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Supporting Material

DNA Hairpins Containing the Cytidine Analog Pyrrolo-dC: Structural, Thermodynamic, and Spectroscopic Studies

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<BELOW IS THE AMBER .frcmod FILE FOR MD SIMULATIONS OF DNA CONTAINING PdC>

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remark goes here
MASS
C* 12.010         0.360              same as c2
HA 1.008          0.135              same as hc
CC 12.010         0.360              same as c2
CT 12.010         0.878              same as c3
HC 1.008          0.135              same as hc
H2 1.008          0.135              same as hc
N* 14.010         0.530              same as na
CM 12.010         0.360              same as c2
H4 1.008          0.135              same as ha
CB 12.010         0.360              same as c2
NA 14.010         0.530              same as na
H  1.008          0.161              same as hn
NC 14.010         0.530              same as n2
C  12.010         0.616              same as c
O  16.000         0.434              same as o
OS 16.000         0.465              same as os
H1 1.008          0.135              same as hc
P  30.970         1.538              same as p4
O2 16.000         0.434              same as o
OH 16.000         0.465              same as oh
HO 1.008          0.135              same as ho

BOND
C*-HA  344.30   1.087       same as c2-hc
C*-CC  418.30   1.429       same as cc-cc
C*-CB  418.30   1.429       same as cc-cc
CC-CT  328.30   1.508       same as c2-c3
CC-NA  411.10   1.391       same as c2-na
CT-HC  337.30   1.092       same as c3-hc
CT-H2  337.30   1.092       same as c3-hc
CT-N*  334.70   1.456       same as c3-na
CT-OS  301.50   1.439       same as c3-os
CT-CT  303.10   1.535       same as c3-c3
N*-CM  411.10   1.391       same as c2-na
N*-C   424.00   1.383       entered by Randy from parm99.dat
CM-H4  344.30   1.087       same as c2-ha
CM-CB  418.30   1.429       same as cc-cc
CB-CB  418.30   1.429       same as cc-cc
CB-NA  411.10   1.391       same as c2-na
CB-NC  431.60   1.376       same as cc-nc
NA-H   406.60   1.011       same as hn-na
NC-C   374.60   1.420       same as c -n2
C -O   648.00   1.214       same as c -o
CT-H1  337.30   1.092       same as c3-hc
OS-P   311.60   1.636       same as os-p4
P -O2  456.40   1.503       same as o -p4
P -OH  307.40   1.641       same as oh-p4
CT-OH  314.10   1.426       same as c3-oh
OH-HO  369.60   0.974       same as ho-oh

ANGLE
C*-CC-CT   64.300     123.420   same as c2-c2-c3
C*-CC-NA   69.800     121.380   same as c2-c2-na
C*-CB-CM   67.900     110.700   same as cc-cc-cc
C*-CB-CB   67.900     110.700   same as cc-cc-cc
HA-C*-CC   50.300     119.700   same as c2-c2-hc
HA-C*-CB   50.300     119.700   same as c2-c2-hc
CC-C*-CB   67.900     110.700   same as cc-cc-cc
CC-CT-HC   47.000     110.490   same as c2-c3-hc
CC-NA-CB   67.800     110.370   same as c2-na-c2
CC-NA-H    47.600     119.280   same as c2-na-hn
CT-CC-NA   65.000     122.540   same as c3-c2-na
HC-CT-HC   39.400     108.350   same as hc-c3-hc
CT-N*-CM   64.200     117.200   same as c2-na-c3
CT-N*-C    64.700     117.600   same as c -na-c3
CT-OS-CT   62.100     113.410   same as c3-os-c3
CT-CT-CT   63.200     110.630   same as c3-c3-c3
CT-CT-HC   33.235     109.490   Calculated with empirical approach
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H2-CT-N*   49.900     109.500   same as hc-c3-na
H2-CT-OS   50.900     108.700   same as hc-c3-os
H2-CT-CT   46.400     110.050   same as c3-c3-hc
N*-CT-OS   71.200     109.190   same as na-c3-os
N*-CT-CT   65.800     112.590   same as c3-c3-na
N*-CM-H4   51.200     112.420   same as ha-c2-na
N*-CM-CB   69.800     121.380   same as c2-c2-na
N*-C -NC   70.700     118.600   same as n2-c -na
N*-C -O    75.000     122.850   same as na-c -o
CM-N*-C    64.300     125.090   same as c -na-c2
CM-CB-CB   67.900     110.700   same as cc-cc-cc
H4-CM-CB   50.000     120.940   same as c2-c2-ha
CB-CB-NA   69.800     121.380   same as c2-c2-na
CB-CB-NC   70.000     113.420   same as cc-cc-nc
CB-NA-H    47.600     119.280   same as c2-na-hn
CB-NC-C    66.200     120.970   same as c -n2-c2
NA-CB-NC   71.700     123.620   same as n2-c2-na
NC-C -O    73.000     122.500   same as n2-c -o
OS-CT-CT   67.800     108.420   same as c3-c3-os
OS-CT-H1   50.900     108.700   same as hc-c3-os
CT-CT-H1   46.400     110.050   same as c3-c3-hc
CT-CT-OH   67.700     109.430   same as c3-c3-oh
CT-OS-P    77.600     117.480   same as c3-os-p4
H1-CT-H1   39.400     108.350   same as hc-c3-hc
OS-P -O2   43.100     116.670   same as o -p4-os
OS-P -OH   72.232      98.025   Calculated with empirical approach
P -OH-HO   55.300     110.190   same as ho-oh-p4
O2-P -O2   45.100     117.220   same as o -p4-o
O2-P -OH   42.900     117.390   same as o -p4-oh
CT-OH-HO   47.100     108.160   same as c3-oh-ho
H1-CT-OH   51.100     109.500   same as hc-c3-oh

DIHE
C*-CC-CT-HC   1    0.000         0.000          2.000      same as X -c2-c3-X
C*-CC-NA-CB   1    0.625       180.000          2.000      same as X -c2-na-X
C*-CC-NA-H    1    0.625       180.000          2.000      same as X -c2-na-X
C*-CB-CM-N*   1    6.650       180.000          2.000      same as X -c2-c2-X
C*-CB-CM-H4   1    4.000       180.000          2.000      same as X -cc-cc-X
C*-CB-CB-NA   1    6.650       180.000          2.000      same as X -c2-c2-X
C*-CB-CB-NC   1    4.000       180.000          2.000      same as X -cc-cc-X
HA-C*-CC-CT   1    6.650       180.000          2.000      same as X -c2-c2-X
HA-C*-CC-NA   1    6.650       180.000          2.000      same as X -c2-c2-X
HA-C*-CB-CM   1    6.650       180.000          2.000      same as X -c2-c2-X
HA-C*-CB-CB   1    6.650       180.000          2.000      same as X -c2-c2-X
CC-C*-CB-CM   1    4.000       180.000          2.000      same as X -cc-cc-X
CC-C*-CB-CB   1    4.000       180.000          2.000      same as X -cc-cc-X
CC-NA-CB-CB   1    0.625       180.000          2.000      same as X -c2-na-X
CC-NA-CB-NC   1    0.625       180.000          2.000      same as X -c2-na-X
CT-CC-C*-CB   1    6.650       180.000          2.000      same as X -c2-c2-X
CT-CC-NA-CB   1    0.625       180.000          2.000      same as X -c2-na-X
CT-CC-NA-H    1    0.625       180.000          2.000      same as X -c2-na-X
HC-CT-CC-NA   1    0.000         0.000          2.000      same as X -c2-c3-X
CT-N*-CM-H4   1    0.625       180.000          2.000      same as X -c2-na-X
CT-N*-CM-CB   1    0.625       180.000          2.000      same as X -c2-na-X
CT-N*-C -NC   1    1.450       180.000          2.000      same as X -c -na-X
CT-N*-C -NC   1    0.350       180.000          4.000      same as X -c -na-X
CT-N*-C -O    1    1.450       180.000          2.000      same as X -c -na-X
CT-N*-C -O    1    0.350       180.000          4.000      same as X -c -na-X
CT-OS-CT-H1   1    0.383         0.000          3.000      same as X -c3-os-X
CT-OS-CT-CT   1    0.383         0.000          3.000      same as X -c3-os-X
CT-CT-CT-CT   1    0.156         0.000          3.000      same as X -c3-c3-X
CT-CT-CT-H1   1    0.156         0.000          3.000      same as X -c3-c3-X
CT-CT-CT-OH   1    0.156         0.000          3.000      same as X -c3-c3-X
H2-CT-N*-CM   1    0.000         0.000          2.000      same as X -c3-na-X
H2-CT-N*-C    1    0.000         0.000          2.000      same as X -c3-na-X
H2-CT-OS-CT   1    0.383         0.000          3.000      same as X -c3-os-X
H2-CT-CT-CT   1    0.156         0.000          3.000      same as X -c3-c3-X
H2-CT-CT-HC   1    0.156         0.000          3.000      same as X -c3-c3-X
N*-CT-OS-CT   1    0.383         0.000          3.000      same as X -c3-os-X
N*-CT-CT-CT   1    0.156         0.000          3.000      same as X -c3-c3-X
N*-CT-CT-HC   1    0.156         0.000          3.000      same as X -c3-c3-X
N*-CM-CB-CB   1    6.650       180.000          2.000      same as X -c2-c2-X
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N*-C -NC-CB   1    4.150       180.000          2.000      same as X -c -n2-X
CM-N*-CT-OS   1    0.000         0.000          2.000      same as X -c3-na-X
CM-N*-CT-CT   1    0.000         0.000          2.000      same as X -c3-na-X
CM-N*-C -NC   1    1.450       180.000          2.000      same as X -c -na-X
CM-N*-C -NC   1    0.350       180.000          4.000      same as X -c -na-X
CM-N*-C -O    1    1.450       180.000          2.000      same as X -c -na-X
CM-N*-C -O    1    0.350       180.000          4.000      same as X -c -na-X
CM-CB-CB-NA   1    6.650       180.000          2.000      same as X -c2-c2-X
CM-CB-CB-NC   1    4.000       180.000          2.000      same as X -cc-cc-X
H4-CM-N*-C    1    0.625       180.000          2.000      same as X -c2-na-X
H4-CM-CB-CB   1    4.000       180.000          2.000      same as X -cc-cc-X
CB-C*-CC-NA   1    6.650       180.000          2.000      same as X -c2-c2-X
CB-CM-N*-C    1    0.625       180.000          2.000      same as X -c2-na-X
CB-CB-NA-H    1    0.625       180.000          2.000      same as X -c2-na-X
CB-CB-NC-C    1    4.150       180.000          2.000      same as X -c2-n2-X
CB-NC-C -O    1    4.150       180.000          2.000      same as X -c -n2-X
NA-CB-NC-C    1    4.150       180.000          2.000      same as X -c2-n2-X
H -NA-CB-NC   1    0.625       180.000          2.000      same as X -c2-na-X
C -N*-CT-OS   1    0.000         0.000          2.000      same as X -c3-na-X
C -N*-CT-CT   1    0.000         0.000          2.000      same as X -c3-na-X
OS-CT-CT-CT   1    0.156         0.000          3.000      same as X -c3-c3-X
OS-CT-CT-HC   1    0.156         0.000          3.000      same as X -c3-c3-X
OS-CT-CT-H1   1    0.156         0.000          3.000      same as X -c3-c3-X
OS-CT-CT-OS   1    0.156         0.000          3.000      same as X -c3-c3-X
OS-CT-CT-OH   1    0.156         0.000          3.000      same as X -c3-c3-X
CT-CT-OS-P    1    0.383         0.000          3.000      same as X -c3-os-X
CT-CT-OH-HO   1    0.167         0.000          3.000      same as X -c3-oh-X
CT-CT-CT-HC   1    0.156         0.000          3.000      same as X -c3-c3-X
H1-CT-CT-H1   1    0.156         0.000          3.000      same as X -c3-c3-X
H1-CT-CT-OH   1    0.156         0.000          3.000      same as X -c3-c3-X
CT-OS-P -O2   1    1.050       180.000          2.000      same as X -os-p4-X
CT-OS-P -OH   1    1.050       180.000          2.000      same as X -os-p4-X
H1-CT-OS-P    1    0.383         0.000          3.000      same as X -c3-os-X
OS-P -OH-HO   1    0.700         0.000          1.000      same as X -oh-p4-X
O2-P -OH-HO   1    0.700         0.000          1.000      same as X -oh-p4-X
H1-CT-OH-HO   1    0.167         0.000          3.000      same as X -c3-oh-X
H1-CT-CT-HC   1    0.156         0.000          3.000      same as X -c3-c3-X
OH-CT-CT-HC   1    0.156         0.000          3.000      same as X -c3-c3-X

IMPROPER
CB-CC-C*-HA          1.1         180.0          2.0        Using default value
C*-CT-CC-NA          1.1         180.0          2.0        Using default value
C -CM-N*-CT          1.1         180.0          2.0        Using default value
CB-H4-CM-N*          1.1         180.0          2.0        Using default value
C*-CB-CB-CM          1.1         180.0          2.0        Using default value
CB-NA-CB-NC          1.1         180.0          2.0        Using default value
CB-CC-NA-H           1.1         180.0          2.0        Using default value
N*-NC-C -O           1.1         180.0          2.0        Using default value

NONBON
  C*          1.9080  0.0860           same as cc
  HA          1.4870  0.0157           same as hc
  CC          1.9080  0.0860           same as cc
  CT          1.9080  0.1094           same as c3
  HC          1.4870  0.0157           same as hc
  H2          1.4870  0.0157           same as hc
  N*          1.8240  0.1700           same as na
  CM          1.9080  0.0860           same as cc
  H4          1.4870  0.0157           same as hc
  CB          1.9080  0.0860           same as cc
  NA          1.8240  0.1700           same as na
  H           0.6000  0.0157           same as hn
  NC          1.8240  0.1700           same as nc
  C           1.9080  0.0860           same as c
  O           1.6612  0.2100           same as o
  OS          1.6837  0.1700           same as os
  H1          1.4870  0.0157           same as hc
  P           2.1000  0.2000           same as p4
  O2          1.6612  0.2100           same as o
  OH          1.7210  0.2104           same as oh
  HO          0.0000  0.0000           same as ho
```

<END OF .frcmod FILE. DO NOT INCLUDE THE LINES WITH <>, INCLUDING THIS ONE>

<BELOW IS THE AMBER .lib FILE FOR DNA CONTAINING PdC>

```
!!index array str
 "PDC"
!entry.PDC.unit.atoms table  str name  str type  int typex  int resx  int flags  int
seq  int elmnt  dbl chg
 "C9" "C*" 0 1 131072 1 6 -0.080300
 "H9" "HA" 0 1 131072 2 1 0.233800
 "C8" "CC" 0 1 131072 3 6 0.198900
 "CM" "CT" 0 1 131072 4 6 -0.126100
 "HM1" "HC" 0 1 131072 5 1 0.134200
 "HM2" "HC" 0 1 131072 6 1 0.136300
 "HM3" "HC" 0 1 131072 7 1 0.106800
 "C1'" "CT" 0 1 131072 8 6 0.298200
 "H1'" "H2" 0 1 131072 9 1 0.114300
 "N3" "N*" 0 1 131072 10 7 -0.285000
 "C4" "CM" 0 1 131072 11 6 0.009200
 "H4" "H4" 0 1 131072 12 1 0.290300
 "C5" "CB" 0 1 131072 13 6 -0.074300
 "C6" "CB" 0 1 131072 14 6 0.017600
 "N7" "NA" 0 1 131072 15 7 -0.146100
 "H7" "H" 0 1 131072 16 1 0.364200
 "N1" "NC" 0 1 131072 17 7 -0.199800
 "C2" "C" 0 1 131072 18 6 0.766900
 "O2" "O" 0 1 131072 19 8 -0.414900
 "O4'" "OS" 0 1 131072 20 8 -0.396000
 "C4'" "CT" 0 1 131072 21 6 0.072900
 "H4'" "H1" 0 1 131072 22 1 0.104800
 "C5'" "CT" 0 1 131072 23 6 0.167600
 "H5'2" "H1" 0 1 131072 24 1 0.070700
 "H5'1" "H1" 0 1 131072 25 1 0.077300
 "O5'" "OS" 0 1 131072 26 8 -0.596700
 "P" "P" 0 1 131072 27 15 1.507300
 "O2P" "O2" 0 1 131072 28 8 -0.509500
 "O1P" "O2" 0 1 131072 29 8 -0.739200
 "C3'" "CT" 0 1 131072 30 6 0.112400
 "H3'" "H1" 0 1 131072 31 1 0.150100
 "O3'" "OS" 0 1 131072 32 8 -0.565500
 "C2'" "CT" 0 1 131072 33 6 -0.145400
 "H2'2" "HC" 0 1 131072 34 1 0.096400
 "H2'1" "HC" 0 1 131072 35 1 0.093300
!entry.PDC.unit.atomspertinfo table  str pname  str ptype  int ptypex  int pelmnt  dbl
pchg
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 "H9" "HA" 0 -1 0.0
 "C8" "CC" 0 -1 0.0
 "CM" "CT" 0 -1 0.0
 "HM1" "HC" 0 -1 0.0
 "HM2" "HC" 0 -1 0.0
 "HM3" "HC" 0 -1 0.0
 "C1'" "CT" 0 -1 0.0
 "H1'" "H2" 0 -1 0.0
 "N3" "N*" 0 -1 0.0
 "C4" "CM" 0 -1 0.0
 "H4" "H4" 0 -1 0.0
 "C5" "CB" 0 -1 0.0
 "C6" "CB" 0 -1 0.0
 "N7" "NA" 0 -1 0.0
 "H7" "H" 0 -1 0.0
 "N1" "NC" 0 -1 0.0
 "C2" "C" 0 -1 0.0
 "O2" "O" 0 -1 0.0
 "O4'" "OS" 0 -1 0.0
 "C4'" "CT" 0 -1 0.0
 "H4'" "H1" 0 -1 0.0
 "C5'" "CT" 0 -1 0.0
 "H5'2" "H1" 0 -1 0.0
 "H5'1" "H1" 0 -1 0.0
 "O5'" "OS" 0 -1 0.0
 "P" "P" 0 -1 0.0
 "O2P" "O2" 0 -1 0.0
 "O1P" "O2" 0 -1 0.0
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 "C3'" "CT" 0 -1 0.0
 "H3'" "H1" 0 -1 0.0
 "O3'" "OS" 0 -1 0.0
 "C2'" "CT" 0 -1 0.0
 "H2'2" "HC" 0 -1 0.0
 "H2'1" "HC" 0 -1 0.0
!entry.PDC.unit.boundbox array dbl
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 0.0
 0.0
 0.0
!entry.PDC.unit.childsequence single int
 2
!entry.PDC.unit.connect array int
 27
 32
!entry.PDC.unit.connectivity table  int atom1x  int atom2x  int flags
 1 2 1
 1 3 2
 1 13 1
 3 4 1
 3 15 1
 4 5 1
 4 6 1
 4 7 1
 8 9 1
 8 10 1
 8 20 1
 8 33 1
 10 11 1
 10 18 4
 11 12 1
 11 13 2
 13 14 1
 14 15 1
 14 17 2
 15 16 1
 17 18 1
 18 19 2
 20 21 1
 21 22 1
 21 23 1
 21 30 1
 23 24 1
 23 25 1
 23 26 1
 26 27 1
 27 28 1
 27 29 1
 30 31 1
 30 32 1
 30 33 1
 33 34 1
 33 35 1
!entry.PDC.unit.hierarchy table  str abovetype  int abovex  str belowtype  int belowx
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 "R" 1 "A" 1
 "R" 1 "A" 2
 "R" 1 "A" 3
 "R" 1 "A" 4
 "R" 1 "A" 5
 "R" 1 "A" 6
 "R" 1 "A" 7
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 "R" 1 "A" 10
 "R" 1 "A" 11
 "R" 1 "A" 12
 "R" 1 "A" 13
 "R" 1 "A" 14
 "R" 1 "A" 15
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 "R" 1 "A" 17
 "R" 1 "A" 18
 "R" 1 "A" 19
 "R" 1 "A" 20
 "R" 1 "A" 21
 "R" 1 "A" 22
 "R" 1 "A" 23
 "R" 1 "A" 24
 "R" 1 "A" 25
 "R" 1 "A" 26
 "R" 1 "A" 27
 "R" 1 "A" 28
 "R" 1 "A" 29
 "R" 1 "A" 30
 "R" 1 "A" 31
 "R" 1 "A" 32
 "R" 1 "A" 33
 "R" 1 "A" 34
 "R" 1 "A" 35
!entry.PDC.unit.name single str
 "PDC"
!entry.PDC.unit.positions table  dbl x  dbl y  dbl z
 4.466000 -1.891000 -8.681000
 5.115000 -1.251000 -8.075000
 3.279000 -1.557000 -9.215000
 2.598000 -0.216000 -9.075000
 1.672000 -0.330000 -8.492000
 3.263000 0.487000 -8.553000
 2.343000 0.198000 -10.061000
 6.698000 -6.249000 -8.889000
 6.478000 -7.283000 -9.207000
 5.639000 -5.299000 -9.258000
 5.690000 -4.025000 -8.772000
 6.518000 -3.670000 -8.168000
 4.702000 -3.158000 -9.010000
 3.571000 -3.575000 -9.808000
 2.720000 -2.560000 -9.926000
 1.871000 -2.537000 -10.439000
 3.496000 -4.745000 -10.288000
 4.575000 -5.674000 -10.022000
 4.456000 -6.779000 -10.528000
 6.802000 -6.213000 -7.458000
 8.048000 -6.814000 -7.065000
 7.866000 -7.860000 -6.757000
 8.634000 -5.994000 -5.901000
 9.545000 -6.482000 -5.524000
 7.906000 -5.915000 -5.079000
 8.961000 -4.701000 -6.420000
 9.614000 -3.596000 -5.476000
 9.787000 -2.305000 -6.199000
 10.925000 -4.076000 -4.959000
 8.976000 -6.730000 -8.306000
 9.965000 -6.279000 -8.115000
 9.228000 -8.073000 -8.737000
 8.145000 -5.883000 -9.293000
 8.356000 -4.823000 -9.101000
 8.397000 -6.098000 -10.331000
!entry.PDC.unit.residueconnect table  int c1x  int c2x  int c3x  int c4x  int c5x  int
c6x
 27 32 0 0 0 0
!entry.PDC.unit.residues table  str name  int seq  int childseq  int startatomx  str
restype  int imagingx
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!entry.PDC.unit.velocities table  dbl x  dbl y  dbl z
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<END OF .lib FILE. DO NOT INCLUDE THE LINES WITH <>, INCLUDING THIS ONE>
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<BELOW IS THE PDB FILE FOR THE 6PdC HAIRPIN>

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REMARK
ATOM      1 H5T  DA5     1      11.166  -0.403  14.164
ATOM      2 O5'  DA5     1      10.698  -0.960  13.512
ATOM      3 C5'  DA5     1      10.404  -2.289  14.012
ATOM      4 H5'1 DA5     1       9.823  -2.195  14.939
ATOM      5 H5'2 DA5     1      11.324  -2.752  14.308
ATOM      6 C4'  DA5     1       9.649  -3.226  13.032
ATOM      7 H4'  DA5     1       9.453  -4.157  13.591
ATOM      8 O4'  DA5     1       8.405  -2.618  12.552
ATOM      9 C1'  DA5     1       8.414  -2.323  11.149
ATOM     10 H1'  DA5     1       7.853  -3.079  10.636
ATOM     11 N9   DA5     1       7.826  -0.991  10.937
ATOM     12 C8   DA5     1       8.367   0.237  11.298
ATOM     13 H8   DA5     1       9.328   0.315  11.756
ATOM     14 N7   DA5     1       7.597   1.256  10.996
ATOM     15 C5   DA5     1       6.451   0.658  10.414
ATOM     16 C6   DA5     1       5.207   1.152   9.945
ATOM     17 N6   DA5     1       4.894   2.439   9.933
ATOM     18 H61  DA5     1       3.987   2.708   9.515
ATOM     19 H62  DA5     1       5.542   3.090  10.367
ATOM     20 N1   DA5     1       4.284   0.340   9.411
ATOM     21 C2   DA5     1       4.498  -0.950   9.487
ATOM     22 H2   DA5     1       3.718  -1.603   9.083
ATOM     23 N3   DA5     1       5.585  -1.576   9.968
ATOM     24 C4   DA5     1       6.562  -0.725  10.459
ATOM     25 C3'  DA5     1      10.417  -3.539  11.721
ATOM     26 H3'  DA5     1      11.494  -3.444  11.852
ATOM     27 C2'  DA5     1       9.871  -2.531  10.708
ATOM     28 H2'1 DA5     1      10.427  -1.564  10.785
ATOM     29 H2'2 DA5     1       9.944  -2.853   9.693
ATOM     30 O3'  DA5     1      10.162  -4.921  11.283
ATOM     31 P    DT      2      10.872  -5.486   9.897
ATOM     32 O1P  DT      2      11.173  -6.972  10.038
ATOM     33 O2P  DT      2      12.093  -4.704   9.439
ATOM     34 O5'  DT      2       9.680  -5.266   8.802
ATOM     35 C5'  DT      2       8.498  -6.046   8.971
ATOM     36 H5'1 DT      2       8.155  -5.936   9.983
ATOM     37 H5'2 DT      2       8.709  -7.109   8.796
ATOM     38 C4'  DT      2       7.403  -5.617   7.970
ATOM     39 H4'  DT      2       6.480  -6.154   8.224
ATOM     40 O4'  DT      2       7.169  -4.204   8.124
ATOM     41 C1'  DT      2       6.589  -3.653   6.914
ATOM     42 H1'  DT      2       5.524  -3.883   6.867
ATOM     43 N1   DT      2       6.869  -2.180   6.833
ATOM     44 C6   DT      2       8.131  -1.674   7.206
ATOM     45 H6   DT      2       8.826  -2.436   7.459
ATOM     46 C5   DT      2       8.366  -0.317   7.262
ATOM     47 C7   DT      2       9.673   0.263   7.775
ATOM     48 H71  DT      2      10.152   0.819   6.984
ATOM     49 H72  DT      2       9.491   0.952   8.579
ATOM     50 H73  DT      2      10.379  -0.556   8.063
ATOM     51 C4   DT      2       7.293   0.614   6.954
ATOM     52 O4   DT      2       7.348   1.820   6.930
ATOM     53 N3   DT      2       6.075   0.026   6.607
ATOM     54 H3   DT      2       5.296   0.650   6.419
ATOM     55 C2   DT      2       5.822  -1.323   6.450
ATOM     56 O2   DT      2       4.758  -1.660   5.990
ATOM     57 C3'  DT      2       7.789  -5.792   6.496
ATOM     58 H3'  DT      2       8.855  -5.939   6.359
ATOM     59 C2'  DT      2       7.300  -4.464   5.821
ATOM     60 H2'1 DT      2       8.175  -3.868   5.545
ATOM     61 H2'2 DT      2       6.624  -4.556   4.960
ATOM     62 O3'  DT      2       7.031  -6.943   6.009
ATOM     63 P    DA      3       7.371  -7.605   4.548
ATOM     64 O1P  DA      3       7.116  -9.089   4.570
ATOM     65 O2P  DA      3       8.779  -7.302   4.097
ATOM     66 O5'  DA      3       6.262  -6.755   3.663
ATOM     67 C5'  DA      3       4.839  -6.884   3.946
ATOM     68 H5'1 DA      3       4.667  -6.574   5.024
ATOM     69 H5'2 DA      3       4.444  -7.890   3.871
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ATOM     70 C4'  DA      3       3.975  -5.956   3.055
ATOM     71 H4'  DA      3       2.972  -6.112   3.328
ATOM     72 O4'  DA      3       4.300  -4.595   3.405
ATOM     73 C1'  DA      3       4.558  -3.788   2.248
ATOM     74 H1'  DA      3       3.632  -3.307   1.883
ATOM     75 N9   DA      3       5.544  -2.759   2.593
ATOM     76 C8   DA      3       6.884  -2.945   2.896
ATOM     77 H8   DA      3       7.304  -3.943   2.831
ATOM     78 N7   DA      3       7.602  -1.892   3.212
ATOM     79 C5   DA      3       6.660  -0.832   3.100
ATOM     80 C6   DA      3       6.741   0.550   3.293
ATOM     81 N6   DA      3       7.789   1.277   3.634
ATOM     82 H61  DA      3       7.658   2.296   3.688
ATOM     83 H62  DA      3       8.674   0.854   3.865
ATOM     84 N1   DA      3       5.646   1.282   3.078
ATOM     85 C2   DA      3       4.527   0.740   2.666
ATOM     86 H2   DA      3       3.675   1.380   2.497
ATOM     87 N3   DA      3       4.299  -0.563   2.491
ATOM     88 C4   DA      3       5.402  -1.374   2.683
ATOM     89 C3'  DA      3       4.157  -6.099   1.529
ATOM     90 H3'  DA      3       4.600  -7.022   1.187
ATOM     91 C2'  DA      3       5.016  -4.855   1.202
ATOM     92 H2'1 DA      3       6.063  -5.160   1.367
ATOM     93 H2'2 DA      3       4.896  -4.497   0.164
ATOM     94 O3'  DA      3       2.854  -6.025   0.852
ATOM     95 P    DT      4       2.641  -6.107  -0.789
ATOM     96 O1P  DT      4       1.360  -6.788  -1.136
ATOM     97 O2P  DT      4       3.780  -6.754  -1.503
ATOM     98 O5'  DT      4       2.547  -4.513  -1.109
ATOM     99 C5'  DT      4       1.284  -3.865  -0.770
ATOM    100 H5'1 DT      4       1.035  -4.021   0.278
ATOM    101 H5'2 DT      4       0.421  -4.277  -1.317
ATOM    102 C4'  DT      4       1.314  -2.361  -1.085
ATOM    103 H4'  DT      4       0.422  -1.834  -0.693
ATOM    104 O4'  DT      4       2.501  -1.786  -0.505
ATOM    105 C1'  DT      4       2.982  -0.658  -1.308
ATOM    106 H1'  DT      4       2.456   0.232  -0.925
ATOM    107 N1   DT      4       4.402  -0.421  -1.130
ATOM    108 C6   DT      4       5.260  -1.540  -1.059
ATOM    109 H6   DT      4       4.810  -2.484  -1.328
ATOM    110 C5   DT      4       6.571  -1.415  -0.736
ATOM    111 C7   DT      4       7.507  -2.647  -0.750
ATOM    112 H71  DT      4       8.338  -2.461  -1.435
ATOM    113 H72  DT      4       7.906  -2.833   0.234
ATOM    114 H73  DT      4       6.964  -3.584  -0.973
ATOM    115 C4   DT      4       7.096  -0.087  -0.357
ATOM    116 O4   DT      4       8.212   0.140   0.044
ATOM    117 N3   DT      4       6.226   0.951  -0.553
ATOM    118 H3   DT      4       6.603   1.841  -0.351
ATOM    119 C2   DT      4       4.857   0.878  -0.844
ATOM    120 O2   DT      4       4.228   1.906  -0.939
ATOM    121 C3'  DT      4       1.407  -2.063  -2.603
ATOM    122 H3'  DT      4       1.739  -2.942  -3.153
ATOM    123 C2'  DT      4       2.519  -0.968  -2.715
ATOM    124 H2'1 DT      4       3.305  -1.380  -3.297
ATOM    125 H2'2 DT      4       2.153  -0.012  -3.125
ATOM    126 O3'  DT      4       0.114  -1.555  -3.060
ATOM    127 P    DA      5      -0.183  -1.325  -4.652
ATOM    128 O1P  DA      5      -1.663  -1.441  -4.942
ATOM    129 O2P  DA      5       0.530  -2.340  -5.529
ATOM    130 O5'  DA      5       0.395   0.179  -4.919
ATOM    131 C5'  DA      5      -0.409   1.299  -4.419
ATOM    132 H5'1 DA      5      -0.611   1.170  -3.373
ATOM    133 H5'2 DA      5      -1.343   1.283  -5.000
ATOM    134 C4'  DA      5       0.359   2.606  -4.625
ATOM    135 H4'  DA      5      -0.178   3.410  -4.128
ATOM    136 O4'  DA      5       1.701   2.472  -4.023
ATOM    137 C1'  DA      5       2.699   3.075  -4.906
ATOM    138 H1'  DA      5       2.787   4.150  -4.670
ATOM    139 N9   DA      5       3.945   2.409  -4.706
ATOM    140 C8   DA      5       4.229   1.068  -4.892
ATOM    141 H8   DA      5       3.527   0.372  -5.306
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ATOM    142 N7   DA      5       5.442   0.649  -4.654
ATOM    143 C5   DA      5       6.038   1.821  -4.156
ATOM    144 C6   DA      5       7.313   2.152  -3.658
ATOM    145 N6   DA      5       8.298   1.308  -3.421
ATOM    146 H61  DA      5       9.106   1.628  -2.907
ATOM    147 H62  DA      5       8.188   0.350  -3.614
ATOM    148 N1   DA      5       7.603   3.420  -3.286
ATOM    149 C2   DA      5       6.668   4.342  -3.436
ATOM    150 H2   DA      5       6.965   5.365  -3.146
ATOM    151 N3   DA      5       5.451   4.198  -3.890
ATOM    152 C4   DA      5       5.137   2.903  -4.261
ATOM    153 C3'  DA      5       0.581   2.994  -6.072
ATOM    154 H3'  DA      5       0.033   2.349  -6.767
ATOM    155 C2'  DA      5       2.096   2.873  -6.302
ATOM    156 H2'1 DA      5       2.352   1.879  -6.682
ATOM    157 H2'2 DA      5       2.471   3.609  -7.012
ATOM    158 O3'  DA      5       0.104   4.385  -6.137
ATOM    159 C9   PDC     6       5.798   2.248  -8.062
ATOM    160 H9   PDC     6       4.880   1.886  -8.557
ATOM    161 C8   PDC     6       7.008   1.494  -7.731
ATOM    162 CM   PDC     6       7.146   0.017  -8.002
ATOM    163 HM1  PDC     6       6.132  -0.400  -8.069
ATOM    164 HM2  PDC     6       7.627  -0.476  -7.144
ATOM    165 HM3  PDC     6       7.673  -0.226  -8.907
ATOM    166 C1'  PDC     6       4.968   7.129  -6.984
ATOM    167 H1'  PDC     6       5.488   7.981  -6.470
ATOM    168 N3   PDC     6       5.794   5.907  -7.011
ATOM    169 C4   PDC     6       5.234   4.730  -7.568
ATOM    170 H4   PDC     6       4.242   4.770  -7.960
ATOM    171 C5   PDC     6       6.070   3.567  -7.582
ATOM    172 C6   PDC     6       7.374   3.548  -7.002
ATOM    173 N7   PDC     6       7.968   2.296  -7.082
ATOM    174 H7   PDC     6       8.834   1.989  -6.640
ATOM    175 N1   PDC     6       7.790   4.691  -6.365
ATOM    176 C2   PDC     6       7.034   5.883  -6.362
ATOM    177 O2   PDC     6       7.516   6.872  -5.818
ATOM    178 O4'  PDC     6       3.761   6.914  -6.213
ATOM    179 C4'  PDC     6       2.787   7.916  -6.596
ATOM    180 H4'  PDC     6       2.804   8.671  -5.800
ATOM    181 C5'  PDC     6       1.398   7.262  -6.729
ATOM    182 H5'2 PDC     6       0.669   7.940  -7.157
ATOM    183 H5'1 PDC     6       1.067   7.033  -5.683
ATOM    184 O5'  PDC     6       1.449   6.048  -7.543
ATOM    185 P    PDC     6       0.059   5.144  -7.591
ATOM    186 O2P  PDC     6       0.127   4.247  -8.789
ATOM    187 O1P  PDC     6      -1.108   6.080  -7.621
ATOM    188 C3'  PDC     6       3.329   8.574  -7.902
ATOM    189 H3'  PDC     6       2.529   8.658  -8.633
ATOM    190 O3'  PDC     6       3.878   9.899  -7.586
ATOM    191 C2'  PDC     6       4.447   7.653  -8.327
ATOM    192 H2'2 PDC     6       4.093   6.859  -8.984
ATOM    193 H2'1 PDC     6       5.216   8.156  -8.856
ATOM    194 P    DC      7       4.369  10.936  -8.765
ATOM    195 O1P  DC      7       4.096  12.338  -8.292
ATOM    196 O2P  DC      7       3.639  10.576 -10.029
ATOM    197 O5'  DC      7       5.959  10.571  -8.845
ATOM    198 C5'  DC      7       6.789  10.884  -7.692
ATOM    199 H5'1 DC      7       6.252  10.542  -6.820
ATOM    200 H5'2 DC      7       6.925  11.982  -7.658
ATOM    201 C4'  DC      7       8.191  10.242  -7.861
ATOM    202 H4'  DC      7       8.711  10.379  -6.915
ATOM    203 O4'  DC      7       7.943   8.818  -8.112
ATOM    204 C1'  DC      7       8.752   8.373  -9.204
ATOM    205 H1'  DC      7       9.757   8.235  -8.851
ATOM    206 N1   DC      7       8.210   7.105  -9.751
ATOM    207 C6   DC      7       7.074   7.085 -10.598
ATOM    208 H6   DC      7       6.529   8.030 -10.732
ATOM    209 C5   DC      7       6.563   5.907 -11.069
ATOM    210 H5   DC      7       5.633   5.918 -11.613
ATOM    211 C4   DC      7       7.303   4.743 -10.775
ATOM    212 N4   DC      7       6.907   3.567 -11.164
ATOM    213 H41  DC      7       7.510   2.810 -10.896
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ATOM    214 H42  DC      7       6.072   3.437 -11.729
ATOM    215 N3   DC      7       8.285   4.678  -9.891
ATOM    216 C2   DC      7       8.789   5.904  -9.354
ATOM    217 O2   DC      7       9.695   5.825  -8.533
ATOM    218 C3'  DC      7       8.986  10.734  -9.129
ATOM    219 H3'  DC      7       8.623  11.689  -9.470
ATOM    220 C2'  DC      7       8.748   9.576 -10.119
ATOM    221 H2'1 DC      7       7.759   9.795 -10.564
ATOM    222 H2'2 DC      7       9.477   9.469 -10.926
ATOM    223 O3'  DC      7      10.424  10.817  -8.785
ATOM    224 P    DC      8      11.441  11.463  -9.868
ATOM    225 O1P  DC      8      12.576  12.200  -9.226
ATOM    226 O2P  DC      8      10.698  12.430 -10.748
ATOM    227 O5'  DC      8      11.914  10.080 -10.606
ATOM    228 C5'  DC      8      12.689   9.084  -9.852
ATOM    229 H5'1 DC      8      12.224   8.991  -8.894
ATOM    230 H5'2 DC      8      13.728   9.472  -9.724
ATOM    231 C4'  DC      8      12.698   7.644 -10.404
ATOM    232 H4'  DC      8      13.159   7.002  -9.637
ATOM    233 O4'  DC      8      11.357   7.142 -10.662
ATOM    234 C1'  DC      8      11.423   6.089 -11.660
ATOM    235 H1'  DC      8      11.251   5.147 -11.126
ATOM    236 N1   DC      8      10.359   6.290 -12.683
ATOM    237 C6   DC      8      10.051   7.619 -13.062
ATOM    238 H6   DC      8      10.711   8.369 -12.677
ATOM    239 C5   DC      8       9.005   7.837 -13.899
ATOM    240 H5   DC      8       8.782   8.866 -14.175
ATOM    241 C4   DC      8       8.233   6.700 -14.319
ATOM    242 N4   DC      8       7.141   6.878 -14.993
ATOM    243 H41  DC      8       6.678   6.036 -15.315
ATOM    244 H42  DC      8       6.947   7.805 -15.361
ATOM    245 N3   DC      8       8.546   5.439 -14.046
ATOM    246 C2   DC      8       9.709   5.181 -13.295
ATOM    247 O2   DC      8       9.977   4.003 -13.022
ATOM    248 C3'  DC      8      13.498   7.481 -11.728
ATOM    249 H3'  DC      8      13.271   8.281 -12.405
ATOM    250 C2'  DC      8      12.876   6.141 -12.201
ATOM    251 H2'1 DC      8      12.886   6.014 -13.320
ATOM    252 H2'2 DC      8      13.364   5.283 -11.724
ATOM    253 O3'  DC      8      14.931   7.398 -11.395
ATOM    254 P    DC      9      15.990   6.957 -12.549
ATOM    255 O1P  DC      9      17.388   7.461 -12.242
ATOM    256 O2P  DC      9      15.595   7.315 -13.981
ATOM    257 O5'  DC      9      15.906   5.370 -12.189
ATOM    258 C5'  DC      9      16.096   4.446 -13.274
ATOM    259 H5'1 DC      9      17.118   4.532 -13.656
ATOM    260 H5'2 DC      9      15.404   4.666 -14.091
ATOM    261 C4'  DC      9      15.722   3.048 -12.727
ATOM    262 H4'  DC      9      16.194   2.789 -11.782
ATOM    263 O4'  DC      9      14.264   3.042 -12.575
ATOM    264 C1'  DC      9      13.719   1.742 -12.914
ATOM    265 H1'  DC      9      13.337   1.297 -11.960
ATOM    266 N1   DC      9      12.612   1.853 -13.867
ATOM    267 C6   DC      9      11.516   0.997 -13.690
ATOM    268 H6   DC      9      11.561   0.324 -12.835
ATOM    269 C5   DC      9      10.476   0.954 -14.556
ATOM    270 H5   DC      9       9.654   0.250 -14.430
ATOM    271 C4   DC      9      10.512   1.927 -15.610
ATOM    272 N4   DC      9       9.560   2.006 -16.507
ATOM    273 H41  DC      9       9.600   2.790 -17.156
ATOM    274 H42  DC      9       8.732   1.427 -16.413
ATOM    275 N3   DC      9      11.514   2.741 -15.854
ATOM    276 C2   DC      9      12.650   2.714 -14.979
ATOM    277 O2   DC      9      13.612   3.377 -15.352
ATOM    278 C3'  DC      9      15.996   1.889 -13.729
ATOM    279 H3'  DC      9      15.836   2.228 -14.737
ATOM    280 C2'  DC      9      14.907   0.877 -13.359
ATOM    281 H2'1 DC      9      14.652   0.239 -14.168
ATOM    282 H2'2 DC      9      15.142   0.261 -12.479
ATOM    283 O3'  DC      9      17.370   1.472 -13.687
ATOM    284 P    DC     10      17.939   0.241 -12.751
ATOM    285 O1P  DC     10      19.388   0.047 -13.106
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ATOM    286 O2P  DC     10      17.257  -1.053 -13.083
ATOM    287 O5'  DC     10      17.645   0.819 -11.247
ATOM    288 C5'  DC     10      18.697   1.628 -10.644
ATOM    289 H5'1 DC     10      19.028   2.401 -11.384
ATOM    290 H5'2 DC     10      19.561   0.996 -10.491
ATOM    291 C4'  DC     10      18.316   2.316  -9.312
ATOM    292 H4'  DC     10      19.061   3.136  -9.107
ATOM    293 O4'  DC     10      17.010   2.936  -9.487
ATOM    294 C1'  DC     10      16.275   2.898  -8.270
ATOM    295 H1'  DC     10      16.568   3.783  -7.633
ATOM    296 N1   DC     10      14.835   2.974  -8.594
ATOM    297 C6   DC     10      14.162   1.854  -9.128
ATOM    298 H6   DC     10      14.808   1.012  -9.378
ATOM    299 C5   DC     10      12.824   1.902  -9.326
ATOM    300 H5   DC     10      12.292   1.062  -9.720
ATOM    301 C4   DC     10      12.139   3.077  -8.957
ATOM    302 N4   DC     10      10.859   3.149  -9.062
ATOM    303 H41  DC     10      10.437   4.055  -8.808
ATOM    304 H42  DC     10      10.326   2.420  -9.477
ATOM    305 N3   DC     10      12.705   4.167  -8.487
ATOM    306 C2   DC     10      14.116   4.155  -8.337
ATOM    307 O2   DC     10      14.645   5.187  -7.933
ATOM    308 C3'  DC     10      18.200   1.357  -8.134
ATOM    309 H3'  DC     10      18.368   0.307  -8.473
ATOM    310 C2'  DC     10      16.760   1.586  -7.589
ATOM    311 H2'1 DC     10      16.215   0.670  -7.883
ATOM    312 H2'2 DC     10      16.701   1.683  -6.518
ATOM    313 O3'  DC     10      19.239   1.728  -7.174
ATOM    314 P    DG     11      19.291   1.170  -5.650
ATOM    315 O1P  DG     11      20.748   1.076  -5.278
ATOM    316 O2P  DG     11      18.558  -0.116  -5.338
ATOM    317 O5'  DG     11      18.506   2.426  -4.949
ATOM    318 C5'  DG     11      19.021   3.766  -5.087
ATOM    319 H5'1 DG     11      19.293   3.907  -6.118
ATOM    320 H5'2 DG     11      19.983   3.839  -4.532
ATOM    321 C4'  DG     11      18.073   4.911  -4.617
ATOM    322 H4'  DG     11      18.476   5.854  -4.953
ATOM    323 O4'  DG     11      16.763   4.676  -5.202
ATOM    324 C1'  DG     11      15.709   4.700  -4.217
ATOM    325 H1'  DG     11      15.298   5.732  -4.093
ATOM    326 N9   DG     11      14.616   3.811  -4.598
ATOM    327 C8   DG     11      14.612   2.442  -4.650
ATOM    328 H8   DG     11      15.484   1.851  -4.373
ATOM    329 N7   DG     11      13.475   1.932  -5.104
ATOM    330 C5   DG     11      12.619   3.003  -5.298
ATOM    331 C6   DG     11      11.209   3.076  -5.624
ATOM    332 O6   DG     11      10.437   2.178  -5.916
ATOM    333 N1   DG     11      10.765   4.383  -5.738
ATOM    334 H1   DG     11       9.855   4.486  -6.146
ATOM    335 C2   DG     11      11.479   5.480  -5.408
ATOM    336 N2   DG     11      10.850   6.633  -5.442
ATOM    337 H21  DG     11       9.857   6.671  -5.626
ATOM    338 H22  DG     11      11.370   7.492  -5.292
ATOM    339 N3   DG     11      12.768   5.480  -5.053
ATOM    340 C4   DG     11      13.366   4.218  -5.007
ATOM    341 C3'  DG     11      17.822   4.938  -3.090
ATOM    342 H3'  DG     11      18.584   4.372  -2.544
ATOM    343 C2'  DG     11      16.414   4.313  -2.922
ATOM    344 H2'1 DG     11      16.575   3.244  -2.896
ATOM    345 H2'2 DG     11      15.791   4.610  -2.054
ATOM    346 O3'  DG     11      17.845   6.328  -2.630
ATOM    347 P    DT     12      17.547   6.779  -1.090
ATOM    348 O1P  DT     12      18.404   7.929  -0.642
ATOM    349 O2P  DT     12      17.548   5.652  -0.113
ATOM    350 O5'  DT     12      15.983   7.288  -1.323
ATOM    351 C5'  DT     12      15.726   8.490  -2.086
ATOM    352 H5'1 DT     12      16.068   8.351  -3.116
ATOM    353 H5'2 DT     12      16.224   9.341  -1.624
ATOM    354 C4'  DT     12      14.222   8.751  -2.059
ATOM    355 H4'  DT     12      13.988   9.576  -2.715
ATOM    356 O4'  DT     12      13.454   7.606  -2.511
ATOM    357 C1'  DT     12      12.204   7.490  -1.761
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ATOM    358 H1'  DT     12      11.494   8.141  -2.226
ATOM    359 N1   DT     12      11.761   6.071  -1.723
ATOM    360 C6   DT     12      12.715   5.103  -1.437
ATOM    361 H6   DT     12      13.725   5.473  -1.165
ATOM    362 C5   DT     12      12.404   3.799  -1.515
ATOM    363 C7   DT     12      13.425   2.718  -1.120
ATOM    364 H71  DT     12      12.949   1.942  -0.513
ATOM    365 H72  DT     12      13.751   2.186  -2.030
ATOM    366 H73  DT     12      14.268   3.144  -0.581
ATOM    367 C4   DT     12      11.092   3.404  -2.006
ATOM    368 O4   DT     12      10.717   2.234  -2.136
ATOM    369 N3   DT     12      10.199   4.425  -2.280
ATOM    370 H3   DT     12       9.363   4.152  -2.780
ATOM    371 C2   DT     12      10.450   5.743  -2.124
ATOM    372 O2   DT     12       9.570   6.581  -2.366
ATOM    373 C3'  DT     12      13.684   9.084  -0.657
ATOM    374 H3'  DT     12      14.504   9.118   0.118
ATOM    375 C2'  DT     12      12.637   8.016  -0.376
ATOM    376 H2'1 DT     12      13.123   7.256   0.259
ATOM    377 H2'2 DT     12      11.779   8.365   0.228
ATOM    378 O3'  DT     12      13.040  10.399  -0.713
ATOM    379 P    DA     13      12.522  11.143   0.632
ATOM    380 O1P  DA     13      12.689  12.638   0.440
ATOM    381 O2P  DA     13      13.202  10.682   1.919
ATOM    382 O5'  DA     13      10.934  10.705   0.562
ATOM    383 C5'  DA     13      10.102  11.365  -0.364
ATOM    384 H5'1 DA     13      10.504  11.201  -1.417
ATOM    385 H5'2 DA     13      10.156  12.418  -0.229
ATOM    386 C4'  DA     13       8.618  10.894  -0.331
ATOM    387 H4'  DA     13       8.074  11.435  -1.130
ATOM    388 O4'  DA     13       8.599   9.445  -0.553
ATOM    389 C1'  DA     13       7.920   8.788   0.539
ATOM    390 H1'  DA     13       6.829   8.681   0.279
ATOM    391 N9   DA     13       8.501   7.453   0.752
ATOM    392 C8   DA     13       9.695   7.125   1.335
ATOM    393 H8   DA     13      10.379   7.854   1.683
ATOM    394 N7   DA     13       9.974   5.843   1.404
ATOM    395 C5   DA     13       8.827   5.237   0.885
ATOM    396 C6   DA     13       8.385   3.915   0.680
ATOM    397 N6   DA     13       9.097   2.844   0.909
ATOM    398 H61  DA     13       8.667   1.928   0.781
ATOM    399 H62  DA     13      10.008   2.908   1.340
ATOM    400 N1   DA     13       7.206   3.641   0.141
ATOM    401 C2   DA     13       6.449   4.645  -0.270
ATOM    402 H2   DA     13       5.511   4.323  -0.741
ATOM    403 N3   DA     13       6.670   5.933  -0.128
ATOM    404 C4   DA     13       7.929   6.267   0.441
ATOM    405 C3'  DA     13       7.986  11.163   1.078
ATOM    406 H3'  DA     13       8.541  11.856   1.683
ATOM    407 C2'  DA     13       7.982   9.767   1.734
ATOM    408 H2'1 DA     13       8.920   9.641   2.279
ATOM    409 H2'2 DA     13       7.148   9.616   2.407
ATOM    410 O3'  DA     13       6.645  11.623   0.883
ATOM    411 P    DT     14       5.696  11.974   2.160
ATOM    412 O1P  DT     14       4.903  13.231   1.953
ATOM    413 O2P  DT     14       6.437  12.101   3.454
ATOM    414 O5'  DT     14       4.670  10.702   2.103
ATOM    415 C5'  DT     14       3.753  10.591   0.960
ATOM    416 H5'1 DT     14       4.279  10.732  -0.003
ATOM    417 H5'2 DT     14       3.023  11.359   1.037
ATOM    418 C4'  DT     14       3.062   9.186   0.996
ATOM    419 H4'  DT     14       2.489   9.061   0.092
ATOM    420 O4'  DT     14       4.093   8.187   1.113
ATOM    421 C1'  DT     14       3.491   7.006   1.780
ATOM    422 H1'  DT     14       2.937   6.414   1.012
ATOM    423 N1   DT     14       4.546   6.231   2.509
ATOM    424 C6   DT     14       5.554   6.926   3.179
ATOM    425 H6   DT     14       5.448   7.987   3.222
ATOM    426 C5   DT     14       6.587   6.262   3.761
ATOM    427 C7   DT     14       7.638   6.983   4.545
ATOM    428 H71  DT     14       7.699   6.548   5.584
ATOM    429 H72  DT     14       8.606   6.826   4.111
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ATOM    430 H73  DT     14       7.450   8.053   4.634
ATOM    431 C4   DT     14       6.635   4.787   3.697
ATOM    432 O4   DT     14       7.509   4.060   4.096
ATOM    433 N3   DT     14       5.511   4.200   3.154
ATOM    434 H3   DT     14       5.464   3.196   3.281
ATOM    435 C2   DT     14       4.491   4.838   2.462
ATOM    436 O2   DT     14       3.622   4.189   1.919
ATOM    437 C3'  DT     14       2.152   9.005   2.234
ATOM    438 H3'  DT     14       2.479   9.750   2.999
ATOM    439 C2'  DT     14       2.461   7.596   2.735
ATOM    440 H2'1 DT     14       2.860   7.695   3.755
ATOM    441 H2'2 DT     14       1.571   6.926   2.753
ATOM    442 O3'  DT     14       0.766   9.176   1.828
ATOM    443 P    DA     15      -0.430   9.160   2.950
ATOM    444 O1P  DA     15      -1.615   9.905   2.465
ATOM    445 O2P  DA     15      -0.085   9.743   4.296
ATOM    446 O5'  DA     15      -0.705   7.580   3.013
ATOM    447 C5'  DA     15      -1.234   6.898   1.818
ATOM    448 H5'1 DA     15      -0.522   6.980   0.982
ATOM    449 H5'2 DA     15      -2.203   7.297   1.496
ATOM    450 C4'  DA     15      -1.415   5.424   2.204
ATOM    451 H4'  DA     15      -1.756   4.829   1.332
ATOM    452 O4'  DA     15      -0.170   4.832   2.673
ATOM    453 C1'  DA     15      -0.363   4.142   3.922
ATOM    454 H1'  DA     15      -0.580   3.069   3.735
ATOM    455 N9   DA     15       0.869   4.327   4.705
ATOM    456 C8   DA     15       1.379   5.508   5.164
ATOM    457 H8   DA     15       0.863   6.441   5.026
ATOM    458 N7   DA     15       2.565   5.447   5.744
ATOM    459 C5   DA     15       2.893   4.070   5.659
ATOM    460 C6   DA     15       3.943   3.229   6.089
ATOM    461 N6   DA     15       4.978   3.666   6.776
ATOM    462 H61  DA     15       5.749   3.061   6.989
ATOM    463 H62  DA     15       5.030   4.633   7.101
ATOM    464 N1   DA     15       3.974   1.936   5.849
ATOM    465 C2   DA     15       2.967   1.409   5.197
ATOM    466 H2   DA     15       3.032   0.332   5.057
ATOM    467 N3   DA     15       1.838   1.987   4.746
ATOM    468 C4   DA     15       1.842   3.362   4.957
ATOM    469 C3'  DA     15      -2.466   5.250   3.351
ATOM    470 H3'  DA     15      -3.044   6.150   3.569
ATOM    471 C2'  DA     15      -1.617   4.786   4.523
ATOM    472 H2'1 DA     15      -1.349   5.646   5.106
ATOM    473 H2'2 DA     15      -2.218   4.192   5.239
ATOM    474 O3'  DA     15      -3.378   4.213   2.889
ATOM    475 P    DT3    16      -4.648   3.717   3.802
ATOM    476 O1P  DT3    16      -5.706   3.284   2.819
ATOM    477 O2P  DT3    16      -5.231   4.703   4.791
ATOM    478 O5'  DT3    16      -3.969   2.438   4.592
ATOM    479 C5'  DT3    16      -3.624   1.242   3.838
ATOM    480 H5'1 DT3    16      -2.963   1.587   3.063
ATOM    481 H5'2 DT3    16      -4.528   0.739   3.397
ATOM    482 C4'  DT3    16      -2.841   0.248   4.741
ATOM    483 H4'  DT3    16      -2.478  -0.595   4.118
ATOM    484 O4'  DT3    16      -1.645   0.949   5.260
ATOM    485 C1'  DT3    16      -1.227   0.239   6.460
ATOM    486 H1'  DT3    16      -0.668  -0.642   6.068
ATOM    487 N1   DT3    16      -0.335   1.040   7.284
ATOM    488 C6   DT3    16      -0.689   2.408   7.483
ATOM    489 H6   DT3    16      -1.623   2.724   7.108
ATOM    490 C5   DT3    16       0.169   3.209   8.164
ATOM    491 C7   DT3    16      -0.187   4.691   8.381
ATOM    492 H71  DT3    16      -0.348   4.891   9.445
ATOM    493 H72  DT3    16       0.606   5.325   8.003
ATOM    494 H73  DT3    16      -1.137   4.919   7.895
ATOM    495 C4   DT3    16       1.401   2.684   8.725
ATOM    496 O4   DT3    16       2.200   3.329   9.364
ATOM    497 N3   DT3    16       1.652   1.345   8.457
ATOM    498 H3   DT3    16       2.519   0.953   8.771
ATOM    499 C2   DT3    16       0.831   0.463   7.786
ATOM    500 O2   DT3    16       1.242  -0.676   7.600
ATOM    501 C3'  DT3    16      -3.600  -0.273   6.007
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ATOM    502 H3'  DT3    16      -4.469   0.347   6.176
ATOM    503 C2'  DT3    16      -2.564  -0.141   7.137
ATOM    504 H2'1 DT3    16      -2.900   0.672   7.795
ATOM    505 H2'2 DT3    16      -2.459  -1.033   7.700
ATOM    506 O3'  DT3    16      -3.941  -1.670   5.780
ATOM    507 H3T  DT3    16      -4.550  -1.920   6.499
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END
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