end
#
#   9 DC    H6  8 DT  H2'2    2.000   2.840
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 291, r1= 1.50, r2= 2.00, r3= 2.84, r4= 3.34,  &end
#
#   9 DC    H6  8 DT  H1'     2.830   3.490
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 272, r1= 2.33, r2= 2.83, r3= 3.49, r4= 3.99,  &end
#
#   9 DC    H6  8 DT  H6      4.900   5.300
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 275, r1= 4.40, r2= 4.90, r3= 5.30, r4= 5.80,  &end
#
#   9 DC    H5  8 DT  H3'     5.000   5.500
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 288, r1= 4.50, r2= 5.00, r3= 5.50, r4= 6.00,  &end
#
#   9 DC    H5  8 DT  H2'2    2.410   3.360
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 291, r1= 1.91, r2= 2.41, r3= 3.36, r4= 3.86,  &end
#
#   9 DC    H5  8 DT  H1'     3.320   4.050
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 272, r1= 2.82, r2= 3.32, r3= 4.05, r4= 4.55,  &end
#
#   9 DC    H5  8 DT  Q5      2.810   3.900
 &rst
  ixpk= 0, nxpk= 0, iat= 309,  -1, r1= 2.31, r2= 2.81, r3= 4.68, r4= 5.18,
 igr2= 278, 279, 280,
 &end
#
#   9 DC    H5  8 DT  H6      3.590   4.080
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 275, r1= 3.09, r2= 3.59, r3= 4.08, r4= 4.58,  &end
#
#   9 DC    H1'   9 DC  H3'     3.730   4.290
 &rst
  ixpk= 0, nxpk= 0, iat= 304, 318, r1= 3.23, r2= 3.73, r3= 4.29, r4= 4.79,  &end
#
#   9 DC    H1'   9 DC  H2'1    2.780   3.270
 &rst
  ixpk= 0, nxpk= 0, iat= 304, 320, r1= 2.28, r2= 2.78, r3= 3.27, r4= 3.77,  &end
#
#   9 DC    H1'   9 DC  H2'2    2.120   2.660
 &rst
  ixpk= 0, nxpk= 0, iat= 304, 321, r1= 1.62, r2= 2.12, r3= 2.66, r4= 3.16,  &end
#
#   9 DC    H5    9 DC  H2'1    4.100   4.680
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 320, r1= 3.60, r2= 4.10, r3= 4.68, r4= 5.18,  &end
#
#   9 DC    H5    9 DC  H2'2    5.300   5.740
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 321, r1= 4.80, r2= 5.30, r3= 5.74, r4= 6.24,  &end
#
#   9 DC    H6    9 DC  H2'1    1.700   2.160
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 320, r1= 1.20, r2= 1.70, r3= 2.16, r4= 2.66,  &end
#
#   9 DC    H6    9 DC  H2'2    3.220   3.730
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 321, r1= 2.72, r2= 3.22, r3= 3.73, r4= 4.23,  &end
#
#   9 DC    H6    9 DC  H1'     3.500   4.210
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 304, r1= 3.00, r2= 3.50, r3= 4.21, r4= 4.71,  &end
#
#  10 DA3   H8    9 DC  H2'1    3.590   4.290
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 320, r1= 3.09, r2= 3.59, r3= 4.29, r4= 4.79,  &end
#
#  10 DA3   H8    9 DC  H2'2    2.480   2.980
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 321, r1= 1.98, r2= 2.48, r3= 2.98, r4= 3.48,  &end
#
#  10 DA3   H8    9 DC  H6      4.430   5.240
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 307, r1= 3.93, r2= 4.43, r3= 5.24, r4= 5.74,  &end
#
#  10 DA3   H8    9 DC  H1'     3.590   4.390
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 304, r1= 3.09, r2= 3.59, r3= 4.39, r4= 4.89,  &end
#
#  10 DA3   H2'1 10 DA3 H3'     2.270   2.770
 &rst
  ixpk= 0, nxpk= 0, iat= 352, 350, r1= 1.77, r2= 2.27, r3= 2.77, r4= 3.27,  &end
#
#  10 DA3   H2'2 10 DA3 H3'     2.510   3.070
 &rst
  ixpk= 0, nxpk= 0, iat= 353, 350, r1= 2.01, r2= 2.51, r3= 3.07, r4= 3.57,  &end
#
#  10 DA3   H1'  10 DA3 H3'     3.550   4.060
 &rst
  ixpk= 0, nxpk= 0, iat= 334, 350, r1= 3.05, r2= 3.55, r3= 4.06, r4= 4.56,  &end
#
#  10 DA3   H1'  10 DA3 H2'1    2.710   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 334, 352, r1= 2.21, r2= 2.71, r3= 3.20, r4= 3.70,  &end
#
#  10 DA3   H1'  10 DA3 H2'2    1.980   2.550
 &rst
  ixpk= 0, nxpk= 0, iat= 334, 353, r1= 1.48, r2= 1.98, r3= 2.55, r4= 3.05,  &end
#
#  10 DA3   H8   10 DA3 H3'     4.150   4.730
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 350, r1= 3.65, r2= 4.15, r3= 4.73, r4= 5.23,  &end
#
#  10 DA3   H8   10 DA3 H2'2    3.460   3.960
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 353, r1= 2.96, r2= 3.46, r3= 3.96, r4= 4.46,  &end
#
#  10 DA3   H8   10 DA3 H1'     3.570   4.070
 &rst
  ixpk= 0, nxpk= 0, iat= 337, 334, r1= 3.07, r2= 3.57, r3= 4.07, r4= 4.57,  &end
```

```
#
#  11 DT5   H1'  11 DT5 H3'     3.740   4.280
 &rst
  ixpk= 0, nxpk= 0, iat= 365, 381, r1= 3.24, r2= 3.74, r3= 4.28, r4= 4.78,  &end
#
#  11 DT5   H1'  11 DT5 H2'1    2.720   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 365, 383, r1= 2.22, r2= 2.72, r3= 3.20, r4= 3.70,  &end
#
#  11 DT5   H1'  11 DT5 H2'2    2.120   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 365, 384, r1= 1.62, r2= 2.12, r3= 2.61, r4= 3.11,  &end
#
#  11 DT5   Q5   11 DT5 H1'     3.410   5.850
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 365, r1= 2.91, r2= 3.41, r3= 7.03, r4= 7.53,
 igr1= 371, 372, 373,
 &end
#
#  11 DT5   H6   11 DT5 H3'     3.820   4.280
 &rst
  ixpk= 0, nxpk= 0, iat= 368, 381, r1= 3.32, r2= 3.82, r3= 4.28, r4= 4.78,  &end
#
#  11 DT5   H6   11 DT5 H2'1    1.730   2.340
 &rst
  ixpk= 0, nxpk= 0, iat= 368, 383, r1= 1.23, r2= 1.73, r3= 2.34, r4= 2.84,  &end
#
#  11 DT5   H6   11 DT5 H2'2    3.110   3.810
 &rst
  ixpk= 0, nxpk= 0, iat= 368, 384, r1= 2.61, r2= 3.11, r3= 3.81, r4= 4.31,  &end
#
#  11 DT5   H6   11 DT5 H1'     2.730   4.390
 &rst
  ixpk= 0, nxpk= 0, iat= 368, 365, r1= 2.23, r2= 2.73, r3= 4.39, r4= 4.89,  &end
#
#  11 DT5   H6   11 DT5 Q5      2.020   2.850
 &rst
  ixpk= 0, nxpk= 0, iat= 368,  -1, r1= 1.52, r2= 2.02, r3= 3.42, r4= 3.92,
 igr2= 371, 372, 373,
 &end
#
#  12 DG    H8   11 DT5 H3'     4.990   5.480
 &rst
  ixpk= 0, nxpk= 0, iat= 400, 381, r1= 4.49, r2= 4.99, r3= 5.48, r4= 5.98,  &end
#
#  12 DG    H8   11 DT5 H2'1    3.590   4.680
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 400, 383, r1= 3.09, r2= 3.59, r3= 4.68, r4= 5.18,  &end
#
#  12 DG    H8   11 DT5 H2'2    2.570   3.640
 &rst
  ixpk= 0, nxpk= 0, iat= 400, 384, r1= 2.07, r2= 2.57, r3= 3.64, r4= 4.14,  &end
#
#  12 DG    H8   11 DT5 H1'     3.550   4.420
 &rst
  ixpk= 0, nxpk= 0, iat= 400, 365, r1= 3.05, r2= 3.55, r3= 4.42, r4= 4.92,  &end
#
#  12 DG    H8   11 DT5 H6      4.660   5.240
 &rst
  ixpk= 0, nxpk= 0, iat= 400, 368, r1= 4.16, r2= 4.66, r3= 5.24, r4= 5.74,  &end
#
#  12 DG    H8   12 DG  H1'     3.700   5.260
 &rst
  ixpk= 0, nxpk= 0, iat= 400, 397, r1= 3.20, r2= 3.70, r3= 5.26, r4= 5.76,  &end
#
#  13 DA    H8   12 DG  H1'     3.240   4.180
 &rst
  ixpk= 0, nxpk= 0, iat= 433, 397, r1= 2.74, r2= 3.24, r3= 4.18, r4= 4.68,  &end
#
#  13 DA    H8   12 DG  H8      5.180   5.790
 &rst
  ixpk= 0, nxpk= 0, iat= 433, 400, r1= 4.68, r2= 5.18, r3= 5.79, r4= 6.29,  &end
#
#  13 DA    H8   12 DG  H2'1    4.500   5.000
 &rst
  ixpk= 0, nxpk= 0, iat= 433, 416, r1= 4.00, r2= 4.50, r3= 5.00, r4= 5.50,  &end
#
#  13 DA    H8   12 DG  H2'2    2.980   3.600
 &rst
  ixpk= 0, nxpk= 0, iat= 433, 417, r1= 2.48, r2= 2.98, r3= 3.60, r4= 4.10,  &end
#
#  13 DA    H1'  13 DA  H3'     3.630   4.150
 &rst
  ixpk= 0, nxpk= 0, iat= 430, 446, r1= 3.13, r2= 3.63, r3= 4.15, r4= 4.65,  &end
#
#  13 DA    H1'  13 DA  H2'1    2.750   3.230
 &rst
  ixpk= 0, nxpk= 0, iat= 430, 448, r1= 2.25, r2= 2.75, r3= 3.23, r4= 3.73,  &end
#
#  13 DA    H1'  13 DA  H2'2    2.120   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 430, 449, r1= 1.62, r2= 2.12, r3= 2.61, r4= 3.11,  &end
```

```
#
#  13 DA    H8   13 DA  H1'     3.680   4.180
 &rst
  ixpk= 0, nxpk= 0, iat= 433, 430, r1= 3.18, r2= 3.68, r3= 4.18, r4= 4.68,  &end
#
#  13 DA    H8   13 DA  H2'2    3.480   3.980
 &rst
  ixpk= 0, nxpk= 0, iat= 433, 449, r1= 2.98, r2= 3.48, r3= 3.98, r4= 4.48,  &end
#
#  14 DA    H8   13 DA  H1'     2.410   3.490
 &rst
  ixpk= 0, nxpk= 0, iat= 465, 430, r1= 1.91, r2= 2.41, r3= 3.49, r4= 3.99,  &end
#
#  14 DA    H8   13 DA  H8      4.490   4.990
 &rst
  ixpk= 0, nxpk= 0, iat= 465, 433, r1= 3.99, r2= 4.49, r3= 4.99, r4= 5.49,  &end
#
#  14 DA    H8   13 DA  H2'1    3.800   4.300
 &rst
  ixpk= 0, nxpk= 0, iat= 465, 448, r1= 3.30, r2= 3.80, r3= 4.30, r4= 4.80,  &end
#
#  14 DA    H8   13 DA  H2'2    2.300   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 465, 449, r1= 1.80, r2= 2.30, r3= 2.90, r4= 3.40,  &end
#
#  14 DA    H1'  14 DA  H2'1    2.800   3.310
 &rst
  ixpk= 0, nxpk= 0, iat= 462, 480, r1= 2.30, r2= 2.80, r3= 3.31, r4= 3.81,  &end
#
#  14 DA    H1'  14 DA  H2'2    2.120   2.630
 &rst
  ixpk= 0, nxpk= 0, iat= 462, 481, r1= 1.62, r2= 2.12, r3= 2.63, r4= 3.13,  &end
#
#  14 DA    H8   14 DA  H2'1    2.030   2.510
 &rst
  ixpk= 0, nxpk= 0, iat= 465, 480, r1= 1.53, r2= 2.03, r3= 2.51, r4= 3.01,  &end
#
#  14 DA    H8   14 DA  H1'     3.650   4.130
 &rst
  ixpk= 0, nxpk= 0, iat= 465, 462, r1= 3.15, r2= 3.65, r3= 4.13, r4= 4.63,  &end
#
#  15 DA    H8   14 DA  H3'     4.680   5.130
 &rst
  ixpk= 0, nxpk= 0, iat= 497, 478, r1= 4.18, r2= 4.68, r3= 5.13, r4= 5.63,  &end
#
#  15 DA    H8   14 DA  H2'1    3.790   4.300
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 497, 480, r1= 3.29, r2= 3.79, r3= 4.30, r4= 4.80,  &end
#
#  15 DA    H8   14 DA  H1'     3.260   3.720
 &rst
  ixpk= 0, nxpk= 0, iat= 497, 462, r1= 2.76, r2= 3.26, r3= 3.72, r4= 4.22,  &end
#
#  15 DA    H8   14 DA  H8      4.960   5.440
 &rst
  ixpk= 0, nxpk= 0, iat= 497, 465, r1= 4.46, r2= 4.96, r3= 5.44, r4= 5.94,  &end
#
#  15 DA    H2'1 15 DA  H3'     2.270   2.730
 &rst
  ixpk= 0, nxpk= 0, iat= 512, 510, r1= 1.77, r2= 2.27, r3= 2.73, r4= 3.23,  &end
#
#  15 DA    H2'2 15 DA  H3'     2.390   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 513, 510, r1= 1.89, r2= 2.39, r3= 2.90, r4= 3.40,  &end
#
#  15 DA    H1'  15 DA  H3'     3.560   4.020
 &rst
  ixpk= 0, nxpk= 0, iat= 494, 510, r1= 3.06, r2= 3.56, r3= 4.02, r4= 4.52,  &end
#
#  15 DA    H1'  15 DA  H2'2    2.100   2.590
 &rst
  ixpk= 0, nxpk= 0, iat= 494, 513, r1= 1.60, r2= 2.10, r3= 2.59, r4= 3.09,  &end
#
#  15 DA    H8   15 DA  H3'     4.190   4.650
 &rst
  ixpk= 0, nxpk= 0, iat= 497, 510, r1= 3.69, r2= 4.19, r3= 4.65, r4= 5.15,  &end
#
#  15 DA    H8   15 DA  H2'1    1.990   2.590
 &rst
  ixpk= 0, nxpk= 0, iat= 497, 512, r1= 1.49, r2= 1.99, r3= 2.59, r4= 3.09,  &end
#
#  15 DA    H8   15 DA  H1'     3.690   4.210
 &rst
  ixpk= 0, nxpk= 0, iat= 497, 494, r1= 3.19, r2= 3.69, r3= 4.21, r4= 4.71,  &end
#
#  16 DC    H2'1  5 FAG H2B     1.840   2.980
 &rst
  ixpk= 0, nxpk= 0, iat= 542, 172, r1= 1.34, r2= 1.84, r3= 2.98, r4= 3.48,  &end
#
#  16 DC    H2'2  5 FAG H2B     2.040   3.380
 &rst
  ixpk= 0, nxpk= 0, iat= 543, 172, r1= 1.54, r2= 2.04, r3= 3.38, r4= 3.88,  &end
```

```
#
#  16 DC    H1'   5 FAG H2B     2.750   3.890
 &rst
  ixpk= 0, nxpk= 0, iat= 526, 172, r1= 2.25, r2= 2.75, r3= 3.89, r4= 4.39,  &end
#
#  16 DC    H6    5 FAG H2B     2.250   3.090
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 172, r1= 1.75, r2= 2.25, r3= 3.09, r4= 3.59,  &end
#
#  16 DC    H5   15 DA  H1'     4.290   4.970
 &rst
  ixpk= 0, nxpk= 0, iat= 531, 494, r1= 3.79, r2= 4.29, r3= 4.97, r4= 5.47,  &end
#
#  16 DC    H5   15 DA  H8      3.510   4.060
 &rst
  ixpk= 0, nxpk= 0, iat= 531, 497, r1= 3.01, r2= 3.51, r3= 4.06, r4= 4.56,  &end
#
#  16 DC    H6   15 DA  H2'1    3.060   3.590
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 512, r1= 2.56, r2= 3.06, r3= 3.59, r4= 4.09,  &end
#
#  16 DC    H6   15 DA  H2'2    2.110   2.630
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 513, r1= 1.61, r2= 2.11, r3= 2.63, r4= 3.13,  &end
#
#  16 DC    H6   15 DA  H1'     3.820   4.380
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 494, r1= 3.32, r2= 3.82, r3= 4.38, r4= 4.88,  &end
#
#  16 DC    H6   15 DA  H8      4.690   5.200
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 497, r1= 4.19, r2= 4.69, r3= 5.20, r4= 5.70,  &end
#
#  16 DC    H5   15 DA  H2'1    3.050   3.540
 &rst
  ixpk= 0, nxpk= 0, iat= 531, 512, r1= 2.55, r2= 3.05, r3= 3.54, r4= 4.04,  &end
#
#  16 DC    H1'  16 DC  H2'2    2.130   2.630
 &rst
  ixpk= 0, nxpk= 0, iat= 526, 543, r1= 1.63, r2= 2.13, r3= 2.63, r4= 3.13,  &end
#
#  16 DC    H5   16 DC  H2'1    4.050   4.530
 &rst
  ixpk= 0, nxpk= 0, iat= 531, 542, r1= 3.55, r2= 4.05, r3= 4.53, r4= 5.03,  &end
#
#  16 DC    H5   16 DC  H2'2    5.260   5.750
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 531, 543, r1= 4.76, r2= 5.26, r3= 5.75, r4= 6.25,  &end
#
#  16 DC    H6   16 DC  H3'     3.760   4.270
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 540, r1= 3.26, r2= 3.76, r3= 4.27, r4= 4.77,  &end
#
#  16 DC    H6   16 DC  H2'1    1.740   2.260
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 542, r1= 1.24, r2= 1.74, r3= 2.26, r4= 2.76,  &end
#
#  16 DC    H6   16 DC  H2'2    3.120   3.710
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 543, r1= 2.62, r2= 3.12, r3= 3.71, r4= 4.21,  &end
#
#  16 DC    H6   16 DC  H1'     3.520   4.040
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 526, r1= 3.02, r2= 3.52, r3= 4.04, r4= 4.54,  &end
#
#  17 DT    H6    5 FAG H3A     3.570   3.970
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 174, r1= 3.07, r2= 3.57, r3= 3.97, r4= 4.47,  &end
#
#  17 DT    H6    5 FAG H3B     4.470   4.970
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 175, r1= 3.97, r2= 4.47, r3= 4.97, r4= 5.47,  &end
#
#  17 DT    H6    5 FAG H2A     3.670   4.070
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 171, r1= 3.17, r2= 3.67, r3= 4.07, r4= 4.57,  &end
#
#  17 DT    H6    5 FAG H2B     4.570   5.070
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 172, r1= 4.07, r2= 4.57, r3= 5.07, r4= 5.57,  &end
#
#  17 DT    H2'2 17 DT  H3'     2.470   2.970
 &rst
  ixpk= 0, nxpk= 0, iat= 575, 572, r1= 1.97, r2= 2.47, r3= 2.97, r4= 3.47,  &end
#
#  17 DT    H1'  17 DT  H3'     3.660   4.210
 &rst
  ixpk= 0, nxpk= 0, iat= 556, 572, r1= 3.16, r2= 3.66, r3= 4.21, r4= 4.71,  &end
#
#  17 DT    H1'  17 DT  H2'2    2.110   2.650
 &rst
  ixpk= 0, nxpk= 0, iat= 556, 575, r1= 1.61, r2= 2.11, r3= 2.65, r4= 3.15,  &end
```

```
#
#  17 DT    H6   17 DT  H3'     3.770   4.570
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 572, r1= 3.27, r2= 3.77, r3= 4.57, r4= 5.07,  &end
#
#  17 DT    H6   17 DT  H2'1    1.740   2.290
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 574, r1= 1.24, r2= 1.74, r3= 2.29, r4= 2.79,  &end
#
#  17 DT    H6   17 DT  H2'2    2.940   3.690
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 575, r1= 2.44, r2= 2.94, r3= 3.69, r4= 4.19,  &end
#
#  17 DT    H6   17 DT  H1'     3.430   3.940
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 556, r1= 2.93, r2= 3.43, r3= 3.94, r4= 4.44,  &end
#
#  17 DT    Q5   17 DT  H2'2    1.930   5.280
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 575, r1= 1.43, r2= 1.93, r3= 6.34, r4= 6.84,
 igr1= 562, 563, 564,
 &end
#
#  17 DT    Q5   17 DT  H1'     2.890   5.510
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 556, r1= 2.39, r2= 2.89, r3= 6.62, r4= 7.12,
 igr1= 562, 563, 564,
 &end
#
#  17 DT    Q5   17 DT  H6      2.570   3.830
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 559, r1= 2.07, r2= 2.57, r3= 4.60, r4= 5.10,
 igr1= 562, 563, 564,
 &end
#
#  18 DT    H3   17 DT  H3      4.330   4.850
 &rst
  ixpk= 0, nxpk= 0, iat= 600, 568, r1= 3.83, r2= 4.33, r3= 4.85, r4= 5.35,  &end
#
#  18 DT    H1'  17 DT  H1'     5.110   5.690
 &rst
  ixpk= 0, nxpk= 0, iat= 588, 556, r1= 4.61, r2= 5.11, r3= 5.69, r4= 6.19,  &end
#
#  18 DT    Q5   17 DT  H2'1    1.990   3.580
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 574, r1= 1.49, r2= 1.99, r3= 4.30, r4= 4.80,
```

```
 igr1= 594, 595, 596,
 &end
#
#  18 DT    Q5   17 DT  H2'2    2.580   4.260
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 575, r1= 2.08, r2= 2.58, r3= 5.12, r4= 5.62,
 igr1= 594, 595, 596,
 &end
#
#  18 DT    Q5   17 DT  H6      2.720   4.310
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 559, r1= 2.22, r2= 2.72, r3= 5.18, r4= 5.68,
 igr1= 594, 595, 596,
 &end
#
#  18 DT    H6   17 DT  H2'1    3.970   4.330
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 574, r1= 3.47, r2= 3.97, r3= 4.33, r4= 4.83,  &end
#
#  18 DT    H6   17 DT  H2'2    2.470   2.730
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 575, r1= 1.97, r2= 2.47, r3= 2.73, r4= 3.23,  &end
#
#  18 DT    H6   17 DT  H1'     2.920   3.190
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 556, r1= 2.42, r2= 2.92, r3= 3.19, r4= 3.69,  &end
#
#  18 DT    H6   17 DT  H6      5.100   5.370
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 559, r1= 4.60, r2= 5.10, r3= 5.37, r4= 5.87,  &end
#
#  18 DT    H1'  18 DT  H3'     3.630   4.160
 &rst
  ixpk= 0, nxpk= 0, iat= 588, 604, r1= 3.13, r2= 3.63, r3= 4.16, r4= 4.66,  &end
#
#  18 DT    H1'  18 DT  H2'1    2.820   3.360
 &rst
  ixpk= 0, nxpk= 0, iat= 588, 606, r1= 2.32, r2= 2.82, r3= 3.36, r4= 3.86,  &end
#
#  18 DT    H1'  18 DT  H2'2    2.110   2.640
 &rst
  ixpk= 0, nxpk= 0, iat= 588, 607, r1= 1.61, r2= 2.11, r3= 2.64, r4= 3.14,  &end
#
#  18 DT    Q5   18 DT  H1'     3.940   5.610
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 588, r1= 3.44, r2= 3.94, r3= 6.74, r4= 7.24,
```

```
 igr1= 594, 595, 596,
 &end
#
#  18 DT    H6   18 DT  H2'1    1.640   2.210
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 606, r1= 1.14, r2= 1.64, r3= 2.21, r4= 2.71,  &end
#
#  18 DT    H6   18 DT  H1'     3.460   3.940
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 588, r1= 2.96, r2= 3.46, r3= 3.94, r4= 4.44,  &end
#
#  19 DA    H2   18 DT  H3      4.130   4.650
 &rst
  ixpk= 0, nxpk= 0, iat= 632, 600, r1= 3.63, r2= 4.13, r3= 4.65, r4= 5.15,  &end
#
#  19 DA    H8   18 DT  H2'1    4.860   5.110
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 606, r1= 4.36, r2= 4.86, r3= 5.11, r4= 5.61,  &end
#
#  19 DA    H8   18 DT  H2'2    3.100   3.390
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 607, r1= 2.60, r2= 3.10, r3= 3.39, r4= 3.89,  &end
#
#  19 DA    H8   18 DT  H1'     3.820   4.190
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 588, r1= 3.32, r2= 3.82, r3= 4.19, r4= 4.69,  &end
#
#  19 DA    H8   18 DT  H6      6.200   6.470
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 591, r1= 5.70, r2= 6.20, r3= 6.47, r4= 6.97,  &end
#
#  19 DA    H2'2 19 DA  H3'     2.390   2.920
 &rst
  ixpk= 0, nxpk= 0, iat= 639, 636, r1= 1.89, r2= 2.39, r3= 2.92, r4= 3.42,  &end
#
#  19 DA    H1'  19 DA  H3'     3.660   4.110
 &rst
  ixpk= 0, nxpk= 0, iat= 620, 636, r1= 3.16, r2= 3.66, r3= 4.11, r4= 4.61,  &end
#
#  19 DA    H1'  19 DA  H2'1    2.730   3.280
 &rst
  ixpk= 0, nxpk= 0, iat= 620, 638, r1= 2.23, r2= 2.73, r3= 3.28, r4= 3.78,  &end
#
#  19 DA    H1'  19 DA  H2'2    2.120   2.690
 &rst
  ixpk= 0, nxpk= 0, iat= 620, 639, r1= 1.62, r2= 2.12, r3= 2.69, r4= 3.19,  &end
```

```
#
#  19 DA    H8   19 DA  H3'     4.130   4.660
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 636, r1= 3.63, r2= 4.13, r3= 4.66, r4= 5.16,  &end
#
#  19 DA    H8   19 DA  H2'2    3.340   3.990
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 639, r1= 2.84, r2= 3.34, r3= 3.99, r4= 4.49,  &end
#
#  19 DA    H8   19 DA  H1'     3.630   4.130
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 620, r1= 3.13, r2= 3.63, r3= 4.13, r4= 4.63,  &end
#
#  20 DG3   H1   19 DA  H2      4.130   4.650
 &rst
  ixpk= 0, nxpk= 0, iat= 661, 632, r1= 3.63, r2= 4.13, r3= 4.65, r4= 5.15,  &end
#
#  20 DG3   H3'  19 DA  H1'     5.130   5.650
 &rst
  ixpk= 0, nxpk= 0, iat= 669, 620, r1= 4.63, r2= 5.13, r3= 5.65, r4= 6.15,  &end
#
#  20 DG3   H8   19 DA  H3'     5.170   5.490
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 636, r1= 4.67, r2= 5.17, r3= 5.49, r4= 5.99,  &end
#
#  20 DG3   H8   19 DA  H2'1    3.880   4.220
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 638, r1= 3.38, r2= 3.88, r3= 4.22, r4= 4.72,  &end
#
#  20 DG3   H8   19 DA  H2'2    2.550   2.840
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 639, r1= 2.05, r2= 2.55, r3= 2.84, r4= 3.34,  &end
#
#  20 DG3   H8   19 DA  H1'     3.330   3.610
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 620, r1= 2.83, r2= 3.33, r3= 3.61, r4= 4.11,  &end
#
#  20 DG3   H8   19 DA  H8      4.370   4.990
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 623, r1= 3.87, r2= 4.37, r3= 4.99, r4= 5.49,  &end
#
#  20 DG3   H8   20 DG3 H3'     4.180   4.670
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 669, r1= 3.68, r2= 4.18, r3= 4.67, r4= 5.17,  &end
#
#  20 DG3   H8   20 DG3 H2'1    2.040   2.500
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 671, r1= 1.54, r2= 2.04, r3= 2.50, r4= 3.00,  &end
#
#  20 DG3   H8   20 DG3 H2'2    3.510   4.050
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 672, r1= 3.01, r2= 3.51, r3= 4.05, r4= 4.55,  &end
#
#  20 DG3   H2'1 20 DG3 H3'     2.210   2.720
 &rst
  ixpk= 0, nxpk= 0, iat= 671, 669, r1= 1.71, r2= 2.21, r3= 2.72, r4= 3.22,  &end
#
#  20 DG3   H2'2 20 DG3 H3'     2.430   2.990
 &rst
  ixpk= 0, nxpk= 0, iat= 672, 669, r1= 1.93, r2= 2.43, r3= 2.99, r4= 3.49,  &end
#
#  20 DG3   H1'  20 DG3 H3'     3.640   4.100
 &rst
  ixpk= 0, nxpk= 0, iat= 652, 669, r1= 3.14, r2= 3.64, r3= 4.10, r4= 4.60,  &end
#
#  20 DG3   H1'  20 DG3 H2'1    2.700   3.270
 &rst
  ixpk= 0, nxpk= 0, iat= 652, 671, r1= 2.20, r2= 2.70, r3= 3.27, r4= 3.77,  &end
#
#  20 DG3   H1'  20 DG3 H2'2    1.990   2.520
 &rst
  ixpk= 0, nxpk= 0, iat= 652, 672, r1= 1.49, r2= 1.99, r3= 2.52, r4= 3.02,  &end
#
#  20 DG3   H8   20 DG3 H1'     3.650   4.140
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 652, r1= 3.15, r2= 3.65, r3= 4.14, r4= 4.64,  &end
#
#  1  DC5  H42           20  DG3  O6     1.80    2.00
 &rst
  ixpk= 0, nxpk= 0, iat=  19, 659, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,
     rk2=20.0, rk3=20.0, ir6=1, ialtd=0,
 &end
#
#  1  DC5  N3  20  DG3  H1    1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  20, 661, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#  1  DC5  N3  20  DG3  N1    2.85    3.05
 &rst
  ixpk= 0, nxpk= 0, iat=  20, 660, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#  1  DC5  N4  20  DG3  O6    2.81    3.01
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  17, 659, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
# 1  DC5  O2  20  DG3  H22   1.75    1.95
 &rst
  ixpk= 0, nxpk= 0, iat=  22, 665, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
# 2  DT   H3   19  DA   N1     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat=  52, 630, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 2  DT   N3   19  DA   N1     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat=  51, 630, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 2  DT   O4   19  DA   H61    1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  50, 628, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 3  DA   H61 18  DT   O4     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  80, 598, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 3  DA   N1   18  DT   H3     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat=  82, 600, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 3  DA   N1   18  DT   N3     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat=  82, 599, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 4  DA   H61 17  DT   O4     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 112, 566, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 4  DA   N1   17  DT   H3     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 114, 568, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 4  DA   N1   17  DT   N3     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 114, 567, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 5  FAG  H1 16  DC   N3     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 146, 536, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
```

```
#
# 5  FAG  H22          16  DC   O2     1.75    1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 144, 538, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
# 5  FAG  N1 16  DC   N3     2.85    3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 145, 536, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
# 5  FAG  O6 16  DC   H42    1.80    2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 148, 535, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
# 5  FAG  O6 16  DC   N4     2.81    3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 148, 533, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
# 6  DT   O4     15  DA   H61 1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 218, 502, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 6  DT   H3     15  DA   N1   1.71   1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 220, 504, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 6  DT   N3     15  DA   N1   2.72   2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 219, 504, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 7  DT   H3   14  DA   N1     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 252, 472, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 7  DT   N3   14  DA   N1     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 251, 472, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 7  DT   O4   14  DA   H61    1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 250, 470, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 8  DT   H3   13  DA   N1     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 284, 440, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 8  DT   N3   13  DA   N1     2.72    2.92
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 283, 440, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 8  DT   O4   13  DA   H61    1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 282, 438, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 9  DC   H42 12  DG   O6     1.80    2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 313, 404, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
# 9  DC   N3   12  DG   H1     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 314, 406, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 9  DC   N3   12  DG   N1     2.85    3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 314, 405, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
# 9  DC   N4   12  DG   O6     2.81    3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 311, 404, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
# 9  DC   O2   12  DG   H22    1.75    1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 316, 410, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
# 10 DA3  H61          11  DT5  O4     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 342, 375, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 10 DA3  N1 11  DT5  H3     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 344, 377, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 10 DA3  N1 11  DT5  N3     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 344, 376, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
# 674 atoms read from pdb file AGT_amber.pdb.
# 2 DT ALPHA:  (1 DC5 O3')-(2 DT P)-(2 DT O5')-(2 DT C5') -90.0 -30.0
 &rst     iat =    28,    29,    32,    33,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
           rk2 =   2.0, rk3 =   2.0,                                    &end

# 3 DA ALPHA:  (2 DT O3')-(3 DA P)-(3 DA O5')-(3 DA C5') -90.0 -30.0
 &rst     iat =    60,    61,    64,    65,
```

```
  r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
 &end

# 4 DA ALPHA:  (3 DA O3')-(4 DA P)-(4 DA O5')-(4 DA C5') -90.0 -30.0
 &rst    iat =   92,   93,   96,   97,
  r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
 &end

# 6 DT ALPHA:  (5 FAG O3')-(6 DT P)-(6 DT O5')-(6 DT C5') -90.0 -30.0
 &rst    iat =  196,  197,  200,  201,
  r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
 &end

# 7 DT ALPHA:  (6 DT O3')-(7 DT P)-(7 DT O5')-(7 DT C5') -90.0 -30.0
 &rst    iat =  228,  229,  232,  233,
  r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
 &end

# 8 DT ALPHA:  (7 DT O3')-(8 DT P)-(8 DT O5')-(8 DT C5') -90.0 -30.0
 &rst    iat =  260,  261,  264,  265,
  r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
 &end

# 9 DC ALPHA:  (8 DT O3')-(9 DC P)-(9 DC O5')-(9 DC C5') -90.0 -30.0
 &rst    iat =  292,  293,  296,  297,
  r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
 &end

# 12 DG ALPHA:  (11 DT5 O3')-(12 DG P)-(12 DG O5')-(12 DG C5') -90.0 -30.0
 &rst    iat =  385,  386,  389,  390,
  r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
 &end

# 13 DA ALPHA:  (12 DG O3')-(13 DA P)-(13 DA O5')-(13 DA C5') -90.0 -30.0
 &rst    iat =  418,  419,  422,  423,
  r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
 &end

# 14 DA ALPHA:  (13 DA O3')-(14 DA P)-(14 DA O5')-(14 DA C5') -90.0 -30.0
 &rst    iat =  450,  451,  454,  455,
  r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
 &end

# 15 DA ALPHA:  (14 DA O3')-(15 DA P)-(15 DA O5')-(15 DA C5') -90.0 -30.0
 &rst    iat =  482,  483,  486,  487,
  r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
```

```
        &end

# 17 DT ALPHA:  (16 DC O3')-(17 DT P)-(17 DT O5')-(17 DT C5') -90.0 -30.0
 &rst    iat =   544,   545,   548,   549,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 18 DT ALPHA:  (17 DT O3')-(18 DT P)-(18 DT O5')-(18 DT C5') -90.0 -30.0
 &rst    iat =   576,   577,   580,   581,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 19 DA ALPHA:  (18 DT O3')-(19 DA P)-(19 DA O5')-(19 DA C5') -90.0 -30.0
 &rst    iat =   608,   609,   612,   613,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 2 DT BETA:  (2 DT P)-(2 DT O5')-(2 DT C5')-(2 DT C4') 150.0 210.0
 &rst    iat =    29,    32,    33,    36,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
        &end

# 3 DA BETA:  (3 DA P)-(3 DA O5')-(3 DA C5')-(3 DA C4') 150.0 210.0
 &rst    iat =    61,    64,    65,    68,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
        &end

# 4 DA BETA:  (4 DA P)-(4 DA O5')-(4 DA C5')-(4 DA C4') 150.0 210.0
 &rst    iat =    93,    96,    97,   100,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
        &end

# 6 DT BETA:  (6 DT P)-(6 DT O5')-(6 DT C5')-(6 DT C4') 150.0 210.0
 &rst    iat =   197,   200,   201,   204,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
        &end

# 7 DT BETA:  (7 DT P)-(7 DT O5')-(7 DT C5')-(7 DT C4') 150.0 210.0
 &rst    iat =   229,   232,   233,   236,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
        &end

# 8 DT BETA:  (8 DT P)-(8 DT O5')-(8 DT C5')-(8 DT C4') 150.0 210.0
 &rst    iat =   261,   264,   265,   268,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
        &end
```

```
# 9 DC BETA:  (9 DC P)-(9 DC O5')-(9 DC C5')-(9 DC C4') 150.0 210.0
 &rst     iat =   293,   296,   297,   300,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 12 DG BETA:  (12 DG P)-(12 DG O5')-(12 DG C5')-(12 DG C4') 150.0 210.0
 &rst     iat =   386,   389,   390,   393,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 13 DA BETA:  (13 DA P)-(13 DA O5')-(13 DA C5')-(13 DA C4') 150.0 210.0
 &rst     iat =   419,   422,   423,   426,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 14 DA BETA:  (14 DA P)-(14 DA O5')-(14 DA C5')-(14 DA C4') 150.0 210.0
 &rst     iat =   451,   454,   455,   458,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 15 DA BETA:  (15 DA P)-(15 DA O5')-(15 DA C5')-(15 DA C4') 150.0 210.0
 &rst     iat =   483,   486,   487,   490,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 17 DT BETA:  (17 DT P)-(17 DT O5')-(17 DT C5')-(17 DT C4') 150.0 210.0
 &rst     iat =   545,   548,   549,   552,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 18 DT BETA:  (18 DT P)-(18 DT O5')-(18 DT C5')-(18 DT C4') 150.0 210.0
 &rst     iat =   577,   580,   581,   584,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 19 DA BETA:  (19 DA P)-(19 DA O5')-(19 DA C5')-(19 DA C4') 150.0 210.0
 &rst     iat =   609,   612,   613,   616,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 2 DT GAMMA:  (2 DT O5')-(2 DT C5')-(2 DT C4')-(2 DT C3')  30.0  90.0
 &rst     iat =    32,    33,    36,    55,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end
```

```
# 3 DA GAMMA:  (3 DA O5')-(3 DA C5')-(3 DA C4')-(3 DA C3')  30.0  90.0
 &rst     iat =    64,    65,    68,    87,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 4 DA GAMMA:  (4 DA O5')-(4 DA C5')-(4 DA C4')-(4 DA C3')  30.0  90.0
 &rst     iat =    96,    97,   100,   119,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 6 DT GAMMA:  (6 DT O5')-(6 DT C5')-(6 DT C4')-(6 DT C3')  30.0  90.0
 &rst     iat =   200,   201,   204,   223,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 7 DT GAMMA:  (7 DT O5')-(7 DT C5')-(7 DT C4')-(7 DT C3')  30.0  90.0
 &rst     iat =   232,   233,   236,   255,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 8 DT GAMMA:  (8 DT O5')-(8 DT C5')-(8 DT C4')-(8 DT C3')  30.0  90.0
 &rst     iat =   264,   265,   268,   287,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 9 DC GAMMA:  (9 DC O5')-(9 DC C5')-(9 DC C4')-(9 DC C3')  30.0  90.0
 &rst     iat =   296,   297,   300,   317,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 12 DG GAMMA:  (12 DG O5')-(12 DG C5')-(12 DG C4')-(12 DG C3')  30.0  90.0
 &rst     iat =   389,   390,   393,   413,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 13 DA GAMMA:  (13 DA O5')-(13 DA C5')-(13 DA C4')-(13 DA C3')  30.0  90.0
 &rst     iat =   422,   423,   426,   445,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 14 DA GAMMA:  (14 DA O5')-(14 DA C5')-(14 DA C4')-(14 DA C3')  30.0  90.0
 &rst     iat =   454,   455,   458,   477,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 15 DA GAMMA:  (15 DA O5')-(15 DA C5')-(15 DA C4')-(15 DA C3')  30.0  90.0
```

```
 &rst     iat =   486,   487,   490,   509,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 17 DT GAMMA:  (17 DT O5')-(17 DT C5')-(17 DT C4')-(17 DT C3')  30.0  90.0
 &rst     iat =   548,   549,   552,   571,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 18 DT GAMMA:  (18 DT O5')-(18 DT C5')-(18 DT C4')-(18 DT C3')  30.0  90.0
 &rst     iat =   580,   581,   584,   603,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 19 DA GAMMA:  (19 DA O5')-(19 DA C5')-(19 DA C4')-(19 DA C3')  30.0  90.0
 &rst     iat =   612,   613,   616,   635,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 2 DT EPSILN:  (2 DT C4')-(2 DT C3')-(2 DT O3')-(3 DA P) 165.0 225.0
 &rst     iat =    36,    55,    60,    61,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 3 DA EPSILN:  (3 DA C4')-(3 DA C3')-(3 DA O3')-(4 DA P) 165.0 225.0
 &rst     iat =    68,    87,    92,    93,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 4 DA EPSILN:  (4 DA C4')-(4 DA C3')-(4 DA O3')-(5 FAG P) 165.0 225.0
 &rst     iat =   100,   119,   124,   125,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 6 DT EPSILN:  (6 DT C4')-(6 DT C3')-(6 DT O3')-(7 DT P) 165.0 225.0
 &rst     iat =   204,   223,   228,   229,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 7 DT EPSILN:  (7 DT C4')-(7 DT C3')-(7 DT O3')-(8 DT P) 165.0 225.0
 &rst     iat =   236,   255,   260,   261,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 8 DT EPSILN:  (8 DT C4')-(8 DT C3')-(8 DT O3')-(9 DC P) 165.0 225.0
 &rst     iat =   268,   287,   292,   293,
```

```
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 9 DC EPSILN:  (9 DC C4')-(9 DC C3')-(9 DC O3')-(10 DA3 P) 165.0 225.0
 &rst    iat =   300,   317,   322,   323,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 12 DG EPSILN:  (12 DG C4')-(12 DG C3')-(12 DG O3')-(13 DA P) 165.0 225.0
 &rst    iat =   393,   413,   418,   419,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 13 DA EPSILN:  (13 DA C4')-(13 DA C3')-(13 DA O3')-(14 DA P) 165.0 225.0
 &rst    iat =   426,   445,   450,   451,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 14 DA EPSILN:  (14 DA C4')-(14 DA C3')-(14 DA O3')-(15 DA P) 165.0 225.0
 &rst    iat =   458,   477,   482,   483,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 15 DA EPSILN:  (15 DA C4')-(15 DA C3')-(15 DA O3')-(16 DC P) 165.0 225.0
 &rst    iat =   490,   509,   514,   515,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 17 DT EPSILN:  (17 DT C4')-(17 DT C3')-(17 DT O3')-(18 DT P) 165.0 225.0
 &rst    iat =   552,   571,   576,   577,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 18 DT EPSILN:  (18 DT C4')-(18 DT C3')-(18 DT O3')-(19 DA P) 165.0 225.0
 &rst    iat =   584,   603,   608,   609,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 19 DA EPSILN:  (19 DA C4')-(19 DA C3')-(19 DA O3')-(20 DG3 P) 165.0 225.0
 &rst    iat =   616,   635,   640,   641,
  r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
 &end

# 2 DT ZETA:  (2 DT C3')-(2 DT O3')-(3 DA P)-(3 DA O5') -135.0 -75.0
 &rst    iat =    55,    60,    61,    64,
  r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
```

```
        &end

# 3 DA ZETA:  (3 DA C3')-(3 DA O3')-(4 DA P)-(4 DA O5') -135.0 -75.0
 &rst    iat =   87,   92,   93,   96,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end

# 4 DA ZETA:  (4 DA C3')-(4 DA O3')-(5 FAG P)-(5 FAG O5') -135.0 -75.0
 &rst    iat =  119,  124,  125,  128,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end

# 6 DT ZETA:  (6 DT C3')-(6 DT O3')-(7 DT P)-(7 DT O5') -135.0 -75.0
 &rst    iat =  223,  228,  229,  232,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end

# 7 DT ZETA:  (7 DT C3')-(7 DT O3')-(8 DT P)-(8 DT O5') -135.0 -75.0
 &rst    iat =  255,  260,  261,  264,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end

# 8 DT ZETA:  (8 DT C3')-(8 DT O3')-(9 DC P)-(9 DC O5') -135.0 -75.0
 &rst    iat =  287,  292,  293,  296,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end

# 9 DC ZETA:  (9 DC C3')-(9 DC O3')-(10 DA3 P)-(10 DA3 O5') -135.0 -75.0
 &rst    iat =  317,  322,  323,  326,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end

# 12 DG ZETA:  (12 DG C3')-(12 DG O3')-(13 DA P)-(13 DA O5') -135.0 -75.0
 &rst    iat =  413,  418,  419,  422,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end

# 13 DA ZETA:  (13 DA C3')-(13 DA O3')-(14 DA P)-(14 DA O5') -135.0 -75.0
 &rst    iat =  445,  450,  451,  454,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end

# 14 DA ZETA:  (14 DA C3')-(14 DA O3')-(15 DA P)-(15 DA O5') -135.0 -75.0
 &rst    iat =  477,  482,  483,  486,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end
```

```
# 15 DA ZETA:  (15 DA C3')-(15 DA O3')-(16 DC P)-(16 DC O5') -135.0 -75.0
 &rst    iat =   509,   514,   515,   518,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 17 DT ZETA:  (17 DT C3')-(17 DT O3')-(18 DT P)-(18 DT O5') -135.0 -75.0
 &rst    iat =   571,   576,   577,   580,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 18 DT ZETA:  (18 DT C3')-(18 DT O3')-(19 DA P)-(19 DA O5') -135.0 -75.0
 &rst    iat =   603,   608,   609,   612,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 19 DA ZETA:  (19 DA C3')-(19 DA O3')-(20 DG3 P)-(20 DG3 O5') -135.0 -75.0
 &rst    iat =   635,   640,   641,   644,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 674 atoms read from pdb file AGT_amber.pdb.
# 2 DT NU0:  (2 DT C4')-(2 DT O4')-(2 DT C1')-(2 DT C2') -52.1 -22.1
 &rst    iat =    36,    38,    39,    57,
          r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
          rk2 =   2.0, rk3 =   2.0,                                  &end

# 2 DT NU1:  (2 DT O4')-(2 DT C1')-(2 DT C2')-(2 DT C3')  15.0  45.0
 &rst    iat =    38,    39,    57,    55,
          r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 2 DT NU2:  (2 DT C1')-(2 DT C2')-(2 DT C3')-(2 DT C4') -27.4   2.6
 &rst    iat =    39,    57,    55,    36,
          r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 2 DT NU3:  (2 DT C2')-(2 DT C3')-(2 DT C4')-(2 DT O4') -25.0   5.0
 &rst    iat =    57,    55,    36,    38,
          r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 2 DT NU4:  (2 DT C3')-(2 DT C4')-(2 DT O4')-(2 DT C1')  13.5  43.5
 &rst    iat =    55,    36,    38,    39,
          r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end
```

```
# 3 DA NU0:  (3 DA C4')-(3 DA O4')-(3 DA C1')-(3 DA C2') -43.9 -13.9
 &rst     iat =    68,    70,    71,    89,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
         &end

# 3 DA NU1:  (3 DA O4')-(3 DA C1')-(3 DA C2')-(3 DA C3')  22.2  52.2
 &rst     iat =    70,    71,    89,    87,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
         &end

# 3 DA NU2:  (3 DA C1')-(3 DA C2')-(3 DA C3')-(3 DA C4') -44.6 -14.6
 &rst     iat =    71,    89,    87,    68,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
         &end

# 3 DA NU3:  (3 DA C2')-(3 DA C3')-(3 DA C4')-(3 DA O4')  -3.2  26.8
 &rst     iat =    89,    87,    68,    70,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
         &end

# 3 DA NU4:  (3 DA C3')-(3 DA C4')-(3 DA O4')-(3 DA C1')  -4.4  25.6
 &rst     iat =    87,    68,    70,    71,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
         &end

# 4 DA NU0:  (4 DA C4')-(4 DA O4')-(4 DA C1')-(4 DA C2') -43.9 -13.9
 &rst     iat =   100,   102,   103,   121,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
         &end

# 4 DA NU1:  (4 DA O4')-(4 DA C1')-(4 DA C2')-(4 DA C3')  22.2  52.2
 &rst     iat =   102,   103,   121,   119,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
         &end

# 4 DA NU2:  (4 DA C1')-(4 DA C2')-(4 DA C3')-(4 DA C4') -44.6 -14.6
 &rst     iat =   103,   121,   119,   100,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
         &end

# 4 DA NU3:  (4 DA C2')-(4 DA C3')-(4 DA C4')-(4 DA O4')  -3.2  26.8
 &rst     iat =   121,   119,   100,   102,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
         &end
```

```
# 4 DA NU4:  (4 DA C3')-(4 DA C4')-(4 DA O4')-(4 DA C1')  -4.4  25.6
 &rst     iat =   119,   100,   102,   103,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
         &end

# 6 DT NU0:  (6 DT C4')-(6 DT O4')-(6 DT C1')-(6 DT C2') -52.1 -22.1
 &rst     iat =   204,   206,   207,   225,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
         &end

# 6 DT NU1:  (6 DT O4')-(6 DT C1')-(6 DT C2')-(6 DT C3')  15.0  45.0
 &rst     iat =   206,   207,   225,   223,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 6 DT NU2:  (6 DT C1')-(6 DT C2')-(6 DT C3')-(6 DT C4') -27.4   2.6
 &rst     iat =   207,   225,   223,   204,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 6 DT NU3:  (6 DT C2')-(6 DT C3')-(6 DT C4')-(6 DT O4') -25.0   5.0
 &rst     iat =   225,   223,   204,   206,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 6 DT NU4:  (6 DT C3')-(6 DT C4')-(6 DT O4')-(6 DT C1')  13.5  43.5
 &rst     iat =   223,   204,   206,   207,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end

# 7 DT NU0:  (7 DT C4')-(7 DT O4')-(7 DT C1')-(7 DT C2') -52.1 -22.1
 &rst     iat =   236,   238,   239,   257,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
         &end

# 7 DT NU1:  (7 DT O4')-(7 DT C1')-(7 DT C2')-(7 DT C3')  15.0  45.0
 &rst     iat =   238,   239,   257,   255,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 7 DT NU2:  (7 DT C1')-(7 DT C2')-(7 DT C3')-(7 DT C4') -27.4   2.6
 &rst     iat =   239,   257,   255,   236,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 7 DT NU3:  (7 DT C2')-(7 DT C3')-(7 DT C4')-(7 DT O4') -25.0   5.0
```

```
 &rst     iat =   257,   255,   236,   238,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
          &end

# 7 DT NU4:  (7 DT C3')-(7 DT C4')-(7 DT O4')-(7 DT C1')  13.5  43.5
 &rst     iat =   255,   236,   238,   239,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
          &end

# 8 DT NU0:  (8 DT C4')-(8 DT O4')-(8 DT C1')-(8 DT C2') -52.1 -22.1
 &rst     iat =   268,   270,   271,   289,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
          &end

# 8 DT NU1:  (8 DT O4')-(8 DT C1')-(8 DT C2')-(8 DT C3')  15.0  45.0
 &rst     iat =   270,   271,   289,   287,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
          &end

# 8 DT NU2:  (8 DT C1')-(8 DT C2')-(8 DT C3')-(8 DT C4') -27.4   2.6
 &rst     iat =   271,   289,   287,   268,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
          &end

# 8 DT NU3:  (8 DT C2')-(8 DT C3')-(8 DT C4')-(8 DT O4') -25.0   5.0
 &rst     iat =   289,   287,   268,   270,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
          &end

# 8 DT NU4:  (8 DT C3')-(8 DT C4')-(8 DT O4')-(8 DT C1')  13.5  43.5
 &rst     iat =   287,   268,   270,   271,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
          &end

# 9 DC NU0:  (9 DC C4')-(9 DC O4')-(9 DC C1')-(9 DC C2') -44.7 -14.7
 &rst     iat =   300,   302,   303,   319,
           r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
          &end

# 9 DC NU1:  (9 DC O4')-(9 DC C1')-(9 DC C2')-(9 DC C3')  18.1  48.1
 &rst     iat =   302,   303,   319,   317,
           r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
          &end

# 9 DC NU2:  (9 DC C1')-(9 DC C2')-(9 DC C3')-(9 DC C4') -37.2  -6.7
 &rst     iat =   303,   319,   317,   300,
```

```
  r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
 &end

# 9 DC NU3:  (9 DC C2')-(9 DC C3')-(9 DC C4')-(9 DC O4') -16.9  24.2
 &rst    iat =   319,   317,   300,   302,
  r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
 &end

# 9 DC NU4:  (9 DC C3')-(9 DC C4')-(9 DC O4')-(9 DC C1')  -1.9  34.0
 &rst    iat =   317,   300,   302,   303,
  r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
 &end

# 12 DG NU0:  (12 DG C4')-(12 DG O4')-(12 DG C1')-(12 DG C2') -44.7 -14.7
 &rst    iat =   393,   395,   396,   415,
  r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
 &end

# 12 DG NU1:  (12 DG O4')-(12 DG C1')-(12 DG C2')-(12 DG C3')  18.1  48.1
 &rst    iat =   395,   396,   415,   413,
  r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
 &end

# 12 DG NU2:  (12 DG C1')-(12 DG C2')-(12 DG C3')-(12 DG C4') -37.2  -6.7
 &rst    iat =   396,   415,   413,   393,
  r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
 &end

# 12 DG NU3:  (12 DG C2')-(12 DG C3')-(12 DG C4')-(12 DG O4') -16.9  24.2
 &rst    iat =   415,   413,   393,   395,
  r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
 &end

# 12 DG NU4:  (12 DG C3')-(12 DG C4')-(12 DG O4')-(12 DG C1')  -1.9  34.0
 &rst    iat =   413,   393,   395,   396,
  r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
 &end

# 13 DA NU0:  (13 DA C4')-(13 DA O4')-(13 DA C1')-(13 DA C2') -43.9 -13.9
 &rst    iat =   426,   428,   429,   447,
  r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
 &end

# 13 DA NU1:  (13 DA O4')-(13 DA C1')-(13 DA C2')-(13 DA C3')  22.2  52.2
 &rst    iat =   428,   429,   447,   445,
  r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
```

```
        &end

# 13 DA NU2:  (13 DA C1')-(13 DA C2')-(13 DA C3')-(13 DA C4') -44.6 -14.6
 &rst    iat =   429,   447,   445,   426,
          r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
        &end

# 13 DA NU3:  (13 DA C2')-(13 DA C3')-(13 DA C4')-(13 DA O4')  -3.2  26.8
 &rst    iat =   447,   445,   426,   428,
          r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
        &end

# 13 DA NU4:  (13 DA C3')-(13 DA C4')-(13 DA O4')-(13 DA C1')  -4.4  25.6
 &rst    iat =   445,   426,   428,   429,
          r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
        &end

# 14 DA NU0:  (14 DA C4')-(14 DA O4')-(14 DA C1')-(14 DA C2') -43.9 -13.9
 &rst    iat =   458,   460,   461,   479,
          r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
        &end

# 14 DA NU1:  (14 DA O4')-(14 DA C1')-(14 DA C2')-(14 DA C3')  22.2  52.2
 &rst    iat =   460,   461,   479,   477,
          r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
        &end

# 14 DA NU2:  (14 DA C1')-(14 DA C2')-(14 DA C3')-(14 DA C4') -44.6 -14.6
 &rst    iat =   461,   479,   477,   458,
          r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
        &end

# 14 DA NU3:  (14 DA C2')-(14 DA C3')-(14 DA C4')-(14 DA O4')  -3.2  26.8
 &rst    iat =   479,   477,   458,   460,
          r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
        &end

# 14 DA NU4:  (14 DA C3')-(14 DA C4')-(14 DA O4')-(14 DA C1')  -4.4  25.6
 &rst    iat =   477,   458,   460,   461,
          r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
        &end

# 15 DA NU0:  (15 DA C4')-(15 DA O4')-(15 DA C1')-(15 DA C2') -43.9 -13.9
 &rst    iat =   490,   492,   493,   511,
          r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
        &end
```

```
# 15 DA NU1:  (15 DA O4')-(15 DA C1')-(15 DA C2')-(15 DA C3')  22.2  52.2
 &rst     iat =   492,   493,   511,   509,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
         &end

# 15 DA NU2:  (15 DA C1')-(15 DA C2')-(15 DA C3')-(15 DA C4') -44.6 -14.6
 &rst     iat =   493,   511,   509,   490,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
         &end

# 15 DA NU3:  (15 DA C2')-(15 DA C3')-(15 DA C4')-(15 DA O4')  -3.2  26.8
 &rst     iat =   511,   509,   490,   492,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
         &end

# 15 DA NU4:  (15 DA C3')-(15 DA C4')-(15 DA O4')-(15 DA C1')  -4.4  25.6
 &rst     iat =   509,   490,   492,   493,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
         &end

# 17 DT NU0:  (17 DT C4')-(17 DT O4')-(17 DT C1')-(17 DT C2') -52.1 -22.1
 &rst     iat =   552,   554,   555,   573,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
         &end

# 17 DT NU1:  (17 DT O4')-(17 DT C1')-(17 DT C2')-(17 DT C3')  15.0  45.0
 &rst     iat =   554,   555,   573,   571,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 17 DT NU2:  (17 DT C1')-(17 DT C2')-(17 DT C3')-(17 DT C4') -27.4   2.6
 &rst     iat =   555,   573,   571,   552,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 17 DT NU3:  (17 DT C2')-(17 DT C3')-(17 DT C4')-(17 DT O4') -25.0   5.0
 &rst     iat =   573,   571,   552,   554,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 17 DT NU4:  (17 DT C3')-(17 DT C4')-(17 DT O4')-(17 DT C1')  13.5  43.5
 &rst     iat =   571,   552,   554,   555,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end
```

```
# 18 DT NU0:  (18 DT C4')-(18 DT O4')-(18 DT C1')-(18 DT C2') -52.1 -22.1
 &rst     iat =   584,   586,   587,   605,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
          &end

# 18 DT NU1:  (18 DT O4')-(18 DT C1')-(18 DT C2')-(18 DT C3')  15.0  45.0
 &rst     iat =   586,   587,   605,   603,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
          &end

# 18 DT NU2:  (18 DT C1')-(18 DT C2')-(18 DT C3')-(18 DT C4') -27.4   2.6
 &rst     iat =   587,   605,   603,   584,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
          &end

# 18 DT NU3:  (18 DT C2')-(18 DT C3')-(18 DT C4')-(18 DT O4') -25.0   5.0
 &rst     iat =   605,   603,   584,   586,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
          &end

# 18 DT NU4:  (18 DT C3')-(18 DT C4')-(18 DT O4')-(18 DT C1')  13.5  43.5
 &rst     iat =   603,   584,   586,   587,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
          &end

# 19 DA NU0:  (19 DA C4')-(19 DA O4')-(19 DA C1')-(19 DA C2') -43.9 -13.9
 &rst     iat =   616,   618,   619,   637,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
          &end

# 19 DA NU1:  (19 DA O4')-(19 DA C1')-(19 DA C2')-(19 DA C3')  22.2  52.2
 &rst     iat =   618,   619,   637,   635,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
          &end

# 19 DA NU2:  (19 DA C1')-(19 DA C2')-(19 DA C3')-(19 DA C4') -44.6 -14.6
 &rst     iat =   619,   637,   635,   616,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
          &end

# 19 DA NU3:  (19 DA C2')-(19 DA C3')-(19 DA C4')-(19 DA O4')  -3.2  26.8
 &rst     iat =   637,   635,   616,   618,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
          &end

# 19 DA NU4:  (19 DA C3')-(19 DA C4')-(19 DA O4')-(19 DA C1')  -4.4  25.6
```

```
&rst     iat =   635,   616,   618,   619,
          r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
         &end
```

Table C-7. Experimental distance and torsion angle restraints used in the rMD calculations of the AFB1-β-FAPY modified AXY adduct.

```
#
#   1 DC5   H2'1  1 DC5 H3'     1.660   2.380
 &rst
  ixpk= 0, nxpk= 0, iat=  26,  24, r1= 1.16, r2= 1.66, r3= 2.38, r4= 2.88,
     rk2=32.0, rk3=32.0, ir6=1, ialtd=0,
 &end
#
#   1 DC5   H2'2  1 DC5 H3'     2.090   2.850
 &rst
  ixpk= 0, nxpk= 0, iat=  27,  24, r1= 1.59, r2= 2.09, r3= 2.85, r4= 3.35,  &end
#
#   1 DC5   H1'   1 DC5 H3'     2.990   3.870
 &rst
  ixpk= 0, nxpk= 0, iat=  10,  24, r1= 2.49, r2= 2.99, r3= 3.87, r4= 4.37,  &end
#
#   1 DC5   H1'   1 DC5 H2'1    2.440   3.030
 &rst
  ixpk= 0, nxpk= 0, iat=  10,  26, r1= 1.94, r2= 2.44, r3= 3.03, r4= 3.53,  &end
#
#   1 DC5   H5    1 DC5 H3'     6.190   6.590
 &rst
  ixpk= 0, nxpk= 0, iat=  15,  24, r1= 5.69, r2= 6.19, r3= 6.59, r4= 7.09,  &end
#
#   1 DC5   H5    1 DC5 H2'1    4.060   4.500
 &rst
  ixpk= 0, nxpk= 0, iat=  15,  26, r1= 3.56, r2= 4.06, r3= 4.50, r4= 5.00,  &end
#
#   1 DC5   H5    1 DC5 H2'2    5.260   5.700
 &rst
  ixpk= 0, nxpk= 0, iat=  15,  27, r1= 4.76, r2= 5.26, r3= 5.70, r4= 6.20,  &end
#
#   1 DC5   H6    1 DC5 H3'     3.440   4.280
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  24, r1= 2.94, r2= 3.44, r3= 4.28, r4= 4.78,  &end
#
#   1 DC5   H6    1 DC5 H2'1    1.670   2.340
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  26, r1= 1.17, r2= 1.67, r3= 2.34, r4= 2.84,  &end
```

```
#
#   1 DC5   H6    1 DC5 H2'2    3.160   3.820
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  27, r1= 2.66, r2= 3.16, r3= 3.82, r4= 4.32,  &end
#
#   1 DC5   H6    1 DC5 H1'     3.160   3.790
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  10, r1= 2.66, r2= 3.16, r3= 3.79, r4= 4.29,  &end
#
#   2 DT    Q5    1 DC5 H3'     2.840   3.580
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  24, r1= 2.34, r2= 2.84, r3= 4.30, r4= 4.80,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H2'1    2.000   3.010
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  26, r1= 1.50, r2= 2.00, r3= 3.61, r4= 4.11,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H2'2    2.010   3.090
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  27, r1= 1.51, r2= 2.01, r3= 3.71, r4= 4.21,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H1'     2.960   4.530
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  10, r1= 2.46, r2= 2.96, r3= 5.44, r4= 5.94,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H5      1.570   2.930
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  15, r1= 1.07, r2= 1.57, r3= 3.52, r4= 4.02,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H6      2.010   2.560
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  13, r1= 1.51, r2= 2.01, r3= 3.07, r4= 3.57,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    H6    1 DC5 H1'     3.980   4.180
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  10, r1= 3.48, r2= 3.98, r3= 4.18, r4= 4.68,  &end
#
#   2 DT    H6    1 DC5 H2'2    2.500   2.710
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  27, r1= 2.00, r2= 2.50, r3= 2.71, r4= 3.21,  &end
#
#   2 DT    H6    1 DC5 H2'1    3.810   4.290
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  26, r1= 3.31, r2= 3.81, r3= 4.29, r4= 4.79,  &end
#
#   2 DT    H6    1 DC5 H3'     4.980   5.280
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  24, r1= 4.48, r2= 4.98, r3= 5.28, r4= 5.78,  &end
#
#   2 DT    H6    1 DC5 H6      5.000   5.320
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  13, r1= 4.50, r2= 5.00, r3= 5.32, r4= 5.82,  &end
#
#   2 DT    Q5    2 DT  H3'     3.250   6.510
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  56, r1= 2.75, r2= 3.25, r3= 7.82, r4= 8.32,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    2 DT  H1'     3.800   5.670
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  40, r1= 3.30, r2= 3.80, r3= 6.81, r4= 7.31,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    H2'2  2 DT  H3'     2.290   2.950
 &rst
  ixpk= 0, nxpk= 0, iat=  59,  56, r1= 1.79, r2= 2.29, r3= 2.95, r4= 3.45,  &end
#
#   2 DT    H1'   2 DT  H3'     3.590   4.010
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  56, r1= 3.09, r2= 3.59, r3= 4.01, r4= 4.51,  &end
#
#   2 DT    H1'   2 DT  H2'1    2.510   3.080
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  58, r1= 2.01, r2= 2.51, r3= 3.08, r4= 3.58,  &end
#
#   2 DT    H1'   2 DT  H2'2    1.870   2.490
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  59, r1= 1.37, r2= 1.87, r3= 2.49, r4= 2.99,  &end
```

```
#
#   2 DT    H6    2 DT  H1'     3.540   3.960
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  40, r1= 3.04, r2= 3.54, r3= 3.96, r4= 4.46,  &end
#
#   3 DA    H61   2 DT  H3      3.570   3.720
 &rst
  ixpk= 0, nxpk= 0, iat=  80,  52, r1= 3.07, r2= 3.57, r3= 3.72, r4= 4.22,  &end
#
#   3 DA    H62   2 DT  H3      4.270   4.520
 &rst
  ixpk= 0, nxpk= 0, iat=  81,  52, r1= 3.77, r2= 4.27, r3= 4.52, r4= 5.02,  &end
#
#   3 DA    H2    2 DT  H3      3.770   4.220
 &rst
  ixpk= 0, nxpk= 0, iat=  84,  52, r1= 3.27, r2= 3.77, r3= 4.22, r4= 4.72,  &end
#
#   3 DA    H61  18 DT  H3      2.370   2.620
 &rst
  ixpk= 0, nxpk= 0, iat=  80, 600, r1= 1.87, r2= 2.37, r3= 2.62, r4= 3.12,  &end
#
#   3 DA    H62  18 DT  H3      3.770   4.120
 &rst
  ixpk= 0, nxpk= 0, iat=  81, 600, r1= 3.27, r2= 3.77, r3= 4.12, r4= 4.62,  &end
#
#   3 DA    H2   19 DA  H2      2.570   3.020
 &rst
  ixpk= 0, nxpk= 0, iat=  84, 632, r1= 2.07, r2= 2.57, r3= 3.02, r4= 3.52,  &end
#
#   3 DA    H8    2 DT  H3'     4.970   5.220
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  56, r1= 4.47, r2= 4.97, r3= 5.22, r4= 5.72,  &end
#
#   3 DA    H8    2 DT  H2'1    4.400   4.660
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  58, r1= 3.90, r2= 4.40, r3= 4.66, r4= 5.16,  &end
#
#   3 DA    H8    2 DT  H2'2    2.650   3.060
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  59, r1= 2.15, r2= 2.65, r3= 3.06, r4= 3.56,  &end
#
#   3 DA    H8    2 DT  H1'     3.640   3.950
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  40, r1= 3.14, r2= 3.64, r3= 3.95, r4= 4.45,  &end
#
#   3 DA    H1'   3 DA  H2'2    2.260   2.960
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  72,  91, r1= 1.76, r2= 2.26, r3= 2.96, r4= 3.46,  &end
#
#   3 DA    H1'   3 DA  H2'1    3.070   3.850
 &rst
  ixpk= 0, nxpk= 0, iat=  72,  90, r1= 2.57, r2= 3.07, r3= 3.85, r4= 4.35,  &end
#
#   3 DA    H8    3 DA  H1'     3.710   4.120
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  72, r1= 3.21, r2= 3.71, r3= 4.12, r4= 4.62,  &end
#
#   3 DA    H8    3 DA  H2'2    3.310   4.320
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  91, r1= 2.81, r2= 3.31, r3= 4.32, r4= 4.82,  &end
#
#   4 DA    H2    3 DA  H2      4.470   4.820
 &rst
  ixpk= 0, nxpk= 0, iat= 116,  84, r1= 3.97, r2= 4.47, r3= 4.82, r4= 5.32,  &end
#
#   4 DA    H2   18 DT  H3      4.270   4.420
 &rst
  ixpk= 0, nxpk= 0, iat= 116, 600, r1= 3.77, r2= 4.27, r3= 4.42, r4= 4.92,  &end
#
#   4 DA    H61  18 DT  H3      4.870   5.120
 &rst
  ixpk= 0, nxpk= 0, iat= 112, 600, r1= 4.37, r2= 4.87, r3= 5.12, r4= 5.62,  &end
#
#   4 DA    H62  18 DT  H3      5.770   6.120
 &rst
  ixpk= 0, nxpk= 0, iat= 113, 600, r1= 5.27, r2= 5.77, r3= 6.12, r4= 6.62,  &end
#
#   4 DA    H2   17 DT  H3      2.370   2.620
 &rst
  ixpk= 0, nxpk= 0, iat= 116, 568, r1= 1.87, r2= 2.37, r3= 2.62, r4= 3.12,  &end
#
#   4 DA    H61  17 DT  H3      2.770   3.020
 &rst
  ixpk= 0, nxpk= 0, iat= 112, 568, r1= 2.27, r2= 2.77, r3= 3.02, r4= 3.52,  &end
#
#   4 DA    H62  17 DT  H3      4.170   4.620
 &rst
  ixpk= 0, nxpk= 0, iat= 113, 568, r1= 3.67, r2= 4.17, r3= 4.62, r4= 5.12,  &end
#
#   4 DA    H1'   3 DA  H1'     5.410   5.610
 &rst
  ixpk= 0, nxpk= 0, iat= 104,  72, r1= 4.91, r2= 5.41, r3= 5.61, r4= 6.11,  &end
```

```
#
#   4 DA    H8    3 DA  H2'1    3.820   4.010
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  90, r1= 3.32, r2= 3.82, r3= 4.01, r4= 4.51,  &end
#
#   4 DA    H8    3 DA  H2'2    2.420   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  91, r1= 1.92, r2= 2.42, r3= 2.61, r4= 3.11,  &end
#
#   4 DA    H8    3 DA  H1'     3.860   4.060
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  72, r1= 3.36, r2= 3.86, r3= 4.06, r4= 4.56,  &end
#
#   4 DA    H8    3 DA  H8      4.670   4.980
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  75, r1= 4.17, r2= 4.67, r3= 4.98, r4= 5.48,  &end
#
#   4 DA    H1'   4 DA  H3'     3.580   4.240
 &rst
  ixpk= 0, nxpk= 0, iat= 104, 120, r1= 3.08, r2= 3.58, r3= 4.24, r4= 4.74,  &end
#
#   4 DA    H1'   4 DA  H2'1    2.700   3.090
 &rst
  ixpk= 0, nxpk= 0, iat= 104, 122, r1= 2.20, r2= 2.70, r3= 3.09, r4= 3.59,  &end
#
#   4 DA    H1'   4 DA  H2'2    2.040   2.500
 &rst
  ixpk= 0, nxpk= 0, iat= 104, 123, r1= 1.54, r2= 2.04, r3= 2.50, r4= 3.00,  &end
#
#   4 DA    H8    4 DA  H2'1    1.800   2.290
 &rst
  ixpk= 0, nxpk= 0, iat= 107, 122, r1= 1.30, r2= 1.80, r3= 2.29, r4= 2.79,  &end
#
#   4 DA    H8    4 DA  H2'2    3.340   3.500
 &rst
  ixpk= 0, nxpk= 0, iat= 107, 123, r1= 2.84, r2= 3.34, r3= 3.50, r4= 4.00,  &end
#
#   4 DA    H8    4 DA  H1'     3.160   3.740
 &rst
  ixpk= 0, nxpk= 0, iat= 107, 104, r1= 2.66, r2= 3.16, r3= 3.74, r4= 4.24,  &end
#
#   5 FAG   H9A   4 DA  H8      3.150   3.670
 &rst
  ixpk= 0, nxpk= 0, iat= 161, 107, r1= 2.65, r2= 3.15, r3= 3.67, r4= 4.17,  &end
#
#   5 FAG   H6A   4 DA  H3'     4.070   4.620
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 120, r1= 3.57, r2= 4.07, r3= 4.62, r4= 5.12,  &end
#
#   5 FAG   H6A   4 DA  H2'1    2.370   3.840
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 122, r1= 1.87, r2= 2.37, r3= 3.84, r4= 4.34,  &end
#
#   5 FAG   H6A   4 DA  H2'2    1.870   2.240
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 123, r1= 1.37, r2= 1.87, r3= 2.24, r4= 2.74,  &end
#
#   5 FAG   H6A   4 DA  H1'     2.340   3.160
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 104, r1= 1.84, r2= 2.34, r3= 3.16, r4= 3.66,  &end
#
#   5 FAG   H6A   4 DA  H8      2.310   2.890
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 107, r1= 1.81, r2= 2.31, r3= 2.89, r4= 3.39,  &end
#
#   5 FAG   H5    4 DA  H2'1    5.450   5.860
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 122, r1= 4.95, r2= 5.45, r3= 5.86, r4= 6.36,  &end
#
#   5 FAG   H5    4 DA  H2'2    4.420   4.830
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 123, r1= 3.92, r2= 4.42, r3= 4.83, r4= 5.33,  &end
#
#   5 FAG   H5    4 DA  H1'     3.070   3.480
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 104, r1= 2.57, r2= 3.07, r3= 3.48, r4= 3.98,  &end
#
#   5 FAG   H5    4 DA  H8      5.070   6.200
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 107, r1= 4.57, r2= 5.07, r3= 6.20, r4= 6.70,  &end
#
#   5 FAG   MA   17 DT  H3      2.500   5.500
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 568, r1= 2.00, r2= 2.50, r3= 6.61, r4= 7.11,
 igr1= 181, 182, 183,
 &end
#
#   5 FAG   MA          4 DA  H2      2.000   3.000
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 116, r1= 1.50, r2= 2.00, r3= 3.60, r4= 4.10,
 igr1= 181, 182, 183,
 &end
```

```
#
#   5 FAG   H2A   5 FAG H3A     2.190   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 171, 174, r1= 1.69, r2= 2.19, r3= 2.61, r4= 3.11,  &end
#
#   5 FAG   H2B   5 FAG H3A     2.970   3.440
 &rst
  ixpk= 0, nxpk= 0, iat= 172, 174, r1= 2.47, r2= 2.97, r3= 3.44, r4= 3.94,  &end
#
#   5 FAG   H2'1  5 FAG H1'     2.690   3.230
 &rst
  ixpk= 0, nxpk= 0, iat= 194, 136, r1= 2.19, r2= 2.69, r3= 3.23, r4= 3.73,  &end
#
#   5 FAG   H2'2  5 FAG H1'     2.080   2.600
 &rst
  ixpk= 0, nxpk= 0, iat= 195, 136, r1= 1.58, r2= 2.08, r3= 2.60, r4= 3.10,  &end
#
#   5 FAG   H3'   5 FAG H1'     3.630   4.150
 &rst
  ixpk= 0, nxpk= 0, iat= 192, 136, r1= 3.13, r2= 3.63, r3= 4.15, r4= 4.65,  &end
#
#   5 FAG   H3'   5 FAG H2'1    2.430   3.070
 &rst
  ixpk= 0, nxpk= 0, iat= 192, 194, r1= 1.93, r2= 2.43, r3= 3.07, r4= 3.57,  &end
#
#   5 FAG   H8    5 FAG H1'     5.230   5.990
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 136, r1= 4.73, r2= 5.23, r3= 5.99, r4= 6.49,  &end
#
#   5 FAG   H8    5 FAG H8A     3.440   4.200
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 155, r1= 2.94, r2= 3.44, r3= 4.20, r4= 4.70,  &end
#
#   5 FAG   H9    5 FAG H8A     2.420   2.950
 &rst
  ixpk= 0, nxpk= 0, iat= 159, 155, r1= 1.92, r2= 2.42, r3= 2.95, r4= 3.45,  &end
#
#   5 FAG   H9    5 FAG H8      2.540   3.690
 &rst
  ixpk= 0, nxpk= 0, iat= 159, 152, r1= 2.04, r2= 2.54, r3= 3.69, r4= 4.19,  &end
#
#   5 FAG   H9A   5 FAG H9      2.490   2.960
 &rst
  ixpk= 0, nxpk= 0, iat= 161, 159, r1= 1.99, r2= 2.49, r3= 2.96, r4= 3.46,  &end
#
#   5 FAG   H6A   5 FAG H9A     1.600   2.420
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 161, r1= 1.10, r2= 1.60, r3= 2.42, r4= 2.92,  &end
#
#   5 FAG   H5    5 FAG H3A     4.710   5.360
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 174, r1= 4.21, r2= 4.71, r3= 5.36, r4= 5.86,  &end
#
#   5 FAG   H5    5 FAG H3B     4.710   5.260
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 175, r1= 4.21, r2= 4.71, r3= 5.26, r4= 5.76,  &end
#
#   5 FAG   H5    5 FAG H1'     5.030   5.500
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 136, r1= 4.53, r2= 5.03, r3= 5.50, r4= 6.00,  &end
#
#   5 FAG   H5    5 FAG H6A     4.100   4.590
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 189, r1= 3.60, r2= 4.10, r3= 4.59, r4= 5.09,  &end
#
#   6 7dG  H1' 5 FAG H1'    3.310   4.810
 &rst
  ixpk= 0, nxpk= 0, iat= 208, 136, r1= 2.81, r2= 3.31, r3= 4.81, r4= 5.31,  &end
#
#   6 7dG  H8  5 FAG H1'    2.440   3.510
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 136, r1= 1.94, r2= 2.44, r3= 3.51, r4= 4.01,  &end
#
#   6 7dG  H8  5 FAG H2'1   3.160   5.190
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 194, r1= 2.66, r2= 3.16, r3= 5.19, r4= 5.69,  &end
#
#   6 7dG  H8  5 FAG H2'2   3.570   5.080
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 195, r1= 3.07, r2= 3.57, r3= 5.08, r4= 5.58,  &end
#
#   6 7dG  H8  5 FAG H3'    3.850   5.670
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 192, r1= 3.35, r2= 3.85, r3= 5.67, r4= 6.17,  &end
#
#   6 7dG  H8  6 7dG  H2'1   2.020   3.720
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 228, r1= 1.52, r2= 2.02, r3= 3.72, r4= 4.22,  &end
#
#   6 7dG  H8  6 7dG  H1'    3.140   4.610
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 208, r1= 2.64, r2= 3.14, r3= 4.61, r4= 5.11,  &end
```

```
#
#   6 7dG  H7   6 7dG  H2'1   2.720   4.890
 &rst
  ixpk= 0, nxpk= 0, iat= 213, 228, r1= 2.22, r2= 2.72, r3= 4.89, r4= 5.39,  &end
#
#   6 7dG  H7   6 7dG  H8     2.570   5.350
 &rst
  ixpk= 0, nxpk= 0, iat= 213, 211, r1= 2.07, r2= 2.57, r3= 5.35, r4= 5.85,  &end
#
#   6 7dG  H2'2          6 7dG  H8     2.700   4.130
 &rst
  ixpk= 0, nxpk= 0, iat= 229, 211, r1= 2.20, r2= 2.70, r3= 4.13, r4= 4.63,  &end
#
#   7 DT   Q5   6 7dG   H2'1   2.970   3.920
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 228, r1= 2.47, r2= 2.97, r3= 4.71, r4= 5.21,
 igr1= 248, 249, 250,
 &end
#
#   7 DT   Q5   6 7dG   H1'    3.050   4.150
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 208, r1= 2.55, r2= 3.05, r3= 4.98, r4= 5.48,
 igr1= 248, 249, 250,
 &end
#
#   7 DT   Q5   6 7dG   H8     3.010   3.800
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 211, r1= 2.51, r2= 3.01, r3= 4.56, r4= 5.06,
 igr1= 248, 249, 250,
 &end
#
#   7 DT   Q5   6 7dG   H7     3.290   4.570
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 213, r1= 2.79, r2= 3.29, r3= 5.49, r4= 5.99,
 igr1= 248, 249, 250,
 &end
#
#   7 DT   Q5   6 7dG   H2'2   2.900   4.200
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 229, r1= 2.40, r2= 2.90, r3= 5.04, r4= 5.54,
 igr1= 248, 249, 250,
 &end
#
#   7 DT   H6   6 7dG   H8     3.390   5.550
 &rst
  ixpk= 0, nxpk= 0, iat= 245, 211, r1= 2.89, r2= 3.39, r3= 5.55, r4= 6.05,  &end
```

```
#
#   7 DT   H6   6 7dG   H7     3.560   6.090
 &rst
  ixpk= 0, nxpk= 0, iat= 245, 213, r1= 3.06, r2= 3.56, r3= 6.09, r4= 6.59,  &end
#
#   7 DT   H6   6 7dG   H2'2   1.660   2.230
 &rst
  ixpk= 0, nxpk= 0, iat= 245, 229, r1= 1.16, r2= 1.66, r3= 2.23, r4= 2.73,  &end
#
#   7 DT    H2'1  7 DT  H3'     2.200   2.820
 &rst
  ixpk= 0, nxpk= 0, iat= 260, 258, r1= 1.70, r2= 2.20, r3= 2.82, r4= 3.32,  &end
#
#   7 DT    H2'2  7 DT  H3'     2.470   3.090
 &rst
  ixpk= 0, nxpk= 0, iat= 261, 258, r1= 1.97, r2= 2.47, r3= 3.09, r4= 3.59,  &end
#
#   7 DT    H1'   7 DT  H2'1    2.780   3.220
 &rst
  ixpk= 0, nxpk= 0, iat= 242, 260, r1= 2.28, r2= 2.78, r3= 3.22, r4= 3.72,  &end
#
#   7 DT    H1'   7 DT  H2'2    2.020   2.520
 &rst
  ixpk= 0, nxpk= 0, iat= 242, 261, r1= 1.52, r2= 2.02, r3= 2.52, r4= 3.02,  &end
#
#   7 DT    H6    7 DT  H2'1    1.710   2.250
 &rst
  ixpk= 0, nxpk= 0, iat= 245, 260, r1= 1.21, r2= 1.71, r3= 2.25, r4= 2.75,  &end
#
#   7 DT    H6    7 DT  H2'2    3.220   3.730
 &rst
  ixpk= 0, nxpk= 0, iat= 245, 261, r1= 2.72, r2= 3.22, r3= 3.73, r4= 4.23,  &end
#
#   8 DT    H6    7 DT  H2'1    3.650   4.120
 &rst
  ixpk= 0, nxpk= 0, iat= 277, 260, r1= 3.15, r2= 3.65, r3= 4.12, r4= 4.62,  &end
#
#   8 DT    H6    7 DT  H2'2    2.180   2.660
 &rst
  ixpk= 0, nxpk= 0, iat= 277, 261, r1= 1.68, r2= 2.18, r3= 2.66, r4= 3.16,  &end
#
#   8 DT    H6    7 DT  H1'     2.800   3.590
 &rst
  ixpk= 0, nxpk= 0, iat= 277, 242, r1= 2.30, r2= 2.80, r3= 3.59, r4= 4.09,  &end
#
#   8 DT    H6    7 DT  H6      4.710   5.390
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 277, 245, r1= 4.21, r2= 4.71, r3= 5.39, r4= 5.89,  &end
#
#   8 DT    Q5  7 DT  H3'     2.380   4.510
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 258, r1= 1.88, r2= 2.38, r3= 5.42, r4= 5.92,
 igr1= 280, 281, 282,
 &end
#
#   8 DT    Q5  7 DT  H2'1    2.170   3.000
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 260, r1= 1.67, r2= 2.17, r3= 3.60, r4= 4.10,
 igr1= 280, 281, 282,
 &end
#
#   8 DT    Q5  7 DT  H2'2    2.130   3.040
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 261, r1= 1.63, r2= 2.13, r3= 3.65, r4= 4.15,
 igr1= 280, 281, 282,
 &end
#
#   8 DT    Q5  7 DT  H1'     2.910   4.410
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 242, r1= 2.41, r2= 2.91, r3= 5.30, r4= 5.80,
 igr1= 280, 281, 282,
 &end
#
#   8 DT    Q5  7 DT  H6      2.520   3.470
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 245, r1= 2.02, r2= 2.52, r3= 4.17, r4= 4.67,
 igr1= 280, 281, 282,
 &end
#
#   8 DT    H3'   7 DT  H1'     4.610   5.490
 &rst
  ixpk= 0, nxpk= 0, iat= 290, 242, r1= 4.11, r2= 4.61, r3= 5.49, r4= 5.99,  &end
#
#   8 DT    H2'1  8 DT  H3'     2.300   3.230
 &rst
  ixpk= 0, nxpk= 0, iat= 292, 290, r1= 1.80, r2= 2.30, r3= 3.23, r4= 3.73,  &end
#
#   8 DT    H2'2  8 DT  H3'     2.400   3.060
 &rst
  ixpk= 0, nxpk= 0, iat= 293, 290, r1= 1.90, r2= 2.40, r3= 3.06, r4= 3.56,  &end
#
#   8 DT    H1'   8 DT  H3'     3.500   5.100
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 274, 290, r1= 3.00, r2= 3.50, r3= 5.10, r4= 5.60,  &end
#
#   8 DT    H1'   8 DT  H2'1    2.720   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 274, 292, r1= 2.22, r2= 2.72, r3= 3.20, r4= 3.70,  &end
#
#   8 DT    Q5    8 DT  H3'     3.050   5.940
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 290, r1= 2.55, r2= 3.05, r3= 7.13, r4= 7.63,
 igr1= 280, 281, 282,
 &end
#
#   8 DT    Q5    8 DT  H1'     3.190   5.960
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 274, r1= 2.69, r2= 3.19, r3= 7.16, r4= 7.66,
 igr1= 280, 281, 282,
 &end
#
#   8 DT    H6    8 DT  H2'1    2.000   2.880
 &rst
  ixpk= 0, nxpk= 0, iat= 277, 292, r1= 1.50, r2= 2.00, r3= 2.88, r4= 3.38,  &end
#
#   8 DT    H6    8 DT  H2'2    3.770   4.280
 &rst
  ixpk= 0, nxpk= 0, iat= 277, 293, r1= 3.27, r2= 3.77, r3= 4.28, r4= 4.78,  &end
#
#   8 DT    H6    8 DT  H1'     3.530   4.220
 &rst
  ixpk= 0, nxpk= 0, iat= 277, 274, r1= 3.03, r2= 3.53, r3= 4.22, r4= 4.72,  &end
#
#   9 DC    H6  8 DT  H2'1    3.600   4.310
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 292, r1= 3.10, r2= 3.60, r3= 4.31, r4= 4.81,  &end
#
#   9 DC    H6  8 DT  H2'2    2.000   2.840
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 293, r1= 1.50, r2= 2.00, r3= 2.84, r4= 3.34,  &end
#
#   9 DC    H6  8 DT  H1'     2.830   3.490
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 274, r1= 2.33, r2= 2.83, r3= 3.49, r4= 3.99,  &end
#
#   9 DC    H6  8 DT  H6      4.900   5.300
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 277, r1= 4.40, r2= 4.90, r3= 5.30, r4= 5.80,  &end
```

```
#
#   9 DC    H5  8 DT  H3'     5.000   5.500
 &rst
  ixpk= 0, nxpk= 0, iat= 311, 290, r1= 4.50, r2= 5.00, r3= 5.50, r4= 6.00,  &end
#
#   9 DC    H5  8 DT  H2'2    2.410   3.360
 &rst
  ixpk= 0, nxpk= 0, iat= 311, 293, r1= 1.91, r2= 2.41, r3= 3.36, r4= 3.86,  &end
#
#   9 DC    H5  8 DT  H1'     3.320   4.050
 &rst
  ixpk= 0, nxpk= 0, iat= 311, 274, r1= 2.82, r2= 3.32, r3= 4.05, r4= 4.55,  &end
#
#   9 DC    H5  8 DT  Q5      2.810   3.900
 &rst
  ixpk= 0, nxpk= 0, iat= 311,  -1, r1= 2.31, r2= 2.81, r3= 4.68, r4= 5.18,
 igr2= 280, 281, 282,
 &end
#
#   9 DC    H5  8 DT  H6      3.590   4.080
 &rst
  ixpk= 0, nxpk= 0, iat= 311, 277, r1= 3.09, r2= 3.59, r3= 4.08, r4= 4.58,  &end
#
#   9 DC    H1'   9 DC  H3'     3.730   4.290
 &rst
  ixpk= 0, nxpk= 0, iat= 306, 320, r1= 3.23, r2= 3.73, r3= 4.29, r4= 4.79,  &end
#
#   9 DC    H1'   9 DC  H2'1    2.780   3.270
 &rst
  ixpk= 0, nxpk= 0, iat= 306, 322, r1= 2.28, r2= 2.78, r3= 3.27, r4= 3.77,  &end
#
#   9 DC    H1'   9 DC  H2'2    2.120   2.660
 &rst
  ixpk= 0, nxpk= 0, iat= 306, 323, r1= 1.62, r2= 2.12, r3= 2.66, r4= 3.16,  &end
#
#   9 DC    H5    9 DC  H2'1    4.100   4.680
 &rst
  ixpk= 0, nxpk= 0, iat= 311, 322, r1= 3.60, r2= 4.10, r3= 4.68, r4= 5.18,  &end
#
#   9 DC    H5    9 DC  H2'2    5.300   5.740
 &rst
  ixpk= 0, nxpk= 0, iat= 311, 323, r1= 4.80, r2= 5.30, r3= 5.74, r4= 6.24,  &end
#
#   9 DC    H6    9 DC  H2'1    1.700   2.160
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 322, r1= 1.20, r2= 1.70, r3= 2.16, r4= 2.66,  &end
```

```
#
#   9 DC    H6    9 DC  H2'2    3.220   3.730
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 323, r1= 2.72, r2= 3.22, r3= 3.73, r4= 4.23,  &end
#
#   9 DC    H6    9 DC  H1'     3.500   4.210
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 306, r1= 3.00, r2= 3.50, r3= 4.21, r4= 4.71,  &end
#
#  10 DA3   H8    9 DC  H2'1    3.590   4.290
 &rst
  ixpk= 0, nxpk= 0, iat= 339, 322, r1= 3.09, r2= 3.59, r3= 4.29, r4= 4.79,  &end
#
#  10 DA3   H8    9 DC  H2'2    2.480   2.980
 &rst
  ixpk= 0, nxpk= 0, iat= 339, 323, r1= 1.98, r2= 2.48, r3= 2.98, r4= 3.48,  &end
#
#  10 DA3   H8    9 DC  H6      4.430   5.240
 &rst
  ixpk= 0, nxpk= 0, iat= 339, 309, r1= 3.93, r2= 4.43, r3= 5.24, r4= 5.74,  &end
#
#  10 DA3   H8    9 DC  H1'     3.590   4.390
 &rst
  ixpk= 0, nxpk= 0, iat= 339, 306, r1= 3.09, r2= 3.59, r3= 4.39, r4= 4.89,  &end
#
#  10 DA3   H2'1 10 DA3 H3'     2.270   2.770
 &rst
  ixpk= 0, nxpk= 0, iat= 354, 352, r1= 1.77, r2= 2.27, r3= 2.77, r4= 3.27,  &end
#
#  10 DA3   H2'2 10 DA3 H3'     2.510   3.070
 &rst
  ixpk= 0, nxpk= 0, iat= 355, 352, r1= 2.01, r2= 2.51, r3= 3.07, r4= 3.57,  &end
#
#  10 DA3   H1'  10 DA3 H3'     3.550   4.060
 &rst
  ixpk= 0, nxpk= 0, iat= 336, 352, r1= 3.05, r2= 3.55, r3= 4.06, r4= 4.56,  &end
#
#  10 DA3   H1'  10 DA3 H2'1    2.710   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 336, 354, r1= 2.21, r2= 2.71, r3= 3.20, r4= 3.70,  &end
#
#  10 DA3   H1'  10 DA3 H2'2    1.980   2.550
 &rst
  ixpk= 0, nxpk= 0, iat= 336, 355, r1= 1.48, r2= 1.98, r3= 2.55, r4= 3.05,  &end
#
#  10 DA3   H8   10 DA3 H3'     4.150   4.730
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 339, 352, r1= 3.65, r2= 4.15, r3= 4.73, r4= 5.23,  &end
#
#  10 DA3   H8   10 DA3 H2'2    3.460   3.960
 &rst
  ixpk= 0, nxpk= 0, iat= 339, 355, r1= 2.96, r2= 3.46, r3= 3.96, r4= 4.46,  &end
#
#  10 DA3   H8   10 DA3 H1'     3.570   4.070
 &rst
  ixpk= 0, nxpk= 0, iat= 339, 336, r1= 3.07, r2= 3.57, r3= 4.07, r4= 4.57,  &end
#
#  11 DT5   H1'  11 DT5 H3'     3.740   4.280
 &rst
  ixpk= 0, nxpk= 0, iat= 367, 383, r1= 3.24, r2= 3.74, r3= 4.28, r4= 4.78,  &end
#
#  11 DT5   H1'  11 DT5 H2'1    2.720   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 367, 385, r1= 2.22, r2= 2.72, r3= 3.20, r4= 3.70,  &end
#
#  11 DT5   H1'  11 DT5 H2'2    2.120   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 367, 386, r1= 1.62, r2= 2.12, r3= 2.61, r4= 3.11,  &end
#
#  11 DT5   Q5   11 DT5 H1'     3.410   5.850
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 367, r1= 2.91, r2= 3.41, r3= 7.03, r4= 7.53,
 igr1= 373, 374, 375,
 &end
#
#  11 DT5   H6   11 DT5 H3'     3.820   4.280
 &rst
  ixpk= 0, nxpk= 0, iat= 370, 383, r1= 3.32, r2= 3.82, r3= 4.28, r4= 4.78,  &end
#
#  11 DT5   H6   11 DT5 H2'1    1.730   2.340
 &rst
  ixpk= 0, nxpk= 0, iat= 370, 385, r1= 1.23, r2= 1.73, r3= 2.34, r4= 2.84,  &end
#
#  11 DT5   H6   11 DT5 H2'2    3.110   3.810
 &rst
  ixpk= 0, nxpk= 0, iat= 370, 386, r1= 2.61, r2= 3.11, r3= 3.81, r4= 4.31,  &end
#
#  11 DT5   H6   11 DT5 H1'     2.730   4.390
 &rst
  ixpk= 0, nxpk= 0, iat= 370, 367, r1= 2.23, r2= 2.73, r3= 4.39, r4= 4.89,  &end
#
#  11 DT5   H6   11 DT5 Q5      2.020   2.850
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 370,  -1, r1= 1.52, r2= 2.02, r3= 3.42, r4= 3.92,
 igr2= 373, 374, 375,
 &end
#
#  12 DG    H8   11 DT5 H3'     4.990   5.480
 &rst
  ixpk= 0, nxpk= 0, iat= 402, 383, r1= 4.49, r2= 4.99, r3= 5.48, r4= 5.98,  &end
#
#  12 DG    H8   11 DT5 H2'1    3.590   4.680
 &rst
  ixpk= 0, nxpk= 0, iat= 402, 385, r1= 3.09, r2= 3.59, r3= 4.68, r4= 5.18,  &end
#
#  12 DG    H8   11 DT5 H2'2    2.570   3.640
 &rst
  ixpk= 0, nxpk= 0, iat= 402, 386, r1= 2.07, r2= 2.57, r3= 3.64, r4= 4.14,  &end
#
#  12 DG    H8   11 DT5 H1'     3.550   4.420
 &rst
  ixpk= 0, nxpk= 0, iat= 402, 367, r1= 3.05, r2= 3.55, r3= 4.42, r4= 4.92,  &end
#
#  12 DG    H8   11 DT5 H6      4.660   5.240
 &rst
  ixpk= 0, nxpk= 0, iat= 402, 370, r1= 4.16, r2= 4.66, r3= 5.24, r4= 5.74,  &end
#
#  12 DG    H8   12 DG  H1'     3.700   5.260
 &rst
  ixpk= 0, nxpk= 0, iat= 402, 399, r1= 3.20, r2= 3.70, r3= 5.26, r4= 5.76,  &end
#
#  13 DA    H8   12 DG  H1'     3.240   4.180
 &rst
  ixpk= 0, nxpk= 0, iat= 435, 399, r1= 2.74, r2= 3.24, r3= 4.18, r4= 4.68,  &end
#
#  13 DA    H8   12 DG  H8      5.180   5.790
 &rst
  ixpk= 0, nxpk= 0, iat= 435, 402, r1= 4.68, r2= 5.18, r3= 5.79, r4= 6.29,  &end
#
#  13 DA    H8   12 DG  H2'1    4.500   5.000
 &rst
  ixpk= 0, nxpk= 0, iat= 435, 418, r1= 4.00, r2= 4.50, r3= 5.00, r4= 5.50,  &end
#
#  13 DA    H8   12 DG  H2'2    2.980   3.600
 &rst
  ixpk= 0, nxpk= 0, iat= 435, 419, r1= 2.48, r2= 2.98, r3= 3.60, r4= 4.10,  &end
#
#  13 DA    H1'  13 DA  H3'     3.630   4.150
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 432, 448, r1= 3.13, r2= 3.63, r3= 4.15, r4= 4.65,  &end
#
#  13 DA    H1'  13 DA  H2'1    2.750   3.230
 &rst
  ixpk= 0, nxpk= 0, iat= 432, 450, r1= 2.25, r2= 2.75, r3= 3.23, r4= 3.73,  &end
#
#  13 DA    H1'  13 DA  H2'2    2.120   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 432, 451, r1= 1.62, r2= 2.12, r3= 2.61, r4= 3.11,  &end
#
#  13 DA    H8   13 DA  H1'     3.680   4.180
 &rst
  ixpk= 0, nxpk= 0, iat= 435, 432, r1= 3.18, r2= 3.68, r3= 4.18, r4= 4.68,  &end
#
#  13 DA    H8   13 DA  H2'2    3.480   3.980
 &rst
  ixpk= 0, nxpk= 0, iat= 435, 451, r1= 2.98, r2= 3.48, r3= 3.98, r4= 4.48,  &end
#
#  14 DA    H8   13 DA  H1'     2.410   3.490
 &rst
  ixpk= 0, nxpk= 0, iat= 467, 432, r1= 1.91, r2= 2.41, r3= 3.49, r4= 3.99,  &end
#
#  14 DA    H8   13 DA  H8      4.490   4.990
 &rst
  ixpk= 0, nxpk= 0, iat= 467, 435, r1= 3.99, r2= 4.49, r3= 4.99, r4= 5.49,  &end
#
#  14 DA    H8   13 DA  H2'1    3.800   4.300
 &rst
  ixpk= 0, nxpk= 0, iat= 467, 450, r1= 3.30, r2= 3.80, r3= 4.30, r4= 4.80,  &end
#
#  14 DA    H8   13 DA  H2'2    2.300   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 467, 451, r1= 1.80, r2= 2.30, r3= 2.90, r4= 3.40,  &end
#
#  14 DA    H1'  14 DA  H2'1    2.800   3.310
 &rst
  ixpk= 0, nxpk= 0, iat= 464, 482, r1= 2.30, r2= 2.80, r3= 3.31, r4= 3.81,  &end
#
#  14 DA    H1'  14 DA  H2'2    2.120   2.630
 &rst
  ixpk= 0, nxpk= 0, iat= 464, 483, r1= 1.62, r2= 2.12, r3= 2.63, r4= 3.13,  &end
#
#  14 DA    H8   14 DA  H2'1    2.030   2.510
 &rst
  ixpk= 0, nxpk= 0, iat= 467, 482, r1= 1.53, r2= 2.03, r3= 2.51, r4= 3.01,  &end
```

```
#
#  14 DA    H8   14 DA  H1'     3.650   4.130
 &rst
  ixpk= 0, nxpk= 0, iat= 467, 464, r1= 3.15, r2= 3.65, r3= 4.13, r4= 4.63,  &end
#
#  15 DC   H2'1  15 DC    H3'    2.200   3.450
 &rst
  ixpk= 0, nxpk= 0, iat= 512, 510, r1= 1.70, r2= 2.20, r3= 3.45, r4= 3.95,  &end
#
#  15 DC   H1'   15 DC    H3'    3.030   4.410
 &rst
  ixpk= 0, nxpk= 0, iat= 496, 510, r1= 2.53, r2= 3.03, r3= 4.41, r4= 4.91,  &end
#
#  15 DC   H1'   15 DC    H2'1   3.200   4.980
 &rst
  ixpk= 0, nxpk= 0, iat= 496, 512, r1= 2.70, r2= 3.20, r3= 4.98, r4= 5.48,  &end
#
#  15 DC   H6    14 DA    H2'1   2.570   4.770
 &rst
  ixpk= 0, nxpk= 0, iat= 499, 482, r1= 2.07, r2= 2.57, r3= 4.77, r4= 5.27,  &end
#
#  15 DC   H6    14 DA    H2'2   1.550   2.620
 &rst
  ixpk= 0, nxpk= 0, iat= 499, 483, r1= 1.05, r2= 1.55, r3= 2.62, r4= 3.12,  &end
#
#  15 DC   H6    14 DA    H1'    3.080   3.860
 &rst
  ixpk= 0, nxpk= 0, iat= 499, 464, r1= 2.58, r2= 3.08, r3= 3.86, r4= 4.36,  &end
#
#  15 DC   H6    14 DA    H8     3.280   5.690
 &rst
  ixpk= 0, nxpk= 0, iat= 499, 467, r1= 2.78, r2= 3.28, r3= 5.69, r4= 6.19,  &end
#
#  15 DC   H6    15 DC    H3'    2.850   3.910
 &rst
  ixpk= 0, nxpk= 0, iat= 499, 510, r1= 2.35, r2= 2.85, r3= 3.91, r4= 4.41,  &end
#
#  15 DC   H6    15 DC    H2'1   2.090   3.240
 &rst
  ixpk= 0, nxpk= 0, iat= 499, 512, r1= 1.59, r2= 2.09, r3= 3.24, r4= 3.74,  &end
#
#  15 DC   H6    15 DC    H1'    3.020   3.820
 &rst
  ixpk= 0, nxpk= 0, iat= 499, 496, r1= 2.52, r2= 3.02, r3= 3.82, r4= 4.32,  &end
#
#  15 DC   H5    14 DA    H2'1   1.770   3.290
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 501, 482, r1= 1.27, r2= 1.77, r3= 3.29, r4= 3.79,  &end
#
#  15 DC   H5    14 DA    H2'2   2.090   3.190
 &rst
  ixpk= 0, nxpk= 0, iat= 501, 483, r1= 1.59, r2= 2.09, r3= 3.19, r4= 3.69,  &end
#
#  15 DC   H2'2  15 DC    H3'    2.290   3.710
 &rst
  ixpk= 0, nxpk= 0, iat= 513, 510, r1= 1.79, r2= 2.29, r3= 3.71, r4= 4.21,  &end
#
#  15 DC   H2'2  15 DC    H1'    2.110   3.160
 &rst
  ixpk= 0, nxpk= 0, iat= 513, 496, r1= 1.61, r2= 2.11, r3= 3.16, r4= 3.66,  &end
#
#  15 DC   H2'2  15 DC    H6     2.740   4.560
 &rst
  ixpk= 0, nxpk= 0, iat= 513, 499, r1= 2.24, r2= 2.74, r3= 4.56, r4= 5.06,  &end
#
#  16 DC   H5    15 DC    H3'    3.310   4.590
 &rst
  ixpk= 0, nxpk= 0, iat= 531, 510, r1= 2.81, r2= 3.31, r3= 4.59, r4= 5.09,  &end
#
#  16 DC   H5    15 DC    H1'    3.530   5.290
 &rst
  ixpk= 0, nxpk= 0, iat= 531, 496, r1= 3.03, r2= 3.53, r3= 5.29, r4= 5.79,  &end
#
#  16 DC   H5    15 DC    H2'2   2.800   4.250
 &rst
  ixpk= 0, nxpk= 0, iat= 531, 513, r1= 2.30, r2= 2.80, r3= 4.25, r4= 4.75,  &end
#
#  16 DC   H6    15 DC    H3'    3.160   4.780
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 510, r1= 2.66, r2= 3.16, r3= 4.78, r4= 5.28,  &end
#
#  16 DC   H6    15 DC    H2'1   2.260   3.560
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 512, r1= 1.76, r2= 2.26, r3= 3.56, r4= 4.06,  &end
#
#  16 DC   H6    15 DC    H1'    3.070   4.370
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 496, r1= 2.57, r2= 3.07, r3= 4.37, r4= 4.87,  &end
#
#  16 DC   H6    15 DC    H6     3.340   4.910
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 499, r1= 2.84, r2= 3.34, r3= 4.91, r4= 5.41,  &end
```

```
#
#  16 DC   H6    15 DC    H2'2   2.310   3.640
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 513, r1= 1.81, r2= 2.31, r3= 3.64, r4= 4.14,  &end
#
#  16 DC    H1'  16 DC  H2'2    2.130   2.630
 &rst
  ixpk= 0, nxpk= 0, iat= 526, 543, r1= 1.63, r2= 2.13, r3= 2.63, r4= 3.13,  &end
#
#  16 DC    H5   16 DC  H2'1    4.050   4.530
 &rst
  ixpk= 0, nxpk= 0, iat= 531, 542, r1= 3.55, r2= 4.05, r3= 4.53, r4= 5.03,  &end
#
#  16 DC    H5   16 DC  H2'2    5.260   5.750
 &rst
  ixpk= 0, nxpk= 0, iat= 531, 543, r1= 4.76, r2= 5.26, r3= 5.75, r4= 6.25,  &end
#
#  16 DC    H6   16 DC  H3'     3.760   4.270
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 540, r1= 3.26, r2= 3.76, r3= 4.27, r4= 4.77,  &end
#
#  16 DC    H6   16 DC  H2'1    1.740   2.260
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 542, r1= 1.24, r2= 1.74, r3= 2.26, r4= 2.76,  &end
#
#  16 DC    H6   16 DC  H2'2    3.120   3.710
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 543, r1= 2.62, r2= 3.12, r3= 3.71, r4= 4.21,  &end
#
#  16 DC    H6   16 DC  H1'     3.520   4.040
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 526, r1= 3.02, r2= 3.52, r3= 4.04, r4= 4.54,  &end
#
#  16 DC    H2'1  5 FAG H2B     1.840   2.980
 &rst
  ixpk= 0, nxpk= 0, iat= 542, 172, r1= 1.34, r2= 1.84, r3= 2.98, r4= 3.48,  &end
#
#  16 DC    H2'2  5 FAG H2B     2.040   3.380
 &rst
  ixpk= 0, nxpk= 0, iat= 543, 172, r1= 1.54, r2= 2.04, r3= 3.38, r4= 3.88,  &end
#
#  16 DC    H1'   5 FAG H2B     2.750   3.890
 &rst
  ixpk= 0, nxpk= 0, iat= 526, 172, r1= 2.25, r2= 2.75, r3= 3.89, r4= 4.39,  &end
#
#  16 DC    H6    5 FAG H2B     2.250   3.090
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 529, 172, r1= 1.75, r2= 2.25, r3= 3.09, r4= 3.59,  &end
#
#  17 DT    H6    5 FAG H3A     3.570   3.970
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 174, r1= 3.07, r2= 3.57, r3= 3.97, r4= 4.47,  &end
#
#  17 DT    H6    5 FAG H3B     4.470   4.970
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 175, r1= 3.97, r2= 4.47, r3= 4.97, r4= 5.47,  &end
#
#  17 DT    H6    5 FAG H2A     3.670   4.070
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 171, r1= 3.17, r2= 3.67, r3= 4.07, r4= 4.57,  &end
#
#  17 DT    H6    5 FAG H2B     4.570   5.070
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 172, r1= 4.07, r2= 4.57, r3= 5.07, r4= 5.57,  &end
#
#  17 DT    H2'2 17 DT  H3'     2.470   2.970
 &rst
  ixpk= 0, nxpk= 0, iat= 575, 572, r1= 1.97, r2= 2.47, r3= 2.97, r4= 3.47,  &end
#
#  17 DT    H1'  17 DT  H3'     3.660   4.210
 &rst
  ixpk= 0, nxpk= 0, iat= 556, 572, r1= 3.16, r2= 3.66, r3= 4.21, r4= 4.71,  &end
#
#  17 DT    H1'  17 DT  H2'2    2.110   2.650
 &rst
  ixpk= 0, nxpk= 0, iat= 556, 575, r1= 1.61, r2= 2.11, r3= 2.65, r4= 3.15,  &end
#
#  17 DT    H6   17 DT  H3'     3.770   4.570
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 572, r1= 3.27, r2= 3.77, r3= 4.57, r4= 5.07,  &end
#
#  17 DT    H6   17 DT  H2'1    1.740   2.290
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 574, r1= 1.24, r2= 1.74, r3= 2.29, r4= 2.79,  &end
#
#  17 DT    H6   17 DT  H2'2    2.940   3.690
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 575, r1= 2.44, r2= 2.94, r3= 3.69, r4= 4.19,  &end
#
#  17 DT    H6   17 DT  H1'     3.430   3.940
 &rst
  ixpk= 0, nxpk= 0, iat= 559, 556, r1= 2.93, r2= 3.43, r3= 3.94, r4= 4.44,  &end
```

```
#
#  17 DT    Q5   17 DT  H2'2    1.930   5.280
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 575, r1= 1.43, r2= 1.93, r3= 6.34, r4= 6.84,
 igr1= 562, 563, 564,
 &end
#
#  17 DT    Q5   17 DT  H1'     2.890   5.510
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 556, r1= 2.39, r2= 2.89, r3= 6.62, r4= 7.12,
 igr1= 562, 563, 564,
 &end
#
#  17 DT    Q5   17 DT  H6      2.570   3.830
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 559, r1= 2.07, r2= 2.57, r3= 4.60, r4= 5.10,
 igr1= 562, 563, 564,
 &end
#
#  18 DT    H3   17 DT  H3      4.330   4.850
 &rst
  ixpk= 0, nxpk= 0, iat= 600, 568, r1= 3.83, r2= 4.33, r3= 4.85, r4= 5.35,  &end
#
#  18 DT    H1'  17 DT  H1'     5.110   5.690
 &rst
  ixpk= 0, nxpk= 0, iat= 588, 556, r1= 4.61, r2= 5.11, r3= 5.69, r4= 6.19,  &end
#
#  18 DT    Q5   17 DT  H2'1    1.990   3.080
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 574, r1= 1.49, r2= 1.99, r3= 3.70, r4= 4.20,
 igr1= 594, 595, 596,
 &end
#
#  18 DT    Q5   17 DT  H2'2    2.580   3.560
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 575, r1= 2.08, r2= 2.58, r3= 4.28, r4= 4.78,
 igr1= 594, 595, 596,
 &end
#
#  18 DT    Q5   17 DT  H6      2.720   3.810
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 559, r1= 2.22, r2= 2.72, r3= 4.58, r4= 5.08,
 igr1= 594, 595, 596,
 &end
#
#  18 DT    H6   17 DT  H2'1    3.970   4.330
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 574, r1= 3.47, r2= 3.97, r3= 4.33, r4= 4.83,  &end
#
#  18 DT    H6   17 DT  H2'2    2.470   2.730
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 575, r1= 1.97, r2= 2.47, r3= 2.73, r4= 3.23,  &end
#
#  18 DT    H6   17 DT  H1'     2.920   3.190
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 556, r1= 2.42, r2= 2.92, r3= 3.19, r4= 3.69,  &end
#
#  18 DT    H6   17 DT  H6      5.100   5.370
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 559, r1= 4.60, r2= 5.10, r3= 5.37, r4= 5.87,  &end
#
#  18 DT    H1'  18 DT  H3'     3.630   4.160
 &rst
  ixpk= 0, nxpk= 0, iat= 588, 604, r1= 3.13, r2= 3.63, r3= 4.16, r4= 4.66,  &end
#
#  18 DT    H1'  18 DT  H2'1    2.820   3.360
 &rst
  ixpk= 0, nxpk= 0, iat= 588, 606, r1= 2.32, r2= 2.82, r3= 3.36, r4= 3.86,  &end
#
#  18 DT    H1'  18 DT  H2'2    2.110   2.640
 &rst
  ixpk= 0, nxpk= 0, iat= 588, 607, r1= 1.61, r2= 2.11, r3= 2.64, r4= 3.14,  &end
#
#  18 DT    Q5   18 DT  H1'     3.940   5.610
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 588, r1= 3.44, r2= 3.94, r3= 6.74, r4= 7.24,
 igr1= 594, 595, 596,
 &end
#
#  18 DT    H6   18 DT  H2'1    1.640   2.210
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 606, r1= 1.14, r2= 1.64, r3= 2.21, r4= 2.71,  &end
#
#  18 DT    H6   18 DT  H1'     3.460   3.940
 &rst
  ixpk= 0, nxpk= 0, iat= 591, 588, r1= 2.96, r2= 3.46, r3= 3.94, r4= 4.44,  &end
#
#  19 DA    H2   18 DT  H3      4.130   4.650
 &rst
  ixpk= 0, nxpk= 0, iat= 632, 600, r1= 3.63, r2= 4.13, r3= 4.65, r4= 5.15,  &end
#
#  19 DA    H8   18 DT  H2'1    4.860   5.110
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 606, r1= 4.36, r2= 4.86, r3= 5.11, r4= 5.61,  &end
#
#  19 DA    H8   18 DT  H2'2    3.100   3.390
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 607, r1= 2.60, r2= 3.10, r3= 3.39, r4= 3.89,  &end
#
#  19 DA    H8   18 DT  H1'     3.820   4.190
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 588, r1= 3.32, r2= 3.82, r3= 4.19, r4= 4.69,  &end
#
#  19 DA    H8   18 DT  H6      6.200   6.470
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 591, r1= 5.70, r2= 6.20, r3= 6.47, r4= 6.97,  &end
#
#  19 DA    H2'2 19 DA  H3'     2.390   2.920
 &rst
  ixpk= 0, nxpk= 0, iat= 639, 636, r1= 1.89, r2= 2.39, r3= 2.92, r4= 3.42,  &end
#
#  19 DA    H1'  19 DA  H3'     3.660   4.110
 &rst
  ixpk= 0, nxpk= 0, iat= 620, 636, r1= 3.16, r2= 3.66, r3= 4.11, r4= 4.61,  &end
#
#  19 DA    H1'  19 DA  H2'1    2.730   3.280
 &rst
  ixpk= 0, nxpk= 0, iat= 620, 638, r1= 2.23, r2= 2.73, r3= 3.28, r4= 3.78,  &end
#
#  19 DA    H1'  19 DA  H2'2    2.120   2.690
 &rst
  ixpk= 0, nxpk= 0, iat= 620, 639, r1= 1.62, r2= 2.12, r3= 2.69, r4= 3.19,  &end
#
#  19 DA    H8   19 DA  H3'     4.130   4.660
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 636, r1= 3.63, r2= 4.13, r3= 4.66, r4= 5.16,  &end
#
#  19 DA    H8   19 DA  H2'2    3.340   3.990
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 639, r1= 2.84, r2= 3.34, r3= 3.99, r4= 4.49,  &end
#
#  19 DA    H8   19 DA  H1'     3.630   4.130
 &rst
  ixpk= 0, nxpk= 0, iat= 623, 620, r1= 3.13, r2= 3.63, r3= 4.13, r4= 4.63,  &end
#
#  20 DG3   H1   19 DA  H2      4.130   4.650
 &rst
  ixpk= 0, nxpk= 0, iat= 661, 632, r1= 3.63, r2= 4.13, r3= 4.65, r4= 5.15,  &end
```

```
#
#  20 DG3   H3'  19 DA  H1'     5.130   5.650
 &rst
  ixpk= 0, nxpk= 0, iat= 669, 620, r1= 4.63, r2= 5.13, r3= 5.65, r4= 6.15,  &end
#
#  20 DG3   H8   19 DA  H3'     5.170   5.490
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 636, r1= 4.67, r2= 5.17, r3= 5.49, r4= 5.99,  &end
#
#  20 DG3   H8   19 DA  H2'1    3.880   4.220
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 638, r1= 3.38, r2= 3.88, r3= 4.22, r4= 4.72,  &end
#
#  20 DG3   H8   19 DA  H2'2    2.550   2.840
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 639, r1= 2.05, r2= 2.55, r3= 2.84, r4= 3.34,  &end
#
#  20 DG3   H8   19 DA  H1'     3.330   3.610
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 620, r1= 2.83, r2= 3.33, r3= 3.61, r4= 4.11,  &end
#
#  20 DG3   H8   19 DA  H8      4.370   4.990
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 623, r1= 3.87, r2= 4.37, r3= 4.99, r4= 5.49,  &end
#
#  20 DG3   H8   20 DG3 H3'     4.180   4.670
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 669, r1= 3.68, r2= 4.18, r3= 4.67, r4= 5.17,  &end
#
#  20 DG3   H8   20 DG3 H2'1    2.040   2.500
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 671, r1= 1.54, r2= 2.04, r3= 2.50, r4= 3.00,  &end
#
#  20 DG3   H8   20 DG3 H2'2    3.510   4.050
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 672, r1= 3.01, r2= 3.51, r3= 4.05, r4= 4.55,  &end
#
#  20 DG3   H2'1 20 DG3 H3'     2.210   2.720
 &rst
  ixpk= 0, nxpk= 0, iat= 671, 669, r1= 1.71, r2= 2.21, r3= 2.72, r4= 3.22,  &end
#
#  20 DG3   H2'2 20 DG3 H3'     2.430   2.990
 &rst
  ixpk= 0, nxpk= 0, iat= 672, 669, r1= 1.93, r2= 2.43, r3= 2.99, r4= 3.49,  &end
#
#  20 DG3   H1'  20 DG3 H3'     3.640   4.100
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 652, 669, r1= 3.14, r2= 3.64, r3= 4.10, r4= 4.60,  &end
#
#  20 DG3   H1'  20 DG3 H2'1    2.700   3.270
 &rst
  ixpk= 0, nxpk= 0, iat= 652, 671, r1= 2.20, r2= 2.70, r3= 3.27, r4= 3.77,  &end
#
#  20 DG3   H1'  20 DG3 H2'2    1.990   2.520
 &rst
  ixpk= 0, nxpk= 0, iat= 652, 672, r1= 1.49, r2= 1.99, r3= 2.52, r4= 3.02,  &end
#
#  20 DG3   H8   20 DG3 H1'     3.650   4.140
 &rst
  ixpk= 0, nxpk= 0, iat= 655, 652, r1= 3.15, r2= 3.65, r3= 4.14, r4= 4.64,  &end
#
#  1  DC5  H42           20  DG3  O6     1.80    2.00
 &rst
  ixpk= 0, nxpk= 0, iat=  19, 659, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,
     rk2=20.0, rk3=20.0, ir6=1, ialtd=0,
 &end
#
#  1  DC5  N3 20  DG3  H1    1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  20, 661, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#  1  DC5  N3 20  DG3  N1    2.85    3.05
 &rst
  ixpk= 0, nxpk= 0, iat=  20, 660, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#  1  DC5  N4 20  DG3  O6    2.81    3.01
 &rst
  ixpk= 0, nxpk= 0, iat=  17, 659, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#  1  DC5  O2 20  DG3  H22   1.75    1.95
 &rst
  ixpk= 0, nxpk= 0, iat=  22, 665, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#  2  DT   H3   19  DA   N1     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat=  52, 630, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
#  2  DT   N3   19  DA   N1     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat=  51, 630, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
#  2  DT   O4   19  DA   H61    1.84    2.04
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  50, 628, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 3 DA   H61 18  DT   O4     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  80, 598, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 3 DA   N1  18  DT   H3     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat=  82, 600, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 3 DA   N1  18  DT   N3     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat=  82, 599, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 4 DA   H61 17  DT   O4     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 112, 566, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 4 DA   N1  17  DT   H3     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 114, 568, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 4 DA   N1  17  DT   N3     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 114, 567, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 5 FAG  H1 16  DC   N3     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 146, 536, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 5 FAG  H22          16  DC   O2     1.75    1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 144, 538, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
# 5 FAG  N1 16  DC   N3     2.85    3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 145, 536, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
# 5 FAG  O6 16  DC   H42    1.80    2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 148, 535, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
# 5 FAG  O6 16  DC   N4     2.81    3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 148, 533, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
```

```
#
# 6 7dG H1 15 DC N3 1.84 2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 218, 506, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 6 7dG H2215 DC O2 1.75 1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 222, 508, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
# 6 7dG N1 15 DC N3 2.85 3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 217, 506, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
# 6 7dG O6 15 DC H42 1.80 2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 216, 505, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
# 6 7dG O6 15 DC N4 2.81 3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 216, 503, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
# 7 DT H3 14 DA N1 1.71 1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 254, 474, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 7 DT N3 14 DA N1 2.72 2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 253, 474, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 7 DT O4 14 DA H61 1.84 2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 252, 472, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 8 DT H3 13 DA N1 1.71 1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 286, 442, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 8 DT N3 13 DA N1 2.72 2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 285, 442, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 8 DT O4 13 DA H61 1.84 2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 284, 440, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 9 DC H42 12 DG O6 1.80 2.00
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 315, 406, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
#  9  DC   N3   12  DG   H1     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 316, 408, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#  9  DC   N3   12  DG   N1     2.85    3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 316, 407, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#  9  DC   N4   12  DG   O6     2.81    3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 313, 406, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#  9  DC   O2   12  DG   H22    1.75    1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 318, 412, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#  10 DA3  H61          11  DT5  O4     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 344, 377, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#  10 DA3  N1 11  DT5  H3     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 346, 379, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
#  10 DA3  N1 11  DT5  N3     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 346, 378, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
# 674 atoms read from pdb file AGdG_amber.pdb.
# 2 DT ALPHA:  (1 DC5 O3')-(2 DT P)-(2 DT O5')-(2 DT C5') -90.0 -30.0
 &rst     iat =    28,    29,    32,    33,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
           rk2 =   2.0, rk3 =   2.0,                                  &end

# 3 DA ALPHA:  (2 DT O3')-(3 DA P)-(3 DA O5')-(3 DA C5') -90.0 -30.0
 &rst     iat =    60,    61,    64,    65,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 4 DA ALPHA:  (3 DA O3')-(4 DA P)-(4 DA O5')-(4 DA C5') -90.0 -30.0
 &rst     iat =    92,    93,    96,    97,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end
```

```
# 6 7dG ALPHA:  (5 FAG O3')-(6 7dG P)-(6 7dG O5')-(6 7dG C5') -90.0 -30.0
 &rst    iat =   196,   197,   200,   201,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 7 DT ALPHA:  (6 7dG O3')-(7 DT P)-(7 DT O5')-(7 DT C5') -90.0 -30.0
 &rst    iat =   230,   231,   234,   235,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 8 DT ALPHA:  (7 DT O3')-(8 DT P)-(8 DT O5')-(8 DT C5') -90.0 -30.0
 &rst    iat =   262,   263,   266,   267,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 9 DC ALPHA:  (8 DT O3')-(9 DC P)-(9 DC O5')-(9 DC C5') -90.0 -30.0
 &rst    iat =   294,   295,   298,   299,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 12 DG ALPHA:  (11 DT5 O3')-(12 DG P)-(12 DG O5')-(12 DG C5') -90.0 -30.0
 &rst    iat =   387,   388,   391,   392,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 13 DA ALPHA:  (12 DG O3')-(13 DA P)-(13 DA O5')-(13 DA C5') -90.0 -30.0
 &rst    iat =   420,   421,   424,   425,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 14 DA ALPHA:  (13 DA O3')-(14 DA P)-(14 DA O5')-(14 DA C5') -90.0 -30.0
 &rst    iat =   452,   453,   456,   457,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 15 DC ALPHA:  (14 DA O3')-(15 DC P)-(15 DC O5')-(15 DC C5') -90.0 -30.0
 &rst    iat =   484,   485,   488,   489,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 17 DT ALPHA:  (16 DC O3')-(17 DT P)-(17 DT O5')-(17 DT C5') -90.0 -30.0
 &rst    iat =   544,   545,   548,   549,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 18 DT ALPHA:  (17 DT O3')-(18 DT P)-(18 DT O5')-(18 DT C5') -90.0 -30.0
```

```
 &rst    iat =   576,   577,   580,   581,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 19 DA ALPHA:  (18 DT O3')-(19 DA P)-(19 DA O5')-(19 DA C5') -90.0 -30.0
 &rst    iat =   608,   609,   612,   613,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 2 DT BETA:  (2 DT P)-(2 DT O5')-(2 DT C5')-(2 DT C4') 150.0 210.0
 &rst    iat =    29,    32,    33,    36,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 3 DA BETA:  (3 DA P)-(3 DA O5')-(3 DA C5')-(3 DA C4') 150.0 210.0
 &rst    iat =    61,    64,    65,    68,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 4 DA BETA:  (4 DA P)-(4 DA O5')-(4 DA C5')-(4 DA C4') 150.0 210.0
 &rst    iat =    93,    96,    97,   100,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 6 7dG BETA:  (6 7dG P)-(6 7dG O5')-(6 7dG C5')-(6 7dG C4') 150.0 210.0
 &rst    iat =   197,   200,   201,   204,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 7 DT BETA:  (7 DT P)-(7 DT O5')-(7 DT C5')-(7 DT C4') 150.0 210.0
 &rst    iat =   231,   234,   235,   238,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 8 DT BETA:  (8 DT P)-(8 DT O5')-(8 DT C5')-(8 DT C4') 150.0 210.0
 &rst    iat =   263,   266,   267,   270,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 9 DC BETA:  (9 DC P)-(9 DC O5')-(9 DC C5')-(9 DC C4') 150.0 210.0
 &rst    iat =   295,   298,   299,   302,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 12 DG BETA:  (12 DG P)-(12 DG O5')-(12 DG C5')-(12 DG C4') 150.0 210.0
 &rst    iat =   388,   391,   392,   395,
```

```
  r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
 &end

# 13 DA BETA:  (13 DA P)-(13 DA O5')-(13 DA C5')-(13 DA C4') 150.0 210.0
 &rst    iat =   421,   424,   425,   428,
  r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
 &end

# 14 DA BETA:  (14 DA P)-(14 DA O5')-(14 DA C5')-(14 DA C4') 150.0 210.0
 &rst    iat =   453,   456,   457,   460,
  r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
 &end

# 15 DC BETA:  (15 DC P)-(15 DC O5')-(15 DC C5')-(15 DC C4') 150.0 210.0
 &rst    iat =   485,   488,   489,   492,
  r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
 &end

# 17 DT BETA:  (17 DT P)-(17 DT O5')-(17 DT C5')-(17 DT C4') 150.0 210.0
 &rst    iat =   545,   548,   549,   552,
  r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
 &end

# 18 DT BETA:  (18 DT P)-(18 DT O5')-(18 DT C5')-(18 DT C4') 150.0 210.0
 &rst    iat =   577,   580,   581,   584,
  r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
 &end

# 19 DA BETA:  (19 DA P)-(19 DA O5')-(19 DA C5')-(19 DA C4') 150.0 210.0
 &rst    iat =   609,   612,   613,   616,
  r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
 &end

# 2 DT GAMMA:  (2 DT O5')-(2 DT C5')-(2 DT C4')-(2 DT C3')  30.0  90.0
 &rst    iat =    32,    33,    36,    55,
  r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
 &end

# 3 DA GAMMA:  (3 DA O5')-(3 DA C5')-(3 DA C4')-(3 DA C3')  30.0  90.0
 &rst    iat =    64,    65,    68,    87,
  r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
 &end

# 4 DA GAMMA:  (4 DA O5')-(4 DA C5')-(4 DA C4')-(4 DA C3')  30.0  90.0
 &rst    iat =    96,    97,   100,   119,
  r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
```

```
        &end

# 6 7dG GAMMA:  (6 7dG O5')-(6 7dG C5')-(6 7dG C4')-(6 7dG C3')  30.0  90.0
 &rst    iat =   200,   201,   204,   225,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
        &end

# 7 DT GAMMA:  (7 DT O5')-(7 DT C5')-(7 DT C4')-(7 DT C3')  30.0  90.0
 &rst    iat =   234,   235,   238,   257,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
        &end

# 8 DT GAMMA:  (8 DT O5')-(8 DT C5')-(8 DT C4')-(8 DT C3')  30.0  90.0
 &rst    iat =   266,   267,   270,   289,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
        &end

# 9 DC GAMMA:  (9 DC O5')-(9 DC C5')-(9 DC C4')-(9 DC C3')  30.0  90.0
 &rst    iat =   298,   299,   302,   319,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
        &end

# 12 DG GAMMA:  (12 DG O5')-(12 DG C5')-(12 DG C4')-(12 DG C3')  30.0  90.0
 &rst    iat =   391,   392,   395,   415,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
        &end

# 13 DA GAMMA:  (13 DA O5')-(13 DA C5')-(13 DA C4')-(13 DA C3')  30.0  90.0
 &rst    iat =   424,   425,   428,   447,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
        &end

# 14 DA GAMMA:  (14 DA O5')-(14 DA C5')-(14 DA C4')-(14 DA C3')  30.0  90.0
 &rst    iat =   456,   457,   460,   479,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
        &end

# 15 DC GAMMA:  (15 DC O5')-(15 DC C5')-(15 DC C4')-(15 DC C3')  30.0  90.0
 &rst    iat =   488,   489,   492,   509,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
        &end

# 17 DT GAMMA:  (17 DT O5')-(17 DT C5')-(17 DT C4')-(17 DT C3')  30.0  90.0
 &rst    iat =   548,   549,   552,   571,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
        &end
```

```
# 18 DT GAMMA:  (18 DT O5')-(18 DT C5')-(18 DT C4')-(18 DT C3')  30.0  90.0
 &rst     iat =   580,   581,   584,   603,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 19 DA GAMMA:  (19 DA O5')-(19 DA C5')-(19 DA C4')-(19 DA C3')  30.0  90.0
 &rst     iat =   612,   613,   616,   635,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 2 DT EPSILN:  (2 DT C4')-(2 DT C3')-(2 DT O3')-(3 DA P) 165.0 225.0
 &rst     iat =    36,    55,    60,    61,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 3 DA EPSILN:  (3 DA C4')-(3 DA C3')-(3 DA O3')-(4 DA P) 165.0 225.0
 &rst     iat =    68,    87,    92,    93,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 4 DA EPSILN:  (4 DA C4')-(4 DA C3')-(4 DA O3')-(5 FAG P) 165.0 225.0
 &rst     iat =   100,   119,   124,   125,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 6 7dG EPSILN:  (6 7dG C4')-(6 7dG C3')-(6 7dG O3')-(7 DT P) 165.0 225.0
 &rst     iat =   204,   225,   230,   231,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 7 DT EPSILN:  (7 DT C4')-(7 DT C3')-(7 DT O3')-(8 DT P) 165.0 225.0
 &rst     iat =   238,   257,   262,   263,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 8 DT EPSILN:  (8 DT C4')-(8 DT C3')-(8 DT O3')-(9 DC P) 165.0 225.0
 &rst     iat =   270,   289,   294,   295,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 9 DC EPSILN:  (9 DC C4')-(9 DC C3')-(9 DC O3')-(10 DA3 P) 165.0 225.0
 &rst     iat =   302,   319,   324,   325,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end
```

```
# 12 DG EPSILN:  (12 DG C4')-(12 DG C3')-(12 DG O3')-(13 DA P) 165.0 225.0
 &rst    iat =   395,   415,   420,   421,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 13 DA EPSILN:  (13 DA C4')-(13 DA C3')-(13 DA O3')-(14 DA P) 165.0 225.0
 &rst    iat =   428,   447,   452,   453,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 14 DA EPSILN:  (14 DA C4')-(14 DA C3')-(14 DA O3')-(15 DC P) 165.0 225.0
 &rst    iat =   460,   479,   484,   485,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 15 DC EPSILN:  (15 DC C4')-(15 DC C3')-(15 DC O3')-(16 DC P) 165.0 225.0
 &rst    iat =   492,   509,   514,   515,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 17 DT EPSILN:  (17 DT C4')-(17 DT C3')-(17 DT O3')-(18 DT P) 165.0 225.0
 &rst    iat =   552,   571,   576,   577,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 18 DT EPSILN:  (18 DT C4')-(18 DT C3')-(18 DT O3')-(19 DA P) 165.0 225.0
 &rst    iat =   584,   603,   608,   609,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 19 DA EPSILN:  (19 DA C4')-(19 DA C3')-(19 DA O3')-(20 DG3 P) 165.0 225.0
 &rst    iat =   616,   635,   640,   641,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 2 DT ZETA:  (2 DT C3')-(2 DT O3')-(3 DA P)-(3 DA O5') -135.0 -75.0
 &rst    iat =    55,    60,    61,    64,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 3 DA ZETA:  (3 DA C3')-(3 DA O3')-(4 DA P)-(4 DA O5') -135.0 -75.0
 &rst    iat =    87,    92,    93,    96,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 4 DA ZETA:  (4 DA C3')-(4 DA O3')-(5 FAG P)-(5 FAG O5') -135.0 -75.0
```

```
 &rst    iat =   119,   124,   125,   128,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 6 7dG ZETA:  (6 7dG C3')-(6 7dG O3')-(7 DT P)-(7 DT O5') -135.0 -75.0
 &rst    iat =   225,   230,   231,   234,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 7 DT ZETA:  (7 DT C3')-(7 DT O3')-(8 DT P)-(8 DT O5') -135.0 -75.0
 &rst    iat =   257,   262,   263,   266,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 8 DT ZETA:  (8 DT C3')-(8 DT O3')-(9 DC P)-(9 DC O5') -135.0 -75.0
 &rst    iat =   289,   294,   295,   298,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 9 DC ZETA:  (9 DC C3')-(9 DC O3')-(10 DA3 P)-(10 DA3 O5') -135.0 -75.0
 &rst    iat =   319,   324,   325,   328,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 12 DG ZETA:  (12 DG C3')-(12 DG O3')-(13 DA P)-(13 DA O5') -135.0 -75.0
 &rst    iat =   415,   420,   421,   424,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 13 DA ZETA:  (13 DA C3')-(13 DA O3')-(14 DA P)-(14 DA O5') -135.0 -75.0
 &rst    iat =   447,   452,   453,   456,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 14 DA ZETA:  (14 DA C3')-(14 DA O3')-(15 DC P)-(15 DC O5') -135.0 -75.0
 &rst    iat =   479,   484,   485,   488,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 15 DC ZETA:  (15 DC C3')-(15 DC O3')-(16 DC P)-(16 DC O5') -135.0 -75.0
 &rst    iat =   509,   514,   515,   518,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 17 DT ZETA:  (17 DT C3')-(17 DT O3')-(18 DT P)-(18 DT O5') -135.0 -75.0
 &rst    iat =   571,   576,   577,   580,
```

```
  r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
 &end

# 18 DT ZETA:  (18 DT C3')-(18 DT O3')-(19 DA P)-(19 DA O5') -135.0 -75.0
 &rst    iat =   603,   608,   609,   612,
  r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
 &end

# 19 DA ZETA:  (19 DA C3')-(19 DA O3')-(20 DG3 P)-(20 DG3 O5') -135.0 -75.0
 &rst    iat =   635,   640,   641,   644,
  r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
 &end

# 674 atoms read from pdb file AGdG_amber.pdb.
# 2 DT NU0:  (2 DT C4')-(2 DT O4')-(2 DT C1')-(2 DT C2') -52.1 -22.1
 &rst    iat =    36,    38,    39,    57,
  r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
  rk2 =   2.0, rk3 =   2.0,                                  &end

# 2 DT NU1:  (2 DT O4')-(2 DT C1')-(2 DT C2')-(2 DT C3')  15.0  45.0
 &rst    iat =    38,    39,    57,    55,
  r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
 &end

# 2 DT NU2:  (2 DT C1')-(2 DT C2')-(2 DT C3')-(2 DT C4') -27.4   2.6
 &rst    iat =    39,    57,    55,    36,
  r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
 &end

# 2 DT NU3:  (2 DT C2')-(2 DT C3')-(2 DT C4')-(2 DT O4') -25.0   5.0
 &rst    iat =    57,    55,    36,    38,
  r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
 &end

# 2 DT NU4:  (2 DT C3')-(2 DT C4')-(2 DT O4')-(2 DT C1')  13.5  43.5
 &rst    iat =    55,    36,    38,    39,
  r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
 &end

# 3 DA NU0:  (3 DA C4')-(3 DA O4')-(3 DA C1')-(3 DA C2') -43.9 -13.9
 &rst    iat =    68,    70,    71,    89,
  r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
 &end

# 3 DA NU1:  (3 DA O4')-(3 DA C1')-(3 DA C2')-(3 DA C3')  22.2  52.2
 &rst    iat =    70,    71,    89,    87,
```

```
  r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
 &end

# 3 DA NU2:  (3 DA C1')-(3 DA C2')-(3 DA C3')-(3 DA C4') -44.6 -14.6
 &rst    iat =   71,   89,   87,   68,
  r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
 &end

# 3 DA NU3:  (3 DA C2')-(3 DA C3')-(3 DA C4')-(3 DA O4')  -3.2  26.8
 &rst    iat =   89,   87,   68,   70,
  r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
 &end

# 3 DA NU4:  (3 DA C3')-(3 DA C4')-(3 DA O4')-(3 DA C1')  -4.4  25.6
 &rst    iat =   87,   68,   70,   71,
  r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
 &end

# 4 DA NU0:  (4 DA C4')-(4 DA O4')-(4 DA C1')-(4 DA C2') -43.9 -13.9
 &rst    iat =  100,  102,  103,  121,
  r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
 &end

# 4 DA NU1:  (4 DA O4')-(4 DA C1')-(4 DA C2')-(4 DA C3')  22.2  52.2
 &rst    iat =  102,  103,  121,  119,
  r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
 &end

# 4 DA NU2:  (4 DA C1')-(4 DA C2')-(4 DA C3')-(4 DA C4') -44.6 -14.6
 &rst    iat =  103,  121,  119,  100,
  r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
 &end

# 4 DA NU3:  (4 DA C2')-(4 DA C3')-(4 DA C4')-(4 DA O4')  -3.2  26.8
 &rst    iat =  121,  119,  100,  102,
  r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
 &end

# 4 DA NU4:  (4 DA C3')-(4 DA C4')-(4 DA O4')-(4 DA C1')  -4.4  25.6
 &rst    iat =  119,  100,  102,  103,
  r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
 &end

# 6 7dG NU0:  (6 7dG C4')-(6 7dG O4')-(6 7dG C1')-(6 7dG C2') -52.1 -22.1
 &rst    iat =  204,  206,  207,  227,
  r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
```

```
        &end

# 6 7dG NU1:  (6 7dG O4')-(6 7dG C1')-(6 7dG C2')-(6 7dG C3')  15.0  45.0
 &rst    iat =   206,   207,   227,   225,
          r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
        &end

# 6 7dG NU2:  (6 7dG C1')-(6 7dG C2')-(6 7dG C3')-(6 7dG C4') -27.4   2.6
 &rst    iat =   207,   227,   225,   204,
          r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
        &end

# 6 7dG NU3:  (6 7dG C2')-(6 7dG C3')-(6 7dG C4')-(6 7dG O4') -25.0   5.0
 &rst    iat =   227,   225,   204,   206,
          r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
        &end

# 6 7dG NU4:  (6 7dG C3')-(6 7dG C4')-(6 7dG O4')-(6 7dG C1')  13.5  43.5
 &rst    iat =   225,   204,   206,   207,
          r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
        &end

# 7 DT NU0:  (7 DT C4')-(7 DT O4')-(7 DT C1')-(7 DT C2') -52.1 -22.1
 &rst    iat =   238,   240,   241,   259,
          r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
        &end

# 7 DT NU1:  (7 DT O4')-(7 DT C1')-(7 DT C2')-(7 DT C3')  15.0  45.0
 &rst    iat =   240,   241,   259,   257,
          r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
        &end

# 7 DT NU2:  (7 DT C1')-(7 DT C2')-(7 DT C3')-(7 DT C4') -27.4   2.6
 &rst    iat =   241,   259,   257,   238,
          r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
        &end

# 7 DT NU3:  (7 DT C2')-(7 DT C3')-(7 DT C4')-(7 DT O4') -25.0   5.0
 &rst    iat =   259,   257,   238,   240,
          r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
        &end

# 7 DT NU4:  (7 DT C3')-(7 DT C4')-(7 DT O4')-(7 DT C1')  13.5  43.5
 &rst    iat =   257,   238,   240,   241,
          r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
        &end
```

```
# 8 DT NU0:  (8 DT C4')-(8 DT O4')-(8 DT C1')-(8 DT C2') -52.1 -22.1
 &rst     iat =   270,   272,   273,   291,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
         &end

# 8 DT NU1:  (8 DT O4')-(8 DT C1')-(8 DT C2')-(8 DT C3')  15.0  45.0
 &rst     iat =   272,   273,   291,   289,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 8 DT NU2:  (8 DT C1')-(8 DT C2')-(8 DT C3')-(8 DT C4') -27.4   2.6
 &rst     iat =   273,   291,   289,   270,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 8 DT NU3:  (8 DT C2')-(8 DT C3')-(8 DT C4')-(8 DT O4') -25.0   5.0
 &rst     iat =   291,   289,   270,   272,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 8 DT NU4:  (8 DT C3')-(8 DT C4')-(8 DT O4')-(8 DT C1')  13.5  43.5
 &rst     iat =   289,   270,   272,   273,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end

# 9 DC NU0:  (9 DC C4')-(9 DC O4')-(9 DC C1')-(9 DC C2') -44.7 -14.7
 &rst     iat =   302,   304,   305,   321,
           r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
         &end

# 9 DC NU1:  (9 DC O4')-(9 DC C1')-(9 DC C2')-(9 DC C3')  18.1  48.1
 &rst     iat =   304,   305,   321,   319,
           r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
         &end

# 9 DC NU2:  (9 DC C1')-(9 DC C2')-(9 DC C3')-(9 DC C4') -37.2  -6.7
 &rst     iat =   305,   321,   319,   302,
           r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
         &end

# 9 DC NU3:  (9 DC C2')-(9 DC C3')-(9 DC C4')-(9 DC O4') -16.9  24.2
 &rst     iat =   321,   319,   302,   304,
           r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
         &end
```

```
# 9 DC NU4:  (9 DC C3')-(9 DC C4')-(9 DC O4')-(9 DC C1')  -1.9  34.0
 &rst     iat =   319,   302,   304,   305,
           r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
          &end

# 12 DG NU0:  (12 DG C4')-(12 DG O4')-(12 DG C1')-(12 DG C2') -44.7 -14.7
 &rst     iat =   395,   397,   398,   417,
           r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
          &end

# 12 DG NU1:  (12 DG O4')-(12 DG C1')-(12 DG C2')-(12 DG C3')  18.1  48.1
 &rst     iat =   397,   398,   417,   415,
           r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
          &end

# 12 DG NU2:  (12 DG C1')-(12 DG C2')-(12 DG C3')-(12 DG C4') -37.2  -6.7
 &rst     iat =   398,   417,   415,   395,
           r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
          &end

# 12 DG NU3:  (12 DG C2')-(12 DG C3')-(12 DG C4')-(12 DG O4') -16.9  24.2
 &rst     iat =   417,   415,   395,   397,
           r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
          &end

# 12 DG NU4:  (12 DG C3')-(12 DG C4')-(12 DG O4')-(12 DG C1')  -1.9  34.0
 &rst     iat =   415,   395,   397,   398,
           r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
          &end

# 13 DA NU0:  (13 DA C4')-(13 DA O4')-(13 DA C1')-(13 DA C2') -43.9 -13.9
 &rst     iat =   428,   430,   431,   449,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
          &end

# 13 DA NU1:  (13 DA O4')-(13 DA C1')-(13 DA C2')-(13 DA C3')  22.2  52.2
 &rst     iat =   430,   431,   449,   447,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
          &end

# 13 DA NU2:  (13 DA C1')-(13 DA C2')-(13 DA C3')-(13 DA C4') -44.6 -14.6
 &rst     iat =   431,   449,   447,   428,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
          &end

# 13 DA NU3:  (13 DA C2')-(13 DA C3')-(13 DA C4')-(13 DA O4')  -3.2  26.8
```

```
 &rst     iat =   449,   447,   428,   430,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
          &end

# 13 DA NU4:  (13 DA C3')-(13 DA C4')-(13 DA O4')-(13 DA C1')  -4.4  25.6
 &rst     iat =   447,   428,   430,   431,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
          &end

# 14 DA NU0:  (14 DA C4')-(14 DA O4')-(14 DA C1')-(14 DA C2') -43.9 -13.9
 &rst     iat =   460,   462,   463,   481,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
          &end

# 14 DA NU1:  (14 DA O4')-(14 DA C1')-(14 DA C2')-(14 DA C3')  22.2  52.2
 &rst     iat =   462,   463,   481,   479,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
          &end

# 14 DA NU2:  (14 DA C1')-(14 DA C2')-(14 DA C3')-(14 DA C4') -44.6 -14.6
 &rst     iat =   463,   481,   479,   460,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
          &end

# 14 DA NU3:  (14 DA C2')-(14 DA C3')-(14 DA C4')-(14 DA O4')  -3.2  26.8
 &rst     iat =   481,   479,   460,   462,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
          &end

# 14 DA NU4:  (14 DA C3')-(14 DA C4')-(14 DA O4')-(14 DA C1')  -4.4  25.6
 &rst     iat =   479,   460,   462,   463,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
          &end

# 15 DC NU0:  (15 DC C4')-(15 DC O4')-(15 DC C1')-(15 DC C2') -43.9 -13.9
 &rst     iat =   492,   494,   495,   511,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
          &end

# 15 DC NU1:  (15 DC O4')-(15 DC C1')-(15 DC C2')-(15 DC C3')  22.2  52.2
 &rst     iat =   494,   495,   511,   509,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
          &end

# 15 DC NU2:  (15 DC C1')-(15 DC C2')-(15 DC C3')-(15 DC C4') -44.6 -14.6
 &rst     iat =   495,   511,   509,   492,
```

```
  r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
 &end

# 15 DC NU3:  (15 DC C2')-(15 DC C3')-(15 DC C4')-(15 DC O4')  -3.2  26.8
 &rst   iat =  511,  509,  492,  494,
  r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
 &end

# 15 DC NU4:  (15 DC C3')-(15 DC C4')-(15 DC O4')-(15 DC C1')  -4.4  25.6
 &rst   iat =  509,  492,  494,  495,
  r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
 &end

# 17 DT NU0:  (17 DT C4')-(17 DT O4')-(17 DT C1')-(17 DT C2') -52.1 -22.1
 &rst   iat =  552,  554,  555,  573,
  r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
 &end

# 17 DT NU1:  (17 DT O4')-(17 DT C1')-(17 DT C2')-(17 DT C3')  15.0  45.0
 &rst   iat =  554,  555,  573,  571,
  r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
 &end

# 17 DT NU2:  (17 DT C1')-(17 DT C2')-(17 DT C3')-(17 DT C4') -27.4   2.6
 &rst   iat =  555,  573,  571,  552,
  r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
 &end

# 17 DT NU3:  (17 DT C2')-(17 DT C3')-(17 DT C4')-(17 DT O4') -25.0   5.0
 &rst   iat =  573,  571,  552,  554,
  r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
 &end

# 17 DT NU4:  (17 DT C3')-(17 DT C4')-(17 DT O4')-(17 DT C1')  13.5  43.5
 &rst   iat =  571,  552,  554,  555,
  r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
 &end

# 18 DT NU0:  (18 DT C4')-(18 DT O4')-(18 DT C1')-(18 DT C2') -52.1 -22.1
 &rst   iat =  584,  586,  587,  605,
  r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
 &end

# 18 DT NU1:  (18 DT O4')-(18 DT C1')-(18 DT C2')-(18 DT C3')  15.0  45.0
 &rst   iat =  586,  587,  605,  603,
  r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
```

```
        &end

# 18 DT NU2:  (18 DT C1')-(18 DT C2')-(18 DT C3')-(18 DT C4') -27.4   2.6
 &rst    iat =   587,   605,   603,   584,
          r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
        &end

# 18 DT NU3:  (18 DT C2')-(18 DT C3')-(18 DT C4')-(18 DT O4') -25.0   5.0
 &rst    iat =   605,   603,   584,   586,
          r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
        &end

# 18 DT NU4:  (18 DT C3')-(18 DT C4')-(18 DT O4')-(18 DT C1')  13.5  43.5
 &rst    iat =   603,   584,   586,   587,
          r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
        &end

# 19 DA NU0:  (19 DA C4')-(19 DA O4')-(19 DA C1')-(19 DA C2') -43.9 -13.9
 &rst    iat =   616,   618,   619,   637,
          r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
        &end

# 19 DA NU1:  (19 DA O4')-(19 DA C1')-(19 DA C2')-(19 DA C3')  22.2  52.2
 &rst    iat =   618,   619,   637,   635,
          r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
        &end

# 19 DA NU2:  (19 DA C1')-(19 DA C2')-(19 DA C3')-(19 DA C4') -44.6 -14.6
 &rst    iat =   619,   637,   635,   616,
          r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
        &end

# 19 DA NU3:  (19 DA C2')-(19 DA C3')-(19 DA C4')-(19 DA O4')  -3.2  26.8
 &rst    iat =   637,   635,   616,   618,
          r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
        &end

# 19 DA NU4:  (19 DA C3')-(19 DA C4')-(19 DA O4')-(19 DA C1')  -4.4  25.6
 &rst    iat =   635,   616,   618,   619,
          r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
        &end
```

Table C-8. Experimental distance and torsion angle restraints used in the rMD calculations of the AFB1-β-FAPY modified AXC adduct.

```
#
#   1 DC5   H2'1  1 DC5 H3'     1.660   2.380
 &rst
  ixpk= 0, nxpk= 0, iat=  26,  24, r1= 1.16, r2= 1.66, r3= 2.38, r4= 2.88,
     rk2=32.0, rk3=32.0, ir6=1, ialtd=0,
 &end
#
#   1 DC5   H2'2  1 DC5 H3'     2.090   2.850
 &rst
  ixpk= 0, nxpk= 0, iat=  27,  24, r1= 1.59, r2= 2.09, r3= 2.85, r4= 3.35,  &end
#
#   1 DC5   H1'   1 DC5 H3'     2.990   3.870
 &rst
  ixpk= 0, nxpk= 0, iat=  10,  24, r1= 2.49, r2= 2.99, r3= 3.87, r4= 4.37,  &end
#
#   1 DC5   H1'   1 DC5 H2'1    2.440   3.030
 &rst
  ixpk= 0, nxpk= 0, iat=  10,  26, r1= 1.94, r2= 2.44, r3= 3.03, r4= 3.53,  &end
#
#   1 DC5   H5    1 DC5 H3'     6.190   6.590
 &rst
  ixpk= 0, nxpk= 0, iat=  15,  24, r1= 5.69, r2= 6.19, r3= 6.59, r4= 7.09,  &end
#
#   1 DC5   H5    1 DC5 H2'1    4.060   4.500
 &rst
  ixpk= 0, nxpk= 0, iat=  15,  26, r1= 3.56, r2= 4.06, r3= 4.50, r4= 5.00,  &end
#
#   1 DC5   H5    1 DC5 H2'2    5.260   5.700
 &rst
  ixpk= 0, nxpk= 0, iat=  15,  27, r1= 4.76, r2= 5.26, r3= 5.70, r4= 6.20,  &end
#
#   1 DC5   H6    1 DC5 H3'     3.440   4.280
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  24, r1= 2.94, r2= 3.44, r3= 4.28, r4= 4.78,  &end
#
#   1 DC5   H6    1 DC5 H2'1    1.670   2.340
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  26, r1= 1.17, r2= 1.67, r3= 2.34, r4= 2.84,  &end
#
#   1 DC5   H6    1 DC5 H2'2    3.160   3.820
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  27, r1= 2.66, r2= 3.16, r3= 3.82, r4= 4.32,  &end
#
#   1 DC5   H6    1 DC5 H1'     3.160   3.790
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  10, r1= 2.66, r2= 3.16, r3= 3.79, r4= 4.29,  &end
#
#   2 DT    H3   20 DG3 H1      3.100   3.510
 &rst
  ixpk= 0, nxpk= 0, iat=  52, 660, r1= 2.60, r2= 3.10, r3= 3.51, r4= 4.01,  &end
#
#   2 DT    Q5    1 DC5 H2'1    2.500   3.510
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  26, r1= 2.00, r2= 2.50, r3= 4.22, r4= 4.72,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H2'2    2.610   3.590
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  27, r1= 2.11, r2= 2.61, r3= 4.31, r4= 4.81,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H1'     2.960   4.530
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  10, r1= 2.46, r2= 2.96, r3= 5.44, r4= 5.94,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H5      1.570   2.930
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  15, r1= 1.07, r2= 1.57, r3= 3.52, r4= 4.02,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    1 DC5 H6      2.010   3.060
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  13, r1= 1.51, r2= 2.01, r3= 3.67, r4= 4.17,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    H6    1 DC5 H1'     3.980   4.180
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  10, r1= 3.48, r2= 3.98, r3= 4.18, r4= 4.68,  &end
#
#   2 DT    H6    1 DC5 H2'2    2.500   2.710
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  27, r1= 2.00, r2= 2.50, r3= 2.71, r4= 3.21,  &end
#
#   2 DT    H6    1 DC5 H2'1    3.810   4.290
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  26, r1= 3.31, r2= 3.81, r3= 4.29, r4= 4.79,  &end
#
#   2 DT    H6    1 DC5 H3'     4.980   5.280
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  24, r1= 4.48, r2= 4.98, r3= 5.28, r4= 5.78,  &end
#
#   2 DT    H6    1 DC5 H6      5.000   5.320
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  13, r1= 4.50, r2= 5.00, r3= 5.32, r4= 5.82,  &end
#
#   2 DT    Q5    2 DT  H3'     3.250   6.510
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  56, r1= 2.75, r2= 3.25, r3= 7.82, r4= 8.32,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    Q5    2 DT  H1'     3.800   5.670
 &rst
  ixpk= 0, nxpk= 0, iat=  -1,  40, r1= 3.30, r2= 3.80, r3= 6.81, r4= 7.31,
 igr1=  46,  47,  48,
 &end
#
#   2 DT    H2'2  2 DT  H3'     2.290   2.950
 &rst
  ixpk= 0, nxpk= 0, iat=  59,  56, r1= 1.79, r2= 2.29, r3= 2.95, r4= 3.45,  &end
#
#   2 DT    H1'   2 DT  H3'     3.590   4.010
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  56, r1= 3.09, r2= 3.59, r3= 4.01, r4= 4.51,  &end
#
#   2 DT    H1'   2 DT  H2'1    2.510   3.080
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  58, r1= 2.01, r2= 2.51, r3= 3.08, r4= 3.58,  &end
#
#   2 DT    H1'   2 DT  H2'2    1.870   2.490
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  59, r1= 1.37, r2= 1.87, r3= 2.49, r4= 2.99,  &end
#
#   2 DT    H6    2 DT  H1'     3.540   3.960
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  40, r1= 3.04, r2= 3.54, r3= 3.96, r4= 4.46,  &end
```

```
#
#   3 DA    H61   2 DT  H3      3.570   3.720
 &rst
  ixpk= 0, nxpk= 0, iat=  80,  52, r1= 3.07, r2= 3.57, r3= 3.72, r4= 4.22,  &end
#
#   3 DA    H62   2 DT  H3      4.270   4.520
 &rst
  ixpk= 0, nxpk= 0, iat=  81,  52, r1= 3.77, r2= 4.27, r3= 4.52, r4= 5.02,  &end
#
#   3 DA    H2    2 DT  H3      3.770   4.220
 &rst
  ixpk= 0, nxpk= 0, iat=  84,  52, r1= 3.27, r2= 3.77, r3= 4.22, r4= 4.72,  &end
#
#   3 DA    H61  18 DT  H3      2.370   2.620
 &rst
  ixpk= 0, nxpk= 0, iat=  80, 599, r1= 1.87, r2= 2.37, r3= 2.62, r4= 3.12,  &end
#
#   3 DA    H62  18 DT  H3      3.770   4.120
 &rst
  ixpk= 0, nxpk= 0, iat=  81, 599, r1= 3.27, r2= 3.77, r3= 4.12, r4= 4.62,  &end
#
#   3 DA    H2   19 DA  H2      2.570   3.020
 &rst
  ixpk= 0, nxpk= 0, iat=  84, 631, r1= 2.07, r2= 2.57, r3= 3.02, r4= 3.52,  &end
#
#   3 DA    H8    2 DT  H3'     4.970   5.220
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  56, r1= 4.47, r2= 4.97, r3= 5.22, r4= 5.72,  &end
#
#   3 DA    H8    2 DT  H2'1    4.400   4.660
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  58, r1= 3.90, r2= 4.40, r3= 4.66, r4= 5.16,  &end
#
#   3 DA    H8    2 DT  H2'2    2.650   3.060
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  59, r1= 2.15, r2= 2.65, r3= 3.06, r4= 3.56,  &end
#
#   3 DA    H8    2 DT  H1'     3.640   3.950
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  40, r1= 3.14, r2= 3.64, r3= 3.95, r4= 4.45,  &end
#
#   3 DA    H1'   3 DA  H2'2    2.260   2.960
 &rst
  ixpk= 0, nxpk= 0, iat=  72,  91, r1= 1.76, r2= 2.26, r3= 2.96, r4= 3.46,  &end
#
#   3 DA    H1'   3 DA  H2'1    3.070   3.850
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  72,  90, r1= 2.57, r2= 3.07, r3= 3.85, r4= 4.35,  &end
#
#   3 DA    H8    3 DA  H1'     3.710   4.120
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  72, r1= 3.21, r2= 3.71, r3= 4.12, r4= 4.62,  &end
#
#   3 DA    H8    3 DA  H2'2    3.310   4.320
 &rst
  ixpk= 0, nxpk= 0, iat=  75,  91, r1= 2.81, r2= 3.31, r3= 4.32, r4= 4.82,  &end
#
#   4 DA    H2    3 DA  H2      4.470   4.820
 &rst
  ixpk= 0, nxpk= 0, iat= 116,  84, r1= 3.97, r2= 4.47, r3= 4.82, r4= 5.32,  &end
#
#   4 DA    H2   18 DT  H3      4.270   4.420
 &rst
  ixpk= 0, nxpk= 0, iat= 116, 599, r1= 3.77, r2= 4.27, r3= 4.42, r4= 4.92,  &end
#
#   4 DA    H61  18 DT  H3      4.870   5.120
 &rst
  ixpk= 0, nxpk= 0, iat= 112, 599, r1= 4.37, r2= 4.87, r3= 5.12, r4= 5.62,  &end
#
#   4 DA    H62  18 DT  H3      5.770   6.120
 &rst
  ixpk= 0, nxpk= 0, iat= 113, 599, r1= 5.27, r2= 5.77, r3= 6.12, r4= 6.62,  &end
#
#   4 DA    H2   17 DT  H3      2.370   2.620
 &rst
  ixpk= 0, nxpk= 0, iat= 116, 567, r1= 1.87, r2= 2.37, r3= 2.62, r4= 3.12,  &end
#
#   4 DA    H61  17 DT  H3      2.770   3.020
 &rst
  ixpk= 0, nxpk= 0, iat= 112, 567, r1= 2.27, r2= 2.77, r3= 3.02, r4= 3.52,  &end
#
#   4 DA    H62  17 DT  H3      4.170   4.620
 &rst
  ixpk= 0, nxpk= 0, iat= 113, 567, r1= 3.67, r2= 4.17, r3= 4.62, r4= 5.12,  &end
#
#   4 DA    H1'   3 DA  H1'     5.410   5.610
 &rst
  ixpk= 0, nxpk= 0, iat= 104,  72, r1= 4.91, r2= 5.41, r3= 5.61, r4= 6.11,  &end
#
#   4 DA    H8    3 DA  H2'1    3.820   4.010
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  90, r1= 3.32, r2= 3.82, r3= 4.01, r4= 4.51,  &end
```

```
#
#   4 DA    H8    3 DA  H2'2    2.420   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  91, r1= 1.92, r2= 2.42, r3= 2.61, r4= 3.11,  &end
#
#   4 DA    H8    3 DA  H1'     3.860   4.060
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  72, r1= 3.36, r2= 3.86, r3= 4.06, r4= 4.56,  &end
#
#   4 DA    H8    3 DA  H8      4.670   4.980
 &rst
  ixpk= 0, nxpk= 0, iat= 107,  75, r1= 4.17, r2= 4.67, r3= 4.98, r4= 5.48,  &end
#
#   4 DA    H1'   4 DA  H3'     3.580   4.240
 &rst
  ixpk= 0, nxpk= 0, iat= 104, 120, r1= 3.08, r2= 3.58, r3= 4.24, r4= 4.74,  &end
#
#   4 DA    H1'   4 DA  H2'1    2.700   3.090
 &rst
  ixpk= 0, nxpk= 0, iat= 104, 122, r1= 2.20, r2= 2.70, r3= 3.09, r4= 3.59,  &end
#
#   4 DA    H1'   4 DA  H2'2    2.040   2.500
 &rst
  ixpk= 0, nxpk= 0, iat= 104, 123, r1= 1.54, r2= 2.04, r3= 2.50, r4= 3.00,  &end
#
#   4 DA    H8    4 DA  H2'1    1.800   2.290
 &rst
  ixpk= 0, nxpk= 0, iat= 107, 122, r1= 1.30, r2= 1.80, r3= 2.29, r4= 2.79,  &end
#
#   4 DA    H8    4 DA  H2'2    3.340   3.500
 &rst
  ixpk= 0, nxpk= 0, iat= 107, 123, r1= 2.84, r2= 3.34, r3= 3.50, r4= 4.00,  &end
#
#   4 DA    H8    4 DA  H1'     3.160   3.740
 &rst
  ixpk= 0, nxpk= 0, iat= 107, 104, r1= 2.66, r2= 3.16, r3= 3.74, r4= 4.24,  &end
#
#   5 FAG   H9A   4 DA  H8      3.150   3.670
 &rst
  ixpk= 0, nxpk= 0, iat= 161, 107, r1= 2.65, r2= 3.15, r3= 3.67, r4= 4.17,  &end
#
#   5 FAG   H6A   4 DA  H3'     4.070   4.620
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 120, r1= 3.57, r2= 4.07, r3= 4.62, r4= 5.12,  &end
#
#   5 FAG   H6A   4 DA  H2'1    2.370   3.840
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 122, r1= 1.87, r2= 2.37, r3= 3.84, r4= 4.34,  &end
#
#   5 FAG   H6A   4 DA  H2'2    1.870   2.240
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 123, r1= 1.37, r2= 1.87, r3= 2.24, r4= 2.74,  &end
#
#   5 FAG   H6A   4 DA  H1'     2.340   3.160
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 104, r1= 1.84, r2= 2.34, r3= 3.16, r4= 3.66,  &end
#
#   5 FAG   H6A   4 DA  H8      2.310   2.890
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 107, r1= 1.81, r2= 2.31, r3= 2.89, r4= 3.39,  &end
#
#   5 FAG   H5    4 DA  H2'1    5.450   5.860
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 122, r1= 4.95, r2= 5.45, r3= 5.86, r4= 6.36,  &end
#
#   5 FAG   H5    4 DA  H2'2    4.420   4.830
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 123, r1= 3.92, r2= 4.42, r3= 4.83, r4= 5.33,  &end
#
#   5 FAG   H5    4 DA  H1'     3.070   3.480
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 104, r1= 2.57, r2= 3.07, r3= 3.48, r4= 3.98,  &end
#
#   5 FAG   H5    4 DA  H8      5.070   6.200
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 107, r1= 4.57, r2= 5.07, r3= 6.20, r4= 6.70,  &end
#
#   5 FAG   MA   17 DT  H3      2.500   5.500
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 567, r1= 2.00, r2= 2.50, r3= 6.61, r4= 7.11,
 igr1= 181, 182, 183,
 &end
#
#   5 FAG   MA          4 DA  H2      2.000   3.000
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 116, r1= 1.50, r2= 2.00, r3= 3.60, r4= 4.10,
 igr1= 181, 182, 183,
 &end
#
#   5 FAG   H2'1  5 FAG H1'     2.690   3.230
 &rst
  ixpk= 0, nxpk= 0, iat= 194, 136, r1= 2.19, r2= 2.69, r3= 3.23, r4= 3.73,  &end
```

```
#
#   5 FAG   H2'2  5 FAG H1'     2.080   2.600
 &rst
  ixpk= 0, nxpk= 0, iat= 195, 136, r1= 1.58, r2= 2.08, r3= 2.60, r4= 3.10,  &end
#
#   5 FAG   H3'   5 FAG H1'     3.630   4.150
 &rst
  ixpk= 0, nxpk= 0, iat= 192, 136, r1= 3.13, r2= 3.63, r3= 4.15, r4= 4.65,  &end
#
#   5 FAG   H3'   5 FAG H2'1    2.430   3.070
 &rst
  ixpk= 0, nxpk= 0, iat= 192, 194, r1= 1.93, r2= 2.43, r3= 3.07, r4= 3.57,  &end
#
#   5 FAG   H3'           5 FAG H2'2    2.700   3.100
 &rst
  ixpk= 0, nxpk= 0, iat= 192, 195, r1= 2.20, r2= 2.70, r3= 3.10, r4= 3.60,  &end
#
#   5 FAG   H2A   5 FAG H3A     2.190   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 171, 174, r1= 1.69, r2= 2.19, r3= 2.61, r4= 3.11,  &end
#
#   5 FAG   H2B   5 FAG H3A     2.970   3.440
 &rst
  ixpk= 0, nxpk= 0, iat= 172, 174, r1= 2.47, r2= 2.97, r3= 3.44, r4= 3.94,  &end
#
#   5 FAG  H8 5 FAG H8A    1.800   2.400
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 155, r1= 1.30, r2= 1.80, r3= 2.40, r4= 2.90,  &end
#
#   5 FAG  H9A          5 FAG H8A    3.600   4.000
 &rst
  ixpk= 0, nxpk= 0, iat= 161, 155, r1= 3.10, r2= 3.60, r3= 4.00, r4= 4.50,  &end
#
#   5 FAG  H9A          5 FAG H8     5.200   6.800
 &rst
  ixpk= 0, nxpk= 0, iat= 161, 152, r1= 4.70, r2= 5.20, r3= 6.80, r4= 7.30,  &end
#
#   5 FAG  H9A          5 FAG H9     2.500   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 161, 159, r1= 2.00, r2= 2.50, r3= 2.90, r4= 3.40,  &end
#
#   5 FAG  H6A          5 FAG H8A    3.400   3.900
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 155, r1= 2.90, r2= 3.40, r3= 3.90, r4= 4.40,  &end
#
#   5 FAG  H6A          5 FAG H9     3.800   4.200
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 159, r1= 3.30, r2= 3.80, r3= 4.20, r4= 4.70,  &end
#
#   5 FAG  H6A          5 FAG H9A    2.300   2.600
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 161, r1= 1.80, r2= 2.30, r3= 2.60, r4= 3.10,  &end
#
#   5 FAG  H6A          5 FAG H8     5.000   5.700
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 152, r1= 4.50, r2= 5.00, r3= 5.70, r4= 6.20,  &end
#
#   5 FAG  H5 5 FAG H1'    4.680   5.530
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 136, r1= 4.18, r2= 4.68, r3= 5.53, r4= 6.03,  &end
#
#   5 FAG   H8    5 FAG HN9     1.990   2.710
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 138, r1= 1.49, r2= 1.99, r3= 2.71, r4= 3.21,  &end
#
#   5 FAG   H2'1  5 FAG HN9     2.050   3.370
 &rst
  ixpk= 0, nxpk= 0, iat= 194, 138, r1= 1.55, r2= 2.05, r3= 3.37, r4= 3.87,  &end
#
#   5 FAG   H2'2  5 FAG HN9     2.130   3.810
 &rst
  ixpk= 0, nxpk= 0, iat= 195, 138, r1= 1.63, r2= 2.13, r3= 3.81, r4= 4.31,  &end
#
#   6 DC    H6    5 FAG H1'     2.180   3.240
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 136, r1= 1.68, r2= 2.18, r3= 3.24, r4= 3.74,  &end
#
#   6 DT            H6    5 FAG H2'2    2.900   3.690
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 195, r1= 2.40, r2= 2.90, r3= 3.69, r4= 4.19,  &end
#
#   6 DC    H6    5 FAG H3'     2.820   4.540
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 192, r1= 2.32, r2= 2.82, r3= 4.54, r4= 5.04,  &end
#
#   6 DC    H5    5 FAG H1'     1.980   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 213, 136, r1= 1.48, r2= 1.98, r3= 2.90, r4= 3.40,  &end
#
#   6 DC    H5    5 FAG H2'1    2.830   3.920
 &rst
  ixpk= 0, nxpk= 0, iat= 213, 194, r1= 2.33, r2= 2.83, r3= 3.92, r4= 4.42,  &end
```

```
#
#   6 DC    H5    5 FAG H2'2    2.570   3.610
 &rst
  ixpk= 0, nxpk= 0, iat= 213, 195, r1= 2.07, r2= 2.57, r3= 3.61, r4= 4.11,  &end
#
#   6 DC    H5    5 FAG H3'     2.860   5.810
 &rst
  ixpk= 0, nxpk= 0, iat= 213, 192, r1= 2.36, r2= 2.86, r3= 5.81, r4= 6.31,  &end
#
#   6 DC    H1'   6 DC  H2'1    1.930   3.730
 &rst
  ixpk= 0, nxpk= 0, iat= 208, 224, r1= 1.43, r2= 1.93, r3= 3.73, r4= 4.23,  &end
#
#   6 DC    H1'   6 DC  H2'2    1.660   2.450
 &rst
  ixpk= 0, nxpk= 0, iat= 208, 225, r1= 1.16, r2= 1.66, r3= 2.45, r4= 2.95,  &end
#
#   6 DC    H6    6 DC  H2'1    1.850   2.310
 &rst
  ixpk= 0, nxpk= 0, iat= 211, 224, r1= 1.35, r2= 1.85, r3= 2.31, r4= 2.81,  &end
#
#   7 DT    Q5  6 DC  H2'1    2.840   3.850
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 224, r1= 2.34, r2= 2.84, r3= 4.62, r4= 5.12,
 igr1= 244, 245, 246,
 &end
#
#   7 DT    Q5  6 DC  H2'2    2.010   3.500
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 225, r1= 1.51, r2= 2.01, r3= 4.20, r4= 4.70,
 igr1= 244, 245, 246,
 &end
#
#   7 DT    Q5  6 DC  H3'     2.180   3.690
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 222, r1= 1.68, r2= 2.18, r3= 4.43, r4= 4.93,
 igr1= 244, 245, 246,
 &end
#
#   7 DT    Q5  6 DC  H1'     2.100   3.140
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 208, r1= 1.60, r2= 2.10, r3= 3.77, r4= 4.27,
 igr1= 244, 245, 246,
 &end
#
#   7 DT    Q5  6 DC  H6      2.460   3.640
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 211, r1= 1.96, r2= 2.46, r3= 4.37, r4= 4.87,
 igr1= 244, 245, 246,
 &end
#
#   7 DT    H6  6 DC  H2'1    3.320   3.870
 &rst
  ixpk= 0, nxpk= 0, iat= 241, 224, r1= 2.82, r2= 3.32, r3= 3.87, r4= 4.37,  &end
#
#   7 DT    H6  6 DC  H2'2    1.900   2.400
 &rst
  ixpk= 0, nxpk= 0, iat= 241, 225, r1= 1.40, r2= 1.90, r3= 2.40, r4= 2.90,  &end
#
#   7 DT    H6  6 DC  H1'     2.900   3.800
 &rst
  ixpk= 0, nxpk= 0, iat= 241, 208, r1= 2.40, r2= 2.90, r3= 3.80, r4= 4.30,  &end
#
#   7 DT    H6  6 DC  H3'     4.600   5.000
 &rst
  ixpk= 0, nxpk= 0, iat= 241, 222, r1= 4.10, r2= 4.60, r3= 5.00, r4= 5.50,  &end
#
#   7 DT    H2'1  7 DT  H3'     2.200   2.820
 &rst
  ixpk= 0, nxpk= 0, iat= 256, 254, r1= 1.70, r2= 2.20, r3= 2.82, r4= 3.32,  &end
#
#   7 DT    H2'2  7 DT  H3'     2.470   3.090
 &rst
  ixpk= 0, nxpk= 0, iat= 257, 254, r1= 1.97, r2= 2.47, r3= 3.09, r4= 3.59,  &end
#
#   7 DT    H1'   7 DT  H2'1    2.780   3.220
 &rst
  ixpk= 0, nxpk= 0, iat= 238, 256, r1= 2.28, r2= 2.78, r3= 3.22, r4= 3.72,  &end
#
#   7 DT    H1'   7 DT  H2'2    2.020   2.520
 &rst
  ixpk= 0, nxpk= 0, iat= 238, 257, r1= 1.52, r2= 2.02, r3= 2.52, r4= 3.02,  &end
#
#   7 DT    H6    7 DT  H2'1    1.710   2.250
 &rst
  ixpk= 0, nxpk= 0, iat= 241, 256, r1= 1.21, r2= 1.71, r3= 2.25, r4= 2.75,  &end
#
#   7 DT    H6    7 DT  H2'2    3.220   3.730
 &rst
  ixpk= 0, nxpk= 0, iat= 241, 257, r1= 2.72, r2= 3.22, r3= 3.73, r4= 4.23,  &end
#
#   8 DT    H6    7 DT  H2'1    3.650   4.120
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 273, 256, r1= 3.15, r2= 3.65, r3= 4.12, r4= 4.62,  &end
#
#   8 DT    H6    7 DT  H2'2    2.180   2.660
 &rst
  ixpk= 0, nxpk= 0, iat= 273, 257, r1= 1.68, r2= 2.18, r3= 2.66, r4= 3.16,  &end
#
#   8 DT    H6    7 DT  H1'     2.800   3.590
 &rst
  ixpk= 0, nxpk= 0, iat= 273, 238, r1= 2.30, r2= 2.80, r3= 3.59, r4= 4.09,  &end
#
#   8 DT    H6    7 DT  H6      4.710   5.390
 &rst
  ixpk= 0, nxpk= 0, iat= 273, 241, r1= 4.21, r2= 4.71, r3= 5.39, r4= 5.89,  &end
#
#   8 DT    Q5  7 DT  H3'     2.380   4.510
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 254, r1= 1.88, r2= 2.38, r3= 5.42, r4= 5.92,
 igr1= 276, 277, 278,
 &end
#
#   8 DT    Q5  7 DT  H2'1    2.170   3.000
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 256, r1= 1.67, r2= 2.17, r3= 3.60, r4= 4.10,
 igr1= 276, 277, 278,
 &end
#
#   8 DT    Q5  7 DT  H2'2    2.130   3.040
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 257, r1= 1.63, r2= 2.13, r3= 3.65, r4= 4.15,
 igr1= 276, 277, 278,
 &end
#
#   8 DT    Q5  7 DT  H1'     2.910   4.410
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 238, r1= 2.41, r2= 2.91, r3= 5.30, r4= 5.80,
 igr1= 276, 277, 278,
 &end
#
#   8 DT    Q5  7 DT  H6      2.520   3.470
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 241, r1= 2.02, r2= 2.52, r3= 4.17, r4= 4.67,
 igr1= 276, 277, 278,
 &end
#
#   8 DT    H3'   7 DT  H1'     4.610   5.490
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 286, 238, r1= 4.11, r2= 4.61, r3= 5.49, r4= 5.99,  &end
#
#   8 DT    H2'1  8 DT  H3'     2.300   3.230
 &rst
  ixpk= 0, nxpk= 0, iat= 288, 286, r1= 1.80, r2= 2.30, r3= 3.23, r4= 3.73,  &end
#
#   8 DT    H2'2  8 DT  H3'     2.400   3.060
 &rst
  ixpk= 0, nxpk= 0, iat= 289, 286, r1= 1.90, r2= 2.40, r3= 3.06, r4= 3.56,  &end
#
#   8 DT    H1'   8 DT  H3'     3.500   5.100
 &rst
  ixpk= 0, nxpk= 0, iat= 270, 286, r1= 3.00, r2= 3.50, r3= 5.10, r4= 5.60,  &end
#
#   8 DT    H1'   8 DT  H2'1    2.720   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 270, 288, r1= 2.22, r2= 2.72, r3= 3.20, r4= 3.70,  &end
#
#   8 DT    Q5    8 DT  H3'     3.050   5.940
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 286, r1= 2.55, r2= 3.05, r3= 7.13, r4= 7.63,
 igr1= 276, 277, 278,
 &end
#
#   8 DT    Q5    8 DT  H1'     3.190   5.960
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 270, r1= 2.69, r2= 3.19, r3= 7.16, r4= 7.66,
 igr1= 276, 277, 278,
 &end
#
#   8 DT    H6    8 DT  H2'1    2.000   2.880
 &rst
  ixpk= 0, nxpk= 0, iat= 273, 288, r1= 1.50, r2= 2.00, r3= 2.88, r4= 3.38,  &end
#
#   8 DT    H6    8 DT  H2'2    3.770   4.280
 &rst
  ixpk= 0, nxpk= 0, iat= 273, 289, r1= 3.27, r2= 3.77, r3= 4.28, r4= 4.78,  &end
#
#   8 DT    H6    8 DT  H1'     3.530   4.220
 &rst
  ixpk= 0, nxpk= 0, iat= 273, 270, r1= 3.03, r2= 3.53, r3= 4.22, r4= 4.72,  &end
#
#   9 DC    H6  8 DT  H2'1    3.600   4.310
 &rst
  ixpk= 0, nxpk= 0, iat= 305, 288, r1= 3.10, r2= 3.60, r3= 4.31, r4= 4.81,  &end
```

```
#
#   9 DC    H6  8 DT  H2'2    2.000   2.840
 &rst
  ixpk= 0, nxpk= 0, iat= 305, 289, r1= 1.50, r2= 2.00, r3= 2.84, r4= 3.34,  &end
#
#   9 DC    H6  8 DT  H1'     2.830   3.490
 &rst
  ixpk= 0, nxpk= 0, iat= 305, 270, r1= 2.33, r2= 2.83, r3= 3.49, r4= 3.99,  &end
#
#   9 DC    H6  8 DT  H6      4.900   5.300
 &rst
  ixpk= 0, nxpk= 0, iat= 305, 273, r1= 4.40, r2= 4.90, r3= 5.30, r4= 5.80,  &end
#
#   9 DC    H5  8 DT  H3'     5.000   5.500
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 286, r1= 4.50, r2= 5.00, r3= 5.50, r4= 6.00,  &end
#
#   9 DC    H5  8 DT  H2'2    2.410   3.360
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 289, r1= 1.91, r2= 2.41, r3= 3.36, r4= 3.86,  &end
#
#   9 DC    H5  8 DT  H1'     3.320   4.050
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 270, r1= 2.82, r2= 3.32, r3= 4.05, r4= 4.55,  &end
#
#   9 DC    H5  8 DT  Q5      2.810   3.900
 &rst
  ixpk= 0, nxpk= 0, iat= 307,  -1, r1= 2.31, r2= 2.81, r3= 4.68, r4= 5.18,
 igr2= 276, 277, 278,
 &end
#
#   9 DC    H5  8 DT  H6      3.590   4.080
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 273, r1= 3.09, r2= 3.59, r3= 4.08, r4= 4.58,  &end
#
#   9 DC    H1'   9 DC  H3'     3.730   4.290
 &rst
  ixpk= 0, nxpk= 0, iat= 302, 316, r1= 3.23, r2= 3.73, r3= 4.29, r4= 4.79,  &end
#
#   9 DC    H1'   9 DC  H2'1    2.780   3.270
 &rst
  ixpk= 0, nxpk= 0, iat= 302, 318, r1= 2.28, r2= 2.78, r3= 3.27, r4= 3.77,  &end
#
#   9 DC    H1'   9 DC  H2'2    2.120   2.660
 &rst
  ixpk= 0, nxpk= 0, iat= 302, 319, r1= 1.62, r2= 2.12, r3= 2.66, r4= 3.16,  &end
```

```
#
#   9 DC    H5    9 DC  H2'1    4.100   4.680
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 318, r1= 3.60, r2= 4.10, r3= 4.68, r4= 5.18,  &end
#
#   9 DC    H5    9 DC  H2'2    5.300   5.740
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 319, r1= 4.80, r2= 5.30, r3= 5.74, r4= 6.24,  &end
#
#   9 DC    H6    9 DC  H2'1    1.700   2.160
 &rst
  ixpk= 0, nxpk= 0, iat= 305, 318, r1= 1.20, r2= 1.70, r3= 2.16, r4= 2.66,  &end
#
#   9 DC    H6    9 DC  H2'2    3.220   3.730
 &rst
  ixpk= 0, nxpk= 0, iat= 305, 319, r1= 2.72, r2= 3.22, r3= 3.73, r4= 4.23,  &end
#
#   9 DC    H6    9 DC  H1'     3.500   4.210
 &rst
  ixpk= 0, nxpk= 0, iat= 305, 302, r1= 3.00, r2= 3.50, r3= 4.21, r4= 4.71,  &end
#
#  10 DA3   H8    9 DC  H2'1    3.590   4.290
 &rst
  ixpk= 0, nxpk= 0, iat= 335, 318, r1= 3.09, r2= 3.59, r3= 4.29, r4= 4.79,  &end
#
#  10 DA3   H8    9 DC  H2'2    2.480   2.980
 &rst
  ixpk= 0, nxpk= 0, iat= 335, 319, r1= 1.98, r2= 2.48, r3= 2.98, r4= 3.48,  &end
#
#  10 DA3   H8    9 DC  H6      4.430   5.240
 &rst
  ixpk= 0, nxpk= 0, iat= 335, 305, r1= 3.93, r2= 4.43, r3= 5.24, r4= 5.74,  &end
#
#  10 DA3   H8    9 DC  H1'     3.590   4.390
 &rst
  ixpk= 0, nxpk= 0, iat= 335, 302, r1= 3.09, r2= 3.59, r3= 4.39, r4= 4.89,  &end
#
#  10 DA3   H2'1 10 DA3 H3'     2.270   2.770
 &rst
  ixpk= 0, nxpk= 0, iat= 350, 348, r1= 1.77, r2= 2.27, r3= 2.77, r4= 3.27,  &end
#
#  10 DA3   H2'2 10 DA3 H3'     2.510   3.070
 &rst
  ixpk= 0, nxpk= 0, iat= 351, 348, r1= 2.01, r2= 2.51, r3= 3.07, r4= 3.57,  &end
#
#  10 DA3   H1'  10 DA3 H3'     3.550   4.060
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 332, 348, r1= 3.05, r2= 3.55, r3= 4.06, r4= 4.56,  &end
#
#  10 DA3   H1'  10 DA3 H2'1    2.710   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 332, 350, r1= 2.21, r2= 2.71, r3= 3.20, r4= 3.70,  &end
#
#  10 DA3   H1'  10 DA3 H2'2    1.980   2.550
 &rst
  ixpk= 0, nxpk= 0, iat= 332, 351, r1= 1.48, r2= 1.98, r3= 2.55, r4= 3.05,  &end
#
#  10 DA3   H8   10 DA3 H3'     4.150   4.730
 &rst
  ixpk= 0, nxpk= 0, iat= 335, 348, r1= 3.65, r2= 4.15, r3= 4.73, r4= 5.23,  &end
#
#  10 DA3   H8   10 DA3 H2'2    3.460   3.960
 &rst
  ixpk= 0, nxpk= 0, iat= 335, 351, r1= 2.96, r2= 3.46, r3= 3.96, r4= 4.46,  &end
#
#  10 DA3   H8   10 DA3 H1'     3.570   4.070
 &rst
  ixpk= 0, nxpk= 0, iat= 335, 332, r1= 3.07, r2= 3.57, r3= 4.07, r4= 4.57,  &end
#
#  11 DT5   H1'  11 DT5 H3'     3.740   4.280
 &rst
  ixpk= 0, nxpk= 0, iat= 363, 379, r1= 3.24, r2= 3.74, r3= 4.28, r4= 4.78,  &end
#
#  11 DT5   H1'  11 DT5 H2'1    2.720   3.200
 &rst
  ixpk= 0, nxpk= 0, iat= 363, 381, r1= 2.22, r2= 2.72, r3= 3.20, r4= 3.70,  &end
#
#  11 DT5   H1'  11 DT5 H2'2    2.120   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 363, 382, r1= 1.62, r2= 2.12, r3= 2.61, r4= 3.11,  &end
#
#  11 DT5   Q5   11 DT5 H1'     3.410   5.850
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 363, r1= 2.91, r2= 3.41, r3= 7.03, r4= 7.53,
 igr1= 369, 370, 371,
 &end
#
#  11 DT5   H6   11 DT5 H3'     3.820   4.280
 &rst
  ixpk= 0, nxpk= 0, iat= 366, 379, r1= 3.32, r2= 3.82, r3= 4.28, r4= 4.78,  &end
#
#  11 DT5   H6   11 DT5 H2'1    1.730   2.340
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 366, 381, r1= 1.23, r2= 1.73, r3= 2.34, r4= 2.84,  &end
#
#  11 DT5   H6   11 DT5 H2'2    3.110   3.810
 &rst
  ixpk= 0, nxpk= 0, iat= 366, 382, r1= 2.61, r2= 3.11, r3= 3.81, r4= 4.31,  &end
#
#  11 DT5   H6   11 DT5 H1'     2.730   4.390
 &rst
  ixpk= 0, nxpk= 0, iat= 366, 363, r1= 2.23, r2= 2.73, r3= 4.39, r4= 4.89,  &end
#
#  11 DT5   H6   11 DT5 Q5      2.020   2.850
 &rst
  ixpk= 0, nxpk= 0, iat= 366,  -1, r1= 1.52, r2= 2.02, r3= 3.42, r4= 3.92,
 igr2= 369, 370, 371,
 &end
#
#  12 DG    H8   11 DT5 H3'     4.990   5.480
 &rst
  ixpk= 0, nxpk= 0, iat= 398, 379, r1= 4.49, r2= 4.99, r3= 5.48, r4= 5.98,  &end
#
#  12 DG    H8   11 DT5 H2'1    3.590   4.680
 &rst
  ixpk= 0, nxpk= 0, iat= 398, 381, r1= 3.09, r2= 3.59, r3= 4.68, r4= 5.18,  &end
#
#  12 DG    H8   11 DT5 H2'2    2.570   3.640
 &rst
  ixpk= 0, nxpk= 0, iat= 398, 382, r1= 2.07, r2= 2.57, r3= 3.64, r4= 4.14,  &end
#
#  12 DG    H8   11 DT5 H1'     3.550   4.420
 &rst
  ixpk= 0, nxpk= 0, iat= 398, 363, r1= 3.05, r2= 3.55, r3= 4.42, r4= 4.92,  &end
#
#  12 DG    H8   11 DT5 H6      4.660   5.240
 &rst
  ixpk= 0, nxpk= 0, iat= 398, 366, r1= 4.16, r2= 4.66, r3= 5.24, r4= 5.74,  &end
#
#  12 DG    H8   12 DG  H1'     3.700   5.260
 &rst
  ixpk= 0, nxpk= 0, iat= 398, 395, r1= 3.20, r2= 3.70, r3= 5.26, r4= 5.76,  &end
#
#  13 DA    H8   12 DG  H1'     3.240   4.180
 &rst
  ixpk= 0, nxpk= 0, iat= 431, 395, r1= 2.74, r2= 3.24, r3= 4.18, r4= 4.68,  &end
#
#  13 DA    H8   12 DG  H8      5.180   5.790
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 431, 398, r1= 4.68, r2= 5.18, r3= 5.79, r4= 6.29,  &end
#
#  13 DA    H8   12 DG  H2'1    4.500   5.000
 &rst
  ixpk= 0, nxpk= 0, iat= 431, 414, r1= 4.00, r2= 4.50, r3= 5.00, r4= 5.50,  &end
#
#  13 DA    H8   12 DG  H2'2    2.980   3.600
 &rst
  ixpk= 0, nxpk= 0, iat= 431, 415, r1= 2.48, r2= 2.98, r3= 3.60, r4= 4.10,  &end
#
#  13 DA    H1'  13 DA  H3'     3.630   4.150
 &rst
  ixpk= 0, nxpk= 0, iat= 428, 444, r1= 3.13, r2= 3.63, r3= 4.15, r4= 4.65,  &end
#
#  13 DA    H1'  13 DA  H2'1    2.750   3.230
 &rst
  ixpk= 0, nxpk= 0, iat= 428, 446, r1= 2.25, r2= 2.75, r3= 3.23, r4= 3.73,  &end
#
#  13 DA    H1'  13 DA  H2'2    2.120   2.610
 &rst
  ixpk= 0, nxpk= 0, iat= 428, 447, r1= 1.62, r2= 2.12, r3= 2.61, r4= 3.11,  &end
#
#  13 DA    H8   13 DA  H1'     3.680   4.180
 &rst
  ixpk= 0, nxpk= 0, iat= 431, 428, r1= 3.18, r2= 3.68, r3= 4.18, r4= 4.68,  &end
#
#  13 DA    H8   13 DA  H2'2    3.480   3.980
 &rst
  ixpk= 0, nxpk= 0, iat= 431, 447, r1= 2.98, r2= 3.48, r3= 3.98, r4= 4.48,  &end
#
#  14 DA    H8   13 DA  H1'     2.410   3.490
 &rst
  ixpk= 0, nxpk= 0, iat= 463, 428, r1= 1.91, r2= 2.41, r3= 3.49, r4= 3.99,  &end
#
#  14 DA    H8   13 DA  H8      4.490   4.990
 &rst
  ixpk= 0, nxpk= 0, iat= 463, 431, r1= 3.99, r2= 4.49, r3= 4.99, r4= 5.49,  &end
#
#  14 DA    H8   13 DA  H2'1    3.800   4.300
 &rst
  ixpk= 0, nxpk= 0, iat= 463, 446, r1= 3.30, r2= 3.80, r3= 4.30, r4= 4.80,  &end
#
#  14 DA    H8   13 DA  H2'2    2.300   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 463, 447, r1= 1.80, r2= 2.30, r3= 2.90, r4= 3.40,  &end
```

```
#
#  14 DA    H1'  14 DA  H2'1    2.800   3.310
 &rst
  ixpk= 0, nxpk= 0, iat= 460, 478, r1= 2.30, r2= 2.80, r3= 3.31, r4= 3.81,  &end
#
#  14 DA    H1'  14 DA  H2'2    2.120   2.630
 &rst
  ixpk= 0, nxpk= 0, iat= 460, 479, r1= 1.62, r2= 2.12, r3= 2.63, r4= 3.13,  &end
#
#  14 DA    H8   14 DA  H2'1    2.030   2.510
 &rst
  ixpk= 0, nxpk= 0, iat= 463, 478, r1= 1.53, r2= 2.03, r3= 2.51, r4= 3.01,  &end
#
#  14 DA    H8   14 DA  H1'     3.650   4.130
 &rst
  ixpk= 0, nxpk= 0, iat= 463, 460, r1= 3.15, r2= 3.65, r3= 4.13, r4= 4.63,  &end
#
#  15 DA    H8   14 DA  H3'     4.680   5.130
 &rst
  ixpk= 0, nxpk= 0, iat= 495, 476, r1= 4.18, r2= 4.68, r3= 5.13, r4= 5.63,  &end
#
#  15 DA    H8   14 DA  H2'1    3.790   4.300
 &rst
  ixpk= 0, nxpk= 0, iat= 495, 478, r1= 3.29, r2= 3.79, r3= 4.30, r4= 4.80,  &end
#
#  15 DA    H8   14 DA  H1'     3.260   3.720
 &rst
  ixpk= 0, nxpk= 0, iat= 495, 460, r1= 2.76, r2= 3.26, r3= 3.72, r4= 4.22,  &end
#
#  15 DA    H8   14 DA  H8      4.960   5.440
 &rst
  ixpk= 0, nxpk= 0, iat= 495, 463, r1= 4.46, r2= 4.96, r3= 5.44, r4= 5.94,  &end
#
#  15 DA    H2'1 15 DA  H3'     2.270   2.730
 &rst
  ixpk= 0, nxpk= 0, iat= 511, 509, r1= 1.77, r2= 2.27, r3= 2.73, r4= 3.23,  &end
#
#  15 DA    H2'2 15 DA  H3'     2.390   2.900
 &rst
  ixpk= 0, nxpk= 0, iat= 512, 509, r1= 1.89, r2= 2.39, r3= 2.90, r4= 3.40,  &end
#
#  15 DA    H1'  15 DA  H3'     3.560   4.020
 &rst
  ixpk= 0, nxpk= 0, iat= 492, 509, r1= 3.06, r2= 3.56, r3= 4.02, r4= 4.52,  &end
#
#  15 DA    H1'  15 DA  H2'2    2.100   2.590
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 492, 512, r1= 1.60, r2= 2.10, r3= 2.59, r4= 3.09,  &end
#
#  15 DA    H8   15 DA  H3'     4.190   4.650
 &rst
  ixpk= 0, nxpk= 0, iat= 495, 509, r1= 3.69, r2= 4.19, r3= 4.65, r4= 5.15,  &end
#
#  15 DA    H8   15 DA  H2'1    1.990   2.590
 &rst
  ixpk= 0, nxpk= 0, iat= 495, 511, r1= 1.49, r2= 1.99, r3= 2.59, r4= 3.09,  &end
#
#  15 DA    H8   15 DA  H1'     3.690   4.210
 &rst
  ixpk= 0, nxpk= 0, iat= 495, 492, r1= 3.19, r2= 3.69, r3= 4.21, r4= 4.71,  &end
#
#  16 DC    H2'1  5 FAG H2B     1.840   2.980
 &rst
  ixpk= 0, nxpk= 0, iat= 541, 172, r1= 1.34, r2= 1.84, r3= 2.98, r4= 3.48,  &end
#
#  16 DC    H2'2  5 FAG H2B     2.040   3.380
 &rst
  ixpk= 0, nxpk= 0, iat= 542, 172, r1= 1.54, r2= 2.04, r3= 3.38, r4= 3.88,  &end
#
#  16 DC    H1'   5 FAG H2B     2.750   3.890
 &rst
  ixpk= 0, nxpk= 0, iat= 525, 172, r1= 2.25, r2= 2.75, r3= 3.89, r4= 4.39,  &end
#
#  16 DC    H6    5 FAG H2B     2.250   3.090
 &rst
  ixpk= 0, nxpk= 0, iat= 528, 172, r1= 1.75, r2= 2.25, r3= 3.09, r4= 3.59,  &end
#
#  16 DC    H5   15 DA  H1'     4.290   4.970
 &rst
  ixpk= 0, nxpk= 0, iat= 530, 492, r1= 3.79, r2= 4.29, r3= 4.97, r4= 5.47,  &end
#
#  16 DC    H5   15 DA  H8      3.510   4.060
 &rst
  ixpk= 0, nxpk= 0, iat= 530, 495, r1= 3.01, r2= 3.51, r3= 4.06, r4= 4.56,  &end
#
#  16 DC    H6   15 DA  H2'1    3.060   3.590
 &rst
  ixpk= 0, nxpk= 0, iat= 528, 511, r1= 2.56, r2= 3.06, r3= 3.59, r4= 4.09,  &end
#
#  16 DC    H6   15 DA  H2'2    2.110   2.630
 &rst
  ixpk= 0, nxpk= 0, iat= 528, 512, r1= 1.61, r2= 2.11, r3= 2.63, r4= 3.13,  &end
```

```
#
#  16 DC    H6   15 DA  H1'     3.820   4.380
 &rst
  ixpk= 0, nxpk= 0, iat= 528, 492, r1= 3.32, r2= 3.82, r3= 4.38, r4= 4.88,  &end
#
#  16 DC    H6   15 DA  H8      4.690   5.200
 &rst
  ixpk= 0, nxpk= 0, iat= 528, 495, r1= 4.19, r2= 4.69, r3= 5.20, r4= 5.70,  &end
#
#  16 DC    H5   15 DA  H2'1    3.050   3.540
 &rst
  ixpk= 0, nxpk= 0, iat= 530, 511, r1= 2.55, r2= 3.05, r3= 3.54, r4= 4.04,  &end
#
#  16 DC    H1'  16 DC  H2'2    2.130   2.630
 &rst
  ixpk= 0, nxpk= 0, iat= 525, 542, r1= 1.63, r2= 2.13, r3= 2.63, r4= 3.13,  &end
#
#  16 DC    H5   16 DC  H2'1    4.050   4.530
 &rst
  ixpk= 0, nxpk= 0, iat= 530, 541, r1= 3.55, r2= 4.05, r3= 4.53, r4= 5.03,  &end
#
#  16 DC    H5   16 DC  H2'2    5.260   5.750
 &rst
  ixpk= 0, nxpk= 0, iat= 530, 542, r1= 4.76, r2= 5.26, r3= 5.75, r4= 6.25,  &end
#
#  16 DC    H6   16 DC  H3'     3.760   4.270
 &rst
  ixpk= 0, nxpk= 0, iat= 528, 539, r1= 3.26, r2= 3.76, r3= 4.27, r4= 4.77,  &end
#
#  16 DC    H6   16 DC  H2'1    1.740   2.260
 &rst
  ixpk= 0, nxpk= 0, iat= 528, 541, r1= 1.24, r2= 1.74, r3= 2.26, r4= 2.76,  &end
#
#  16 DC    H6   16 DC  H2'2    3.120   3.710
 &rst
  ixpk= 0, nxpk= 0, iat= 528, 542, r1= 2.62, r2= 3.12, r3= 3.71, r4= 4.21,  &end
#
#  16 DC    H6   16 DC  H1'     3.520   4.040
 &rst
  ixpk= 0, nxpk= 0, iat= 528, 525, r1= 3.02, r2= 3.52, r3= 4.04, r4= 4.54,  &end
#
#  17 DT    H6    5 FAG H3A     3.570   3.970
 &rst
  ixpk= 0, nxpk= 0, iat= 558, 174, r1= 3.07, r2= 3.57, r3= 3.97, r4= 4.47,  &end
#
#  17 DT    H6    5 FAG H3B     4.470   4.970
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 558, 175, r1= 3.97, r2= 4.47, r3= 4.97, r4= 5.47,  &end
#
#  17 DT    H6    5 FAG H2A     3.670   4.070
 &rst
  ixpk= 0, nxpk= 0, iat= 558, 171, r1= 3.17, r2= 3.67, r3= 4.07, r4= 4.57,  &end
#
#  17 DT    H6    5 FAG H2B     4.570   5.070
 &rst
  ixpk= 0, nxpk= 0, iat= 558, 172, r1= 4.07, r2= 4.57, r3= 5.07, r4= 5.57,  &end
#
#  17 DT    H2'2 17 DT  H3'     2.470   2.970
 &rst
  ixpk= 0, nxpk= 0, iat= 574, 571, r1= 1.97, r2= 2.47, r3= 2.97, r4= 3.47,  &end
#
#  17 DT    H1'  17 DT  H3'     3.660   4.210
 &rst
  ixpk= 0, nxpk= 0, iat= 555, 571, r1= 3.16, r2= 3.66, r3= 4.21, r4= 4.71,  &end
#
#  17 DT    H1'  17 DT  H2'2    2.110   2.650
 &rst
  ixpk= 0, nxpk= 0, iat= 555, 574, r1= 1.61, r2= 2.11, r3= 2.65, r4= 3.15,  &end
#
#  17 DT    H6   17 DT  H3'     3.770   4.570
 &rst
  ixpk= 0, nxpk= 0, iat= 558, 571, r1= 3.27, r2= 3.77, r3= 4.57, r4= 5.07,  &end
#
#  17 DT    H6   17 DT  H2'1    1.740   2.290
 &rst
  ixpk= 0, nxpk= 0, iat= 558, 573, r1= 1.24, r2= 1.74, r3= 2.29, r4= 2.79,  &end
#
#  17 DT    H6   17 DT  H2'2    2.940   3.690
 &rst
  ixpk= 0, nxpk= 0, iat= 558, 574, r1= 2.44, r2= 2.94, r3= 3.69, r4= 4.19,  &end
#
#  17 DT    H6   17 DT  H1'     3.430   3.940
 &rst
  ixpk= 0, nxpk= 0, iat= 558, 555, r1= 2.93, r2= 3.43, r3= 3.94, r4= 4.44,  &end
#
#  17 DT    Q5   17 DT  H2'2    1.930   5.280
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 574, r1= 1.43, r2= 1.93, r3= 6.34, r4= 6.84,
 igr1= 561, 562, 563,
 &end
#
#  17 DT    Q5   17 DT  H1'     2.890   5.510
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 555, r1= 2.39, r2= 2.89, r3= 6.62, r4= 7.12,
 igr1= 561, 562, 563,
 &end
#
#  17 DT    Q5   17 DT  H6      2.570   3.830
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 558, r1= 2.07, r2= 2.57, r3= 4.60, r4= 5.10,
 igr1= 561, 562, 563,
 &end
#
#  18 DT    H3   17 DT  H3      4.330   4.850
 &rst
  ixpk= 0, nxpk= 0, iat= 599, 567, r1= 3.83, r2= 4.33, r3= 4.85, r4= 5.35,  &end
#
#  18 DT    H1'  17 DT  H1'     5.110   5.690
 &rst
  ixpk= 0, nxpk= 0, iat= 587, 555, r1= 4.61, r2= 5.11, r3= 5.69, r4= 6.19,  &end
#
#  18 DT    Q5   17 DT  H2'1    1.990   3.580
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 573, r1= 1.49, r2= 1.99, r3= 4.30, r4= 4.80,
 igr1= 593, 594, 595,
 &end
#
#  18 DT    Q5   17 DT  H2'2    2.580   4.260
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 574, r1= 2.08, r2= 2.58, r3= 5.12, r4= 5.62,
 igr1= 593, 594, 595,
 &end
#
#  18 DT    Q5   17 DT  H6      2.720   4.310
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 558, r1= 2.22, r2= 2.72, r3= 5.18, r4= 5.68,
 igr1= 593, 594, 595,
 &end
#
#  18 DT    H6   17 DT  H2'1    3.970   4.330
 &rst
  ixpk= 0, nxpk= 0, iat= 590, 573, r1= 3.47, r2= 3.97, r3= 4.33, r4= 4.83,  &end
#
#  18 DT    H6   17 DT  H2'2    2.470   2.730
 &rst
  ixpk= 0, nxpk= 0, iat= 590, 574, r1= 1.97, r2= 2.47, r3= 2.73, r4= 3.23,  &end
#
#  18 DT    H6   17 DT  H1'     2.920   3.190
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 590, 555, r1= 2.42, r2= 2.92, r3= 3.19, r4= 3.69,  &end
#
#  18 DT    H6   17 DT  H6      5.100   5.370
 &rst
  ixpk= 0, nxpk= 0, iat= 590, 558, r1= 4.60, r2= 5.10, r3= 5.37, r4= 5.87,  &end
#
#  18 DT    H1'  18 DT  H3'     3.630   4.160
 &rst
  ixpk= 0, nxpk= 0, iat= 587, 603, r1= 3.13, r2= 3.63, r3= 4.16, r4= 4.66,  &end
#
#  18 DT    H1'  18 DT  H2'1    2.820   3.360
 &rst
  ixpk= 0, nxpk= 0, iat= 587, 605, r1= 2.32, r2= 2.82, r3= 3.36, r4= 3.86,  &end
#
#  18 DT    H1'  18 DT  H2'2    2.110   2.640
 &rst
  ixpk= 0, nxpk= 0, iat= 587, 606, r1= 1.61, r2= 2.11, r3= 2.64, r4= 3.14,  &end
#
#  18 DT    Q5   18 DT  H1'     3.940   5.610
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 587, r1= 3.44, r2= 3.94, r3= 6.74, r4= 7.24,
 igr1= 593, 594, 595,
 &end
#
#  18 DT    H6   18 DT  H2'1    1.640   2.210
 &rst
  ixpk= 0, nxpk= 0, iat= 590, 605, r1= 1.14, r2= 1.64, r3= 2.21, r4= 2.71,  &end
#
#  18 DT    H6   18 DT  H1'     3.460   3.940
 &rst
  ixpk= 0, nxpk= 0, iat= 590, 587, r1= 2.96, r2= 3.46, r3= 3.94, r4= 4.44,  &end
#
#  19 DA    H2   18 DT  H3      4.130   4.650
 &rst
  ixpk= 0, nxpk= 0, iat= 631, 599, r1= 3.63, r2= 4.13, r3= 4.65, r4= 5.15,  &end
#
#  19 DA    H8   18 DT  H2'1    4.860   5.110
 &rst
  ixpk= 0, nxpk= 0, iat= 622, 605, r1= 4.36, r2= 4.86, r3= 5.11, r4= 5.61,  &end
#
#  19 DA    H8   18 DT  H2'2    3.100   3.390
 &rst
  ixpk= 0, nxpk= 0, iat= 622, 606, r1= 2.60, r2= 3.10, r3= 3.39, r4= 3.89,  &end
#
#  19 DA    H8   18 DT  H1'     3.820   4.190
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 622, 587, r1= 3.32, r2= 3.82, r3= 4.19, r4= 4.69,  &end
#
#  19 DA    H8   18 DT  H6      6.200   6.470
 &rst
  ixpk= 0, nxpk= 0, iat= 622, 590, r1= 5.70, r2= 6.20, r3= 6.47, r4= 6.97,  &end
#
#  19 DA    H2'2 19 DA  H3'     2.390   2.920
 &rst
  ixpk= 0, nxpk= 0, iat= 638, 635, r1= 1.89, r2= 2.39, r3= 2.92, r4= 3.42,  &end
#
#  19 DA    H1'  19 DA  H3'     3.660   4.110
 &rst
  ixpk= 0, nxpk= 0, iat= 619, 635, r1= 3.16, r2= 3.66, r3= 4.11, r4= 4.61,  &end
#
#  19 DA    H1'  19 DA  H2'1    2.730   3.280
 &rst
  ixpk= 0, nxpk= 0, iat= 619, 637, r1= 2.23, r2= 2.73, r3= 3.28, r4= 3.78,  &end
#
#  19 DA    H1'  19 DA  H2'2    2.120   2.690
 &rst
  ixpk= 0, nxpk= 0, iat= 619, 638, r1= 1.62, r2= 2.12, r3= 2.69, r4= 3.19,  &end
#
#  19 DA    H8   19 DA  H3'     4.130   4.660
 &rst
  ixpk= 0, nxpk= 0, iat= 622, 635, r1= 3.63, r2= 4.13, r3= 4.66, r4= 5.16,  &end
#
#  19 DA    H8   19 DA  H2'2    3.340   3.990
 &rst
  ixpk= 0, nxpk= 0, iat= 622, 638, r1= 2.84, r2= 3.34, r3= 3.99, r4= 4.49,  &end
#
#  19 DA    H8   19 DA  H1'     3.630   4.130
 &rst
  ixpk= 0, nxpk= 0, iat= 622, 619, r1= 3.13, r2= 3.63, r3= 4.13, r4= 4.63,  &end
#
#  20 DG3   H1   19 DA  H2      4.130   4.650
 &rst
  ixpk= 0, nxpk= 0, iat= 660, 631, r1= 3.63, r2= 4.13, r3= 4.65, r4= 5.15,  &end
#
#  20 DG3   H3'  19 DA  H1'     5.130   5.650
 &rst
  ixpk= 0, nxpk= 0, iat= 668, 619, r1= 4.63, r2= 5.13, r3= 5.65, r4= 6.15,  &end
#
#  20 DG3   H8   19 DA  H3'     5.170   5.490
 &rst
  ixpk= 0, nxpk= 0, iat= 654, 635, r1= 4.67, r2= 5.17, r3= 5.49, r4= 5.99,  &end
```

```
#
#  20 DG3   H8   19 DA  H2'1    3.880   4.220
 &rst
  ixpk= 0, nxpk= 0, iat= 654, 637, r1= 3.38, r2= 3.88, r3= 4.22, r4= 4.72,  &end
#
#  20 DG3   H8   19 DA  H2'2    2.550   2.840
 &rst
  ixpk= 0, nxpk= 0, iat= 654, 638, r1= 2.05, r2= 2.55, r3= 2.84, r4= 3.34,  &end
#
#  20 DG3   H8   19 DA  H1'     3.330   3.610
 &rst
  ixpk= 0, nxpk= 0, iat= 654, 619, r1= 2.83, r2= 3.33, r3= 3.61, r4= 4.11,  &end
#
#  20 DG3   H8   19 DA  H8      4.370   4.990
 &rst
  ixpk= 0, nxpk= 0, iat= 654, 622, r1= 3.87, r2= 4.37, r3= 4.99, r4= 5.49,  &end
#
#  20 DG3   H8   20 DG3 H3'     4.180   4.670
 &rst
  ixpk= 0, nxpk= 0, iat= 654, 668, r1= 3.68, r2= 4.18, r3= 4.67, r4= 5.17,  &end
#
#  20 DG3   H8   20 DG3 H2'1    2.040   2.500
 &rst
  ixpk= 0, nxpk= 0, iat= 654, 670, r1= 1.54, r2= 2.04, r3= 2.50, r4= 3.00,  &end
#
#  20 DG3   H8   20 DG3 H2'2    3.510   4.050
 &rst
  ixpk= 0, nxpk= 0, iat= 654, 671, r1= 3.01, r2= 3.51, r3= 4.05, r4= 4.55,  &end
#
#  20 DG3   H2'1 20 DG3 H3'     2.210   2.720
 &rst
  ixpk= 0, nxpk= 0, iat= 670, 668, r1= 1.71, r2= 2.21, r3= 2.72, r4= 3.22,  &end
#
#  20 DG3   H2'2 20 DG3 H3'     2.430   2.990
 &rst
  ixpk= 0, nxpk= 0, iat= 671, 668, r1= 1.93, r2= 2.43, r3= 2.99, r4= 3.49,  &end
#
#  20 DG3   H1'  20 DG3 H3'     3.640   4.100
 &rst
  ixpk= 0, nxpk= 0, iat= 651, 668, r1= 3.14, r2= 3.64, r3= 4.10, r4= 4.60,  &end
#
#  20 DG3   H1'  20 DG3 H2'1    2.700   3.270
 &rst
  ixpk= 0, nxpk= 0, iat= 651, 670, r1= 2.20, r2= 2.70, r3= 3.27, r4= 3.77,  &end
#
#  20 DG3   H1'  20 DG3 H2'2    1.990   2.520
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 651, 671, r1= 1.49, r2= 1.99, r3= 2.52, r4= 3.02,  &end
#
#  20 DG3   H8   20 DG3 H1'     3.650   4.140
 &rst
  ixpk= 0, nxpk= 0, iat= 654, 651, r1= 3.15, r2= 3.65, r3= 4.14, r4= 4.64,  &end
#
#  1  DC5  H42          20  DG3  O6    1.80    2.00
 &rst
  ixpk= 0, nxpk= 0, iat=  19, 658, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,
     rk2=20.0, rk3=20.0, ir6=1, ialtd=0,
 &end
#
#  1  DC5  N3  20  DG3  H1    1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  20, 660, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#  1  DC5  N3  20  DG3  N1    2.85    3.05
 &rst
  ixpk= 0, nxpk= 0, iat=  20, 659, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#  1  DC5  N4  20  DG3  O6    2.81    3.01
 &rst
  ixpk= 0, nxpk= 0, iat=  17, 658, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#  1  DC5  O2  20  DG3  H22   1.75    1.95
 &rst
  ixpk= 0, nxpk= 0, iat=  22, 664, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#  2  DT   H3   19  DA   N1     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat=  52, 629, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
#  2  DT   N3   19  DA   N1     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat=  51, 629, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
#  2  DT   O4   19  DA   H61    1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  50, 627, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#  3  DA   H61 18  DT   O4     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  80, 597, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#  3  DA   N1   18  DT   H3     1.71    1.91
```

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 &rst
  ixpk= 0, nxpk= 0, iat=  82, 599, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 3 DA   N1  18 DT   N3     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat=  82, 598, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 4 DA   H61 17 DT   O4     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 112, 565, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 4 DA   N1  17 DT   H3     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 114, 567, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 4 DA   N1  17 DT   N3     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 114, 566, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 5 FAG  H1 16 DC   N3     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 146, 535, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 5 FAG  H22          16 DC   O2     1.75    1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 144, 537, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
# 5 FAG  N1 16 DC   N3     2.85    3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 145, 535, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
# 5 FAG  O6 16 DC   H42    1.80    2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 148, 534, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
# 5 FAG  O6 16 DC   N4     2.81    3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 148, 532, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
# 6 DC   H42 15 DG   O6     1.80    2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 217, 499, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
# 6 DC   N3  15 DG   H1     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 218, 501, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
```

```
#
# 6 DC   N3  15 DG   N1    2.85   3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 218, 500, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
# 6 DC   N4  15 DG   O6    2.81   3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 215, 499, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
# 6 DC   O2  15 DG   H22   1.75   1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 220, 505, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
# 7 DT   H3  14 DA   N1    1.71   1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 250, 470, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 7 DT   N3  14 DA   N1    2.72   2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 249, 470, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 7 DT   O4  14 DA   H61   1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 248, 468, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 8 DT   H3  13 DA   N1    1.71   1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 282, 438, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
# 8 DT   N3  13 DA   N1    2.72   2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 281, 438, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
# 8 DT   O4  13 DA   H61   1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 280, 436, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 9 DC   H42 12 DG   O6    1.80   2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 311, 402, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
# 9 DC   N3  12 DG   H1    1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 312, 404, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
# 9 DC   N3  12 DG   N1    2.85   3.05
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 312, 403, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#  9  DC   N4   12  DG   O6     2.81    3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 309, 402, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#  9  DC   O2   12  DG   H22    1.75    1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 314, 408, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#  10 DA3  H61          11  DT5  O4     1.84    2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 340, 373, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#  10 DA3  N1 11  DT5  H3     1.71    1.91
 &rst
  ixpk= 0, nxpk= 0, iat= 342, 375, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
#  10 DA3  N1 11  DT5  N3     2.72    2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 342, 374, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
# 673 atoms read from pdb file AGC_amber.pdb.
# 2 DT ALPHA:  (1 DC5 O3')-(2 DT P)-(2 DT O5')-(2 DT C5') -90.0 -30.0
 &rst     iat =    28,    29,    32,    33,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
           rk2 =   2.0, rk3 =   2.0,                                    &end

# 3 DA ALPHA:  (2 DT O3')-(3 DA P)-(3 DA O5')-(3 DA C5') -90.0 -30.0
 &rst     iat =    60,    61,    64,    65,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 4 DA ALPHA:  (3 DA O3')-(4 DA P)-(4 DA O5')-(4 DA C5') -90.0 -30.0
 &rst     iat =    92,    93,    96,    97,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 6 DC ALPHA:  (5 FAG O3')-(6 DC P)-(6 DC O5')-(6 DC C5') -90.0 -30.0
 &rst     iat =   196,   197,   200,   201,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 7 DT ALPHA:  (6 DC O3')-(7 DT P)-(7 DT O5')-(7 DT C5') -90.0 -30.0
 &rst     iat =   226,   227,   230,   231,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
```

```
        &end

# 8 DT ALPHA:  (7 DT O3')-(8 DT P)-(8 DT O5')-(8 DT C5') -90.0 -30.0
 &rst    iat =   258,   259,   262,   263,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 9 DC ALPHA:  (8 DT O3')-(9 DC P)-(9 DC O5')-(9 DC C5') -90.0 -30.0
 &rst    iat =   290,   291,   294,   295,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 12 DG ALPHA:  (11 DT5 O3')-(12 DG P)-(12 DG O5')-(12 DG C5') -90.0 -30.0
 &rst    iat =   383,   384,   387,   388,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 13 DA ALPHA:  (12 DG O3')-(13 DA P)-(13 DA O5')-(13 DA C5') -90.0 -30.0
 &rst    iat =   416,   417,   420,   421,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 14 DA ALPHA:  (13 DA O3')-(14 DA P)-(14 DA O5')-(14 DA C5') -90.0 -30.0
 &rst    iat =   448,   449,   452,   453,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 15 DG ALPHA:  (14 DA O3')-(15 DG P)-(15 DG O5')-(15 DG C5') -90.0 -30.0
 &rst    iat =   480,   481,   484,   485,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 17 DT ALPHA:  (16 DC O3')-(17 DT P)-(17 DT O5')-(17 DT C5') -90.0 -30.0
 &rst    iat =   543,   544,   547,   548,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 18 DT ALPHA:  (17 DT O3')-(18 DT P)-(18 DT O5')-(18 DT C5') -90.0 -30.0
 &rst    iat =   575,   576,   579,   580,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end

# 19 DA ALPHA:  (18 DT O3')-(19 DA P)-(19 DA O5')-(19 DA C5') -90.0 -30.0
 &rst    iat =   607,   608,   611,   612,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
        &end
```

```
# 2 DT BETA:  (2 DT P)-(2 DT O5')-(2 DT C5')-(2 DT C4') 150.0 210.0
 &rst     iat =    29,    32,    33,    36,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 3 DA BETA:  (3 DA P)-(3 DA O5')-(3 DA C5')-(3 DA C4') 150.0 210.0
 &rst     iat =    61,    64,    65,    68,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 4 DA BETA:  (4 DA P)-(4 DA O5')-(4 DA C5')-(4 DA C4') 150.0 210.0
 &rst     iat =    93,    96,    97,   100,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 6 DC BETA:  (6 DC P)-(6 DC O5')-(6 DC C5')-(6 DC C4') 150.0 210.0
 &rst     iat =   197,   200,   201,   204,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 7 DT BETA:  (7 DT P)-(7 DT O5')-(7 DT C5')-(7 DT C4') 150.0 210.0
 &rst     iat =   227,   230,   231,   234,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 8 DT BETA:  (8 DT P)-(8 DT O5')-(8 DT C5')-(8 DT C4') 150.0 210.0
 &rst     iat =   259,   262,   263,   266,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 9 DC BETA:  (9 DC P)-(9 DC O5')-(9 DC C5')-(9 DC C4') 150.0 210.0
 &rst     iat =   291,   294,   295,   298,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 12 DG BETA:  (12 DG P)-(12 DG O5')-(12 DG C5')-(12 DG C4') 150.0 210.0
 &rst     iat =   384,   387,   388,   391,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 13 DA BETA:  (13 DA P)-(13 DA O5')-(13 DA C5')-(13 DA C4') 150.0 210.0
 &rst     iat =   417,   420,   421,   424,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end
```

```
# 14 DA BETA:  (14 DA P)-(14 DA O5')-(14 DA C5')-(14 DA C4') 150.0 210.0
 &rst     iat =   449,   452,   453,   456,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 15 DG BETA:  (15 DG P)-(15 DG O5')-(15 DG C5')-(15 DG C4') 150.0 210.0
 &rst     iat =   481,   484,   485,   488,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 17 DT BETA:  (17 DT P)-(17 DT O5')-(17 DT C5')-(17 DT C4') 150.0 210.0
 &rst     iat =   544,   547,   548,   551,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 18 DT BETA:  (18 DT P)-(18 DT O5')-(18 DT C5')-(18 DT C4') 150.0 210.0
 &rst     iat =   576,   579,   580,   583,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 19 DA BETA:  (19 DA P)-(19 DA O5')-(19 DA C5')-(19 DA C4') 150.0 210.0
 &rst     iat =   608,   611,   612,   615,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 2 DT GAMMA:  (2 DT O5')-(2 DT C5')-(2 DT C4')-(2 DT C3')  30.0  90.0
 &rst     iat =    32,    33,    36,    55,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 3 DA GAMMA:  (3 DA O5')-(3 DA C5')-(3 DA C4')-(3 DA C3')  30.0  90.0
 &rst     iat =    64,    65,    68,    87,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 4 DA GAMMA:  (4 DA O5')-(4 DA C5')-(4 DA C4')-(4 DA C3')  30.0  90.0
 &rst     iat =    96,    97,   100,   119,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 6 DC GAMMA:  (6 DC O5')-(6 DC C5')-(6 DC C4')-(6 DC C3')  30.0  90.0
 &rst     iat =   200,   201,   204,   221,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 7 DT GAMMA:  (7 DT O5')-(7 DT C5')-(7 DT C4')-(7 DT C3')  30.0  90.0
```

```
 &rst    iat =   230,   231,   234,   253,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
         &end

# 8 DT GAMMA:  (8 DT O5')-(8 DT C5')-(8 DT C4')-(8 DT C3')  30.0  90.0
 &rst    iat =   262,   263,   266,   285,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
         &end

# 9 DC GAMMA:  (9 DC O5')-(9 DC C5')-(9 DC C4')-(9 DC C3')  30.0  90.0
 &rst    iat =   294,   295,   298,   315,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
         &end

# 12 DG GAMMA:  (12 DG O5')-(12 DG C5')-(12 DG C4')-(12 DG C3')  30.0  90.0
 &rst    iat =   387,   388,   391,   411,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
         &end

# 13 DA GAMMA:  (13 DA O5')-(13 DA C5')-(13 DA C4')-(13 DA C3')  30.0  90.0
 &rst    iat =   420,   421,   424,   443,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
         &end

# 14 DA GAMMA:  (14 DA O5')-(14 DA C5')-(14 DA C4')-(14 DA C3')  30.0  90.0
 &rst    iat =   452,   453,   456,   475,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
         &end

# 15 DG GAMMA:  (15 DG O5')-(15 DG C5')-(15 DG C4')-(15 DG C3')  30.0  90.0
 &rst    iat =   484,   485,   488,   508,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
         &end

# 17 DT GAMMA:  (17 DT O5')-(17 DT C5')-(17 DT C4')-(17 DT C3')  30.0  90.0
 &rst    iat =   547,   548,   551,   570,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
         &end

# 18 DT GAMMA:  (18 DT O5')-(18 DT C5')-(18 DT C4')-(18 DT C3')  30.0  90.0
 &rst    iat =   579,   580,   583,   602,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
         &end

# 19 DA GAMMA:  (19 DA O5')-(19 DA C5')-(19 DA C4')-(19 DA C3')  30.0  90.0
 &rst    iat =   611,   612,   615,   634,
```

```
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
         &end

# 2 DT EPSILN:  (2 DT C4')-(2 DT C3')-(2 DT O3')-(3 DA P) 165.0 225.0
 &rst    iat =   36,   55,   60,   61,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 3 DA EPSILN:  (3 DA C4')-(3 DA C3')-(3 DA O3')-(4 DA P) 165.0 225.0
 &rst    iat =   68,   87,   92,   93,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 4 DA EPSILN:  (4 DA C4')-(4 DA C3')-(4 DA O3')-(5 FAG P) 165.0 225.0
 &rst    iat =  100,  119,  124,  125,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 6 DC EPSILN:  (6 DC C4')-(6 DC C3')-(6 DC O3')-(7 DT P) 165.0 225.0
 &rst    iat =  204,  221,  226,  227,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 7 DT EPSILN:  (7 DT C4')-(7 DT C3')-(7 DT O3')-(8 DT P) 165.0 225.0
 &rst    iat =  234,  253,  258,  259,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 8 DT EPSILN:  (8 DT C4')-(8 DT C3')-(8 DT O3')-(9 DC P) 165.0 225.0
 &rst    iat =  266,  285,  290,  291,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 9 DC EPSILN:  (9 DC C4')-(9 DC C3')-(9 DC O3')-(10 DA3 P) 165.0 225.0
 &rst    iat =  298,  315,  320,  321,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 12 DG EPSILN:  (12 DG C4')-(12 DG C3')-(12 DG O3')-(13 DA P) 165.0 225.0
 &rst    iat =  391,  411,  416,  417,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 13 DA EPSILN:  (13 DA C4')-(13 DA C3')-(13 DA O3')-(14 DA P) 165.0 225.0
 &rst    iat =  424,  443,  448,  449,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
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```
        &end

# 14 DA EPSILN:  (14 DA C4')-(14 DA C3')-(14 DA O3')-(15 DG P) 165.0 225.0
 &rst    iat =   456,   475,   480,   481,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
        &end

# 15 DG EPSILN:  (15 DG C4')-(15 DG C3')-(15 DG O3')-(16 DC P) 165.0 225.0
 &rst    iat =   488,   508,   513,   514,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
        &end

# 17 DT EPSILN:  (17 DT C4')-(17 DT C3')-(17 DT O3')-(18 DT P) 165.0 225.0
 &rst    iat =   551,   570,   575,   576,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
        &end

# 18 DT EPSILN:  (18 DT C4')-(18 DT C3')-(18 DT O3')-(19 DA P) 165.0 225.0
 &rst    iat =   583,   602,   607,   608,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
        &end

# 19 DA EPSILN:  (19 DA C4')-(19 DA C3')-(19 DA O3')-(20 DG3 P) 165.0 225.0
 &rst    iat =   615,   634,   639,   640,
          r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
        &end

# 2 DT ZETA:  (2 DT C3')-(2 DT O3')-(3 DA P)-(3 DA O5') -135.0 -75.0
 &rst    iat =    55,    60,    61,    64,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end

# 3 DA ZETA:  (3 DA C3')-(3 DA O3')-(4 DA P)-(4 DA O5') -135.0 -75.0
 &rst    iat =    87,    92,    93,    96,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end

# 4 DA ZETA:  (4 DA C3')-(4 DA O3')-(5 FAG P)-(5 FAG O5') -135.0 -75.0
 &rst    iat =   119,   124,   125,   128,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end

# 6 DC ZETA:  (6 DC C3')-(6 DC O3')-(7 DT P)-(7 DT O5') -135.0 -75.0
 &rst    iat =   221,   226,   227,   230,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
        &end
```

```
# 7 DT ZETA:  (7 DT C3')-(7 DT O3')-(8 DT P)-(8 DT O5') -135.0 -75.0
 &rst    iat =   253,   258,   259,   262,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 8 DT ZETA:  (8 DT C3')-(8 DT O3')-(9 DC P)-(9 DC O5') -135.0 -75.0
 &rst    iat =   285,   290,   291,   294,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 9 DC ZETA:  (9 DC C3')-(9 DC O3')-(10 DA3 P)-(10 DA3 O5') -135.0 -75.0
 &rst    iat =   315,   320,   321,   324,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 12 DG ZETA:  (12 DG C3')-(12 DG O3')-(13 DA P)-(13 DA O5') -135.0 -75.0
 &rst    iat =   411,   416,   417,   420,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 13 DA ZETA:  (13 DA C3')-(13 DA O3')-(14 DA P)-(14 DA O5') -135.0 -75.0
 &rst    iat =   443,   448,   449,   452,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 14 DA ZETA:  (14 DA C3')-(14 DA O3')-(15 DG P)-(15 DG O5') -135.0 -75.0
 &rst    iat =   475,   480,   481,   484,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 15 DG ZETA:  (15 DG C3')-(15 DG O3')-(16 DC P)-(16 DC O5') -135.0 -75.0
 &rst    iat =   508,   513,   514,   517,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 17 DT ZETA:  (17 DT C3')-(17 DT O3')-(18 DT P)-(18 DT O5') -135.0 -75.0
 &rst    iat =   570,   575,   576,   579,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 18 DT ZETA:  (18 DT C3')-(18 DT O3')-(19 DA P)-(19 DA O5') -135.0 -75.0
 &rst    iat =   602,   607,   608,   611,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end
```

```
# 19 DA ZETA:  (19 DA C3')-(19 DA O3')-(20 DG3 P)-(20 DG3 O5') -135.0 -75.0
 &rst    iat =   634,   639,   640,   643,
          r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 673 atoms read from pdb file AGC_amber.pdb.
# 2 DT NU0:  (2 DT C4')-(2 DT O4')-(2 DT C1')-(2 DT C2') -52.1 -22.1
 &rst    iat =    36,    38,    39,    57,
          r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
          rk2 =   2.0, rk3 =   2.0,                                  &end

# 2 DT NU1:  (2 DT O4')-(2 DT C1')-(2 DT C2')-(2 DT C3')  15.0  45.0
 &rst    iat =    38,    39,    57,    55,
          r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 2 DT NU2:  (2 DT C1')-(2 DT C2')-(2 DT C3')-(2 DT C4') -27.4   2.6
 &rst    iat =    39,    57,    55,    36,
          r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 2 DT NU3:  (2 DT C2')-(2 DT C3')-(2 DT C4')-(2 DT O4') -25.0   5.0
 &rst    iat =    57,    55,    36,    38,
          r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 2 DT NU4:  (2 DT C3')-(2 DT C4')-(2 DT O4')-(2 DT C1')  13.5  43.5
 &rst    iat =    55,    36,    38,    39,
          r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end

# 3 DA NU0:  (3 DA C4')-(3 DA O4')-(3 DA C1')-(3 DA C2') -43.9 -13.9
 &rst    iat =    68,    70,    71,    89,
          r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
         &end

# 3 DA NU1:  (3 DA O4')-(3 DA C1')-(3 DA C2')-(3 DA C3')  22.2  52.2
 &rst    iat =    70,    71,    89,    87,
          r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
         &end

# 3 DA NU2:  (3 DA C1')-(3 DA C2')-(3 DA C3')-(3 DA C4') -44.6 -14.6
 &rst    iat =    71,    89,    87,    68,
          r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
         &end
```

```
# 3 DA NU3:  (3 DA C2')-(3 DA C3')-(3 DA C4')-(3 DA O4')  -3.2  26.8
 &rst     iat =    89,    87,    68,    70,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
          &end

# 3 DA NU4:  (3 DA C3')-(3 DA C4')-(3 DA O4')-(3 DA C1')  -4.4  25.6
 &rst     iat =    87,    68,    70,    71,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
          &end

# 4 DA NU0:  (4 DA C4')-(4 DA O4')-(4 DA C1')-(4 DA C2') -43.9 -13.9
 &rst     iat =   100,   102,   103,   121,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
          &end

# 4 DA NU1:  (4 DA O4')-(4 DA C1')-(4 DA C2')-(4 DA C3')  22.2  52.2
 &rst     iat =   102,   103,   121,   119,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
          &end

# 4 DA NU2:  (4 DA C1')-(4 DA C2')-(4 DA C3')-(4 DA C4') -44.6 -14.6
 &rst     iat =   103,   121,   119,   100,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
          &end

# 4 DA NU3:  (4 DA C2')-(4 DA C3')-(4 DA C4')-(4 DA O4')  -3.2  26.8
 &rst     iat =   121,   119,   100,   102,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
          &end

# 4 DA NU4:  (4 DA C3')-(4 DA C4')-(4 DA O4')-(4 DA C1')  -4.4  25.6
 &rst     iat =   119,   100,   102,   103,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
          &end

# 6 DC NU0:  (6 DC C4')-(6 DC O4')-(6 DC C1')-(6 DC C2') -44.7 -14.7
 &rst     iat =   204,   206,   207,   223,
           r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
          &end

# 6 DC NU1:  (6 DC O4')-(6 DC C1')-(6 DC C2')-(6 DC C3')  18.1  48.1
 &rst     iat =   206,   207,   223,   221,
           r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
          &end

# 6 DC NU2:  (6 DC C1')-(6 DC C2')-(6 DC C3')-(6 DC C4') -37.2  -6.7
```

```
 &rst     iat =   207,   223,   221,   204,
           r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
          &end

# 6 DC NU3:  (6 DC C2')-(6 DC C3')-(6 DC C4')-(6 DC O4') -16.9  24.2
 &rst     iat =   223,   221,   204,   206,
           r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
          &end

# 6 DC NU4:  (6 DC C3')-(6 DC C4')-(6 DC O4')-(6 DC C1')  -1.9  34.0
 &rst     iat =   221,   204,   206,   207,
           r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
          &end

# 7 DT NU0:  (7 DT C4')-(7 DT O4')-(7 DT C1')-(7 DT C2') -52.1 -22.1
 &rst     iat =   234,   236,   237,   255,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
          &end

# 7 DT NU1:  (7 DT O4')-(7 DT C1')-(7 DT C2')-(7 DT C3')  15.0  45.0
 &rst     iat =   236,   237,   255,   253,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
          &end

# 7 DT NU2:  (7 DT C1')-(7 DT C2')-(7 DT C3')-(7 DT C4') -27.4   2.6
 &rst     iat =   237,   255,   253,   234,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
          &end

# 7 DT NU3:  (7 DT C2')-(7 DT C3')-(7 DT C4')-(7 DT O4') -25.0   5.0
 &rst     iat =   255,   253,   234,   236,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
          &end

# 7 DT NU4:  (7 DT C3')-(7 DT C4')-(7 DT O4')-(7 DT C1')  13.5  43.5
 &rst     iat =   253,   234,   236,   237,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
          &end

# 8 DT NU0:  (8 DT C4')-(8 DT O4')-(8 DT C1')-(8 DT C2') -52.1 -22.1
 &rst     iat =   266,   268,   269,   287,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
          &end

# 8 DT NU1:  (8 DT O4')-(8 DT C1')-(8 DT C2')-(8 DT C3')  15.0  45.0
 &rst     iat =   268,   269,   287,   285,
```

```
          r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 8 DT NU2:  (8 DT C1')-(8 DT C2')-(8 DT C3')-(8 DT C4') -27.4   2.6
 &rst     iat =   269,   287,   285,   266,
          r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 8 DT NU3:  (8 DT C2')-(8 DT C3')-(8 DT C4')-(8 DT O4') -25.0   5.0
 &rst     iat =   287,   285,   266,   268,
          r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 8 DT NU4:  (8 DT C3')-(8 DT C4')-(8 DT O4')-(8 DT C1')  13.5  43.5
 &rst     iat =   285,   266,   268,   269,
          r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end

# 9 DC NU0:  (9 DC C4')-(9 DC O4')-(9 DC C1')-(9 DC C2') -44.7 -14.7
 &rst     iat =   298,   300,   301,   317,
          r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
         &end

# 9 DC NU1:  (9 DC O4')-(9 DC C1')-(9 DC C2')-(9 DC C3')  18.1  48.1
 &rst     iat =   300,   301,   317,   315,
          r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
         &end

# 9 DC NU2:  (9 DC C1')-(9 DC C2')-(9 DC C3')-(9 DC C4') -37.2  -6.7
 &rst     iat =   301,   317,   315,   298,
          r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
         &end

# 9 DC NU3:  (9 DC C2')-(9 DC C3')-(9 DC C4')-(9 DC O4') -16.9  24.2
 &rst     iat =   317,   315,   298,   300,
          r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
         &end

# 9 DC NU4:  (9 DC C3')-(9 DC C4')-(9 DC O4')-(9 DC C1')  -1.9  34.0
 &rst     iat =   315,   298,   300,   301,
          r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
         &end

# 12 DG NU0:  (12 DG C4')-(12 DG O4')-(12 DG C1')-(12 DG C2') -44.7 -14.7
 &rst     iat =   391,   393,   394,   413,
          r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
```

```
        &end

# 12 DG NU1:  (12 DG O4')-(12 DG C1')-(12 DG C2')-(12 DG C3')  18.1  48.1
 &rst    iat =   393,   394,   413,   411,
          r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
        &end

# 12 DG NU2:  (12 DG C1')-(12 DG C2')-(12 DG C3')-(12 DG C4') -37.2  -6.7
 &rst    iat =   394,   413,   411,   391,
          r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
        &end

# 12 DG NU3:  (12 DG C2')-(12 DG C3')-(12 DG C4')-(12 DG O4') -16.9  24.2
 &rst    iat =   413,   411,   391,   393,
          r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
        &end

# 12 DG NU4:  (12 DG C3')-(12 DG C4')-(12 DG O4')-(12 DG C1')  -1.9  34.0
 &rst    iat =   411,   391,   393,   394,
          r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
        &end

# 13 DA NU0:  (13 DA C4')-(13 DA O4')-(13 DA C1')-(13 DA C2') -43.9 -13.9
 &rst    iat =   424,   426,   427,   445,
          r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
        &end

# 13 DA NU1:  (13 DA O4')-(13 DA C1')-(13 DA C2')-(13 DA C3')  22.2  52.2
 &rst    iat =   426,   427,   445,   443,
          r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
        &end

# 13 DA NU2:  (13 DA C1')-(13 DA C2')-(13 DA C3')-(13 DA C4') -44.6 -14.6
 &rst    iat =   427,   445,   443,   424,
          r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
        &end

# 13 DA NU3:  (13 DA C2')-(13 DA C3')-(13 DA C4')-(13 DA O4')  -3.2  26.8
 &rst    iat =   445,   443,   424,   426,
          r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
        &end

# 13 DA NU4:  (13 DA C3')-(13 DA C4')-(13 DA O4')-(13 DA C1')  -4.4  25.6
 &rst    iat =   443,   424,   426,   427,
          r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
        &end
```

```
# 14 DA NU0:  (14 DA C4')-(14 DA O4')-(14 DA C1')-(14 DA C2') -43.9 -13.9
 &rst     iat =   456,   458,   459,   477,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
         &end

# 14 DA NU1:  (14 DA O4')-(14 DA C1')-(14 DA C2')-(14 DA C3')  22.2  52.2
 &rst     iat =   458,   459,   477,   475,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
         &end

# 14 DA NU2:  (14 DA C1')-(14 DA C2')-(14 DA C3')-(14 DA C4') -44.6 -14.6
 &rst     iat =   459,   477,   475,   456,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
         &end

# 14 DA NU3:  (14 DA C2')-(14 DA C3')-(14 DA C4')-(14 DA O4')  -3.2  26.8
 &rst     iat =   477,   475,   456,   458,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
         &end

# 14 DA NU4:  (14 DA C3')-(14 DA C4')-(14 DA O4')-(14 DA C1')  -4.4  25.6
 &rst     iat =   475,   456,   458,   459,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
         &end

# 15 DG NU0:  (15 DG C4')-(15 DG O4')-(15 DG C1')-(15 DG C2') -44.7 -14.7
 &rst     iat =   488,   490,   491,   510,
           r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
         &end

# 15 DG NU1:  (15 DG O4')-(15 DG C1')-(15 DG C2')-(15 DG C3')  18.1  48.1
 &rst     iat =   490,   491,   510,   508,
           r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
         &end

# 15 DG NU2:  (15 DG C1')-(15 DG C2')-(15 DG C3')-(15 DG C4') -37.2  -6.7
 &rst     iat =   491,   510,   508,   488,
           r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
         &end

# 15 DG NU3:  (15 DG C2')-(15 DG C3')-(15 DG C4')-(15 DG O4') -16.9  24.2
 &rst     iat =   510,   508,   488,   490,
           r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
         &end
```

```
# 15 DG NU4:  (15 DG C3')-(15 DG C4')-(15 DG O4')-(15 DG C1')  -1.9  34.0
 &rst     iat =   508,   488,   490,   491,
           r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
         &end

# 17 DT NU0:  (17 DT C4')-(17 DT O4')-(17 DT C1')-(17 DT C2') -52.1 -22.1
 &rst     iat =   551,   553,   554,   572,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
         &end

# 17 DT NU1:  (17 DT O4')-(17 DT C1')-(17 DT C2')-(17 DT C3')  15.0  45.0
 &rst     iat =   553,   554,   572,   570,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 17 DT NU2:  (17 DT C1')-(17 DT C2')-(17 DT C3')-(17 DT C4') -27.4   2.6
 &rst     iat =   554,   572,   570,   551,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 17 DT NU3:  (17 DT C2')-(17 DT C3')-(17 DT C4')-(17 DT O4') -25.0   5.0
 &rst     iat =   572,   570,   551,   553,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 17 DT NU4:  (17 DT C3')-(17 DT C4')-(17 DT O4')-(17 DT C1')  13.5  43.5
 &rst     iat =   570,   551,   553,   554,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end

# 18 DT NU0:  (18 DT C4')-(18 DT O4')-(18 DT C1')-(18 DT C2') -52.1 -22.1
 &rst     iat =   583,   585,   586,   604,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
         &end

# 18 DT NU1:  (18 DT O4')-(18 DT C1')-(18 DT C2')-(18 DT C3')  15.0  45.0
 &rst     iat =   585,   586,   604,   602,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 18 DT NU2:  (18 DT C1')-(18 DT C2')-(18 DT C3')-(18 DT C4') -27.4   2.6
 &rst     iat =   586,   604,   602,   583,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 18 DT NU3:  (18 DT C2')-(18 DT C3')-(18 DT C4')-(18 DT O4') -25.0   5.0
```

```
 &rst     iat =   604,   602,   583,   585,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
          &end

# 18 DT NU4:  (18 DT C3')-(18 DT C4')-(18 DT O4')-(18 DT C1')  13.5  43.5
 &rst     iat =   602,   583,   585,   586,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
          &end

# 19 DA NU0:  (19 DA C4')-(19 DA O4')-(19 DA C1')-(19 DA C2') -43.9 -13.9
 &rst     iat =   615,   617,   618,   636,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
          &end

# 19 DA NU1:  (19 DA O4')-(19 DA C1')-(19 DA C2')-(19 DA C3')  22.2  52.2
 &rst     iat =   617,   618,   636,   634,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
          &end

# 19 DA NU2:  (19 DA C1')-(19 DA C2')-(19 DA C3')-(19 DA C4') -44.6 -14.6
 &rst     iat =   618,   636,   634,   615,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
          &end

# 19 DA NU3:  (19 DA C2')-(19 DA C3')-(19 DA C4')-(19 DA O4')  -3.2  26.8
 &rst     iat =   636,   634,   615,   617,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
          &end

# 19 DA NU4:  (19 DA C3')-(19 DA C4')-(19 DA O4')-(19 DA C1') -4.4  25.6
 &rst     iat =   634,   615,   617,   618,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
          &end
```

APPENDIX D

MOLECULAR DYNAMICS FILES

File D1. Energy minimization protocol (initial minimisation prior to MD GB model)

```
&cntrl
imin = 1,
maxcyc = 500,
ncyc = 250,
ntb = 0,
igb = 1,
cut = 12
```

File D2. Simulated annealing protocol, 100 ps

```
 &cntrl
   imin=0, ntr=0, ntc=2, ntf=2,
   cut=18.0, igb=1, saltcon=0.1, gbsa=0, offset=0.13,
   ntpr=1000, ntwx=1000, nstlim=100000, dt=0.001,
   ntt=1, ntx=1, irest=0, ntb=0, vlimit=20,
   pencut=-0.001, nmropt=1,
 &end

#
#Simple simulated annealing algorithm:
#
#from steps 0 to 5000: heat the system to 600K with short tautp
#from steps 5001 to 10000: keep the temperature at 600K
```

```
#from steps 10001 to 90000: cool down the system to 100K with long tautp
#from steps 90001 to 100000: cool down the system to 0K with short tautp
#
 &wt type='TEMP0', istep1=0,istep2=5000,value1=0.0,
          value2=600.0,    &end
 &wt type='TEMP0', istep1=5000,istep2=10000,value1=600.0,
          value2=600.0,    &end
 &wt type='TEMP0', istep1=10001, istep2=90000, value1=600.0,
          value2=100.0,     &end
 &wt type='TEMP0', istep1=90001, istep2=100000, value1=100.0,
          value2=0.0,     &end

 &wt type='TAUTP', istep1=0,istep2=10000,value1=0.5,
          value2=0.5,     &end
 &wt type='TAUTP', istep1=10001,istep2=90000,value1=4.0,
          value2=4.0,     &end
 &wt type='TAUTP', istep1=90001,istep2=100000,value1=1.0,
          value2=1.0,     &end

 &wt type='REST', istep1=0,istep2=20000,value1=0.1,
          value2=1.0,  &end
 &wt type='REST', istep1=20001,istep2=100000,value1=1.0,
          value2=1.0,  &end

 &wt type='END'  &end
LISTOUT=POUT
```

File D3. Control script for explicit solvent production calculations, 1 ns

```
&cntrl
  imin = 0, irest = 1, ntx = 7,
```

```
  ntb = 2, pres0 = 1.0, ntp = 1,
  taup = 2.0,
  cut = 10.0,
  pencut=-0.001, nmropt=1,
  ntr = 0,
  ntc = 2, ntf = 2,
  tempi = 300.0, temp0 = 300.0,
  ntt = 3, gamma_ln = 1.0,
  nstlim = 500000, dt = 0.002,
  ntpr = 100, ntwx = 100, ntwr = 1000
/

 &wt type='REST', istep1=0,istep2=30000,value1=0.1,
          value2=1.0, /
 &wt type='REST', istep1=30001,istep2=20000,value1=1.0,
          value2=1.0,  /

 &wt type='END'  /
LISTOUT=POUT
```

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