Constrained Bonding Environment in the Michaelis Complex of *Trypanosoma cruzi* Uridine Phosphorylase

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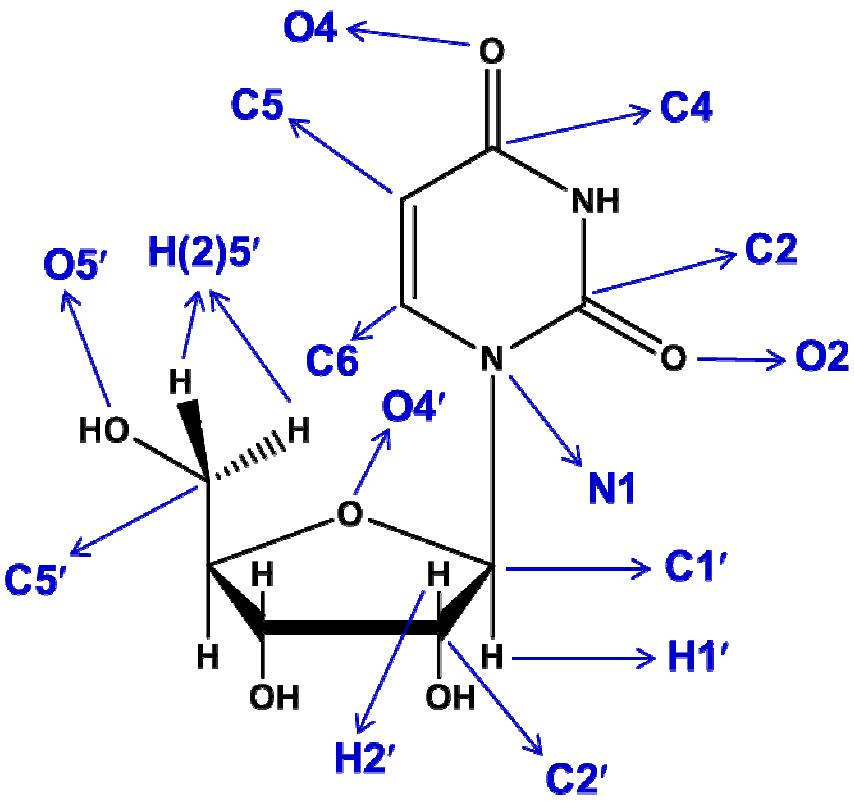
Scheme S1. Atom numbering of uridine.



EXPERIMENTAL PROCEDURES

Materials. D-[1-^{3}H]Ribose and D-[6-$^{3}H_2$]Glucose were purchased from American Radiolabeled Chemicals, Inc., and D-[6-^{14}C]glucose was from Perkin Elmer, Inc. Pyruvate kinase, myokinase, hexokinase, glucose-6-phosphate dehydrogenase, glutamic acid dehydrogenase, 6-phosphogluconic acid dehydrogenase, and phosphoriboisomerase were from Sigma-Aldrich. Alkaline phosphatase was from Roche. Ribokinase and phosphoribosyl-α-1-pyrophosphate synthetase were prepared as previously described.[1] UMP synthase was kindly provided by Dr. Keith Hazleton of this laboratory. All other chemicals and reagents were obtained from commercial sources and were used without further purification. *Trypanosoma cruzi* uridine phosphorylase was expressed and purified as published.[2]

Synthesis and purification of radiolabeled uridines. [1′-^{3}H]Uridine, [5′-$^{3}H_2$]uridine, and [5′-^{14}C]uridine were synthesized and purified as previously reported.[2]

Measurement of 1′-^{3}H and 5′-$^{3}H_2$ BIE's. BIE's were determined by the competitive radiolabel method. Incubation mixtures (100 μL) consisted of 20 μM TcUP, 50 μM uridine ([5′-^{14}C]uridine and either [1′-^{3}H]uridine or [5′-$^{3}H_2$]uridine), 50 mM $(NH_4)_2SO_4$ pH 7.5, and 100 mM HEPES pH 7.5. The incubation mixture was loaded onto an ultrafiltration apparatus, and an argon pressure of 30 psi was applied until approximately half the volume had passed through a semi-permeable membrane (10 kDa molecular weight retention), when 30 μL were removed from top and bottom wells. The total ^{3}H signal was assessed by eq 1, and the total ^{14}C signal by eq 2.[3] Tritium BIE's were calculated with eq 3.[4] In eqs 1−3, ^{3}H is the total number of cpm for this isotope, ^{14}C is the total number of cpm for this isotope, channel 1 and channel 2 are the number of cpm in each channel, r is the channel 1 to channel 2 ratio of ^{14}C standard, $^{14}C_T$ and $^{14}C_B$ are the total ^{14}C counts in the top and bottom wells, respectively, and $^{3}H_T$ and $^{3}H_B$ are the total ^{3}H counts in the top and bottom wells, respectively. BIE values are expressed as averages and their standard errors for at least 10 replicates in 2 independent experiments. The effect of sulfate ion on the 1′-

^{3}H BIE was assessed by excluding $(NH_4)_2SO_4$ from the incubation mixture. Controls were performed by the same procedure, except that enzyme was omitted.

$$^3H = \text{channel 1} - (\text{channel 2} \times r) \quad (1)$$

$$^{14}C = \text{channel 2} \times (1 + r) \quad (2)$$

$$\text{BIE} = (^{14}C_T / {}^{14}C_B - 1) / (^3H_T / {}^3H_B - 1) \quad (3)$$

Computational methods. Uridine conformations were optimized in vacuo at the B3LYP level of theory and the 6-31G** basis set, as implemented in Gaussian 09[5], by varying the O4′-C1′-N1-C6 dihedral angle with either 2′-endo-3′-exo or 2′-exo-3′-endo ribosyl pucker. Isotope effects for each structure were calculated from scaled vibrational frequencies using ISOEFF98.[6]

By testing two opposite ribosyl conformations and varying the O4′-C1′-N1-C6 dihedral angle to search for a theoretical model of enzyme-bound uridine, several possible degrees of freedom of uridine were not explored in this study. It should be pointed out, therefore, that the proposed model of uridine in the Michaelis complex provides a solution whose calculated BIE's best match the experimental ones, but it may not necessarily be a unique solution.

HPLC analysis. A reaction mixture (100 μL) containing 50 mM $(NH_4)_2SO_4$ pH 7.5, 10 μM TcUP, 100 μM uridine, and 100 mM HEPES pH 7.5 was allowed to proceed for 90 min. Standards contained either 100 μM uridine or 100 μM uracil, and 50 mM $(NH_4)_2SO_4$ pH 7.5 and 100 mM HEPES pH 7.5. Each sample was injected and run at 1.0 mL min^{-1} in an HPLC C_{18} Delta Pak column (Waters) pre-equilibrated with 10 column volumes of 50 mM of triethylamine:acetic acid pH 5.0, and base and nucleoside elution were followed by monitoring the increase in absorbance at 262 nm.

RESULTS

Table S1. Calculated BIE's for DFT-optimized uridine conformations.

O4′-C1′-N1-C6 Dihedral Angle (°) (2′-endo-3′-exo sugar pucker)	1′-^{3}H BIE	5′-$^3H_2$ BIE	O4′-C1′-N1-C6 Dihedral Angle (°) (2′-exo-3′-endo sugar pucker)	1′-^{3}H BIE	5′-$^3H_2$ BIE
-180.0000	1.0450	0.9853	**-180.0000**	1.0196	0.9802
-160.0000	1.0288	0.9954	**-140.0000**	1.0052	0.9890
-140.0000	1.0246	0.9970	**-120.0000**	0.9706	0.9793
-120.0000	1.0019	1.0001	**-100.0000**	0.9611	0.9826
-100.0000	0.9912	0.9986	**-75.0000**	0.9487	0.9720
-80.0000	0.9814	0.9937	**-50.0000**	0.9624	0.9689
-60.0000	0.9634	0.9933	**-30.0000**	1.0220	0.9543
-40.0000	1.0248	0.9693	**-20.0000**	1.0166	0.9571
-20.0000	1.0232	0.9737	**0.0000**	0.9957	0.9499
0.0000	1.0050	0.9767	**20.0000**	0.9617	0.9367
20.0000	0.9806	0.9558	**40.0000**	0.9290	0.9438
40.0000	0.9486	1.0150	**47.0000**	0.9360	0.9433
65.0000	0.9190	1.0067	**60.0000**	0.9082	0.9487
80.0000	0.9112	1.0050	**80.0000**	0.9072	0.9551
90.0000	0.9106	1.0097	**100.0000**	0.9136	0.9601
120.0000	0.9906	1.0204	**120.0000**	0.9445	0.9582
140.0000	1.0528	1.0218	**145.0000**	0.9901	0.9868
150.0000	1.0660	1.0195	**170.0000**	1.0173	0.9811
180.0000	1.0450	0.9853	**180.0000**	1.0196	0.9802

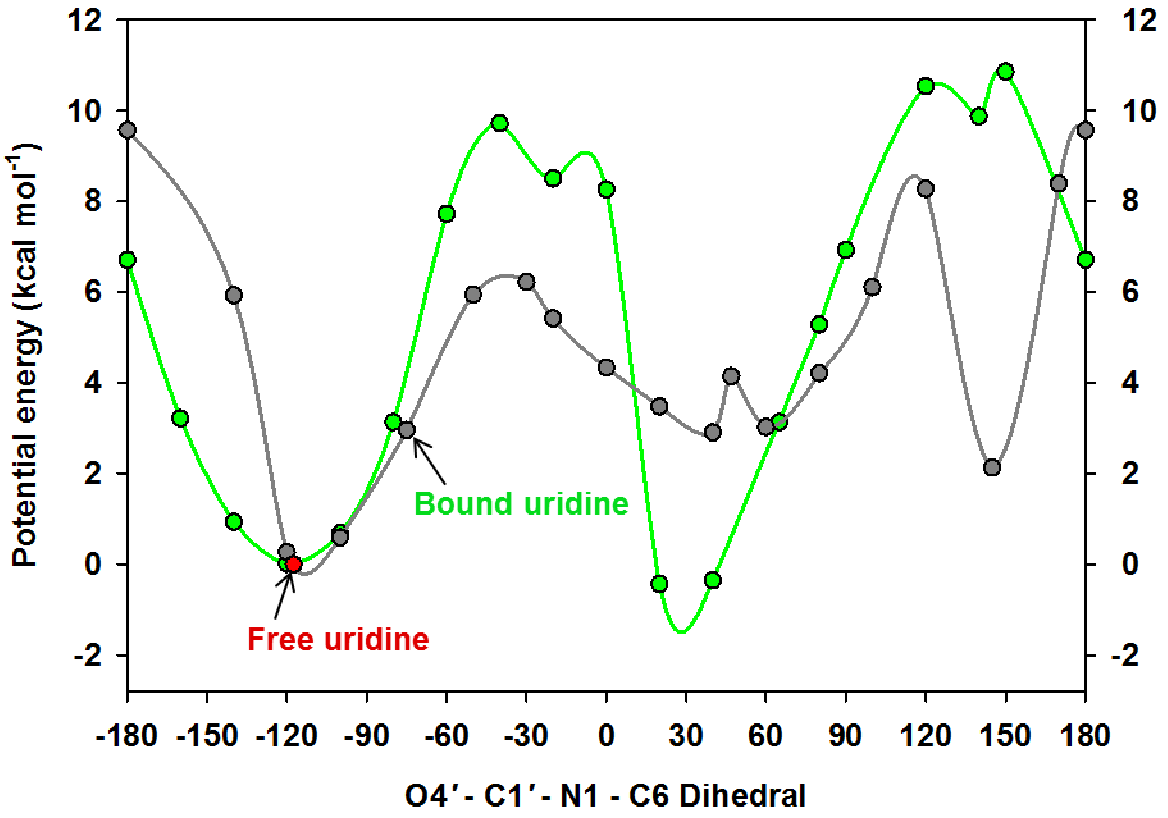


Figure S1. Potential energy dependence on O4′-C1′-N1-C6 dihedral angles of 2′-endo-3′-exo (green) and 2′-exo-3′-endo (gray) optimized uridine conformers. The red circle denotes the potential energy of optimized free uridine.

Caution should be exercised when analyzing the potential energy data presented in Figure S1. As described under Experimental Procedures, these are energies were derived from calculations performed *in vacuo*, in the absence of any implicit or explicit models of solvent or of enzyme active site. While they serve a comparative purpose, since all structures were treated in the same manner, the energies obtained here are in no way intended to represent the actual potential energies of the free substrate and the Michaelis complex as found in solution.

Atomic coordinates of optimized uridine

2′-endo-3′-exo ribosyl pucker

O4′-C1′-N1-C6 dihedral = −180°

C	-1.31875500	-1.05129400	0.53356800
C	-0.60573800	-0.53818000	-0.75544800
O	-1.28083600	0.61305500	-1.15146500
C	-2.51314500	0.80146800	-0.42005000
C	-2.73975500	-0.50473700	0.35202200
N	0.85674500	-0.30246900	-0.51067100
C	1.45458100	0.95615300	-0.37613200
N	2.82411100	0.90000900	-0.18065600
C	3.63377000	-0.20992400	0.13929400
C	2.87028300	-1.44532300	0.19110800
C	1.55628700	-1.43580000	-0.11370300
O	0.87851500	2.03804500	-0.42169500
O	4.82575500	-0.06823000	0.35486000
C	-2.38473700	2.06161900	0.43853900
O	-1.30737700	1.98083700	1.34564100
O	-3.42079900	-1.48776100	-0.43550100
O	-1.26282000	-2.44589600	0.70977000
H	-0.85821700	-0.56600000	1.39738000
H	-3.31449800	0.94057300	-1.15784100
H	-2.28365600	2.92424500	-0.23485700
H	-3.30748100	2.20059200	1.01666300
H	-4.37024500	-1.31968100	-0.40481000
H	-0.64352900	-1.30558900	-1.54141700
H	-2.01745800	-2.80045300	0.21012600
H	-3.24617000	-0.34560600	1.31048700
H	3.26967200	1.80796900	-0.11862000
H	3.37466300	-2.35652800	0.48117400
H	0.95533900	-2.33783900	-0.08129800
H	-0.50065600	2.13123400	0.81424100

O4′-C1′-N1-C6 dihedral = −160°

C	-1.22973100	-0.93691700	0.67415400
C	-0.52273500	-0.60995700	-0.66504700
O	-1.21669700	0.46646200	-1.22325600
C	-2.54892500	0.56917600	-0.66068700
C	-2.68701500	-0.59786000	0.33384800
N	0.92134900	-0.30758800	-0.50579800
C	1.39176500	0.95680400	-0.12494500
N	2.76416400	1.01783200	0.02612900

C	3.69908400	-0.03859500	0.08192200
C	3.07387300	-1.33582600	-0.11536800
C	1.75344200	-1.41143900	-0.37799800
O	0.69798600	1.94988700	0.05653000
O	4.87824800	0.18784800	0.29316000
C	-2.70696200	1.95261800	-0.03297000
O	-1.88902000	2.12504900	1.10208300
O	-3.21250200	-1.78093500	-0.28041900
O	-1.02181600	-2.25546600	1.11195400
H	-0.87314500	-0.24506300	1.44114200
H	-3.26979100	0.44697600	-1.48061900
H	-2.50537800	2.70700500	-0.80776600
H	-3.74938900	2.07881300	0.28673400
H	-4.17546300	-1.72756100	-0.29988400
H	-0.55686600	-1.49223100	-1.32075000
H	-1.72020300	-2.78067200	0.68653100
H	-3.26472900	-0.32065900	1.22154500
H	3.11801000	1.93827600	0.25921900
H	3.68654900	-2.22347600	-0.04338400
H	1.25421100	-2.36208700	-0.52087100
H	-0.96875600	2.17818900	0.77791500

O4′-C1′-N1-C6 dihedral = –140°

C	-1.22976500	-0.84597600	0.77074000
C	-0.48013500	-0.66907000	-0.57011200
O	-1.15297000	0.34535900	-1.26788300
C	-2.52308100	0.45030800	-0.80272400
C	-2.67880200	-0.58508200	0.32933300
N	0.95114100	-0.34541200	-0.43698800
C	1.36280700	0.88738100	0.08488200
N	2.72997500	1.01834000	0.21311400
C	3.73590700	0.04250200	0.03524800
C	3.19333000	-1.23808000	-0.38708400
C	1.86695400	-1.37302000	-0.59064200
O	0.60619200	1.79442000	0.40866500
O	4.90593500	0.31638200	0.23928400
C	-2.78526300	1.88993400	-0.36662800
O	-2.13582700	2.22112800	0.83953300
O	-3.15956400	-1.84785000	-0.14999100
O	-1.01619900	-2.09899100	1.36596500
H	-0.91826600	-0.06240600	1.46399100
H	-3.18457700	0.18682300	-1.63950100
H	-2.49935000	2.55767900	-1.19356200
H	-3.86281200	2.01520600	-0.20068600
H	-4.12360800	-1.83066800	-0.17381000
H	-0.51045400	-1.62096000	-1.11892800
H	-1.69196000	-2.68356400	0.98392800

H	-3.29718400	-0.20887000	1.14981200
H	3.03645700	1.91685000	0.56741800
H	3.87356400	-2.06533500	-0.53314800
H	1.43375200	-2.31344800	-0.90954800
H	-1.17563300	2.20124000	0.66849900

O4′-C1′-N1-C6 dihedral = –120°

C	-1.30781000	-0.78136600	0.84016200
C	-0.46878000	-0.72643600	-0.45823000
O	-1.06878600	0.24004000	-1.28733700
C	-2.45662300	0.43226200	-0.90991500
C	-2.71605000	-0.51181400	0.28023300
N	0.95906100	-0.42336500	-0.29114700
C	1.36430300	0.78942600	0.27546600
N	2.73007700	0.94639400	0.36707000
C	3.75519100	0.05220300	-0.01554300
C	3.23102400	-1.17714800	-0.58770300
C	1.89851300	-1.35309000	-0.70107300
O	0.59440100	1.65530200	0.67490100
O	4.92600100	0.34986200	0.14491100
C	-2.69003600	1.90830100	-0.59220600
O	-2.14768400	2.30021300	0.64852000
O	-3.20624000	-1.79184600	-0.14154900
O	-1.18336100	-1.99664100	1.53100700
H	-1.01792500	0.03563500	1.50097200
H	-3.08022100	0.13364700	-1.76361700
H	-2.29774100	2.50536800	-1.42981300
H	-3.77142000	2.08732300	-0.54004500
H	-4.16667900	-1.75172000	-0.21951000
H	-0.49796800	-1.72205900	-0.92209400
H	-1.85058000	-2.58498400	1.14012200
H	-3.37411900	-0.06028200	1.02848000
H	3.03008800	1.82264700	0.77810800
H	3.93025500	-1.93154200	-0.91998800
H	1.47781000	-2.25524300	-1.12912800
H	-1.17850700	2.21054000	0.59428800

O4′-C1′-N1-C6 dihedral = –100°

C	-1.40242000	-0.71702100	0.89101100
C	-0.47629900	-0.77662200	-0.34696500
O	-0.98350100	0.13458000	-1.29736000
C	-2.36992200	0.44705400	-1.00245200
C	-2.75426000	-0.41652700	0.21309000

N	0.95341200	-0.51828200	-0.13631500
C	1.37382400	0.67633700	0.45924800
N	2.74031700	0.84010600	0.50854900
C	3.75027200	0.03413500	-0.06405300
C	3.20628900	-1.11943900	-0.76225800
C	1.87435900	-1.32854600	-0.78140300
O	0.61284600	1.51821800	0.92360100
O	4.92374000	0.34283600	0.04649800
C	-2.51730600	1.95048800	-0.76678000
O	-2.05368500	2.37023300	0.49718200
O	-3.27337300	-1.69479900	-0.17879900
O	-1.39126600	-1.90069700	1.64532200
H	-1.12363400	0.11493300	1.53489300
H	-2.96819000	0.15202300	-1.87494700
H	-2.01684800	2.47614100	-1.59466000
H	-3.58321300	2.20673500	-0.81308700
H	-4.22467500	-1.61946900	-0.31810900
H	-0.51931000	-1.80484200	-0.73206800
H	-2.05075200	-2.47968400	1.22827100
H	-3.44099300	0.10254600	0.88802600
H	3.05029500	1.69052400	0.96418900
H	3.89060800	-1.78928800	-1.26380900
H	1.43863500	-2.17702000	-1.29589400
H	-1.09334700	2.21249400	0.54336900

O4′-C1′-N1-C6 dihedral = –80°

C	-1.49466800	-0.64719300	0.92235400
C	-0.50009400	-0.82419000	-0.25019700
O	-0.91614100	0.01058300	-1.31251300
C	-2.27133700	0.47806700	-1.08263400
C	-2.78158100	-0.29879000	0.14270900
N	0.93623900	-0.61722700	-0.01174800
C	1.38521800	0.54076000	0.63963600
N	2.75365600	0.69553200	0.65215000
C	3.72368800	-0.00043100	-0.10446400
C	3.13257900	-1.03762500	-0.93521700
C	1.80745800	-1.27462300	-0.87290500
O	0.64735800	1.35655300	1.18226700
O	4.90023900	0.30719100	-0.03443400
C	-2.28318100	1.99820800	-0.90237600
O	-1.88121900	2.42736000	0.38074000
O	-3.35626400	-1.55923400	-0.22688100
O	-1.61039600	-1.79684900	1.71968800
H	-1.21026300	0.18869000	1.55539200
H	-2.86019500	0.21391300	-1.97061000
H	-1.67319000	2.44037700	-1.70504600
H	-3.31173300	2.35451700	-1.03934400

H	-4.29330900	-1.43458700	-0.41757500
H	-0.56862000	-1.87856400	-0.55368700
H	-2.26868100	-2.35638700	1.27501700
H	-3.47315800	0.29244700	0.74995600
H	3.08429200	1.50295000	1.16783200
H	3.77681200	-1.59807000	-1.59818700
H	1.33723200	-2.04052300	-1.47874200
H	-0.94555200	2.19717400	0.51979900

O4′-C1′-N1-C6 dihedral = –60°

C	-1.57687700	-0.57224700	0.92922200
C	-0.54723900	-0.86908000	-0.19232200
O	-0.91887400	-0.15590600	-1.35756300
C	-2.18079900	0.52759400	-1.14352000
C	-2.80274700	-0.15325200	0.08401400
N	0.90436000	-0.68956100	0.03612200
C	1.39915100	0.37242200	0.81026000
N	2.77202900	0.49656900	0.79515500
C	3.68548700	-0.04753700	-0.13648300
C	3.02660200	-0.89764000	-1.11568700
C	1.70752000	-1.14781100	-1.00759800
O	0.70132100	1.13533000	1.47094200
O	4.86918400	0.23405000	-0.08078100
C	-1.98010200	2.04055200	-0.97943800
O	-1.63254000	2.45506000	0.32687700
O	-3.46616700	-1.37345700	-0.26705700
O	-1.81744100	-1.68574500	1.74987700
H	-1.26170300	0.25387600	1.55686600
H	-2.78849400	0.34462800	-2.03802700
H	-1.24963300	2.36848600	-1.73439000
H	-2.93114800	2.53700200	-1.20754000
H	-4.38854400	-1.18272200	-0.47354200
H	-0.63537000	-1.94457800	-0.40004400
H	-2.49029100	-2.21101700	1.28538000
H	-3.46339200	0.51528200	0.64375500
H	3.13747100	1.21709400	1.40718700
H	3.61609400	-1.30988000	-1.92274800
H	1.18852500	-1.77856100	-1.71979400
H	-0.73807200	2.14867800	0.55491900

O4′-C1′-N1-C6 dihedral = –40°

C	1.57224200	1.03376200	0.21223900
C	0.62827300	0.35839100	-0.83324600

O	1.20461400	-0.87690600	-1.18039100
C	2.23866600	-1.26659300	-0.24300900
C	2.77126600	0.04279300	0.32953200
N	-0.77435200	0.09018200	-0.34628300
C	-1.47391700	1.09858800	0.35405600
N	-2.81715900	0.81957100	0.54690400
C	-3.60663900	-0.18332900	-0.05146300
C	-2.82765400	-1.05678000	-0.91729800
C	-1.49781200	-0.87412400	-1.04517700
O	-0.95539500	2.11320600	0.78218900
O	-4.80481100	-0.24505100	0.16519000
C	1.70103300	-2.22829900	0.81407800
O	0.84375900	-1.60345000	1.75759900
O	3.86461800	0.47639300	-0.48346700
O	1.99345900	2.31298700	-0.18973400
H	1.06997200	1.13890900	1.16922100
H	3.01258000	-1.76727900	-0.83315500
H	1.21055400	-3.07368600	0.31041400
H	2.54646600	-2.62901200	1.38428900
H	4.34810000	1.14592200	0.01907300
H	0.55125600	0.98137800	-1.73071600
H	2.64596100	2.16137600	-0.89266200
H	3.08392600	-0.07034300	1.37223800
H	-3.31521900	1.51549000	1.08963000
H	-3.34291100	-1.83988500	-1.45632700
H	-0.88538300	-1.50486500	-1.67630900
H	0.01257600	-1.39018900	1.31059100

O4′-C1′-N1-C6 dihedral = –20°

C	1.54518000	1.02907300	0.31641600
C	0.65524800	0.47879000	-0.84224900
O	1.23739300	-0.71554500	-1.29420200
C	2.19355000	-1.24046400	-0.33904900
C	2.68284300	-0.03514800	0.46119600
N	-0.76421200	0.19849200	-0.43257700
C	-1.49455400	1.24827100	0.14659100
N	-2.81635400	0.93456100	0.41620500
C	-3.53864700	-0.22167100	0.05568700
C	-2.72057500	-1.18457900	-0.66814800
C	-1.41352400	-0.92848000	-0.90138100
O	-1.00460300	2.33389100	0.40335500
O	-4.72042700	-0.33109500	0.33707600
C	1.59530200	-2.34223900	0.53494500
O	0.70560300	-1.85148400	1.52824300
O	3.89289300	0.43320900	-0.13754700
O	2.07017700	2.30267500	0.04113500
H	0.96688000	1.10366700	1.23523000

H	3.01449300	-1.65742000	-0.93090400
H	1.12142400	-3.09865700	-0.10555000
H	2.41684000	-2.83436200	1.06846500
H	4.29752400	1.05479900	0.48324000
H	0.62295100	1.20117600	-1.66385400
H	2.78765200	2.15670300	-0.59655500
H	2.84531800	-0.29156200	1.51246500
H	-3.34587900	1.67379200	0.86311700
H	-3.19205700	-2.08598100	-1.03473500
H	-0.77798200	-1.60262600	-1.46083800
H	-0.17042000	-1.74543400	1.13600300

O4′-C1′-N1-C6 dihedral = 0°

C	-1.47993200	0.96999600	-0.45740600
C	-0.65518200	0.53813500	0.79748700
O	-1.25606400	-0.61095800	1.33383500
C	-2.24578400	-1.17068100	0.43308000
C	-2.68625800	-0.01957700	-0.46674800
N	0.78186300	0.23885800	0.49797300
C	1.56312300	1.30167700	0.02858800
N	2.86900500	0.95176800	-0.27309100
C	3.50254600	-0.29905600	-0.12190500
C	2.61871300	-1.30665400	0.44822500
C	1.33470400	-0.99611800	0.74404700
O	1.12138600	2.42911200	-0.10607900
O	4.67158000	-0.44766700	-0.43790300
C	-1.70958100	-2.36883000	-0.34966300
O	-0.80637000	-1.99279600	-1.38321900
O	-3.83617500	0.58805500	0.12013500
O	-1.91427800	2.30522700	-0.42190300
H	-0.87827200	0.84710400	-1.35811300
H	-3.07982700	-1.49834100	1.06186300
H	-1.26304100	-3.09115600	0.34624800
H	-2.56124800	-2.86589000	-0.83034000
H	-4.18246200	1.21819500	-0.52712700
H	-0.65949400	1.34147600	1.54083700
H	-2.55370800	2.36037600	0.30504400
H	-2.90366800	-0.36312700	-1.48353400
H	3.44290700	1.70692600	-0.62903300
H	3.02723600	-2.28440300	0.66359800
H	0.66065200	-1.69405400	1.22327400
H	0.10011700	-2.07263200	-1.06003300

O4′-C1′-N1-C6 dihedral = 20°

C	1.26234200	0.82708200	0.68944700
C	0.50499700	0.39098700	-0.57930100
O	1.18559500	-0.73858700	-1.06901600
C	2.58801600	-0.67306600	-0.66524000
C	2.71612600	0.55153500	0.25617600
N	-0.91799100	0.02706300	-0.38430500
C	-1.79694900	1.08539300	-0.17662700
N	-3.10923900	0.71925500	-0.01000700
C	-3.64431900	-0.58937800	0.09809700
C	-2.62783400	-1.62011900	-0.04071600
C	-1.33947600	-1.28145600	-0.26709200
O	-1.42123600	2.25798300	-0.14217400
O	-4.83591800	-0.75015700	0.29225900
C	2.96779900	-2.00208100	-0.02735800
O	2.30659500	-2.23307800	1.20943300
O	3.19424200	1.64279600	-0.50611500
O	1.11610400	2.18817500	1.02166900
H	0.98802400	0.16448700	1.52241400
H	3.19371700	-0.50537200	-1.56298300
H	2.78071100	-2.81440000	-0.74426800
H	4.04052600	-1.99296800	0.19083100
H	2.79558900	2.42860100	-0.09263000
H	0.51566300	1.21360100	-1.30432700
H	0.23616300	2.47802700	0.71213200
H	3.36337900	0.34419300	1.11874100
H	-3.75915700	1.48334400	0.13432700
H	-2.93519100	-2.65439000	0.02695900
H	-0.55816500	-2.01190600	-0.42472500
H	1.38209100	-2.42787600	1.01095000

O4′-C1′-N1-C6 dihedral = 40°

C	-1.26821200	-0.77549500	0.74327900
C	-0.54040600	-0.49078700	-0.58021200
O	-1.24034300	0.53145200	-1.24499600
C	-2.56400500	0.68022300	-0.67317900
C	-2.72365900	-0.44664400	0.36466900
N	0.87101900	-0.09061200	-0.42600800
C	1.78223400	-1.13442100	-0.27942000
N	3.08732000	-0.73096200	-0.13271200
C	3.56591500	0.58332700	0.10396600
C	2.49951100	1.57154300	0.13774000
C	1.22078100	1.20660700	-0.10344300
O	1.43728000	-2.31629300	-0.27401600
O	4.75668500	0.77691200	0.27884400
C	-2.72437100	2.09324300	-0.13784000
O	-1.80783000	2.28496800	0.93743300
O	-3.31358100	-1.56251700	-0.27190300

O	-1.15777000	-2.12584900	1.15271500
H	-0.91625600	-0.08560300	1.52021000
H	-3.29795800	0.52387000	-1.47145500
H	-2.53263500	2.80297400	-0.95513400
H	-3.76581400	2.22517000	0.19210300
H	-2.90661200	-2.33788000	0.15284000
H	-0.52106100	-1.40367400	-1.18415400
H	-0.31493100	-2.47538400	0.81017800
H	-3.31205600	-0.11946900	1.23330900
H	3.76868200	-1.47625400	-0.04994400
H	2.76110900	2.59533400	0.36643000
H	0.38660900	1.89735900	-0.08161700
H	-1.93970100	3.16962300	1.30029200

O4′-C1′-N1-C6 dihedral = 65°

C	-1.36522300	-0.57285800	0.94330300
C	-0.52116200	-0.62561200	-0.34451100
O	-1.16367000	0.21541900	-1.28901600
C	-2.51125300	0.51048500	-0.86478000
C	-2.77692400	-0.36069400	0.37466200
N	0.87222300	-0.20591200	-0.20378500
C	1.88209500	-1.12805800	-0.52933400
N	3.16109400	-0.64290000	-0.33470100
C	3.56376300	0.60367200	0.19212300
C	2.43814800	1.46358700	0.52656200
C	1.17358400	1.03857000	0.32100700
O	1.65669700	-2.25824300	-0.93056500
O	4.74819200	0.86341100	0.32500800
C	-2.66677000	2.00787700	-0.64642300
O	-1.91427700	2.39819200	0.50352900
O	-3.31856400	-1.59307300	-0.06063400
O	-1.34644100	-1.78008700	1.68844900
H	-1.08444600	0.28325600	1.56622500
H	-3.19833900	0.20384300	-1.66167000
H	-2.31429000	2.52814400	-1.54740200
H	-3.73506300	2.23493300	-0.51219700
H	-3.00881600	-2.25858800	0.57489200
H	-0.47922000	-1.65480000	-0.71044500
H	-0.43667600	-2.09738800	1.76181800
H	-3.43788700	0.13833500	1.09667200
H	3.90419300	-1.28956700	-0.57067100
H	2.64679200	2.44629400	0.92638000
H	0.30801000	1.66577400	0.50798600
H	-1.99050800	3.35468400	0.60800100

O4′-C1′-N1-C6 dihedral = 80°

C	-1.39767400	-0.46926700	1.00765600
C	-0.52949900	-0.64248100	-0.25451500
O	-1.17306600	0.06156500	-1.30674900
C	-2.50546500	0.44305800	-0.91264900
C	-2.79807900	-0.31052200	0.39440100
N	0.86350700	-0.20397800	-0.15488800
C	1.85616300	-1.08143200	-0.63578900
N	3.14732700	-0.63164300	-0.42865100
C	3.58309000	0.54049900	0.22369700
C	2.47907900	1.36566400	0.69079300
C	1.20353500	0.97328300	0.48749900
O	1.60811500	-2.14655100	-1.17295700
O	4.77411400	0.77628200	0.34293300
C	-2.61123500	1.95863800	-0.81809100
O	-1.85594000	2.42050200	0.30383300
O	-3.33808600	-1.57496600	0.06148900
O	-1.40028100	-1.60719200	1.85519800
H	-1.14199700	0.43717700	1.56364800
H	-3.20306600	0.09641600	-1.68349500
H	-2.23297900	2.38866200	-1.75527200
H	-3.67200800	2.23355500	-0.71535900
H	-3.05842300	-2.18312100	0.76383400
H	-0.47519700	-1.70469700	-0.50499500
H	-0.49464200	-1.80917100	2.12324300
H	-3.46922100	0.25290000	1.05744100
H	3.87319000	-1.24733600	-0.77528600
H	2.71090900	2.30042000	1.18232800
H	0.35963500	1.59731400	0.75799200
H	-1.87038100	3.38546400	0.30270500

O4′-C1′-N1-C6 dihedral = 90°

C	-1.42691600	-0.40697400	1.04124500
C	-0.53673800	-0.64372300	-0.19528000
O	-1.17041100	-0.01884500	-1.30142200
C	-2.49623900	0.41107700	-0.94079000
C	-2.81613700	-0.27638700	0.39506900
N	0.85801300	-0.19726700	-0.10785500
C	1.82575300	-1.03840800	-0.69725100
N	3.12918900	-0.61848500	-0.50283400
C	3.60289500	0.48663500	0.23296400
C	2.52596500	1.27484000	0.81275700
C	1.23906900	0.91311800	0.62263200
O	1.54537800	-2.05122800	-1.31234700
O	4.80001100	0.70239400	0.32715700

C	-2.56857000	1.93171100	-0.91464600
O	-1.80582700	2.42628900	0.18765300
O	-3.35591500	-1.55341600	0.11545400
O	-1.44693600	-1.50354500	1.94199900
H	-1.18941200	0.52522900	1.55905200
H	-3.19276300	0.04543700	-1.70370000
H	-2.17663200	2.30845100	-1.86888100
H	-3.62322000	2.23605000	-0.83037900
H	-3.09643300	-2.12717800	0.85331800
H	-0.47684300	-1.71866600	-0.38215500
H	-0.55273600	-1.66743300	2.26773100
H	-3.49600900	0.32130200	1.01819500
H	3.83375800	-1.20886700	-0.92848500
H	2.78507900	2.15998000	1.37710000
H	0.42011400	1.52299300	0.98135900
H	-1.77021200	3.38844200	0.12352900

O4′-C1′-N1-C6 dihedral = 120°

C	-1.38655400	0.92819700	-0.66799900
C	-0.48110100	0.39868000	0.45381200
O	-1.09132800	-0.79904400	0.89246500
C	-2.50621400	-0.75796600	0.60815400
C	-2.76975700	0.58531600	-0.09347700
N	0.91677000	0.11939900	0.09408000
C	1.77720900	-0.12231300	1.18855700
N	3.10180600	-0.31348000	0.83355100
C	3.70665600	-0.16183600	-0.42948200
C	2.75070400	0.20100800	-1.46555500
C	1.43940000	0.32662800	-1.16683900
O	1.38626000	-0.15476600	2.33855900
O	4.90790800	-0.32215500	-0.56936900
C	-2.88817400	-1.98415700	-0.20578800
O	-2.35997300	-1.85011600	-1.52150300
O	-3.15240600	1.53638800	0.88355200
O	-1.31448100	2.32681600	-0.88975000
H	-1.25116300	0.34882100	-1.58779000
H	-3.05937900	-0.77400500	1.55482300
H	-2.48513400	-2.87063600	0.30290200
H	-3.98649700	-2.06760200	-0.22183300
H	-2.90522200	2.40439600	0.52849200
H	-0.45700100	1.12630100	1.27356300
H	-0.40125700	2.58530800	-1.06726900
H	-3.52109700	0.49861700	-0.88903800
H	3.72382700	-0.51408000	1.60760500
H	3.11659300	0.35782700	-2.47065400
H	0.71944900	0.57113700	-1.93708600
H	-2.48399600	-2.68584200	-1.98706800

O4′-C1′-N1-C6 dihedral = 140°

C	1.35564400	1.12164800	0.27834700
C	0.47162100	0.23201300	-0.62013700
O	1.07364000	-1.04757900	-0.55555400
C	2.48027300	-0.92215100	-0.28359000
C	2.75113300	0.57898000	-0.06106700
N	-0.92728500	0.12708500	-0.18193900
C	-1.74234300	-0.77233600	-0.90331600
N	-3.05467500	-0.81125300	-0.45992200
C	-3.71026400	0.07296900	0.42071000
C	-2.82239000	1.10117800	0.93839700
C	-1.51145000	1.09943000	0.61212600
O	-1.33460000	-1.45537100	-1.82238200
O	-4.90102500	-0.05649100	0.65779800
C	2.83775600	-1.80519200	0.90424600
O	2.35532800	-1.19514900	2.09498200
O	3.13723100	1.25304100	-1.26202500
O	1.21535800	2.50580200	0.08350200
H	1.14385900	0.88889300	1.32505000
H	3.04284700	-1.27168500	-1.16086700
H	2.38631900	-2.79195400	0.73796000
H	3.93250300	-1.93252000	0.93847500
H	4.08512100	1.13962700	-1.40019300
H	0.48016100	0.60012200	-1.65588100
H	1.75040700	2.71933200	-0.69822800
H	3.46624600	0.76529600	0.74634600
H	-3.64319300	-1.48208700	-0.93898600
H	-3.24045600	1.87006000	1.57300900
H	-0.84539300	1.87825100	0.95858300
H	2.28796900	-1.86742700	2.78289600

O4′-C1′-N1-C6 dihedral = 150°

C	1.36694000	1.11788900	0.29761100
C	0.49285300	0.26173200	-0.64779600
O	1.10049900	-1.01272300	-0.66278400
C	2.48377900	-0.92456000	-0.27756900
C	2.76570100	0.56330400	-0.00612900
N	-0.90698000	0.13466100	-0.19727200
C	-1.71326200	-0.82647000	-0.84817500
N	-3.02351100	-0.84799100	-0.39197000
C	-3.69614500	0.11043600	0.39193900
C	-2.82521700	1.19997000	0.80161700
C	-1.51292700	1.18041900	0.48242700
O	-1.31021500	-1.57454000	-1.71638300
O	-4.88585800	-0.01195400	0.63845500

C	2.73746600	-1.84052700	0.91284500
O	2.18160800	-1.25001900	2.08111200
O	3.20111000	1.26064000	-1.17658800
O	1.25828300	2.50871900	0.12325500
H	1.11273500	0.87220700	1.33143100
H	3.09921800	-1.27193400	-1.11895600
H	2.28133900	-2.81356200	0.68943200
H	3.82432400	-1.99057200	1.02323400
H	4.14951300	1.12783400	-1.29238100
H	0.49269900	0.68866400	-1.66157900
H	1.82310800	2.72605500	-0.63628200
H	3.45500900	0.72021400	0.82981600
H	-3.60280700	-1.56380000	-0.81385300
H	-3.25590800	2.02587200	1.35042700
H	-0.85596400	1.99847200	0.74888300
H	2.03163000	-1.94028500	2.73736500

O4′-C1′-N1-C6 dihedral = 180°

C	-1.31875500	-1.05129400	0.53356800
C	-0.60573800	-0.53818000	-0.75544800
O	-1.28083600	0.61305500	-1.15146500
C	-2.51314500	0.80146800	-0.42005000
C	-2.73975500	-0.50473700	0.35202200
N	0.85674500	-0.30246900	-0.51067100
C	1.45458100	0.95615300	-0.37613200
N	2.82411100	0.90000900	-0.18065600
C	3.63377000	-0.20992400	0.13929400
C	2.87028300	-1.44532300	0.19110800
C	1.55628700	-1.43580000	-0.11370300
O	0.87851500	2.03804500	-0.42169500
O	4.82575500	-0.06823000	0.35486000
C	-2.38473700	2.06161900	0.43853900
O	-1.30737700	1.98083700	1.34564100
O	-3.42079900	-1.48776100	-0.43550100
O	-1.26282000	-2.44589600	0.70977000
H	-0.85821700	-0.56600000	1.39738000
H	-3.31449800	0.94057300	-1.15784100
H	-2.28365600	2.92424500	-0.23485700
H	-3.30748100	2.20059200	1.01666300
H	-4.37024500	-1.31968100	-0.40481000
H	-0.64352900	-1.30558900	-1.54141700
H	-2.01745800	-2.80045300	0.21012600
H	-3.24617000	-0.34560600	1.31048700
H	3.26967200	1.80796900	-0.11862000
H	3.37466300	-2.35652800	0.48117400
H	0.95533900	-2.33783900	-0.08129800
H	-0.50065600	2.13123400	0.81424100

2′-exo-3′-endo ribosyl pucker

O4′-C1′-N1-C6 dihedral = –180°

O	-1.29044900	0.37314500	-1.27473800
C	-0.51525300	-0.73624700	-0.94757800
C	-1.32905900	-1.51103100	0.11379700
C	-2.10068700	-0.38669600	0.82652400
C	-2.37811400	0.58899300	-0.32940100
C	-2.44146400	2.06044300	0.06614000
O	-1.33238000	2.47690400	0.82439700
H	-0.72883900	-2.11071900	0.79808400
O	-2.23407900	-2.42509200	-0.50555700
O	-3.25052600	-0.84158900	1.49690700
H	-3.32051500	0.31760800	-0.82973000
H	-2.57402400	2.66466000	-0.84412600
H	-3.33611400	2.19312200	0.68610300
H	-0.55701900	2.45774300	0.23244000
H	-1.45711900	0.11605900	1.55523800
H	-3.56215300	-1.61397700	0.99788200
H	-0.36272800	-1.34579700	-1.84755600
H	-2.64810600	-1.98637800	-1.26351100
C	1.44126200	0.87391100	-0.42826300
C	1.64931000	-1.51135100	-0.11919100
C	3.60055200	-0.16411500	0.38394600
N	0.87421800	-0.40779600	-0.44609900
O	4.74871400	0.04369700	0.73536400
C	2.93387800	-1.45330800	0.28469100
N	2.75739300	0.89727100	0.00222100
O	0.87884700	1.91107100	-0.75251000
H	3.16402600	1.82514400	0.03156800
H	1.14686100	-2.46512100	-0.23233300
H	3.49088000	-2.34734600	0.52819600

O4′-C1′-N1-C6 dihedral = –140°

O	-1.09252000	-0.17367800	1.29246800
C	-0.34167000	0.86016900	0.71549200
C	-1.12044400	1.36371500	-0.53290900
C	-2.21677000	0.29699600	-0.73966900
C	-2.40442600	-0.25835900	0.68538600
C	-2.87943100	-1.70383100	0.77598500
O	-2.18343400	-2.58217800	-0.07588600
H	-0.47320000	1.49429900	-1.40157000
O	-1.69639800	2.65212500	-0.29936900
O	-3.39880700	0.81205700	-1.30728700

H	-3.10834900	0.38325200	1.24246400
H	-2.82102300	-2.01467200	1.83212600
H	-3.93428900	-1.73150400	0.48059600
H	-1.23374500	-2.38777200	-0.00658100
H	-1.83960500	-0.50898500	-1.37274800
H	-3.34699300	1.77706100	-1.21590600
H	-0.23376600	1.70284200	1.41337000
H	-2.18085100	2.62939100	0.53941100
C	1.29902100	-0.77221000	-0.23508200
C	2.07600000	1.30874300	0.71520700
C	3.75064100	-0.19368000	-0.19774700
N	1.04636200	0.41635900	0.46340400
O	4.87521000	-0.55287100	-0.49755700
C	3.37005400	1.06533400	0.42576000
N	2.63776600	-1.02514600	-0.45320900
O	0.42644000	-1.53090900	-0.63331700
H	2.83042000	-1.89555600	-0.93546600
H	1.76553600	2.23228300	1.19132500
H	4.14518800	1.78323800	0.65465400

O4′-C1′-N1-C6 dihedral = –120°

O	0.99574200	0.11156500	1.30660400
C	0.33970700	-0.93026600	0.61926700
C	1.19871200	-1.31021600	-0.61433200
C	2.29970800	-0.22135600	-0.64085000
C	2.33132800	0.29833800	0.80241500
C	2.69011900	1.77476900	0.94092500
O	2.02937200	2.60592300	0.01027800
H	0.59631600	-1.32054900	-1.53205500
O	1.76889200	-2.58008800	-0.37005900
O	3.57268500	-0.77680900	-0.97638600
H	3.03613300	-0.31227300	1.38601900
H	2.48975000	2.07697800	1.98092800
H	3.76576400	1.88775100	0.76488300
H	1.09676000	2.33566600	-0.03285400
H	2.02755600	0.59210500	-1.31357600
H	3.75227200	-0.58711200	-1.90563400
H	0.26176200	-1.82527600	1.24640200
H	2.70290400	-2.49329200	-0.63272900
C	-1.28688100	0.60632400	-0.44217800
C	-2.09939800	-1.26942000	0.84367100
C	-3.75375400	0.20157500	-0.15696100
N	-1.04906700	-0.52564900	0.33909800
O	-4.87558600	0.59483300	-0.42413300
C	-3.39752400	-0.96737300	0.63210700
N	-2.61875700	0.90329000	-0.62665000
O	-0.39005400	1.28000400	-0.93886200

H	-2.80156000	1.72550100	-1.19008700
H	-1.80038600	-2.12815300	1.43385000
H	-4.19302300	-1.57251400	1.04380000

O4′-C1′-N1-C6 dihedral = –100°

O	0.91465100	0.07674000	1.29713000
C	0.36017300	-0.97991100	0.53878800
C	1.30615100	-1.28186900	-0.64703400
C	2.34873900	-0.13703800	-0.58245600
C	2.25854300	0.36651200	0.86576900
C	2.49606800	1.86444800	1.02996200
O	1.82524200	2.65072200	0.06551000
H	0.76531800	-1.30101800	-1.60050700
O	1.92755000	-2.52664000	-0.39184600
O	3.66967400	-0.62017400	-0.83491900
H	2.97425100	-0.19463000	1.48418200
H	2.21534000	2.14463400	2.05721700
H	3.56732100	2.06239300	0.91287400
H	0.92426300	2.30493700	-0.03910900
H	2.08088300	0.66818400	-1.26600700
H	3.90052900	-0.41050700	-1.74845200
H	0.30592900	-1.89576600	1.13751400
H	2.87125000	-2.38355400	-0.58582600
C	-1.28654500	0.43438300	-0.63215200
C	-2.06034200	-1.20952100	0.95411500
C	-3.73482700	0.18521500	-0.11971800
N	-1.03527900	-0.65185300	0.20987500
O	-4.85861300	0.59455500	-0.35120700
C	-3.35610600	-0.85864100	0.82024800
N	-2.61862200	0.74376300	-0.78664200
O	-0.39463900	1.05678100	-1.19945500
H	-2.81215700	1.51537400	-1.41444200
H	-1.74438200	-1.97956000	1.64868500
H	-4.13327900	-1.33120400	1.40439800

O4′-C1′-N1-C6 dihedral = –75°

O	-0.90994100	0.37168200	-1.23186500
C	-0.39471700	-0.86042500	-0.72482300
C	-1.38956200	-1.38563900	0.32970900
C	-2.27439800	-0.15095300	0.60571500
C	-2.24801100	0.58294300	-0.73893800
C	-2.48665900	2.08382400	-0.66484600
O	-1.57198300	2.72870900	0.20197800

H	-0.89601800	-1.77203100	1.22467600
O	-2.16560400	-2.38573000	-0.31290300
O	-3.61577800	-0.52087100	0.91916400
H	-2.97987300	0.11828900	-1.41519200
H	-2.44862800	2.50475100	-1.68126000
H	-3.49090800	2.25915900	-0.26593600
H	-0.68957200	2.46246800	-0.09398500
H	-1.82701700	0.47830300	1.37722000
H	-3.70671300	-0.54284500	1.88015100
H	-0.36874200	-1.59956900	-1.53235600
H	-3.06679000	-2.26745000	0.03348400
C	1.34693000	-0.16163500	0.92718100
C	1.92775000	-0.58561500	-1.37889700
C	3.69811300	0.18469700	0.09266500
N	1.00926300	-0.66478600	-0.34085200
O	4.83004300	0.52997900	0.38343200
C	3.21219000	-0.20886600	-1.22150700
N	2.68491900	0.14636900	1.07538900
O	0.54369900	-0.02451200	1.83692400
H	2.94589500	0.47149600	1.99892500
H	1.53403900	-0.88003900	-2.34508700
H	3.90177000	-0.18766000	-2.05379100

O4′-C1′-N1-C6 dihedral = –50°

O	1.07883100	0.73017600	1.27039100
C	0.61445900	-0.60245000	1.10014400
C	1.65186200	-1.30753000	0.22113100
C	2.13675600	-0.14982500	-0.67009200
C	2.09210100	1.05014700	0.28731300
C	1.73216900	2.37499900	-0.37336700
O	0.46573400	2.32835500	-1.00926500
H	1.25186600	-2.15419000	-0.33573800
O	2.69858800	-1.69402300	1.09912200
O	3.47956200	-0.33724600	-1.11021100
H	3.06088200	1.13447600	0.79547500
H	1.77925800	3.18133000	0.37315700
H	2.47348300	2.59367000	-1.14894200
H	-0.18711100	2.19289500	-0.30834200
H	1.44947000	0.00103200	-1.50742400
H	3.45740700	-0.83399000	-1.93871600
H	0.59543100	-1.07380100	2.08674400
H	3.51786200	-1.54999600	0.59690700
C	-1.25666600	-1.00963800	-0.60811000
C	-1.62265700	0.26154600	1.41367200
C	-3.49242900	0.05678400	-0.12053400
N	-0.80681100	-0.55667100	0.64266800
O	-4.62964100	0.24226800	-0.51827200

C	-2.89733800	0.57320100	1.10327900
N	-2.58578200	-0.72207200	-0.86638100
O	-0.57151900	-1.61786500	-1.41600200
H	-2.92164600	-1.06832400	-1.75735300
H	-1.15085200	0.63402600	2.31493200
H	-3.49988200	1.19734800	1.74856800

O4′-C1′-N1-C6 dihedral = –30°

O	1.17237700	0.62141500	1.21634900
C	0.47734700	-0.58425900	0.94547500
C	1.37439700	-1.37802300	-0.02254400
C	2.17263200	-0.26350400	-0.72076200
C	2.36036900	0.75245400	0.40387600
C	2.50001100	2.19881600	-0.04934500
O	1.45956600	2.61197800	-0.92004100
H	0.80357200	-2.00938600	-0.70462100
O	2.25026400	-2.14317800	0.78734800
O	3.44793800	-0.71484500	-1.16771700
H	3.23490600	0.46776700	1.00292400
H	2.57459200	2.85064500	0.83326400
H	3.43440600	2.28997800	-0.61221200
H	0.63448800	2.58394000	-0.41736900
H	1.59523600	0.19154800	-1.53297200
H	3.35720900	-1.03854700	-2.07318700
H	0.32921700	-1.14254400	1.87439000
H	3.09070900	-2.17498400	0.30141700
C	-1.68530600	-1.22578000	-0.15363400
C	-1.43927000	0.97898300	0.79113300
C	-3.57695900	0.43766300	-0.23204000
N	-0.86606200	-0.21607200	0.38355300
O	-4.72867600	0.64212300	-0.57663000
C	-2.70675500	1.34295600	0.50195200
N	-2.94979100	-0.79410700	-0.51298000
O	-1.32552300	-2.38113100	-0.31286100
H	-3.53181500	-1.50538100	-0.93949100
H	-0.77149200	1.61632500	1.35507300
H	-3.10642200	2.29515700	0.82251100

O4′-C1′-N1-C6 dihedral = –20°

O	-1.16976700	0.56425500	-1.21932100
C	-0.44207000	-0.60848500	-0.89775900
C	-1.29754000	-1.38237800	0.12430700
C	-2.16832600	-0.27063800	0.73684200

C	-2.39430600	0.65405700	-0.45724400
C	-2.66345200	2.10965200	-0.10438800
O	-1.70652500	2.65468000	0.79027100
H	-0.68752600	-1.92029100	0.85390500
O	-2.11925800	-2.26347400	-0.61806000
O	-3.42224000	-0.76232800	1.20090900
H	-3.22315300	0.26370700	-1.06203300
H	-2.73943300	2.70051500	-1.02854500
H	-3.63054900	2.16009500	0.40561700
H	-0.85880700	2.68291400	0.32788500
H	-1.63072000	0.27352200	1.52099300
H	-3.33240500	-0.99941200	2.13279600
H	-0.28593900	-1.21572600	-1.79401800
H	-2.95884900	-2.30818500	-0.13147500
C	1.76796100	-1.21356700	0.04933600
C	1.38958800	1.06919600	-0.63556800
C	3.58115900	0.52026800	0.26608200
N	0.89556500	-0.19382400	-0.36546300
O	4.73202700	0.74213200	0.60338400
C	2.64641700	1.46042600	-0.33231500
N	3.02452400	-0.76803100	0.41604600
O	1.44473000	-2.38960500	0.09687800
H	3.65096500	-1.49101700	0.74968700
H	0.67668800	1.72716900	-1.11299600
H	2.99079200	2.46321500	-0.54414500

O4′-C1′-N1-C6 dihedral = 0°

O	-1.18288500	0.41967100	-1.25005900
C	-0.41012900	-0.68814000	-0.82880700
C	-1.21997900	-1.39931300	0.27078300
C	-2.11367900	-0.25700900	0.79332800
C	-2.40743100	0.50781900	-0.49774700
C	-2.81710600	1.96171800	-0.32698100
O	-1.86671400	2.72120400	0.41397400
H	-0.56685700	-1.83992100	1.03241000
O	-2.02809000	-2.37744400	-0.35079300
O	-3.33459800	-0.73253300	1.35086800
H	-3.20696000	-0.01955000	-1.03661900
H	-3.00686700	2.40620200	-1.31163500
H	-3.76200700	1.97154700	0.22908300
H	-1.33084300	3.22188500	-0.21118700
H	-1.57213600	0.38989000	1.49282800
H	-3.20467000	-0.87669900	2.29697800
H	-0.21667200	-1.36906900	-1.66085200
H	-2.85101100	-2.40445100	0.16468600
C	1.87665300	-1.19679600	-0.12320500
C	1.24553200	1.13171000	-0.29932500

C	3.55275200	0.63217600	0.29634700
N	0.90830000	-0.20368300	-0.32134500
O	4.70874700	0.89562300	0.58551500
C	2.48572800	1.57545400	0.00483600
N	3.12608300	-0.71194800	0.21109200
O	1.62323400	-2.38666100	-0.23130200
H	3.83331300	-1.41913300	0.37174400
H	0.41841300	1.79233600	-0.51196500
H	2.71400500	2.63177600	0.03530300

O4′-C1′-N1-C6 dihedral = 20°

O	-1.17608000	0.32266100	-1.24231800
C	-0.39377400	-0.74931000	-0.74049300
C	-1.18815900	-1.37412900	0.42402500
C	-2.12606200	-0.21715800	0.82995100
C	-2.42298900	0.41281500	-0.53239900
C	-2.90139600	1.85685100	-0.51375700
O	-1.95672700	2.75434700	0.06178600
H	-0.52010400	-1.70850500	1.22865500
O	-1.95858100	-2.43969400	-0.08937100
O	-3.33966100	-0.67897700	1.41348700
H	-3.18502100	-0.20205800	-1.03235600
H	-3.17178100	2.16701400	-1.53095400
H	-3.80860500	1.89917200	0.09869900
H	-1.36940200	3.04280500	-0.64765700
H	-1.61933900	0.50947400	1.47585200
H	-3.22319800	-0.72734200	2.37106400
H	-0.20651700	-1.50041200	-1.50959400
H	-2.78729200	-2.43472900	0.41786900
C	1.97165900	-1.16701600	-0.29134300
C	1.15225200	1.09894200	-0.03039900
C	3.52605100	0.70687300	0.34605300
N	0.92917400	-0.23083600	-0.31128300
O	4.67383100	1.01748300	0.62083100
C	2.36989900	1.58766900	0.29551400
N	3.20302800	-0.63265700	0.03619000
O	1.79385000	-2.34949600	-0.53668200
H	3.96812400	-1.29615800	0.05780400
H	0.26590000	1.71653600	-0.07119400
H	2.51387500	2.63484600	0.52267900

O4′-C1′-N1-C6 dihedral = 40°

O	-1.14520800	0.20957200	-1.23442200

C	-0.38940300	-0.81854300	-0.59927200
C	-1.22096900	-1.29673700	0.61309200
C	-2.20992800	-0.13075700	0.82796500
C	-2.42781100	0.35552600	-0.60733500
C	-2.87771500	1.80368700	-0.74739400
O	-1.91152300	2.72306500	-0.25196500
H	-0.57861000	-1.49427900	1.48302300
O	-1.93599400	-2.45041200	0.22533000
O	-3.45046800	-0.56480500	1.37619900
H	-3.16642200	-0.30402200	-1.08513000
H	-3.12207300	2.01544200	-1.79675700
H	-3.78885000	1.94070300	-0.15648100
H	-1.19637500	2.74137300	-0.90209600
H	-1.76812100	0.67073600	1.43066100
H	-3.40198600	-0.50280300	2.33887900
H	-0.21016700	-1.65784400	-1.27184000
H	-2.80037000	-2.38585000	0.66528000
C	2.04224100	-1.12749200	-0.45928000
C	1.09482400	0.99096800	0.25356300
C	3.50856000	0.72635800	0.41266800
N	0.93728700	-0.28664400	-0.24348300
O	4.64890000	1.07430500	0.67150800
C	2.29604200	1.51280900	0.58450800
N	3.25375600	-0.55768200	-0.11392100
O	1.94112100	-2.25842500	-0.90343400
H	4.06169100	-1.15105000	-0.25984600
H	0.17722500	1.55845200	0.34741400
H	2.38708500	2.51810800	0.97189900

O4′-C1′-N1-C6 dihedral = 47°

O	-1.15619200	0.16869200	-1.24626800
C	-0.40696900	-0.82642300	-0.55442300
C	-1.25419400	-1.25195800	0.66713500
C	-2.24620700	-0.08282400	0.84147300
C	-2.43458600	0.38160500	-0.61441800
C	-2.82181700	1.84562300	-0.78644200
O	-1.80274800	2.72492000	-0.32946300
H	-0.64036000	-1.44013500	1.54958800
O	-1.98044200	-2.45991800	0.43154300
O	-3.44094500	-0.45151400	1.48069100
H	-3.20385400	-0.24786100	-1.09108000
H	-3.07406500	2.04696000	-1.83646400
H	-3.71356100	2.03802100	-0.18182100
H	-1.08697100	2.66858400	-0.97699900
H	-1.79096400	0.72822000	1.42002600
H	-3.54574800	-1.40202300	1.30416100
H	-0.20846500	-1.68792300	-1.19760500

H	-2.22407300	-2.51234600	-0.50319500
C	2.02772000	-1.11507900	-0.50800100
C	1.07711300	0.95517600	0.34409000
C	3.49646700	0.70331300	0.42865200
N	0.92046200	-0.29803900	-0.21826100
O	4.63936600	1.04688800	0.67750700
C	2.28185600	1.46852600	0.67188600
N	3.24049200	-0.55334900	-0.16313100
O	1.92354400	-2.22122600	-1.01244800
H	4.05066200	-1.12897800	-0.35965000
H	0.15892600	1.51376900	0.48135200
H	2.37484200	2.45294200	1.10923200

O4′-C1′-N1-C6 dihedral = 60°

O	-1.10629500	0.11594700	-1.22926000
C	-0.39076100	-0.85415500	-0.45900600
C	-1.26379800	-1.18400800	0.77514600
C	-2.31070200	-0.04665600	0.78570000
C	-2.42248600	0.31729000	-0.69847500
C	-2.81343900	1.76650400	-0.96329000
O	-1.85730000	2.67062600	-0.42695800
H	-0.65865600	-1.22437800	1.69269200
O	-1.90692700	-2.41685600	0.53432900
O	-3.57854800	-0.48396100	1.26645200
H	-3.14324400	-0.36346900	-1.17395700
H	-2.94818300	1.92206400	-2.04247000
H	-3.76852800	1.97297000	-0.47026600
H	-1.04388800	2.52202800	-0.92962900
H	-1.95658400	0.82337500	1.34903500
H	-3.62787800	-0.30953500	2.21517000
H	-0.22602200	-1.76404700	-1.03652500
H	-2.81132200	-2.31388400	0.87666900
C	2.05586800	-1.05193900	-0.62349600
C	1.09609700	0.84678200	0.55023200
C	3.52043600	0.68435900	0.46914200
N	0.94063700	-0.32657900	-0.16200800
O	4.66393900	1.03945500	0.70072800
C	2.29870100	1.36437500	0.87789600
N	3.26936700	-0.48953400	-0.27043700
O	1.96669700	-2.08172000	-1.26756300
H	4.08393300	-0.99962600	-0.59058500
H	0.17225600	1.35507000	0.80061700
H	2.38606500	2.28897800	1.43143600

O4′-C1′-N1-C6 dihedral = 80°

O	1.06757000	0.09824700	1.19543100
C	0.38464400	-0.85862700	0.37412400
C	1.29287100	-1.13731500	-0.84514100
C	2.34239400	-0.00374600	-0.77074100
C	2.40989800	0.28993500	0.73123900
C	2.81497100	1.71844000	1.07452400
O	1.91656800	2.65996100	0.50994500
H	0.72519300	-1.14202700	-1.78716000
O	1.92476400	-2.38215700	-0.63656900
O	3.61942000	-0.42356300	-1.24031300
H	3.09574300	-0.42778300	1.20417100
H	2.88022200	1.82713300	2.16647800
H	3.80520000	1.91981800	0.65409600
H	1.04931800	2.45022100	0.88639500
H	2.00399000	0.89935300	-1.29153100
H	3.70132000	-0.18852200	-2.17342700
H	0.23520900	-1.78365700	0.93116500
H	2.83839600	-2.26806500	-0.95018000
C	-2.02409100	-0.87593500	0.82842400
C	-1.16885800	0.58811300	-0.91078900
C	-3.56791700	0.58953600	-0.52126700
N	-0.95148800	-0.35338900	0.07639000
O	-4.72167000	0.93428000	-0.71276600
C	-2.38908300	1.06495400	-1.23322100
N	-3.25721200	-0.35910000	0.47420900
O	-1.88227500	-1.70891500	1.70417000
H	-4.03977800	-0.72513400	1.00330100
H	-0.27629800	0.94666600	-1.40902900
H	-2.52159900	1.80447500	-2.01056900

O4′-C1′-N1-C6 dihedral = 100°

O	1.09047900	0.10205900	1.23061900
C	0.43270000	-0.88860800	0.43479300
C	1.38523400	-1.23185700	-0.72427000
C	2.31065100	0.00255300	-0.78370300
C	2.37632400	0.43418900	0.68563800
C	2.59176800	1.92937900	0.88747600
O	1.55637000	2.68411200	0.28005300
H	0.85612300	-1.43193700	-1.66654400
O	2.13542900	-2.36189100	-0.33053900
O	3.61625800	-0.32892300	-1.24473800
H	3.16637200	-0.13953400	1.18972900
H	2.67108100	2.14369200	1.96284900
H	3.53293000	2.22459000	0.41278200
H	0.73597700	2.37722900	0.69406000
H	1.86884600	0.81402300	-1.37416400
H	3.65318900	-0.19527400	-2.20052400

H	0.26610600	-1.77284700	1.04972200
H	3.03439500	-2.20879800	-0.66838200
C	-1.91963800	-0.62339900	1.01449200
C	-1.20032600	0.15327600	-1.16848000
C	-3.55668200	0.38784200	-0.61121000
N	-0.90139600	-0.39863000	0.06233700
O	-4.71770300	0.70080000	-0.81346900
C	-2.44001300	0.54374800	-1.53273900
N	-3.17063300	-0.18955300	0.61521500
O	-1.71343000	-1.15389800	2.08965200
H	-3.90884600	-0.33845900	1.29291100
H	-0.35947900	0.28350500	-1.83695800
H	-2.63182300	0.98028000	-2.50294800

O4′-C1′-N1-C6 dihedral = 120°

O	1.12315000	0.56876400	1.12463900
C	0.48021600	-0.65803400	0.79479700
C	1.46195200	-1.43384500	-0.09582200
C	2.27853600	-0.30070500	-0.74850900
C	2.33781000	0.74230000	0.37332200
C	2.39091300	2.18426400	-0.11671000
O	1.26810800	2.49947500	-0.92254900
H	0.97275000	-2.09935800	-0.81899600
O	2.29650600	-2.18162000	0.76426100
O	3.59931600	-0.71647300	-1.08052200
H	3.20398700	0.52547800	1.01278400
H	2.47090400	2.85845800	0.74796700
H	3.28399000	2.32019000	-0.73536200
H	0.49350400	2.35360500	-0.35954900
H	1.75651400	0.12511500	-1.61367600
H	3.60655100	-1.03473400	-1.99236200
H	0.29897600	-1.20157700	1.72291700
H	3.18189600	-2.14500700	0.36414200
C	-1.80599800	0.08187700	1.15122900
C	-1.25345600	-0.73345000	-1.06018300
C	-3.55210800	-0.04091300	-0.65863700
N	-0.85026700	-0.36480400	0.20967900
O	-4.72054500	0.14818800	-0.95191400
C	-2.51472800	-0.58891600	-1.51975100
N	-3.07306400	0.27234200	0.62916800
O	-1.53243600	0.28321000	2.31880300
H	-3.75922100	0.61129900	1.29311500
H	-0.47737000	-1.12237000	-1.70437400
H	-2.78077200	-0.87168700	-2.52869100

O4′-C1′-N1-C6 dihedral = 145°

O	1.09606100	0.18097300	1.30328100
C	0.33281000	-0.86040100	0.75016800
C	1.07687500	-1.37278300	-0.51238200
C	2.19322100	-0.32154000	-0.71721600
C	2.39802200	0.24148900	0.69278200
C	2.89067200	1.68342600	0.75017600
O	2.21631300	2.54544100	-0.13847500
H	0.39665000	-1.44554300	-1.37310700
O	1.64189600	-2.63057000	-0.20633700
O	3.40042500	-0.92775300	-1.17742300
H	3.09536000	-0.41032000	1.24007200
H	2.82031200	2.02436800	1.79533300
H	3.95008800	1.69437900	0.47013900
H	1.26129400	2.38498800	-0.04700900
H	1.86470100	0.48108500	-1.37998700
H	3.47810500	-0.77410600	-2.12709500
H	0.24326100	-1.69860700	1.45088100
H	2.53459400	-2.60976400	-0.59497500
C	-1.29916200	0.78990500	-0.18691400
C	-2.07726300	-1.31538600	0.69115000
C	-3.74639000	0.19585200	-0.21515300
N	-1.05451600	-0.39890800	0.51062800
O	-4.86670600	0.55472100	-0.53303800
C	-3.36663700	-1.07923300	0.37316600
N	-2.63588300	1.04536000	-0.41711200
O	-0.42523900	1.55307300	-0.57865600
H	-2.82385500	1.92109200	-0.89114900
H	-1.76564400	-2.25125300	1.14190200
H	-4.13696700	-1.81653700	0.55090000

O4′-C1′-N1-C6 dihedral = 170°

O	-1.28810900	0.46748800	-1.23269800
C	-0.54590300	-0.69117700	-1.03134100
C	-1.32283600	-1.50663300	0.03567100
C	-2.07710600	-0.40343500	0.80550100
C	-2.36076900	0.62715000	-0.28469000
C	-2.38111000	2.07550600	0.19334400
O	-1.20541500	2.42891500	0.88599100
H	-0.67156400	-2.09169100	0.69705200
O	-2.23724800	-2.33978900	-0.64042400
O	-3.30526400	-0.88747700	1.34280300
H	-3.31083000	0.37987700	-0.77770900

H	-2.56297000	2.72893900	-0.67237800
H	-3.22522300	2.19547200	0.88284800
H	-0.48021500	2.42892400	0.23245300
H	-1.44254000	0.04782200	1.57565700
H	-3.15178600	-1.17713700	2.25120000
H	-0.46759100	-1.25164500	-1.96884200
H	-3.05223900	-2.31354800	-0.10964400
C	1.46247700	0.85685100	-0.52211000
C	1.60009600	-1.52159900	-0.15050000
C	3.54776600	-0.20517400	0.44219300
N	0.87774600	-0.41692600	-0.57434900
O	4.67540700	-0.01070300	0.86361700
C	2.85804300	-1.47988700	0.33522500
N	2.75582600	0.86120900	-0.02365900
O	0.93536400	1.90422500	-0.87318100
H	3.17681000	1.78219800	0.01480400
H	1.09481800	-2.47031800	-0.28374900
H	3.37649100	-2.37977100	0.63573600

O4′-C1′-N1-C6 dihedral = 180°

O	-1.29044900	0.37314500	-1.27473800
C	-0.51525300	-0.73624700	-0.94757800
C	-1.32905900	-1.51103100	0.11379700
C	-2.10068700	-0.38669600	0.82652400
C	-2.37811400	0.58899300	-0.32940100
C	-2.44146400	2.06044300	0.06614000
O	-1.33238000	2.47690400	0.82439700
H	-0.72883900	-2.11071900	0.79808400
O	-2.23407900	-2.42509200	-0.50555700
O	-3.25052600	-0.84158900	1.49690700
H	-3.32051500	0.31760800	-0.82973000
H	-2.57402400	2.66466000	-0.84412600
H	-3.33611400	2.19312200	0.68610300
H	-0.55701900	2.45774300	0.23244000
H	-1.45711900	0.11605900	1.55523800
H	-3.56215300	-1.61397700	0.99788200
H	-0.36272800	-1.34579700	-1.84755600
H	-2.64810600	-1.98637800	-1.26351100
C	1.44126200	0.87391100	-0.42826300
C	1.64931000	-1.51135100	-0.11919100
C	3.60055200	-0.16411500	0.38394600
N	0.87421800	-0.40779600	-0.44609900
O	4.74871400	0.04369700	0.73536400
C	2.93387800	-1.45330800	0.28469100
N	2.75739300	0.89727100	0.00222100
O	0.87884700	1.91107100	-0.75251000

H	3.16402600	1.82514400	0.03156800
H	1.14686100	-2.46512100	-0.23233300
H	3.49088000	-2.34734600	0.52819600

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