Structures of the 3,4-Epoxybutene-Derived *R*- and *S*-N1-(2-Hydroxy-buten-2-yl) - 2' Deoxyinosine DNA Adducts: Regiochemical Control of Glycosidic Torsion Angle Conformation

BY

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To my parents Mon-Lin and Carol and my sister Angie for always being there for me

To my friends who have shared my journey and made it meaningful

To my teachers, past and present, who have helped me explore my curiousity of the world

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Introduction

1.1 **Butadiene: evidence for toxicity in rodents and humans**

Chemicals in the environment are a constant exogenous challenge to the human body. People can be exposed through ingestion of contaminated food and water or inhalation of contaminated air. Some of these chemicals are known to be carcinogens, including polycyclic aromatic hydrocarbons, the mold-produced aflatoxin, and aromatic or heterocyclic amines. 1,3-Butadiene (BD), a colorless gas, has been classified as a known carcinogen by the National Toxicology Program, but the mechanism and degree of carcinogenicity is the subject of debate[1].

BD is primarily obtained through petrochemical extraction and is used for a wide variety of applications including the synthesis of various plastics and styrene-butadiene rubber (SBR), and is produced in excess of a million tons per year in the United States alone[2]. Additionally, the EPA estimates that over 200 million pounds are released into the environment as emissions from vehicles and industry[3]. Other sources of BD include combustion products[4] such as cigarette smoke[5], and contamination through release of BD from plastic containers[,] . Exposure to high concentrations of BD primarily occurs in industrial settings. The National Toxicology Program has classified BD a human carcinogen based on: 1) evidence of multi-organ carcinogenicity in animal models, and 2) epidemiological data that shows an increased incidence of leukemia related mortality in BD workers compared to the general population[6].

Human Epidemiology of BD

Epidemiological evidence of BD toxicity is primarily derived from three study groups of exposed workers. First, the works of Meinhardt et al[7] and Matanoski et al[8,9], examined SBR factories in operation in 1976. Exposure in these facilities was estimated to be .1-4.2 ppm over 8 h. Results obtained by Meinhardt et al[7] showed that the mortality due to cancers in BD workers was actually lower compared with the general population except in the case of lymphohematopoietic cancers (LHCs), suggesting that BD exposure could lead to LHC outcomes; however, the sample size of this study was too small to be statistically significant. In order to correct this deficiency, Matanoski et al[8] examined a cohort of 12,110 North American SBR workers and again found that mortality due to cancers was lower in the sample population than the control, excepting LHCs. These studies pointed toward LHC's as a possible outcome due to BD exposures. The second study group, including the works of Downs et al[10], Divine et al[11,12], and Divine and Hartman[13], studied butadiene monomer workers belonging to a WWII era BD manufacturing facility which was the top producing factory of the time. Similar to the above mentioned studies, Downs, Divine, Hartman and collaborators observed an overall lower mortality rate due to cancer in the observed population compared to the general population, but average rates of mortality due to LHCs. The third study group, examined by Matanoski and Santos Burgos et al[14,15], attempted to control examined cases by age, employment duration, years of employment, facility of employment, and exposure level[14, 15]. Worker exposure data was not available; instead, exposure was estimated by a panel of engineers based on the specific jobs held by each individual. These studies found a correlation between high exposure levels and increased risk of leukemia. Finally, a follow up study done by Delzell et al[16,17] found a clear increase in leukemia over the general population, especially in workers employed for at least 10 years and followed for at least 20 years. These results suggested that there was a long incubation period between BD exposure and leukemia related mortality. Overall, although some critics disagree[18], these studies[14,15,16,17] found that BD exposed workers may have higher risk of developing LHCs than other cancers.

Animal models of BD toxicity

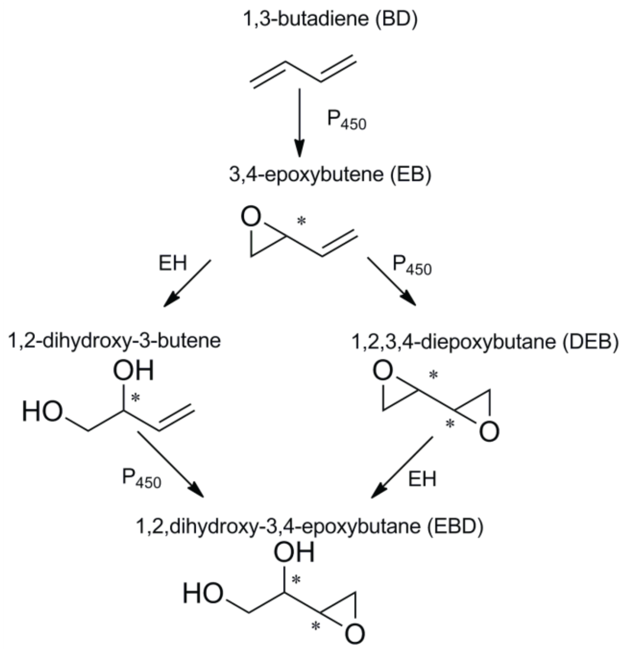
Rodents exposed to BD and its metabolites exhibit genotoxicity, mutagenicity, and multi-organ carcinogenicity. Mice had a higher sensitivity to BD toxicity than rats. Melnick and coworkers[19] found that B6C3F$_1$ mice exposed to inhaled BD had higher incidences of tumors in multiple organs compared to the control; control mice had tumor incidences of 20 and 12 percent in males and females respectively, while BD exposed mice had 80 and 94 percent incidences. These tumors occurred in multiple organs, including lymphomas in the thymus, spleen, lymph nodes, lung, liver, kidney, heart, pancreas and stomach. Of particular note in this study was the absence of tumors in the nasal cavity, which suggested that metabolic activation was a prerequisite of BD mediated toxicity. The BD concentrations examined in this study were 625 and 1250 ppm(compared to the contemporary OSHA standard of 1000 ppm) over 104 weeks, but the study length was shortened to 65 weeks due to cancer related mortality. In order to investigate lower dosages of BD, Melnick et al[20] chose concentrations of 6.25, 20, 62.5, 200, and 625 ppm in their next study. Over 65 weeks of exposure, it was found that lymphocytic lymphomas occurred in mice exposed to as low as 62.5 ppm. At the dosage of 625 ppm, 24 male and 59 female mice died before 65 weeks. Of these mice, 75% of males and 33% of females had lymphocytic lymphoma. Other tissues found to have significant tumorigenesis included heart, forestomach, lung, harderian gland, and liver. Owen et al[21] observed that Sprague-Dawley rats were also sensitive to chronic BD inhalation. Subjects were exposed to either 1000 or 8000 ppm BD over 111 or 105 weeks for males and females respectively. Increased BD concentration was associated with increased mortality in both males and females, which the authors attributed to renal lesions and sacrifice due to subcutaneous masses respectively. Tumors were most common in the mammary gland, the pancreas, the thyroid, and the testes. Through these three studies, Melnick, Owen and coworkers[19,20,21] show that chronic inhaled BD induces tumorigenesis in $B6C3F_1$ mice and Sprague-Dawley rats. Comparing these three studies, however, one may notice a large difference in the BD dosage necessary to induce tumorigenesis; rats were exposed 1000 and 8000 ppm of BD, while mice were sensitive to doses as low as 6.25 ppm.

Noticing the species differences between mice and rats leads to two important questions: what are the causes of these species differences in BD toxicity, and do these differences have relevance in human BD toxicity? The differences in toxicity between rats and mice is likely due to species differences in the metabolism of BD[27]. Mouse and human response to BD toxicity is similar in the type of cancers observed. BD exposure induces lymphatic, hematopoietic, and lung cancers in mice[22], which may indicate a better model for studying human cancers caused by BD. In addition, studies have shown that rat models tend to be insensitive to leukemia and lymphomas[23]. On the other hand, rat metabolism of BD is more similar to humans, producing similar levels of metabolites at both low at high exposure levels, and concentrations of BD metabolites deposited in various tissues were more similar between rat and human models than in mouse and human models[24]. Therefore, it is unclear whether the rat or mouse model is superior, and both must be considered.

Metabolism of 1,3-butadiene

The mutagenicity of BD towards *Salmonella typhimurium* increases when co-incubated with rat liver microsomes or S-9 rat liver fractions, suggesting that BD is more potent after metabolic activation[25]. The key step behind BD metabolism and toxicity is oxidation by cytochrome P450 to form reactive epoxide intermediates. Either vinyl carbon is first oxidized by cytochrome P450 2E1 or 2A6 to *R*- or *S*- 3,4-epoxybutene (EB)[26]. EB is subsequently oxidized to form 1,2,3,4-diepoxybutane (DEB), or hydrolyzed by epoxide hydrolase to form 1,2-dihydroxy-3-butene. The metabolite 1,2-dihydroxy-3,4-epoxybutane (EB-diol) may be produced by the hydrolysis of DEB by epoxide hydrolase or the oxidation of 1,2-dihydroxy-3-butene by cytochrome P450. These epoxides are highly reactive and can alkylate macromolecules including protein and DNA.

Scheme 1[a] Cytochrome P_{450} Mediated Oxidation



[a] EH is Epoxide Hydrolase, and P_{450} is cytochrome P_{450}

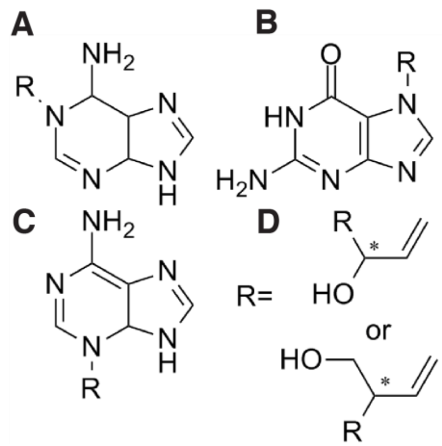
The secondary metabolite DEB is observed to be the most mutagenic epoxide, followed by EB-diol and EB[27]. Mice uptake BD more readily and have a higher rate of both EB and DEB production than both rats and humans. In addition, rats have a higher rate of detoxification of epoxides by hydrolysis and glutathione conjugation than mice[28]. As a consequence, mice have higher tissue accumulation of reactive BD metabolites than rats: EB concentration can be 15 times higher in mice compared to rats, while estimates of relative DEB concentrations range from 3 times higher in mice to 100 times higher in mice[29, 30]. These differences in epoxide production and clearance and tissue concentrations of reactive epoxides are thought to be the primary factors in the relative increase in BD carcinogenicity in mice compared to rats.

Up to 20% of observed mutations in mice chronically exposed to BD occur at A:T pairs[22]. 3,4-epoxybutene has been observed to induce A:T to G:C transitions and A:T to C:G transversions in the splenic T-cells from B6C3F_1 mice. These A to G transitions have been found to be particularly common at codon 61 of the oncogene H-*ras*, occurring in 75% of Harderian gland tumors examined[31]. Taken together, these two studies may implicate EB induced DNA adducts as a culprit for A to G transitions caused by BD. As human *ras* mutations are associated with leukemia, EB induced mutations may represent crucial targets in the search for the mechanism for BD induced carcinogenicity.

1.2 **3,4-epoxybutene alkylation of Adenine**

EB can alkylate at epoxide carbon 3 (C-3) or carbon 4 (C-4), and has been shown to react with guanine and adenine *in vitro*[32]. The direction of ring opening may depend on the mechanism of substitution: S_n1 like reactions are more likely to occur at the more substituted C-3 position, while S_n2 like reactions are more likely to occur at the less sterically hindered C-4 position[32,33]. All EB adducts can be sorted by product stereochemistry (*R- vs S-*), epoxide regiochemistry (C-3 vs C-4), and nucleotide regiochemistry. The differences in biological processing caused by adduct stereochemistry and regiochemistry are largely unresolved.

Scheme 2[a]

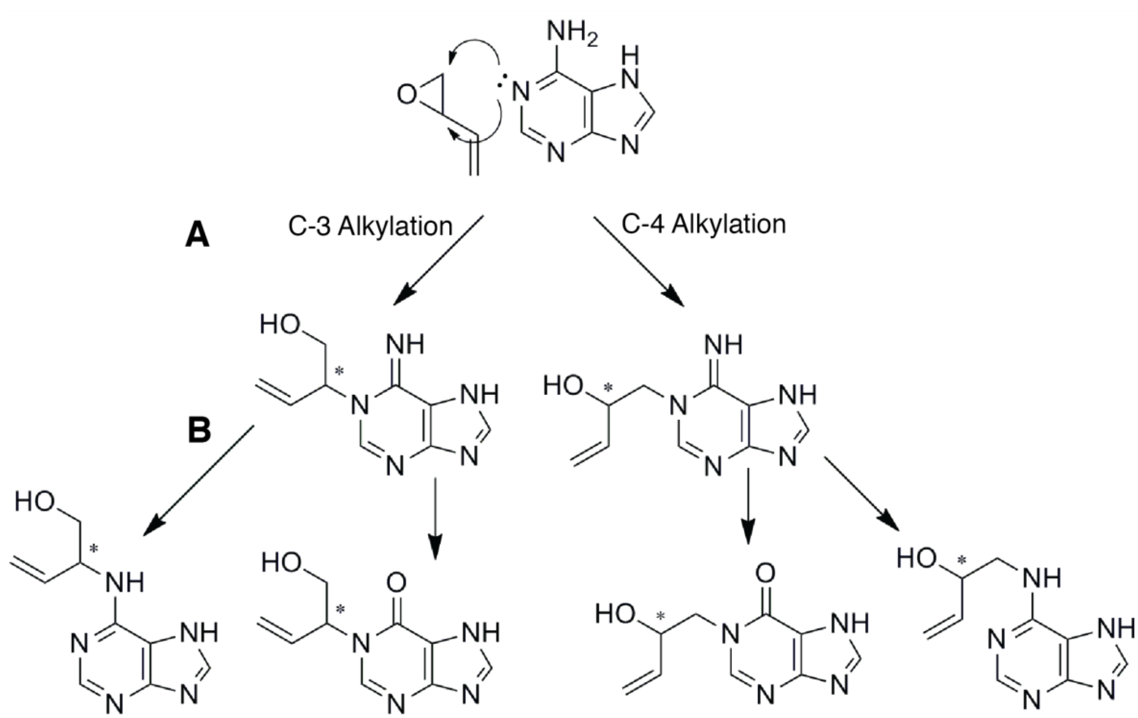


[a] (A) N1 EB adenine adducts (B) N7 EB guanine adducts (C) N3 EB adenine adducts

When reacted with calf thymus DNA under physiologically relevant conditions, EB-dG adducts were more common than EB-dA adducts[32]. The most prevalent dG adducts were identified as the regioisomeric pair 7-(2-hydroxy-3-buten-1-yl) guanine and 7-(1-hydroxy-3-buten-2-yl), which result from alkylation of the carbon-4 (C-4) and carbon-3 (C-3) of EB respectively[32]. The most abundant dA adducts were identified as the regioisomeric pair of N-3 substituted adducts 3-(2-hydroxy-3-buten-1-yl) adenine and 3-(1-hydroxy-3-buten-1-yl)[32]. The least common adducts were the regioisomeric pair 1-(2-hydroxy-3-buten-1-yl) adenine and 1-(1-hydroxy-3-buten-1-yl) (Scheme 2)[32].

The N-3 EB-dA adducts are unlikely to be responsible for A to G transitions because they are unstable and depurinate to form abasic sites. Some evidence shows that adenine is preferentially inserted across from abasic sites, a hypothesis known as the “A rule”, while studies done with human Y-family polymerases showed a preference for thymine and cytosine[34, 35]. Therefore, the N-1 EB adenine adducts may be the most likely suspects in EB related A to G and A to C mutations. Under physiological conditions, EB reacts with adenine at the N-1 position to form two regioisomeric pairs of enantiomers, the C-3 adducts *R*- and *S*- 1-(1-hydroxy-3-buten-2-yl) adenine and the C-4 adducts *R*- and *S*- 1-(2-hydroxy-3-buten-2-yl) adenine, which are unstable and have half-lives of 7 and 9.5 hours respectively[36](Scheme 4). These adducts can either undergo base catalyzed Dimroth rearrangement to form N-6 adenine adducts or deamination to form N-1 inosine adducts.

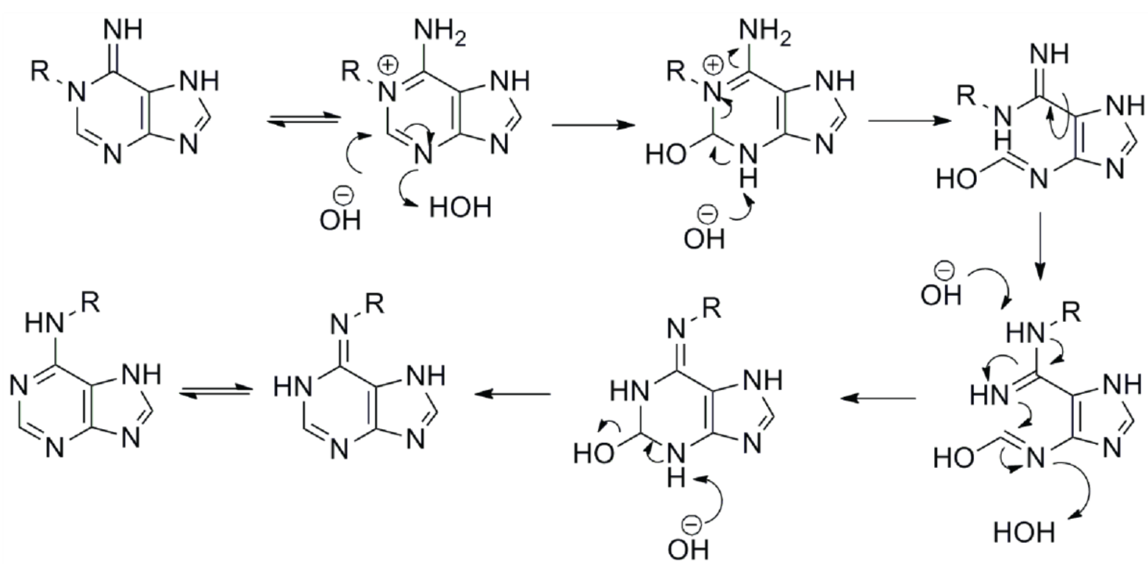
Scheme 3[a]



[a] (A) Regioselective alkylation of adenine by EB at either carbon 3 (C-3_ or carbon 4 (C-4) to form initial N1 adenine products (B) Formation of N6 adenine adducts through Dimroth rearrangement or formation of N1 inosine adducts through deamination

Dimroth rearrangement of adenine adducts is initialized by hydroxide attack at the N3 position, causing the heterocyclic ring to open at the C-2-N-1 bond[29]. The C-5-C-6 bond can rotated 180^0, and upon ring closure, the N-1 alkyl groups have migrated to the exocyclic N6 position. This mechanism has been confirmed by labeling the exocyclic nitrogen in adenosine with ^{15}N, allowing the monitoring of the rearrangement by NMR. Deamination of N1 adenine adducts can occur by acid catalyzed hydrolysis, where a water attacks the electrophilic C-6 and displaces the exocyclic amine[29].

Scheme 4[a]



[a] Proposed mechanism of Dimroth rearrangement of N1 adenine adducts into N6 adenine adducts

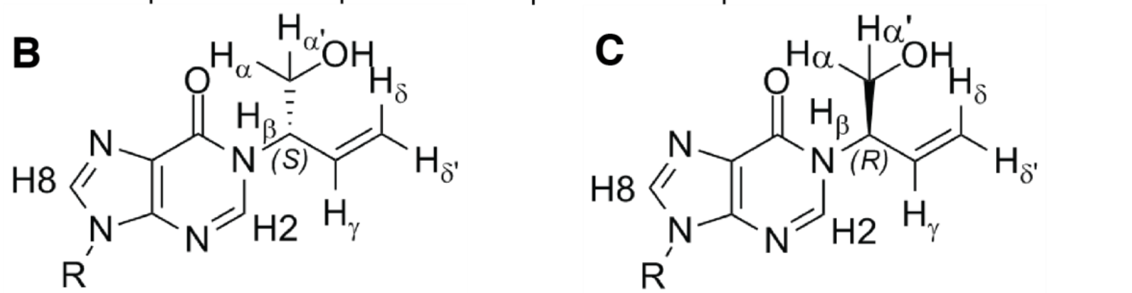
1.3 **Properties of adenine adducts**

EB alkylation of adenine results in two regioisomeric pairs of stable adducts- The N6 adenine and N1 inosine adducts. In order to determine the role of these EB adenine adducts in BD toxicity, the mutagenic spectra of both C-3 N1 and N6 adducts were determined in the *ras* 61 sequence contex[37, 38]. The Lloyd group investigated these adducts by ligating 11mer *ras* sequences with modified oligonucleotide at the 6th position into bacterial plasmid M13mp7L2[37]. The modified plasmid was transformed into repair deficient *E. coli* or COS-7 systems, and resulting plaques were probed for misincorporation across from the modified nucleotide.

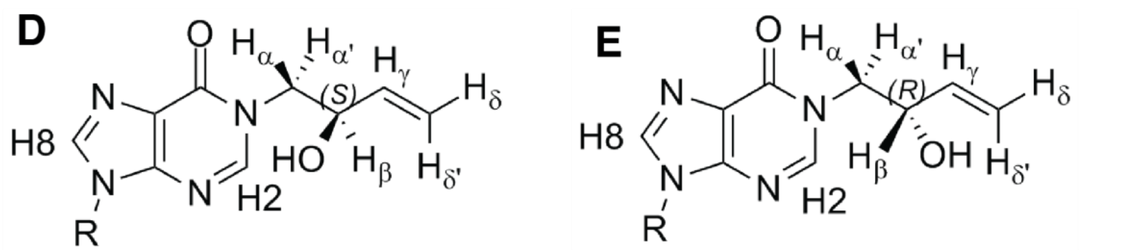
Scheme 5[a]

A

$$
\begin{array}{lcccl}
 & 60 & 61 & 62 & \\
5'\text{-}C^{1} & |\,G^{2}\ G^{3}\ A^{4} & |\,C^{5}\ X^{6}\ G^{7} & |\,G^{8}\ A^{9}\ A^{10} & |\,G^{11}\text{-}3' \\
3'\text{-}G^{22} & |\,C^{21}C^{20}T^{19} & |\,G^{18}T^{17}T^{16} & |\,C^{15}T^{14}T^{13} & |\,C^{12}\text{-}5'
\end{array}
$$



N1-[1(*S*)-hydroxy-3-buten-2-yl]-2'-deoxyinosine Adduct **N1-[1(*R*)-hydroxy-3-buten-2-yl]-2'-deoxyinosine Adduct**



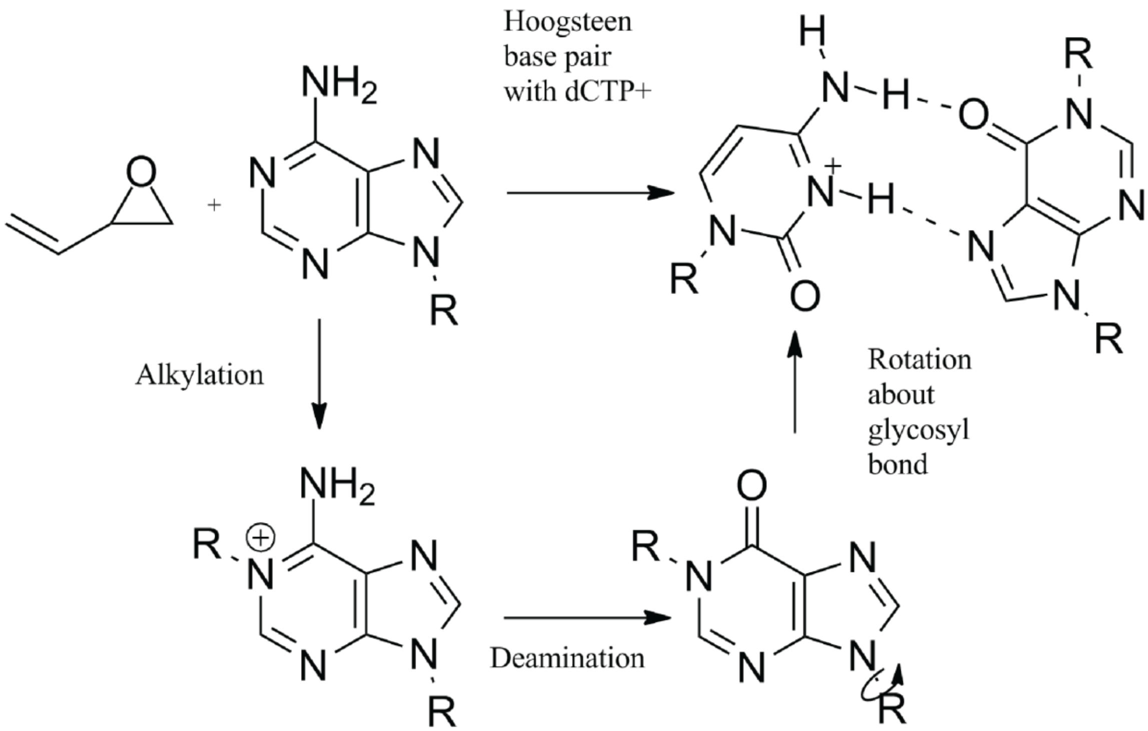
N1-[2(*S*)-hydroxy-3-buten-2-yl]-2'-deoxyinosine Adduct **N1-[2(*R*)-hydroxy-3-buten-2-yl]-2'-deoxyinosine Adduct**

[a] (A) The *ras61* oligodeoxynucleotide (B) The chemical structure of the N1-[1(S)-hydroxy-3-buten-2-yl]-2'-deoxyinosine adduct (C) The chemical structure of the N1-[1(R)-hydroxy-3-buten-2-yl]-2'-deoxyinosine adduct (D) The chemical structure of the N1-[2(S)-hydroxy-3-buten-2-yl]-2'-deoxyinosine adduct (E) The chemical structure of the N1-[2(R)-hydroxy-3-buten-2-yl]-2'-deoxyinosine adduct

Both *R*- and *S*- N-6 adducts been observed to be non-mutagenic in *E. coli* models[39]. In contrast, C-3 regioisomers of N-1 inosine adducts have been shown to be very mutagenic in both E coli and COS-7 cell models[37,38]. Both stereoisomers of C-3 N1 inosine adducts cause primarily A to G mutations in the *ras* codon 61 sequence context[37,38]. In the bacterial model, Rodriguez et al discovered that these inosine adducts caused A to G mutations over 50% of the time, with the *S*- isomer being more mutatgenic at 67%[37]. These results were mirrored in COS-7 cells, which are a line derived from African green monkeys and presumably more accurate to human response. The *S*- isomer adduct caused A to G point mutations at 79%, while the *R*- isomer produced A to G mutations as 48% of products[38]. The next most common mutation observed in these experiments was A to C at 10% in *S*- isomers and 7% in *R*- isomers[38].

In order to explain the high prevalence of the observed mutations, the Lloyd group postulated that the deamination of adenine into inosine would change the preferred base-pairing partners of the modified base to I-C> I-A > I-G[38]. However, the presence of a bulky alkyl chain at the N1 position would block Watson-Crick base pairing between the modified base and a deoxycytidine. Therefore, it was proposed that N1 adducted nucleotides would rotate into the *syn* conformation to allow Hoogsteen base pairing with an opposite dC[38]. These observations led to a three step mechanistic hypothesis of A to G mutations caused by EB adducts of adenine: 1) the alkylation of adenine by EB at the N1 position, 2) the deamination of EB adenine adducts to form inosine adducts, and 3) rotation about the glycosyl bond to from a Hoogsteen base pair with a protonated dC (Scheme 7)[38].

Scheme 6[a]



[a] Proposed mutation mechanism of carbon 3 (C-3) N1-dI adducts leading to A to G mutations

To test this hypothesis, Scholdberg et al[40] and Merritt et al[41] determined the solution structures of the C-3 inosine adducts in the *ras* codon 61 sequence context using NMR methods. Both isomers were found to closely resemble standard B-type DNA. In both isomers, the BD moiety was found to significantly disrupt DNA conformation at the lesion site, where the modified base X^6 flipped into the *syn* conformation. This conformation pointed the BD moiety into the major groove of the duplex, which disrupted the 3' neighbor base pair A^7:T^{16}. The primary piece of evidence for this conformation was the relatively high intensity of the observed NOE between the base proton X^6H8 and sugar proton X^6H1', which indicates that the purine has flipped about the glycosyl bond to bring those two protons closer in space. The presence of the BD moiety at the N1 position also severely destabilized the DNA duplex, causing the melting temperature to fall to 33^0C, a 24^0 shift. The causes of this dramatic shift in melting temperature include a disruption base stacking around lesion and the loss of base pairing between X^6 and T^{17}.

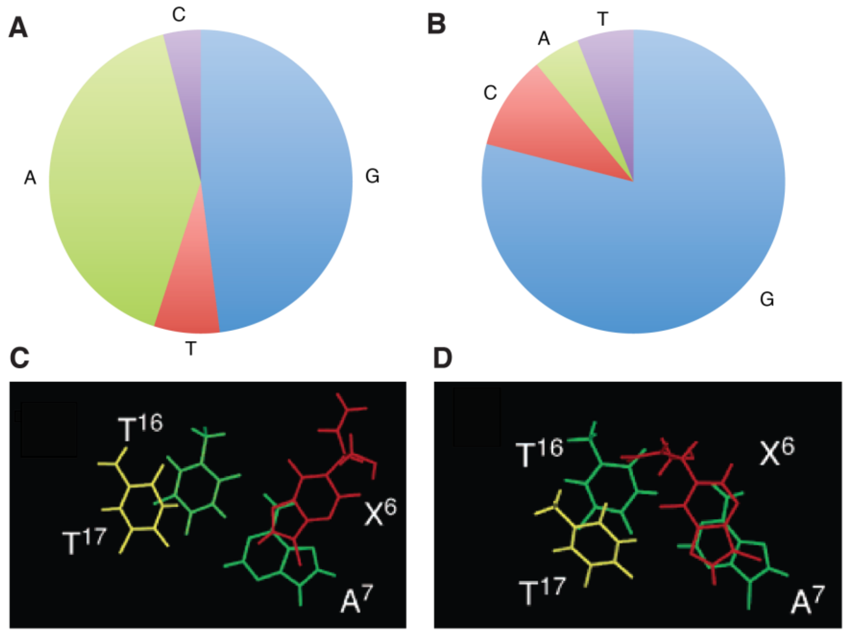


Figure 1. Mutagenic spectra and lesion structure of carbon 3 (C-3) N1 EB inosine adducts. (A) Mutation percentage of the site specifically modified S- N1 EB inosine adduct. (B) Mutation percentage of the site specifically modified R- N1 EB inosine adduct. (C) Lesion site in the S- N1 EB insoine adduct. (D) Lesion site in the R- N1 EB insoine adduct

These structure observations supported the hypothesis proposed by Lloyd and coworkers[38] that A to G mutations may be the result of a mispairing between an N1 inosine adduct and a protonated dCTP. The N1 inosine adducted nucleotide assumed the *syn* conformation even without the ability to form a favorable hydrogen bond with a suitable base pairing partner. Translesion synthesis could provide a favorable environment for misincorporation to occur at these lesions.

Stereochemical differences between the *R*- and *S*- isomers resulted in small conformational differences between the isomers. Merritt[41] observed that the primary difference between the isomers was the orientation of the hydroxyl group from the BD moiety. The *R*- hydroxyl was oriented toward the complementary base T[17] across the major groove, while the *S*- hydroxyl was pointed away from the duplex and into solution. This difference creates a more solvent accessible lesion site in the *S*- adduct, which may contribute to differential biological processing by repair mechanisms. This speculation is corroborated by a number of studies that observed stereoselective processing by DNA binding proteins, including phosphodiesterases, Y-family polymerases, and RNA polymerases[36,37,38].

1.4 **Statement of Problem**

Research into BD related toxicity has shown that mutations at A:T pairs cause around 20% of all point mutations observed in mouse models, including mutations at codon 61 in the *ras* oncogene[22]. These mutations are particularly interesting in the context of BD carcinogenicity because mutations in the *ras* oncogene are commonly found in hematopoietic and lymphoid cancers. EB has been shown to cause mutations at A:T pairs *in vitro*, and can form a variety of adducts on adenine, including the N1 inosine adducts[36]. There are four unique

N1 inosine adducts as a result of stereo and regioselective alkylation by EB. Research done by the Lloyd group has shown that the C-3 regioisomers are extremely mutagenic and tended to cause A to G adducts[37,38], with the *S*-adducts causing mutations at a higher rate than the *R*- isomer. Subsequent work done by the Stone group[40,41] supported the hypothesis that these C-3 adducts caused the A to G mutations by forming Hoogsteen base pairs with incoming dCTP. These studies beg the question: do the C-4 and C-3 adducts behave in similar ways? To answer that question, this work used NMR methods to determine the solution structure of the C-4 *R*- and *S*- N1 inosine isomers in the *ras* codon 61 sequence context (scheme 6).

Chapter 2

Structure determination of C4 N1-dI adducts using NMR and rMD

2.1 Introduction to NMR based structure determination

There are two primary techniques that can be used to obtain atomic resolution structural information from DNA duplexes: X-ray crystallography and nuclear magnetic resonance (NMR). NMR based techniques. X-ray crystallography has been used to study various biological macromolecules, can sometimes achieve resolutions as fine as 1.5 Å, and can be used to study complexes between different macromolecules. This technique requires the sample to be in the form of large and stable crystals organized into a uniform lattice[42]. Not all macromolecules will crystalize in such a way, and finding the correct conditions can be a challenging process. In addition, as a result of confining macromolecules to a rigid lattice, information about the conformational flexibility and dynamics about the sample can be lost using X-ray crystallography. On the other hand, NMR techniques can be used reliably with small soluble macromolecules (<40 kDA), and can give give information about dynamics in solution[43, 44]. Due to these advantages, NMR was used to determine the structures of these modified DNA duplexes.

The most powerful 2-D NMR experiment for structure determination is the Nuclear Overhauser Effect spectroscopy (NOESY)[45]. This experiment measures the dipolar interactions of spins through space within ~5Å, and is the most widely used technique in the determination of oligodeoxynucleotide structure. To obtain the best quality spectrum for analysis of non-exchangeable protons, samples were prepared in deuterated solvent to eliminate detection of solvent signals. Labile protons involved in base pairing can be detected in H_2O solvent with 5% D_2O[45, 46, 47].

Identification of proton signals in NOESY spectra can be done using a method known as sequential assignment[48]. In this method, cross peaks between protons on spatially adjacent bases are identified and used to propagate assignment throughout the duplex. The first step is usually to identify aromatic protons H6 and H8 and the cross peaks to their own H2' sugar protons. Going from the 5' to 3' end, these H2' protons are within 5Å of the 3' neighbor's H6 or H8. This process is continued until the whole strand is assigned. The entire 5' to 3' assignment of cross peaks between aromatic and sugar protons is known as the NOESY walk. These initial assignments can be used as references to assign the rest of the unidentified sugar, aromatic, and exchangeable protons within a DNA duplex. These assignments are useful tools in studying DNA damage, as perturbation of native DNA conformation may lead to breaks in the NOESY walk or other assignments that can be easily observed.

Assignment of the initial NOESY walk can be challenging, especially in duplexes where the "walking region" is disrupted by lesions, or when the target sequence has repeating nucleotides. In order to provide reference points to aid in the assignment of NOESY spectra, 2-D correlation spectroscopy (COSY) is used. In ^{1}H COSY spectra, through bond interactions less than 3 bonds are observed[49]. In the context of DNA duplexes, these spectra reveal cytosine H5-H6 cross peaks and thymine methyl signals.

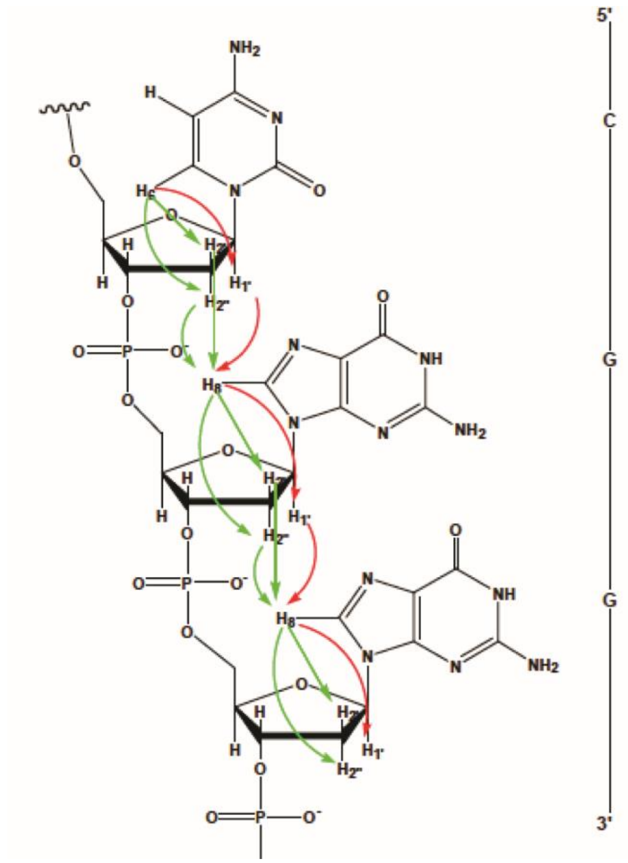


Figure 2. Depiction of the observable NOEs between adjacent nucleotides in DNA. Red arrows represent the initial NOESY walk between sugar H1' protons and aromatic H6/8 protons. Green arrows represent sequential connectivity between aromatic H6/8 protons and sugar H2'/2'' protons.

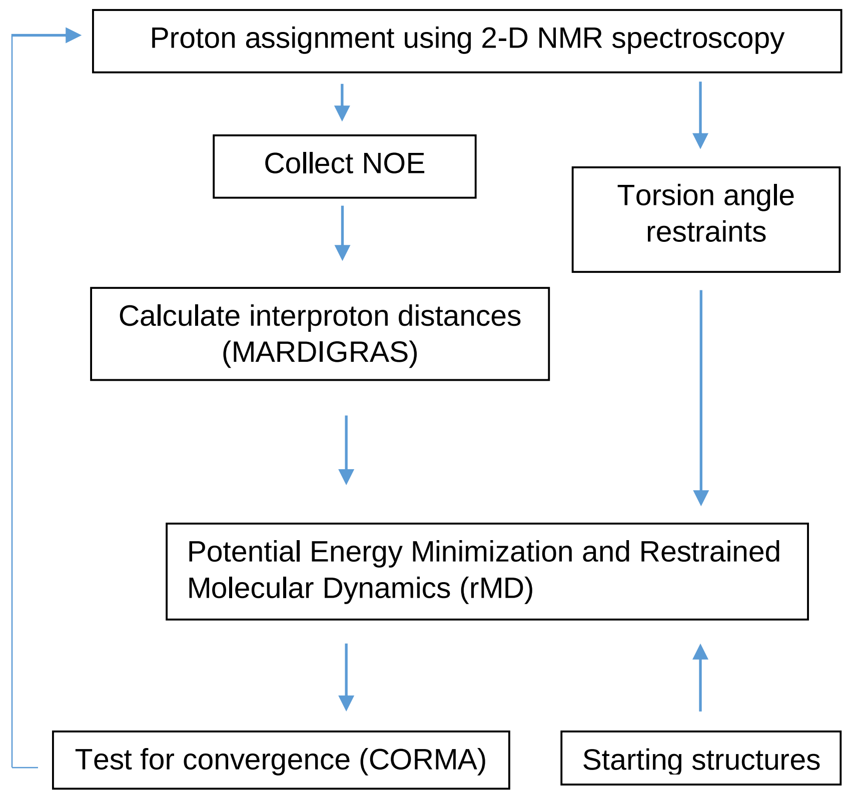


Figure 3. The method of NMR based structural refinement for oligodeoxynucleotides

After assignment of NMR spectra, the data is processed by integrating cross peaks to find the intensity of the signal. These volumes can be converted to proton-proton distances using programs such as Matrix Analysis of Relaxation for Discerning Geometry of an Aqueous Solution (MARDIGRAS)[50]. These distances are used as restraints in a restrained molecular dynamics simulation (rMD) using simulated annealing method in order to determine the solution structure[51]. This method works by heating up the simulated DNA duplex so that it may overcome energy barriers to conformational movement, so that it may explore many different conformations. The system is then cooled to find the lowest energy structure. These low energy stable structures are verified using the program complete relaxation matrix analysis (CORMA)[52,53], which compares the calculated NOESY intensities of the refined structure to the experimentally obtained intensities(Figure 3).

2.2 **Methods**

Preparation and Characterization of Oligodeoxynucleotide.

The unmodified oligodeoxynucleotides 5'-d(CGGACAAGAAG)-3' and 5'-d(CTTCTTGTCCG)-3', purified by anion exchange HPLC, were purchased from the Midland Certified Reagent Co. (Midland, TX). The concentrations of the single stranded oligodeoxynucleotides were determined from their calculated extinction coefficients[54]. The *R*- and *S*- modified oligodeoxynucleotides were synthesized via the phosphoramidite method courtesy of Kowalczyk et al[55] and were purified with reverse-phase HPLC using a C8(2) column in .1M ammonium formate with the following acetonitrile gradient: 1 to 4% over 5 min, 4 to 6.6% over 30 min, 6.6 to 90% over 3 min. These purified oligonucleotides were annealed to their complements in 10 mM Na_2HPO_4, 0.1M NaCl, and 50 μM Na_2EDTA (pH 7.0). The modified duplexes were annealed by heating to 80 ºC for 15 min and cooled to room temperature. The duplexes were separated from excess single strand DNA using Biogel hydroxyapatite using a 10 to 200 mM NaH_2PO_4 gradient (pH 7.0). The duplex was desalted by passing over a Sephadex G-25 column.

DNA Melting Studies

The thermal stabilities of unmodified and modified duplexes were determined by measuring UV absorption at 260 nm vs. temperatures using a Varian Cary 100 Biospectrophotometer (Varian Associates, Palo Alto, CA). The concentrations of the duplexes were 1.5 uM. Samples were prepared in 10 mM NaH_2PO_4, 1M NaCl, and 50□M Na_2EDTA (pH 7). The temperature was increased from 5 to 90 ºC at a rate of 0.7 ºC/min. The UV absorbance was monitored at 260 nm. The T_m values were determined by taking the first derivatives of the melting curves.

NMR Spectroscopy

The duplexes containing the modified *R*- and *S*- adducts were prepared at 1 mM concentration in 10mM NaH_2PO_4, 0.1M NaCl, and 50 □M EDTA (pH 7.0). To observe non-exchangable protons, the duplexes were exchanged with D_2O and dissolved in 99.996% D_2O. To observe exchangeable protons, the duplexes were dissolved in 9:1 H_2O:D_2O. ^1H NMR spectra were recorded using 900, 800, and 600 MHz spectrometers equipped with cryogenic probes (Bruker Biospin Inc., Billerica, MA). Chemical shifts were referenced to the chemical shift of the water resonance at the corresponding temperature, with respect to 4,4-dimethyl-4-silapentane-1-sulfonic acid (DSS). Data were processed using the program TOPSPIN (Bruker Biospin Inc., Billerica, MA). NOESY spectra in D_2O were collected at 15 ºC at 900 MHz at mixing times 150, 200, and 250 ms with a relaxation delay of 2.0 s.[27, 28] The *R*-isomer spectrum was recorded at a digital resolution of 2048 by 1024, zero filled to 2048 by 2048. The *S*-isomer spectrum was recorded at a digital resolution of 2048 by 512, zero filled to 2048 by 1024.

NOESY spectra in 9:1 H_2O:D_2O were collected at 5 ºC at 800 MHz with a relaxation delay of 1.2s and 250 ms mixing time. Water suppression was achieved using the WATERGATE pulse sequence. A skewed sine-bell square apodization function with a skew factor of 3.0 was used in both dimensions. Spectra were assigned using the program SPARKY[56].

NMR Distance Restraints

NOESY spectra peak intensities were determined by volume integrations of crosspeaks using the program SPARKY.[56] The unmodified B-type DNA duplex[51] 5'-d($C^1G^2G^3A^4C^5X^6A^7G^8A^9A^{10}G^{11}$)-3':5'-d($C^{12}T^{13}T^{14}C^{15}T^{16}T^{17}G^{18}T^{19}C^{20}C^{21}G^{22}$)-3', containing the *H-ras* codon 60-62 sequence context was constructed using the program INSIGHT II (ThermoFisher Scientific, Inc., Waltham, MA). To construct the starting structures adenine A^6 was replaced by either the *R*- or *S*- C4 adducts. Partial charges for the *R*- or *S*-C4 adducts were calculated with the B3LYP/6-31G* basis set in Gaussian 09[57] and used to prepare the parameter files in the program XLEAP[58]. These starting structures were minimized through 1000 cycles of potential energy calculations using the AMBER suite[59]. The NOESY peak intensities, the starting structures, and the AMBER parameter files were used to generate a refined hybrid intensity matrix. The program MARDIGRAS was used to calculate interproton distance vectors with upper and lower bounds at 2, 3, and 4 ns isotropic correlation times.[50,52,53] The JUMP 3 model was used for methyl protons.[60]

Restrained Molecular Dynamics Calculations

The interproton distance vectors calculated by MARDIGRAS were used to provide distance restraints used in restrained molecular dynamics (rMD) calculations. NOE crosspeaks were sorted into classes based on the confidence in the volume integrations. Class 1 peaks were defined as strong, well-resolved peaks with no overlap, and were assigned 10% error to the obtained volumes. Class 2 peaks were defined as strong peaks with minor overlap or broadening, and volumes obtained were assigned 20% errors. Class 3 peaks were defined as strong, overlapped cross-peaks, and obtained volumes were assigned 30% error. Class 4 and 5 cross-peaks were defined as highly overlapped and/or weak peaks closer to the level of noise, and the volumes obtained were assigned 40% and 50% error respectively. Empirical phosphodiester and deoxyribose pseudorotations restraints from B-DNA were also used[61]. For the modified base X^6 and its complement T^{17}, square energy potential wells of ±120º were used. For all other nucleotides, square energy potential wells of ± 60º were used. Pseudorotation restraints for the modified base X^6 and terminal bases C^1, G^{11}, C^{12}, and G^{22} were not employed. Watson-Crick base pair restraints were used for all base pairs except for the base pair X^6:T^{17}. Base pair restraints on base pair A^7:T^{16} were increased by ± 0.2 Å.

The AMBER[59] suite was used to perform simulated annealing calculations[62] using the parm99 force field.[63] Force constants of 32 kcal mol^{-1} $Å^{-2}$ were used for all restraints. The generalized Born model was used to simulate solvation, and the salt concentration was 1.0 M[64]. The duplex was coupled to the bath temperature to heat the duplex during simulated annealing[64]. Initial refinements were performed using a 20 ps protocol. For the first ps, the system was heated to 1000 K with a coupling of 0.5 ps, followed by 1 ps at 1000 K. Then, the system was cooled to 100 K over 16 ps with a coupling of 4 ps. Finally, the system was cooled to 0 K over the last 2 ps with a coupling of 1 ps. After initial refinements, a 100 ps protocol was used. The first 5 ps consisted of system heating from 0 K to 1000 K with a coupling of 0.5 ps, followed by 5 ps at 1000 K, followed by cooling to 100 K over 80 ps with a coupling of 4 ps. Finally, the system was allowed to cool to 0 K over the last 10 ps with a coupling of 1 ps. The output structure coordinates were saved after each iteration. To validate these structures, complete relaxation matrix analysis (CORMA) was used to compare experimentally obtained NOE intensities to intensities calculated from the output structure coordinates.[52,53] The nine best structures were chosen and subjected to potential energy minimization to compile an average refined structure.

2.3 **Results**

Thermal Melting Studies

The thermal melting temperatures (T_m values) of the duplexes were determined by temperature-dependent UV spectroscopy at 260 nm. The adducts reduced the T_m values compared to the *ras61* unmodified duplex by 22 ºC for the *S*- isomer and 20 ºC for the *R*- isomer. In ^{1}H NMR collected at 10 ºC increments from 5 ºC to 35 ºC, resonances were severely broadened by 25 ºC (Figure 4). At 5 ºC, the *R*- isomer spectrum had ten observed resonances, where the A^7:T^{16}

and A^4:T^{19} were completely overlapped, and the modified base pair was missing. When the temperature was increased to 15 ºC, the A^7:T^{16} cross-peak was observable but still overlapped with the A^4:T^{19} cross-peak. At 25 ºC, all resonances were broadened, with the A^7:T^{16} cross-peak severely broadened and the terminal base pairs not observed. For the *S*- isomer, ten distinct resonances were observed at 5 ºC, with the modified base pair missing. At 15 ºC, the A^7:T^{16} cross-peak was broadened and completely separated from the A^4:T^{19} cross peak. At 25 ºC, the terminal bases were not observable, and the A^7:T^{16} cross-peak was severely broadened.

Table 1 Melting temperature changes as comparted to wild type *ras61* DNA duplex in carbon 3 (C-3) and carbon 4 (C-4) adducted sequences

	Regioisomer	**S- Isomer**	**R- Isomer**
ΔT_m (from WT)	Carbon 4	-22.0	-19.5
ΔT_m (from WT	Carbon 3	-22.0	-22.0

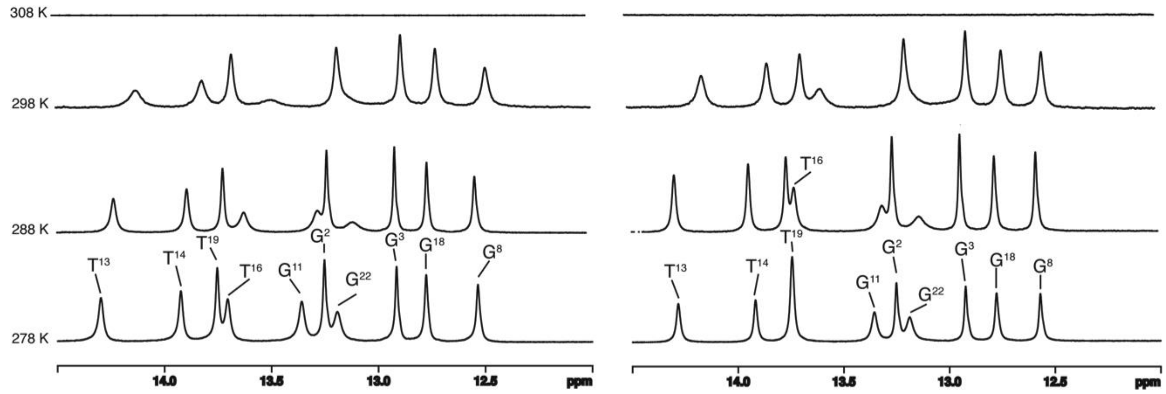


Figure 4. 1-D ^{1}H NMR of *S*- isomer (left) and *R*- isomer (right) carbon 4 (C-4) duplexes at 278, 288, 298 and 308 K at 800.13 MHz.

NMR spectroscopy. (a) Base Proton Assignment

Figure 5 shows a representative region of the NOESY spectra exhibiting cross-peaks between deoxyribose anomeric H1' and base aromatic protons of the *R*- and *S*- isomers and the unmodified duplex. These assignments were completed with the help of COSY data (Figure 6). The *R*- isomer adduct induced observable changes in the sequential NOEs between the sugar H1' and base aromatic protons. Especially of note is weak C^5 H1'- X^6 H8 NOE compared to the unmodified spectrum, indicating that the conformation of neighbor bases were affected by the adduct. The relative intensity of the X^6 H1' - A^7 H8 cross-peak was also comparatively weak, but overlap with the A^7 H1' - A^7 H8 cross-peak obscures this difference in the shown spectra.

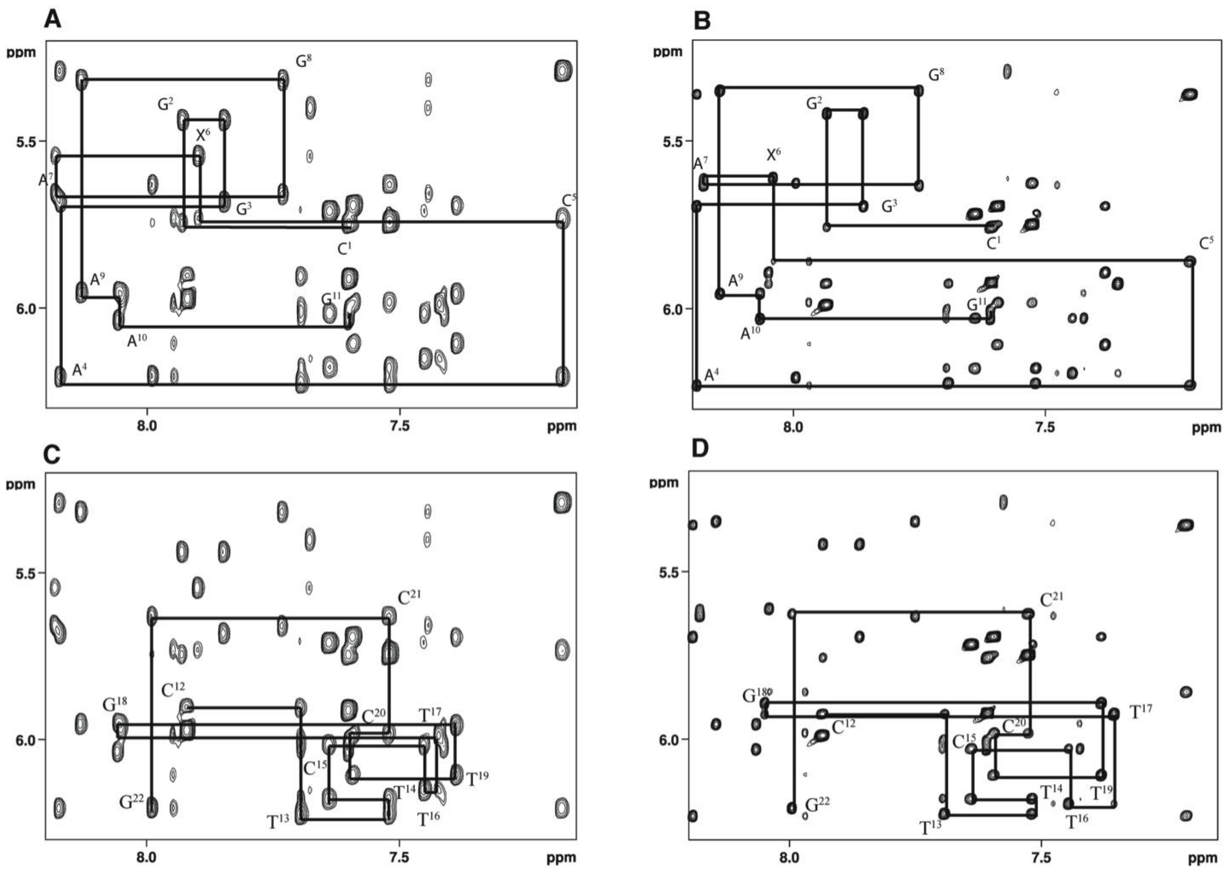


Figure 5. Expanded plots of NOESY spectra at a mixing time of 250 ms showing sequential NOE connectivites from the anomeric to aromatic protons. Nucleotides C^1 to G^{11} of the modified strand of the (A) N1-[2(S)-hydroxy-3-buten-2-yl]-2'-deoxyinosine duplex and (B) N1-[2(R)-hydroxy-3-buten-2-yl]-2'-deoxyinosine duplex. Nucleotides C^{12} to G^{22} of the (C) N1-[2(S)-hydroxy-3-buten-2-yl]-2'-deoxyinosine duplex and (D) N1-[2(R)-hydroxy-3-buten-2-yl]-2'-deoxyinosine duplex.

The complementary strand of the modified duplex exhibited similar disruptions between the T^{16}H1' – T^{17} H6 and T^{17} H1' – G^{18} H6 NOEs compared to the unmodified duplex.

The *S*- isomer adduct spectrum was similar to the *R*- isomer spectrum. In the walking region of the spectrum, the *S*- isomer adduct induced changes compared to the unmodified *ras61* sequence. The biggest change occurred at C^5 H1'- X^6 H8 and X^6 H1' - A^7 H8, where the NOEs were weak compared to the unmodified sequence. Similarly, interactions of the complement of the modified nucleotide with its neighbor bases were notably weak. The T^{16} H1' – T^{17} H6 and T^{17} H1' – G^{18} H6 cross-peaks were weak compared with the unmodified *ras61* sequence.

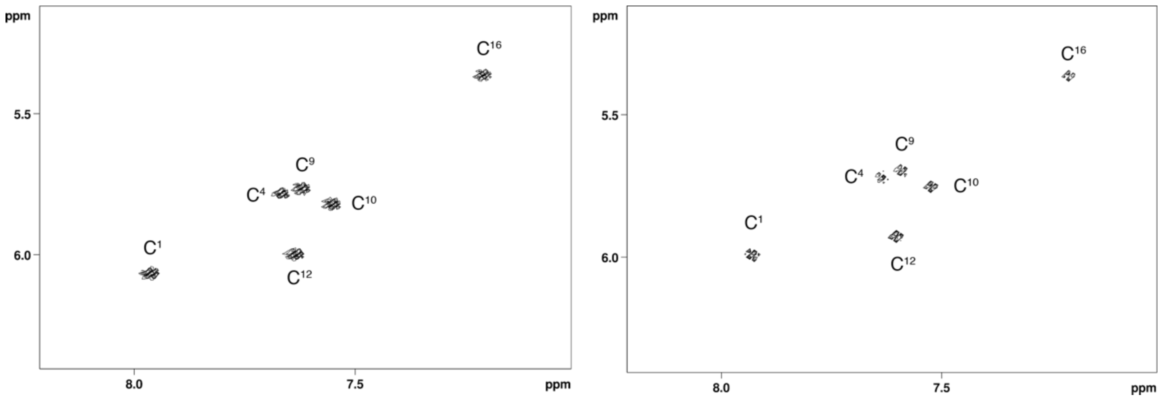


Figure 6. Expanded plots of the COSY spectra for the N1-[2(S)-hydroxy-3-buten-2-yl]-2'-deoxyinosine duplex (left) and the N1-[2(R)-hydroxy-3-buten-2-yl]-2'-deoxyinosine duplex (right).

The remainder of the NOESY spectra were assigned based on these initial sugar H1' to base aromatic cross-peaks. The adenine H2 protons were assigned based on relative intensities to the base aromatic protons and NOEs to thymine N1H protons on their respective complementary bases.

(b) Imino and Amino Proton Assignments

Figure 7 shows a representative plot of the downfield regions of the NOESY spectra containing the hydrogen bonding thymine N1H and guanine N3H resonances. The *R*- isomer spectrum exhibited sequential connectivity from G^2:C^{21} – G^3:C^{20} – A^4:T^{19} –C^5:G^{18} and A^7:T^{16} - G^8:C^{15} – A^9:T^{14} – A^{10}:T^{13}. Imino protons for the modified base pair X^6:T^{17} and terminal base pairs C^1:G^{22} and G^{11}:C^{12} were not observed. Imino proton resonance of the pair A^7:T^{16} was heavily overlapped with that of the pair A^4:T^{19}. The identity of these peaks was confirmed by the assignment of their respective adenine H2 protons to the opposite base N1H.

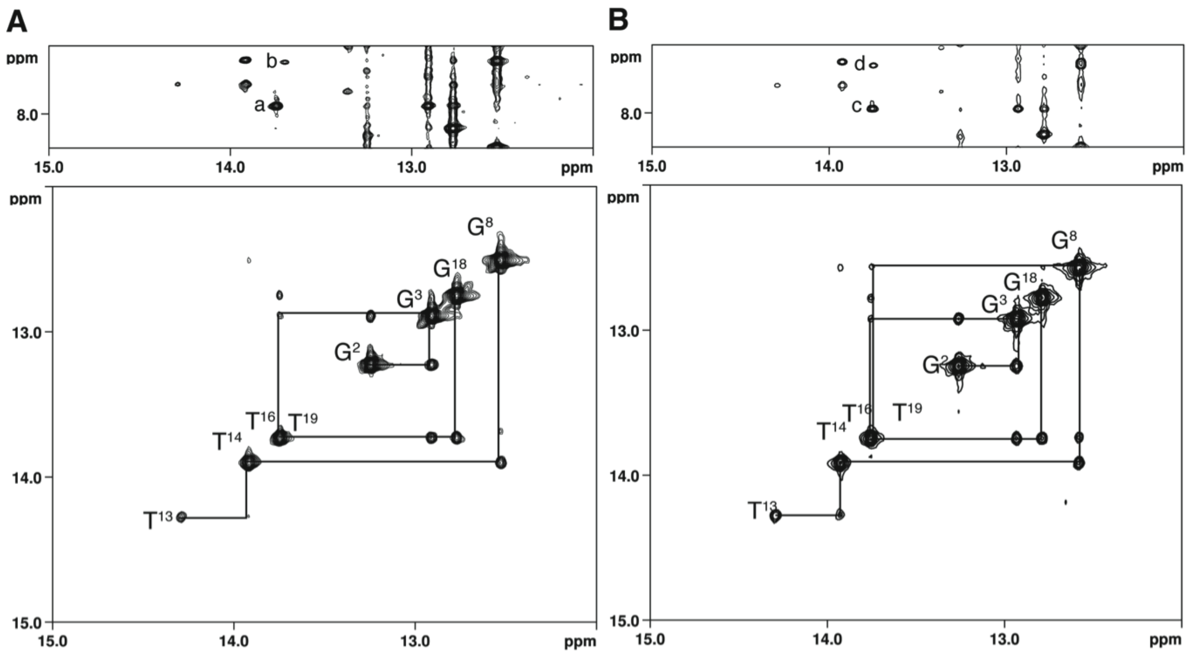


Figure 7. Explanded plot of a NOESY spectrum at a mixing time of 250 ms showing NOE connectivities for imino protons, and upfield interactions. (A) NOE connectivites for the The chemical structure of the N1-[1(S)-hydroxy-3-buten-2-yl]-2'-deoxyinosine adduct from G^2:C^{21} to A^{10}:T^{13}. No resonance was observed for base pairs X^6:T^{17} and A^7:T^{16}. (a) NOE between T^{19} N1H and A^4H2. (b) NOE between T^{16} N1H and A^7 H2. (B) NOE connectivities for the *R*- adduct from G^2:C^{21} to A^{10}:T^{13}. (c) NOE between T^{19} N1H and A^4 H2. (c) NOE between T^{16} N1H and A^7 H2.

For the *S*- isomer, sequential connectivity between imino protons was observed for base pairs G^2:C^{21} – G^3:C^{20} – A^4:T^{19} –C^5:G^{18} and G^8:C^{15} – A^9:T^{14} – A^{10}:T^{13}. Although the sequential connectivity for the A^7:T^{16} base pair was not observed, the assignment of the A^7 H2 – T^{16} N1H cross-peak indicated that these bases were still within hydrogen bonding range. Imino protons belonging to terminal base pairs C^1:G^{22} and G^{11}:C^{12} and modified base pair X^6:T^{17} were not observed.

Adduct Proton Assignments

Adduct protons were assigned using a combination of NOESY spectra and restrained molecular dynamics (rMD) calculations (Figure 8). Relative chemical shifts were first determined by knowledge of the chemical structure. The fully substituted H_α carbons were reasoned to be the most upfield, followed by the fully substituted H_β, which is geminal to the electronegative hydroxyl group. Next downfield was reasoned to be the H_δ protons, as they are the terminal protons in an alkene. Finally, the most downfield proton was reasoned to be the H_γ proton, as it is an internal alkene proton viscinal to a hydroxyl group. In the *R*- isomer, The H_α and $H_{\alpha'}$ protons were assigned as the most upfield at 3.64 and 3.08 ppm respectively. H_β was assigned at 3.79 ppm, while H_γ was assigned at 5.29 ppm. Finally, H_δ and $H_{\delta'}$ were assigned at 4.78 ppm and 4.80 ppm respectively. The initial reasoning for these assignments was consistent with the pattern of observed cross peaks in the spectra. Specifically, the base proton X^6H2 was observed to have the most intense NOEs to the closest adduct protons H_α and $H_{\alpha'}$, a moderately intense NOE to H_β, a smaller NOE to H_γ, and the smallest NOE to the distant H_δ and $H_{\delta'}$.

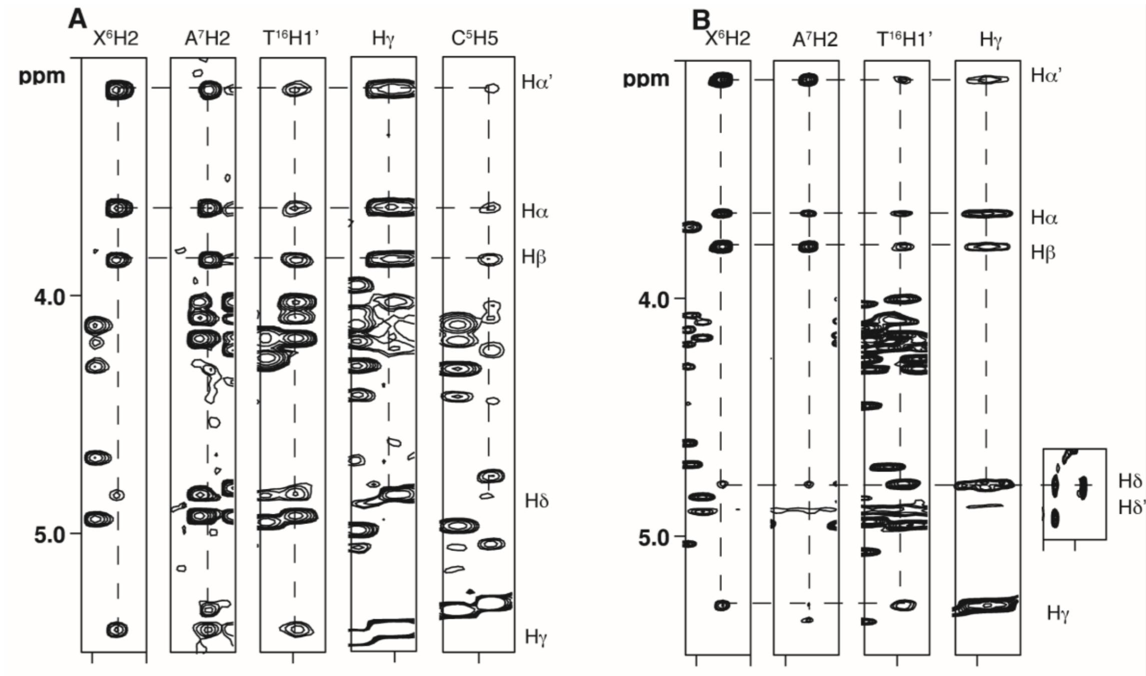


Figure 8. Assignment of adduct protons in NOESY spectra at 250 ms mixing time for (A) *S*- isomer and (B) *R*- isomer adducts. Experiments were at 900 MHz and 15^0C.

In the *S*- isomer, The H_α and $H_{\alpha'}$ protons were assigned as the most upfield at 3.64 and 3.14 ppm, respectively. H_β was assigned at 3.85 ppm, while H_γ was assigned at 5.40 ppm. Finally, H_δ and $H_{\delta'}$ were assigned at 4.84 ppm and 4.85 ppm respectively.

The H_α and $H_{\alpha'}$ protons were tentatively assigned by concurrent rMD calculations utilizing swapped assignments of the α and α' protons. The assignments that led to more validated structures as according to structural corroboration with observed chemical shift changes and CORMA analysis (as described later in this work) were selected as the tentative assignments.

Glycosidic Torsion Angle Assessment

Glycosidic torsion angle conformations of both *R*- and *S*- adducts were evaluated by comparing relative intensities of intrabase anomeric H1' to aromatic base proton NOEs (Figure 9). In both isomers, the intrabase NOEs on the modified base X^6 were of similar intensity to the rest of the duplex, indicating that the glycosyl torsion angles for all nucleotides remained in the *anti* conformational range.

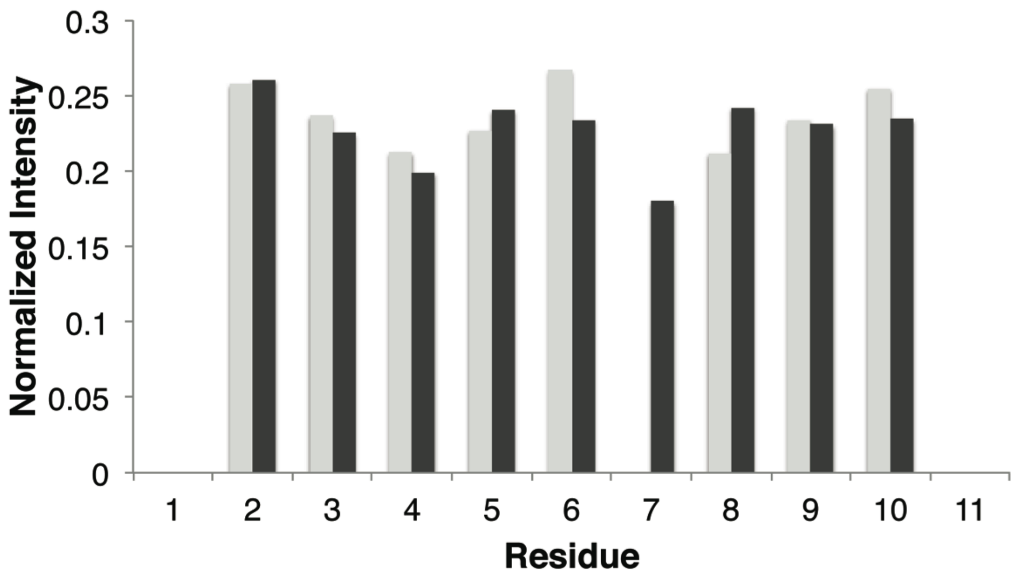
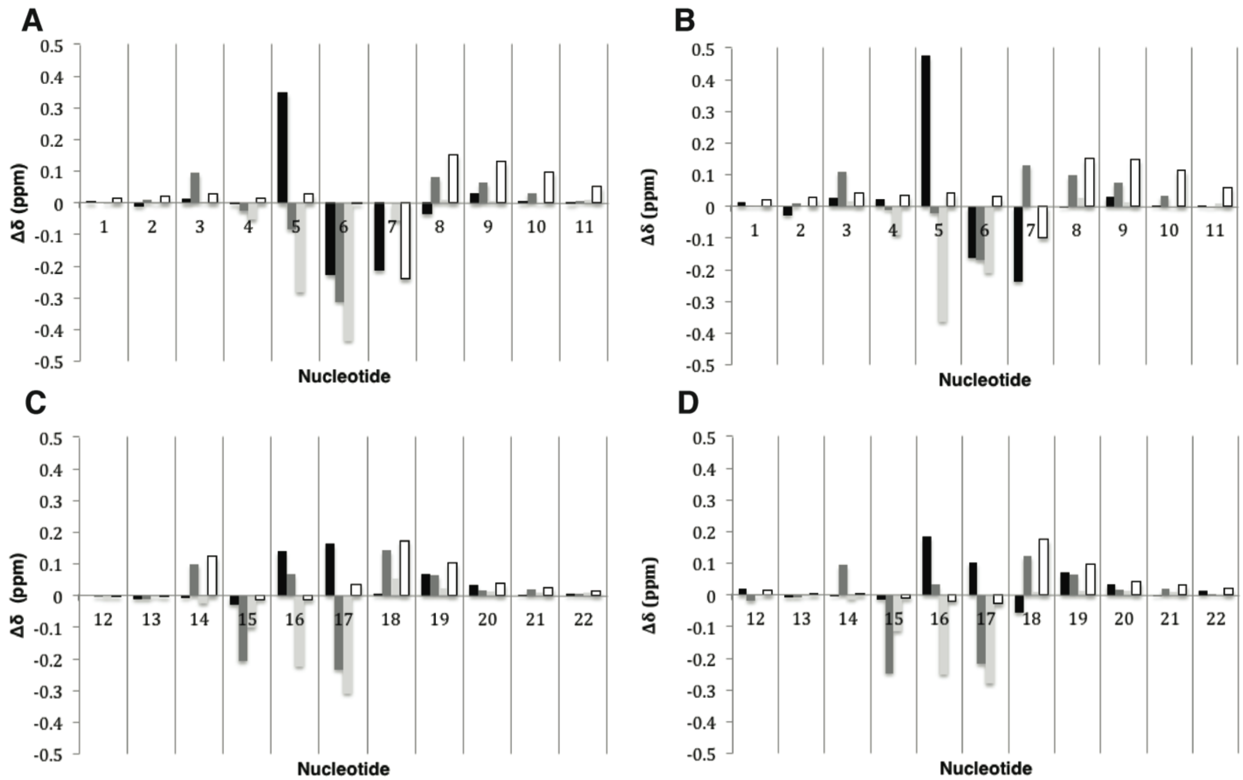


Figure 9. Resonance intensities of intranucleotide H1' and H6/8 ^{1}H NOE cross peaks at 900 MHz and 15^{o}C. Grey bars represent the *S*- adducts, while black bars represent the *R*- adducts.

Chemical Shift Perturbations

Chemical shifts were compared between the *R*- and *S*- isomer adducts and the unmodified sequence by subtracting chemical shifts observed in the unmodified spectrum from those observed in the modified spectra(Figure 10). Changes were observed in both isomers, with the largest perturbations occurring the bases neighboring the BD modification and diminishing toward the 3' end of each respective strand. The largest observed difference in the *R*- isomer spectrum was the C^{5} H1' resonance, which showed a 0.48 ppm shift downfield. On the same nucleotide, the H2'' proton showed a strong upfield shift at 0.36 ppm. The 3' neighbor base X^{6} exhibited upfield shifts on the H1', H2', and H2'' protons, at 0.16, 0.17, and 0.21 ppm, respectively. Continuing in the 3' direction, base A^{7} showed both downfield and upfield shifts, with the H1' and H8 protons shifted upfield 0.24 and 0.10 ppm respectively, while the H2' proton was shifted downfield 0.13 ppm. Base G^{8} exhibited moderate shifts downfield, with H2' proton shifted 0.01 ppm, and the H8 proton shifted 0.15 ppm. The observed trend continued to base A^{9}, which showed a moderate downfield shift on its H8 proton at 0.13 ppm, and smaller shifts on its H1' and H2' protons. Base A^{10} displayed a 0.11 shift downfield on its H8 proton, and terminal base G^{11} showed a 0.05 shift downfield on its H8 proton. The complementary strand of the *R*- isomer also exhibited strong shift changes starting on nucleotide C^{15}, with upfield shifts to the sugar H2' and H2'' protons of 0.25 and 0.11 ppm respectively. 3' neighbor T^{16} showed a downfield shift to its H1' proton 0.18 ppm, and a large upfield shift to its H2'' proton of 0.25 ppm. Similarly, the H1' proton of base T^{17} showed a small downfield shift to proton H1' of 0.10 ppm, and large upfield shifts to protons H2' and H2'' of 0.22 and 0.28 ppm, respectively. Continuing to A^{18}, the H2' and H8 protons showed downfield shifts of 0.12 and 0.18 ppm. G^{19} protons H1', H2', and H8 all exhibited small shifts (< 0.10 ppm) downfield. These small downfield shifts continued diminishing to the terminal base C^{22}.

Figure 10. Chemical shift differences of the protons of the carbon 4 (C-4) N1-dI EB



adducts relative to the unmodified *ras61* oligodeoxynucleotide. (A) The modified strand of the *S*- adduct. (B) The modified strand of the *R*- adduct. (C) The complementary strand of the *S*- adduct. (D) The complementary strand of the *R*- adduct. Black bars represent H1' protons, dark grey bars represent H2' protons, light grey bars represent H2'' protons, and white bars represent H3' protons.

The *S*- isomer spectrum largely exhibited similar chemical shift perturbations. On the modified strand, the largest chemical shift change with respect to the unmodified *ras61* duplex, the C^5 H1' proton showed a downfield shift of 0.35 ppm. On the same base, the H2'' proton showed a large upfield shift of 0.28 ppm. The modified base X^6 showed large upfield shifts of its sugar protons, with H1', H2', and H2'' chemical shifts changing upfield by 0.23, 0.31, and 0.44 ppm. Upfield shifts were observed on 3' neighbor A^{8} on protons H1' and H8 of 0.21 and 0.24 ppm respectively. Base G^{8} showed a moderate shift downfield on its H8 proton of 0.15 ppm. The trend of downfield shifts on the aromatic proton continued diminishing to the 3' terminal base G^{11}. The complementary strand of the *S*- isomer similarly displayed chemical shift changes starting on C^{15}, with its H2' and H2'' protons shifted upfield 0.21 and 0.10 ppm respectively. Nucleotide T^{16} exhibited both upfield and downfield shifts, as protons H1' and H2' shifted downfield 0.14 and 0.07 ppm, and proton H2'' shifted upfield 0.22 ppm. The complement of the modified base, T^{17}, showed a moderate shift downfield on its H1' proton of 0.16 ppm, and a large upfield shift on the H2' and H2'' protons of 0.23 and 0.31 ppm respectively. 3' neighbor G^{18} showed moderate downfield shifts, with protons H2' and H8 shifting 0.14 and 0.17 ppm. This pattern of downfield shifts continued on base T^{19}, with its H6 proton shifting 0.10 ppm, continuing diminishing to the terminal base G^{22} (Figure 10).

Structural Refinement

Assignment of the C4 *S*- NOESY spectra led to the generation of 384 distance restraints for use in retrained molecular dynamics (rMD) calculations, of which 201 were intranucleotide restrains, and 183 were internucleotide. The C4 *R*- NOESY spectra led to the generation of 313 distance restraints, of which 182 were intranucelotide and 131 were internucelotide. 16 deoxyribose pseudorotations, 90 backbone torsion angles, and 42 hydrogen bonding restraints derived from B-DNA were included as empirical restraints. Resulting structures from rMD calculations (Figure 11) were analyzed using CORMA (Figure 12)[52,53]. The sixth root residuals (R_1^x) were mostly below 15%, and generally below 10%, showing good agreement between the calculated structure and experimental data. Residuals above 15% were the result of very low sample sizes (two or fewer cross-peaks).

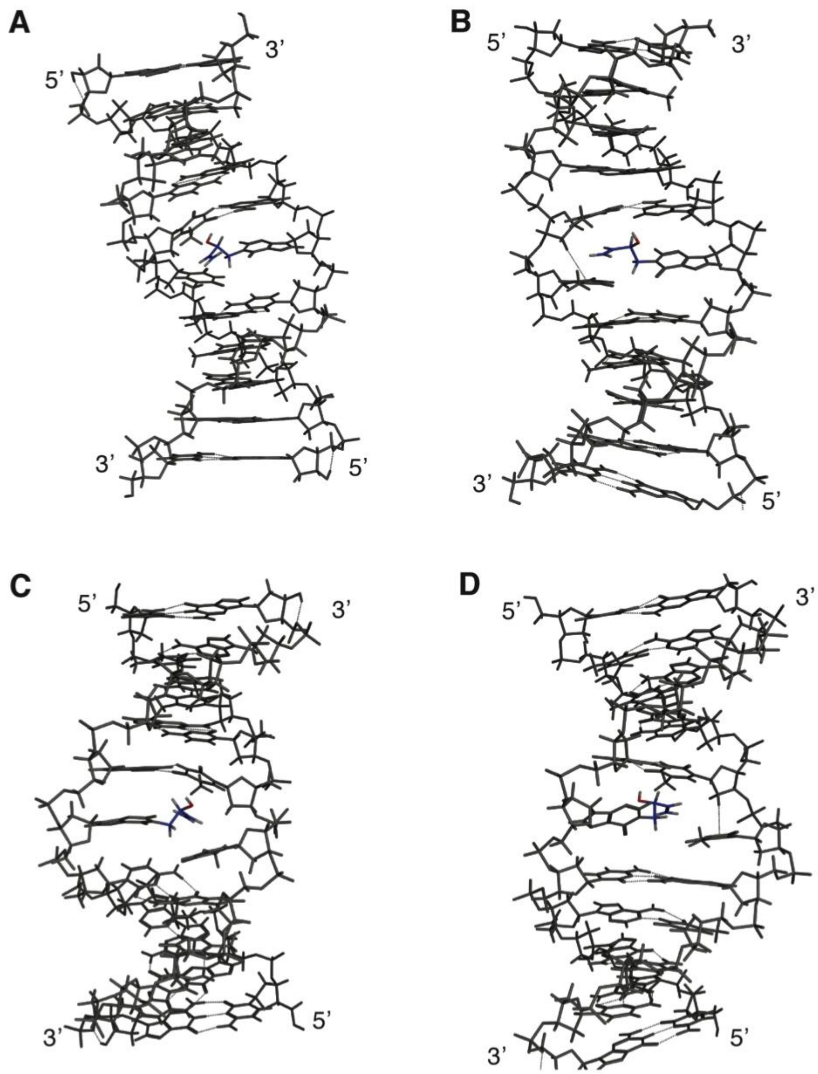


Figure 11. Views of the calculated structures obtained from the rMD calculations for the (A: major groove, C: minor groove) N1-[2(S)-hydroxy-3-buten-2-yl]-2'-deoxyinosine duplex and the (B: major groove, D: minor groove) N1-[2(R)-hydroxy-3-buten-2-yl]-2'-deoxyinosine duplex.

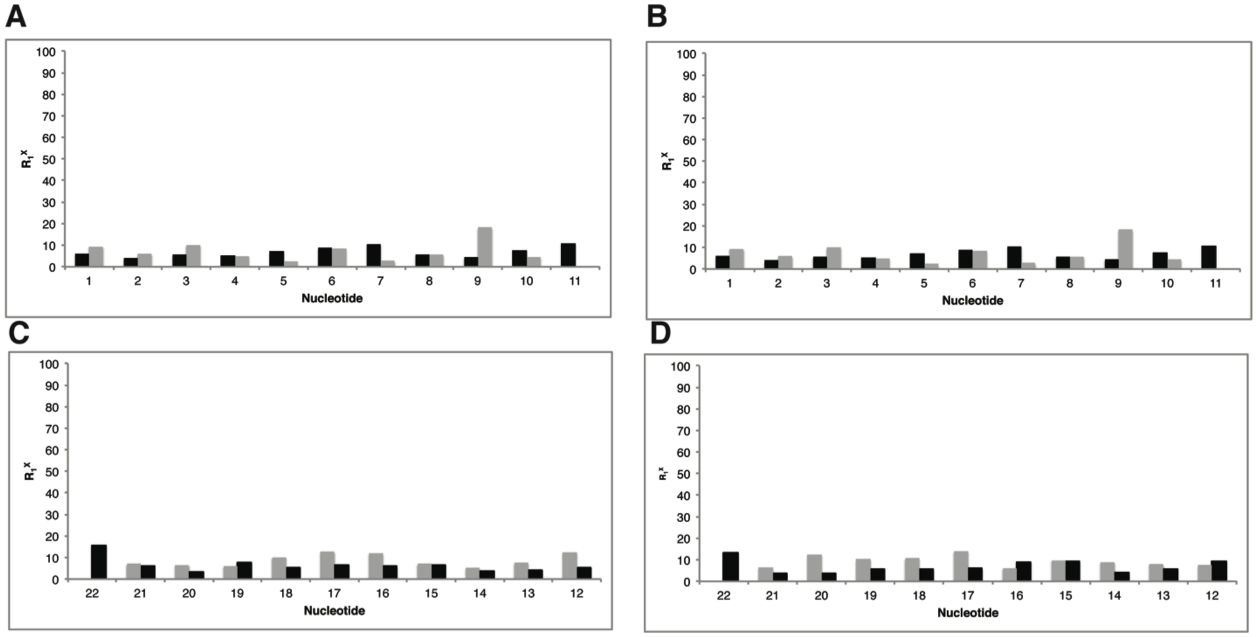


Figure 12. Distribution of R_1x values calculated using CORMA. (A) The modified strand of the *S*- duplex. (B) The modified strand of the *R*- duplex. (C) The complementary strand of the *S*- duplex. (D) The complementary strand of the *R*- duplex. The dark bars represent intranucleotide values. The light bars represent internucleotide values.

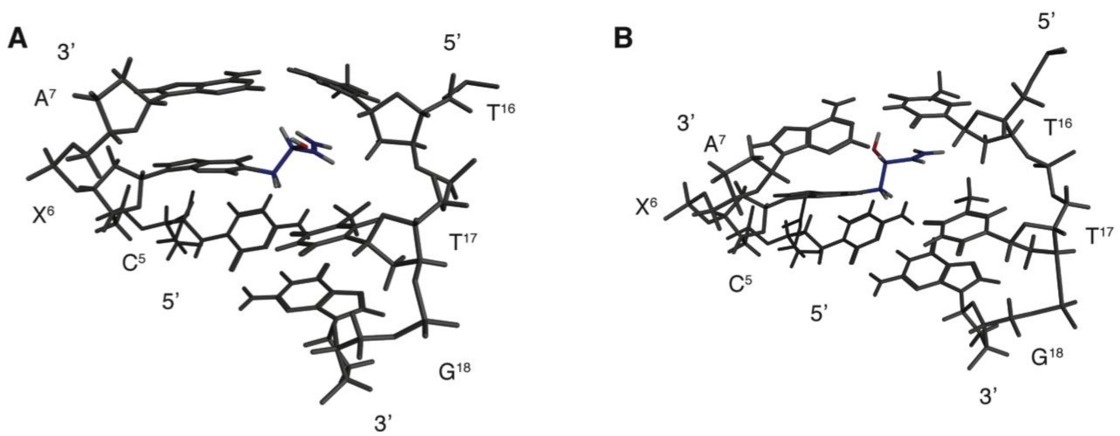


Figure 13. Structure of the (A) N1-[2(S)-hydroxy-buten-2-yl] duplex and (B) N1-[2(R)-hydroxy-buten-2-yl] duplex in the region of the C^5:G^{18}, X^6:T^{17}, and A^7:T^{16} base pairs. The butadiene moiety is highlighted in blue. The hydroxyl group is shown in red.

Structures of the Duplexes

The orientation of the BD moiety was very similar for the *R*- and *S*-adducts. Watson-Crick base pairing was disrupted, as the BD moiety was oriented into the duplex, extending between T^{16} and T^{17} (Figure 13) and extending toward its 3' side. The alkene in the BD moiety in both *R*- and *S*-isomers stacked with the T^{16} base, causing the H_{α} protons in both isomers to be oriented toward the 5' base T^{16}. The stereoisomeric carbon C_{β} was oriented close to A^{7}, corroborated by strong NOEs observed between H_{β} and A^{7} H2. T^{17} was displaced toward the major groove on its 3' side, interrupting its base stacking with T^{16} and interfering with 5' base stacking with C^{15}. The modified base maintained the *anti* conformation about the glycosidic bond. Base stacking was disrupted for base pairs C^{5}:G^{18}, X^{6}:T^{17}, and A^{7}:T^{16} (Figure 14). In the *R*- isomer, the minor groove widened from 6 to 14 Å, while the major widened from 12 to 16 Å. In the *S*- isomer, the minor groove widened from 7 to 11 Å, while the major widened from 9 to 15 Å.

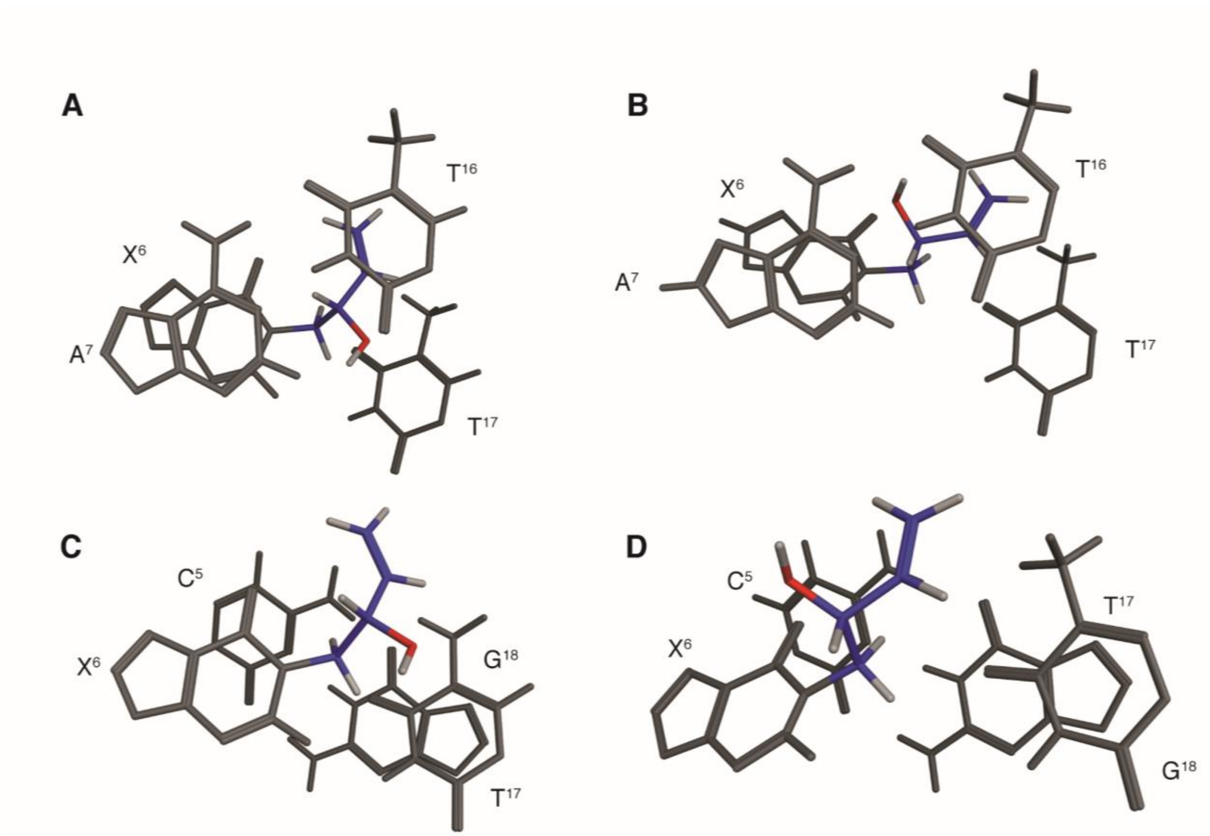


Figure 14. Stacking interactions for the (A, C) N1-[2(S)-hydroxy-buten-2-yl] duplex (B,D) N1-[2(R)-hydroxy-buten-2-yl] duplex. (A, B) Stacking of the A^7:T^{16} base pair above the X^6:T^{17} base pair. (C, D) Stacking of the X^6:T^{17} above the C^5G^{18} base pair.

Chapter 3

The structure of the C-4 EB N1 inosine adducts and implications

3.1 **Discussion of results**

Inhalation of the primary metabolite of BD, EB, was observed to cause A to G transitions at the first A:T pair in codon 61 of the *H-ras* oncogene in harderian gland tumors in mice.[31] The C4 adducts investigated in this work are of interest due to the mutagenicity of regioisomeric pair, the C3 adducts.[36,37] These N1-dI adducts were initially studied because they necessarily disrupt Watson-Crick base pairing due to the presence of the BD moiety at the N1 position, which could indicate mutagenic outcomes. The C3 adducts induce predominantly A to G transitions in both *E. coli* and COS-7 cells[37,38]. It was proposed that these adducts induce A to G transitions by causing a rotation about the glycosyl bond of the modified base, allowing Hoogsteen base pairing with an incoming protonated dCTP during translesion synthesis[37,38]. Structures of the C3 adducts determined using NMR reveal that the BD moiety induces a rotation about the glycosidic bond into the *syn* conformation, which exposes the Hoogsteen face of the modified nucleotide to its base pairing partner, supporting the Hoogsteen base pairing mechanistic proposal[40,41]. As both C3 and C4 regioisomers can be expected to form upon EB reaction with DNA, we have investigated the structures of the R and S isomers in the *H-ras* codon 61sequence context.

Structures of the R-and S -N1-dI Adducts

Overall, both *R*- and *S*- diastereomers adopt similar conformations. In both diastereomers, the cross-peak intensity between X^6 H8 and H1' is comparable to other nucleotides in the duplex (Figure 5). This indicates that the modified base H8 protons remained oriented toward the major groove in the anti conformation. NOEs from H_β to A^7 H2, T^{16} H1', and C^5 H5 confirm that the modified base remains in the anti conformation, causing the BD moiety to be oriented into the duplex (Figure 8). In the *R*- isomer, H_δ protons interact with T^{17} CH_3 and T^{16} CH_3, as well as T^{16} H2', confirming the orientation of the vinyl group. In the *S*- isomer, these peaks overlap with the solvent peak and are therefore not observable (Figure 8). For both diastereomers, NMR resonances of T^{17} imino protons are not observed, which suggests rapid exchange with solvent and provides evidence for the disruption of Watson-Crick base pairing at the modified base pairs (Figure 7). In addition, the T^{16} imino resonance in the *S*-N1-dI adduct is not observed, and in the *R*-N1-dI adduct, this resonance is broad and overlaps with the T^{19} imino resonance. However, NOEs from A^7 H2 to T^{16} N3H are observed, suggesting that these two bases are remain Watson-Crick base paired. Both adducts are thermally destabilized relative to the unmodified duplex, which is consistent with the proposed orientation of the BD moiety into the duplex causing a local disruption in base stacking. In particular, T^{17} is forced toward its 3' side and into the major groove by the BD moiety, disrupting its base stacking with T^{16}. By assuming this conformation, T^{17} is placed near T^{16} H2', which is corroborated by the large upfield shift observed for this resonance (Figure 10). In addition, this 3' displacement of T^{17} could explain the chemical shift perturbations extending to the terminal 3' base (Figure 10). The T^{17} residue is twisted toward the 3' side, which shields the H2' and H2'' protons. C^5 H1' is shifted especially far downfield, as the stacking of the modified base X^6 base with C^5 is disrupted and the minor groove is widened, deshielding the H1' proton. The BD moiety is oriented toward its 3' side, explaining the chemical shifts of its 3' neighbors diminishing to the terminal base. Of particular interest is the fact that the BD vinyl group has a base stacking interaction with T^{16}. This provides a possible explanation for the difference in conformation between the C3 and C4 regioisomers, as the geometry of the C4 adducts allows for this favorable stacking interaction to occur.

3.2 **Structure-Activity Relationships**

(a) Implications of the Glycosidic Torsion Angle.

Unlike the C3 adducts, the C4 N1-dI adducts do not undergo a rotation about the glycosidic bond, instead remaining in the anti conformation. The finding that the glycosidic torsion angle for the N1 adducted dI nucleotide for both the *R*- and *S*- C4 adducts remains in the *anti* conformation is significant. This establishes that the regiochemistry of N1-dI adducts affects adduct conformation in DNA. The C3 adducts cause predominantly A to G mutations in cellular models[37,38]. Structural data for these C3 adducts indicated that the modified bases of both stereoisomers were flipped into the syn conformation, supporting the hypothesis that the glycosidic bond angle is the primary factor for mutagenic outcome in these N1-dI adducts by facilitating Hoogsteen base pairing with an incoming protonated dCTP[40,41]. By not initially adopting the syn conformation, the conformation of the C4 adducts may be an indicator that the biological processing of these regioisomers will differ.

There are no obvious structural interactions observed in the determined C4 structures that would stabilize the *anti* conformation in the modified base instead of the *syn* conformation. The hydroxyl groups in both *R*- and *S*- isomers are oriented into the solvent accessible lesion site, away from potential hydrogen bonding interactions with the duplex. Although the vinyl group of the BD moiety in both *R*- and *S*- isomers stack well with the nucleotide T^{16}, melting temperature studies indicate that the thermal stability of the C4 adducts are very similar to the thermal stability of the C3 adducts, suggesting that the C4 adducts are no more stable than the C3 adducts due to this stacking interaction. With these two possibilities eliminated, we speculate that the primary contributor to conformational selection between *syn* and *anti* is the addition of an sp^3 hybridized carbon in between the N1 of the modified base and the vinyl group of the BD moiety, allowing the BD moiety the conformational flexibility to find a favorable orientation. In the C4 structures, the vinyl group of the BD moiety is intercalated between T^{16} and T^{17} (Figure 8). The presence of an additional carbon between N1 and the vinyl group allows the BD moiety to be more flexible and extend “over” the opposite base T^{17} to insert the vinyl group in between two nucleotides. In contrast, the C3 adducts do not have this flexibility; if the C3 adducts assumed the *anti* conformation, the BD moiety would extend directly into the opposite base.

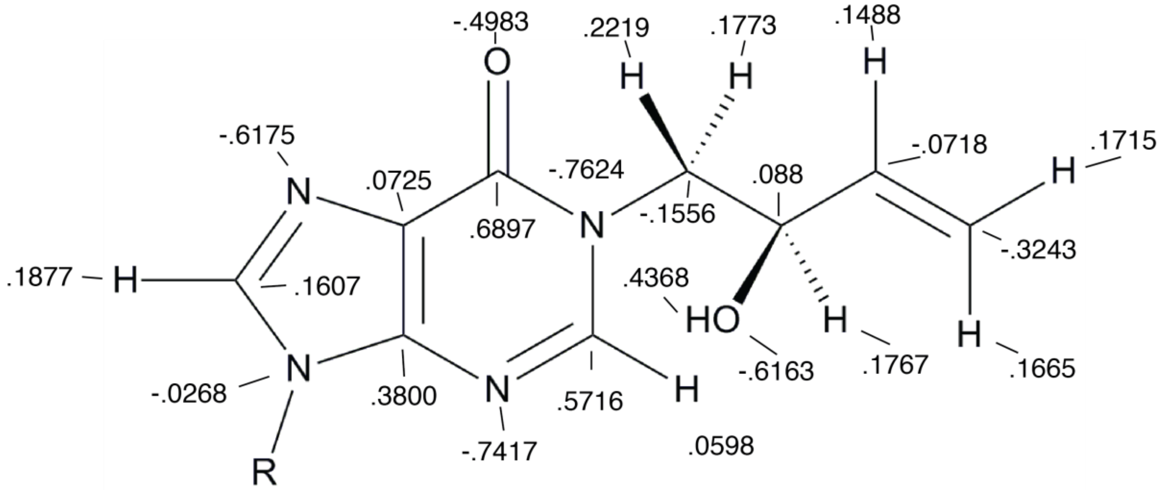
(b) Implications for Biological Processing.

Studies of BD toxicity in B6c3F1 *lacI* transgenic mice induced point mutations at dG and dA.[65,66,67] Mutations at A:T base pairs comprised 20% of total mutations, a significant contribution to overall mutagenicity. The mutations observed at these base pairs were primarily A to T transitions[37,38]. However, A to G mutations were observed in *H-ras* codon 61[31]. Interestingly, *ras* codo*n* 61 is highly conserved in mammals, and (61,2) A to G transitions are prevalent in several studies of human cancers[68,69]. The C3 adducts induce A to G transitions in bacterial and mammalian cell models[37,38], and their structures provide strong evidence toward a possible mutation mechanism. The results from this study indicate that the C4 adducts may be differently processed due to differential rotation of the glycosyl bond. The recent observation of hpol ι using Hoogsteen type pairing to bypass a 1,N^6 –ethenodA adduct is consistent with the proposed mutation mechanism for the C3 adducts[70,71]. In addition, it has been observed that hpol κ and hpol η preferentially insert dCTP across from dI lesions[72]. The structural data obtained in this study suggest that comparison of translesion synthesis polymerase processing between the C3 and C4 adducts may lead to further understanding of BD induced mutations at A:T pairs. Evidence suggests that DNA damage resulting from 3,4-epoxybutene is repaired through the NER pathway in mice, of which the DNA damage recognition protein XPC is vital[73]. As XPC complexes are known to recognize DNA damage by helical distortion and disruption of Watson-Crick base pairs, these N1-dI adducts are likely to be good binding partners, suggesting that further investigation into NER processing of these adducts may yield useful information[74].

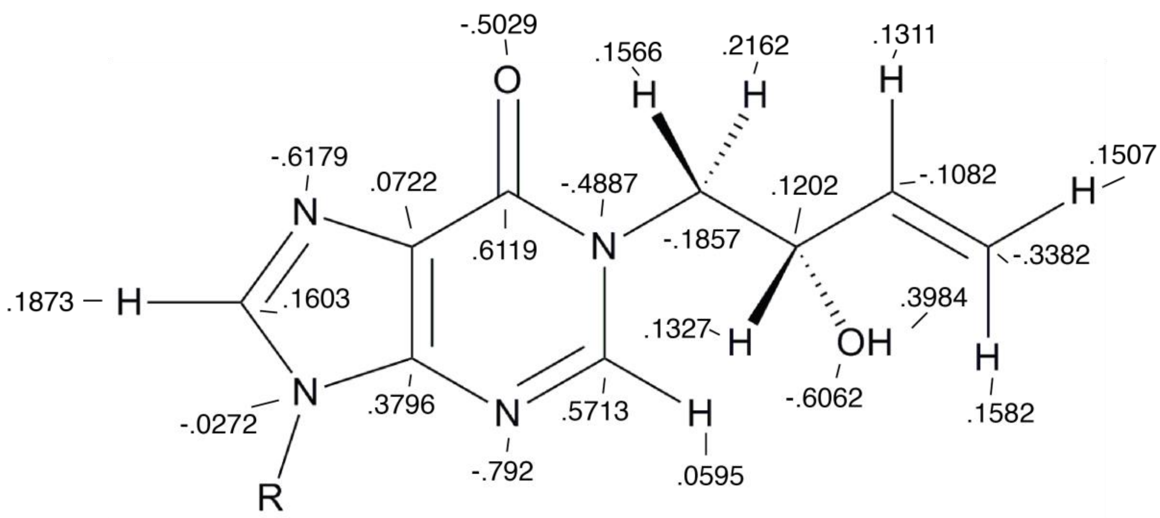
APPENDIX A

ATOMIC CHARGES

Calculated Charges for the *S*-N1-(2-Hydroxy-buten-2-yl) -2' Deoxyinosine DNA Adducts



Calculated Charges for the *R*-N1-(2-Hydroxy-buten-2-yl) -2' Deoxyinosine DNA Adducts



Atomic partial charges calculated using GAUSSIAN 09 and the B3LYP/6-31G* basis set

*Partial charges expected to be identical in both enantiomers. The source of the differences in partial charges is unknown. When *R*- and *S*- charges are swapped during rMD calculations, the resulting structures are unchanged from their presented forms.

APPENDIX B

CHEMICAL SHIFT ASSIGNMENTS

Chemical Shift Assignments for the N1-[2(S)-hydroxy-3-buten-2-yl]-2'-deoxyinosine duplex

	H1'	H2'	H2''	H3'	H5	H6	H8	Me
C^{1}	5.91	2.33	2.63	4.69	5.97	7.92		
T^{2}	6.22	2.30	2.68	4.94		7.70		1.71
T^{3}	6.18	2.29	2.62	4.95		7.52		1.70
C^{4}	6.02	2.12	2.49	4.84	5.71	7.64		
T^{5}	6.15	2.24	2.32	4.93		7.46		1.74
T^{6}	5.99	1.98	2.28	4.81		7.43		1.71
G^{7}	5.96	2.75	2.84	4.95			8.05	
T^{8}	6.11	2.24	2.56	4.91		7.39		1.42
C^{9}	5.98	2.16	2.44	4.84	5.70	7.60		
C^{10}	5.63	2.03	2.36	4.85	5.75	7.52		
G^{11}	6.20	2.40	2.67	4.71			7.99	
C^{12}	5.75	1.85	2.35	4.70	5.92	7.60		
G^{13}	5.44	2.70	2.74	4.99			7.93	
G^{14}	5.68	2.66	2.81	5.07			7.85	
A^{15}	6.21	2.62	2.86	5.05			8.17	
C^{16}	5.74	1.77	1.96	4.76	5.30	7.18		
X^{17}	5.55	2.35	2.39				7.90	
A^{18}	5.66		2.72	4.99			8.18	
G^{19}	5.32	2.56	2.63	4.97			7.74	
A^{20}	5.96	2.56	2.63	4.97			8.13	
A^{21}	6.03	2.59	2.89	5.04			8.06	
G^{22}	6.00	2.27	2.37	4.61			7.60	

Adduct Proton Assignments

Hα'	3.64
Hα''	3.14
Hβ	3.86
Hγ	5.40
Hδ'	4.84

Chemical Shift Assignments for the N1-[2(R)-hydroxy-3-buten-2-yl]-2’-deoxyinosine duplex

	H1'	H2'	H2''	H3'	H5	H6	H8	Me
C[1]	5.93	2.32	2.64	4.69	5.99	7.94		
T[2]	6.23	2.30	2.68	4.94		7.70		1.71
T[3]	6.18	2.28	2.64	4.95		7.52		1.69
C[4]	6.03	2.08	2.48	4.86	5.72	7.64		
T[5]	6.19	2.20	2.29	4.96		7.45		1.77
T[6]	5.93	2.00	2.31	4.79		7.36		1.68
G[7]	5.90	2.73	2.80	4.94			8.05	
T[8]	6.11	2.24	2.55	4.90		7.38		1.42
C[9]	5.99	2.15	2.44	4.84		7.60		
C[10]	5.63	2.03	2.36	4.85	5.75	7.53		
G[11]	6.21	2.40	2.67	4.71			8.00	
C[12]	5.76	1.86	2.36	4.70	5.92	7.61		
G[13]	5.42	2.70	2.75	4.99			7.92	
G[14]	5.70	2.71	2.82	5.07			7.86	
A[15]	6.23	2.64	2.89	5.07				
C[16]	5.86	1.83	1.88	4.84	5.36	7.22		
X[17]	5.61	2.49	2.62	4.91			8.04	
A[18]	5.63	2.70		4.99			8.18	
G[19]	5.35	2.58	2.65	4.98			7.75	
A[20]	5.96	2.67	2.89	5.07			8.15	
A[21]	6.03	2.59	2.87	5.04			8.07	
G[22]	6.01	2.26	2.37	4.61			7.61	

Adduct Proton Assignments

Hα'	3.64
Hα''	3.08
Hβ	3.79
Hγ	5.29
Hδ'	4.78
Hδ''	4.80

APPENDIX C

RESTRAINT FILES

Combined distance and torsion restraints used in the rMD calculations for the R adduct

```
#
#   1 DC5 H6     1 DC5 H1'   3.360   3.840
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  10, r1= 2.86, r2= 3.36, r3= 3.84, r4= 4.34,
      rk2=32.0, rk3=32.0, ir6=1, ialtd=1,
 &end
#
#   1 DC5 H3'    1 DC5 H1'   3.010   4.760
 &rst
  ixpk= 0, nxpk= 0, iat=  24,  10, r1= 2.51, r2= 3.01, r3= 4.76, r4= 5.26,  &end
#
#   1 DC5 H3'    1 DC5 H5    4.520   7.140  (#4.520   6.540 22 37)
 &rst
  ixpk= 6, nxpk= 0, iat=  24,  15, r1= 4.02, r2= 4.52, r3= 7.14, r4= 7.64,  &end
#
#   1 DC5 H2'1   1 DC5 H1'   2.530   3.860
 &rst
  ixpk= 6, nxpk= 0, iat=  26,  10, r1= 2.03, r2= 2.53, r3= 3.86, r4= 4.36,  &end
#
#   1 DC5 H2'1   1 DC5 H3'   1.850   2.790  (#1.850   2.490 26)
 &rst
  ixpk= 2, nxpk= 0, iat=  26,  24, r1= 1.35, r2= 1.85, r3= 2.79, r4= 3.29,  &end
#
#   1 DC5 H2'2   1 DC5 H1'   1.990   2.740  (#1.990   2.440 19)
 &rst
  ixpk= 2, nxpk= 0, iat=  27,  10, r1= 1.49, r2= 1.99, r3= 2.74, r4= 3.24,  &end
#
#   1 DC5 H2'2   1 DC5 H6    2.920   5.070
 &rst
  ixpk= 2, nxpk= 0, iat=  27,  13, r1= 2.42, r2= 2.92, r3= 5.07, r4= 5.57,  &end
#
#   1 DC5 H2'2   1 DC5 H3'   2.590   4.200  (#2.890   4.200 4)
 &rst
  ixpk= 4, nxpk= 0, iat=  27,  24, r1= 2.09, r2= 2.59, r3= 4.20, r4= 4.70,  &end
#
#   2 DT  H6     1 DC5 H1'   3.010   5.640
 &rst
  ixpk= 4, nxpk= 0, iat=  43,  10, r1= 2.51, r2= 3.01, r3= 5.64, r4= 6.14,  &end
#
#   2 DT  H6     1 DC5 H6    4.500   6.480
 &rst
  ixpk= 4, nxpk= 0, iat=  43,  13, r1= 4.00, r2= 4.50, r3= 6.48, r4= 6.98,  &end
#
```

```
#   2 DT  H6     1 DC5 H3'   2.940   4.810  (#2.940   4.210 7 43)
 &rst
  ixpk= 4, nxpk= 0, iat=  43,  24, r1= 2.44, r2= 2.94, r3= 4.81, r4= 5.31,  &end
#
#   2 DT  H6     1 DC5 H2'2  2.170   3.350  (#2.170   3.050 40)
 &rst
  ixpk= 3, nxpk= 0, iat=  43,  27, r1= 1.67, r2= 2.17, r3= 3.35, r4= 3.85,  &end
#
#   2 DT  H6     2 DT  H1'   2.540   4.510
 &rst
  ixpk= 3, nxpk= 0, iat=  43,  40, r1= 2.04, r2= 2.54, r3= 4.51, r4= 5.01,  &end
#
#   2 DT  Q5     1 DC5 H1'   3.310   4.830
 &rst
  ixpk= 3, nxpk= 0, iat=  -1,  10, r1= 2.81, r2= 3.31, r3= 5.80, r4= 6.30,
 igr1=  46,  47,  48,
 &end
#
#   2 DT  Q5     1 DC5 H6    2.740   3.200
 &rst
  ixpk= 3, nxpk= 0, iat=  -1,  13, r1= 2.24, r2= 2.74, r3= 3.84, r4= 4.34,
 igr1=  46,  47,  48,
 &end
#
#   2 DT  Q5     1 DC5 H5    2.730   4.180  (#2.730   3.580 10 13)
 &rst
  ixpk= 3, nxpk= 0, iat=  -1,  15, r1= 2.23, r2= 2.73, r3= 5.02, r4= 5.52,
 igr1=  46,  47,  48,
 &end
#
#   2 DT  Q5     1 DC5 H3'   2.980   4.200  (#2.980   3.600 23 25 )
 &rst
  ixpk= 3, nxpk= 0, iat=  -1,  24, r1= 2.48, r2= 2.98, r3= 5.04, r4= 5.54,
 igr1=  46,  47,  48,
 &end
#
#   2 DT  Q5     1 DC5 H2'2  2.650   4.040
 &rst
  ixpk= 3, nxpk= 0, iat=  -1,  27, r1= 2.15, r2= 2.65, r3= 4.85, r4= 5.35,
 igr1=  46,  47,  48,
 &end
#
#   2 DT  Q5     2 DT  H6    2.180   2.910
 &rst
  ixpk= 3, nxpk= 0, iat=  -1,  43, r1= 1.68, r2= 2.18, r3= 3.49, r4= 3.99,
 igr1=  46,  47,  48,
 &end
#
#   2 DT  H3'    2 DT  H1'   3.060   4.420
 (#2 DT  H3'    1 DC5 H1'   3.660   6.730 # 3.660   5.830 1 14 15 38(removed))
 &rst
```

```
  ixpk= 3, nxpk= 0, iat=  56,  40, r1= 2.56, r2= 3.06, r3= 4.42, r4= 4.92,  &end
#
#   2 DT  H3'    2 DT  H6    2.880   4.870
 &rst
  ixpk= 3, nxpk= 0, iat=  56,  43, r1= 2.38, r2= 2.88, r3= 4.87, r4= 5.37,  &end
#
#   2 DT  H2'1   2 DT  H1'   2.070   4.370
 &rst
  ixpk= 3, nxpk= 0, iat=  58,  40, r1= 1.57, r2= 2.07, r3= 4.37, r4= 4.87,  &end
#
#   2 DT  H2'1   2 DT  H6    1.760   2.760  (#1.760   2.160 24 39)
 &rst
  ixpk= 2, nxpk= 0, iat=  58,  43, r1= 1.26, r2= 1.76, r3= 2.76, r4= 3.26,  &end
#
#   2 DT  H2'2   2 DT  H1'   1.670   2.550  (#1.670   2.250 2)
 &rst
  ixpk= 2, nxpk= 0, iat=  59,  40, r1= 1.17, r2= 1.67, r3= 2.55, r4= 3.05,  &end
#
#   2 DT  H2'2   2 DT  H6    2.000   4.660
 &rst
  ixpk= 2, nxpk= 0, iat=  59,  43, r1= 1.50, r2= 2.00, r3= 4.66, r4= 5.16,  &end
#
#   2 DT  H2'2   2 DT  H3'   2.400   3.260
 &rst
  ixpk= 2, nxpk= 0, iat=  59,  56, r1= 1.90, r2= 2.40, r3= 3.26, r4= 3.76,  &end
#
#   3 DT  H6     2 DT  H1'   2.460   5.030  (#2.460   4.730 18)
 &rst
  ixpk= 4, nxpk= 0, iat=  75,  40, r1= 1.96, r2= 2.46, r3= 5.03, r4= 5.53,  &end
#
#   3 DT  H6     2 DT  H6    2.840   6.270  (#2.840   5.970 28)
 &rst
  ixpk= 5, nxpk= 0, iat=  75,  43, r1= 2.34, r2= 2.84, r3= 6.27, r4= 6.77,  &end
#
#   3 DT  H6     2 DT  H2'2  2.160   3.390  (#2.160   3.090 35)
 &rst
  ixpk= 3, nxpk= 0, iat=  75,  59, r1= 1.66, r2= 2.16, r3= 3.39, r4= 3.89,  &end
#
#   3 DT  H6     3 DT  H1'   2.870   4.560
 &rst
  ixpk= 3, nxpk= 0, iat=  75,  72, r1= 2.37, r2= 2.87, r3= 4.56, r4= 5.06,  &end
#
#   3 DT  Q5     2 DT  H1'   2.940   5.550
 &rst
  ixpk= 3, nxpk= 0, iat=  -1,  40, r1= 2.44, r2= 2.94, r3= 6.67, r4= 7.17,
 igr1=  78,  79,  80,
 &end
#
#   3 DT  Q5     2 DT  H3'   3.320   5.130  (#3.320   4.830 34)
 &rst
  ixpk= 4, nxpk= 0, iat=  -1,  56, r1= 2.82, r2= 3.32, r3= 6.16, r4= 6.66,
```

```
 igr1=  78,  79,  80,
 &end
#
#   3 DT  Q5     2 DT  H2'2  2.700   4.490
 &rst
  ixpk= 4, nxpk= 0, iat=  -1,  59, r1= 2.20, r2= 2.70, r3= 5.39, r4= 5.89,
 igr1=  78,  79,  80,
 &end
#
#   3 DT  Q5     3 DT  H1'   4.160   6.220
 &rst
  ixpk= 4, nxpk= 0, iat=  -1,  72, r1= 3.66, r2= 4.16, r3= 7.47, r4= 7.97,
 igr1=  78,  79,  80,
 &end
#
#   3 DT  Q5     3 DT  H6    2.460   3.170
 &rst
  ixpk= 4, nxpk= 0, iat=  -1,  75, r1= 1.96, r2= 2.46, r3= 3.81, r4= 4.31,
 igr1=  78,  79,  80,
 &end
#
#   3 DT  H3'    3 DT  H1'   3.190   5.600
 &rst
  ixpk= 4, nxpk= 0, iat=  88,  72, r1= 2.69, r2= 3.19, r3= 5.60, r4= 6.10,  &end
#
#   3 DT  H3'    3 DT  H6    2.700   4.660
 &rst
  ixpk= 4, nxpk= 0, iat=  88,  75, r1= 2.20, r2= 2.70, r3= 4.66, r4= 5.16,  &end
#
#   3 DT  H2'1   3 DT  H1'   2.510   4.010
 &rst
  ixpk= 4, nxpk= 0, iat=  90,  72, r1= 2.01, r2= 2.51, r3= 4.01, r4= 4.51,  &end
#
#   3 DT  H2'1   3 DT  H6    1.840   2.510
 &rst
  ixpk= 4, nxpk= 0, iat=  90,  75, r1= 1.34, r2= 1.84, r3= 2.51, r4= 3.01,  &end
#
#   3 DT  H2'2   3 DT  H1'   1.820   2.780  (#1.820   2.780 27 36)
 &rst
  ixpk= 2, nxpk= 0, iat=  91,  72, r1= 1.32, r2= 1.82, r3= 2.78, r4= 3.28,  &end
#
#   3 DT  H2'2   3 DT  H6    2.220   3.800  (#2.220   3.500 32)
 &rst
  ixpk= 3, nxpk= 0, iat=  91,  75, r1= 1.72, r2= 2.22, r3= 3.80, r4= 4.30,  &end
#
#   3 DT  H2'2   3 DT  H3'   1.650   3.020  (#1.650   2.420 5 16)
 &rst
  ixpk= 2, nxpk= 0, iat=  91,  88, r1= 1.15, r2= 1.65, r3= 3.02, r4= 3.52,  &end
#
#   4 DC  H1'    3 DT  H1'   3.800   4.870  (#3.800   4.570 1 11)
 &rst
```

```
 ixpk= 4, nxpk= 0, iat= 104,  72, r1= 3.30, r2= 3.80, r3= 4.87, r4= 5.37,  &end
#
#   4 DC  H6     3 DT  H1'   2.770   3.410  (#3.070   3.410 12)
 &rst
 ixpk= 3, nxpk= 0, iat= 107,  72, r1= 2.27, r2= 2.77, r3= 3.41, r4= 3.91,  &end
#
#   4 DC  H6     3 DT  H6    3.300   5.970
 &rst
 ixpk= 3, nxpk= 0, iat= 107,  75, r1= 2.80, r2= 3.30, r3= 5.97, r4= 6.47,  &end
#
#   4 DC  H6     3 DT  Q5    3.460   6.830
 &rst
 ixpk= 3, nxpk= 0, iat= 107,  -1, r1= 2.96, r2= 3.46, r3= 8.20, r4= 8.70,
 igr2=  78,  79,  80,
 &end
#
#   4 DC  H6     3 DT  H3'   3.370   6.150
 &rst
 ixpk= 3, nxpk= 0, iat= 107,  88, r1= 2.87, r2= 3.37, r3= 6.15, r4= 6.65,  &end
#
#   4 DC  H6     3 DT  H2'1  2.660   3.800
 &rst
 ixpk= 3, nxpk= 0, iat= 107,  90, r1= 2.16, r2= 2.66, r3= 3.80, r4= 4.30,  &end
#
#   4 DC  H6     3 DT  H2'2  2.170   2.900  (#2.470   2.900 14)
 &rst
 ixpk= 2, nxpk= 0, iat= 107,  91, r1= 1.67, r2= 2.17, r3= 2.90, r4= 3.40,  &end
#
#   4 DC  H6     4 DC  H1'   3.220   4.100
 &rst
 ixpk= 2, nxpk= 0, iat= 107, 104, r1= 2.72, r2= 3.22, r3= 4.10, r4= 4.60,  &end
#
#   4 DC  H5     3 DT  H1'   3.500   4.990  (#3.500   4.090 2 26 30)
 &rst
 ixpk= 4, nxpk= 0, iat= 109,  72, r1= 3.00, r2= 3.50, r3= 4.99, r4= 5.49,  &end
#
#   4 DC  H5     3 DT  Q5    2.650   3.800  (#2.650   3.500 10)
 &rst
 ixpk= 3, nxpk= 0, iat= 109,  -1, r1= 2.15, r2= 2.65, r3= 4.56, r4= 5.06,
 igr2=  78,  79,  80,
 &end
#
#   4 DC  H5     3 DT  H3'   3.830   6.260
 &rst
 ixpk= 3, nxpk= 0, iat= 109,  88, r1= 3.33, r2= 3.83, r3= 6.26, r4= 6.76,  &end
#
#   4 DC  H5     3 DT  H2'1  2.970   4.380  (#2.970   4.080 39 41)
 &rst
 ixpk= 4, nxpk= 0, iat= 109,  90, r1= 2.47, r2= 2.97, r3= 4.38, r4= 4.88,  &end
#
#   4 DC  H5     3 DT  H2'2  2.630   4.700  (#2.930   4.700 17)
```

```
 &rst
  ixpk= 4, nxpk= 0, iat= 109,  91, r1= 2.13, r2= 2.63, r3= 4.70, r4= 5.20,  &end
#
#   4 DC  H5     4 DC  H1'   3.640   5.610  (#3.640   5.010 8 29)
 &rst
  ixpk= 5, nxpk= 0, iat= 109, 104, r1= 3.14, r2= 3.64, r3= 5.61, r4= 6.11,  &end
#
#   4 DC  H3'    3 DT  H1'   4.260   5.840
 &rst
  ixpk= 5, nxpk= 0, iat= 118,  72, r1= 3.76, r2= 4.26, r3= 5.84, r4= 6.34,  &end
#
#   4 DC  H3'    4 DC  H1'   3.000   4.940
 &rst
  ixpk= 5, nxpk= 0, iat= 118, 104, r1= 2.50, r2= 3.00, r3= 4.94, r4= 5.44,  &end
#
#   4 DC  H3'    4 DC  H6    3.110   4.350
 &rst
  ixpk= 5, nxpk= 0, iat= 118, 107, r1= 2.61, r2= 3.11, r3= 4.35, r4= 4.85,  &end
#
#   4 DC  H3'    4 DC  H5    3.470   6.570  (#3.470   5.970 16 32)
 &rst
  ixpk= 5, nxpk= 0, iat= 118, 109, r1= 2.97, r2= 3.47, r3= 6.57, r4= 7.07,  &end
#
#   4 DC  H2'1   3 DT  H1'   3.020   5.830
 &rst
  ixpk= 5, nxpk= 0, iat= 120,  72, r1= 2.52, r2= 3.02, r3= 5.83, r4= 6.33,  &end
#
#   4 DC  H2'1   3 DT  H2'2  2.350   4.290  (#2.350   4.290 9 23)
 &rst
  ixpk= 4, nxpk= 0, iat= 120,  91, r1= 1.85, r2= 2.35, r3= 4.29, r4= 4.79,  &end
#
#   4 DC  H2'1   4 DC  H1'   2.400   4.140
 &rst
  ixpk= 4, nxpk= 0, iat= 120, 104, r1= 1.90, r2= 2.40, r3= 4.14, r4= 4.64,  &end
#
#   4 DC  H2'1   4 DC  H6    2.080   2.850
 &rst
  ixpk= 4, nxpk= 0, iat= 120, 107, r1= 1.58, r2= 2.08, r3= 2.85, r4= 3.35,  &end
#
#   4 DC  H2'1   4 DC  H5    2.650   4.450  (#2.650   3.550 4 7 28)
 &rst
  ixpk= 3, nxpk= 0, iat= 120, 109, r1= 2.15, r2= 2.65, r3= 4.45, r4= 4.95,  &end
#
#   4 DC  H2'1   4 DC  H3'   1.780   2.510
 &rst
  ixpk= 3, nxpk= 0, iat= 120, 118, r1= 1.28, r2= 1.78, r3= 2.51, r4= 3.01,  &end
#
#   4 DC  H2'2   3 DT  H1'   3.730   5.970
 &rst
  ixpk= 3, nxpk= 0, iat= 121,  72, r1= 3.23, r2= 3.73, r3= 5.97, r4= 6.47,  &end
#
```

```
#   4 DC  H2'2   4 DC  H1'   2.010   2.740
 &rst
  ixpk= 3, nxpk= 0, iat= 121, 104, r1= 1.51, r2= 2.01, r3= 2.74, r4= 3.24,  &end
#
#   4 DC  H2'2   4 DC  H6    2.460   3.980  (#2.460   3.380 13 33)
 &rst
  ixpk= 3, nxpk= 0, iat= 121, 107, r1= 1.96, r2= 2.46, r3= 3.98, r4= 4.48,  &end
#
#   4 DC  H2'2   4 DC  H5    3.120   5.580  (#3.120   4.680 6 19 22)
 &rst
  ixpk= 4, nxpk= 0, iat= 121, 109, r1= 2.62, r2= 3.12, r3= 5.58, r4= 6.08,  &end
#
#   4 DC  H2'2   4 DC  H3'   2.260   4.080
 &rst
  ixpk= 4, nxpk= 0, iat= 121, 118, r1= 1.76, r2= 2.26, r3= 4.08, r4= 4.58,  &end
#
#   5 DT  H1'    4 DC  H2'1  3.700   5.800  (#3.700   5.500 42)
 &rst
  ixpk= 5, nxpk= 0, iat= 134, 120, r1= 3.20, r2= 3.70, r3= 5.80, r4= 6.30,  &end
#
#   5 DT  H1'    4 DC  H2'2  3.920   5.710
 &rst
  ixpk= 5, nxpk= 0, iat= 134, 121, r1= 3.42, r2= 3.92, r3= 5.71, r4= 6.21,  &end
#
#   5 DT  H6     4 DC  H1'   3.530   6.140
 &rst
  ixpk= 5, nxpk= 0, iat= 137, 104, r1= 3.03, r2= 3.53, r3= 6.14, r4= 6.64,  &end
#
#   5 DT  H6     4 DC  H6    3.840   5.890
 &rst
  ixpk= 5, nxpk= 0, iat= 137, 107, r1= 3.34, r2= 3.84, r3= 5.89, r4= 6.39,  &end
#
#   5 DT  H6     4 DC  H5    4.650   6.660
 &rst
  ixpk= 5, nxpk= 0, iat= 137, 109, r1= 4.15, r2= 4.65, r3= 6.66, r4= 7.16,  &end
#
#   5 DT  H6     4 DC  H3'   3.550   5.840
 &rst
  ixpk= 5, nxpk= 0, iat= 137, 118, r1= 3.05, r2= 3.55, r3= 5.84, r4= 6.34,  &end
#
#   5 DT  H6     4 DC  H2'1  2.620   3.590
 &rst
  ixpk= 5, nxpk= 0, iat= 137, 120, r1= 2.12, r2= 2.62, r3= 3.59, r4= 4.09,  &end
#
#   5 DT  H6     4 DC  H2'2  2.410   3.140  (#2.410   2.840 21)
 &rst
  ixpk= 2, nxpk= 0, iat= 137, 121, r1= 1.91, r2= 2.41, r3= 3.14, r4= 3.64,  &end
#
#   5 DT  H6     5 DT  H1'   2.690   4.430
 &rst
  ixpk= 2, nxpk= 0, iat= 137, 134, r1= 2.19, r2= 2.69, r3= 4.43, r4= 4.93,  &end
```

```
#
#   5 DT  Q5     4 DC  H1'   3.450   5.280  (#3.450   4.380 5 15 18)
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 104, r1= 2.95, r2= 3.45, r3= 6.34, r4= 6.84,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  Q5     4 DC  H6    2.770   3.780
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 107, r1= 2.27, r2= 2.77, r3= 4.54, r4= 5.04,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  Q5     4 DC  H5    2.820   3.870
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 109, r1= 2.32, r2= 2.82, r3= 4.65, r4= 5.15,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  Q5     4 DC  H3'   3.070   4.270  (#3.070   3.970 24)
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 118, r1= 2.57, r2= 3.07, r3= 5.13, r4= 5.63,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  Q5     4 DC  H2'1  2.980   4.170
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 120, r1= 2.48, r2= 2.98, r3= 5.01, r4= 5.51,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  Q5     4 DC  H2'2  3.120   3.850
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 121, r1= 2.62, r2= 3.12, r3= 4.62, r4= 5.12,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  Q5     5 DT  H6    2.510   3.390
 (#5 DT  Q5     5 DT  H1'   2.820   3.530)
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 137, r1= 2.01, r2= 2.51, r3= 4.07, r4= 4.57,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  H3'    4 DC  H2'1  3.940   5.910
 &rst
  ixpk= 3, nxpk= 0, iat= 150, 120, r1= 3.44, r2= 3.94, r3= 5.91, r4= 6.41,  &end
#
#   5 DT  H3'    4 DC  H2'2  3.530   4.690  (#3.530   4.090 31 44)
 &rst
  ixpk= 4, nxpk= 0, iat= 150, 121, r1= 3.03, r2= 3.53, r3= 4.69, r4= 5.19,  &end
```

```
#
#   5 DT  H3'    5 DT  H1'   3.240   4.450
 &rst
  ixpk= 4, nxpk= 0, iat= 150, 134, r1= 2.74, r2= 3.24, r3= 4.45, r4= 4.95,  &end
#
#   5 DT  H3'    5 DT  H6    2.610   3.800  (#2.610   3.200 23 40)
 &rst
  ixpk= 3, nxpk= 0, iat= 150, 137, r1= 2.11, r2= 2.61, r3= 3.80, r4= 4.30,  &end
#
#   5 DT  H2'1   5 DT  H1'   2.490   4.540
 &rst
  ixpk= 3, nxpk= 0, iat= 152, 134, r1= 1.99, r2= 2.49, r3= 4.54, r4= 5.04,  &end
#
#   5 DT  H2'1   5 DT  H6    2.130   2.860  (#1.830   2.860 46)
 &rst
  ixpk= 2, nxpk= 0, iat= 152, 137, r1= 1.63, r2= 2.13, r3= 2.86, r4= 3.36,  &end
#
#   5 DT  H2'1   5 DT  H3'   1.830   3.160  (#2.430   3.160 6 22)
 &rst
  ixpk= 3, nxpk= 0, iat= 152, 150, r1= 1.33, r2= 1.83, r3= 3.16, r4= 3.66,  &end
#
#   5 DT  H2'2   5 DT  H1'   2.260   2.610  (#1.960   2.610 48)
 &rst
  ixpk= 2, nxpk= 0, iat= 153, 134, r1= 1.76, r2= 2.26, r3= 2.61, r4= 3.11,  &end
#
#   5 DT  H2'2   5 DT  H6    2.240   4.140  (#2.240   3.840 39)
 &rst
  ixpk= 3, nxpk= 0, iat= 153, 137, r1= 1.74, r2= 2.24, r3= 4.14, r4= 4.64,  &end
#
#   6 DT  H6     5 DT  H1'   4.060   5.600  (#4.960   5.600 1 8 9)
 &rst
  ixpk= 5, nxpk= 0, iat= 169, 134, r1= 3.56, r2= 4.06, r3= 5.60, r4= 6.10,  &end
#
#   6 DT  H6     5 DT  H3'   3.860   6.230
 &rst
  ixpk= 5, nxpk= 0, iat= 169, 150, r1= 3.36, r2= 3.86, r3= 6.23, r4= 6.73,  &end
#
#   6 DT  H6     5 DT  H2'1  2.090   4.020  (#2.090   3.720 29)
 &rst
  ixpk= 3, nxpk= 0, iat= 169, 152, r1= 1.59, r2= 2.09, r3= 4.02, r4= 4.52,  &end
#
#   6 DT  H6     5 DT  H2'2  1.860   2.860  (#1.860   2.560 28)
 &rst
  ixpk= 2, nxpk= 0, iat= 169, 153, r1= 1.36, r2= 1.86, r3= 2.86, r4= 3.36,  &end
#
#   6 DT  H6     6 DT  H1'   2.780   4.200
 &rst
  ixpk= 2, nxpk= 0, iat= 169, 166, r1= 2.28, r2= 2.78, r3= 4.20, r4= 4.70,  &end
#
#   6 DT  Q5     5 DT  H1'   2.860   4.550  (#2.860   4.250 37)
 &rst
```

```
  ixpk= 4, nxpk= 0, iat=  -1, 134, r1= 2.36, r2= 2.86, r3= 5.46, r4= 5.96,
 igr1= 172, 173, 174,
 &end
#
#   6 DT  Q5     5 DT  H3'   3.040   4.480  (#3.040   4.180 16)
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 150, r1= 2.54, r2= 3.04, r3= 5.38, r4= 5.88,
 igr1= 172, 173, 174,
 &end
#
#   6 DT  Q5     6 DT  H6    2.230   3.100  (#2.530   3.100 35)
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 169, r1= 1.73, r2= 2.23, r3= 3.72, r4= 4.22,
 igr1= 172, 173, 174,
 &end
#
#   6 DT  H3'    6 DT  H1'   2.330   3.880  (#2.330   3.280 3 6)
 &rst
  ixpk= 3, nxpk= 0, iat= 182, 166, r1= 1.83, r2= 2.33, r3= 3.88, r4= 4.38,  &end
#
#   6 DT  H3'    6 DT  H6    2.970   4.600  (#2.970   4.000 4 20)
 &rst
  ixpk= 4, nxpk= 0, iat= 182, 169, r1= 2.47, r2= 2.97, r3= 4.60, r4= 5.10,  &end
#
#   6 DT  H3'    6 DT  Q5    4.470   6.820
 &rst
  ixpk= 4, nxpk= 0, iat= 182,  -1, r1= 3.97, r2= 4.47, r3= 8.19, r4= 8.69,
 igr2= 172, 173, 174,
 &end
#
#   6 DT  H2'1   5 DT  H1'   3.140   6.670  (#3.140   5.170 2 11 14 26 41)
 &rst
  ixpk= 5, nxpk= 0, iat= 184, 134, r1= 2.64, r2= 3.14, r3= 6.67, r4= 7.17,  &end
#
#   6 DT  H2'1   6 DT  H1'   2.680   3.760
 &rst
  ixpk= 5, nxpk= 0, iat= 184, 166, r1= 2.18, r2= 2.68, r3= 3.76, r4= 4.26,  &end
#
#   6 DT  H2'1   6 DT  H6    1.970   2.620
 &rst
  ixpk= 5, nxpk= 0, iat= 184, 169, r1= 1.47, r2= 1.97, r3= 2.62, r4= 3.12,  &end
#
#   6 DT  H2'1   6 DT  Q5    2.820   5.690
 &rst
  ixpk= 5, nxpk= 0, iat= 184,  -1, r1= 2.32, r2= 2.82, r3= 6.83, r4= 7.33,
 igr2= 172, 173, 174,
 &end
#
#   6 DT  H2'1   6 DT  H3'   2.080   2.670  (#2.380   2.670 19)
 &rst
  ixpk= 2, nxpk= 0, iat= 184, 182, r1= 1.58, r2= 2.08, r3= 2.67, r4= 3.17,  &end
```

```
#
#   6 DT  H2'2   6 DT  H6    2.200   4.090  (#2.200   3.190 12 22 39)
 &rst
  ixpk= 3, nxpk= 0, iat= 185, 169, r1= 1.70, r2= 2.20, r3= 4.09, r4= 4.59,  &end
#
#   6 DT  H2'2   6 DT  H3'   2.510   3.500
 &rst
  ixpk= 3, nxpk= 0, iat= 185, 182, r1= 2.01, r2= 2.51, r3= 3.50, r4= 4.00,  &end
#
#   7 DG  H8     6 DT  Q5    4.100   6.510  (#4.100   6.210 15)
 &rst
  ixpk= 6, nxpk= 0, iat= 201,  -1, r1= 3.60, r2= 4.10, r3= 7.82, r4= 8.32,
 igr2= 172, 173, 174,
 &end
#
#   7 DG  H8     6 DT  H3'   3.720   4.710  (#3.720   4.410 17)
 &rst
  ixpk= 4, nxpk= 0, iat= 201, 182, r1= 3.22, r2= 3.72, r3= 4.71, r4= 5.21,  &end
#
#   7 DG  H8     6 DT  H2'1  3.380   4.470  (#3.380   3.870 24 32 40)
 &rst
  ixpk= 3, nxpk= 0, iat= 201, 184, r1= 2.88, r2= 3.38, r3= 4.47, r4= 4.97,  &end
#
#   7 DG  H8     6 DT  H2'2  3.050   3.540  (#3.050   3.540 5 7 10 45 47 51)
 &rst
  ixpk= 3, nxpk= 0, iat= 201, 185, r1= 2.55, r2= 3.05, r3= 3.54, r4= 4.04,  &end
#
#   7 DG  H3'    7 DG  H1'   3.270   4.270
 &rst
  ixpk= 3, nxpk= 0, iat= 215, 198, r1= 2.77, r2= 3.27, r3= 4.27, r4= 4.77,  &end
#
#   7 DG  H3'    7 DG  H8    3.140   4.730
 &rst
  ixpk= 3, nxpk= 0, iat= 215, 201, r1= 2.64, r2= 3.14, r3= 4.73, r4= 5.23,  &end
#
#   7 DG  H2'1   7 DG  H1'   2.640   4.450
 &rst
  ixpk= 3, nxpk= 0, iat= 217, 198, r1= 2.14, r2= 2.64, r3= 4.45, r4= 4.95,  &end
#
#   7 DG  H2'1   7 DG  H8    1.830   2.980  (#2.130   2.680 25 44)
 &rst
  ixpk= 2, nxpk= 0, iat= 217, 201, r1= 1.33, r2= 1.83, r3= 2.98, r4= 3.48,  &end
#
#   7 DG  H2'1   7 DG  H3'   2.270   3.280  (#2.270   3.280 30 48)
 &rst
  ixpk= 3, nxpk= 0, iat= 217, 215, r1= 1.77, r2= 2.27, r3= 3.28, r4= 3.78,  &end
#
#   7 DG  H2'2   7 DG  H1'   1.860   2.580
 &rst
  ixpk= 3, nxpk= 0, iat= 218, 198, r1= 1.36, r2= 1.86, r3= 2.58, r4= 3.08,  &end
#
```

```
#   7 DG  H2'2   7 DG  H3'   2.330   3.350
 &rst
  ixpk= 3, nxpk= 0, iat= 218, 215, r1= 1.83, r2= 2.33, r3= 3.35, r4= 3.85,  &end
#
#   8 DT  H6     7 DG  H1'   2.780   4.250  (#2.780   3.650 16 23)
 &rst
  ixpk= 3, nxpk= 0, iat= 234, 198, r1= 2.28, r2= 2.78, r3= 4.25, r4= 4.75,  &end
#
#   8 DT  H6     7 DG  H8    3.540   5.850
 &rst
  ixpk= 3, nxpk= 0, iat= 234, 201, r1= 3.04, r2= 3.54, r3= 5.85, r4= 6.35,  &end
#
#   8 DT  H6     7 DG  H3'   3.690   5.670
 &rst
  ixpk= 3, nxpk= 0, iat= 234, 215, r1= 3.19, r2= 3.69, r3= 5.67, r4= 6.17,  &end
#
#   8 DT  H6     7 DG  H2'1  2.930   4.770
 &rst
  ixpk= 3, nxpk= 0, iat= 234, 217, r1= 2.43, r2= 2.93, r3= 4.77, r4= 5.27,  &end
#
#   8 DT  H6     7 DG  H2'2  2.300   3.290  (#2.600   3.290 11)
 &rst
  ixpk= 3, nxpk= 0, iat= 234, 218, r1= 1.80, r2= 2.30, r3= 3.29, r4= 3.79,  &end
#
#   8 DT  H6     8 DT  H1'   3.090   4.250
 &rst
  ixpk= 3, nxpk= 0, iat= 234, 231, r1= 2.59, r2= 3.09, r3= 4.25, r4= 4.75,  &end
#
#   8 DT  Q5     7 DG  H1'   3.230   4.840
 (#8 DT  Q5     6 DT  H1'   3.580   6.820)
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 198, r1= 2.73, r2= 3.23, r3= 5.81, r4= 6.31,
 igr1= 237, 238, 239,
 &end
#
#   8 DT  Q5     7 DG  H8    2.870   3.670  (#2.870   3.370 27)
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 201, r1= 2.37, r2= 2.87, r3= 4.41, r4= 4.91,
 igr1= 237, 238, 239,
 &end
#
#   8 DT  Q5     7 DG  H3'   3.410   5.240  (#3.410   4.340 18 33 42)
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 215, r1= 2.91, r2= 3.41, r3= 6.29, r4= 6.79,
 igr1= 237, 238, 239,
 &end
#
#   8 DT  Q5     7 DG  H2'1  2.700   4.440  (#3.000   4.440 28)
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 217, r1= 2.20, r2= 2.70, r3= 5.33, r4= 5.83,
 igr1= 237, 238, 239,
```

```
 &end
#
#   8 DT  Q5     7 DG  H2'2  2.560   3.870  (#2.860   3.870 12)
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 218, r1= 2.06, r2= 2.56, r3= 4.65, r4= 5.15,
 igr1= 237, 238, 239,
 &end
#
#   8 DT  Q5     8 DT  H1'   3.960   6.280
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 231, r1= 3.46, r2= 3.96, r3= 7.54, r4= 8.04,
 igr1= 237, 238, 239,
 &end
#
#   8 DT  Q5     8 DT  H6    2.380   3.160  (#2.680   3.160 13)
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 234, r1= 1.88, r2= 2.38, r3= 3.79, r4= 4.29,
 igr1= 237, 238, 239,
 &end
#
#   8 DT  H3'    7 DG  H2'2  3.760   5.260
 &rst
  ixpk= 3, nxpk= 0, iat= 247, 218, r1= 3.26, r2= 3.76, r3= 5.26, r4= 5.76,  &end
#
#   8 DT  H3'    8 DT  H1'   3.260   4.530
 &rst
  ixpk= 3, nxpk= 0, iat= 247, 231, r1= 2.76, r2= 3.26, r3= 4.53, r4= 5.03,  &end
#
#   8 DT  H3'    8 DT  H6    2.980   4.900
 &rst
  ixpk= 3, nxpk= 0, iat= 247, 234, r1= 2.48, r2= 2.98, r3= 4.90, r4= 5.40,  &end
#
#   8 DT  H3'    8 DT  Q5    3.630   6.280  (#3.630   5.380 9 14 30)
 &rst
  ixpk= 5, nxpk= 0, iat= 247,  -1, r1= 3.13, r2= 3.63, r3= 7.54, r4= 8.04,
 igr2= 237, 238, 239,
 &end
#
#   8 DT  H2'1   7 DG  H1'   3.450   5.180  (#3.450   4.880 21)
 &rst
  ixpk= 4, nxpk= 0, iat= 249, 198, r1= 2.95, r2= 3.45, r3= 5.18, r4= 5.68,  &end
#
#   8 DT  H2'1   8 DT  H1'   2.430   3.440
 &rst
  ixpk= 4, nxpk= 0, iat= 249, 231, r1= 1.93, r2= 2.43, r3= 3.44, r4= 3.94,  &end
#
#   8 DT  H2'1   8 DT  H6    1.890   2.810
 &rst
  ixpk= 4, nxpk= 0, iat= 249, 234, r1= 1.39, r2= 1.89, r3= 2.81, r4= 3.31,  &end
#
#   8 DT  H2'1   8 DT  Q5    2.660   5.460
```

```
 &rst
  ixpk= 4, nxpk= 0, iat= 249,  -1, r1= 2.16, r2= 2.66, r3= 6.56, r4= 7.06,
 igr2= 237, 238, 239,
 &end
#
#   8 DT  H2'1   8 DT  H3'   1.960   2.810
 &rst
  ixpk= 4, nxpk= 0, iat= 249, 247, r1= 1.46, r2= 1.96, r3= 2.81, r4= 3.31,  &end
#
#   8 DT  H2'2   8 DT  H1'   1.880   2.800  (#2.180   2.500 25 29)
 &rst
  ixpk= 2, nxpk= 0, iat= 250, 231, r1= 1.38, r2= 1.88, r3= 2.80, r4= 3.30,  &end
#
#   8 DT  H2'2   8 DT  H6    2.350   3.970
 &rst
  ixpk= 2, nxpk= 0, iat= 250, 234, r1= 1.85, r2= 2.35, r3= 3.97, r4= 4.47,  &end
#
#   8 DT  H2'2   8 DT  Q5    2.700   6.260  (#2.700   6.560 46)
 &rst
  ixpk= 6, nxpk= 0, iat= 250,  -1, r1= 2.20, r2= 2.70, r3= 7.52, r4= 8.02,
 igr2= 237, 238, 239,
 &end
#
#   8 DT  H2'2   8 DT  H3'   2.640   4.430
 &rst
  ixpk= 6, nxpk= 0, iat= 250, 247, r1= 2.14, r2= 2.64, r3= 4.43, r4= 4.93,  &end
#
#   9 DC  H6     8 DT  H1'   3.240   5.790
 &rst
  ixpk= 6, nxpk= 0, iat= 266, 231, r1= 2.74, r2= 3.24, r3= 5.79, r4= 6.29,  &end
#
#   9 DC  H6     8 DT  H6    3.200   5.390
 &rst
  ixpk= 6, nxpk= 0, iat= 266, 234, r1= 2.70, r2= 3.20, r3= 5.39, r4= 5.89,  &end
#
#   9 DC  H6     8 DT  Q5    2.900   6.060
 &rst
  ixpk= 6, nxpk= 0, iat= 266,  -1, r1= 2.40, r2= 2.90, r3= 7.28, r4= 7.78,
 igr2= 237, 238, 239,
 &end
#
#   9 DC  H6     8 DT  H3'   3.770   5.800
 &rst
  ixpk= 6, nxpk= 0, iat= 266, 247, r1= 3.27, r2= 3.77, r3= 5.80, r4= 6.30,  &end
#
#   9 DC  H6     8 DT  H2'1  2.580   4.530
 &rst
  ixpk= 6, nxpk= 0, iat= 266, 249, r1= 2.08, r2= 2.58, r3= 4.53, r4= 5.03,  &end
#
#   9 DC  H6     8 DT  H2'2  2.100   2.880
 &rst
```

```
  ixpk= 6, nxpk= 0, iat= 266, 250, r1= 1.60, r2= 2.10, r3= 2.88, r4= 3.38,  &end
#
#   9 DC  H5     8 DT  H1'   3.320   4.700  (#3.320   3.700 1 15 31)
 &rst
  ixpk= 3, nxpk= 0, iat= 268, 231, r1= 2.82, r2= 3.32, r3= 4.70, r4= 5.20,  &end
#
#   9 DC  H5     8 DT  H6    2.960   4.030  (#3.260   3.730 19 34)
 &rst
  ixpk= 3, nxpk= 0, iat= 268, 234, r1= 2.46, r2= 2.96, r3= 4.03, r4= 4.53,  &end
#
#   9 DC  H5     8 DT  Q5    3.650   4.600
 &rst
  ixpk= 3, nxpk= 0, iat= 268,  -1, r1= 3.15, r2= 3.65, r3= 5.52, r4= 6.02,
 igr2= 237, 238, 239,
 &end
#
#   9 DC  H5     8 DT  H3'   4.280   6.100
 &rst
  ixpk= 3, nxpk= 0, iat= 268, 247, r1= 3.78, r2= 4.28, r3= 6.10, r4= 6.60,  &end
#
#   9 DC  H5     8 DT  H2'1  2.690   5.490  (#2.990   5.490 8)
 &rst
  ixpk= 5, nxpk= 0, iat= 268, 249, r1= 2.19, r2= 2.69, r3= 5.49, r4= 5.99,  &end
#
#   9 DC  H5     8 DT  H2'2  2.870   4.330
 &rst
  ixpk= 5, nxpk= 0, iat= 268, 250, r1= 2.37, r2= 2.87, r3= 4.33, r4= 4.83,  &end
#
#   9 DC  H5     9 DC  H1'   3.950   5.470  (#3.950   4.870 5 7)
 &rst
  ixpk= 4, nxpk= 0, iat= 268, 263, r1= 3.45, r2= 3.95, r3= 5.47, r4= 5.97,  &end
#
#   9 DC  H3'    9 DC  H1'   3.520   5.440
 &rst
  ixpk= 4, nxpk= 0, iat= 277, 263, r1= 3.02, r2= 3.52, r3= 5.44, r4= 5.94,  &end
#
#   9 DC  H3'    9 DC  H6    3.120   4.280  (#3.120   3.680 22 28)
 &rst
  ixpk= 3, nxpk= 0, iat= 277, 266, r1= 2.62, r2= 3.12, r3= 4.28, r4= 4.78,  &end
#
#   9 DC  H3'    9 DC  H5    4.110   6.690  (#4.110   5.790 9 17 38)
 &rst
  ixpk= 5, nxpk= 0, iat= 277, 268, r1= 3.61, r2= 4.11, r3= 6.69, r4= 7.19,  &end
#
#   9 DC  H2'1   8 DT  H1'   3.940   6.180  (#3.940   5.880 43)
 &rst
  ixpk= 5, nxpk= 0, iat= 279, 231, r1= 3.44, r2= 3.94, r3= 6.18, r4= 6.68,  &end
#
#   9 DC  H2'1   9 DC  H1'   2.570   3.200
 &rst
  ixpk= 5, nxpk= 0, iat= 279, 263, r1= 2.07, r2= 2.57, r3= 3.20, r4= 3.70,  &end
```

```
#
#   9 DC  H2'1   9 DC  H6    1.870   2.740  (#2.170   2.740 25)
 &rst
  ixpk= 2, nxpk= 0, iat= 279, 266, r1= 1.37, r2= 1.87, r3= 2.74, r4= 3.24,  &end
#
#   9 DC  H2'1   9 DC  H5    2.970   4.520  (#2.970   3.920 4 14)
 &rst
  ixpk= 3, nxpk= 0, iat= 279, 268, r1= 2.47, r2= 2.97, r3= 4.52, r4= 5.02,  &end
#
#   9 DC  H2'1   9 DC  H3'   1.890   2.860  (#2.190   2.860 32)
 &rst
  ixpk= 2, nxpk= 0, iat= 279, 277, r1= 1.39, r2= 1.89, r3= 2.86, r4= 3.36,  &end
#
#   9 DC  H2'2   9 DC  H1'   1.910   2.640  (# 2.210   2.640 41)
 &rst
  ixpk= 2, nxpk= 0, iat= 280, 263, r1= 1.41, r2= 1.91, r3= 2.64, r4= 3.14,  &end
#
#   9 DC  H2'2   9 DC  H6    2.230   4.060  (#2.230   2.860 3 6 10 35)
 &rst
  ixpk= 2, nxpk= 0, iat= 280, 266, r1= 1.73, r2= 2.23, r3= 4.06, r4= 4.56,  &end
#
#   9 DC  H2'2   9 DC  H5    3.820   5.780
 &rst
  ixpk= 2, nxpk= 0, iat= 280, 268, r1= 3.32, r2= 3.82, r3= 5.78, r4= 6.28,  &end
#
#   9 DC  H2'2   9 DC  H3'   2.260   3.000
 &rst
  ixpk= 2, nxpk= 0, iat= 280, 277, r1= 1.76, r2= 2.26, r3= 3.00, r4= 3.50,  &end
#
#  10 DC  H1'    9 DC  H1'   4.200   6.510  (#4.200   5.910 33 37)
 &rst
  ixpk= 5, nxpk= 0, iat= 293, 263, r1= 3.70, r2= 4.20, r3= 6.51, r4= 7.01,  &end
#
#  10 DC  H6     9 DC  H1'   3.280   4.100  (#3.280   3.800 20)
 &rst
  ixpk= 3, nxpk= 0, iat= 296, 263, r1= 2.78, r2= 3.28, r3= 4.10, r4= 4.60,  &end
#
#  10 DC  H6     9 DC  H2'1  2.500   5.850
 &rst
  ixpk= 3, nxpk= 0, iat= 296, 279, r1= 2.00, r2= 2.50, r3= 5.85, r4= 6.35,  &end
#
#  10 DC  H6     9 DC  H2'2  2.250   3.900  (#2.850   3.900 2 23)
 &rst
  ixpk= 3, nxpk= 0, iat= 296, 280, r1= 1.75, r2= 2.25, r3= 3.90, r4= 4.40,  &end
#
#  10 DC  H6    10 DC  H1'   3.440   5.560
 &rst
  ixpk= 3, nxpk= 0, iat= 296, 293, r1= 2.94, r2= 3.44, r3= 5.56, r4= 6.06,  &end
#
#  10 DC  H5     9 DC  H1'   3.840   5.900
 &rst
```

```
  ixpk= 3, nxpk= 0, iat= 298, 263, r1= 3.34, r2= 3.84, r3= 5.90, r4= 6.40,  &end
#
#  10 DC  H5    10 DC  H3'   3.560   5.810  (#3.560   4.310 6 8 12 15 25 43)
 &rst
  ixpk= 4, nxpk= 0, iat= 298, 307, r1= 3.06, r2= 3.56, r3= 5.81, r4= 6.31,  &end
#
#  10 DC  H5     9 DC  H2'1  3.200   4.240
 &rst
  ixpk= 4, nxpk= 0, iat= 298, 279, r1= 2.70, r2= 3.20, r3= 4.24, r4= 4.74,  &end
#
#  10 DC  H5     9 DC  H2'2  2.460   3.950  (#2.760   3.350 11 24 26)
 &rst
  ixpk= 3, nxpk= 0, iat= 298, 280, r1= 1.96, r2= 2.46, r3= 3.95, r4= 4.45,  &end
#
#  10 DC  H3'   10 DC  H1'   3.490   5.400
 &rst
  ixpk= 3, nxpk= 0, iat= 307, 293, r1= 2.99, r2= 3.49, r3= 5.40, r4= 5.90,  &end
#
#  10 DC  H3'   10 DC  H6    2.770   3.400  (#2.770   3.100 32)
 &rst
  ixpk= 3, nxpk= 0, iat= 307, 296, r1= 2.27, r2= 2.77, r3= 3.40, r4= 3.90,  &end
#
#  10 DC  H2'1   9 DC  H2'2  2.140   4.970  (#2.140   4.070 12 16 27)
 &rst
  ixpk= 4, nxpk= 0, iat= 309, 280, r1= 1.64, r2= 2.14, r3= 4.97, r4= 5.47,  &end
#
#  10 DC  H2'1  10 DC  H1'   2.530   3.200  (#2.530   2.900 31)
 &rst
  ixpk= 2, nxpk= 0, iat= 309, 293, r1= 2.03, r2= 2.53, r3= 3.20, r4= 3.70,  &end
#
#  10 DC  H2'1  10 DC  H6    2.160   2.660
 &rst
  ixpk= 2, nxpk= 0, iat= 309, 296, r1= 1.66, r2= 2.16, r3= 2.66, r4= 3.16,  &end
#
#  10 DC  H2'1  10 DC  H5    2.950   4.520  (#2.950   4.220 29)
 &rst
  ixpk= 4, nxpk= 0, iat= 309, 298, r1= 2.45, r2= 2.95, r3= 4.52, r4= 5.02,  &end
#
#  10 DC  H2'1  10 DC  H3'   2.140   2.780  (#2.440   2.780 17 41)
 &rst
  ixpk= 2, nxpk= 0, iat= 309, 307, r1= 1.64, r2= 2.14, r3= 2.78, r4= 3.28,  &end
#
#  10 DC  H2'2  10 DC  H1'   1.940   2.340
 &rst
  ixpk= 2, nxpk= 0, iat= 310, 293, r1= 1.44, r2= 1.94, r3= 2.34, r4= 2.84,  &end
#
#  10 DC  H2'2  10 DC  H6    2.190   3.860  (#2.190   2.960 1 3 21)
 &rst
  ixpk= 2, nxpk= 0, iat= 310, 296, r1= 1.69, r2= 2.19, r3= 3.86, r4= 4.36,  &end
#
#  11 DG3 H1'   10 DC  H1'   2.250   5.000
```

```
 &rst
  ixpk= 2, nxpk= 0, iat= 323, 293, r1= 1.75, r2= 2.25, r3= 5.00, r4= 5.50,  &end
#
#  11 DG3 H8    10 DC  H1'   2.730   6.740
 &rst
  ixpk= 2, nxpk= 0, iat= 326, 293, r1= 2.23, r2= 2.73, r3= 6.74, r4= 7.24,  &end
#
#  11 DG3 H8    10 DC  H6    4.070   6.590  (#4.370   6.590 30)
 &rst
  ixpk= 6, nxpk= 0, iat= 326, 296, r1= 3.57, r2= 4.07, r3= 6.59, r4= 7.09,  &end
#
#  11 DG3 H8    10 DC  H5    3.700   6.590
 &rst
  ixpk= 6, nxpk= 0, iat= 326, 298, r1= 3.20, r2= 3.70, r3= 6.59, r4= 7.09,  &end
#
#  11 DG3 H8    10 DC  H2'1  2.300   5.400
 &rst
  ixpk= 6, nxpk= 0, iat= 326, 309, r1= 1.80, r2= 2.30, r3= 5.40, r4= 5.90,  &end
#
#  11 DG3 H8    10 DC  H2'2  1.750   2.540  (#1.750   2.240 44)
 &rst
  ixpk= 2, nxpk= 0, iat= 326, 310, r1= 1.25, r2= 1.75, r3= 2.54, r4= 3.04,  &end
#
#  11 DG3 H8    11 DG3 H1'   2.140   5.450
 &rst
  ixpk= 2, nxpk= 0, iat= 326, 323, r1= 1.64, r2= 2.14, r3= 5.45, r4= 5.95,  &end
#
#  11 DG3 H3'   11 DG3 H1'   3.100   5.440
 (#11 DG3 H3'   10 DC  H2'1  3.210   6.760 #3.210   5.860 9 13 28 40(removed))
 &rst
  ixpk= 2, nxpk= 0, iat= 340, 323, r1= 2.60, r2= 3.10, r3= 5.44, r4= 5.94,  &end
#
#  11 DG3 H3'   11 DG3 H8    2.540   5.180  (#2.540   3.380 3 8 10 11 33 37)
 &rst
  ixpk= 3, nxpk= 0, iat= 340, 326, r1= 2.04, r2= 2.54, r3= 5.18, r4= 5.68,  &end
#
#  11 DG3 H2'1  11 DG3 H1'   1.920   3.060
 &rst
  ixpk= 3, nxpk= 0, iat= 342, 323, r1= 1.42, r2= 1.92, r3= 3.06, r4= 3.56,  &end
#
#  11 DG3 H2'1  11 DG3 H8    2.260   4.360  (#2.260   3.760 35 38)
 &rst
  ixpk= 3, nxpk= 0, iat= 342, 326, r1= 1.76, r2= 2.26, r3= 4.36, r4= 4.86,  &end
#
#  11 DG3 H2'1  11 DG3 H3'   2.170   3.510
 &rst
  ixpk= 3, nxpk= 0, iat= 342, 340, r1= 1.67, r2= 2.17, r3= 3.51, r4= 4.01,  &end
#
#  11 DG3 H2'2  10 DC  H1'   2.740   5.790  (#2.740   4.590 4 14 18 42)
 &rst
  ixpk= 4, nxpk= 0, iat= 343, 293, r1= 2.24, r2= 2.74, r3= 5.79, r4= 6.29,  &end
```

```
#
#  11 DG3 H2'2  11 DG3 H1'   1.640   2.640  (#1.640   2.340 31 )
 &rst
  ixpk= 2, nxpk= 0, iat= 343, 323, r1= 1.14, r2= 1.64, r3= 2.64, r4= 3.14,  &end
#
#  11 DG3 H2'2  11 DG3 H8    1.810   4.100  (#1.810   3.200 1 2 7 11 24 46 47)
 &rst
  ixpk= 3, nxpk= 0, iat= 343, 326, r1= 1.31, r2= 1.81, r3= 4.10, r4= 4.60,  &end
#
#  11 DG3 H2'2  11 DG3 H3'   1.960   2.900
 &rst
  ixpk= 3, nxpk= 0, iat= 343, 340, r1= 1.46, r2= 1.96, r3= 2.90, r4= 3.40,  &end
#
#  12 DC5 H6    12 DC5 H1'   2.580   3.980  (#2.580   3.380 8 18)
 &rst
  ixpk= 3, nxpk= 0, iat= 358, 355, r1= 2.08, r2= 2.58, r3= 3.98, r4= 4.48,  &end
#
#  12 DC5 H3'   12 DC5 H1'   3.610   5.860
 &rst
  ixpk= 3, nxpk= 0, iat= 369, 355, r1= 3.11, r2= 3.61, r3= 5.86, r4= 6.36,  &end
#
#  12 DC5 H3'   12 DC5 H6    3.020   4.400  (#3.020   3.800 23 42)
 &rst
  ixpk= 3, nxpk= 0, iat= 369, 358, r1= 2.52, r2= 3.02, r3= 4.40, r4= 4.90,  &end
#
#  12 DC5 H2'1  12 DC5 H1'   2.640   4.360
 &rst
  ixpk= 3, nxpk= 0, iat= 371, 355, r1= 2.14, r2= 2.64, r3= 4.36, r4= 4.86,  &end
#
#  12 DC5 H2'1  12 DC5 H6    1.880   2.790  (#2.180   2.490 28 29)
 &rst
  ixpk= 2, nxpk= 0, iat= 371, 358, r1= 1.38, r2= 1.88, r3= 2.79, r4= 3.29,  &end
#
#  12 DC5 H2'1  12 DC5 H5    3.080   4.950  (#3.080   4.650 33)
 &rst
  ixpk= 4, nxpk= 0, iat= 371, 360, r1= 2.58, r2= 3.08, r3= 4.95, r4= 5.45,  &end
#
#  12 DC5 H2'1  12 DC5 H3'   2.010   3.140  (#2.310   3.140 20)
 &rst
  ixpk= 3, nxpk= 0, iat= 371, 369, r1= 1.51, r2= 2.01, r3= 3.14, r4= 3.64,  &end
#
#  12 DC5 H2'2  12 DC5 H1'   2.080   2.520
 &rst
  ixpk= 3, nxpk= 0, iat= 372, 355, r1= 1.58, r2= 2.08, r3= 2.52, r4= 3.02,  &end
#
#  12 DC5 H2'2  12 DC5 H3'   2.000   3.250  (#2.000   2.650 13 41)
 &rst
  ixpk= 2, nxpk= 0, iat= 372, 369, r1= 1.50, r2= 2.00, r3= 3.25, r4= 3.75,  &end
#
#  13 DG  H1'   12 DC5 H2'2  3.770   5.290  (#3.770   4.990 31)
 &rst
```

```
  ixpk= 4, nxpk= 0, iat= 385, 372, r1= 3.27, r2= 3.77, r3= 5.29, r4= 5.79,  &end
#
#  13 DG  H8    12 DC5 H1'   3.830   6.120
 &rst
  ixpk= 4, nxpk= 0, iat= 388, 355, r1= 3.33, r2= 3.83, r3= 6.12, r4= 6.62,  &end
#
#  13 DG  H8    12 DC5 H6    3.760   6.500  (#4.360   6.500 24 25)
 &rst
  ixpk= 6, nxpk= 0, iat= 388, 358, r1= 3.26, r2= 3.76, r3= 6.50, r4= 7.00,  &end
#
#  13 DG  H8    12 DC5 H2'1  2.480   3.350  (#2.780   3.350 22)
 &rst
  ixpk= 3, nxpk= 0, iat= 388, 371, r1= 1.98, r2= 2.48, r3= 3.35, r4= 3.85,  &end
#
#  13 DG  H8    13 DG  H1'   3.420   5.210
 &rst
  ixpk= 3, nxpk= 0, iat= 388, 385, r1= 2.92, r2= 3.42, r3= 5.21, r4= 5.71,  &end
#
#  13 DG  H3'   12 DC5 H1'   5.160   6.250  (#5.160   5.950 34)
 &rst
  ixpk= 5, nxpk= 0, iat= 402, 355, r1= 4.66, r2= 5.16, r3= 6.25, r4= 6.75,  &end
#
#  13 DG  H3'   12 DC5 H2'1  4.530   6.110  (#4.530   5.810 40)
 &rst
  ixpk= 5, nxpk= 0, iat= 402, 371, r1= 4.03, r2= 4.53, r3= 6.11, r4= 6.61,  &end
#
#  13 DG  H3'   12 DC5 H2'2  3.470   4.490  (#3.470   3.890 5 35)
 &rst
  ixpk= 3, nxpk= 0, iat= 402, 372, r1= 2.97, r2= 3.47, r3= 4.49, r4= 4.99,  &end
#
#  13 DG  H3'   13 DG  H1'   3.020   4.140
 &rst
  ixpk= 3, nxpk= 0, iat= 402, 385, r1= 2.52, r2= 3.02, r3= 4.14, r4= 4.64,  &end
#
#  13 DG  H3'   13 DG  H8    3.240   5.400
 &rst
  ixpk= 3, nxpk= 0, iat= 402, 388, r1= 2.74, r2= 3.24, r3= 5.40, r4= 5.90,  &end
#
#  13 DG  H2'1  12 DC5 H1'   3.500   5.690  (#.500   4.190 9 11 12 21 43)
 &rst
  ixpk= 4, nxpk= 0, iat= 404, 355, r1= 3.00, r2= 3.50, r3= 5.69, r4= 6.19,  &end
#
#  13 DG  H2'1  12 DC5 H2'1  2.690   5.470
 &rst
  ixpk= 4, nxpk= 0, iat= 404, 371, r1= 2.19, r2= 2.69, r3= 5.47, r4= 5.97,  &end
#
#  13 DG  H2'1  13 DG  H1'   2.050   3.170
 &rst
  ixpk= 4, nxpk= 0, iat= 404, 385, r1= 1.55, r2= 2.05, r3= 3.17, r4= 3.67,  &end
#
#  13 DG  H2'1  13 DG  H8    1.870   2.660
```

```
 &rst
  ixpk= 4, nxpk= 0, iat= 404, 388, r1= 1.37, r2= 1.87, r3= 2.66, r4= 3.16,  &end
#
#  13 DG  H2'2  12 DC5 H2'1  3.110   6.560  (#3.110   4.760 1 4 6 9 15 32)
 &rst
  ixpk= 4, nxpk= 0, iat= 405, 371, r1= 2.61, r2= 3.11, r3= 6.56, r4= 7.06,  &end
#
#  13 DG  H2'2  13 DG  H1'   2.100   3.490
 &rst
  ixpk= 4, nxpk= 0, iat= 405, 385, r1= 1.60, r2= 2.10, r3= 3.49, r4= 3.99,  &end
#
#  13 DG  H2'2  13 DG  H8    2.170   4.140  (#2.170   3.840 38)
 &rst
  ixpk= 3, nxpk= 0, iat= 405, 388, r1= 1.67, r2= 2.17, r3= 4.14, r4= 4.64,  &end
#
#  14 DG  H1'   13 DG  H1'   3.740   5.630  (#3.740   5.330 17)
 &rst
  ixpk= 5, nxpk= 0, iat= 418, 385, r1= 3.24, r2= 3.74, r3= 5.63, r4= 6.13,  &end
#
#  14 DG  H8    13 DG  H1'   3.120   5.390  (#3.120   5.090 27)
 &rst
  ixpk= 5, nxpk= 0, iat= 421, 385, r1= 2.62, r2= 3.12, r3= 5.39, r4= 5.89,  &end
#
#  14 DG  H8    13 DG  H3'   4.900   6.650
 &rst
  ixpk= 5, nxpk= 0, iat= 421, 402, r1= 4.40, r2= 4.90, r3= 6.65, r4= 7.15,  &end
#
#  14 DG  H8    13 DG  H2'1  1.900   3.820  (#1.900   2.620 7 13 23 44)
 &rst
  ixpk= 2, nxpk= 0, iat= 421, 404, r1= 1.40, r2= 1.90, r3= 3.82, r4= 4.32,  &end
#
#  14 DG  H8    13 DG  H2'2  2.480   4.720
 &rst
  ixpk= 2, nxpk= 0, iat= 421, 405, r1= 1.98, r2= 2.48, r3= 4.72, r4= 5.22,  &end
#
#  14 DG  H8    14 DG  H1'   2.970   4.730
 &rst
  ixpk= 2, nxpk= 0, iat= 421, 418, r1= 2.47, r2= 2.97, r3= 4.73, r4= 5.23,  &end
#
#  14 DG  H3'   14 DG  H1'   2.650   4.280  (#2.650   3.380 1 15 22)
 &rst
  ixpk= 3, nxpk= 0, iat= 435, 418, r1= 2.15, r2= 2.65, r3= 4.28, r4= 4.78,  &end
#
#  14 DG  H3'   14 DG  H8    3.070   5.810  (#3.370   5.810 8)
 &rst
  ixpk= 5, nxpk= 0, iat= 435, 421, r1= 2.57, r2= 3.07, r3= 5.81, r4= 6.31,  &end
#
#  14 DG  H2'2  14 DG  H1'   1.920   2.570
 &rst
  ixpk= 5, nxpk= 0, iat= 438, 418, r1= 1.42, r2= 1.92, r3= 2.57, r4= 3.07,  &end
#
```

```
#  14 DG  H2'2  14 DG  H8    2.490   4.430  (#2.490   4.130 31)
 &rst
  ixpk= 4, nxpk= 0, iat= 438, 421, r1= 1.99, r2= 2.49, r3= 4.43, r4= 4.93,  &end
#
#  14 DG  H2'2  14 DG  H3'   2.560   3.430
 &rst
  ixpk= 4, nxpk= 0, iat= 438, 435, r1= 2.06, r2= 2.56, r3= 3.43, r4= 3.93,  &end
#
#  15 DA  H1'   14 DG  H1'   4.460   5.780
 &rst
  ixpk= 4, nxpk= 0, iat= 451, 418, r1= 3.96, r2= 4.46, r3= 5.78, r4= 6.28,  &end
#
#  15 DA  H8    14 DG  H1'   2.250   4.540  (#2.250   3.040 9 10 11 12 18 36)
 &rst
  ixpk= 3, nxpk= 0, iat= 454, 418, r1= 1.75, r2= 2.25, r3= 4.54, r4= 5.04,  &end
#
#  15 DA  H8    14 DG  H8    4.460   6.940
 &rst
  ixpk= 3, nxpk= 0, iat= 454, 421, r1= 3.96, r2= 4.46, r3= 6.94, r4= 7.44,  &end
#
#  15 DA  H8    15 DA  H2'1  1.940   3.960  (#1.940   2.760 6 24 25 33 45)
 &rst
  ixpk= 2, nxpk= 0, iat= 454, 469, r1= 1.44, r2= 1.94, r3= 3.96, r4= 4.46,  &end
#
#  15 DA  H8    14 DG  H2'2  2.190   5.930  (#2.790   5.930 5 16)
 &rst
  ixpk= 5, nxpk= 0, iat= 454, 438, r1= 1.69, r2= 2.19, r3= 5.93, r4= 6.43,  &end
#
#  15 DA  H8    15 DA  H1'   3.150   5.17
 &rst
  ixpk= 5, nxpk= 0, iat= 454, 451, r1= 2.65, r2= 3.15, r3= 5.17, r4= 5.67,  &end
#
#  15 DA  H3'   15 DA  H1'   3.240   5.370
 &rst
  ixpk= 5, nxpk= 0, iat= 467, 451, r1= 2.74, r2= 3.24, r3= 5.37, r4= 5.87,  &end
#
#  15 DA  H3'   15 DA  H8    2.690   4.710  (#2.690   3.210 2 17 26 32 35)
 &rst
  ixpk= 3, nxpk= 0, iat= 467, 454, r1= 2.19, r2= 2.69, r3= 4.71, r4= 5.21,  &end
#
#  15 DA  H2'1  15 DA  H1'   1.790   3.050  (#1.790   2.450 1 21)
 &rst
  ixpk= 2, nxpk= 0, iat= 469, 451, r1= 1.29, r2= 1.79, r3= 3.05, r4= 3.55,  &end
#
#  15 DA  H2'2  15 DA  H1'   1.800   4.090  (#2.100   4.090 38)
 &rst
  ixpk= 4, nxpk= 0, iat= 470, 451, r1= 1.30, r2= 1.80, r3= 4.09, r4= 4.59,  &end
#
#  15 DA  H2'2  15 DA  H8    2.460   4.340  (#2.460   4.040 31)
 &rst
  ixpk= 4, nxpk= 0, iat= 470, 454, r1= 1.96, r2= 2.46, r3= 4.34, r4= 4.84,  &end
```

```
#
# 15 DA  H2'2  15 DA  H3'   2.180   3.330
 &rst
  ixpk= 4, nxpk= 0, iat= 470, 467, r1= 1.68, r2= 2.18, r3= 3.33, r4= 3.83,  &end
#
# 16 DC  H1'   15 DA  H1'   4.580   5.880
 &rst
  ixpk= 4, nxpk= 0, iat= 483, 451, r1= 4.08, r2= 4.58, r3= 5.88, r4= 6.38,  &end
#
# 16 DC  H1'   15 DA  H2'2  3.830   4.760  (#3.830   4.460 30)
 &rst
  ixpk= 4, nxpk= 0, iat= 483, 470, r1= 3.33, r2= 3.83, r3= 4.76, r4= 5.26,  &end
#
# 16 DC  H6    15 DA  H1'   3.200   4.920  (#3.200   3.720 13 37 41 43)
 &rst
  ixpk= 3, nxpk= 0, iat= 486, 451, r1= 2.70, r2= 3.20, r3= 4.92, r4= 5.42,  &end
#
# 16 DC  H6    15 DA  H8    3.410   4.880  (#3.410   3.980 4 7 14)
 &rst
  ixpk= 3, nxpk= 0, iat= 486, 454, r1= 2.91, r2= 3.41, r3= 4.88, r4= 5.38,  &end
#
# 16 DC  H6    15 DA  H3'   3.690   4.970
 &rst
  ixpk= 3, nxpk= 0, iat= 486, 467, r1= 3.19, r2= 3.69, r3= 4.97, r4= 5.47,  &end
#
# 16 DC  H6    15 DA  H2'1  2.680   4.460  (#2.980   4.460 3)
 &rst
  ixpk= 4, nxpk= 0, iat= 486, 469, r1= 2.18, r2= 2.68, r3= 4.46, r4= 4.96,  &end
#
# 16 DC  H6    15 DA  H2'2  2.170   2.980  (#2.470   2.980 8)
 &rst
  ixpk= 2, nxpk= 0, iat= 486, 470, r1= 1.67, r2= 2.17, r3= 2.98, r4= 3.48,  &end
#
# 16 DC  H6    16 DC  H1'   3.390   4.310
 &rst
  ixpk= 2, nxpk= 0, iat= 486, 483, r1= 2.89, r2= 3.39, r3= 4.31, r4= 4.81,  &end
#
# 16 DC  H5     6 DT  Q5    4.530   5.420
 &rst
  ixpk= 2, nxpk= 0, iat= 488,  -1, r1= 4.03, r2= 4.53, r3= 6.51, r4= 7.01,
 igr2= 172, 173, 174,
 &end
#
# 16 DC  H5    15 DA  H1'   3.760   6.580
 (#16 DC  H5    14 DG  H1'   3.850   4.950)
 &rst
  ixpk= 2, nxpk= 0, iat= 488, 451, r1= 3.26, r2= 3.76, r3= 6.58, r4= 7.08,  &end
#
# 16 DC  H5    15 DA  H8    3.230   4.100  (#3.230   3.800  20)
 &rst
  ixpk= 3, nxpk= 0, iat= 488, 454, r1= 2.73, r2= 3.23, r3= 4.10, r4= 4.60,  &end
```

```
#
# 16 DC  H5    15 DA  H3'   4.230   6.670
 &rst
  ixpk= 3, nxpk= 0, iat= 488, 467, r1= 3.73, r2= 4.23, r3= 6.67, r4= 7.17,  &end
#
# 16 DC  H5    15 DA  H2'1  2.360   3.880  (#2.360   2.980 23 34 39)
 &rst
  ixpk= 2, nxpk= 0, iat= 488, 469, r1= 1.86, r2= 2.36, r3= 3.88, r4= 4.38,  &end
#
# 16 DC  H5    15 DA  H2'2  3.220   5.880
 &rst
  ixpk= 2, nxpk= 0, iat= 488, 470, r1= 2.72, r2= 3.22, r3= 5.88, r4= 6.38,  &end
#
# 16 DC  H5    16 DC  H1'   4.450   5.650
 &rst
  ixpk= 2, nxpk= 0, iat= 488, 483, r1= 3.95, r2= 4.45, r3= 5.65, r4= 6.15,  &end
#
# 16 DC  H3'   15 DA  H2'2  2.950   3.760  (#2.950   3.460 44)
 &rst
  ixpk= 3, nxpk= 0, iat= 497, 470, r1= 2.45, r2= 2.95, r3= 3.76, r4= 4.26,  &end
#
# 16 DC  H3'   16 DC  H1'   3.250   4.020
 &rst
  ixpk= 3, nxpk= 0, iat= 497, 483, r1= 2.75, r2= 3.25, r3= 4.02, r4= 4.52,  &end
#
# 16 DC  H3'   16 DC  H6    2.920   3.680  (#2.920   3.380 35)
 &rst
  ixpk= 3, nxpk= 0, iat= 497, 486, r1= 2.42, r2= 2.92, r3= 3.68, r4= 4.18,  &end
#
# 16 DC  H3'   16 DC  H5    4.600   6.630
 &rst
  ixpk= 3, nxpk= 0, iat= 497, 488, r1= 4.10, r2= 4.60, r3= 6.63, r4= 7.13,  &end
#
# 16 DC  H2'1  15 DA  H1'   3.750   5.620  (#3.750   5.320 40)
 &rst
  ixpk= 5, nxpk= 0, iat= 499, 451, r1= 3.25, r2= 3.75, r3= 5.62, r4= 6.12,  &end
#
# 16 DC  H2'1  15 DA  H8    6.570   7.000
 &rst
  ixpk= 5, nxpk= 0, iat= 499, 454, r1= 6.07, r2= 6.57, r3= 7.00, r4= 7.50,  &end
#
# 16 DC  H2'1  15 DA  H3'   4.260   6.170  (#4.260   5.870 27)
 &rst
  ixpk= 5, nxpk= 0, iat= 499, 467, r1= 3.76, r2= 4.26, r3= 6.17, r4= 6.67,  &end
#
# 16 DC  H2'1  15 DA  H2'2  2.740   4.550
 &rst
  ixpk= 5, nxpk= 0, iat= 499, 470, r1= 2.24, r2= 2.74, r3= 4.55, r4= 5.05,  &end
#
# 16 DC  H2'1  16 DC  H1'   2.450   3.240
 &rst
```

```
  ixpk= 5, nxpk= 0, iat= 499, 483, r1= 1.95, r2= 2.45, r3= 3.24, r4= 3.74,  &end
#
#  16 DC  H2'1  16 DC  H6    1.720   2.710  (#2.320   2.710 17 26)
 &rst
  ixpk= 2, nxpk= 0, iat= 499, 486, r1= 1.22, r2= 1.72, r3= 2.71, r4= 3.21,  &end
#
#  16 DC  H2'1  16 DC  H5    3.020   4.510  (#3.020   3.910 5 29)
 &rst
  ixpk= 3, nxpk= 0, iat= 499, 488, r1= 2.52, r2= 3.02, r3= 4.51, r4= 5.01,  &end
#
#  16 DC  H2'1  16 DC  H3'   2.020   2.660  (#2.320   2.660 15)
 &rst
  ixpk= 2, nxpk= 0, iat= 499, 497, r1= 1.52, r2= 2.02, r3= 2.66, r4= 3.16,  &end
#
#  16 DC  H2'2  15 DA  H2'2  2.990   5.280
 &rst
  ixpk= 2, nxpk= 0, iat= 500, 470, r1= 2.49, r2= 2.99, r3= 5.28, r4= 5.78,  &end
#
#  16 DC  H2'2  16 DC  H1'   1.960   2.710  (#2.260   2.710 18)
 &rst
  ixpk= 2, nxpk= 0, iat= 500, 483, r1= 1.46, r2= 1.96, r3= 2.71, r4= 3.21,  &end
#
#  16 DC  H2'2  16 DC  H6    2.670   3.630  (#2.670   3.330 6)
 &rst
  ixpk= 3, nxpk= 0, iat= 500, 486, r1= 2.17, r2= 2.67, r3= 3.63, r4= 4.13,  &end
#
#  16 DC  H2'2  16 DC  H5    3.680   5.960
 &rst
  ixpk= 3, nxpk= 0, iat= 500, 488, r1= 3.18, r2= 3.68, r3= 5.96, r4= 6.46,  &end
#
#  16 DC  H2'2  16 DC  H3'   2.600   3.250
 &rst
  ixpk= 3, nxpk= 0, iat= 500, 497, r1= 2.10, r2= 2.60, r3= 3.25, r4= 3.75,  &end
#
#  17 SDI H2'1  17 SDI H1'   2.260   3.370
 &rst
  ixpk= 3, nxpk= 0, iat= 515, 513, r1= 1.76, r2= 2.26, r3= 3.37, r4= 3.87,  &end
#
#  17 SDI H2'2  17 SDI H1'   2.230   3.660
 &rst
  ixpk= 3, nxpk= 0, iat= 516, 513, r1= 1.73, r2= 2.23, r3= 3.66, r4= 4.16,  &end
#
#  17 SDI HA1    5 DT  H1'   3.920   5.290  (#3.920   4.490 12 25 35)
 &rst
  ixpk= 4, nxpk= 0, iat= 526, 134, r1= 3.42, r2= 3.92, r3= 5.29, r4= 5.79,  &end
#
#  17 SDI HA1   16 DC  H5    4.570   5.360
 &rst
  ixpk= 4, nxpk= 0, iat= 526, 488, r1= 4.07, r2= 4.57, r3= 5.36, r4= 5.86,  &end
#
#  17 SDI HA2    5 DT  H1'   4.050   5.910  (#4.350   5.610 30 49)
```

```
 &rst
  ixpk= 5, nxpk= 0, iat= 527, 134, r1= 3.55, r2= 4.05, r3= 5.91, r4= 6.41,  &end
#
#  17 SDI HA2    6 DT  H1'   4.950   6.160  (#4.950   5.860 27)
 &rst
  ixpk= 5, nxpk= 0, iat= 527, 166, r1= 4.45, r2= 4.95, r3= 6.16, r4= 6.66,  &end
#
#  17 SDI HA2   16 DC  H5    4.650   6.490  (#4.650   5.290 2 16 19 38)
 &rst
  ixpk= 5, nxpk= 0, iat= 527, 488, r1= 4.15, r2= 4.65, r3= 6.49, r4= 6.99,  &end
#
#  17 SDI HB     5 DT  H1'   3.410   4.060  (#3.710   4.060 13)
 &rst
  ixpk= 4, nxpk= 0, iat= 529, 134, r1= 2.91, r2= 3.41, r3= 4.06, r4= 4.56,  &end
#
#  17 SDI HB     6 DT  Q5    3.340   4.610  (#3.340   4.310 18)
 &rst
  ixpk= 4, nxpk= 0, iat= 529,  -1, r1= 2.84, r2= 3.34, r3= 5.54, r4= 6.04,
 igr2= 172, 173, 174,
 &end
#
#  17 SDI HB    16 DC  H5    4.080   6.090  (#4.080   4.590 9 10 11 24 33)
 &rst
  ixpk= 4, nxpk= 0, iat= 529, 488, r1= 3.58, r2= 4.08, r3= 6.09, r4= 6.59,  &end
#
#  17 SDI HC     5 DT  H1'   3.810   4.510  (#4.110   4.510 36)
 &rst
  ixpk= 4, nxpk= 0, iat= 531, 134, r1= 3.31, r2= 3.81, r3= 4.51, r4= 5.01,  &end
#
#  17 SDI H8    16 DC  H1'   4.510   6.400
 &rst
  ixpk= 4, nxpk= 0, iat= 540, 483, r1= 4.01, r2= 4.51, r3= 6.40, r4= 6.90,  &end
#
#  17 SDI H8    16 DC  H6    4.890   6.740
 &rst
  ixpk= 4, nxpk= 0, iat= 540, 486, r1= 4.39, r2= 4.89, r3= 6.74, r4= 7.24,  &end
#
#  17 SDI H8    16 DC  H3'   3.970   5.810  (#4.270   5.810 22)
 &rst
  ixpk= 5, nxpk= 0, iat= 540, 497, r1= 3.47, r2= 3.97, r3= 5.81, r4= 6.31,  &end
#
#  17 SDI H8    16 DC  H2'1  2.930   3.570  (#2.930   3.270 28)
 &rst
  ixpk= 3, nxpk= 0, iat= 540, 499, r1= 2.43, r2= 2.93, r3= 3.57, r4= 4.07,  &end
#
#  17 SDI H8    16 DC  H2'2  2.660   3.620  (#2.960   3.320 21 31)
 &rst
  ixpk= 3, nxpk= 0, iat= 540, 500, r1= 2.16, r2= 2.66, r3= 3.62, r4= 4.12,  &end
#
#  17 SDI H8    17 SDI H1'   3.210   4.110  (#3.210   3.810 29)
 &rst
```

```
  ixpk= 3, nxpk= 0, iat= 540, 513, r1= 2.71, r2= 3.21, r3= 4.11, r4= 4.61,  &end
#
#  17 SDI H8    17 SDI H2'1  1.990   3.090  (#2.290   3.090 17)
 &rst
  ixpk= 3, nxpk= 0, iat= 540, 515, r1= 1.49, r2= 1.99, r3= 3.09, r4= 3.59,  &end
#
#  17 SDI H8    17 SDI H2'2  2.720   5.120
 &rst
  ixpk= 3, nxpk= 0, iat= 540, 516, r1= 2.22, r2= 2.72, r3= 5.12, r4= 5.62,  &end
#
#  18 DA  H8    17 SDI H1'   3.790   4.780  (#3.790   4.480 15)
 &rst
  ixpk= 4, nxpk= 0, iat= 558, 513, r1= 3.29, r2= 3.79, r3= 4.78, r4= 5.28,  &end
#
#  18 DA  H8    17 SDI H2'1  3.140   4.790
 &rst
  ixpk= 4, nxpk= 0, iat= 558, 515, r1= 2.64, r2= 3.14, r3= 4.79, r4= 5.29,  &end
#
#  18 DA  H8    17 SDI H2'2  3.000   3.970  (#3.000   3.970 44)
 &rst
  ixpk= 3, nxpk= 0, iat= 558, 516, r1= 2.50, r2= 3.00, r3= 3.97, r4= 4.47,  &end
#
#  18 DA  H8    17 SDI H8    4.810   6.770  (#4.810   6.170 1 6)
 &rst
  ixpk= 6, nxpk= 0, iat= 558, 540, r1= 4.31, r2= 4.81, r3= 6.77, r4= 7.27,  &end
#
#  18 DA  H8    18 DA  H1'   2.610   4.800
 &rst
  ixpk= 6, nxpk= 0, iat= 558, 555, r1= 2.11, r2= 2.61, r3= 4.80, r4= 5.30,  &end
#
#  18 DA  H3'   17 SDI H1'   4.100   5.930  (#4.100   5.030 20 39 40)
 &rst
  ixpk= 5, nxpk= 0, iat= 571, 513, r1= 3.60, r2= 4.10, r3= 5.93, r4= 6.43,  &end
#
#  18 DA  H3'   18 DA  H1'   3.040   5.520
 &rst
  ixpk= 5, nxpk= 0, iat= 571, 555, r1= 2.54, r2= 3.04, r3= 5.52, r4= 6.02,  &end
#
#  18 DA  H3'   18 DA  H8    4.090   6.400
 &rst
  ixpk= 5, nxpk= 0, iat= 571, 558, r1= 3.59, r2= 4.09, r3= 6.40, r4= 6.90,  &end
#
#  18 DA  H2'2  17 SDI H1'   4.510   6.110  (#4.510   5.810 32)
 &rst
  ixpk= 5, nxpk= 0, iat= 574, 513, r1= 4.01, r2= 4.51, r3= 6.11, r4= 6.61,  &end
#
#  18 DA  H2'2  18 DA  H1'   1.960   2.610
 &rst
  ixpk= 5, nxpk= 0, iat= 574, 555, r1= 1.46, r2= 1.96, r3= 2.61, r4= 3.11,  &end
#
#  18 DA  H2'2  18 DA  H8    1.800   3.850  (#1.800   2.650 3 18 21 23)
```

```
 &rst
  ixpk= 2, nxpk= 0, iat= 574, 558, r1= 1.30, r2= 1.80, r3= 3.85, r4= 4.35,  &end
#
#  18 DA  H2'2  18 DA  H3'   1.710   2.600  (#1.710   2.300 7 24 47 48 50)
 &rst
  ixpk= 2, nxpk= 0, iat= 574, 571, r1= 1.21, r2= 1.71, r3= 2.60, r4= 3.10,  &end
#
#  19 DG  H1'   18 DA  H2'2  3.740   6.070  (#3.740   5.170 12 30 33)
 &rst
  ixpk= 5, nxpk= 0, iat= 587, 574, r1= 3.24, r2= 3.74, r3= 6.07, r4= 6.57,  &end
#
#  19 DG  H8    18 DA  H1'   3.220   4.080
 &rst
  ixpk= 5, nxpk= 0, iat= 590, 555, r1= 2.72, r2= 3.22, r3= 4.08, r4= 4.58,  &end
#
#  19 DG  H8    18 DA  H8    4.350   6.640
 &rst
  ixpk= 5, nxpk= 0, iat= 590, 558, r1= 3.85, r2= 4.35, r3= 6.64, r4= 7.14,  &end
#
#  19 DG  H8    18 DA  H2'2  2.380   3.260  (#2.380   3.260 42)
 &rst
  ixpk= 3, nxpk= 0, iat= 590, 574, r1= 1.88, r2= 2.38, r3= 3.26, r4= 3.76,  &end
#
#  19 DG  H8    19 DG  H1'   3.160   5.020
 &rst
  ixpk= 3, nxpk= 0, iat= 590, 587, r1= 2.66, r2= 3.16, r3= 5.02, r4= 5.52,  &end
#
#  19 DG  H3'   19 DG  H1'   2.860   4.310  (#2.860   3.710 27 44)
 &rst
  ixpk= 3, nxpk= 0, iat= 604, 587, r1= 2.36, r2= 2.86, r3= 4.31, r4= 4.81,  &end
#
#  19 DG  H2'1  18 DA  H1'   3.960   5.750  (#3.960   5.450 36)
 &rst
  ixpk= 5, nxpk= 0, iat= 606, 555, r1= 3.46, r2= 3.96, r3= 5.75, r4= 6.25,  &end
#
#  19 DG  H2'1  19 DG  H1'   2.410   4.250
 &rst
  ixpk= 5, nxpk= 0, iat= 606, 587, r1= 1.91, r2= 2.41, r3= 4.25, r4= 4.75,  &end
#
#  19 DG  H2'1  19 DG  H8    1.920   3.340  (#2.220   3.340 29)
 &rst
  ixpk= 3, nxpk= 0, iat= 606, 590, r1= 1.42, r2= 1.92, r3= 3.34, r4= 3.84,  &end
#
#  19 DG  H2'1  19 DG  H3'   2.070   3.190
 &rst
  ixpk= 3, nxpk= 0, iat= 606, 604, r1= 1.57, r2= 2.07, r3= 3.19, r4= 3.69,  &end
#
#  19 DG  H2'2  18 DA  H1'   3.670   6.950  (#3.670   5.150 9 10 11 19 34 35)
 &rst
  ixpk= 5, nxpk= 0, iat= 607, 555, r1= 3.17, r2= 3.67, r3= 6.95, r4= 7.45,  &end
#
```

```
# 19 DG  H2'2  19 DG  H1'   2.000   3.240
 &rst
  ixpk= 5, nxpk= 0, iat= 607, 587, r1= 1.50, r2= 2.00, r3= 3.24, r4= 3.74,  &end
#
# 19 DG  H2'2  19 DG  H8    2.420   4.120  (#2.420   3.820 40)
 &rst
  ixpk= 3, nxpk= 0, iat= 607, 590, r1= 1.92, r2= 2.42, r3= 4.12, r4= 4.62,  &end
#
# 19 DG  H2'2  19 DG  H3'   2.340   3.940
 &rst
  ixpk= 3, nxpk= 0, iat= 607, 604, r1= 1.84, r2= 2.34, r3= 3.94, r4= 4.44,  &end
#
# 20 DA  H1'   19 DG  H1'   4.790   5.830
 &rst
  ixpk= 3, nxpk= 0, iat= 620, 587, r1= 4.29, r2= 4.79, r3= 5.83, r4= 6.33,  &end
#
# 20 DA  H8    19 DG  H1'   2.710   3.790  (#3.010   3.790 7)
 &rst
  ixpk= 3, nxpk= 0, iat= 623, 587, r1= 2.21, r2= 2.71, r3= 3.79, r4= 4.29,  &end
#
# 20 DA  H8    19 DG  H8    3.590   5.750  (#3.890   5.750 4)
 &rst
  ixpk= 5, nxpk= 0, iat= 623, 590, r1= 3.09, r2= 3.59, r3= 5.75, r4= 6.25,  &end
#
# 20 DA  H8    19 DG  H3'   3.200   5.350  (#3.200   3.850 14 22 23 25 28)
 &rst
  ixpk= 3, nxpk= 0, iat= 623, 604, r1= 2.70, r2= 3.20, r3= 5.35, r4= 5.85,  &end
#
# 20 DA  H8    19 DG  H2'1  2.480   4.530  (#2.780   4.230 38 41)
 &rst
  ixpk= 4, nxpk= 0, iat= 623, 606, r1= 1.98, r2= 2.48, r3= 4.53, r4= 5.03,  &end
#
# 20 DA  H8    20 DA  H1'   2.710   4.560
 &rst
  ixpk= 4, nxpk= 0, iat= 623, 620, r1= 2.21, r2= 2.71, r3= 4.56, r4= 5.06,  &end
#
# 20 DA  H3'   19 DG  H1'   4.040   6.420  (#4.040   5.820 16 26)
 &rst
  ixpk= 5, nxpk= 0, iat= 636, 587, r1= 3.54, r2= 4.04, r3= 6.42, r4= 6.92,  &end
#
# 20 DA  H3'   20 DA  H1'   2.890   4.130
 &rst
  ixpk= 5, nxpk= 0, iat= 636, 620, r1= 2.39, r2= 2.89, r3= 4.13, r4= 4.63,  &end
#
# 20 DA  H3'   20 DA  H8    3.290   5.690
 &rst
  ixpk= 5, nxpk= 0, iat= 636, 623, r1= 2.79, r2= 3.29, r3= 5.69, r4= 6.19,  &end
#
# 20 DA  H2'1  20 DA  H1'   2.510   3.860
 &rst
  ixpk= 5, nxpk= 0, iat= 638, 620, r1= 2.01, r2= 2.51, r3= 3.86, r4= 4.36,  &end
```

```
#
#  20 DA  H2'1  20 DA  H8    1.840   2.560
 &rst
  ixpk= 5, nxpk= 0, iat= 638, 623, r1= 1.34, r2= 1.84, r3= 2.56, r4= 3.06,  &end
#
#  20 DA  H2'1  20 DA  H3'   1.850   2.720  (#1.850   2.420 20)
 &rst
  ixpk= 2, nxpk= 0, iat= 638, 636, r1= 1.35, r2= 1.85, r3= 2.72, r4= 3.22,  &end
#
#  20 DA  H2'2  19 DG  H1'   3.500   6.520  (#3.500   5.320 2 13 17 31)
 &rst
  ixpk= 5, nxpk= 0, iat= 639, 587, r1= 3.00, r2= 3.50, r3= 6.52, r4= 7.02,  &end
#
#  20 DA  H2'2  20 DA  H1'   1.970   2.840  (#1.970   2.540 27)
 &rst
  ixpk= 2, nxpk= 0, iat= 639, 620, r1= 1.47, r2= 1.97, r3= 2.84, r4= 3.34,  &end
#
#  20 DA  H2'2  20 DA  H8    2.530   3.980
 &rst
  ixpk= 2, nxpk= 0, iat= 639, 623, r1= 2.03, r2= 2.53, r3= 3.98, r4= 4.48,  &end
#
#  20 DA         H2'2  20 DA  H3'   2.230   4.170
 &rst
  ixpk= 2, nxpk= 0, iat= 639, 636, r1= 1.73, r2= 2.23, r3= 4.17, r4= 4.67,  &end
#
#  21 DA         H8    20 DA  H2'1  2.920   4.800
 &rst
  ixpk= 2, nxpk= 0, iat= 655, 638, r1= 2.42, r2= 2.92, r3= 4.80, r4= 5.30,  &end
#
#  21 DA         H8    21 DA  H1'   2.380   4.250  (#2.380   3.050 3 5 19 20)
 &rst
  ixpk= 3, nxpk= 0, iat= 655, 652, r1= 1.88, r2= 2.38, r3= 4.25, r4= 4.75,  &end
#
#  21 DA         H3'   21 DA  H1'   2.810   4.190  (#2.810   3.890 21)
 &rst
  ixpk= 3, nxpk= 0, iat= 668, 652, r1= 2.31, r2= 2.81, r3= 4.19, r4= 4.69,  &end
#
#  21 DA         H3'   21 DA  H8    2.750   4.800  (#2.750   4.200 27 33)
 &rst
  ixpk= 4, nxpk= 0, iat= 668, 655, r1= 2.25, r2= 2.75, r3= 4.80, r4= 5.30,  &end
#
#  21 DA         H2'1  21 DA  H1'   2.230   3.610
 &rst
  ixpk= 4, nxpk= 0, iat= 670, 652, r1= 1.73, r2= 2.23, r3= 3.61, r4= 4.11,  &end
#
#  21 DA         H2'1  21 DA  H8    1.970   3.040  (#1.970   2.740 43)
 &rst
  ixpk= 2, nxpk= 0, iat= 670, 655, r1= 1.47, r2= 1.97, r3= 3.04, r4= 3.54,  &end
#
#  21 DA         H2'1  21 DA  H3'   2.000   2.670
 &rst
```

```
  ixpk= 2, nxpk= 0, iat= 670, 668, r1= 1.50, r2= 2.00, r3= 2.67, r4= 3.17,  &end
#
#  21 DA         H2'2  21 DA  H1'   2.000   2.550
 &rst
  ixpk= 2, nxpk= 0, iat= 671, 652, r1= 1.50, r2= 2.00, r3= 2.55, r4= 3.05,  &end
#
#  22 DG3       H8    21 DA  H1'   2.270   4.790  (#2.270   2.990 7 8 10 17 35 39)
 &rst
  ixpk= 2, nxpk= 0, iat= 687, 652, r1= 1.77, r2= 2.27, r3= 4.79, r4= 5.29,  &end
#
#  22 DG3       H8    21 DA  H8    3.880   6.420
 &rst
  ixpk= 2, nxpk= 0, iat= 687, 655, r1= 3.38, r2= 3.88, r3= 6.42, r4= 6.92,  &end
#
#  22 DG3       H8    21 DA  H3'   3.710   5.880
 &rst
  ixpk= 2, nxpk= 0, iat= 687, 668, r1= 3.21, r2= 3.71, r3= 5.88, r4= 6.38,  &end
#
#  22 DG3       H8    21 DA  H2'1  1.970   3.740  (#1.970   2.840 6 18 25)
 &rst
  ixpk= 2, nxpk= 0, iat= 687, 670, r1= 1.47, r2= 1.97, r3= 3.74, r4= 4.24,  &end
#
#  22 DG3       H8    21 DA  H2'2  2.400   4.370
 &rst
  ixpk= 2, nxpk= 0, iat= 687, 671, r1= 1.90, r2= 2.40, r3= 4.37, r4= 4.87,  &end
#
#  22 DG3       H3'   21 DA  H1'   4.110   6.390  (#4.110   4.590 2 13 24 28 32 34)
 &rst
  ixpk= 4, nxpk= 0, iat= 701, 652, r1= 3.61, r2= 4.11, r3= 6.39, r4= 6.89,  &end
#
#  22 DG3       H3'   21 DA  H2'1  3.180   6.840  (#3.180   5.940 12 29 41)
 &rst
  ixpk= 5, nxpk= 0, iat= 701, 670, r1= 2.68, r2= 3.18, r3= 6.84, r4= 7.34,  &end
#
#  22 DG3       H3'   21 DA  H2'2  3.210   5.380  (#3.210   4.480 14 31 42)
 &rst
  ixpk= 4, nxpk= 0, iat= 701, 671, r1= 2.71, r2= 3.21, r3= 5.38, r4= 5.88,  &end
#
#  22 DG3       H3'   22 DG3 H1'   2.020   4.190  (#3.220   4.190 3 4 19 38)
 &rst
  ixpk= 4, nxpk= 0, iat= 701, 684, r1= 1.52, r2= 2.02, r3= 4.19, r4= 4.69,  &end
#
#  22 DG3       H2'1  22 DG3 H8    1.970   4.290  (#2.570   4.290 15 20)
 &rst
  ixpk= 4, nxpk= 0, iat= 703, 687, r1= 1.47, r2= 1.97, r3= 4.29, r4= 4.79,  &end
#
#  22 DG3       H2'1  22 DG3 H3'   2.710   4.430
 &rst
  ixpk= 4, nxpk= 0, iat= 703, 701, r1= 2.21, r2= 2.71, r3= 4.43, r4= 4.93,  &end
#
#  22 DG3       H2'2  21 DA  H1'   2.960   6.010  (#2.960   5.710 37)
```

```
 &rst
  ixpk= 5, nxpk= 0, iat= 704, 652, r1= 2.46, r2= 2.96, r3= 6.01, r4= 6.51,  &end
#
#  22 DG3       H2'2  21 DA  H3'   3.290   6.710  (#3.290   5.510 9 11 16 26)
 &rst
  ixpk= 5, nxpk= 0, iat= 704, 668, r1= 2.79, r2= 3.29, r3= 6.71, r4= 7.21,  &end
#
#  22 DG3       H2'2  21 DA  H2'2  2.570   4.860
 &rst
  ixpk= 5, nxpk= 0, iat= 704, 671, r1= 2.07, r2= 2.57, r3= 4.86, r4= 5.36,  &end
#
#  22 DG3       H2'2  22 DG3 H1'   2.350   2.940
 &rst
  ixpk= 5, nxpk= 0, iat= 704, 684, r1= 1.85, r2= 2.35, r3= 2.94, r4= 3.44,  &end
#
#  22 DG3       H2'2  22 DG3 H8    1.830   3.720  (#1.830   2.520 21 22 36 40)
 &rst
  ixpk= 2, nxpk= 0, iat= 704, 687, r1= 1.33, r2= 1.83, r3= 3.72, r4= 4.22,  &end
#
#  22 DG3       H2'2  22 DG3 H3'   1.960   2.700  (#2.260   2.700 33)
 &rst
  ixpk= 2, nxpk= 0, iat= 704, 701, r1= 1.46, r2= 1.96, r3= 2.70, r4= 3.20,  &end
#
#  17 SDI       HA1   17 SDI H2    2.420   4.190  (#AH2)
 &rst
  ixpk= 2, nxpk= 0, iat= 526, 524, r1= 1.92, r2= 2.42, r3= 4.19, r4= 4.69,  &end
#
#  17 SDI       HA2   17 SDI H2    2.150   2.530  (#AH2)
 &rst
  ixpk= 2, nxpk= 0, iat= 527, 524, r1= 1.65, r2= 2.15, r3= 2.53, r4= 3.03,  &end
#
#  17 SDI       HB    17 SDI H2    2.830   3.810  (#AH2 2.830   3.210 8 26)
 &rst
  ixpk= 2, nxpk= 0, iat= 529, 524, r1= 2.33, r2= 2.83, r3= 3.81, r4= 4.31,  &end
#
#  18 DA        H2    17 SDI HA1   3.650   6.780  (#AH2)
 &rst
  ixpk= 2, nxpk= 0, iat= 567, 526, r1= 3.15, r2= 3.65, r3= 6.78, r4= 7.28,  &end
#
#  18 DA        H2    17 SDI HA2   2.950   4.690  (#AH2 2.950   3.490 4 14 37 43)
 &rst
  ixpk= 2, nxpk= 0, iat= 567, 527, r1= 2.45, r2= 2.95, r3= 4.69, r4= 5.19,  &end
#
#  18 DA        H2    17 SDI HB    2.700   3.560  (#AH2 2.700   3.260 5)
 &rst
  ixpk= 2, nxpk= 0, iat= 567, 529, r1= 2.20, r2= 2.70, r3= 3.56, r4= 4.06,  &end
#
#   1  DC5  H42    22  DG3  O6      1.80   2.00
 &rst
  ixpk= 0, nxpk= 0, iat=  19, 691, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,
      rk2=32.0, rk3=32.0, ir6=1, ialtd=0,
```

```
 &end
#
#   1  DC5  N3     22  DG3  H1      1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  20, 693, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   1  DC5  N3     22  DG3  N1      2.85   3.05
 &rst
  ixpk= 0, nxpk= 0, iat=  20, 692, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#   1  DC5  N4     22  DG3  O6      2.81   3.01
 &rst
  ixpk= 0, nxpk= 0, iat=  17, 691, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#   1  DC5  O2     22  DG3  H22     1.75   1.95
 &rst
  ixpk= 0, nxpk= 0, iat=  22, 697, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#   2  DT   H3     21  DA   N1      1.71   1.91
 &rst
  ixpk= 0, nxpk= 0, iat=  52, 662, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
#   2  DT   N3     21  DA   N1      2.72   2.92
 &rst
  ixpk= 0, nxpk= 0, iat=  51, 662, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
#   2  DT   O4     21  DA   H61     1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  50, 660, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   3  DT   H3     20  DA   N1      1.71   1.91
 &rst
  ixpk= 0, nxpk= 0, iat=  84, 630, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
#   3  DT   N3     20  DA   N1      2.72   2.92
 &rst
  ixpk= 0, nxpk= 0, iat=  83, 630, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
#   3  DT   O4     20  DA   H61     1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  82, 628, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   4  DC   H42    19  DG   O6      1.80   2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 113, 594, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
#   4  DC   N3     19  DG   H1      1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 114, 596, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   4  DC   N3     19  DG   N1      2.85   3.05
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 114, 595, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#   4  DC   N4     19  DG   O6      2.81   3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 111, 594, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#   4  DC   O2     19  DG   H22     1.75   1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 116, 600, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#   5  DT   H3     18  DA   N1      1.61   2.01  (#1.71   1.91 )
 &rst
  ixpk= 1, nxpk= 0, iat= 146, 565, r1= 1.11, r2= 1.61, r3= 2.01, r4= 2.51,  &end
#
#   5  DT   N3     18  DA   N1      2.62   3.02  (#2.72   2.92 )
 &rst
  ixpk= 2, nxpk= 0, iat= 145, 565, r1= 2.12, r2= 2.62, r3= 3.02, r4= 3.52,  &end
#
#   5  DT   O4     18  DA   H61     1.74   2.14  (#1.84   2.04)
 &rst
  ixpk= 2, nxpk= 0, iat= 144, 563, r1= 1.24, r2= 1.74, r3= 2.14, r4= 2.64,  &end
#
#   7  DG   H1     16  DC   N3      1.84   2.04
 &rst
  ixpk= 2, nxpk= 0, iat= 207, 493, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   7  DG   H22    16  DC   O2      1.75   1.95
 &rst
  ixpk= 2, nxpk= 0, iat= 211, 495, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#   7  DG   N1     16  DC   N3      2.85   3.05
 &rst
  ixpk= 2, nxpk= 0, iat= 206, 493, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#   7  DG   O6     16  DC   H42     1.80   2.00
 &rst
  ixpk= 2, nxpk= 0, iat= 205, 492, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
#   7  DG   O6     16  DC   N4      2.81   3.01
 &rst
  ixpk= 2, nxpk= 0, iat= 205, 490, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#   8  DT   H3     15  DA   N1      1.71   1.91
 &rst
  ixpk= 2, nxpk= 0, iat= 243, 461, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
#   8  DT   N3     15  DA   N1      2.72   2.92
 &rst
  ixpk= 2, nxpk= 0, iat= 242, 461, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
```

```
#   8  DT   O4    15  DA   H61    1.84   2.04
 &rst
  ixpk= 2, nxpk= 0, iat= 241, 459, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   9  DC   H42    14  DG   O6     1.80   2.00
 &rst
  ixpk= 2, nxpk= 0, iat= 272, 425, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
#   9  DC   N3    14  DG   H1     1.84   2.04
 &rst
  ixpk= 2, nxpk= 0, iat= 273, 427, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   9  DC   N3    14  DG   N1     2.85   3.05
 &rst
  ixpk= 2, nxpk= 0, iat= 273, 426, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#   9  DC   N4    14  DG   O6     2.81   3.01
 &rst
  ixpk= 2, nxpk= 0, iat= 270, 425, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#   9  DC   O2    14  DG   H22    1.75   1.95
 &rst
  ixpk= 2, nxpk= 0, iat= 275, 431, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#  10  DC   H42    13  DG   O6     1.80   2.00
 &rst
  ixpk= 2, nxpk= 0, iat= 302, 392, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
#  10  DC   N3    13  DG   H1     1.84   2.04
 &rst
  ixpk= 2, nxpk= 0, iat= 303, 394, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#  10  DC   N3    13  DG   N1     2.85   3.05
 &rst
  ixpk= 2, nxpk= 0, iat= 303, 393, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#  10  DC   N4    13  DG   O6     2.81   3.01
 &rst
  ixpk= 2, nxpk= 0, iat= 300, 392, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#  10  DC   O2    13  DG   H22    1.75   1.95
 &rst
  ixpk= 2, nxpk= 0, iat= 305, 398, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#  11  DG3  H1    12  DC5  N3     1.84   2.04
 &rst
  ixpk= 2, nxpk= 0, iat= 332, 365, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#  11  DG3  H22    12  DC5  O2     1.75   1.95
 &rst
  ixpk= 2, nxpk= 0, iat= 336, 367, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
```

```
#
# 11  DG3  N1     12  DC5  N3      2.85   3.05
 &rst
  ixpk= 2, nxpk= 0, iat= 331, 365, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
# 11  DG3  O6     12  DC5  H42     1.80   2.00
 &rst
  ixpk= 2, nxpk= 0, iat= 330, 364, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
# 11  DG3  O6     12  DC5  N4      2.81   3.01
 &rst
  ixpk= 2, nxpk= 0, iat= 330, 362, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
# 706 atoms read from pdb file SdI_Major_New_v4.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 = 100.0, rk3 = 100.0,                                &end

# 3 DT ALPHA:  (2 DT O3')-(3 DT P)-(3 DT O5')-(3 DT 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 DC ALPHA:  (3 DT O3')-(4 DC P)-(4 DC O5')-(4 DC C5') -90.0 -30.0
 &rst    iat =    92,    93,    96,    97,
            r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 5 DT ALPHA:  (4 DC O3')-(5 DT P)-(5 DT O5')-(5 DT C5') -90.0 -30.0
 &rst    iat =   122,   123,   126,   127,
            r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 6 DT ALPHA:  (5 DT O3')-(6 DT P)-(6 DT O5')-(6 DT C5') -90.0 -30.0
 &rst    iat =   154,   155,   158,   159,
            r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 7 DG ALPHA:  (6 DT O3')-(7 DG P)-(7 DG O5')-(7 DG C5') -90.0 -30.0
 &rst    iat =   186,   187,   190,   191,
            r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 8 DT ALPHA:  (7 DG O3')-(8 DT P)-(8 DT O5')-(8 DT C5') -90.0 -30.0
 &rst    iat =   219,   220,   223,   224,
            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 =   251,   252,   255,   256,
            r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
```

```
          &end

# 10 DC ALPHA:  (9 DC O3')-(10 DC P)-(10 DC O5')-(10 DC C5') -90.0 -30.0
 &rst     iat =   281,   282,   285,   286,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 13 DG ALPHA:  (12 DC5 O3')-(13 DG P)-(13 DG O5')-(13 DG C5') -90.0 -30.0
 &rst     iat =   373,   374,   377,   378,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 14 DG ALPHA:  (13 DG O3')-(14 DG P)-(14 DG O5')-(14 DG C5') -90.0 -30.0
 &rst     iat =   406,   407,   410,   411,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 15 DA ALPHA:  (14 DG O3')-(15 DA P)-(15 DA O5')-(15 DA C5') -90.0 -30.0
 &rst     iat =   439,   440,   443,   444,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 16 DC ALPHA:  (15 DA O3')-(16 DC P)-(16 DC O5')-(16 DC C5') -90.0 -30.0
 &rst     iat =   471,   472,   475,   476,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 17 SDI ALPHA:  (16 DC O3')-(17 SDI P)-(17 SDI O5')-(17 SDI C5') -120.0   0.0
 &rst     iat =   501,   502,   505,   506,
           r1 = -121.0, r2 = -120.0, r3 =   0.0, r4 =   1.0,
          &end

# 18 DA ALPHA:  (17 SDI O3')-(18 DA P)-(18 DA O5')-(18 DA C5') -90.0 -30.0
 &rst     iat =   543,   544,   547,   548,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 19 DG ALPHA:  (18 DA O3')-(19 DG P)-(19 DG O5')-(19 DG C5') -90.0 -30.0
 &rst     iat =   575,   576,   579,   580,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
          &end

# 20 DA ALPHA:  (19 DG O3')-(20 DA P)-(20 DA O5')-(20 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

# 21 DA ALPHA:  (20 DA O3')-(21 DA P)-(21 DA O5')-(21 DA C5') -90.0 -30.0
 &rst     iat =   640,   641,   644,   645,
           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 DT BETA:  (3 DT P)-(3 DT O5')-(3 DT C5')-(3 DT 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 DC BETA:  (4 DC P)-(4 DC O5')-(4 DC C5')-(4 DC C4') 150.0 210.0
 &rst     iat =    93,    96,    97,   100,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 5 DT BETA:  (5 DT P)-(5 DT O5')-(5 DT C5')-(5 DT C4') 150.0 210.0
 &rst     iat =   123,   126,   127,   130,
           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 =   155,   158,   159,   162,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 7 DG BETA:  (7 DG P)-(7 DG O5')-(7 DG C5')-(7 DG C4') 150.0 210.0
 &rst     iat =   187,   190,   191,   194,
           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 =   220,   223,   224,   227,
           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 =   252,   255,   256,   259,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 10 DC BETA:  (10 DC P)-(10 DC O5')-(10 DC C5')-(10 DC C4') 150.0 210.0
 &rst     iat =   282,   285,   286,   289,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 13 DG BETA:  (13 DG P)-(13 DG O5')-(13 DG C5')-(13 DG C4') 150.0 210.0
 &rst     iat =   374,   377,   378,   381,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end
```

```
# 14 DG BETA:  (14 DG P)-(14 DG O5')-(14 DG C5')-(14 DG C4') 150.0 210.0
 &rst     iat =   407,   410,   411,   414,
           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 =   440,   443,   444,   447,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 16 DC BETA:  (16 DC P)-(16 DC O5')-(16 DC C5')-(16 DC C4') 150.0 210.0
 &rst     iat =   472,   475,   476,   479,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 17 SDI BETA:  (17 SDI P)-(17 SDI O5')-(17 SDI C5')-(17 SDI C4') 120.0 240.0
 &rst     iat =   502,   505,   506,   509,
           r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,
          &end

# 18 DA BETA:  (18 DA P)-(18 DA O5')-(18 DA C5')-(18 DA C4') 150.0 210.0
 &rst     iat =   544,   547,   548,   551,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 19 DG BETA:  (19 DG P)-(19 DG O5')-(19 DG C5')-(19 DG C4') 150.0 210.0
 &rst     iat =   576,   579,   580,   583,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 20 DA BETA:  (20 DA P)-(20 DA O5')-(20 DA C5')-(20 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

# 21 DA BETA:  (21 DA P)-(21 DA O5')-(21 DA C5')-(21 DA C4') 150.0 210.0
 &rst     iat =   641,   644,   645,   648,
           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 DT GAMMA:  (3 DT O5')-(3 DT C5')-(3 DT C4')-(3 DT 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 DC GAMMA:  (4 DC O5')-(4 DC C5')-(4 DC C4')-(4 DC C3')  30.0  90.0
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```
 &rst     iat =    96,    97,   100,   117,
            r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 5 DT GAMMA:  (5 DT O5')-(5 DT C5')-(5 DT C4')-(5 DT C3')  30.0  90.0
 &rst     iat =   126,   127,   130,   149,
            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 =   158,   159,   162,   181,
            r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 7 DG GAMMA:  (7 DG O5')-(7 DG C5')-(7 DG C4')-(7 DG C3')  30.0  90.0
 &rst     iat =   190,   191,   194,   214,
            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 =   223,   224,   227,   246,
            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 =   255,   256,   259,   276,
            r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 10 DC GAMMA:  (10 DC O5')-(10 DC C5')-(10 DC C4')-(10 DC C3')  30.0  90.0
 &rst     iat =   285,   286,   289,   306,
            r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 13 DG GAMMA:  (13 DG O5')-(13 DG C5')-(13 DG C4')-(13 DG C3')  30.0  90.0
 &rst     iat =   377,   378,   381,   401,
            r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 14 DG GAMMA:  (14 DG O5')-(14 DG C5')-(14 DG C4')-(14 DG C3')  30.0  90.0
 &rst     iat =   410,   411,   414,   434,
            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 =   443,   444,   447,   466,
            r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 16 DC GAMMA:  (16 DC O5')-(16 DC C5')-(16 DC C4')-(16 DC C3')  30.0  90.0
 &rst     iat =   475,   476,   479,   496,
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```
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 17 SDI GAMMA:  (17 SDI O5')-(17 SDI C5')-(17 SDI C4')-(17 SDI C3')   0.0 120.0
 &rst     iat =   505,   506,   509,   541,
           r1 =  -1.0, r2 =   0.0, r3 = 120.0, r4 = 121.0,
          &end

# 18 DA GAMMA:  (18 DA O5')-(18 DA C5')-(18 DA C4')-(18 DA C3')  30.0  90.0
 &rst     iat =   547,   548,   551,   570,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 19 DG GAMMA:  (19 DG O5')-(19 DG C5')-(19 DG C4')-(19 DG C3')  30.0  90.0
 &rst     iat =   579,   580,   583,   603,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 20 DA GAMMA:  (20 DA O5')-(20 DA C5')-(20 DA C4')-(20 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

# 21 DA GAMMA:  (21 DA O5')-(21 DA C5')-(21 DA C4')-(21 DA C3')  30.0  90.0
 &rst     iat =   644,   645,   648,   667,
           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 DT 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 DT EPSILN:  (3 DT C4')-(3 DT C3')-(3 DT O3')-(4 DC 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 DC EPSILN:  (4 DC C4')-(4 DC C3')-(4 DC O3')-(5 DT P) 165.0 225.0
 &rst     iat =   100,   117,   122,   123,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 5 DT EPSILN:  (5 DT C4')-(5 DT C3')-(5 DT O3')-(6 DT P) 165.0 225.0
 &rst     iat =   130,   149,   154,   155,
           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 DG P) 165.0 225.0
 &rst     iat =   162,   181,   186,   187,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
```

```
          &end

# 7 DG EPSILN:  (7 DG C4')-(7 DG C3')-(7 DG O3')-(8 DT P) 165.0 225.0
 &rst     iat =   194,   214,   219,   220,
           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 =   227,   246,   251,   252,
           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 DC P) 165.0 225.0
 &rst     iat =   259,   276,   281,   282,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 10 DC EPSILN:  (10 DC C4')-(10 DC C3')-(10 DC O3')-(11 DG3 P) 165.0 225.0
 &rst     iat =   289,   306,   311,   312,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 13 DG EPSILN:  (13 DG C4')-(13 DG C3')-(13 DG O3')-(14 DG P) 165.0 225.0
 &rst     iat =   381,   401,   406,   407,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 14 DG EPSILN:  (14 DG C4')-(14 DG C3')-(14 DG O3')-(15 DA P) 165.0 225.0
 &rst     iat =   414,   434,   439,   440,
           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 =   447,   466,   471,   472,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 16 DC EPSILN:  (16 DC C4')-(16 DC C3')-(16 DC O3')-(17 SDI P) 165.0 225.0
 &rst     iat =   479,   496,   501,   502,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 17 SDI EPSILN:  (17 SDI C4')-(17 SDI C3')-(17 SDI O3')-(18 DA P) 135.0 255.0
 &rst     iat =   509,   541,   543,   544,
           r1 = 134.0, r2 = 135.0, r3 = 255.0, r4 = 256.0,
          &end

# 18 DA EPSILN:  (18 DA C4')-(18 DA C3')-(18 DA O3')-(19 DG P) 165.0 225.0
 &rst     iat =   551,   570,   575,   576,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end
```

19 DG EPSILN: (19 DG C4')-(19 DG C3')-(19 DG O3')-(20 DA P) 165.0 225.0
&rst   iat =   583,   603,   608,   609,
   r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
  &end

20 DA EPSILN: (20 DA C4')-(20 DA C3')-(20 DA O3')-(21 DA P) 165.0 225.0
&rst   iat =   616,   635,   640,   641,
   r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
  &end

21 DA EPSILN: (21 DA C4')-(21 DA C3')-(21 DA O3')-(22 DG3 P) 165.0 225.0
&rst   iat =   648,   667,   672,   673,
   r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
  &end

2 DT ZETA: (2 DT C3')-(2 DT O3')-(3 DT P)-(3 DT 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 DT ZETA: (3 DT C3')-(3 DT O3')-(4 DC P)-(4 DC 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 DC ZETA: (4 DC C3')-(4 DC O3')-(5 DT P)-(5 DT O5') -135.0 -75.0
&rst   iat =   117,   122,   123,   126,
   r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
  &end

5 DT ZETA: (5 DT C3')-(5 DT O3')-(6 DT P)-(6 DT O5') -135.0 -75.0
&rst   iat =   149,   154,   155,   158,
   r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
  &end

6 DT ZETA: (6 DT C3')-(6 DT O3')-(7 DG P)-(7 DG O5') -135.0 -75.0
&rst   iat =   181,   186,   187,   190,
   r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
  &end

7 DG ZETA: (7 DG C3')-(7 DG O3')-(8 DT P)-(8 DT O5') -135.0 -75.0
&rst   iat =   214,   219,   220,   223,
   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 =   246,   251,   252,   255,
   r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
  &end

```
# 9 DC ZETA:  (9 DC C3')-(9 DC O3')-(10 DC P)-(10 DC O5') -135.0 -75.0
 &rst    iat =   276,   281,   282,   285,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 10 DC ZETA:  (10 DC C3')-(10 DC O3')-(11 DG3 P)-(11 DG3 O5') -135.0 -75.0
 &rst    iat =   306,   311,   312,   315,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 13 DG ZETA:  (13 DG C3')-(13 DG O3')-(14 DG P)-(14 DG O5') -135.0 -75.0
 &rst    iat =   401,   406,   407,   410,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 14 DG ZETA:  (14 DG C3')-(14 DG O3')-(15 DA P)-(15 DA O5') -135.0 -75.0
 &rst    iat =   434,   439,   440,   443,
           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 =   466,   471,   472,   475,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 16 DC ZETA:  (16 DC C3')-(16 DC O3')-(17 SDI P)-(17 SDI O5') -135.0 -75.0
 &rst    iat =   496,   501,   502,   505,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 17 SDI ZETA:  (17 SDI C3')-(17 SDI O3')-(18 DA P)-(18 DA O5') -165.0 -45.0
 &rst    iat =   541,   543,   544,   547,
           r1 = -166.0, r2 = -165.0, r3 = -45.0, r4 = -44.0,
         &end

# 18 DA ZETA:  (18 DA C3')-(18 DA O3')-(19 DG P)-(19 DG O5') -135.0 -75.0
 &rst    iat =   570,   575,   576,   579,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 19 DG ZETA:  (19 DG C3')-(19 DG O3')-(20 DA P)-(20 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

# 20 DA ZETA:  (20 DA C3')-(20 DA O3')-(21 DA P)-(21 DA O5') -135.0 -75.0
 &rst    iat =   635,   640,   641,   644,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
         &end

# 21 DA ZETA:  (21 DA C3')-(21 DA O3')-(22 DG3 P)-(22 DG3 O5') -135.0 -75.0
```

```
 &rst    iat =   667,   672,   673,   676,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
          &end

# 706 atoms read from pdb file SdI_Major_New_v4.pdb.
# 2 DT NU0:  (2 DT C4')-(2 DT O4')-(2 DT C1')-(2 DT C2') -44.7 -14.7
 &rst    iat =    36,    38,    39,    57,
           r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
           rk2 =  32.0, rk3 =  32.0,                              &end

# 2 DT NU1:  (2 DT O4')-(2 DT C1')-(2 DT C2')-(2 DT C3')  18.1  48.1
 &rst    iat =    38,    39,    57,    55,
           r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
          &end

# 2 DT NU2:  (2 DT C1')-(2 DT C2')-(2 DT C3')-(2 DT C4') -37.2  -6.7
 &rst    iat =    39,    57,    55,    36,
           r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
          &end

# 2 DT NU3:  (2 DT C2')-(2 DT C3')-(2 DT C4')-(2 DT O4') -16.9  24.2
 &rst    iat =    57,    55,    36,    38,
           r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
          &end

# 2 DT NU4:  (2 DT C3')-(2 DT C4')-(2 DT O4')-(2 DT C1')  -1.9  34.0
 &rst    iat =    55,    36,    38,    39,
           r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
          &end

# 3 DT NU0:  (3 DT C4')-(3 DT O4')-(3 DT C1')-(3 DT C2') -52.1 -22.1
 &rst    iat =    68,    70,    71,    89,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
          &end

# 3 DT NU1:  (3 DT O4')-(3 DT C1')-(3 DT C2')-(3 DT C3')  15.0  45.0
 &rst    iat =    70,    71,    89,    87,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
          &end

# 3 DT NU2:  (3 DT C1')-(3 DT C2')-(3 DT C3')-(3 DT C4') -27.4   2.6
 &rst    iat =    71,    89,    87,    68,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
          &end

# 3 DT NU3:  (3 DT C2')-(3 DT C3')-(3 DT C4')-(3 DT O4') -25.0   5.0
 &rst    iat =    89,    87,    68,    70,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
          &end

# 3 DT NU4:  (3 DT C3')-(3 DT C4')-(3 DT O4')-(3 DT C1')  13.5  43.5
```

```
 &rst     iat =    87,    68,    70,    71,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end

# 4 DC NU0:  (4 DC C4')-(4 DC O4')-(4 DC C1')-(4 DC C2') -52.1 -22.1
 &rst     iat =   100,   102,   103,   119,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
         &end

# 4 DC NU1:  (4 DC O4')-(4 DC C1')-(4 DC C2')-(4 DC C3')  15.0  45.0
 &rst     iat =   102,   103,   119,   117,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 4 DC NU2:  (4 DC C1')-(4 DC C2')-(4 DC C3')-(4 DC C4') -27.4   2.6
 &rst     iat =   103,   119,   117,   100,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 4 DC NU3:  (4 DC C2')-(4 DC C3')-(4 DC C4')-(4 DC O4') -25.0   5.0
 &rst     iat =   119,   117,   100,   102,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 4 DC NU4:  (4 DC C3')-(4 DC C4')-(4 DC O4')-(4 DC C1')  13.5  43.5
 &rst     iat =   117,   100,   102,   103,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end

# 5 DT NU0:  (5 DT C4')-(5 DT O4')-(5 DT C1')-(5 DT C2') -52.1 -22.1
 &rst     iat =   130,   132,   133,   151,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
         &end

# 5 DT NU1:  (5 DT O4')-(5 DT C1')-(5 DT C2')-(5 DT C3')  15.0  45.0
 &rst     iat =   132,   133,   151,   149,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 5 DT NU2:  (5 DT C1')-(5 DT C2')-(5 DT C3')-(5 DT C4') -27.4   2.6
 &rst     iat =   133,   151,   149,   130,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 5 DT NU3:  (5 DT C2')-(5 DT C3')-(5 DT C4')-(5 DT O4') -25.0   5.0
 &rst     iat =   151,   149,   130,   132,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 5 DT NU4:  (5 DT C3')-(5 DT C4')-(5 DT O4')-(5 DT C1')  13.5  43.5
 &rst     iat =   149,   130,   132,   133,
```

```
          r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
        &end

# 7 DG NU0:  (7 DG C4')-(7 DG O4')-(7 DG C1')-(7 DG C2') -43.9 -13.9
 &rst     iat =   194,   196,   197,   216,
          r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
        &end

# 7 DG NU1:  (7 DG O4')-(7 DG C1')-(7 DG C2')-(7 DG C3')  22.2  52.2
 &rst     iat =   196,   197,   216,   214,
          r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
        &end

# 7 DG NU2:  (7 DG C1')-(7 DG C2')-(7 DG C3')-(7 DG C4') -44.6 -14.6
 &rst     iat =   197,   216,   214,   194,
          r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
        &end

# 7 DG NU3:  (7 DG C2')-(7 DG C3')-(7 DG C4')-(7 DG O4')  -3.2  26.8
 &rst     iat =   216,   214,   194,   196,
          r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
        &end

# 7 DG NU4:  (7 DG C3')-(7 DG C4')-(7 DG O4')-(7 DG C1')  -4.4  25.6
 &rst     iat =   214,   194,   196,   197,
          r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
        &end

# 8 DT NU0:  (8 DT C4')-(8 DT O4')-(8 DT C1')-(8 DT C2') -52.1 -22.1
 &rst     iat =   227,   229,   230,   248,
          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 =   229,   230,   248,   246,
          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 =   230,   248,   246,   227,
          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 =   248,   246,   227,   229,
          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 =   246,   227,   229,   230,
          r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
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        &end

# 9 DC NU0:  (9 DC C4')-(9 DC O4')-(9 DC C1')-(9 DC C2') -52.1 -22.1
 &rst    iat =   259,   261,   262,   278,
          r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
        &end

# 9 DC NU1:  (9 DC O4')-(9 DC C1')-(9 DC C2')-(9 DC C3')  15.0  45.0
 &rst    iat =   261,   262,   278,   276,
          r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
        &end

# 9 DC NU2:  (9 DC C1')-(9 DC C2')-(9 DC C3')-(9 DC C4') -27.4   2.6
 &rst    iat =   262,   278,   276,   259,
          r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
        &end

# 9 DC NU3:  (9 DC C2')-(9 DC C3')-(9 DC C4')-(9 DC O4') -25.0   5.0
 &rst    iat =   278,   276,   259,   261,
          r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
        &end

# 9 DC NU4:  (9 DC C3')-(9 DC C4')-(9 DC O4')-(9 DC C1')  13.5  43.5
 &rst    iat =   276,   259,   261,   262,
          r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
        &end

# 10 DC NU0:  (10 DC C4')-(10 DC O4')-(10 DC C1')-(10 DC C2') -44.7 -14.7
 &rst    iat =   289,   291,   292,   308,
          r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
        &end

# 10 DC NU1:  (10 DC O4')-(10 DC C1')-(10 DC C2')-(10 DC C3')  18.1  48.1
 &rst    iat =   291,   292,   308,   306,
          r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
        &end

# 10 DC NU2:  (10 DC C1')-(10 DC C2')-(10 DC C3')-(10 DC C4') -37.2  -6.7
 &rst    iat =   292,   308,   306,   289,
          r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
        &end

# 10 DC NU3:  (10 DC C2')-(10 DC C3')-(10 DC C4')-(10 DC O4') -16.9  24.2
 &rst    iat =   308,   306,   289,   291,
          r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
        &end

# 10 DC NU4:  (10 DC C3')-(10 DC C4')-(10 DC O4')-(10 DC C1')  -1.9  34.0
 &rst    iat =   306,   289,   291,   292,
          r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
        &end
```

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# 13 DG NU0:  (13 DG C4')-(13 DG O4')-(13 DG C1')-(13 DG C2') -44.7 -14.7
 &rst    iat =   381,   383,   384,   403,
           r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
         &end

# 13 DG NU1:  (13 DG O4')-(13 DG C1')-(13 DG C2')-(13 DG C3')  18.1  48.1
 &rst    iat =   383,   384,   403,   401,
           r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
         &end

# 13 DG NU2:  (13 DG C1')-(13 DG C2')-(13 DG C3')-(13 DG C4') -37.2  -6.7
 &rst    iat =   384,   403,   401,   381,
           r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
         &end

# 13 DG NU3:  (13 DG C2')-(13 DG C3')-(13 DG C4')-(13 DG O4') -16.9  24.2
 &rst    iat =   403,   401,   381,   383,
           r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
         &end

# 13 DG NU4:  (13 DG C3')-(13 DG C4')-(13 DG O4')-(13 DG C1')  -1.9  34.0
 &rst    iat =   401,   381,   383,   384,
           r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
         &end

# 14 DG NU0:  (14 DG C4')-(14 DG O4')-(14 DG C1')-(14 DG C2') -43.9 -13.9
 &rst    iat =   414,   416,   417,   436,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
         &end

# 14 DG NU1:  (14 DG O4')-(14 DG C1')-(14 DG C2')-(14 DG C3')  22.2  52.2
 &rst    iat =   416,   417,   436,   434,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
         &end

# 14 DG NU2:  (14 DG C1')-(14 DG C2')-(14 DG C3')-(14 DG C4') -44.6 -14.6
 &rst    iat =   417,   436,   434,   414,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
         &end

# 14 DG NU3:  (14 DG C2')-(14 DG C3')-(14 DG C4')-(14 DG O4')  -3.2  26.8
 &rst    iat =   436,   434,   414,   416,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
         &end

# 14 DG NU4:  (14 DG C3')-(14 DG C4')-(14 DG O4')-(14 DG C1')  -4.4  25.6
 &rst    iat =   434,   414,   416,   417,
           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 =   447,   449,   450,   468,
           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 =   449,   450,   468,   466,
           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 =   450,   468,   466,   447,
           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 =   468,   466,   447,   449,
           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 =   466,   447,   449,   450,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
         &end

# 16 DC NU0:  (16 DC C4')-(16 DC O4')-(16 DC C1')-(16 DC C2') -52.1 -22.1
 &rst    iat =   479,   481,   482,   498,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
         &end

# 16 DC NU1:  (16 DC O4')-(16 DC C1')-(16 DC C2')-(16 DC C3')  15.0  45.0
 &rst    iat =   481,   482,   498,   496,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
         &end

# 16 DC NU2:  (16 DC C1')-(16 DC C2')-(16 DC C3')-(16 DC C4') -27.4   2.6
 &rst    iat =   482,   498,   496,   479,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
         &end

# 16 DC NU3:  (16 DC C2')-(16 DC C3')-(16 DC C4')-(16 DC O4') -25.0   5.0
 &rst    iat =   498,   496,   479,   481,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
         &end

# 16 DC NU4:  (16 DC C3')-(16 DC C4')-(16 DC O4')-(16 DC C1')  13.5  43.5
 &rst    iat =   496,   479,   481,   482,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
         &end

# 18 DA NU0:  (18 DA C4')-(18 DA O4')-(18 DA C1')-(18 DA C2') -43.9 -13.9
```

```
 &rst     iat =   551,   553,   554,   572,
            r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
          &end

# 18 DA NU1:  (18 DA O4')-(18 DA C1')-(18 DA C2')-(18 DA C3')  22.2  52.2
 &rst     iat =   553,   554,   572,   570,
            r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
          &end

# 18 DA NU2:  (18 DA C1')-(18 DA C2')-(18 DA C3')-(18 DA C4') -44.6 -14.6
 &rst     iat =   554,   572,   570,   551,
            r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
          &end

# 18 DA NU3:  (18 DA C2')-(18 DA C3')-(18 DA C4')-(18 DA O4')  -3.2  26.8
 &rst     iat =   572,   570,   551,   553,
            r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
          &end

# 18 DA NU4:  (18 DA C3')-(18 DA C4')-(18 DA O4')-(18 DA C1')  -4.4  25.6
 &rst     iat =   570,   551,   553,   554,
            r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
          &end

# 19 DG NU0:  (19 DG C4')-(19 DG O4')-(19 DG C1')-(19 DG C2') -43.9 -13.9
 &rst     iat =   583,   585,   586,   605,
            r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
          &end

# 19 DG NU1:  (19 DG O4')-(19 DG C1')-(19 DG C2')-(19 DG C3')  22.2  52.2
 &rst     iat =   585,   586,   605,   603,
            r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
          &end

# 19 DG NU2:  (19 DG C1')-(19 DG C2')-(19 DG C3')-(19 DG C4') -44.6 -14.6
 &rst     iat =   586,   605,   603,   583,
            r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
          &end

# 19 DG NU3:  (19 DG C2')-(19 DG C3')-(19 DG C4')-(19 DG O4')  -3.2  26.8
 &rst     iat =   605,   603,   583,   585,
            r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
          &end

# 19 DG NU4:  (19 DG C3')-(19 DG C4')-(19 DG O4')-(19 DG C1')  -4.4  25.6
 &rst     iat =   603,   583,   585,   586,
            r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
          &end

# 20 DA NU0:  (20 DA C4')-(20 DA O4')-(20 DA C1')-(20 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

# 20 DA NU1:  (20 DA O4')-(20 DA C1')-(20 DA C2')-(20 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

# 20 DA NU2:  (20 DA C1')-(20 DA C2')-(20 DA C3')-(20 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

# 20 DA NU3:  (20 DA C2')-(20 DA C3')-(20 DA C4')-(20 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

# 20 DA NU4:  (20 DA C3')-(20 DA C4')-(20 DA O4')-(20 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

# 21 DA NU0:  (21 DA C4')-(21 DA O4')-(21 DA C1')-(21 DA C2') -44.7 -14.7
 &rst    iat =   648,   650,   651,   669,
           r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
         &end

# 21 DA NU1:  (21 DA O4')-(21 DA C1')-(21 DA C2')-(21 DA C3')  18.1  48.1
 &rst    iat =   650,   651,   669,   667,
           r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
         &end

# 21 DA NU2:  (21 DA C1')-(21 DA C2')-(21 DA C3')-(21 DA C4') -37.2  -6.7
 &rst    iat =   651,   669,   667,   648,
           r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
         &end

# 21 DA NU3:  (21 DA C2')-(21 DA C3')-(21 DA C4')-(21 DA O4') -16.9  24.2
 &rst    iat =   669,   667,   648,   650,
           r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
         &end

# 21 DA NU4:  (21 DA C3')-(21 DA C4')-(21 DA O4')-(21 DA C1')  -1.9  34.0
 &rst    iat =   667,   648,   650,   651,
           r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
         &end
```

Distance restraints used in the rMD calculations of the R isomer adduct

```
#
#   1 DC5 H6     1 DC5 H1'   3.130   3.810
 &rst
  ixpk= 0, nxpk= 0, iat=  13,  10, r1= 2.63, r2= 3.13, r3= 3.81, r4= 4.31,
      rk2=32.0, rk3=32.0, ir6=1, ialtd=1,
 &end
#
#   1 DC5 H3'    1 DC5 H1'   3.660   5.450
 &rst
  ixpk= 0, nxpk= 0, iat=  24,  10, r1= 3.16, r2= 3.66, r3= 5.45, r4= 5.95,  &end
#
#   1 DC5 H3'    1 DC5 H5    5.030   6.820
 (#1 DC5 H3'    1 DC5 H6    2.590   3.300)
 &rst
  ixpk= 0, nxpk= 0, iat=  24,  15, r1= 4.53, r2= 5.03, r3= 6.82, r4= 7.32,  &end
#
#   1 DC5 H2'1   1 DC5 H6    2.060   3.660  (#2.060   3.060 29 35 44)
 &rst
  ixpk= 3, nxpk= 0, iat=  26,  13, r1= 1.56, r2= 2.06, r3= 3.66, r4= 4.16,  &end
#
#   1 DC5 H2'1   1 DC5 H5    3.460   5.460  (#3.460   5.160 45)
 &rst
  ixpk= 5, nxpk= 0, iat=  26,  15, r1= 2.96, r2= 3.46, r3= 5.46, r4= 5.96,  &end
#
#   1 DC5 H2'2   1 DC5 H1'   2.190   3.260
 &rst
  ixpk= 5, nxpk= 0, iat=  27,  10, r1= 1.69, r2= 2.19, r3= 3.26, r4= 3.76,  &end
#
#   1 DC5 H2'2   1 DC5 H6    2.230   5.990  (#3.130   5.990 13 18 24)
 &rst
  ixpk= 5, nxpk= 0, iat=  27,  13, r1= 1.73, r2= 2.23, r3= 5.99, r4= 6.49,  &end
#
#   1 DC5 H2'2   1 DC5 H3'   2.270   3.410  (#2.870   3.410 6 8)
 &rst
  ixpk= 3, nxpk= 0, iat=  27,  24, r1= 1.77, r2= 2.27, r3= 3.41, r4= 3.91,  &end
#
#   2 DT  H6     1 DC5 H1'   3.850   5.620  (#3.850   5.320 27)
 &rst
  ixpk= 5, nxpk= 0, iat=  43,  10, r1= 3.35, r2= 3.85, r3= 5.62, r4= 6.12,  &end
#
#   2 DT  H6     1 DC5 H3'   2.930   3.940  (#3.230   3.640 17 19)
 &rst
  ixpk= 3, nxpk= 0, iat=  43,  24, r1= 2.43, r2= 2.93, r3= 3.94, r4= 4.44,  &end
#
#   2 DT  H6     1 DC5 H2'2  2.460   3.200
 &rst
  ixpk= 3, nxpk= 0, iat=  43,  27, r1= 1.96, r2= 2.46, r3= 3.20, r4= 3.70,  &end
#
#   2 DT  H6     2 DT  H1'   3.080   3.740  (#3.080   3.440 13)
 &rst
  ixpk= 3, nxpk= 0, iat=  43,  40, r1= 2.58, r2= 3.08, r3= 3.74, r4= 4.24,  &end
```

```
#
#   2 DT  Q5     1 DC5 H6    2.970   3.780  (#3.270   3.780 32)
 &rst
  ixpk= 3, nxpk= 0, iat=  -1,  13, r1= 2.47, r2= 2.97, r3= 4.54, r4= 5.04,
 igr1=  46,  47,  48,
 &end
#
#   2 DT  Q5     1 DC5 H5    3.590   5.330
 &rst
  ixpk= 3, nxpk= 0, iat=  -1,  15, r1= 3.09, r2= 3.59, r3= 6.40, r4= 6.90,
 igr1=  46,  47,  48,
 &end
#
#   2 DT  Q5     1 DC5 H3'   3.410   3.670
 &rst
  ixpk= 3, nxpk= 0, iat=  -1,  24, r1= 2.91, r2= 3.41, r3= 4.41, r4= 4.91,
 igr1=  46,  47,  48,
 &end
#
#   2 DT  Q5     1 DC5 H2'2  2.740   3.780
 &rst
  ixpk= 3, nxpk= 0, iat=  -1,  27, r1= 2.24, r2= 2.74, r3= 4.54, r4= 5.04,
 igr1=  46,  47,  48,
 &end
#
#   2 DT  H3'    2 DT  H1'   3.170   4.040
 &rst
  ixpk= 3, nxpk= 0, iat=  56,  40, r1= 2.67, r2= 3.17, r3= 4.04, r4= 4.54,  &end
#
#   2 DT  H3'    2 DT  H6    2.920   4.020  (#2.920   3.420 20 26)
 &rst
  ixpk= 3, nxpk= 0, iat=  56,  43, r1= 2.42, r2= 2.92, r3= 4.02, r4= 4.52,  &end
#
#   2 DT  H2'1   2 DT  H1'   2.260   3.030
 &rst
  ixpk= 3, nxpk= 0, iat=  58,  40, r1= 1.76, r2= 2.26, r3= 3.03, r4= 3.53,  &end
#
#   2 DT  H2'2   2 DT  H6    1.930   3.370  (#2.230   3.070 25 38)
 &rst
  ixpk= 3, nxpk= 0, iat=  59,  43, r1= 1.43, r2= 1.93, r3= 3.37, r4= 3.87,  &end
#
#   3 DT  H6     2 DT  H1'   3.500   4.790  (#3.500   4.490 23)
 &rst
  ixpk= 4, nxpk= 0, iat=  75,  40, r1= 3.00, r2= 3.50, r3= 4.79, r4= 5.29,  &end
#
#   3 DT  H6     2 DT  H6    3.400   4.360
 &rst
  ixpk= 4, nxpk= 0, iat=  75,  43, r1= 2.90, r2= 3.40, r3= 4.36, r4= 4.86,  &end
#
#   3 DT  H6     2 DT  H2'2  2.160   3.380
 &rst
```

```
  ixpk= 4, nxpk= 0, iat=  75,  59, r1= 1.66, r2= 2.16, r3= 3.38, r4= 3.88,  &end
#
#   3 DT  H6     3 DT  H1'   3.160   4.170
 &rst
  ixpk= 4, nxpk= 0, iat=  75,  72, r1= 2.66, r2= 3.16, r3= 4.17, r4= 4.67,  &end
#
#   3 DT  Q5     2 DT  H1'   4.100   5.310
 &rst
  ixpk= 4, nxpk= 0, iat=  -1,  40, r1= 3.60, r2= 4.10, r3= 6.38, r4= 6.88,
 igr1=  78,  79,  80,
 &end
#
#   3 DT  Q5     2 DT  H2'2  2.770   4.710
 &rst
  ixpk= 4, nxpk= 0, iat=  -1,  59, r1= 2.27, r2= 2.77, r3= 5.66, r4= 6.16,
 igr1=  78,  79,  80,
 &end
#
#   3 DT  Q5     3 DT  H6    2.660   3.360
 &rst
  ixpk= 4, nxpk= 0, iat=  -1,  75, r1= 2.16, r2= 2.66, r3= 4.04, r4= 4.54,
 igr1=  78,  79,  80,
 &end
#
#   3 DT  H3'    3 DT  H6    2.700   3.760  (#2.700   3.160 21 38)
 &rst
  ixpk= 3, nxpk= 0, iat=  88,  75, r1= 2.20, r2= 2.70, r3= 3.76, r4= 4.26,  &end
#
#   3 DT  H2'2   3 DT  H1'   2.150   3.160
 &rst
  ixpk= 3, nxpk= 0, iat=  91,  72, r1= 1.65, r2= 2.15, r3= 3.16, r4= 3.66,  &end
#
#   3 DT  H2'2   3 DT  H6    2.050   3.630  (#2.050   3.030 37 40)
 &rst
  ixpk= 3, nxpk= 0, iat=  91,  75, r1= 1.55, r2= 2.05, r3= 3.63, r4= 4.13,  &end
#
#   4 DC  H1'    3 DT  H1'   3.230   4.270  (#3.230   3.670 30 41)
 &rst
  ixpk= 3, nxpk= 0, iat= 104,  72, r1= 2.73, r2= 3.23, r3= 4.27, r4= 4.77,  &end
#
#   4 DC  H1'    3 DT  H2'1  3.540   5.400
 &rst
  ixpk= 3, nxpk= 0, iat= 104,  90, r1= 3.04, r2= 3.54, r3= 5.40, r4= 5.90,  &end
#
#   4 DC  H6     3 DT  H1'   3.280   4.050
 &rst
  ixpk= 3, nxpk= 0, iat= 107,  72, r1= 2.78, r2= 3.28, r3= 4.05, r4= 4.55,  &end
#
#   4 DC  H6     3 DT  Q5    3.410   5.030  (#3.410   4.730 10)
 &rst
  ixpk= 4, nxpk= 0, iat= 107,  -1, r1= 2.91, r2= 3.41, r3= 6.04, r4= 6.54,
```

```
 igr2=  78,  79,  80,
 &end
#
#   4 DC  H6     3 DT  H3'   3.720   5.170
 &rst
  ixpk= 4, nxpk= 0, iat= 107,  88, r1= 3.22, r2= 3.72, r3= 5.17, r4= 5.67,  &end
#
#   4 DC  H6     3 DT  H2'1  2.090   3.860  (#2.690   3.860  13 29)
 &rst
  ixpk= 3, nxpk= 0, iat= 107,  90, r1= 1.59, r2= 2.09, r3= 3.86, r4= 4.36,  &end
#
#   4 DC  H6     3 DT  H2'2  2.350   3.120
 &rst
  ixpk= 3, nxpk= 0, iat= 107,  91, r1= 1.85, r2= 2.35, r3= 3.12, r4= 3.62,  &end
#
#   4 DC  H6     4 DC  H1'   3.100   3.900
 &rst
  ixpk= 3, nxpk= 0, iat= 107, 104, r1= 2.60, r2= 3.10, r3= 3.90, r4= 4.40,  &end
#
#   4 DC  H5     3 DT  H1'   3.800   4.920  (#3.800   4.620 32)
 &rst
  ixpk= 4, nxpk= 0, iat= 109,  72, r1= 3.30, r2= 3.80, r3= 4.92, r4= 5.42,  &end
#
#   4 DC  H5     3 DT  H6    3.380   5.180
 &rst
  ixpk= 4, nxpk= 0, iat= 109,  75, r1= 2.88, r2= 3.38, r3= 5.18, r4= 5.68,  &end
#
#   4 DC  H5     3 DT  Q5    3.590   4.070
 &rst
  ixpk= 4, nxpk= 0, iat= 109,  -1, r1= 3.09, r2= 3.59, r3= 4.89, r4= 5.39,
 igr2=  78,  79,  80,
 &end
#
#   4 DC  H5     3 DT  H2'1  3.120   3.900  (#3.120   3.600 25)
 &rst
  ixpk= 3, nxpk= 0, iat= 109,  90, r1= 2.62, r2= 3.12, r3= 3.90, r4= 4.40,  &end
#
#   4 DC  H5     3 DT  H2'2  3.120   4.300
 &rst
  ixpk= 3, nxpk= 0, iat= 109,  91, r1= 2.62, r2= 3.12, r3= 4.30, r4= 4.80,  &end
#
#   4 DC  H3'    4 DC  H1'   3.640   5.720  (#4.540   5.720 4 13 22)
 &rst
  ixpk= 5, nxpk= 0, iat= 118, 104, r1= 3.14, r2= 3.64, r3= 5.72, r4= 6.22,  &end
#
#   4 DC  H3'    4 DC  H6    2.910   4.160  (#2.910   3.560 5 18)
 &rst
  ixpk= 3, nxpk= 0, iat= 118, 107, r1= 2.41, r2= 2.91, r3= 4.16, r4= 4.66,  &end
#
#   4 DC  H2'1   3 DT  H1'   3.540   5.620  (#3.540   4.720 9 31)
 &rst
```

```
 ixpk= 4, nxpk= 0, iat= 120,  72, r1= 3.04, r2= 3.54, r3= 5.62, r4= 6.12,  &end
#
#   4 DC  H2'1   4 DC  H1'   2.270   3.550  (#2.870   3.550 11 44)
 &rst
 ixpk= 3, nxpk= 0, iat= 120, 104, r1= 1.77, r2= 2.27, r3= 3.55, r4= 4.05,  &end
#
#   4 DC  H2'1   4 DC  H6    2.100   3.660  (#2.100   2.760 16 21 33)
 &rst
 ixpk= 2, nxpk= 0, iat= 120, 107, r1= 1.60, r2= 2.10, r3= 3.66, r4= 4.16,  &end
#
#   4 DC  H2'1   4 DC  H5    3.290   5.440  (#3.290   4.540 8 20 35)
 &rst
 ixpk= 4, nxpk= 0, iat= 120, 109, r1= 2.79, r2= 3.29, r3= 5.44, r4= 5.94,  &end
#
#   4 DC  H2'1   4 DC  H3'   2.350   3.760  (#2.950   3.760 27 37 47 48)
 &rst
 ixpk= 3, nxpk= 0, iat= 120, 118, r1= 1.85, r2= 2.35, r3= 3.76, r4= 4.26,  &end
#
#   4 DC  H2'2   4 DC  H1'   2.190   3.240  (#2.190   2.640 2 13)
 &rst
 ixpk= 2, nxpk= 0, iat= 121, 104, r1= 1.69, r2= 2.19, r3= 3.24, r4= 3.74,  &end
#
#   4 DC  H2'2   4 DC  H6    2.050   3.550  (#2.650   3.550 3 6)
 &rst
 ixpk= 3, nxpk= 0, iat= 121, 107, r1= 1.55, r2= 2.05, r3= 3.55, r4= 4.05,  &end
#
#   5 DT  H6     4 DC  H1'   3.680   5.380
 (#5 DT  H1'    4 DC  H2'2  2.520   3.090)
 &rst
 ixpk= 3, nxpk= 0, iat= 137, 104, r1= 3.18, r2= 3.68, r3= 5.38, r4= 5.88,  &end
#
#   5 DT  H6     4 DC  H6    2.950   4.290  (#2.950   3.69 17 26)
 &rst
 ixpk= 3, nxpk= 0, iat= 137, 107, r1= 2.45, r2= 2.95, r3= 4.29, r4= 4.79,  &end
#
#   5 DT  H6     4 DC  H3'   4.530   6.990  (#4.830   6.990 23)
 &rst
 ixpk= 6, nxpk= 0, iat= 137, 118, r1= 4.03, r2= 4.53, r3= 6.99, r4= 7.49,  &end
#
#   5 DT  H6     4 DC  H2'1  3.030   3.830
 &rst
 ixpk= 6, nxpk= 0, iat= 137, 120, r1= 2.53, r2= 3.03, r3= 3.83, r4= 4.33,  &end
#
#   5 DT  H6     4 DC  H2'2  2.490   3.210
 &rst
 ixpk= 6, nxpk= 0, iat= 137, 121, r1= 1.99, r2= 2.49, r3= 3.21, r4= 3.71,  &end
#
#   5 DT  H6     5 DT  H1'   3.230   4.900
 &rst
 ixpk= 6, nxpk= 0, iat= 137, 134, r1= 2.73, r2= 3.23, r3= 4.90, r4= 5.40,  &end
#
```

```
#   5 DT  Q5     5 DT  H2'2  2.770   4.790  (#2.770   3.890 37 39 43)
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 153, r1= 2.27, r2= 2.77, r3= 5.75, r4= 6.25,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  Q5     4 DC  H1'   4.170   5.400
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 104, r1= 3.67, r2= 4.17, r3= 6.49, r4= 6.99,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  Q5     4 DC  H6    2.790   3.540
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 107, r1= 2.29, r2= 2.79, r3= 4.25, r4= 4.75,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  Q5     4 DC  H5    2.850   3.520  (#3.150   3.520 22)
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 109, r1= 2.35, r2= 2.85, r3= 4.23, r4= 4.73,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  Q5     4 DC  H2'1  3.300   4.140
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 120, r1= 2.80, r2= 3.30, r3= 4.97, r4= 5.47,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  Q5     4 DC  H2'2  3.250   4.820
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 121, r1= 2.75, r2= 3.25, r3= 5.79, r4= 6.29,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  Q5     5 DT  H1'   3.040   6.040
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 134, r1= 2.54, r2= 3.04, r3= 7.25, r4= 7.75,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  Q5     5 DT  H6    2.400   3.280  (#2.700   3.280 4)
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 137, r1= 1.90, r2= 2.40, r3= 3.94, r4= 4.44,
 igr1= 140, 141, 142,
 &end
#
#   5 DT  H3'    5 DT  H6    2.650   4.290  (#2.650   3.090 2 8 9 13)
 &rst
  ixpk= 3, nxpk= 0, iat= 150, 137, r1= 2.15, r2= 2.65, r3= 4.29, r4= 4.79,  &end
```

```
#
#   5 DT  H3'    5 DT  Q5    3.640   5.760  (#3.640   5.460 13)
 &rst
  ixpk= 5, nxpk= 0, iat= 150,  -1, r1= 3.14, r2= 3.64, r3= 6.92, r4= 7.42,
 igr2= 140, 141, 142,
 &end
#
#   5 DT  H2'1   5 DT  H1'   2.120   3.770
 &rst
  ixpk= 5, nxpk= 0, iat= 152, 134, r1= 1.62, r2= 2.12, r3= 3.77, r4= 4.27,  &end
#
#   5 DT  H2'1   5 DT  H6    2.250   2.980  (#1.950   2.680 46 47)
 &rst
  ixpk= 2, nxpk= 0, iat= 152, 137, r1= 1.75, r2= 2.25, r3= 2.98, r4= 3.48,  &end
#
#   5 DT  H2'1   5 DT  Q5    2.350   4.550
 &rst
  ixpk= 2, nxpk= 0, iat= 152,  -1, r1= 1.85, r2= 2.35, r3= 5.46, r4= 5.96,
 igr2= 140, 141, 142,
 &end
#
#   5 DT  H2'1   5 DT  H3'   2.410   3.440
 &rst
  ixpk= 2, nxpk= 0, iat= 152, 150, r1= 1.91, r2= 2.41, r3= 3.44, r4= 3.94,  &end
#
#   5 DT  H2'2   5 DT  H1'   1.920   3.100  (#1.920   2.800 18)
 &rst
  ixpk= 2, nxpk= 0, iat= 153, 134, r1= 1.42, r2= 1.92, r3= 3.10, r4= 3.60,  &end
#
#   5 DT  H2'2   5 DT  H6    2.020   5.060  (#2.320   5.060 5)
 &rst
  ixpk= 5, nxpk= 0, iat= 153, 137, r1= 1.52, r2= 2.02, r3= 5.06, r4= 5.56,  &end
#
#   1 DC5 H1'    2 DT  Q5    3.980   4.800  (#3.980   4.500 10)
 &rst
  ixpk= 4, nxpk= 0, iat=  10,  -1, r1= 3.48, r2= 3.98, r3= 5.76, r4= 6.26,
 igr2=  46,  47,  48,
 &end
#
#   6 DT  H6     5 DT  H1'   3.850   5.710  (#3.850   5.410 36)
 &rst
  ixpk= 5, nxpk= 0, iat= 169, 134, r1= 3.35, r2= 3.85, r3= 5.71, r4= 6.21,  &end
#
#   6 DT  H6     5 DT  Q5    2.630   6.560
 &rst
  ixpk= 5, nxpk= 0, iat= 169,  -1, r1= 2.13, r2= 2.63, r3= 7.88, r4= 8.38,
 igr2= 140, 141, 142,
 &end
#
#   6 DT  H6     5 DT  H3'   3.830   5.200  (#3.830   4.300 16 21 24)
 &rst
```

```
  ixpk= 4, nxpk= 0, iat= 169, 150, r1= 3.33, r2= 3.83, r3= 5.20, r4= 5.70,  &end
#
#   6 DT  H6     5 DT  H2'1  2.800   4.470
 &rst
  ixpk= 4, nxpk= 0, iat= 169, 152, r1= 2.30, r2= 2.80, r3= 4.47, r4= 4.97,  &end
#
#   6 DT  H6     6 DT  H1'   2.910   5.390
 &rst
  ixpk= 4, nxpk= 0, iat= 169, 166, r1= 2.41, r2= 2.91, r3= 5.39, r4= 5.89,  &end
#
#   6 DT  Q5     5 DT  H1'   3.010   4.370
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 134, r1= 2.51, r2= 3.01, r3= 5.25, r4= 5.75,
 igr1= 172, 173, 174,
 &end
#
#   6 DT  Q5     5 DT  H6    3.000   4.090
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 137, r1= 2.50, r2= 3.00, r3= 4.91, r4= 5.41,
 igr1= 172, 173, 174,
 &end
#
#   6 DT  Q5     5 DT  H2'1  2.510   3.890
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 152, r1= 2.01, r2= 2.51, r3= 4.67, r4= 5.17,
 igr1= 172, 173, 174,
 &end
#
#   6 DT  Q5     6 DT  H1'   3.340   5.580
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 166, r1= 2.84, r2= 3.34, r3= 6.70, r4= 7.20,
 igr1= 172, 173, 174,
 &end
#
#   6 DT  Q5     6 DT  H6    2.550   3.220
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 169, r1= 2.05, r2= 2.55, r3= 3.87, r4= 4.37,
 igr1= 172, 173, 174,
 &end
#
#   6 DT  H3'    6 DT  H1'   3.220   4.580
 &rst
  ixpk= 4, nxpk= 0, iat= 182, 166, r1= 2.72, r2= 3.22, r3= 4.58, r4= 5.08,  &end
#
#   6 DT  H3'    6 DT  H6    3.090   5.190
 &rst
  ixpk= 4, nxpk= 0, iat= 182, 169, r1= 2.59, r2= 3.09, r3= 5.19, r4= 5.69,  &end
#
#   6 DT  H2'1   6 DT  H1'   2.210   4.540  (#2.810   4.540 5 23)
 &rst
  ixpk= 4, nxpk= 0, iat= 184, 166, r1= 1.71, r2= 2.21, r3= 4.54, r4= 5.04,  &end
```

```
#
#   6 DT  H2'1   6 DT  H6    2.300   3.520  (#2.000   3.220 20 49)
 &rst
  ixpk= 3, nxpk= 0, iat= 184, 169, r1= 1.80, r2= 2.30, r3= 3.52, r4= 4.02,  &end
#
#   6 DT  H2'1   6 DT  Q5    3.050   4.810  (#3.050   4.510 32)
 &rst
  ixpk= 4, nxpk= 0, iat= 184,  -1, r1= 2.55, r2= 3.05, r3= 5.78, r4= 6.28,
 igr2= 172, 173, 174,
 &end
#
#   6 DT  H2'1   6 DT  H3'   2.350   2.790
 &rst
  ixpk= 4, nxpk= 0, iat= 184, 182, r1= 1.85, r2= 2.35, r3= 2.79, r4= 3.29,  &end
#
#   6 DT  H2'2   6 DT  H1'   1.950   3.070  (#1.950   2.570 10 16)
 &rst
  ixpk= 2, nxpk= 0, iat= 185, 166, r1= 1.45, r2= 1.95, r3= 3.07, r4= 3.57,  &end
#
#   6 DT  H2'2   6 DT  H6    1.830   3.300  (#1.830   2.400 37 38 41 47 48)
 &rst
  ixpk= 2, nxpk= 0, iat= 185, 169, r1= 1.33, r2= 1.83, r3= 3.30, r4= 3.80,  &end
#
#   7 DG  H8     6 DT  H1'   3.890   5.760
 &rst
  ixpk= 2, nxpk= 0, iat= 201, 166, r1= 3.39, r2= 3.89, r3= 5.76, r4= 6.26,  &end
#
#   7 DG  H8     6 DT  H6    4.260   6.250
 &rst
  ixpk= 2, nxpk= 0, iat= 201, 169, r1= 3.76, r2= 4.26, r3= 6.25, r4= 6.75,  &end
#
#   7 DG  H8     6 DT  H3'   3.660   4.960  (#3.660   4.060 2 8 13)
 &rst
  ixpk= 4, nxpk= 0, iat= 201, 182, r1= 3.16, r2= 3.66, r3= 4.96, r4= 5.46,  &end
#
#   7 DG  H8     6 DT  H2'1  2.160   3.650  (#3.060   3.650 4 17 25)
 &rst
  ixpk= 3, nxpk= 0, iat= 201, 184, r1= 1.66, r2= 2.16, r3= 3.65, r4= 4.15,  &end
#
#   7 DG  H8     6 DT  H2'2  2.700   3.650  (#3.000   3.350 30 39)
 &rst
  ixpk= 3, nxpk= 0, iat= 201, 185, r1= 2.20, r2= 2.70, r3= 3.65, r4= 4.15,  &end
#
#   7 DG  H3'    6 DT  H1'   3.670   5.100  (#3.670   4.200 9 18 27)
 &rst
  ixpk= 4, nxpk= 0, iat= 215, 166, r1= 3.17, r2= 3.67, r3= 5.10, r4= 5.60,  &end
#
#   7 DG  H3'    7 DG  H1'   3.440   3.950
 &rst
  ixpk= 4, nxpk= 0, iat= 215, 198, r1= 2.94, r2= 3.44, r3= 3.95, r4= 4.45,  &end
#
```

```
#   7 DG  H3'    7 DG  H8    3.290   4.430  (#3.290   4.130 26)
 &rst
  ixpk= 4, nxpk= 0, iat= 215, 201, r1= 2.79, r2= 3.29, r3= 4.43, r4= 4.93,  &end
#
#   7 DG  H2'1   7 DG  H1'   2.160   4.440  (#2.760   4.440 13 21)
 &rst
  ixpk= 4, nxpk= 0, iat= 217, 198, r1= 1.66, r2= 2.16, r3= 4.44, r4= 4.94,  &end
#
#   7 DG  H2'1   7 DG  H8    2.120   3.930  (#2.120   2.730 1 3 7 19)
 &rst
  ixpk= 2, nxpk= 0, iat= 217, 201, r1= 1.62, r2= 2.12, r3= 3.93, r4= 4.43,  &end
#
#   7 DG  H2'2   7 DG  H1'   2.240   3.160  (#2.240   2.860 33)
 &rst
  ixpk= 2, nxpk= 0, iat= 218, 198, r1= 1.74, r2= 2.24, r3= 3.16, r4= 3.66,  &end
#
#   7 DG  H2'2   7 DG  H8    2.450   4.430  (#2.750   4.430 6)
 &rst
  ixpk= 4, nxpk= 0, iat= 218, 201, r1= 1.95, r2= 2.45, r3= 4.43, r4= 4.93,  &end
#
#   7 DG  H2'2   7 DG  H3'   2.460   3.030  (#2.460   3.230 20)
 &rst
  ixpk= 3, nxpk= 0, iat= 218, 215, r1= 1.96, r2= 2.46, r3= 3.03, r4= 3.53,  &end
#
#   8 DT  H6     7 DG  H1'   3.050   3.590
 &rst
  ixpk= 3, nxpk= 0, iat= 234, 198, r1= 2.55, r2= 3.05, r3= 3.59, r4= 4.09,  &end
#
#   8 DT  H6     7 DG  H8    4.020   5.970
 &rst
  ixpk= 3, nxpk= 0, iat= 234, 201, r1= 3.52, r2= 4.02, r3= 5.97, r4= 6.47,  &end
#
#   8 DT  H6     7 DG  H2'1  2.170   4.660  (#3.070   4.660 5 13 31)
 &rst
  ixpk= 4, nxpk= 0, iat= 234, 217, r1= 1.67, r2= 2.17, r3= 4.66, r4= 5.16,  &end
#
#   8 DT  H6     7 DG  H2'2  2.540   3.560
 &rst
  ixpk= 4, nxpk= 0, iat= 234, 218, r1= 2.04, r2= 2.54, r3= 3.56, r4= 4.06,  &end
#
#   8 DT  H6     8 DT  H1'   3.190   3.860  (#3.190   3.560 13)
 &rst
  ixpk= 3, nxpk= 0, iat= 234, 231, r1= 2.69, r2= 3.19, r3= 3.86, r4= 4.36,  &end
#
#   8 DT  Q5     7 DG  H1'   3.580   4.250
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 198, r1= 3.08, r2= 3.58, r3= 5.10, r4= 5.60,
 igr1= 237, 238, 239,
 &end
#
#   8 DT  Q5     7 DG  H8    2.950   3.450
```

```
 &rst
  ixpk= 3, nxpk= 0, iat=  -1, 201, r1= 2.45, r2= 2.95, r3= 4.14, r4= 4.64,
 igr1= 237, 238, 239,
 &end
#
#   8 DT  Q5     7 DG  H3'   3.740   4.540  (#3.740   4.240 22)
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 215, r1= 3.24, r2= 3.74, r3= 5.45, r4= 5.95,
 igr1= 237, 238, 239,
 &end
#
#   8 DT  Q5     7 DG  H2'1  2.820   4.610
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 217, r1= 2.32, r2= 2.82, r3= 5.54, r4= 6.04,
 igr1= 237, 238, 239,
 &end
#
#   8 DT  Q5     7 DG  H2'2  2.490   3.510
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 218, r1= 1.99, r2= 2.49, r3= 4.22, r4= 4.72,
 igr1= 237, 238, 239,
 &end
#
#   8 DT  Q5     8 DT  H1'   3.830   5.230
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 231, r1= 3.33, r2= 3.83, r3= 6.28, r4= 6.78,
 igr1= 237, 238, 239,
 &end
#
#   8 DT  Q5     8 DT  H6    2.620   3.170
 &rst
  ixpk= 4, nxpk= 0, iat=  -1, 234, r1= 2.12, r2= 2.62, r3= 3.81, r4= 4.31,
 igr1= 237, 238, 239,
 &end
#
#   8 DT  H3'    8 DT  H1'   3.210   4.690
 &rst
  ixpk= 4, nxpk= 0, iat= 247, 231, r1= 2.71, r2= 3.21, r3= 4.69, r4= 5.19,  &end
#
#   8 DT  H2'1   7 DG  H1'   3.720   4.910  (#3.720   4.610 24)
 &rst
  ixpk= 4, nxpk= 0, iat= 249, 198, r1= 3.22, r2= 3.72, r3= 4.91, r4= 5.41,  &end
#
#   8 DT  H2'1   8 DT  H1'   2.740   3.600
 &rst
  ixpk= 4, nxpk= 0, iat= 249, 231, r1= 2.24, r2= 2.74, r3= 3.60, r4= 4.10,  &end
#
#   8 DT  H2'1   8 DT  H6    2.170   2.680
 &rst
  ixpk= 4, nxpk= 0, iat= 249, 234, r1= 1.67, r2= 2.17, r3= 2.68, r4= 3.18,  &end
#
```

```
#   8 DT  H2'1   8 DT  Q5    2.600   4.050
 &rst
  ixpk= 4, nxpk= 0, iat= 249,  -1, r1= 2.10, r2= 2.60, r3= 4.86, r4= 5.36,
 igr2= 237, 238, 239,
 &end
#
#   8 DT  H2'2   8 DT  H1'   2.300   2.680
 &rst
  ixpk= 4, nxpk= 0, iat= 250, 231, r1= 1.80, r2= 2.30, r3= 2.68, r4= 3.18,  &end
#
#   8 DT  H2'2   8 DT  H6    2.540   3.680  (#2.540   3.380 29)
 &rst
  ixpk= 3, nxpk= 0, iat= 250, 234, r1= 2.04, r2= 2.54, r3= 3.68, r4= 4.18,  &end
#
#   8 DT  H2'2   8 DT  Q5    2.580   6.340
 &rst
  ixpk= 3, nxpk= 0, iat= 250,  -1, r1= 2.08, r2= 2.58, r3= 7.61, r4= 8.11,
 igr2= 237, 238, 239,
 &end
#
#   9 DC  H6     8 DT  H1'   2.830   3.640  (#3.130   3.640)
 &rst
  ixpk= 3, nxpk= 0, iat= 266, 231, r1= 2.33, r2= 2.83, r3= 3.64, r4= 4.14,  &end
#
#   9 DC  H6     8 DT  H3'   3.640   4.810  (#3.640   4.210 17 23)
 &rst
  ixpk= 4, nxpk= 0, iat= 266, 247, r1= 3.14, r2= 3.64, r3= 4.81, r4= 5.31,  &end
#
#   9 DC  H6     8 DT  H2'1  3.350   4.930
 &rst
  ixpk= 4, nxpk= 0, iat= 266, 249, r1= 2.85, r2= 3.35, r3= 4.93, r4= 5.43,  &end
#
#   9 DC  H6     8 DT  H2'2  2.520   3.130  (#2.520   3.130 10 47)
 &rst
  ixpk= 3, nxpk= 0, iat= 266, 250, r1= 2.02, r2= 2.52, r3= 3.13, r4= 3.63,  &end
#
#   9 DC  H5     8 DT  H1'   3.700   4.170
 &rst
  ixpk= 3, nxpk= 0, iat= 268, 231, r1= 3.20, r2= 3.70, r3= 4.17, r4= 4.67,  &end
#
#   9 DC  H5     8 DT  Q5    3.890   4.540
 (#9 DC  H5     8 DT  H6    3.630   4.260)
 &rst
  ixpk= 3, nxpk= 0, iat= 268,  -1, r1= 3.39, r2= 3.89, r3= 5.45, r4= 5.95,
 igr2= 237, 238, 239,
 &end
#
#   9 DC  H5     8 DT  H2'1  3.010   3.370
 &rst
  ixpk= 3, nxpk= 0, iat= 268, 249, r1= 2.51, r2= 3.01, r3= 3.37, r4= 3.87,  &end
#
```

```
#   9 DC  H5     8 DC  H2'2  2.680   3.400  (#2.980   3.400 30)
 &rst
  ixpk= 3, nxpk= 0, iat= 268, 250, r1= 2.18, r2= 2.68, r3= 3.40, r4= 3.90,  &end
#
#   9 DC  H5     9 DC  H1'   3.300   5.590  (#3.300   3.790 1 3 7 9 18 36)
 &rst
  ixpk= 3, nxpk= 0, iat= 268, 263, r1= 2.80, r2= 3.30, r3= 5.59, r4= 6.09,  &end
#
#   9 DC  H3'    9 DC  H1'   3.640   5.390
 &rst
  ixpk= 3, nxpk= 0, iat= 277, 263, r1= 3.14, r2= 3.64, r3= 5.39, r4= 5.89,  &end
#
#   9 DC  H3'    9 DC  H6    3.020   4.230  (#3.020   3.330 13 16 19)
 &rst
  ixpk= 3, nxpk= 0, iat= 277, 266, r1= 2.52, r2= 3.02, r3= 4.23, r4= 4.73,  &end
#
#   9 DC  H3'    9 DC  H5    4.520   6.820
 &rst
  ixpk= 3, nxpk= 0, iat= 277, 268, r1= 4.02, r2= 4.52, r3= 6.82, r4= 7.32,  &end
#
#   9 DC  H2'1   8 DT  H1'   3.720   5.910  (#3.720   5.310 25 44)
 &rst
  ixpk= 5, nxpk= 0, iat= 279, 231, r1= 3.22, r2= 3.72, r3= 5.91, r4= 6.41,  &end
#
#   9 DC  H2'1   9 DC  H1'   2.210   3.820  (#2.810   3.820 5 8)
 &rst
  ixpk= 3, nxpk= 0, iat= 279, 263, r1= 1.71, r2= 2.21, r3= 3.82, r4= 4.32,  &end
#
#   9 DC  H2'1   9 DC  H6    2.120   3.780  (#2.120   2.580 6 13 20 33)
 &rst
  ixpk= 2, nxpk= 0, iat= 279, 266, r1= 1.62, r2= 2.12, r3= 3.78, r4= 4.28,  &end
#
#   9 DC  H2'1   9 DC  H5    3.330   5.540
 &rst
  ixpk= 2, nxpk= 0, iat= 279, 268, r1= 2.83, r2= 3.33, r3= 5.54, r4= 6.04,  &end
#
#   9 DC  H2'1   9 DC  H3'   2.500   2.900
 &rst
  ixpk= 2, nxpk= 0, iat= 279, 277, r1= 2.00, r2= 2.50, r3= 2.90, r4= 3.40,  &end
#
#   9 DC  H2'2   9 DC  H1'   2.240   3.210  (#2.240   2.610 13 27)
 &rst
  ixpk= 2, nxpk= 0, iat= 280, 263, r1= 1.74, r2= 2.24, r3= 3.21, r4= 3.71,  &end
#
#   9 DC  H2'2   9 DC  H6    2.290   3.510  (#2.590   3.21 4 43)
 &rst
  ixpk= 3, nxpk= 0, iat= 280, 266, r1= 1.79, r2= 2.29, r3= 3.51, r4= 4.01,  &end
#
#   9 DC  H2'2   9 DC  H5    3.360   5.400  (#3.360   4.800 40 41 42)
 &rst
  ixpk= 4, nxpk= 0, iat= 280, 268, r1= 2.86, r2= 3.36, r3= 5.40, r4= 5.90,  &end
```

```
#
#  10 DC  H6     9 DC  H1'   3.830   5.300  (#3.830   4.400 11 22)
 &rst
  ixpk= 4, nxpk= 0, iat= 296, 263, r1= 3.33, r2= 3.83, r3= 5.30, r4= 5.80,  &end
#
#  10 DC  H6     9 DC  H2'1  2.480   3.950  (#3.080   3.950 10 35)
 &rst
  ixpk= 3, nxpk= 0, iat= 296, 279, r1= 1.98, r2= 2.48, r3= 3.95, r4= 4.45,  &end
#
#  10 DC  H6     9 DC  H2'2  2.710   3.240
 &rst
  ixpk= 3, nxpk= 0, iat= 296, 280, r1= 2.21, r2= 2.71, r3= 3.24, r4= 3.74,  &end
#
#  10 DC  H6    10 DC  H1'   3.090   3.700
 &rst
  ixpk= 3, nxpk= 0, iat= 296, 293, r1= 2.59, r2= 3.09, r3= 3.70, r4= 4.20,  &end
#
#  10 DC  H5     9 DC  H2'1  3.220   3.470
 &rst
  ixpk= 3, nxpk= 0, iat= 298, 279, r1= 2.72, r2= 3.22, r3= 3.47, r4= 3.97,  &end
#
#  10 DC  H5     9 DC  H2'2  2.670   3.610  (#3.270   3.610 21 29)
 &rst
  ixpk= 3, nxpk= 0, iat= 298, 280, r1= 2.17, r2= 2.67, r3= 3.61, r4= 4.11,  &end
#
#  10 DC  H3'   10 DC  H1'   3.830   5.680
 &rst
  ixpk= 3, nxpk= 0, iat= 307, 293, r1= 3.33, r2= 3.83, r3= 5.68, r4= 6.18,  &end
#
#   9 DC  H3'   10 DC  H5    3.510   5.080  (#3.510   3.880 1 13 20 26 29)
 &rst
  ixpk= 3, nxpk= 0, iat= 277, 298, r1= 3.01, r2= 3.51, r3= 5.08, r4= 5.58,  &end
#
#  10 DC  H2'1  10 DC  H1'   2.250   4.190  (#2.850   4.190 5 9)
 &rst
  ixpk= 4, nxpk= 0, iat= 309, 293, r1= 1.75, r2= 2.25, r3= 4.19, r4= 4.69,  &end
#
#  10 DC  H2'1  10 DC  H6    2.000   3.760  (#2.000   2.560 2 3 6 13)
 &rst
  ixpk= 2, nxpk= 0, iat= 309, 296, r1= 1.50, r2= 2.00, r3= 3.76, r4= 4.26,  &end
#
#  10 DC  H2'1  10 DC  H5    3.150   5.690  (#3.150   5.090 13 24)
 &rst
  ixpk= 5, nxpk= 0, iat= 309, 298, r1= 2.65, r2= 3.15, r3= 5.69, r4= 6.19,  &end
#
#  10 DC  H2'1  10 DC  H3'   2.420   3.440
 &rst
  ixpk= 5, nxpk= 0, iat= 309, 307, r1= 1.92, r2= 2.42, r3= 3.44, r4= 3.94,  &end
#
#  10 DC  H2'2  10 DC  H1'   2.140   3.170  (#2.140   2.570 23 45)
 &rst
```

```
  ixpk= 2, nxpk= 0, iat= 310, 293, r1= 1.64, r2= 2.14, r3= 3.17, r4= 3.67,  &end
#
#  10 DC  H2'2  10 DC  H6    2.380   3.990  (#2.680   3.990 27)
 &rst
  ixpk= 3, nxpk= 0, iat= 310, 296, r1= 1.88, r2= 2.38, r3= 3.99, r4= 4.49,  &end
#
#  11 DG3 H8    10 DC  H1'   3.640   4.710  (#3.640   4.110 17 19)
 &rst
  ixpk= 4, nxpk= 0, iat= 326, 293, r1= 3.14, r2= 3.64, r3= 4.71, r4= 5.21,  &end
#
#  11 DG3 H8    10 DC  H3'   4.050   5.010
 &rst
  ixpk= 4, nxpk= 0, iat= 326, 307, r1= 3.55, r2= 4.05, r3= 5.01, r4= 5.51,  &end
#
#  11 DG3 H8    10 DC  H2'1  2.820   4.160  (#3.120   4.160 33)
 &rst
  ixpk= 4, nxpk= 0, iat= 326, 309, r1= 2.32, r2= 2.82, r3= 4.16, r4= 4.66,  &end
#
#  11 DG3 H8    10 DC  H2'2  2.790   3.490
 &rst
  ixpk= 4, nxpk= 0, iat= 326, 310, r1= 2.29, r2= 2.79, r3= 3.49, r4= 3.99,  &end
#
#  11 DG3 H8    11 DG3 H1'   3.370   4.900
 &rst
  ixpk= 4, nxpk= 0, iat= 326, 323, r1= 2.87, r2= 3.37, r3= 4.90, r4= 5.40,  &end
#
#  11 DG3 H3'   11 DG3 H8    2.500   4.580  (#2.500   3.380 8 18 38 40)
 &rst
  ixpk= 3, nxpk= 0, iat= 340, 326, r1= 2.00, r2= 2.50, r3= 4.58, r4= 5.08,  &end
#
#  11 DG3 H2'1  11 DG3 H1'   1.980   3.080  (#1.980   2.480 37 41)
 &rst
  ixpk= 2, nxpk= 0, iat= 342, 323, r1= 1.48, r2= 1.98, r3= 3.08, r4= 3.58,  &end
#
#  11 DG3 H2'1  11 DG3 H8    2.430   5.230
 &rst
  ixpk= 2, nxpk= 0, iat= 342, 326, r1= 1.93, r2= 2.43, r3= 5.23, r4= 5.73,  &end
#
#  11 DG3 H2'2  11 DG3 H8    2.000   2.520
 &rst
  ixpk= 2, nxpk= 0, iat= 343, 326, r1= 1.50, r2= 2.00, r3= 2.52, r4= 3.02,  &end
#
#  11 DG3 H2'2  11 DG3 H3'   1.800   3.080
 &rst
  ixpk= 2, nxpk= 0, iat= 343, 340, r1= 1.30, r2= 1.80, r3= 3.08, r4= 3.58,  &end
#
#  12 DC5 H6    12 DC5 H1'   2.700   3.770  (# 2.700   3.170 7 13)
 &rst
  ixpk= 2, nxpk= 0, iat= 358, 355, r1= 2.20, r2= 2.70, r3= 3.77, r4= 4.27,  &end
#
#  12 DG5 H3'   12 DC5 H1'   3.610   5.750  (#3.910   5.750 30)
```

```
 &rst
  ixpk= 5, nxpk= 0, iat= 369, 355, r1= 3.11, r2= 3.61, r3= 5.75, r4= 6.25,  &end
#
#  12 DC5 H2'1  12 DC5 H1'   2.390   5.150  (#3.190   5.150 4 16 21)
 &rst
  ixpk= 5, nxpk= 0, iat= 371, 355, r1= 1.89, r2= 2.39, r3= 5.15, r4= 5.65,  &end
#
#  12 DC5 H2'1  12 DC5 H6    2.040   3.830  (#2.040   2.630 19 26 35 46)
 &rst
  ixpk= 2, nxpk= 0, iat= 371, 358, r1= 1.54, r2= 2.04, r3= 3.83, r4= 4.33,  &end
#
#  12 DC5 H2'1  12 DC5 H5    4.060   5.640
 &rst
  ixpk= 2, nxpk= 0, iat= 371, 360, r1= 3.56, r2= 4.06, r3= 5.64, r4= 6.14,  &end
#
#  12 DC5 H2'2  12 DC5 H1'   2.000   3.280  (#2.000   2.680 6 36)
 &rst
  ixpk= 2, nxpk= 0, iat= 372, 355, r1= 1.50, r2= 2.00, r3= 3.28, r4= 3.78,  &end
#
#  12 DC5 H2'2  12 DC5 H5    2.330   5.340  (#2.330   3.040 1 3 5 9 29 39 42 43)
 &rst
  ixpk= 3, nxpk= 0, iat= 372, 360, r1= 1.83, r2= 2.33, r3= 5.34, r4= 5.84,  &end
#
#  13 DG  H8    12 DC5 H1'   3.760   6.470
 &rst
  ixpk= 3, nxpk= 0, iat= 388, 355, r1= 3.26, r2= 3.76, r3= 6.47, r4= 6.97,  &end
#
#  13 DG  H8    12 DC5 H3'   3.190   3.880  (#3.190   3.580 48)
 &rst
  ixpk= 3, nxpk= 0, iat= 388, 369, r1= 2.69, r2= 3.19, r3= 3.88, r4= 4.38,  &end
#
#  13 DG  H8    12 DC5 H2'1  2.670   4.020
 &rst
  ixpk= 3, nxpk= 0, iat= 388, 371, r1= 2.17, r2= 2.67, r3= 4.02, r4= 4.52,  &end
#
#  13 DG  H8    12 DC5 H2'2  2.360   4.170
 &rst
  ixpk= 3, nxpk= 0, iat= 388, 372, r1= 1.86, r2= 2.36, r3= 4.17, r4= 4.67,  &end
#
#  13 DG  H8    13 DG  H1'   3.130   5.100
 &rst
  ixpk= 3, nxpk= 0, iat= 388, 385, r1= 2.63, r2= 3.13, r3= 5.10, r4= 5.60,  &end
#
#  13 DG  H3'   13 DG  H1'   3.390   5.140
 &rst
  ixpk= 3, nxpk= 0, iat= 402, 385, r1= 2.89, r2= 3.39, r3= 5.14, r4= 5.64,  &end
#
#  13 DG  H3'   13 DG  H8    3.290   5.170
 &rst
  ixpk= 3, nxpk= 0, iat= 402, 388, r1= 2.79, r2= 3.29, r3= 5.17, r4= 5.67,  &end
#
```

```
#  13 DG  H2'1  13 DG  H1'   2.340   3.730
 &rst
  ixpk= 3, nxpk= 0, iat= 404, 385, r1= 1.84, r2= 2.34, r3= 3.73, r4= 4.23,  &end
#
#  13 DG  H2'1  13 DG  H8    1.960   3.190  (#1.960   2.890 17)
 &rst
  ixpk= 2, nxpk= 0, iat= 404, 388, r1= 1.46, r2= 1.96, r3= 3.19, r4= 3.69,  &end
#
#  13 DG  H2'2  13 DG  H1'   2.030   3.160
 &rst
  ixpk= 2, nxpk= 0, iat= 405, 385, r1= 1.53, r2= 2.03, r3= 3.16, r4= 3.66,  &end
#
#  13 DG  H2'2  13 DG  H8    2.290   4.250
 &rst
  ixpk= 2, nxpk= 0, iat= 405, 388, r1= 1.79, r2= 2.29, r3= 4.25, r4= 4.75,  &end
#
#  14 DG  H1'   13 DG  H1'   3.250   4.620  (#3.250   3.720 10 24 26)
 &rst
  ixpk= 3, nxpk= 0, iat= 418, 385, r1= 2.75, r2= 3.25, r3= 4.62, r4= 5.12,  &end
#
#  14 DG  H8    13 DG  H1'   3.210   3.920  (#3.210   3.620 32)
 &rst
  ixpk= 3, nxpk= 0, iat= 421, 385, r1= 2.71, r2= 3.21, r3= 3.92, r4= 4.42,  &end
#
#  14 DG  H8    13 DG  H3'   4.400   6.630
 &rst
  ixpk= 3, nxpk= 0, iat= 421, 402, r1= 3.90, r2= 4.40, r3= 6.63, r4= 7.13,  &end
#
#  14 DG  H8    14 DG  H1'   3.490   3.900
 &rst
  ixpk= 3, nxpk= 0, iat= 421, 418, r1= 2.99, r2= 3.49, r3= 3.90, r4= 4.40,  &end
#
#  14 DG  H3'   14 DG  H1'   3.170   4.000  (#3.170   3.400 7 25)
 &rst
  ixpk= 3, nxpk= 0, iat= 435, 418, r1= 2.67, r2= 3.17, r3= 4.00, r4= 4.50,  &end
#
#  14 DG  H3'   14 DG  H8    3.210   4.320  (#3.210   3.420 13 16 21)
 &rst
  ixpk= 3, nxpk= 0, iat= 435, 421, r1= 2.71, r2= 3.21, r3= 4.32, r4= 4.82,  &end
#
#  14 DG  H2'1  14 DG  H1'   2.400   4.770  (#3.000   4.770 5 20)
 &rst
  ixpk= 4, nxpk= 0, iat= 437, 418, r1= 1.90, r2= 2.40, r3= 4.77, r4= 5.27,  &end
#
#  14 DG  H2'2  14 DG  H1'   2.250   3.030  (#2.250   2.730 9)
 &rst
  ixpk= 2, nxpk= 0, iat= 438, 418, r1= 1.75, r2= 2.25, r3= 3.03, r4= 3.53,  &end
#
#  14 DG  H2'2  14 DG  H8    2.570   3.270  (#2.570   2.970 48)
 &rst
  ixpk= 2, nxpk= 0, iat= 438, 421, r1= 2.07, r2= 2.57, r3= 3.27, r4= 3.77,  &end
```

```
#
#  14 DG  H2'2  14 DG  H3'   2.040   3.120  (#2.640   3.120 15 22)
 &rst
  ixpk= 3, nxpk= 0, iat= 438, 435, r1= 1.54, r2= 2.04, r3= 3.12, r4= 3.62,  &end
#
#  15 DA  H8    14 DG  H1'   3.030   4.350  (#3.030   3.450 18 23 31)
 &rst
  ixpk= 3, nxpk= 0, iat= 454, 418, r1= 2.53, r2= 3.03, r3= 4.35, r4= 4.85,  &end
#
#  15 DA  H8    14 DG  H8    3.890   4.550  (#3.890   4.250 19)
 &rst
  ixpk= 4, nxpk= 0, iat= 454, 421, r1= 3.39, r2= 3.89, r3= 4.55, r4= 5.05,  &end
#
#  15 DA  H8    14 DG  H2'2  2.830   3.930
 &rst
  ixpk= 4, nxpk= 0, iat= 454, 438, r1= 2.33, r2= 2.83, r3= 3.93, r4= 4.43,  &end
#
#  15 DA  H8    15 DA  H1'   3.020   3.860
 &rst
  ixpk= 4, nxpk= 0, iat= 454, 451, r1= 2.52, r2= 3.02, r3= 3.86, r4= 4.36,  &end
#
#  15 DA  H3'   15 DA  H1'   3.340   3.980
 &rst
  ixpk= 4, nxpk= 0, iat= 467, 451, r1= 2.84, r2= 3.34, r3= 3.98, r4= 4.48,  &end
#
#  15 DA  H3'   15 DA  H8    2.940   3.930  (#2.940   3.330 27 48)
 &rst
  ixpk= 3, nxpk= 0, iat= 467, 454, r1= 2.44, r2= 2.94, r3= 3.93, r4= 4.43,  &end
#
#  15 DA  H2'1  15 DA  H1'   2.220   4.870  (#2.520   4.870 7)
 &rst
  ixpk= 4, nxpk= 0, iat= 469, 451, r1= 1.72, r2= 2.22, r3= 4.87, r4= 5.37,  &end
#
#  15 DA  H2'1  15 DA  H8    1.970   4.170  (#1.970   2.970 1 2 4 11)
 &rst
  ixpk= 2, nxpk= 0, iat= 469, 454, r1= 1.47, r2= 1.97, r3= 4.17, r4= 4.67,  &end
#
#  15 DA  H2'2  15 DA  H1'   2.030   3.110  (#2.030   2.810 29)
 &rst
  ixpk= 2, nxpk= 0, iat= 470, 451, r1= 1.53, r2= 2.03, r3= 3.11, r4= 3.61,  &end
#
#  15 DA  H2'2  15 DA  H8    2.510   4.490  (#2.810   4.490 33)
 &rst
  ixpk= 4, nxpk= 0, iat= 470, 454, r1= 2.01, r2= 2.51, r3= 4.49, r4= 4.99,  &end
#
#  16 DC  H6    15 DA  H1'   3.380   4.610  (#3.380   3.710 13 20 32)
 &rst
  ixpk= 3, nxpk= 0, iat= 486, 451, r1= 2.88, r2= 3.38, r3= 4.61, r4= 5.11,  &end
#
#  16 DC  H6    15 DA  H8    3.570   4.750  (#3.570   4.450  24)
 &rst
```

```
  ixpk= 4, nxpk= 0, iat= 486, 454, r1= 3.07, r2= 3.57, r3= 4.75, r4= 5.25,  &end
#
#  16 DC  H6    15 DA  H3'   3.880   5.060
 &rst
  ixpk= 4, nxpk= 0, iat= 486, 467, r1= 3.38, r2= 3.88, r3= 5.06, r4= 5.56,  &end
#
#  16 DC  H6    15 DA  H2'1  2.430   5.180  (#3.030   5.180 11 46)
 &rst
  ixpk= 5, nxpk= 0, iat= 486, 469, r1= 1.93, r2= 2.43, r3= 5.18, r4= 5.68,  &end
#
#  16 DC  H6    15 DA  H2'2  2.440   3.080
 &rst
  ixpk= 5, nxpk= 0, iat= 486, 470, r1= 1.94, r2= 2.44, r3= 3.08, r4= 3.58,  &end
#
#  16 DC  H5    15 DA  H1'   4.310   5.760
 (#16 DC  H5     6 DT  Q5    4.990   5.670)
 &rst
  ixpk= 5, nxpk= 0, iat= 488, 451, r1= 3.81, r2= 4.31, r3= 5.76, r4= 6.26,  &end
#
#  16 DC  H5    15 DA  H8    3.350   4.090  (#3.350   4.090 17 25)
 &rst
  ixpk= 4, nxpk= 0, iat= 488, 454, r1= 2.85, r2= 3.35, r3= 4.09, r4= 4.59,  &end
#
#  16 DC  H5    15 DA  H2'2  3.100   3.700
 &rst
  ixpk= 4, nxpk= 0, iat= 488, 470, r1= 2.60, r2= 3.10, r3= 3.70, r4= 4.20,  &end
#
#  16 DC  H3'   16 DC  H1'   2.980   3.810
 &rst
  ixpk= 4, nxpk= 0, iat= 497, 483, r1= 2.48, r2= 2.98, r3= 3.81, r4= 4.31,  &end
#
#  16 DC  H3'   16 DC  H6    2.890   4.180  (#2.890   3.280 16 19 31)
 &rst
  ixpk= 3, nxpk= 0, iat= 497, 486, r1= 2.39, r2= 2.89, r3= 4.18, r4= 4.68,  &end
#
#  16 DC  H3'   16 DC  H5    4.470   6.520
 &rst
  ixpk= 3, nxpk= 0, iat= 497, 488, r1= 3.97, r2= 4.47, r3= 6.52, r4= 7.02,  &end
#
#  16 DC  H2'1  16 DC  H1'   2.310   4.820  (#2.910   4.820 6 23)
 &rst
  ixpk= 4, nxpk= 0, iat= 499, 483, r1= 1.81, r2= 2.31, r3= 4.82, r4= 5.32,  &end
#
#  16 DC  H2'1  16 DC  H6    2.040   3.540  (#2.040   2.940 8 29)
 &rst
  ixpk= 2, nxpk= 0, iat= 499, 486, r1= 1.54, r2= 2.04, r3= 3.54, r4= 4.04,  &end
#
#  16 DC  H2'1  16 DC  H5    2.950   5.390  (# 2.950   4.190 4 9 22 36)
 &rst
  ixpk= 2, nxpk= 0, iat= 499, 488, r1= 2.45, r2= 2.95, r3= 5.39, r4= 5.89,  &end
#
```

```
#  16 DC  H2'1  16 DC  H3'   2.140   3.160
 &rst
  ixpk= 2, nxpk= 0, iat= 499, 497, r1= 1.64, r2= 2.14, r3= 3.16, r4= 3.66,  &end
#
#  16 DC  H2'2  16 DC  H1'   2.060   3.070  (#2.060   2.770 10)
 &rst
  ixpk= 2, nxpk= 0, iat= 500, 483, r1= 1.56, r2= 2.06, r3= 3.07, r4= 3.57,  &end
#
#  16 DC  H2'2  16 DC  H6    1.950   4.580  (#2.550   4.580 3 13)
 &rst
  ixpk= 4, nxpk= 0, iat= 500, 486, r1= 1.45, r2= 1.95, r3= 4.58, r4= 5.08,  &end
#
#  16 DC  H2'2  16 DC  H5    2.930   5.450
 &rst
  ixpk= 4, nxpk= 0, iat= 500, 488, r1= 2.43, r2= 2.93, r3= 5.45, r4= 5.95,  &end
#
#  16 DC  H2'2  16 DC  H3'   2.250   4.940  (#2.850   4.940 7 15)
 &rst
  ixpk= 4, nxpk= 0, iat= 500, 497, r1= 1.75, r2= 2.25, r3= 4.94, r4= 5.44,  &end
#
#  17 RDI H2'1  17 RDI H1'   2.400   4.490  (#2.700   4.490 19)
 &rst
  ixpk= 4, nxpk= 0, iat= 515, 513, r1= 1.90, r2= 2.40, r3= 4.49, r4= 4.99,  &end
#
#  17 RDI H2'2  17 RDI H1'   2.130   3.090
 &rst
  ixpk= 4, nxpk= 0, iat= 516, 513, r1= 1.63, r2= 2.13, r3= 3.09, r4= 3.59,  &end
#
#  17 RDI HA1    5 DT  H1'   3.210   5.770  (#3.210   5.470 26)
 &rst
  ixpk= 5, nxpk= 0, iat= 526, 134, r1= 2.71, r2= 3.21, r3= 5.77, r4= 6.27,  &end
#
#  17 RDI HA1    6 DT  Q5    2.880   4.630
 &rst
  ixpk= 5, nxpk= 0, iat= 526,  -1, r1= 2.38, r2= 2.88, r3= 5.56, r4= 6.06,
 igr2= 172, 173, 174,
 &end
#
#  17 RDI HA1   17 RDI H2    3.340   3.800
 &rst
  ixpk= 5, nxpk= 0, iat= 526, 524, r1= 2.84, r2= 3.34, r3= 3.80, r4= 4.30,  &end
#
#  17 RDI HA2   17 RDI H2    1.800   2.530  (#1.800   2.230  42)
 &rst
  ixpk= 2, nxpk= 0, iat= 527, 524, r1= 1.30, r2= 1.80, r3= 2.53, r4= 3.03,  &end
#
#  17 RDI HB     5 DT  H1'   4.540   6.120
 &rst
  ixpk= 2, nxpk= 0, iat= 529, 134, r1= 4.04, r2= 4.54, r3= 6.12, r4= 6.62,  &end
#
#  17 RDI HB    17 RDI H2    2.080   2.550  (#2.140   2.630 13 34(HA2))
```

```
 &rst
  ixpk= 2, nxpk= 0, iat= 529, 524, r1= 1.58, r2= 2.08, r3= 2.55, r4= 3.05,  &end
#
#  17 RDI HC     5 DT  H1'   2.700   3.360
 &rst
  ixpk= 2, nxpk= 0, iat= 531, 134, r1= 2.20, r2= 2.70, r3= 3.36, r4= 3.86,  &end
#
#  17 RDI HC     6 DT  H6    4.380   5.290
 &rst
  ixpk= 2, nxpk= 0, iat= 531, 169, r1= 3.88, r2= 4.38, r3= 5.29, r4= 5.79,  &end
#
#  17 RDI HC     6 DT  Q5    3.540   6.280  (#3.840   6.280 30)
 &rst
  ixpk= 6, nxpk= 0, iat= 531,  -1, r1= 3.04, r2= 3.54, r3= 7.54, r4= 8.04,
 igr2= 172, 173, 174,
 &end
#
#  17 RDI HC    17 RDI H2    2.300   4.480  (#3.540   5.350 34 37 38 39 40 41 44)
 &rst
  ixpk= 5, nxpk= 0, iat= 531, 524, r1= 1.80, r2= 2.30, r3= 4.48, r4= 4.98,  &end
#
#  17 RDI HD1    5 DT  H6    3.630   4.990  (#3.630   4.690 27)
 &rst
  ixpk= 4, nxpk= 0, iat= 533, 137, r1= 3.13, r2= 3.63, r3= 4.99, r4= 5.49,  &end
#
#  17 RDI HD1    5 DT  Q5    3.120   5.440
 &rst
  ixpk= 4, nxpk= 0, iat= 533,  -1, r1= 2.62, r2= 3.12, r3= 6.53, r4= 7.03,
 igr2= 140, 141, 142,
 &end
#
#  17 RDI HD1    5 DT  H2'1  2.600   3.410
 &rst
  ixpk= 4, nxpk= 0, iat= 533, 152, r1= 2.10, r2= 2.60, r3= 3.41, r4= 3.91,  &end
#
#  17 RDI HD1    5 DT  H1'   3.560   6.240
 &rst
  ixpk= 4, nxpk= 0, iat= 533, 134, r1= 3.06, r2= 3.56, r3= 6.24, r4= 6.74,  &end
#
#  17 RDI HD1    6 DT  Q5    2.540   5.040  (#2.840   5.040 23)
 &rst
  ixpk= 5, nxpk= 0, iat= 533,  -1, r1= 2.04, r2= 2.54, r3= 6.05, r4= 6.55,
 igr2= 172, 173, 174,
 &end
#
#  17 RDI HD2    5 DT  H2'1  3.130   5.560
 (#17 RDI HD1   17 RDI HA2   2.250   3.550)
 &rst
  ixpk= 5, nxpk= 0, iat= 534, 152, r1= 2.63, r2= 3.13, r3= 5.56, r4= 6.06,  &end
#
#  17 RDI HD2    6 DT  Q5    3.310   5.720
```

```
 &rst
  ixpk= 5, nxpk= 0, iat= 534,  -1, r1= 2.81, r2= 3.31, r3= 6.87, r4= 7.37,
 igr2= 172, 173, 174,
 &end
#
#  17 RDI HD2    5 DT  H1'   3.320   5.590
 (#17 RDI HD2   17 RDI H2    2.160   3.470 #2.160   2.870 21 29)
 &rst
  ixpk= 5, nxpk= 0, iat= 534, 134, r1= 2.82, r2= 3.32, r3= 5.59, r4= 6.09,  &end
#
#  17 RDI H8    16 DC  H6    4.540   6.280
 (#17 RDI HD2   17 RDI HA2   2.680   6.090)
 &rst
  ixpk= 5, nxpk= 0, iat= 540, 486, r1= 4.04, r2= 4.54, r3= 6.28, r4= 6.78,  &end
#
#  17 RDI H8    16 DC  H3'   3.760   4.260
 &rst
  ixpk= 5, nxpk= 0, iat= 540, 497, r1= 3.26, r2= 3.76, r3= 4.26, r4= 4.76,  &end
#
#  17 RDI H8    16 DC  H2'1  3.190   4.260
 &rst
  ixpk= 5, nxpk= 0, iat= 540, 499, r1= 2.69, r2= 3.19, r3= 4.26, r4= 4.76,  &end
#
#  17 RDI H8    16 DC  H2'2  3.220   4.130
 &rst
  ixpk= 5, nxpk= 0, iat= 540, 500, r1= 2.72, r2= 3.22, r3= 4.13, r4= 4.63,  &end
#
#  17 RDI H8    17 RDI H1'   2.900   3.860  (#2.900   3.560 48)
 &rst
  ixpk= 3, nxpk= 0, iat= 540, 513, r1= 2.40, r2= 2.90, r3= 3.86, r4= 4.36,  &end
#
#  17 RDI H8    17 RDI H2'1  2.020   3.020  (#2.020   2.720 15)
 &rst
  ixpk= 2, nxpk= 0, iat= 540, 515, r1= 1.52, r2= 2.02, r3= 3.02, r4= 3.52,  &end
#
#  17 RDI H8    17 RDI H2'2  2.330   4.660  (#2.930   4.660 3 10)
 &rst
  ixpk= 4, nxpk= 0, iat= 540, 516, r1= 1.83, r2= 2.33, r3= 4.66, r4= 5.16,  &end
#
#  17 RDI H3'   17 RDI H8    3.260   4.770  (#3.260   4.170 6 33)
 &rst
  ixpk= 4, nxpk= 0, iat= 542, 540, r1= 2.76, r2= 3.26, r3= 4.77, r4= 5.27,  &end
#
#  18 DA  H8    17 RDI H1'   3.300   5.770  (#3.900   5.770 16 31)
 &rst
  ixpk= 5, nxpk= 0, iat= 558, 513, r1= 2.80, r2= 3.30, r3= 5.77, r4= 6.27,  &end
#
#  18 DA  H8    17 RDI H2'1  2.610   4.100  (#2.910   4.100 22)
 &rst
  ixpk= 4, nxpk= 0, iat= 558, 515, r1= 2.11, r2= 2.61, r3= 4.10, r4= 4.60,  &end
#
```

```
# 18 DA  H8    17 RDI H2'2  2.830   4.410
 &rst
  ixpk= 4, nxpk= 0, iat= 558, 516, r1= 2.33, r2= 2.83, r3= 4.41, r4= 4.91,  &end
#
# 18 DA  H8    17 RDI H3'   3.930   5.360  (#3.930   4.460 11 20 25)
 &rst
  ixpk= 4, nxpk= 0, iat= 558, 542, r1= 3.43, r2= 3.93, r3= 5.36, r4= 5.86,  &end
#
# 18 DA  H8    18 DA  H1'   3.210   6.280
 &rst
  ixpk= 4, nxpk= 0, iat= 558, 555, r1= 2.71, r2= 3.21, r3= 6.28, r4= 6.78,  &end
#
# 18 DA  H2    17 RDI HA2   2.730   3.730  (# 2.810   3.210 1 2 4 5 7 24 34 36 45)
 &rst
  ixpk= 2, nxpk= 0, iat= 567, 527, r1= 2.23, r2= 2.73, r3= 3.73, r4= 4.23,  &end
#
# 18 DA  H2    17 RDI HB    2.790   3.710  (#2.790   3.110 43 46)
 &rst
  ixpk= 3, nxpk= 0, iat= 567, 529, r1= 2.29, r2= 2.79, r3= 3.71, r4= 4.21,  &end
#
# 18 DA  H2    17 RDI HC    3.190   4.020  (#3.790   4.020 8 9)
 &rst
  ixpk= 4, nxpk= 0, iat= 567, 531, r1= 2.69, r2= 3.19, r3= 4.02, r4= 4.52,  &end
#
# 18 DA  H2    17 RDI HD1   3.850   6.000
 &rst
  ixpk= 4, nxpk= 0, iat= 567, 533, r1= 3.35, r2= 3.85, r3= 6.00, r4= 6.50,  &end
#
# 18 DA  H2    17 RDI HD2   4.160   6.560
 &rst
  ixpk= 4, nxpk= 0, iat= 567, 534, r1= 3.66, r2= 4.16, r3= 6.56, r4= 7.06,  &end
#
# 18 DA  H3'   18 DA  H1'   3.280   5.370
 &rst
  ixpk= 4, nxpk= 0, iat= 571, 555, r1= 2.78, r2= 3.28, r3= 5.37, r4= 5.87,  &end
#
# 18 DA  H3'   18 DA  H8    3.500   5.450
 &rst
  ixpk= 4, nxpk= 0, iat= 571, 558, r1= 3.00, r2= 3.50, r3= 5.45, r4= 5.95,  &end
#
# 18 DA  H2'1  18 DA  H1'   1.910   3.010  (#1.910   2.710 39)
 &rst
  ixpk= 2, nxpk= 0, iat= 573, 555, r1= 1.41, r2= 1.91, r3= 3.01, r4= 3.51,  &end
#
# 18 DA  H2'1  18 DA  H8    1.850   3.360  (#1.850   2.760 17 18 26 47)
 &rst
  ixpk= 2, nxpk= 0, iat= 573, 558, r1= 1.35, r2= 1.85, r3= 3.36, r4= 3.86,  &end
#
# 19 DG  H8    18 DA  H1'   3.480   5.120
 &rst
  ixpk= 2, nxpk= 0, iat= 590, 555, r1= 2.98, r2= 3.48, r3= 5.12, r4= 5.62,  &end
```

```
#
#  19 DG  H8    18 DA  H8    4.290   6.220
 &rst
  ixpk= 2, nxpk= 0, iat= 590, 558, r1= 3.79, r2= 4.29, r3= 6.22, r4= 6.72,  &end
#
#  19 DG  H8    18 DA  H2'1  2.180   3.000
 &rst
  ixpk= 2, nxpk= 0, iat= 590, 573, r1= 1.68, r2= 2.18, r3= 3.00, r4= 3.50,  &end
#
#  19 DG  H8    19 DG  H1'   3.440   5.470
 &rst
  ixpk= 2, nxpk= 0, iat= 590, 587, r1= 2.94, r2= 3.44, r3= 5.47, r4= 5.97,  &end
#
#  19 DG  H3'   19 DG  H1'   3.420   5.020
 &rst
  ixpk= 2, nxpk= 0, iat= 604, 587, r1= 2.92, r2= 3.42, r3= 5.02, r4= 5.52,  &end
#
#  19 DG  H2'1  19 DG  H1'   2.450   5.660  (#2.750   5.660 6)
 &rst
  ixpk= 5, nxpk= 0, iat= 606, 587, r1= 1.95, r2= 2.45, r3= 5.66, r4= 6.16,  &end
#
#  19 DG  H2'1  19 DG  H8    2.140   3.160  (#2.140   2.860 25)
 &rst
  ixpk= 2, nxpk= 0, iat= 606, 590, r1= 1.64, r2= 2.14, r3= 3.16, r4= 3.66,  &end
#
#  19 DG  H2'2  19 DG  H1'   2.130   3.000  (#2.130   2.700 2)
 &rst
  ixpk= 2, nxpk= 0, iat= 607, 587, r1= 1.63, r2= 2.13, r3= 3.00, r4= 3.50,  &end
#
#  19 DG  H2'2  19 DG  H8    2.260   3.860  (#2.260   3.260 37 42)
 &rst
  ixpk= 3, nxpk= 0, iat= 607, 590, r1= 1.76, r2= 2.26, r3= 3.86, r4= 4.36,  &end
#
#  20 DA  H8    19 DG  H1'   3.040   3.380
 &rst
  ixpk= 3, nxpk= 0, iat= 623, 587, r1= 2.54, r2= 3.04, r3= 3.38, r4= 3.88,  &end
#
#  20 DA  H8    19 DG  H8    4.020   5.610
 &rst
  ixpk= 3, nxpk= 0, iat= 623, 590, r1= 3.52, r2= 4.02, r3= 5.61, r4= 6.11,  &end
#
#  20 DA  H8    19 DG  H3'   3.830   5.620
 &rst
  ixpk= 3, nxpk= 0, iat= 623, 604, r1= 3.33, r2= 3.83, r3= 5.62, r4= 6.12,  &end
#
#  20 DA  H8    19 DG  H2'1  2.930   3.520
 &rst
  ixpk= 3, nxpk= 0, iat= 623, 606, r1= 2.43, r2= 2.93, r3= 3.52, r4= 4.02,  &end
#
#  20 DA  H8    20 DA  H1'   3.490   4.030
 &rst
```

```
  ixpk= 3, nxpk= 0, iat= 623, 620, r1= 2.99, r2= 3.49, r3= 4.03, r4= 4.53,  &end
#
#  20 DA  H3'   20 DA  H1'   3.400   4.660
 &rst
  ixpk= 3, nxpk= 0, iat= 636, 620, r1= 2.90, r2= 3.40, r3= 4.66, r4= 5.16,  &end
#
#  20 DA  H2'1  20 DA  H1'   2.290   4.250  (#2.590   4.250 20)
 &rst
  ixpk= 4, nxpk= 0, iat= 638, 620, r1= 1.79, r2= 2.29, r3= 4.25, r4= 4.75,  &end
#
#  20 DA  H2'2  20 DA  H1'   2.070   3.150  (#2.070   2.850 7)
 &rst
  ixpk= 2, nxpk= 0, iat= 639, 620, r1= 1.57, r2= 2.07, r3= 3.15, r4= 3.65,  &end
#
#  20 DA  H2'2  20 DA  H8    2.170   3.820  (#2.470   2.920 13 38 39 42)
 &rst
  ixpk= 2, nxpk= 0, iat= 639, 623, r1= 1.67, r2= 2.17, r3= 3.82, r4= 4.32,  &end
#
#  20 DA  H2'2  20 DA  H3'   2.100   2.930  (#2.100   2.630 43)
 &rst
  ixpk= 2, nxpk= 0, iat= 639, 636, r1= 1.60, r2= 2.10, r3= 2.93, r4= 3.43,  &end
#
#  21 DA  H8    20 DA  H1'   3.400   4.110
 (#21 DA  H1'   20 DA  H2    3.450   3.970)
 &rst
  ixpk= 2, nxpk= 0, iat= 655, 620, r1= 2.90, r2= 3.40, r3= 4.11, r4= 4.61,  &end
#
#  21 DA  H8    20 DA  H8    3.790   6.410  (#3.790   6.110 29)
 &rst
  ixpk= 6, nxpk= 0, iat= 655, 623, r1= 3.29, r2= 3.79, r3= 6.41, r4= 6.91,  &end
#
#  21 DA  H8    20 DA  H3'   3.650   5.650
 &rst
  ixpk= 6, nxpk= 0, iat= 655, 636, r1= 3.15, r2= 3.65, r3= 5.65, r4= 6.15,  &end
#
#  21 DA  H8    20 DA  H2'1  2.330   3.460  (#2.930   3.460 23 44)
 &rst
  ixpk= 3, nxpk= 0, iat= 655, 638, r1= 1.83, r2= 2.33, r3= 3.46, r4= 3.96,  &end
#
#  21 DA  H8    21 DA  H1'   2.920   4.420
 &rst
  ixpk= 3, nxpk= 0, iat= 655, 652, r1= 2.42, r2= 2.92, r3= 4.42, r4= 4.92,  &end
#
#  21 DA  H3'   21 DA  H1'   3.290   4.040  (#3.290   3.740 21)
 &rst
  ixpk= 3, nxpk= 0, iat= 668, 652, r1= 2.79, r2= 3.29, r3= 4.04, r4= 4.54,  &end
#
#  21 DA  H3'   21 DA  H8    3.280   4.120
 &rst
  ixpk= 3, nxpk= 0, iat= 668, 655, r1= 2.78, r2= 3.28, r3= 4.12, r4= 4.62,  &end
#
```

```
#  21 DA  H2'1  21 DA  H1'   2.090   4.590  (#2.990   4.590 5 10 15)
 &rst
  ixpk= 4, nxpk= 0, iat= 670, 652, r1= 1.59, r2= 2.09, r3= 4.59, r4= 5.09,  &end
#
#  21 DA  H2'1  21 DA  H8    2.000   3.950  (#2.000   2.850 4 7 11 27)
 &rst
  ixpk= 2, nxpk= 0, iat= 670, 655, r1= 1.50, r2= 2.00, r3= 3.95, r4= 4.45,  &end
#
#  21 DA  H2'2  21 DA  H1'   2.000   3.040  (#2.000   2.740 3)
 &rst
  ixpk= 2, nxpk= 0, iat= 671, 652, r1= 1.50, r2= 2.00, r3= 3.04, r4= 3.54,  &end
#
#  21 DA  H2'2  21 DA  H8    2.260   3.960
 &rst
  ixpk= 2, nxpk= 0, iat= 671, 655, r1= 1.76, r2= 2.26, r3= 3.96, r4= 4.46,  &end
#
#  21 DA  H2'2  21 DA  H3'   2.150   3.010  (#2.450   3.010 17)
 &rst
  ixpk= 3, nxpk= 0, iat= 671, 668, r1= 1.65, r2= 2.15, r3= 3.01, r4= 3.51,  &end
#
#  22 DG3 H8    21 DA  H8    3.730   6.240  (#3.730   5.340 30 32 33)
 &rst
  ixpk= 5, nxpk= 0, iat= 687, 655, r1= 3.23, r2= 3.73, r3= 6.24, r4= 6.74,  &end
#
#  22 DG3 H8    21 DA  H3'   3.670   4.480  (#3.670   4.180 36)
 &rst
  ixpk= 4, nxpk= 0, iat= 687, 668, r1= 3.17, r2= 3.67, r3= 4.48, r4= 4.98,  &end
#
#  22 DG3 H8    21 DA  H2'1  2.440   3.430
 &rst
  ixpk= 4, nxpk= 0, iat= 687, 670, r1= 1.94, r2= 2.44, r3= 3.43, r4= 3.93,  &end
#
#  22 DG3 H8    21 DA  H2'2  2.490   3.790  (#2.490   3.190 16 26)
 &rst
  ixpk= 3, nxpk= 0, iat= 687, 671, r1= 1.99, r2= 2.49, r3= 3.79, r4= 4.29,  &end
#
#  22 DG3 H3'   22 DG3 H1'   2.670   3.760  (#3.270   3.460 9 19 40)
 &rst
  ixpk= 3, nxpk= 0, iat= 701, 684, r1= 2.17, r2= 2.67, r3= 3.76, r4= 4.26,  &end
#
#  22 DG3 H3'   22 DG3 H8    2.490   4.970  (#2.490   3.470 2 8 11 18 22)
 &rst
  ixpk= 3, nxpk= 0, iat= 701, 687, r1= 1.99, r2= 2.49, r3= 4.97, r4= 5.47,  &end
#
#  22 DG3 H2'1  22 DG3 H1'   2.150   3.220  (#2.150   2.620 37 41)
 &rst
  ixpk= 2, nxpk= 0, iat= 703, 684, r1= 1.65, r2= 2.15, r3= 3.22, r4= 3.72,  &end
#
#  22 DG3 H2'1  22 DG3 H8    2.180   4.420  (#2.480   4.120 39 45)
 &rst
  ixpk= 4, nxpk= 0, iat= 703, 687, r1= 1.68, r2= 2.18, r3= 4.42, r4= 4.92,  &end
```

```
#
#  22 DG3 H2'2  22 DG3 H1'   2.600   4.650
 &rst
  ixpk= 4, nxpk= 0, iat= 704, 684, r1= 2.10, r2= 2.60, r3= 4.65, r4= 5.15,  &end
#
#  22 DG3 H2'2  22 DG3 H8    2.020   3.120  (#2.020   2.520 42 43)
 &rst
  ixpk= 2, nxpk= 0, iat= 704, 687, r1= 1.52, r2= 2.02, r3= 3.12, r4= 3.62,  &end
#
#  17 RDI        HA2    7 DG  H1    3.250   4.770  (#H2O 27 35 37)
 &rst
  ixpk= 27, nxpk= 0, iat= 527, 207, r1= 2.75, r2= 3.25, r3= 4.77, r4= 5.27,  &end
#
#  17 RDI        HA2   16 DC  H42   4.030   6.070  (#H2O)
 &rst
  ixpk= 27, nxpk= 0, iat= 527, 492, r1= 3.53, r2= 4.03, r3= 6.07, r4= 6.57,  &end
#
#  16 DC  H41    6 DT  Q5    2.590   4.940  (#H2O)
 &rst
  ixpk= 27, nxpk= 0, iat= 491,  -1, r1= 2.09, r2= 2.59, r3= 5.93, r4= 6.43,
 igr2= 172, 173, 174,
 &end
#
#  16 DC  H42    6 DT  Q5        2.600   5.120  (#H2O)
 &rst
  ixpk= 27, nxpk= 0, iat= 492,  -1, r1= 2.10, r2= 2.60, r3= 6.15, r4= 6.65,
 igr2= 172, 173, 174,
 &end
#
#   1  DC5  H42    22  DG3  O6      1.80   2.00
 &rst
  ixpk= 0, nxpk= 0, iat=  19, 691, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,
      rk2=32.0, rk3=32.0, ir6=1, ialtd=0,
 &end
#
#   1  DC5  N3     22  DG3  H1      1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  20, 693, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   1  DC5  N3     22  DG3  N1      2.85   3.05
 &rst
  ixpk= 0, nxpk= 0, iat=  20, 692, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#   1  DC5  N4     22  DG3  O6      2.81   3.01
 &rst
  ixpk= 0, nxpk= 0, iat=  17, 691, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#   1  DC5  O2     22  DG3  H22     1.75   1.95
 &rst
  ixpk= 0, nxpk= 0, iat=  22, 697, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
```

```
#   2  DT   H3     21  DA   N1      1.71   1.91
 &rst
  ixpk= 0, nxpk= 0, iat=  52, 662, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
#   2  DT   N3     21  DA   N1      2.72   2.92
 &rst
  ixpk= 0, nxpk= 0, iat=  51, 662, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
#   2  DT   O4     21  DA   H61     1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  50, 660, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   3  DT   H3     20  DA   N1      1.71   1.91
 &rst
  ixpk= 0, nxpk= 0, iat=  84, 630, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
#   3  DT   N3     20  DA   N1      2.72   2.92
 &rst
  ixpk= 0, nxpk= 0, iat=  83, 630, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
#   3  DT   O4     20  DA   H61     1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat=  82, 628, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   4  DC   H42    19  DG   O6      1.80   2.00
 &rst
  ixpk= 0, nxpk= 0, iat= 113, 594, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
#   4  DC   N3     19  DG   H1      1.84   2.04
 &rst
  ixpk= 0, nxpk= 0, iat= 114, 596, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   4  DC   N3     19  DG   N1      2.85   3.05
 &rst
  ixpk= 0, nxpk= 0, iat= 114, 595, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#   4  DC   N4     19  DG   O6      2.81   3.01
 &rst
  ixpk= 0, nxpk= 0, iat= 111, 594, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#   4  DC   O2     19  DG   H22     1.75   1.95
 &rst
  ixpk= 0, nxpk= 0, iat= 116, 600, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#   5  DT   H3     18  DA   N1      1.61   2.01  (#1.71   1.91 )
 &rst
  ixpk= 1, nxpk= 0, iat= 146, 565, r1= 1.11, r2= 1.61, r3= 2.01, r4= 2.51,  &end
#
#   5  DT   N3     18  DA   N1      2.62   3.02  (#2.72   2.92 )
 &rst
  ixpk= 2, nxpk= 0, iat= 145, 565, r1= 2.12, r2= 2.62, r3= 3.02, r4= 3.52,  &end
```

```
#
#   5  DT   O4     18  DA   H61     1.74   2.14  (#1.84   2.04)
 &rst
  ixpk= 2, nxpk= 0, iat= 144, 563, r1= 1.24, r2= 1.74, r3= 2.14, r4= 2.64,  &end
#
#   7  DG   H1     16  DC   N3      1.84   2.04
 &rst
  ixpk= 2, nxpk= 0, iat= 207, 493, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   7  DG   H22    16  DC   O2      1.75   1.95
 &rst
  ixpk= 2, nxpk= 0, iat= 211, 495, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#   7  DG   N1     16  DC   N3      2.85   3.05
 &rst
  ixpk= 2, nxpk= 0, iat= 206, 493, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#   7  DG   O6     16  DC   H42     1.80   2.00
 &rst
  ixpk= 2, nxpk= 0, iat= 205, 492, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
#   7  DG   O6     16  DC   N4      2.81   3.01
 &rst
  ixpk= 2, nxpk= 0, iat= 205, 490, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#   8  DT   H3     15  DA   N1      1.71   1.91
 &rst
  ixpk= 2, nxpk= 0, iat= 243, 461, r1= 1.21, r2= 1.71, r3= 1.91, r4= 2.41,  &end
#
#   8  DT   N3     15  DA   N1      2.72   2.92
 &rst
  ixpk= 2, nxpk= 0, iat= 242, 461, r1= 2.22, r2= 2.72, r3= 2.92, r4= 3.42,  &end
#
#   8  DT   O4     15  DA   H61     1.84   2.04
 &rst
  ixpk= 2, nxpk= 0, iat= 241, 459, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   9  DC   H42    14  DG   O6      1.80   2.00
 &rst
  ixpk= 2, nxpk= 0, iat= 272, 425, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
#   9  DC   N3     14  DG   H1      1.84   2.04
 &rst
  ixpk= 2, nxpk= 0, iat= 273, 427, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#   9  DC   N3     14  DG   N1      2.85   3.05
 &rst
  ixpk= 2, nxpk= 0, iat= 273, 426, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#   9  DC   N4     14  DG   O6      2.81   3.01
 &rst
```

```
 ixpk= 2, nxpk= 0, iat= 270, 425, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#   9  DC   O2     14  DG   H22     1.75   1.95
 &rst
 ixpk= 2, nxpk= 0, iat= 275, 431, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#  10  DC   H42    13  DG   O6      1.80   2.00
 &rst
 ixpk= 2, nxpk= 0, iat= 302, 392, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
#  10  DC   N3     13  DG   H1      1.84   2.04
 &rst
 ixpk= 2, nxpk= 0, iat= 303, 394, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#  10  DC   N3     13  DG   N1      2.85   3.05
 &rst
 ixpk= 2, nxpk= 0, iat= 303, 393, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#  10  DC   N4     13  DG   O6      2.81   3.01
 &rst
 ixpk= 2, nxpk= 0, iat= 300, 392, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
#
#  10  DC   O2     13  DG   H22     1.75   1.95
 &rst
 ixpk= 2, nxpk= 0, iat= 305, 398, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#  11  DG3  H1     12  DC5  N3      1.84   2.04
 &rst
 ixpk= 2, nxpk= 0, iat= 332, 365, r1= 1.34, r2= 1.84, r3= 2.04, r4= 2.54,  &end
#
#  11  DG3  H22    12  DC5  O2      1.75   1.95
 &rst
 ixpk= 2, nxpk= 0, iat= 336, 367, r1= 1.25, r2= 1.75, r3= 1.95, r4= 2.45,  &end
#
#  11  DG3  N1     12  DC5  N3      2.85   3.05
 &rst
 ixpk= 2, nxpk= 0, iat= 331, 365, r1= 2.35, r2= 2.85, r3= 3.05, r4= 3.55,  &end
#
#  11  DG3  O6     12  DC5  H42     1.80   2.00
 &rst
 ixpk= 2, nxpk= 0, iat= 330, 364, r1= 1.30, r2= 1.80, r3= 2.00, r4= 2.50,  &end
#
#  11  DG3  O6     12  DC5  N4      2.81   3.01
 &rst
 ixpk= 2, nxpk= 0, iat= 330, 362, r1= 2.31, r2= 2.81, r3= 3.01, r4= 3.51,  &end
# 706 atoms read from pdb file RdI_Major_New_v3.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 =64.0, rk3 =64.0,                          &end
```

```
# 3 DT ALPHA:  (2 DT O3')-(3 DT P)-(3 DT O5')-(3 DT 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 DC ALPHA:  (3 DT O3')-(4 DC P)-(4 DC O5')-(4 DC C5') -90.0 -30.0
 &rst    iat =    92,    93,    96,    97,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 5 DT ALPHA:  (4 DC O3')-(5 DT P)-(5 DT O5')-(5 DT C5') -90.0 -30.0
 &rst    iat =   122,   123,   126,   127,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 6 DT ALPHA:  (5 DT O3')-(6 DT P)-(6 DT O5')-(6 DT C5') -120.0  -0.0
 &rst    iat =   154,   155,   158,   159,
          r1 = -121.0, r2 = -120.0, r3 =  -0.0, r4 =   1.0,
         &end

# 7 DG ALPHA:  (6 DT O3')-(7 DG P)-(7 DG O5')-(7 DG C5') -90.0 -30.0
 &rst    iat =   186,   187,   190,   191,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 8 DT ALPHA:  (7 DG O3')-(8 DT P)-(8 DT O5')-(8 DT C5') -90.0 -30.0
 &rst    iat =   219,   220,   223,   224,
          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 =   251,   252,   255,   256,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 10 DC ALPHA:  (9 DC O3')-(10 DC P)-(10 DC O5')-(10 DC C5') -90.0 -30.0
 &rst    iat =   281,   282,   285,   286,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 13 DG ALPHA:  (12 DC5 O3')-(13 DG P)-(13 DG O5')-(13 DG C5') -90.0 -30.0
 &rst    iat =   373,   374,   377,   378,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 14 DG ALPHA:  (13 DG O3')-(14 DG P)-(14 DG O5')-(14 DG C5') -90.0 -30.0
 &rst    iat =   406,   407,   410,   411,
          r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 15 DA ALPHA:  (14 DG O3')-(15 DA P)-(15 DA O5')-(15 DA C5') -90.0 -30.0
```

```
 &rst     iat =   439,   440,   443,   444,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 16 DC ALPHA:  (15 DA O3')-(16 DC P)-(16 DC O5')-(16 DC C5') -90.0 -30.0
 &rst     iat =   471,   472,   475,   476,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 17 RDI ALPHA:  (16 DC O3')-(17 RDI P)-(17 RDI O5')-(17 RDI C5') -120.0   0.0
 &rst     iat =   501,   502,   505,   506,
           r1 = -121.0, r2 = -120.0, r3 =   0.0, r4 =   1.0,
         &end

# 18 DA ALPHA:  (17 RDI O3')-(18 DA P)-(18 DA O5')-(18 DA C5') -90.0 -30.0
 &rst     iat =   543,   544,   547,   548,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 19 DG ALPHA:  (18 DA O3')-(19 DG P)-(19 DG O5')-(19 DG C5') -90.0 -30.0
 &rst     iat =   575,   576,   579,   580,
           r1 = -91.0, r2 = -90.0, r3 = -30.0, r4 = -29.0,
         &end

# 20 DA ALPHA:  (19 DG O3')-(20 DA P)-(20 DA O5')-(20 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

# 21 DA ALPHA:  (20 DA O3')-(21 DA P)-(21 DA O5')-(21 DA C5') -90.0 -30.0
 &rst     iat =   640,   641,   644,   645,
           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 DT BETA:  (3 DT P)-(3 DT O5')-(3 DT C5')-(3 DT 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 DC BETA:  (4 DC P)-(4 DC O5')-(4 DC C5')-(4 DC C4') 150.0 210.0
 &rst     iat =    93,    96,    97,   100,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 5 DT BETA:  (5 DT P)-(5 DT O5')-(5 DT C5')-(5 DT C4') 150.0 210.0
 &rst     iat =   123,   126,   127,   130,
```

```
           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') 120.0 240.0
 &rst     iat =   155,   158,   159,   162,
           r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,
          &end

# 7 DG BETA:  (7 DG P)-(7 DG O5')-(7 DG C5')-(7 DG C4') 150.0 210.0
 &rst     iat =   187,   190,   191,   194,
           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 =   220,   223,   224,   227,
           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 =   252,   255,   256,   259,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 10 DC BETA:  (10 DC P)-(10 DC O5')-(10 DC C5')-(10 DC C4') 150.0 210.0
 &rst     iat =   282,   285,   286,   289,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 13 DG BETA:  (13 DG P)-(13 DG O5')-(13 DG C5')-(13 DG C4') 150.0 210.0
 &rst     iat =   374,   377,   378,   381,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 14 DG BETA:  (14 DG P)-(14 DG O5')-(14 DG C5')-(14 DG C4') 150.0 210.0
 &rst     iat =   407,   410,   411,   414,
           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 =   440,   443,   444,   447,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 16 DC BETA:  (16 DC P)-(16 DC O5')-(16 DC C5')-(16 DC C4') 150.0 210.0
 &rst     iat =   472,   475,   476,   479,
           r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
          &end

# 17 RDI BETA:  (17 RDI P)-(17 RDI O5')-(17 RDI C5')-(17 RDI C4') 120.0 240.0
 &rst     iat =   502,   505,   506,   509,
           r1 = 119.0, r2 = 120.0, r3 = 240.0, r4 = 241.0,
```

```
         &end

# 18 DA BETA:  (18 DA P)-(18 DA O5')-(18 DA C5')-(18 DA C4') 150.0 210.0
 &rst    iat =   544,   547,   548,   551,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 19 DG BETA:  (19 DG P)-(19 DG O5')-(19 DG C5')-(19 DG C4') 150.0 210.0
 &rst    iat =   576,   579,   580,   583,
          r1 = 149.0, r2 = 150.0, r3 = 210.0, r4 = 211.0,
         &end

# 20 DA BETA:  (20 DA P)-(20 DA O5')-(20 DA C5')-(20 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

# 21 DA BETA:  (21 DA P)-(21 DA O5')-(21 DA C5')-(21 DA C4') 150.0 210.0
 &rst    iat =   641,   644,   645,   648,
          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 DT GAMMA:  (3 DT O5')-(3 DT C5')-(3 DT C4')-(3 DT 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 DC GAMMA:  (4 DC O5')-(4 DC C5')-(4 DC C4')-(4 DC C3')  30.0  90.0
 &rst    iat =    96,    97,   100,   117,
          r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
         &end

# 5 DT GAMMA:  (5 DT O5')-(5 DT C5')-(5 DT C4')-(5 DT C3')  30.0  90.0
 &rst    iat =   126,   127,   130,   149,
          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')   0.0 120.0
 &rst    iat =   158,   159,   162,   181,
          r1 =  -1.0, r2 =   0.0, r3 = 120.0, r4 = 121.0,
         &end

# 7 DG GAMMA:  (7 DG O5')-(7 DG C5')-(7 DG C4')-(7 DG C3')  30.0  90.0
 &rst    iat =   190,   191,   194,   214,
          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 =   223,   224,   227,   246,
           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 =   255,   256,   259,   276,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 10 DC GAMMA:  (10 DC O5')-(10 DC C5')-(10 DC C4')-(10 DC C3')  30.0  90.0
 &rst     iat =   285,   286,   289,   306,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 13 DG GAMMA:  (13 DG O5')-(13 DG C5')-(13 DG C4')-(13 DG C3')  30.0  90.0
 &rst     iat =   377,   378,   381,   401,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 14 DG GAMMA:  (14 DG O5')-(14 DG C5')-(14 DG C4')-(14 DG C3')  30.0  90.0
 &rst     iat =   410,   411,   414,   434,
           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 =   443,   444,   447,   466,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 16 DC GAMMA:  (16 DC O5')-(16 DC C5')-(16 DC C4')-(16 DC C3')  30.0  90.0
 &rst     iat =   475,   476,   479,   496,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 17 RDI GAMMA:  (17 RDI O5')-(17 RDI C5')-(17 RDI C4')-(17 RDI C3')   0.0 120.0
 &rst     iat =   505,   506,   509,   541,
           r1 =  -1.0, r2 =   0.0, r3 = 120.0, r4 = 121.0,
          &end

# 18 DA GAMMA:  (18 DA O5')-(18 DA C5')-(18 DA C4')-(18 DA C3')  30.0  90.0
 &rst     iat =   547,   548,   551,   570,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end

# 19 DG GAMMA:  (19 DG O5')-(19 DG C5')-(19 DG C4')-(19 DG C3')  30.0  90.0
 &rst     iat =   579,   580,   583,   603,
           r1 =  29.0, r2 =  30.0, r3 =  90.0, r4 =  91.0,
          &end
```

```
# 20 DA GAMMA:  (20 DA O5')-(20 DA C5')-(20 DA C4')-(20 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

# 21 DA GAMMA:  (21 DA O5')-(21 DA C5')-(21 DA C4')-(21 DA C3')  30.0  90.0
 &rst    iat =   644,   645,   648,   667,
           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 DT 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 DT EPSILN:  (3 DT C4')-(3 DT C3')-(3 DT O3')-(4 DC 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 DC EPSILN:  (4 DC C4')-(4 DC C3')-(4 DC O3')-(5 DT P) 165.0 225.0
 &rst    iat =   100,   117,   122,   123,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 5 DT EPSILN:  (5 DT C4')-(5 DT C3')-(5 DT O3')-(6 DT P) 165.0 225.0
 &rst    iat =   130,   149,   154,   155,
           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 DG P) 135.0 255.0
 &rst    iat =   162,   181,   186,   187,
           r1 = 134.0, r2 = 135.0, r3 = 255.0, r4 = 256.0,
         &end

# 7 DG EPSILN:  (7 DG C4')-(7 DG C3')-(7 DG O3')-(8 DT P) 165.0 225.0
 &rst    iat =   194,   214,   219,   220,
           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 =   227,   246,   251,   252,
           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 DC P) 165.0 225.0
 &rst    iat =   259,   276,   281,   282,
           r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
         &end

# 10 DC EPSILN:  (10 DC C4')-(10 DC C3')-(10 DC O3')-(11 DG3 P) 165.0 225.0
```

```
 &rst     iat =   289,   306,   311,   312,
            r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 13 DG EPSILN:  (13 DG C4')-(13 DG C3')-(13 DG O3')-(14 DG P) 165.0 225.0
 &rst     iat =   381,   401,   406,   407,
            r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 14 DG EPSILN:  (14 DG C4')-(14 DG C3')-(14 DG O3')-(15 DA P) 165.0 225.0
 &rst     iat =   414,   434,   439,   440,
            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 =   447,   466,   471,   472,
            r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 16 DC EPSILN:  (16 DC C4')-(16 DC C3')-(16 DC O3')-(17 RDI P) 165.0 225.0
 &rst     iat =   479,   496,   501,   502,
            r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 17 RDI EPSILN:  (17 RDI C4')-(17 RDI C3')-(17 RDI O3')-(18 DA P) 135.0 255.0
 &rst     iat =   509,   541,   543,   544,
            r1 = 134.0, r2 = 135.0, r3 = 255.0, r4 = 256.0,
          &end

# 18 DA EPSILN:  (18 DA C4')-(18 DA C3')-(18 DA O3')-(19 DG P) 165.0 225.0
 &rst     iat =   551,   570,   575,   576,
            r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 19 DG EPSILN:  (19 DG C4')-(19 DG C3')-(19 DG O3')-(20 DA P) 165.0 225.0
 &rst     iat =   583,   603,   608,   609,
            r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 20 DA EPSILN:  (20 DA C4')-(20 DA C3')-(20 DA O3')-(21 DA P) 165.0 225.0
 &rst     iat =   616,   635,   640,   641,
            r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

# 21 DA EPSILN:  (21 DA C4')-(21 DA C3')-(21 DA O3')-(22 DG3 P) 165.0 225.0
 &rst     iat =   648,   667,   672,   673,
            r1 = 164.0, r2 = 165.0, r3 = 225.0, r4 = 226.0,
          &end

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

# 3 DT ZETA:  (3 DT C3')-(3 DT O3')-(4 DC P)-(4 DC 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 DC ZETA:  (4 DC C3')-(4 DC O3')-(5 DT P)-(5 DT O5') -135.0 -75.0
 &rst    iat =   117,   122,   123,   126,
            r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
           &end

# 5 DT ZETA:  (5 DT C3')-(5 DT O3')-(6 DT P)-(6 DT O5') -135.0 -75.0
 &rst    iat =   149,   154,   155,   158,
            r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
           &end

# 6 DT ZETA:  (6 DT C3')-(6 DT O3')-(7 DG P)-(7 DG O5') -165.0 -45.0
 &rst    iat =   181,   186,   187,   190,
            r1 = -166.0, r2 = -165.0, r3 = -45.0, r4 = -44.0,
           &end

# 7 DG ZETA:  (7 DG C3')-(7 DG O3')-(8 DT P)-(8 DT O5') -135.0 -75.0
 &rst    iat =   214,   219,   220,   223,
            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 =   246,   251,   252,   255,
            r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
           &end

# 9 DC ZETA:  (9 DC C3')-(9 DC O3')-(10 DC P)-(10 DC O5') -135.0 -75.0
 &rst    iat =   276,   281,   282,   285,
            r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
           &end

# 10 DC ZETA:  (10 DC C3')-(10 DC O3')-(11 DG3 P)-(11 DG3 O5') -135.0 -75.0
 &rst    iat =   306,   311,   312,   315,
            r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
           &end

# 13 DG ZETA:  (13 DG C3')-(13 DG O3')-(14 DG P)-(14 DG O5') -135.0 -75.0
 &rst    iat =   401,   406,   407,   410,
            r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
           &end

# 14 DG ZETA:  (14 DG C3')-(14 DG O3')-(15 DA P)-(15 DA O5') -135.0 -75.0
 &rst    iat =   434,   439,   440,   443,
            r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
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          &end

# 15 DA ZETA:  (15 DA C3')-(15 DA O3')-(16 DC P)-(16 DC O5') -135.0 -75.0
 &rst    iat =   466,   471,   472,   475,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
          &end

# 16 DC ZETA:  (16 DC C3')-(16 DC O3')-(17 RDI P)-(17 RDI O5') -135.0 -75.0
 &rst    iat =   496,   501,   502,   505,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
          &end

# 17 RDI ZETA:  (17 RDI C3')-(17 RDI O3')-(18 DA P)-(18 DA O5') -165.0 -45.0
 &rst    iat =   541,   543,   544,   547,
           r1 = -166.0, r2 = -165.0, r3 = -45.0, r4 = -44.0,
          &end

# 18 DA ZETA:  (18 DA C3')-(18 DA O3')-(19 DG P)-(19 DG O5') -135.0 -75.0
 &rst    iat =   570,   575,   576,   579,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
          &end

# 19 DG ZETA:  (19 DG C3')-(19 DG O3')-(20 DA P)-(20 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

# 20 DA ZETA:  (20 DA C3')-(20 DA O3')-(21 DA P)-(21 DA O5') -135.0 -75.0
 &rst    iat =   635,   640,   641,   644,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
          &end

# 21 DA ZETA:  (21 DA C3')-(21 DA O3')-(22 DG3 P)-(22 DG3 O5') -135.0 -75.0
 &rst    iat =   667,   672,   673,   676,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
          &end

# 21 DA ZETA:  (21 DA C3')-(21 DA O3')-(22 DG3 P)-(22 DG3 O5') -135.0 -75.0
 &rst    iat =   667,   672,   673,   676,
           r1 = -136.0, r2 = -135.0, r3 = -75.0, r4 = -74.0,
          &end

# 706 atoms read from pdb file RdI_Major_New_v3.pdb.
# 2 DT NU0:  (2 DT C4')-(2 DT O4')-(2 DT C1')-(2 DT C2') -44.7 -14.7
 &rst    iat =    36,    38,    39,    57,
           r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
           rk2 =  32.0, rk3 =  32.0,                          &end

# 2 DT NU1:  (2 DT O4')-(2 DT C1')-(2 DT C2')-(2 DT C3')  18.1  48.1
 &rst    iat =    38,    39,    57,    55,
           r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
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 &end

# 2 DT NU2:  (2 DT C1')-(2 DT C2')-(2 DT C3')-(2 DT C4') -37.2  -6.7
 &rst     iat =    39,    57,    55,    36,
           r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
          &end

# 2 DT NU3:  (2 DT C2')-(2 DT C3')-(2 DT C4')-(2 DT O4') -16.9  24.2
 &rst     iat =    57,    55,    36,    38,
           r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
          &end

# 2 DT NU4:  (2 DT C3')-(2 DT C4')-(2 DT O4')-(2 DT C1')  -1.9  34.0
 &rst     iat =    55,    36,    38,    39,
           r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
          &end

# 3 DT NU0:  (3 DT C4')-(3 DT O4')-(3 DT C1')-(3 DT C2') -52.1 -22.1
 &rst     iat =    68,    70,    71,    89,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
          &end

# 3 DT NU1:  (3 DT O4')-(3 DT C1')-(3 DT C2')-(3 DT C3')  15.0  45.0
 &rst     iat =    70,    71,    89,    87,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
          &end

# 3 DT NU2:  (3 DT C1')-(3 DT C2')-(3 DT C3')-(3 DT C4') -27.4   2.6
 &rst     iat =    71,    89,    87,    68,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
          &end

# 3 DT NU3:  (3 DT C2')-(3 DT C3')-(3 DT C4')-(3 DT O4') -25.0   5.0
 &rst     iat =    89,    87,    68,    70,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
          &end

# 3 DT NU4:  (3 DT C3')-(3 DT C4')-(3 DT O4')-(3 DT C1')  13.5  43.5
 &rst     iat =    87,    68,    70,    71,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
          &end

# 4 DC NU0:  (4 DC C4')-(4 DC O4')-(4 DC C1')-(4 DC C2') -52.1 -22.1
 &rst     iat =   100,   102,   103,   119,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
          &end

# 4 DC NU1:  (4 DC O4')-(4 DC C1')-(4 DC C2')-(4 DC C3')  15.0  45.0
 &rst     iat =   102,   103,   119,   117,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
          &end
```

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# 4 DC NU2:  (4 DC C1')-(4 DC C2')-(4 DC C3')-(4 DC C4') -27.4   2.6
 &rst     iat =   103,   119,   117,   100,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
          &end

# 4 DC NU3:  (4 DC C2')-(4 DC C3')-(4 DC C4')-(4 DC O4') -25.0   5.0
 &rst     iat =   119,   117,   100,   102,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
          &end

# 4 DC NU4:  (4 DC C3')-(4 DC C4')-(4 DC O4')-(4 DC C1')  13.5  43.5
 &rst     iat =   117,   100,   102,   103,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
          &end

# 5 DT NU0:  (5 DT C4')-(5 DT O4')-(5 DT C1')-(5 DT C2') -52.1 -22.1
 &rst     iat =   130,   132,   133,   151,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
          &end

# 5 DT NU1:  (5 DT O4')-(5 DT C1')-(5 DT C2')-(5 DT C3')  15.0  45.0
 &rst     iat =   132,   133,   151,   149,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
          &end

# 5 DT NU2:  (5 DT C1')-(5 DT C2')-(5 DT C3')-(5 DT C4') -27.4   2.6
 &rst     iat =   133,   151,   149,   130,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
          &end

# 5 DT NU3:  (5 DT C2')-(5 DT C3')-(5 DT C4')-(5 DT O4') -25.0   5.0
 &rst     iat =   151,   149,   130,   132,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
          &end

# 5 DT NU4:  (5 DT C3')-(5 DT C4')-(5 DT O4')-(5 DT C1')  13.5  43.5
 &rst     iat =   149,   130,   132,   133,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
          &end

# 7 DG NU0:  (7 DG C4')-(7 DG O4')-(7 DG C1')-(7 DG C2') -43.9 -13.9
 &rst     iat =   194,   196,   197,   216,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
          &end

# 7 DG NU1:  (7 DG O4')-(7 DG C1')-(7 DG C2')-(7 DG C3')  22.2  52.2
 &rst     iat =   196,   197,   216,   214,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
          &end
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# 7 DG NU2:  (7 DG C1')-(7 DG C2')-(7 DG C3')-(7 DG C4') -44.6 -14.6
 &rst     iat =   197,   216,   214,   194,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
          &end

# 7 DG NU3:  (7 DG C2')-(7 DG C3')-(7 DG C4')-(7 DG O4')  -3.2  26.8
 &rst     iat =   216,   214,   194,   196,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
          &end

# 7 DG NU4:  (7 DG C3')-(7 DG C4')-(7 DG O4')-(7 DG C1')  -4.4  25.6
 &rst     iat =   214,   194,   196,   197,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
          &end

# 8 DT NU0:  (8 DT C4')-(8 DT O4')-(8 DT C1')-(8 DT C2') -52.1 -22.1
 &rst     iat =   227,   229,   230,   248,
           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 =   229,   230,   248,   246,
           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 =   230,   248,   246,   227,
           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 =   248,   246,   227,   229,
           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 =   246,   227,   229,   230,
           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') -52.1 -22.1
 &rst     iat =   259,   261,   262,   278,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
          &end

# 9 DC NU1:  (9 DC O4')-(9 DC C1')-(9 DC C2')-(9 DC C3')  15.0  45.0
 &rst     iat =   261,   262,   278,   276,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
          &end

# 9 DC NU2:  (9 DC C1')-(9 DC C2')-(9 DC C3')-(9 DC C4') -27.4   2.6
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 &rst     iat =   262,   278,   276,   259,
            r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
          &end

# 9 DC NU3:  (9 DC C2')-(9 DC C3')-(9 DC C4')-(9 DC O4') -25.0   5.0
 &rst     iat =   278,   276,   259,   261,
            r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
          &end

# 9 DC NU4:  (9 DC C3')-(9 DC C4')-(9 DC O4')-(9 DC C1')  13.5  43.5
 &rst     iat =   276,   259,   261,   262,
            r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
          &end

# 10 DC NU0:  (10 DC C4')-(10 DC O4')-(10 DC C1')-(10 DC C2') -44.7 -14.7
 &rst     iat =   289,   291,   292,   308,
            r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
          &end

# 10 DC NU1:  (10 DC O4')-(10 DC C1')-(10 DC C2')-(10 DC C3')  18.1  48.1
 &rst     iat =   291,   292,   308,   306,
            r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
          &end

# 10 DC NU2:  (10 DC C1')-(10 DC C2')-(10 DC C3')-(10 DC C4') -37.2  -6.7
 &rst     iat =   292,   308,   306,   289,
            r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
          &end

# 10 DC NU3:  (10 DC C2')-(10 DC C3')-(10 DC C4')-(10 DC O4') -16.9  24.2
 &rst     iat =   308,   306,   289,   291,
            r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
          &end

# 10 DC NU4:  (10 DC C3')-(10 DC C4')-(10 DC O4')-(10 DC C1')  -1.9  34.0
 &rst     iat =   306,   289,   291,   292,
            r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
          &end

# 13 DG NU0:  (13 DG C4')-(13 DG O4')-(13 DG C1')-(13 DG C2') -44.7 -14.7
 &rst     iat =   381,   383,   384,   403,
            r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
          &end

# 13 DG NU1:  (13 DG O4')-(13 DG C1')-(13 DG C2')-(13 DG C3')  18.1  48.1
 &rst     iat =   383,   384,   403,   401,
            r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
          &end

# 13 DG NU2:  (13 DG C1')-(13 DG C2')-(13 DG C3')-(13 DG C4') -37.2  -6.7
 &rst     iat =   384,   403,   401,   381,
```

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

# 13 DG NU3:  (13 DG C2')-(13 DG C3')-(13 DG C4')-(13 DG O4') -16.9  24.2
 &rst    iat =   403,   401,   381,   383,
      r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
     &end

# 13 DG NU4:  (13 DG C3')-(13 DG C4')-(13 DG O4')-(13 DG C1')  -1.9  34.0
 &rst    iat =   401,   381,   383,   384,
      r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
     &end

# 14 DG NU0:  (14 DG C4')-(14 DG O4')-(14 DG C1')-(14 DG C2') -43.9 -13.9
 &rst    iat =   414,   416,   417,   436,
      r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
     &end

# 14 DG NU1:  (14 DG O4')-(14 DG C1')-(14 DG C2')-(14 DG C3')  22.2  52.2
 &rst    iat =   416,   417,   436,   434,
      r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
     &end

# 14 DG NU2:  (14 DG C1')-(14 DG C2')-(14 DG C3')-(14 DG C4') -44.6 -14.6
 &rst    iat =   417,   436,   434,   414,
      r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
     &end

# 14 DG NU3:  (14 DG C2')-(14 DG C3')-(14 DG C4')-(14 DG O4')  -3.2  26.8
 &rst    iat =   436,   434,   414,   416,
      r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
     &end

# 14 DG NU4:  (14 DG C3')-(14 DG C4')-(14 DG O4')-(14 DG C1')  -4.4  25.6
 &rst    iat =   434,   414,   416,   417,
      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 =   447,   449,   450,   468,
      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 =   449,   450,   468,   466,
      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 =   450,   468,   466,   447,
      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 =   468,   466,   447,   449,
           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 =   466,   447,   449,   450,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
          &end

# 16 DC NU0:  (16 DC C4')-(16 DC O4')-(16 DC C1')-(16 DC C2') -52.1 -22.1
 &rst    iat =   479,   481,   482,   498,
           r1 = -53.1, r2 = -52.1, r3 = -22.1, r4 = -21.1,
          &end

# 16 DC NU1:  (16 DC O4')-(16 DC C1')-(16 DC C2')-(16 DC C3')  15.0  45.0
 &rst    iat =   481,   482,   498,   496,
           r1 =  14.0, r2 =  15.0, r3 =  45.0, r4 =  46.0,
          &end

# 16 DC NU2:  (16 DC C1')-(16 DC C2')-(16 DC C3')-(16 DC C4') -27.4   2.6
 &rst    iat =   482,   498,   496,   479,
           r1 = -28.4, r2 = -27.4, r3 =   2.6, r4 =   3.6,
          &end

# 16 DC NU3:  (16 DC C2')-(16 DC C3')-(16 DC C4')-(16 DC O4') -25.0   5.0
 &rst    iat =   498,   496,   479,   481,
           r1 = -26.0, r2 = -25.0, r3 =   5.0, r4 =   6.0,
          &end

# 16 DC NU4:  (16 DC C3')-(16 DC C4')-(16 DC O4')-(16 DC C1')  13.5  43.5
 &rst    iat =   496,   479,   481,   482,
           r1 =  12.5, r2 =  13.5, r3 =  43.5, r4 =  44.5,
          &end

# 18 DA NU0:  (18 DA C4')-(18 DA O4')-(18 DA C1')-(18 DA C2') -43.9 -13.9
 &rst    iat =   551,   553,   554,   572,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
          &end

# 18 DA NU1:  (18 DA O4')-(18 DA C1')-(18 DA C2')-(18 DA C3')  22.2  52.2
 &rst    iat =   553,   554,   572,   570,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
          &end

# 18 DA NU2:  (18 DA C1')-(18 DA C2')-(18 DA C3')-(18 DA C4') -44.6 -14.6
 &rst    iat =   554,   572,   570,   551,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
          &end
```

```
# 18 DA NU3:  (18 DA C2')-(18 DA C3')-(18 DA C4')-(18 DA O4')  -3.2  26.8
 &rst    iat =   572,   570,   551,   553,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
         &end

# 18 DA NU4:  (18 DA C3')-(18 DA C4')-(18 DA O4')-(18 DA C1')  -4.4  25.6
 &rst    iat =   570,   551,   553,   554,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
         &end

# 19 DG NU0:  (19 DG C4')-(19 DG O4')-(19 DG C1')-(19 DG C2') -43.9 -13.9
 &rst    iat =   583,   585,   586,   605,
           r1 = -44.9, r2 = -43.9, r3 = -13.9, r4 = -12.9,
         &end

# 19 DG NU1:  (19 DG O4')-(19 DG C1')-(19 DG C2')-(19 DG C3')  22.2  52.2
 &rst    iat =   585,   586,   605,   603,
           r1 =  21.2, r2 =  22.2, r3 =  52.2, r4 =  53.2,
         &end

# 19 DG NU2:  (19 DG C1')-(19 DG C2')-(19 DG C3')-(19 DG C4') -44.6 -14.6
 &rst    iat =   586,   605,   603,   583,
           r1 = -45.6, r2 = -44.6, r3 = -14.6, r4 = -13.6,
         &end

# 19 DG NU3:  (19 DG C2')-(19 DG C3')-(19 DG C4')-(19 DG O4')  -3.2  26.8
 &rst    iat =   605,   603,   583,   585,
           r1 =  -4.2, r2 =  -3.2, r3 =  26.8, r4 =  27.8,
         &end

# 19 DG NU4:  (19 DG C3')-(19 DG C4')-(19 DG O4')-(19 DG C1')  -4.4  25.6
 &rst    iat =   603,   583,   585,   586,
           r1 =  -5.4, r2 =  -4.4, r3 =  25.6, r4 =  26.6,
         &end

# 20 DA NU0:  (20 DA C4')-(20 DA O4')-(20 DA C1')-(20 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

# 20 DA NU1:  (20 DA O4')-(20 DA C1')-(20 DA C2')-(20 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

# 20 DA NU2:  (20 DA C1')-(20 DA C2')-(20 DA C3')-(20 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
```

```
# 20 DA NU3:  (20 DA C2')-(20 DA C3')-(20 DA C4')-(20 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

# 20 DA NU4:  (20 DA C3')-(20 DA C4')-(20 DA O4')-(20 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

# 21 DA NU0:  (21 DA C4')-(21 DA O4')-(21 DA C1')-(21 DA C2') -44.7 -14.7
 &rst    iat =   648,   650,   651,   669,
          r1 = -45.7, r2 = -44.7, r3 = -14.7, r4 = -13.7,
         &end

# 21 DA NU1:  (21 DA O4')-(21 DA C1')-(21 DA C2')-(21 DA C3')  18.1  48.1
 &rst    iat =   650,   651,   669,   667,
          r1 =  17.1, r2 =  18.1, r3 =  48.1, r4 =  49.1,
         &end

# 21 DA NU2:  (21 DA C1')-(21 DA C2')-(21 DA C3')-(21 DA C4') -37.2  -6.7
 &rst    iat =   651,   669,   667,   648,
          r1 = -38.2, r2 = -37.2, r3 =  -6.7, r4 =  -5.7,
         &end

# 21 DA NU3:  (21 DA C2')-(21 DA C3')-(21 DA C4')-(21 DA O4') -16.9  24.2
 &rst    iat =   669,   667,   648,   650,
          r1 = -17.9, r2 = -16.9, r3 =  24.2, r4 =  25.2,
         &end

# 21 DA NU4:  (21 DA C3')-(21 DA C4')-(21 DA O4')-(21 DA C1')  -1.9  34.0
 &rst    iat =   667,   648,   650,   651,
          r1 =  -2.9, r2 =  -1.9, r3 =  34.0, r4 =  35.0,
         &end
```

APPENDIX D

MOLECULAR DYNAMICS FILES

File D1. Energy minimization protocol

```
&cntrl
  imin   = 1,
  igb    = 0,
  maxcyc = 1000,
  ncyc   = 500,
  ntb     = 0,
  cut     = 18.0,
 &end
```

File D2. Simulated annealing protocol

```
simulated annealing protocol, 18A cut off, 100ps

 &cntrl
   imin=0, ntr=0, ntc=2, ntf=2,
   cut=18.0, igb=1, saltcon=1.0, 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 1000K with short tautp
#from steps 5000 to 10000: keep the temperature at 1000K
#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=1000.0,    &end
 &wt type='TEMP0', istep1=5000,istep2=10000,value1=1000.0,
          value2=1000.0,    &end
 &wt type='TEMP0', istep1=10001, istep2=90000, value1=1000.0,
          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
DISANG=RdIall.rst
```

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