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DUPLEX: A Molecular Mechanics Program in Torsion Angle Space for Computing Structures of DNA and RNA

Brian E. Hingerty

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DUPLEX: A Molecular Mechanics Program In Torsion Angle Space For Computing Structures of DNA and RNA

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Introduction

DUPLEX produces energy minimized structures of DNA and RNA of any base sequence for single and double strands. The smallest subunits are deoxydinucleoside monophosphates, and up to 12 residues, single or double stranded can be treated. In addition, it can incorporate NMR derived interproton distances as constraints in the minimizations. Both upper and lower bounds for these distances can be specified. Details can be found in the references(1-4). The program has been designed to run on a UNICOS Cray supercomputer, but should run, albeit slowly, on a laboratory computer such as a VAX or a workstation.

This program will be available via anonymous ftp on the INTERNET acfcluster.nyu.edu and on the Bitnet from VMSSERV@NYUACF by interactive message. It is also available by electronic mail from MAILSERV@ACFcluster.NYU.EDU and MAILSERV@NYUACF.

The files:

```
README.
d120392.fd
rib40rna.
rib40dna.
```

will be in the [ANONYMOUS.BIOCHEM] directory.

Further information if needed can be obtained from Suse Broyde at broyde@acfcluster.nyu.edu on the internet or at broyde@nyuacf on bitnet.

A more complex version of the program is available from the author which permits computation of DNA structures modified by a selected number of polycyclic aromatic hydrocarbons and amines. If the user is willing to do some fortran programming, additional DNA-adducts can be set up. Contact Dr. Brian Hingerty (internet: BEH@ornl.gov; bitnet BEH@ornlstc) for details. Files can be sent by bitnet or internet on request.

Table 1 gives the atomic names used in the program. These are needed to name the protons, if NMR data is used. Table 2 lists the program files needed to run. Table 3 gives the UNICOS Cray compilation, loading and run steps. Table 4 presents a sample run of questions asked by the program during an actual run. Table 5 gives the 2 needed input files for this sample run: hello and inputd. Table 6 gives the output files: duplexd, outang and moutd.

Table 1

Atomic Names (format A5)

1) Ribose-Phosphate Backbone

HO5′	(for O5′ terminus)
P	(for in chain)
O5′	
C5′	
H1C5′	
H2C5′	
C4′	
HC4′	
C3′	
HC3′	
C2′	
HC2′	
O2′	(for RNA)
HC2"	(for DNA)
HO2′	(for RNA)
C1′	
HC1′	
O1′	
O3′	
HO3′	(for O3′ terminus)
P	(for in chain)
OA	(for phosphate oxygens)
OB	(for phosphate oxygens)

2) Guanine (G) (type 1)

N9	HC8
C8	HN1
N7	HN2A(cis to N1)
C5	HN2B(trans to N1)
C6	
N1	
C2	
N2	
C4	
N3	
O6	

3) Adenine (A) (type 2)

N9	HC8
C8	HC2
N7	HN6A(cis to N1)
C5	HN6B(trans to N1)
C4	
N3	
C2	
N1	
C6	
N6	

3) Cytidine (C) (type 3)

N1	HC6
C6	HC5
C5	HN4A(cis to C5)
C4	HN4B(trans to C5)
N4	
N3	
C2	
O2	

4) Thymine (T) (type 4)

N1	HC6
C6	H1C5A
C5	H2C5A
C4	H3C5A
O4	HN3
N3	
C2	
O2	
C5A(methyl carbon)	

5) Uracil (U) (type 5)

N1	HC6
C6	HC5
C5	HN3
C4	
O4	
N3	
O2	
C2	

6) Cytidine(+) (C+) (type 7)
at HN3

N1	HC6
C6	HC5
C5	HN4A(cis to C5)
C4	HN4B(trans to C5)
N4	HN3
N3	
C2	
O2	

7) Adenine(+) (A+) (type 8)
at HN1

N9	HC8
C8	HN6A(cis to N1)
N7	HN6B(trans to N1)
C5	HN1
C4	HC2
N3	
C2	
N1	
C6	
N6	

8) Inosine (I) (type 10)

N9	HC8
C8	HN1
N7	HC2
C5	
C4	
N3	
C2	
N1	
C6	
O6	

Table 2

Input/Output Files

a) Required Program Files

d120392.fd	-	fortran source code for distribution (date:3/92)
rib40rna	-	sugar puckering table for RNA
rib40dna	-	sugar puckering table for DNA
hello	-	file which answers the first few questions
inputd	-	file which answers the next group of questions if the program is not run interactively

b) Output Files

duplexd	-	initial angles and initial function values followed by final function values and final angles
outang	-	output angles with machine precision decimal places (needed to recreate output results if required at a future time, since roundoff error can be serious)
moutd	-	initial angles and function values followed by final atomic coordinates and then final angles and function values

Table 3

Unicos Cray Compilation, Loading and Run Steps

a) Compilation

```
cft77 -b d120392.o -e m -l d120392.lst d120392.fd
```

From the fortran source code, d120392.fd, a binary object file is created called d120392.o with d120392.lst as the output listing. The -e m command enables vectorization information in the d120392.lst file.

b) Library Creation

```
bld rvz lib.d12 d120392.o (other object files)
```

A library of object files, lib.d12, is created from the d120392.o file. In principle, other object files can be added to the library sequentially after the d120392.o file.

c) Loading

```
segldr -o xd120392 lib.d12
```

The loader will create the executable xd120392 from the library lib.d12 file.

d) Print Out

```
lpr -P hsp -J "box number yourname" d120392.lst
```

This prints out the listing on the high speed printer.

e) Batch Run - Shell Script (C-shell)

file: nqs.d120392

```
#QSUB -s /bin/csh
#QSUB -eo
#QSUB -o mylog
#script steps start here
cd /work1/usernumber
set echo
set timestamp
ja ja.out
chmod u+x xd120392
xd120392
ja -cst ja.out
#end of batch script
```

This is an example of a shell script to submit the program to the NQS batch processor. All the timing information and interactive questions will be printed out in the file mylog.
The interactive questions are printed out here even though they are read by the file inputd.

f) Batch Submission

```
qsub -eo -o mylog -lT 5:00:00 -lM 5MW nqs.d120392
```

The shell script nqs.d120392 is submitted to the batch queue. The time limit is 5 hours and the core limit is 5 megawords. The terminal output and timing information will be in the file called mylog.

Table 4

Questions Asked By The Program During Execution

These questions are the actual questions from a sample run in Tables 5 and 6.

a) The following 4 questions are answered in file: hello.

Do you want to run from tty or inputd?(5=tty,8=inputd). (If the answer to this question is 5, the the next 3 questions are omitted.)

How many trials do you want from unit 8? Multiple trials of different sequences can be
performed but require complete input. A single trial can be run, but the orientation default selection must come after the angle list (see below). Multiple trials of the same sequence must have the questions answered only once followed by the orientation default selections and then repeated lists of the angles in the omega namelist array starting in
column 2 with the angles having decimals and separatedy commas:
&XOMEGA OMEGA = ang1, ang2,....&END

Do you want to run trials for a dinucleoside
monophosphate? (Type in 0)
For repeated calculations of the same sequence? (Type in 0)
For a single trial? (Type in 1)
For multiple trials of different sequences? (Type in 1)

What type of duplex do you want to search for ?
A, B or Z forms where the first base pair is oriented
as in the idealized helix? (answer=0),
or a general helix where the first base pair is in a
Watson-Crick idealized co-planar orientation? (answer=1)

b) The following questions are answered in the file: inputd. If selection 5 was made above these questions will appear on the screen and the program will run interactively. For a single stranded structure questions 6,7,8,9,19 and 21 will be omitted while questions 27 and 28 will be changed slightly to reflect a selection of the default angles for the A,B or Z canonical forms.

1) Type in 1=RNA, 0=DNA

2) Type in 1=Single Strand, 2=Double Strand

3) Type in maximum number of iterations(integer)

4) Type in number of residues per strand (12=Max,2=Min)

5) Do you want to calculate the angle between the base planes of a dinucleoside monophosphate? 1=Yes,0=No (This question is omitted if the molecular structure is larger than a dinucleoside monophosphate.)

6) Type in 1 to use H-bond Forcing Function, 0 to Omit see Hingerty et al,Biopolymers 28,1195-1222(1989) and/or manual

7) Type in weighting factor for H-Bond Forcing Function as floating point number

8) Type in for each base pair separated by commas
1 to accept Hydrogen Bond Forcing Term
0 to omit Hydrogen Bond Forcing Term
example for 5 base pairs 1,0,0,0,1

9) Type in for each base pair separated by commas
0 for Watson-Crick hydrogen bonds
1 for Hoogsteen hydrogen bonds
2 for g(syn)-a+(anti) hydrogen bonds
3 for g(syn)-a+(anti), 1 hb,o6(g)-n1(a+)
4 for no hydrogen bonds
5 for g(syn)-c+(anti), 1 hb,o6(g)-n3(c+)
6 for a(anti)-g(anti),2hbs,n6(a)-o6(g),n1(a)-n1(g)
7 for a(syn)-g(anti),2hbs,n7(a)-n1(g),n6(a)-o6(g)
8 for a(syn)-t(anti),1hb,n6(a)-o2(t)
9 for g(syn)-inosine(anti),1hb,o6(g)-h1n1(i)
10 for g(syn)-g(anti),1hb,o6(g)-h1n1(g)
example for 5 base pairs 0,0,1,0,0

10) Do you want to use NOE upper bound distance constraints (1=Y,0=N)
(If the answer to this question is no, then the next 3 questions are omitted.)

11) Type in weighting factor for NOE upper bound distance constraints so that
if(dcalc .gt. dnoe) FNOE=w*(dcalc-dnoe)**2
(decimal number)

12) Type in number of NOE upper bound distance constraints to be read in as an integer(MAX=1000)

13) For each NOE upper bound distance constraint value type in 7 values
for first atom:strand #,residue #,atom name
for second atom:strand #,residue #,atom name
followed by noe upper bound distance constraint
residue number is from 5 prime end
format:1x,2(2i3,1x,a5,1x),f6.2
example: 1 1 HC8 2 12 HC8 3.80

14) Do you want to use NOE lower bound distance
constraints? (1=YES,0=NO)
(If the answer to this question is no, then the next 3
questions are omitted.)

15) Type in weighting factor for NOE lower bound
distance constraints so that
if(dcalc .lt. dNONOE) FNONOE=w*(dcalc-dNONOE)**2
(decimal)

16) Type in number of NOE lower bound distance
constraints to be read in as an integer (MAX=1000)

17) For each NOE lower bound distance constraint
value type in 7 values
for first atom:strand #,residue #,atom name
for second atom:strand #,residue #,atom name
followed by NOE lower bound distance constraint
residue number is from 5 prime end
format:1x,2(2i3,1x,a5,1x),f6.2
example: 1 1 HC8 2 12 HC8 3.80

18) Type in sequence of first strand
separated by commas with the following code:
1=G,2=A,3=C,4=T,5=U,7=C+,8=A+,10=inosine
6,9,11 are not enabled in this version
start with 5 prime hydroxy terminus

19) Type in 0 if you want second strand sequence
generated automatically,
or type in 1 if you want to type in second strand sequence

20) Which dielectric do you want to use?
0=Olsen dielectric 4*exp(.1*r)
1=Debye dielectric (Hingerty et al Biopolymers 24,423(1985))

21) Type in base sequence on second strand using
the following code:
1=G,2=A,3=C,4=T,5=U,7=C+,8=A+,10=Inosine
6,9,11 are not enabled in this version
starting from 5 prime hydroxy terminal
(This question is omitted if the second strand sequence is
generated automatically.)

22) Type in
2 to output coordinates and minimize energy,
or 1 to output coordinates only (no minimization),
or 0 to minimize energy only

23) Type in 0 for ORTEP format
or 1 for CHEMGRAF
or 2 for Protein Data Bank

24) Do you want to eliminate hydrogens from output
coordinates?(1=YES,0=NO)

25) Type in 1 to type in all angles,
or 0 for A,B or Z defaults
(If you choose the defaults, then the next question is omitted.)

26) Type in 160 angles.
Start with:(begin in column 2; angles separated by commas)
&XOMEGA OMEGA= ang1,ang2...
&END
(160 is the actual number of required angles for this
particular test run.)

(The following 2 questions are omitted if a general helix
orientation (from file hello) is used with the first base-pair
in a Watson-Crick idealized co-planar orientation.)

27) Type in default for first base pair orientation:
0=A or B-DNA,1=Z1-DNA,2=Z2-DNA

28) Type in 1=A-form, 0=B-form

Table 5

Sample Input Files

a) hello

Start in col 1:

```
8
1
1
0
```

b) inputd

Start in col 1. Note: a previous outang file has been used for the input here. The file has been edited using either vi on the Cray or edi on the VAX so that the angles have the convenient format with the glycosidic torsion angle chi being the fourth position of every other line. An extra angle is present in the case of the base thymine because of the methyl group rotation, so an additional line with this angle set off is prepared. This requires manual editing by the user. Note also that &XOMEGA and &END must start in col 2. The last 6 variables at the end correspond to the 6 orientation parameters of strand 2 relative to strand 1 with the first 3 being 100 times the shifts in x,y and z in angstroms (units of hundreths of an angstrom) and the last 3 being Euler shifts in degrees. These 6 terms are not present for single strands.

```
0
2
600
11
1
30.
1,1,1,1,1,1,1,1,1,1,1
0,0,0,0,0,0,0,0,0,0,0
1
15.
1
   1  7 HC1'    1  7 HC1'  3.14
1
15.
1
   1  7 HC1'    1  7 HC1'  2.14
3,3,2,4,3,1,3,4,2,3,3
1
0
1,1,4,2,1,3,1,2,4,1,1
1
2
0
1
```

```
&XOMEGA  OMEGA  =
    184.08140804032, 58.628608067634, 158.18960623278, 65.693817691353,
    183.89500989334, 248.39254555117, 296.07629617745,
    185.13316857181, 46.551812649324, 158.95174924207, 62.476784533507,
    179.27026279015, 246.64449682456, 303.89535798597,
    179.05982657909, 50.089476395344, 154.38614347139, 53.695678915947,
    175.79919916255, 254.6901590582, 296.94955949715,
    194.10791992297, 48.341098653161, 154.77439017367, 61.956098640206,
    62.619967106872,
    185.04299564882, 245.14491698967, 303.88714597169,
    181.38692325807, 41.937710988119, 157.45136540312, 63.843094999703,
    192.19791983759, 248.07088152169, 283.37688587588,
    189.99537564625, 43.81118893548, 161.70873490312, 79.961703061867,
    175.17512432539, 261.87410773669, 304.80555741696,
    182.81211338456, 42.182096092429, 141.30618946506, 53.361390342368,
    187.90665447955, 237.40376105157, 302.84069771313,
    172.36406780473, 52.271959200119, 151.63320787414, 61.270088238426,
    149.06177859919,
    181.64590358616, 254.33984525501, 299.69868622124,
    182.44303691481, 45.262256294132, 154.2926071214, 62.780405942774,
    184.99815612348, 237.41278212721, 301.14655937118,
    172.29319896546, 54.551946907321, 156.91747359315, 56.531095616421,
    183.19246774592, 248.90760103876, 292.78675388306,
    184.98561891273, 52.411686256562, 157.80870231214, 57.803511484923,
    185.90231166743,

    183.76475978146, 58.876464398474, 165.80795137643, 58.276392810489,
    181.78325796161, 250.15192848011, 294.70053033247,
    187.15015810153, 50.244528491316, 159.55444851284, 63.254875319657,
    180.33516178954, 245.25990798403, 299.35922121182,
    179.7984865502, 54.085376495953, 153.30823917836, 60.784555959157,
    35.988782798034,
    183.02530271111, 247.89682307688, 294.54402009517,
    187.46000539499, 46.850540230525, 162.64428799827, 67.423080529856,
    183.90854775955, 244.66854229072, 295.06291326413,
    173.16473184544, 57.614168277981, 150.43886965622, 58.015796467126,
    190.43687725191, 238.05703810395, 287.40157783837,
    192.98554724236, 47.956445240058, 170.38650658461, 59.449448825753,
    192.40020657569, 260.52053584306, 283.62898618457,
    176.78572809577, 49.356687657642, 132.0320940337, 62.293013849181,
    175.49855590174, 248.87140762555, 318.75201126315,
    176.04907232231, 40.891737321157, 157.65613796227, 64.125598065842,
    175.212848148, 252.61194958531, 294.86260694611,
    185.96702731212, 54.555019934274, 144.36189449961, 56.714721852191,
    76.360761461601,
    175.7471526686, 251.46672149925, 305.04842478845,
    186.77945767693, 47.192243044727, 161.31294634904, 59.002541265961,
    177.92620457733, 255.55743757591, 300.06110364495,
    194.42249256795, 41.133128116121, 161.46458480406, 69.519302816881,
    185.55104095329,

    -18.652842541885, 15.627857935655, -106.46152402847,
    -9.8462626941625, -6.3221340987767, -0.99531518693877
 &END
0
0
```

Table 6

Output Files

These files represent the output from the sample run in Table 5.

a) duplexd

```
        1 The Initial Angles Are:
184.      59.     158.      66.     184.     248.     296.  185.
 47.     159.      62.     179.     247.     304.     179.   50.
154.      54.     176.     255.     297.     194.      48.  155.
 62.      63.     185.     245.     304.     181.      42.     157.
 64.     192.     248.     283.     190.      44.     162.      80.
175.     262.     305.     183.      42.     141.      53.     188.
237.     303.     172.      52.     152.      61.     149.     182.
254.     300.     182.      45.     154.      63.     185.     237.
301.     172.      55.     157.      57.     183.     249.     293.
185.      52.     158.      58.     186.     184.      59.     166.
 58.     182.     250.     295.     187.      50.     160.      63.
180.     245.     299.     180.      54.     153.      61.      36.
183.     248.     295.     187.      47.     163.      67.     184.
245.     295.     173.      58.     150.      58.     190.     238.
287.     193.      48.     170.      59.     192.     261.     284.
177.      49.     132.      62.     175.     249.     319.     176.
 41.     158.      64.     175.     253.     295.     186.      55.
144.      57.      76.     176.     251.     305.     187.      47.
161.      59.     178.     256.     300.     194.      41.     161.
 70.     186.     -19.      16.    -106.     -10.      -6.      -1.
Func = -.4602E+03 E = -.5470E+03 FHB = 0.1806E+02
FNOE = 0.0000E+00 FNONOE = 0.6869E+02 FCSTN = 0.0000E+00
FBA = 0.0000E+00 FDH = 0.0000E+00
UNSCALED FHB = 0.6020E+00
strd,res,atom name,strd,res,atom name,dnoe,dcalc
  1  7 HC1'    1  7 HC1'    3.14  0.00
strd,res,atom name,strd,res,atom name,dnonoe,dcalc
  1  7 HC1'    1  7 HC1'    2.14  0.00
FUNC = 0.0000E+00 E = -.5470E+03 FHB = 0.1806E+02
FNOE = 0.0000E+00 FNONOE = 0.6869E+02 FCSTN = 0.0000E+00
FBA = 0.0000E+00 FDH = 0.0000E+00 NFUNC =      1
Angle between base planes of an xpy is =     0.0000
UNSCALED FHB = 0.6020E+00 E(Van der Waals) = -.6970E+03
E(Coulomb) = -.2506E+02 E(Polarization) = 0.0000E+00
E(DNA-DNA) = -.5470E+03 E(DNA-Carc) = 0.0000E+00
E(Carc-Carc) = 0.0000E+00
E(Ribose) = 0.1074E+03
E(Torsion+Anomeric) = 0.6767E+02 E(Metal-DNA) = 0.0000E+00
E(Metal-Carc) = 0.0000E+00E(Metal-Metal) = 0.0000E+00
     184.      59.     158.      66.     184.     248.     296.     185.
      47.     159.      62.     179.     247.     304.     179.      50.
     154.      54.     176.     255.     297.     194.      48.     155.
      62.      63.     185.     245.     304.     181.      42.     157.
      64.     192.     248.     283.     190.      44.     162.      80.
     175.     262.     305.     183.      42.     141.      53.     188.
     237.     303.     172.      52.     152.      61.     149.     182.
     254.     300.     182.      45.     154.      63.     185.     237.
```

```
     301.     172.      55.     157.      57.     183.     249.     293.
     185.      52.     158.      58.     186.     184.      59.     166.
      58.     182.     250.     295.     187.      50.     160.      63.
     180.     245.     299.     180.      54.     153.      61.      36.
     183.     248.     295.     187.      47.     163.      67.     184.
     245.     295.     173.      58.     150.      58.     190.     238.
     287.     193.      48.     170.      59.     192.     261.     284.
     177.      49.     132.      62.     175.     249.     319.     176.
      41.     158.      64.     175.     253.     295.     186.      55.
     144.      57.      76.     176.     251.     305.     187.      47.
     161.      59.     178.     256.     300.     194.      41.     161.
      70.     186.     -19.      16.    -106.     -10.      -6.      -1.
strd,res,atom name,strd,res,atom name,dnoe,dcalc
  1  7 HC1'    1  7 HC1'    3.14  0.00
strd,res,atom name,strd,res,atom name,dnonoe,dcalc
  1  7 HC1'    1  7 HC1'    2.14  0.00

 Explanation of terms:
     Func = E+FHB+FNOE+FNONOE+FCSTN+FBA+FDH
     E = energy of the molecule
     FHB = value of hydrogen bond forcing function
     FNOE = value of NOE upper bound distance constraint function
     FNONOE = value of NOE lower bound distance constraint
              function
     FCSTN,FBA,FDH - not implemented in this version
     UNSCALED FHB = FHB with a weight of 1.
     dnoe is the upper bound NOE distance target
     dnonoe is the lower bound NOE distance target
     dcalc is the calculated distance from the model
     strd is the strand number (1 or 2)
     res is the residue number
     atom name - self explanatory
     Angle between the base planes of an xpy - in degrees
       (This quantity is not calculated unless the molecular structure
        being considered is a dinucleoside monophosphate - an xpy.)

     The second values of FUNC etc. are the results after minimization.
     In this case no minimization was done so the results are the same.
     E(Van-der-Waals) = Van-der-Waals energy (non bonded)
     E(Coulomb) = coulomb energy
     E(Ribose) = ribose strain energy
     E(DNA-DNA)=E in this version of the program
      (This is the energy term for DNA with itself.)
     E(torsion+anomeric) = torsional and anomeric energy terms
     E(DNA-Carc),E(Carc-Carc),E(Polarization) are not implemented.
     E(Metal-DNA),E(Metal-Carc),E(Metal-Metal) are not implemented.

     The final torsion angles, sugar pseudorotation parameters and
     the 6 orientation parameters now appear followed by the NOE upper
     and lower bound target distances compared to the calculated
     values from the model. Torsion angle and pseudorotation parameter
     conventions are those of reference (1). The order of the final
     values in the output are as in reference (1) ie. starting with
     the free 5' end: phi, psi, P, chi, (extra angle if T - methyl
```

rotation), phi′, omega′, omega, phi, psi, P, chi , etc. till phi′(terminal OH rotation). The second strand now follows starting with the 5′ end and ending with the 6 orientation parameters.

b) outang - This file has been edited to fit conveniently on this page and to have the chi glycosidic torsion angle at the end of every other line. In this case you can see it is about 60 degrees.

```
 &XOMEGA   OMEGA =
184.0814080403,  58.62860806763,  158.1896062328, 65.69381769135,
183.8950098933,  248.3925455512, 296.0762961775,
185.1331685718,  46.55181264932,  158.9517492421, 62.47678453351,
179.2702627901,  246.6444968246, 303.895357986,
179.0598265791,  50.08947639534,  154.3861434714, 53.69567891595,
175.7991991626,  254.6901590582, 296.9495594972,
194.107919923,  48.34109865316,  154.7743901737, 61.95609864021,
62.61996710687,
185.0429956488, 245.1449169897,  303.8871459717,
181.3869232581,  41.93771098812, 157.4513654031,  63.8430949997,
192.1979198376, 248.0708815217,  283.3768858759,
189.9953756463,  43.81118893548, 161.7087349031,  79.96170306187,
175.1751243254, 261.8741077367,  304.805557417,
182.8121133846,  42.18209609243, 141.3061894651,  53.36139034237,
187.9066544795, 237.4037610516,  302.8406977131,
172.3640678047,  52.27195920012, 151.6332078741,  61.27008823843,
149.0617785992,
181.6459035862,  254.339845255,  299.6986862212,
182.4430369148,  45.26225629413,  154.2926071214,  62.78040594277,
184.9981561235,  237.4127821272,  301.1465593712,
172.2931989655,  54.55194690732,  156.9174735932,  56.53109561642,
183.1924677459,  248.9076010388,  292.7867538831,
184.9856189127,  52.41168625656,  157.8087023121,  57.80351148492,
185.9023116674,

183.7647597815,  58.87646439847,  165.8079513764,  58.27639281049,
181.7832579616,  250.1519284801, 294.7005303325,
187.1501581015,  50.24452849132,  159.5544485128,  63.25487531966,
180.3351617895,  245.259907984, 299.3592212118,
179.7984865502,  54.08537649595,  153.3082391784,  60.78455595916,
35.98878279803,
183.0253027111, 247.8968230769,  294.5440200952,
187.460005395,  46.85054023052,  162.6442879983,  67.42308052986,
183.9085477595, 244.6685422907,  295.0629132641,
173.1647318454,  57.61416827798,  150.4388696562,  58.01579646713,
190.4368772519, 238.0570381039,  287.4015778384,
192.9855472424,  47.95644524006,  170.3865065846,  59.44944882575,
192.4002065757, 260.5205358431,  283.6289861846,
176.7857280958,  49.35668765764,  132.0320940337,  62.29301384918,
175.4985559017, 248.8714076256,  318.7520112632,
176.0490723223,  40.89173732116,  157.6561379623,  64.12559806584,
175.212848148, 252.6119495853,  294.8626069461,
185.9670273121,  54.55501993427,  144.3618944996,  56.71472185219,
76.3607614616,
```

```
175.7471526686,  251.4667214992,  305.0484247885,
186.7794576769,  47.19224304473,  161.312946349,  59.00254126596,
177.9262045773,  255.5574375759,  300.0611036449,
194.422492568,  41.13312811612,  161.4645848041,  69.51930281688,
185.5510409533,

-18.65284254188,  15.62785793566,  -106.4615240285,
-9.846262694162,  -6.322134098777,  -0.9953151869388,
164*0.
 &END
```

c) moutd - output file with coordinates
This output is essentially the same as duplexd above except that the coordinates are now present in the center. This file can be edited by the user to produce an input file for graphical illustration.

```
     1 The Initial Angles Are:
   184.      59.     158.      66.     184.     248.     296.     185.
    47.     159.      62.     179.     247.     304.     179.      50.
   154.      54.     176.     255.     297.     194.      48.     155.
    62.      63.     185.     245.     304.     181.      42.     157.
    64.     192.     248.     283.     190.      44.     162.      80.
   175.     262.     305.     183.      42.     141.      53.     188.
   237.     303.     172.      52.     152.      61.     149.     182.
   254.     300.     182.      45.     154.      63.     185.     237.
   301.     172.      55.     157.      57.     183.     249.     293.
   185.      52.     158.      58.     186.     184.      59.     166.
    58.     182.     250.     295.     187.      50.     160.      63.
   180.     245.     299.     180.      54.     153.      61.      36.
   183.     248.     295.     187.      47.     163.      67.     184.
   245.     295.     173.      58.     150.      58.     190.     238.
   287.     193.      48.     170.      59.     192.     261.     284.
   177.      49.     132.      62.     175.     249.     319.     176.
    41.     158.      64.     175.     253.     295.     186.      55.
   144.      57.      76.     176.     251.     305.     187.      47.
   161.      59.     178.     256.     300.     194.      41.     161.
    70.     186.     -19.      16.    -106.     -10.      -6.      -1.
Func = -.4602E+03 E = -.5470E+03 FHB = 0.1806E+02
FNOE = 0.0000E+00 FNONOE = 0.6869E+02 FCSTN = 0.0000E+00
FBA = 0.0000E+00 FDH = 0.0000E+00
UNSCALED FHB = 0.6020E+00
strd,res,atom name,strd,res,atom name,dnoe,dcalc
  1  7 HC1'    1  7 HC1'    3.14  0.00
strd,res,atom name,strd,res,atom name,dnonoe,dcalc
  1  7 HC1'    1  7 HC1'    2.14  0.00
Total number of atoms including dummy=   696
ATOM      1  HO5' CYT    1       0.157   8.967   2.056
ATOM      2  O5'  CYT    1       0.688   8.243   1.615
ATOM      3  C5'  CYT    1       1.959   8.248   2.291
ATOM      4  C4'  CYT    1       2.894   7.255   1.642
ATOM      5  C3'  CYT    1       3.172   7.488   0.161
ATOM      6  O3'  CYT    1       4.529   7.131  -0.116
```

ATOM	1	O1′	CYT	1	2.308	5.926	1.732
ATOM	2	C1′	CYT	1	2.284	5.316	0.450
ATOM	3	N1	CYT	1	1.098	4.468	0.370
ATOM	4	C6	CYT	1	-0.136	5.038	0.402
ATOM	5	C5	CYT	1	-1.258	4.291	0.330
ATOM	6	C4	CYT	1	-1.075	2.877	0.220
ATOM	7	N3	CYT	1	0.177	2.320	0.189
ATOM	8	C2	CYT	1	1.222	3.106	0.263
ATOM	9	O2	CYT	1	2.367	2.582	0.234
ATOM	1	C2′	CYT	1	2.249	6.484	-0.522
ATOM	2	HC2"	CYT	1	2.615	6.254	-1.424
ATOM	1	H1C5′	CYT	1	2.362	9.162	2.238
ATOM	2	H2C5′	CYT	1	1.828	7.998	3.250
ATOM	3	HC4′	CYT	1	3.781	7.281	2.103
ATOM	4	HC1′	CYT	1	3.109	4.764	0.328
ATOM	5	HC6	CYT	1	-0.214	6.032	0.480
ATOM	6	HC5	CYT	1	-2.169	4.704	0.353
ATOM	7	N4	CYT	1	-2.116	2.053	0.143
ATOM	8	HN4A	CYT	1	-3.046	2.420	0.162
ATOM	9	HN4B	CYT	1	-1.968	1.067	0.066
ATOM	10	HC3′	CYT	1	3.024	8.452	-0.059
ATOM	11	HC2′	CYT	1	1.338	6.883	-0.623
ATOM	7	P	CYT	2	5.165	7.347	-1.568
ATOM	8	O5′	CYT	2	5.362	5.836	-2.055
ATOM	9	C5′	CYT	2	6.261	4.943	-1.372

atomic coordinates continue here in Protein Data Bank format

ATOM	131	HN2B	GUA	21	2.130	-1.269	-3.787
ATOM	132	HC3′	GUA	21	-3.213	-8.738	-4.594
ATOM	133	HC2′	GUA	21	-3.488	-6.597	-3.599
ATOM	61	P	GUA	22	-0.526	-9.187	-3.653
ATOM	62	O5′	GUA	22	0.500	-8.029	-3.243
ATOM	63	C5′	GUA	22	1.511	-7.569	-4.158
ATOM	64	C4′	GUA	22	2.543	-6.750	-3.420
ATOM	65	C3′	GUA	22	2.956	-7.292	-2.056
ATOM	66	O3′	GUA	22	4.335	-6.985	-1.833
ATOM	67	HO3′	GUA	22	4.567	-7.442	-0.974
ATOM	109	O1′	GUA	22	2.003	-5.422	-3.172
ATOM	110	C1′	GUA	22	2.080	-5.113	-1.788
ATOM	111	N9	GUA	22	0.911	-4.312	-1.435
ATOM	112	C8	GUA	22	-0.354	-4.719	-1.379
ATOM	113	N7	GUA	22	-1.141	-3.709	-1.020
ATOM	114	C5	GUA	22	-0.348	-2.595	-0.835
ATOM	115	C6	GUA	22	-0.617	-1.253	-0.457
ATOM	116	N1	GUA	22	0.555	-0.507	-0.414
ATOM	117	C2	GUA	22	1.802	-0.975	-0.692
ATOM	118	N2	GUA	22	2.796	-0.083	-0.589
ATOM	119	HN2A	GUA	22	3.738	-0.359	-0.780

```
ATOM      21  C2'  GUA   22        2.104  -6.467  -1.097
ATOM      22  HC2" GUA   22        2.542  -6.441  -0.199
ATOM     134  OA   GUA   22       -1.530  -9.477  -2.605
ATOM     135  OB   GUA   22        0.143 -10.445  -4.054
ATOM     136  H1C5'GUA   22        1.959  -8.356  -4.583
ATOM     137  H2C5'GUA   22        1.089  -7.004  -4.867
ATOM     138  HC4' GUA   22        3.379  -6.695  -3.966
ATOM     139  HC1' GUA   22        2.917  -4.598  -1.607
ATOM     140  HC8  GUA   22       -0.667  -5.647  -1.577
ATOM     141  C4   GUA   22        0.943  -2.974  -1.096
ATOM     142  O6   GUA   22       -1.697  -0.730  -0.186
ATOM     143  HN1  GUA   22        0.476   0.456  -0.157
ATOM     144  N3   GUA   22        2.045  -2.224  -1.043
ATOM     145  HN2B GUA   22        2.596   0.860  -0.322
ATOM     146  HC3' GUA   22        2.824  -8.283  -2.036
ATOM     147  HC2' GUA   22        1.198  -6.882  -1.014
Total number of non-h atoms including dummy is=   250
FUNC = 0.0000E+00 E = -.5470E+03 FHB = 0.1806E+02
FNOE = 0.0000E+00 FNONOE = 0.6869E+02 FCSTN = 0.0000E+00
FBA = 0.0000E+00 FDH = 0.0000E+00 NFUNC =      1
Angle between base planes of an xpy is =     0.0000
UNSCALED FHB = 0.6020E+00 E(Van der Waals) = -.6970E+03
E(Coulomb) = -.2506E+02 E(Polarization) = 0.0000E+00
E(DNA-DNA) = -.5470E+03 E(DNA-Carc) = 0.0000E+00
E(Carc-Carc) = 0.0000E+00
E(Ribose) = 0.1074E+03
E(Torsion+Anomeric) = 0.6767E+02 E(Metal-DNA) = 0.0000E+00
E(Metal-Carc) = 0.0000E+00E(Metal-Metal) = 0.0000E+00
     184.      59.     158.      66.     184.     248.     296.     185.
      47.     159.      62.     179.     247.     304.     179.      50.
     154.      54.     176.     255.     297.     194.      48.     155.
      62.      63.     185.     245.     304.     181.      42.     157.
      64.     192.     248.     283.     190.      44.     162.      80.
     175.     262.     305.     183.      42.     141.      53.     188.
     237.     303.     172.      52.     152.      61.     149.     182.
     254.     300.     182.      45.     154.      63.     185.     237.
     301.     172.      55.     157.      57.     183.     249.     293.
     185.      52.     158.      58.     186.     184.      59.     166.
      58.     182.     250.     295.     187.      50.     160.      63.
     180.     245.     299.     180.      54.     153.      61.      36.
     183.     248.     295.     187.      47.     163.      67.     184.
     245.     295.     173.      58.     150.      58.     190.     238.
     287.     193.      48.     170.      59.     192.     261.     284.
     177.      49.     132.      62.     175.     249.     319.     176.
      41.     158.      64.     175.     253.     295.     186.      55.
     144.      57.      76.     176.     251.     305.     187.      47.
     161.      59.     178.     256.     300.     194.      41.     161.
      70.     186.     -19.      16.    -106.     -10.      -6.      -1.
strd,res,atom name,strd,res,atom name,dnoe,dcalc
  1  7 HC1'    1  7 HC1'    3.14  0.00
strd,res,atom name,strd,res,atom name,dnonoe,dcalc
  1  7 HC1'    1  7 HC1'    2.14  0.00
```

Acknowledgements

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