Leap.in

```
source oldff/leaprc.ff99SB

addAtomTypes {
      { "C3"  "C" "sp3" }
        { "CI"  "C" "sp3" }
        { "C1"  "C" "sp2" }
        { "C2"  "C" "sp2" }
        { "OP"  "O" "sp2" }
        { "OR"  "O" "sp3" }
}

addPdbAtomMap {
  { "OP1" "O1P" }
  { "OP2" "O2P" }
}


loadamberprep rna_nuc94bsc0-ez1-ol3_Case-all_Phos.in
ci = loadamberparams frcmod.parmbsc0
chi = loadamberparams frcmod.OL3.chi
case = loadamberparams frcmod.99bsc0-chiol3-CaseP
loadOff ions08.lib
```

rna_nuc94bsc0-ez1-ol3_Case-all_Phos.in

```
    1    0    2
db94.dat
R-ADENOSINE - with 5' - OH end group and 3' - O(minus)

 RA5  INT     1
 CORRECT NOMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00       0.00       0.00        0.0000
   2   DUMM  DU    M    1   0  -1    1.00       0.00       0.00        0.0000
   3   DUMM  DU    M    2   1   0    1.00      90.00       0.00        0.0000
   4   H5T   HO    M    3   2   1    1.00     120.00     180.00        0.4295
   5   O5'   OH    M    4   3   2    0.96     101.43     -98.89       -0.6223
   6   C5'   CI    M    5   4   3    1.44     119.00     -39.22        0.0558
   7   H5'1  H1    E    6   5   4    1.09     109.50      60.00        0.0679
   8   H5'2  H1    E    6   5   4    1.09     109.50     -60.00        0.0679
   9   C4'   CT    M    6   5   4    1.52     110.00     180.00        0.1065
  10   H4'   H1    E    9   6   5    1.09     109.50    -200.00        0.1174
  11   O4'   OS    S    9   6   5    1.46     108.86     -86.31       -0.3548
  12   C1'   CT    B   11   9   6    1.42     110.04     105.60        0.0394
  13   H1'   H2    E   12  11   9    1.09     109.50    -240.00        0.2007
  14   N9    N*    S   12  11   9    1.52     109.59    -127.70       -0.0251
  15   C8    C2    B   14  12  11    1.37     131.20      81.59        0.2006
  16   H8    H5    E   15  14  12    1.08     120.00       0.00        0.1553
  17   N7    NB    S   15  14  12    1.30     113.93     177.00       -0.6073
  18   C5    CB    S   17  15  14    1.39     104.00       0.00        0.0515
  19   C6    CA    B   18  17  15    1.40     132.42     180.00        0.7009
  20   N6    N2    B   19  18  17    1.34     123.50       0.00       -0.9019
  21   H61   H     E   20  19  18    1.01     120.00     180.00        0.4115
  22   H62   H     E   20  19  18    1.01     120.00       0.00        0.4115
  23   N1    NC    S   19  18  17    1.34     117.43     180.00       -0.7615
  24   C2    CQ    B   23  19  18    1.33     118.80       0.00        0.5875
  25   H2    H5    E   24  23  19    1.08     120.00     180.00        0.0473
  26   N3    NC    S   24  23  19    1.32     129.17       0.00       -0.6997
  27   C4    CB    E   26  24  23    1.35     110.80       0.00        0.3053
  28   C3'   C3    M    9   6   5    1.53     115.78    -329.11        0.2022
  29   H3'   H1    E   28   9   6    1.09     109.50      30.00        0.0615
  30   C2'   CT    B   28   9   6    1.53     102.80     -86.30        0.0670
  31   H2'1  H1    E   30  28   9    1.09     109.50     120.00        0.0972
  32   O2'   OH    S   30  28   9    1.43     109.50     240.00       -0.6139
  33   HO'2  HO    E   32  30  28    0.96     107.00     180.00        0.4186
  34   O3'   OR    M   28   9   6    1.42     116.52    -203.47       -0.5246

CHARGE RA5E
  0.4295 -0.6223  0.0558  0.0679  0.0679
  0.1065  0.1174 -0.3548  0.0394  0.2007
 -0.0251  0.2006  0.1553 -0.6073  0.0515
  0.7009 -0.9019  0.4115  0.4115 -0.7615
  0.5875  0.0473 -0.6997  0.3053  0.2022
  0.0615  0.0670  0.0972 -0.6139  0.4186
 -0.5246

IMPROPER
 C8   C4   N9   C1'
 C6   H61  N6   H62
 N7   N9   C8   H8
 N1   N3   C2   H2
 C5   N1   C6   N6

LOOP CLOSING EXPLICIT
```

```
 C1'  C2'
 C4   C5
 C4   N9

DONE
R-ADENOSINE - with 5' - phosphate group and 3' - O(minus) group

 RA   INT     1
 CORRECT OMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00      0.00      0.00       0.0000
   2   DUMM  DU    M    1   0  -1    1.00      0.00      0.00       0.0000
   3   DUMM  DU    M    2   1   0    1.00     90.00      0.00       0.0000
   4   P     P     M    3   2   1    1.60    119.04    200.00       1.1662
   5   O1P   OP    E    4   3   2    1.48    109.61    150.00      -0.7760
   6   O2P   OP    E    4   3   2    1.48    109.58     20.00      -0.7760
   7   O5'   OR    M    4   3   2    1.60    101.43    -98.89      -0.4989
   8   C5'   CI    M    7   4   3    1.44    119.00    -39.22       0.0558
   9   H5'1  H1    E    8   7   4    1.09    109.50     60.00       0.0679
  10   H5'2  H1    E    8   7   4    1.09    109.50    -60.00       0.0679
  11   C4'   CT    M    8   7   4    1.52    110.00    180.00       0.1065
  12   H4'   H1    E   11   8   7    1.09    109.50   -200.00       0.1174
  13   O4'   OS    S   11   8   7    1.46    108.86    -86.31      -0.3548
  14   C1'   CT    B   13  11   8    1.42    110.04    105.60       0.0394
  15   H1'   H2    E   14  13  11    1.09    109.50   -240.00       0.2007
  16   N9    N*    S   14  13  11    1.52    109.59   -127.70      -0.0251
  17   C8    C2    B   16  14  13    1.37    131.20     81.59       0.2006
  18   H8    H5    E   17  16  14    1.08    120.00      0.00       0.1553
  19   N7    NB    S   17  16  14    1.30    113.93    177.00      -0.6073
  20   C5    CB    S   19  17  16    1.39    104.00      0.00       0.0515
  21   C6    CA    B   20  19  17    1.40    132.42    180.00       0.7009
  22   N6    N2    B   21  20  19    1.34    123.50      0.00      -0.9019
  23   H61   H     E   22  21  20    1.01    120.00    180.00       0.4115
  24   H62   H     E   22  21  20    1.01    120.00      0.00       0.4115
  25   N1    NC    S   21  20  19    1.34    117.43    180.00      -0.7615
  26   C2    CQ    B   25  21  20    1.33    118.80      0.00       0.5875
  27   H2    H5    E   26  25  21    1.08    120.00    180.00       0.0473
  28   N3    NC    S   26  25  21    1.32    129.17      0.00      -0.6997
  29   C4    CB    E   28  26  25    1.35    110.80      0.00       0.3053
  30   C3'   C3    M   11   8   7    1.53    115.78   -329.11       0.2022
  31   H3'   H1    E   30  11   8    1.09    109.50     30.00       0.0615
  32   C2'   CT    B   30  11   8    1.53    102.80    -86.30       0.0670
  33   H2'1  H1    E   32  30  11    1.09    109.50    120.00       0.0972
  34   O2'   OH    S   32  30  11    1.43    109.50    240.00      -0.6139
  35   HO'2  HO    E   34  32  30    0.96    107.00    180.00       0.4186
  36   O3'   OR    M   30  11   8    1.42    116.52   -203.47      -0.5246

CHARGE RA
  1.1662 -0.7760 -0.7760 -0.4989  0.0558
  0.0679  0.0679  0.1065  0.1174 -0.3548
  0.0394  0.2007 -0.0251  0.2006  0.1553
 -0.6073  0.0515  0.7009 -0.9019  0.4115
  0.4115 -0.7615  0.5875  0.0473 -0.6997
  0.3053  0.2022  0.0615  0.0670  0.0972
 -0.6139  0.4186 -0.5246

IMPROPER
 C8   C4   N9   C1'
 C6   H61  N6   H62
 N7   N9   C8   H8
```

```
 N1   N3   C2   H2
 C5   N1   C6   N6

LOOP CLOSING EXPLICIT
 C1'  C2'
 C4   C5
 C4   N9

DONE
R-ADENOSINE - with 5' - phosphate group and 3' - OH group

 RA3  INT     1
 CORRECT OMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00      0.00      0.00       0.0000
   2   DUMM  DU    M    1   0  -1    1.00      0.00      0.00       0.0000
   3   DUMM  DU    M    2   1   0    1.00     90.00      0.00       0.0000
   4   P     P     M    3   2   1    1.60    119.04    200.00       1.1662
   5   O1P   OP    E    4   3   2    1.48    109.61    150.00      -0.7760
   6   O2P   OP    E    4   3   2    1.48    109.58     20.00      -0.7760
   7   O5'   OR    M    4   3   2    1.60    101.43    -98.89      -0.4989
   8   C5'   CI    M    7   4   3    1.44    119.00    -39.22       0.0558
   9   H5'1  H1    E    8   7   4    1.09    109.50     60.00       0.0679
  10   H5'2  H1    E    8   7   4    1.09    109.50    -60.00       0.0679
  11   C4'   CT    M    8   7   4    1.52    110.00    180.00       0.1065
  12   H4'   H1    E   11   8   7    1.09    109.50   -200.00       0.1174
  13   O4'   OS    S   11   8   7    1.46    108.86    -86.31      -0.3548
  14   C1'   CT    B   13  11   8    1.42    110.04    105.60       0.0394
  15   H1'   H2    E   14  13  11    1.09    109.50   -240.00       0.2007
  16   N9    N*    S   14  13  11    1.52    109.59   -127.70      -0.0251
  17   C8    C2    B   16  14  13    1.37    131.20     81.59       0.2006
  18   H8    H5    E   17  16  14    1.08    120.00      0.00       0.1553
  19   N7    NB    S   17  16  14    1.30    113.93    177.00      -0.6073
  20   C5    CB    S   19  17  16    1.39    104.00      0.00       0.0515
  21   C6    CA    B   20  19  17    1.40    132.42    180.00       0.7009
  22   N6    N2    B   21  20  19    1.34    123.50      0.00      -0.9019
  23   H61   H     E   22  21  20    1.01    120.00    180.00       0.4115
  24   H62   H     E   22  21  20    1.01    120.00      0.00       0.4115
  25   N1    NC    S   21  20  19    1.34    117.43    180.00      -0.7615
  26   C2    CQ    B   25  21  20    1.33    118.80      0.00       0.5875
  27   H2    H5    E   26  25  21    1.08    120.00    180.00       0.0473
  28   N3    NC    S   26  25  21    1.32    129.17      0.00      -0.6997
  29   C4    CB    E   28  26  25    1.35    110.80      0.00       0.3053
  30   C3'   C3    M   11   8   7    1.53    115.78   -329.11       0.2022
  31   H3'   H1    E   30  11   8    1.09    109.50     30.00       0.0615
  32   C2'   CT    B   30  11   8    1.53    102.80    -86.30       0.0670
  33   H2'1  H1    E   32  30  11    1.09    109.50    120.00       0.0972
  34   O2'   OH    S   32  30  11    1.43    109.50    240.00      -0.6139
  35   HO'2  HO    E   34  32  30    0.96    107.00    180.00       0.4186
  36   O3'   OH    M   30  11   8    1.42    116.52   -203.47      -0.6541
  37   H3T   HO    M   36  30  11    0.96    114.97    180.00       0.4376

CHARGE RA3E
  1.1662 -0.7760 -0.7760 -0.4989  0.0558
  0.0679  0.0679  0.1065  0.1174 -0.3548
  0.0394  0.2007 -0.0251  0.2006  0.1553
 -0.6073  0.0515  0.7009 -0.9019  0.4115
  0.4115 -0.7615  0.5875  0.0473 -0.6997
  0.3053  0.2022  0.0615  0.0670  0.0972
 -0.6139  0.4186 -0.6541  0.4376
```

```
IMPROPER
 C8   C4   N9   C1'
 C6   H61  N6   H62
 N7   N9   C8   H8
 N1   N3   C2   H2
 C5   N1   C6   N6

LOOP CLOSING EXPLICIT
 C1'  C2'
 C4   C5
 C4   N9

DONE
R-ADENOSINE - with 5' - OH group and 3' - OH group

 RAN  INT     1
 CORRECT NOMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00       0.00       0.00        0.0000
   2   DUMM  DU    M    1   0  -1    1.00       0.00       0.00        0.0000
   3   DUMM  DU    M    2   1   0    1.00      90.00       0.00        0.0000
   4   H5T   HO    M    3   2   1    1.00     120.00     180.00        0.4295
   5   O5'   OH    M    4   3   2    0.96     101.43     -98.89       -0.6223
   6   C5'   CI    M    5   4   3    1.44     119.00     -39.22        0.0558
   7   H5'1  H1    E    6   5   4    1.09     109.50      60.00        0.0679
   8   H5'2  H1    E    6   5   4    1.09     109.50     -60.00        0.0679
   9   C4'   CT    M    6   5   4    1.52     110.00     180.00        0.1065
  10   H4'   H1    E    9   6   5    1.09     109.50    -200.00        0.1174
  11   O4'   OS    S    9   6   5    1.46     108.86     -86.31       -0.3548
  12   C1'   CT    B   11   9   6    1.42     110.04     105.60        0.0394
  13   H1'   H2    E   12  11   9    1.09     109.50    -240.00        0.2007
  14   N9    N*    S   12  11   9    1.52     109.59    -127.70       -0.0251
  15   C8    C2    B   14  12  11    1.37     131.20      81.59        0.2006
  16   H8    H5    E   15  14  12    1.08     120.00       0.00        0.1553
  17   N7    NB    S   15  14  12    1.30     113.93     177.00       -0.6073
  18   C5    CB    S   17  15  14    1.39     104.00       0.00        0.0515
  19   C6    CA    B   18  17  15    1.40     132.42     180.00        0.7009
  20   N6    N2    B   19  18  17    1.34     123.50       0.00       -0.9019
  21   H61   H     E   20  19  18    1.01     120.00     180.00        0.4115
  22   H62   H     E   20  19  18    1.01     120.00       0.00        0.4115
  23   N1    NC    S   19  18  17    1.34     117.43     180.00       -0.7615
  24   C2    CQ    B   23  19  18    1.33     118.80       0.00        0.5875
  25   H2    H5    E   24  23  19    1.08     120.00     180.00        0.0473
  26   N3    NC    S   24  23  19    1.32     129.17       0.00       -0.6997
  27   C4    CB    E   26  24  23    1.35     110.80       0.00        0.3053
  28   C3'   C3    M    9   6   5    1.53     115.78    -329.11        0.2022
  29   H3'   H1    E   28   9   6    1.09     109.50      30.00        0.0615
  30   C2'   CT    B   28   9   6    1.53     102.80     -86.30        0.0670
  31   H2'1  H1    E   30  28   9    1.09     109.50     120.00        0.0972
  32   O2'   OH    S   30  28   9    1.43     109.50     240.00       -0.6139
  33   HO'2  HO    E   32  30  28    0.96     107.00     180.00        0.4186
  34   O3'   OH    M   28   9   6    1.42     116.52    -203.47       -0.6541
  35   H3T   HO    M   34  28   9    0.96     114.97     180.00        0.4376

CHARGE  resp RADE
  0.4295 -0.6223  0.0558  0.0679  0.0679
  0.1065  0.1174 -0.3548  0.0394  0.2007
 -0.0251  0.2006  0.1553 -0.6073  0.0515
  0.7009 -0.9019  0.4115  0.4115 -0.7615
```

```
  0.5875  0.0473 -0.6997  0.3053  0.2022
  0.0615  0.0670  0.0972 -0.6139  0.4186
 -0.6541  0.4376

IMPROPER
 C8   C4   N9   C1'
 C6   H61  N6   H62
 N7   N9   C8   H8
 N1   N3   C2   H2
 C5   N1   C6   N6

LOOP CLOSING EXPLICIT
 C1'  C2'
 C4   C5
 C4   N9

DONE
R-URACIL - with 5' - OH end group and 3' - O(minus)

 RU5  INT     1
 CORRECT NOMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00      0.00      0.00       0.0000
   2   DUMM  DU    M    1   0  -1    1.00      0.00      0.00       0.0000
   3   DUMM  DU    M    2   1   0    1.00     90.00      0.00       0.0000
   4   H5T   HO    M    3   2   1    1.00    120.00    180.00       0.4295
   5   O5'   OH    M    4   3   2    0.96    101.43    -98.89      -0.6223
   6   C5'   CI    M    5   4   3    1.44    119.00    -39.22       0.0558
   7   H5'1  H1    E    6   5   4    1.09    109.50     60.00       0.0679
   8   H5'2  H1    E    6   5   4    1.09    109.50    -60.00       0.0679
   9   C4'   CT    M    6   5   4    1.52    110.00   -180.00       0.1065
  10   H4'   H1    E    9   6   5    1.09    109.50   -200.00       0.1174
  11   O4'   OS    S    9   6   5    1.46    108.86    -86.31      -0.3548
  12   C1'   CT    B   11   9   6    1.42    110.04    105.60       0.0674
  13   H1'   H2    E   12  11   9    1.09    109.50   -240.00       0.1824
  14   N1    N*    S   12  11   9    1.53    109.59   -127.70       0.0418
  15   C6    CM    B   14  12  11    1.37    123.04     81.59      -0.1126
  16   H6    H4    E   15  14  12    1.08    120.00      0.00       0.2188
  17   C5    CM    B   15  14  12    1.34    121.22    177.30      -0.3635
  18   H5    HA    E   17  15  14    1.09    120.00    180.00       0.1811
  19   C4    C     B   17  15  14    1.44    120.78      0.00       0.5952
  20   O4    O     E   19  17  15    1.23    125.35    180.00      -0.5761
  21   N3    NA    B   19  17  15    1.38    114.07      0.00      -0.3549
  22   H3    H     E   21  19  17    1.09    116.77    180.00       0.3154
  23   C2    C     S   21  19  17    1.38    126.46      0.00       0.4687
  24   O2    O     E   23  21  19    1.22    121.70    180.00      -0.5477
  25   C3'   C3    M    9   6   5    1.53    115.78   -329.11       0.2022
  26   H3'   H1    E   25   9   6    1.09    109.50     30.00       0.0615
  27   C2'   CT    B   25   9   6    1.53    102.80    -86.30       0.0670
  28   H2'1  H1    E   27  25   9    1.09    109.50    120.00       0.0972
  29   O2'   OH    S   27  25   9    1.43    109.50    240.00      -0.6139
  30   HO'2  HO    E   29  27  25    0.96    107.00    180.00       0.4186
  31   O3'   OR    M   25   9   6    1.42    116.52   -203.47      -0.5246

CHARGE RU5E
  0.4295 -0.6223  0.0558  0.0679  0.0679
  0.1065  0.1174 -0.3548  0.0674  0.1824
  0.0418 -0.1126  0.2188 -0.3635  0.1811
  0.5952 -0.5761 -0.3549  0.3154  0.4687
 -0.5477  0.2022  0.0615  0.0670  0.0972
```

```
 -0.6139  0.4186 -0.5246

IMPROPER
 C6   C2   N1   C1'
 C4   C6   C5   H5
 N1   N3   C2   O2
 C5   N3   C4   O4
 C2   C4   N3   H3
 N1   C5   C6   H6

LOOP CLOSING EXPLICIT
 C1'  C2'
 C2   N1

DONE
R-URACIL - with 5' - phosphate group and 3' - O(minus) group

 RU   INT     1
 CORRECT OMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00      0.00      0.00       0.0000
   2   DUMM  DU    M    1   0  -1    1.00      0.00      0.00       0.0000
   3   DUMM  DU    M    2   1   0    1.00     90.00      0.00       0.0000
   4   P     P     M    3   2   1    1.60    119.04    200.00       1.1662
   5   O1P   OP    E    4   3   2    1.48    109.61    150.00      -0.7760
   6   O2P   OP    E    4   3   2    1.48    109.58     20.00      -0.7760
   7   O5'   OR    M    4   3   2    1.60    101.43    -98.89      -0.4989
   8   C5'   CI    M    7   4   3    1.44    119.00    -39.22       0.0558
   9   H5'1  H1    E    8   7   4    1.09    109.50     60.00       0.0679
  10   H5'2  H1    E    8   7   4    1.09    109.50    -60.00       0.0679
  11   C4'   CT    M    8   7   4    1.52    110.00    180.00       0.1065
  12   H4'   H1    E   11   8   7    1.09    109.50   -200.00       0.1174
  13   O4'   OS    S   11   8   7    1.46    108.86    -86.31      -0.3548
  14   C1'   CT    B   13  11   8    1.42    110.04    105.60       0.0674
  15   H1'   H2    E   14  13  11    1.09    109.50   -240.00       0.1824
  16   N1    N*    S   14  13  11    1.53    109.59   -127.70       0.0418
  17   C6    CM    B   16  14  13    1.37    123.04     81.59      -0.1126
  18   H6    H4    E   17  16  14    1.08    120.00      0.00       0.2188
  19   C5    CM    B   17  16  14    1.34    121.22    177.30      -0.3635
  20   H5    HA    E   19  17  16    1.09    120.00    180.00       0.1811
  21   C4    C     B   19  17  16    1.44    120.78      0.00       0.5952
  22   O4    O     E   21  19  17    1.23    125.35    180.00      -0.5761
  23   N3    NA    B   21  19  17    1.38    114.07      0.00      -0.3549
  24   H3    H     E   23  21  19    1.09    116.77    180.00       0.3154
  25   C2    C     S   23  21  19    1.38    126.46      0.00       0.4687
  26   O2    O     E   25  23  21    1.22    121.70    180.00      -0.5477
  27   C3'   C3    M   11   8   7    1.53    115.78   -329.11       0.2022
  28   H3'   H1    E   27  11   8    1.09    109.50     30.00       0.0615
  29   C2'   CT    B   27  11   8    1.53    102.80    -86.30       0.0670
  30   H2'1  H1    E   29  27  11    1.09    109.50    120.00       0.0972
  31   O2'   OH    S   29  27  11    1.43    109.50    240.00      -0.6139
  32   HO'2  HO    E   31  29  27    0.96    107.00    180.00       0.4186
  33   O3'   OR    M   27  11   8    1.42    116.52   -203.47      -0.5246

CHARGE RU
  1.1662 -0.7760 -0.7760 -0.4989  0.0558
  0.0679  0.0679  0.1065  0.1174 -0.3548
  0.0674  0.1824  0.0418 -0.1126  0.2188
 -0.3635  0.1811  0.5952 -0.5761 -0.3549
  0.3154  0.4687 -0.5477  0.2022  0.0615
```

```
  0.0670  0.0972 -0.6139  0.4186 -0.5246

IMPROPER
 C6   C2   N1   C1'
 C4   C6   C5   H5
 N1   N3   C2   O2
 C5   N3   C4   O4
 C2   C4   N3   H3
 N1   C5   C6   H6

LOOP CLOSING EXPLICIT
 C1'  C2'
 C2   N1

DONE
R-URACIL - with 5' - phosphate group and 3' - OH group

 RU3  INT     1
 CORRECT OMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00       0.00       0.00        0.0000
   2   DUMM  DU    M    1   0  -1    1.00       0.00       0.00        0.0000
   3   DUMM  DU    M    2   1   0    1.00      90.00       0.00        0.0000
   4   P     P     M    3   2   1    1.60     119.04     200.00        1.1662
   5   O1P   OP    E    4   3   2    1.48     109.61     150.00       -0.7760
   6   O2P   OP    E    4   3   2    1.48     109.58      20.00       -0.7760
   7   O5'   OR    M    4   3   2    1.60     101.43     -98.89       -0.4989
   8   C5'   CI    M    7   4   3    1.44     119.00     -39.22        0.0558
   9   H5'1  H1    E    8   7   4    1.09     109.50      60.00        0.0679
  10   H5'2  H1    E    8   7   4    1.09     109.50     -60.00        0.0679
  11   C4'   CT    M    8   7   4    1.52     110.00     180.00        0.1065
  12   H4'   H1    E   11   8   7    1.09     109.50    -200.00        0.1174
  13   O4'   OS    S   11   8   7    1.46     108.86     -86.31       -0.3548
  14   C1'   CT    B   13  11   8    1.42     110.04     105.60        0.0674
  15   H1'   H2    E   14  13  11    1.09     109.50    -240.00        0.1824
  16   N1    N*    S   14  13  11    1.53     109.59    -127.70        0.0418
  17   C6    CM    B   16  14  13    1.37     123.04      81.59       -0.1126
  18   H6    H4    E   17  16  14    1.08     120.00       0.00        0.2188
  19   C5    CM    B   17  16  14    1.34     121.22     177.30       -0.3635
  20   H5    HA    E   19  17  16    1.09     120.00     180.00        0.1811
  21   C4    C     B   19  17  16    1.44     120.78       0.00        0.5952
  22   O4    O     E   21  19  17    1.23     125.35     180.00       -0.5761
  23   N3    NA    B   21  19  17    1.38     114.07       0.00       -0.3549
  24   H3    H     E   23  21  19    1.09     116.77     180.00        0.3154
  25   C2    C     S   23  21  19    1.38     126.46       0.00        0.4687
  26   O2    O     E   25  23  21    1.22     121.70     180.00       -0.5477
  27   C3'   C3    M   11   8   7    1.53     115.78    -329.11        0.2022
  28   H3'   H1    E   27  11   8    1.09     109.50      30.00        0.0615
  29   C2'   CT    B   27  11   8    1.53     102.80     -86.30        0.0670
  30   H2'1  H1    E   29  27  11    1.09     109.50     120.00        0.0972
  31   O2'   OH    S   29  27  11    1.43     109.50     240.00       -0.6139
  32   HO'2  HO    E   31  29  27    0.96     107.00     180.00        0.4186
  33   O3'   OH    M   27  11   8    1.42     116.52    -203.47       -0.6541
  34   H3T   HO    M   33  27  11    0.96     114.97     180.00        0.4376

CHARGE RU3E
  1.1662 -0.7760 -0.7760 -0.4989  0.0558
  0.0679  0.0679  0.1065  0.1174 -0.3548
  0.0674  0.1824  0.0418 -0.1126  0.2188
 -0.3635  0.1811  0.5952 -0.5761 -0.3549
```

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  0.3154  0.4687 -0.5477  0.2022  0.0615
  0.0670  0.0972 -0.6139  0.4186 -0.6541
  0.4376

IMPROPER
 C6   C2   N1   C1'
 C4   C6   C5   H5
 N1   N3   C2   O2
 C5   N3   C4   O4
 C2   C4   N3   H3
 N1   C5   C6   H6

LOOP CLOSING EXPLICIT
 C1'  C2'
 C2   N1

DONE
R-URACIL - with 5' - OH group and 3' - OH group

 RUN  INT     1
 CORRECT NOMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00      0.00      0.00       0.0000
   2   DUMM  DU    M    1   0  -1    1.00      0.00      0.00       0.0000
   3   DUMM  DU    M    2   1   0    1.00     90.00      0.00       0.0000
   4   H5T   HO    M    3   2   1    1.00    120.00    180.00       0.4295
   5   O5'   OH    M    4   3   2    0.96    101.43    -98.89      -0.6223
   6   C5'   CI    M    5   4   3    1.44    119.00    -39.22       0.0558
   7   H5'1  H1    E    6   5   4    1.09    109.50     60.00       0.0679
   8   H5'2  H1    E    6   5   4    1.09    109.50    -60.00       0.0679
   9   C4'   CT    M    6   5   4    1.52    110.00   -180.00       0.1065
  10   H4'   H1    E    9   6   5    1.09    109.50   -200.00       0.1174
  11   O4'   OS    S    9   6   5    1.46    108.86    -86.31      -0.3548
  12   C1'   CT    B   11   9   6    1.42    110.04    105.60       0.0674
  13   H1'   H2    E   12  11   9    1.09    109.50   -240.00       0.1824
  14   N1    N*    S   12  11   9    1.53    109.59   -127.70       0.0418
  15   C6    CM    B   14  12  11    1.37    123.04     81.59      -0.1126
  16   H6    H4    E   15  14  12    1.08    120.00      0.00       0.2188
  17   C5    CM    B   15  14  12    1.34    121.22    177.30      -0.3635
  18   H5    HA    E   17  15  14    1.09    120.00    180.00       0.1811
  19   C4    C     B   17  15  14    1.44    120.78      0.00       0.5952
  20   O4    O     E   19  17  15    1.23    125.35    180.00      -0.5761
  21   N3    NA    B   19  17  15    1.38    114.07      0.00      -0.3549
  22   H3    H     E   21  19  17    1.09    116.77    180.00       0.3154
  23   C2    C     S   21  19  17    1.38    126.46      0.00       0.4687
  24   O2    O     E   23  21  19    1.22    121.70    180.00      -0.5477
  25   C3'   C3    M    9   6   5    1.53    115.78   -329.11       0.2022
  26   H3'   H1    E   25   9   6    1.09    109.50     30.00       0.0615
  27   C2'   CT    B   25   9   6    1.53    102.80    -86.30       0.0670
  28   H2'1  H1    E   27  25   9    1.09    109.50    120.00       0.0972
  29   O2'   OH    S   27  25   9    1.43    109.50    240.00      -0.6139
  30   HO'2  HO    E   29  27  25    0.96    107.00    180.00       0.4186
  31   O3'   OH    M   25   9   6    1.42    116.52   -203.47      -0.6541
  32   H3T   HO    M   31  25   9    0.96    114.97    180.00       0.4376

CHARGE  resp RURA
  0.4295 -0.6223  0.0558  0.0679  0.0679
  0.1065  0.1174 -0.3548  0.0674  0.1824
  0.0418 -0.1126  0.2188 -0.3635  0.1811
  0.5952 -0.5761 -0.3549  0.3154  0.4687
```

```
 -0.5477  0.2022  0.0615  0.0670  0.0972
 -0.6139  0.4186 -0.6541  0.4376

IMPROPER
 C6   C2   N1   C1'
 C4   C6   C5   H5
 N1   N3   C2   O2
 C5   N3   C4   O4
 C2   C4   N3   H3
 N1   C5   C6   H6

LOOP CLOSING EXPLICIT
 C1'  C2'
 C2   N1

DONE
R-GUANOSINE - with 5' - OH end group and 3' - O(minus) group

 RG5  INT     1
 CORRECT NOMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00      0.00      0.00       0.0000
   2   DUMM  DU    M    1   0  -1    1.00      0.00      0.00       0.0000
   3   DUMM  DU    M    2   1   0    1.00     90.00      0.00       0.0000
   4   H5T   HO    M    3   2   1    1.00    120.00    180.00       0.4295
   5   O5'   OH    M    4   3   2    0.96    101.43    -98.89      -0.6223
   6   C5'   CI    M    5   4   3    1.44    119.00    -39.22       0.0558
   7   H5'1  H1    E    6   5   4    1.09    109.50     60.00       0.0679
   8   H5'2  H1    E    6   5   4    1.09    109.50    -60.00       0.0679
   9   C4'   CT    M    6   5   4    1.52    110.00   -180.00       0.1065
  10   H4'   H1    E    9   6   5    1.09    109.50   -200.00       0.1174
  11   O4'   OS    S    9   6   5    1.46    108.86    -86.31      -0.3548
  12   C1'   CT    B   11   9   5    1.42    110.04    105.60       0.0191
  13   H1'   H2    E   12  11   9    1.09    109.50   -240.00       0.2006
  14   N9    N*    S   12  11   9    1.49    108.06   -127.70       0.0492
  15   C8    CK    B   14  12  11    1.38    129.20     81.59       0.1374
  16   H8    H5    E   15  14  12    1.08    120.00      0.00       0.1640
  17   N7    NB    S   15  14  12    1.31    114.00   -179.90      -0.5709
  18   C5    CB    S   17  15  14    1.39    103.90      0.00       0.1744
  19   C6    C     B   18  17  15    1.42    130.40    180.00       0.4770
  20   O6    O     E   19  18  17    1.23    128.80      0.00      -0.5597
  21   N1    NA    B   19  18  17    1.40    111.38    180.00      -0.4787
  22   H1    H     E   21  19  18    1.00    117.36    179.90       0.3424
  23   C2    CA    B   21  19  18    1.38    125.24     -0.10       0.7657
  24   N2    N2    B   23  21  19    1.34    116.02    180.00      -0.9672
  25   H21   H     E   24  23  21    1.01    127.00     -0.82       0.4364
  26   H22   H     E   24  23  21    1.01    116.53   -179.44       0.4364
  27   N3    NC    S   23  21  19    1.33    123.30      0.00      -0.6323
  28   C4    CB    E   27  23  21    1.36    112.20      0.00       0.1222
  29   C3'   C3    M    9   6   5    1.53    115.78   -329.11       0.2022
  30   H3'   H1    E   29   9   6    1.09    109.50     30.00       0.0615
  31   C2'   CT    B   29   9   6    1.53    102.80    -86.30       0.0670
  32   H2'1  H1    E   31  29   9    1.09    109.50    120.00       0.0972
  33   O2'   OH    S   31  29   9    1.43    109.50    240.00      -0.6139
  34   HO'2  HO    E   33  31  29    0.96    107.00    180.00       0.4186
  35   O3'   OR    M   29   9   6    1.42    116.52   -203.47      -0.5246

CHARGE RG5E
  0.4295 -0.6223  0.0558  0.0679  0.0679
  0.1065  0.1174 -0.3548  0.0191  0.2006
```

```
  0.0492  0.1374  0.1640 -0.5709  0.1744
  0.4770 -0.5597 -0.4787  0.3424  0.7657
 -0.9672  0.4364  0.4364 -0.6323  0.1222
  0.2022  0.0615  0.0670  0.0972 -0.6139
  0.4186 -0.5246

IMPROPER
 C8   C4   N9   C1'
 C5   N1   C6   O6
 C6   C2   N1   H1
 C2   H21  N2   H22
 N7   N9   C8   H8
 N1   N3   C2   N2

LOOP CLOSING EXPLICIT
 C1'  C2'
 C4   C5
 C4   N9

DONE
R-GUANOSINE - with 5' - phosphate group and 3' - O(minus) group

 RG   INT     1
 CORRECT OMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00      0.00      0.00       0.0000
   2   DUMM  DU    M    1   0  -1    1.00      0.00      0.00       0.0000
   3   DUMM  DU    M    2   1   0    1.00     90.00      0.00       0.0000
   4   P     P     M    3   2   1    1.60    119.04    200.00       1.1662
   5   O1P   OP    E    4   3   2    1.48    109.61    150.00      -0.7760
   6   O2P   OP    E    4   3   2    1.48    109.58     20.00      -0.7760
   7   O5'   OR    M    4   3   2    1.60    101.43    -98.89      -0.4989
   8   C5'   CI    M    7   4   3    1.44    119.00    -39.22       0.0558
   9   H5'1  H1    E    8   7   4    1.09    109.50     60.00       0.0679
  10   H5'2  H1    E    8   7   4    1.09    109.50    -60.00       0.0679
  11   C4'   CT    M    8   7   4    1.52    110.00    180.00       0.1065
  12   H4'   H1    E   11   8   7    1.09    109.50   -200.00       0.1174
  13   O4'   OS    S   11   8   7    1.46    108.86    -86.31      -0.3548
  14   C1'   CT    B   13  11   8    1.42    110.04    105.60       0.0191
  15   H1'   H2    E   14  13  11    1.09    109.50   -240.00       0.2006
  16   N9    N*    S   14  13  11    1.49    108.06   -127.70       0.0492
  17   C8    CK    B   16  14  13    1.38    129.20     81.59       0.1374
  18   H8    H5    E   17  16  14    1.08    120.00      0.00       0.1640
  19   N7    NB    S   17  16  14    1.31    114.00   -179.90      -0.5709
  20   C5    CB    S   19  17  16    1.39    103.90      0.00       0.1744
  21   C6    C     B   20  19  17    1.42    130.40    180.00       0.4770
  22   O6    O     E   21  20  19    1.23    128.80      0.00      -0.5597
  23   N1    NA    B   21  20  19    1.40    111.38    180.00      -0.4787
  24   H1    H     E   23  21  20    1.00    117.36    179.90       0.3424
  25   C2    CA    B   23  21  20    1.38    125.24     -0.10       0.7657
  26   N2    N2    B   25  23  21    1.34    116.02    180.00      -0.9672
  27   H21   H     E   26  25  23    1.01    127.00     -0.82       0.4364
  28   H22   H     E   26  25  23    1.01    116.53   -179.44       0.4364
  29   N3    NC    S   25  23  21    1.33    123.30      0.00      -0.6323
  30   C4    CB    E   29  25  23    1.36    112.20      0.00       0.1222
  31   C3'   C3    M   11   8   7    1.53    115.78   -329.11       0.2022
  32   H3'   H1    E   31  11   8    1.09    109.50     30.00       0.0615
  33   C2'   CT    B   31  11   8    1.53    102.80    -86.30       0.0670
  34   H2'1  H1    E   33  31  11    1.09    109.50    120.00       0.0972
  35   O2'   OH    S   33  31  11    1.43    109.50    240.00      -0.6139
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  36   HO'2  HO    E   35  33  31    0.96    107.00    180.00       0.4186
  37   O3'   OR    M   31  11   8    1.42    116.52   -203.47      -0.5246

CHARGE RG
  1.1662 -0.7760 -0.7760 -0.4989  0.0558
  0.0679  0.0679  0.1065  0.1174 -0.3548
  0.0191  0.2006  0.0492  0.1374  0.1640
 -0.5709  0.1744  0.4770 -0.5597 -0.4787
  0.3424  0.7657 -0.9672  0.4364  0.4364
 -0.6323  0.1222  0.2022  0.0615  0.0670
  0.0972 -0.6139  0.4186 -0.5246

IMPROPER
 C8   C4   N9   C1'
 C5   N1   C6   O6
 C6   C2   N1   H1
 C2   H21  N2   H22
 N7   N9   C8   H8
 N1   N3   C2   N2

LOOP CLOSING EXPLICIT
 C1'  C2'
 C4   C5
 C4   N9

DONE
R-GUANOSINE - with 5' - phosphate group and 3' - OH group

 RG3  INT     1
 CORRECT OMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00      0.00      0.00       0.0000
   2   DUMM  DU    M    1   0  -1    1.00      0.00      0.00       0.0000
   3   DUMM  DU    M    2   1   0    1.00     90.00      0.00       0.0000
   4   P     P     M    3   2   1    1.60    119.04    200.00       1.1662
   5   O1P   OP    E    4   3   2    1.48    109.61    150.00      -0.7760
   6   O2P   OP    E    4   3   2    1.48    109.58     20.00      -0.7760
   7   O5'   OR    M    4   3   2    1.60    101.43    -98.89      -0.4989
   8   C5'   CI    M    7   4   3    1.44    119.00    -39.22       0.0558
   9   H5'1  H1    E    8   7   4    1.09    109.50     60.00       0.0679
  10   H5'2  H1    E    8   7   4    1.09    109.50    -60.00       0.0679
  11   C4'   CT    M    8   7   4    1.52    110.00    180.00       0.1065
  12   H4'   H1    E   11   8   7    1.09    109.50   -200.00       0.1174
  13   O4'   OS    S   11   8   7    1.46    108.86    -86.31      -0.3548
  14   C1'   CT    B   13  11   8    1.42    110.04    105.60       0.0191
  15   H1'   H2    E   14  13  11    1.09    109.50   -240.00       0.2006
  16   N9    N*    S   14  13  11    1.49    108.06   -127.70       0.0492
  17   C8    CK    B   16  14  13    1.38    129.20     81.59       0.1374
  18   H8    H5    E   17  16  14    1.08    120.00      0.00       0.1640
  19   N7    NB    S   17  16  14    1.31    114.00   -179.90      -0.5709
  20   C5    CB    S   19  17  16    1.39    103.90      0.00       0.1744
  21   C6    C     B   20  19  17    1.42    130.40    180.00       0.4770
  22   O6    O     E   21  20  19    1.23    128.80      0.00      -0.5597
  23   N1    NA    B   21  20  19    1.40    111.38    180.00      -0.4787
  24   H1    H     E   23  21  20    1.00    117.36    179.90       0.3424
  25   C2    CA    B   23  21  20    1.38    125.24     -0.10       0.7657
  26   N2    N2    B   25  23  21    1.34    116.02    180.00      -0.9672
  27   H21   H     E   26  25  23    1.01    127.00     -0.82       0.4364
  28   H22   H     E   26  25  23    1.01    116.53   -179.44       0.4364
  29   N3    NC    S   25  23  21    1.33    123.30      0.00      -0.6323
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  30   C4    CB    E   29  25  23    1.36    112.20      0.00       0.1222
  31   C3'   C3    M   11   8   7    1.53    115.78   -329.11       0.2022
  32   H3'   H1    E   31  11   8    1.09    109.50     30.00       0.0615
  33   C2'   CT    B   31  11   8    1.53    102.80    -86.30       0.0670
  34   H2'1  H1    E   33  31  11    1.09    109.50    120.00       0.0972
  35   O2'   OH    S   33  31  11    1.43    109.50    240.00      -0.6139
  36   HO'2  HO    E   35  33  31    0.96    107.00    180.00       0.4186
  37   O3'   OH    M   31  11   8    1.42    116.52   -203.47      -0.6541
  38   H3T   HO    M   37  31  11    0.96    114.97    180.00       0.4376

CHARGE RG3E
  1.1662 -0.7760 -0.7760 -0.4989  0.0558
  0.0679  0.0679  0.1065  0.1174 -0.3548
  0.0191  0.2006  0.0492  0.1374  0.1640
 -0.5709  0.1744  0.4770 -0.5597 -0.4787
  0.3424  0.7657 -0.9672  0.4364  0.4364
 -0.6323  0.1222  0.2022  0.0615  0.0670
  0.0972 -0.6139  0.4186 -0.6541  0.4376

IMPROPER
 C8   C4   N9   C1'
 C5   N1   C6   O6
 C6   C2   N1   H1
 C2   H21  N2   H22
 N7   N9   C8   H8
 N1   N3   C2   N2

LOOP CLOSING EXPLICIT
 C1'  C2'
 C4   C5
 C4   N9

DONE
R-GUANOSINE - with 5' - OH group and 3' - OH group

 RGN  INT     1
 CORRECT NOMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00      0.00      0.00       0.0000
   2   DUMM  DU    M    1   0  -1    1.00      0.00      0.00       0.0000
   3   DUMM  DU    M    2   1   0    1.00     90.00      0.00       0.0000
   4   H5T   HO    M    3   2   1    1.00    120.00    180.00       0.4295
   5   O5'   OH    M    4   3   2    0.96    101.43    -98.89      -0.6223
   6   C5'   CI    M    5   4   3    1.44    119.00    -39.22       0.0558
   7   H5'1  H1    E    6   5   4    1.09    109.50     60.00       0.0679
   8   H5'2  H1    E    6   5   4    1.09    109.50    -60.00       0.0679
   9   C4'   CT    M    6   5   4    1.52    110.00   -180.00       0.1065
  10   H4'   H1    E    9   6   5    1.09    109.50   -200.00       0.1174
  11   O4'   OS    S    9   6   5    1.46    108.86    -86.31      -0.3548
  12   C1'   CT    B   11   9   5    1.42    110.04    105.60       0.0191
  13   H1'   H2    E   12  11   9    1.09    109.50   -240.00       0.2006
  14   N9    N*    S   12  11   9    1.49    108.06   -127.70       0.0492
  15   C8    CK    B   14  12  11    1.38    129.20     81.59       0.1374
  16   H8    H5    E   15  14  12    1.08    120.00      0.00       0.1640
  17   N7    NB    S   15  14  12    1.31    114.00   -179.90      -0.5709
  18   C5    CB    S   17  15  14    1.39    103.90      0.00       0.1744
  19   C6    C     B   18  17  15    1.42    130.40    180.00       0.4770
  20   O6    O     E   19  18  17    1.23    128.80      0.00      -0.5597
  21   N1    NA    B   19  18  17    1.40    111.38    180.00      -0.4787
  22   H1    H     E   21  19  18    1.00    117.36    179.90       0.3424
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  23   C2    CA    B   21  19  18    1.38    125.24     -0.10       0.7657
  24   N2    N2    B   23  21  19    1.34    116.02    180.00      -0.9672
  25   H21   H     E   24  23  21    1.01    127.00     -0.82       0.4364
  26   H22   H     E   24  23  21    1.01    116.53   -179.44       0.4364
  27   N3    NC    S   23  21  19    1.33    123.30      0.00      -0.6323
  28   C4    CB    E   27  23  21    1.36    112.20      0.00       0.1222
  29   C3'   C3    M    9   6   5    1.53    115.78   -329.11       0.2022
  30   H3'   H1    E   29   9   6    1.09    109.50     30.00       0.0615
  31   C2'   CT    B   29   9   6    1.53    102.80    -86.30       0.0670
  32   H2'1  H1    E   31  29   9    1.09    109.50    120.00       0.0972
  33   O2'   OH    S   31  29   9    1.43    109.50    240.00      -0.6139
  34   HO'2  HO    E   33  31  29    0.96    107.00    180.00       0.4186
  35   O3'   OH    M   29   9   6    1.42    116.52   -203.47      -0.6541
  36   H3T   HO    M   35  29   9    0.96    114.97    180.00       0.4376

CHARGE  resp RGUA
  0.4295 -0.6223  0.0558  0.0679  0.0679
  0.1065  0.1174 -0.3548  0.0191  0.2006
  0.0492  0.1374  0.1640 -0.5709  0.1744
  0.4770 -0.5597 -0.4787  0.3424  0.7657
 -0.9672  0.4364  0.4364 -0.6323  0.1222
  0.2022  0.0615  0.0670  0.0972 -0.6139
  0.4186 -0.6541  0.4376

IMPROPER
 C8   C4   N9   C1'
 C5   N1   C6   O6
 C6   C2   N1   H1
 C2   H21  N2   H22
 N7   N9   C8   H8
 N1   N3   C2   N2

LOOP CLOSING EXPLICIT
 C1'  C2'
 C4   C5
 C4   N9

DONE
R-CYTOSINE - with 5' - OH end group and 3' - O(minus) group

 RC5  INT     1
 CORRECT NOMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00      0.00      0.00       0.0000
   2   DUMM  DU    M    1   0  -1    1.00      0.00      0.00       0.0000
   3   DUMM  DU    M    2   1   0    1.00     90.00      0.00       0.0000
   4   H5T   HO    M    3   2   1    1.00    120.00    180.00       0.4295
   5   O5'   OH    M    4   3   2    0.96    101.43    -98.89      -0.6223
   6   C5'   CI    M    5   4   3    1.44    119.00    -39.22       0.0558
   7   H5'1  H1    E    6   5   4    1.09    109.50     60.00       0.0679
   8   H5'2  H1    E    6   5   4    1.09    109.50    -60.00       0.0679
   9   C4'   CT    M    6   5   4    1.52    110.00   -180.00       0.1065
  10   H4'   H1    E    9   6   5    1.09    109.50   -200.00       0.1174
  11   O4'   OS    S    9   6   5    1.46    108.86    -86.31      -0.3548
  12   C1'   CT    B   11   9   5    1.42    110.04    105.60       0.0066
  13   H1'   H2    E   12  11   9    1.09    109.50   -240.00       0.2029
  14   N1    N*    S   12  11   9    1.49    108.10   -127.70      -0.0484
  15   C6    C1    B   14  12  11    1.36    121.10     81.59       0.0053
  16   H6    H4    E   15  14  12    1.08    120.00      0.00       0.1958
  17   C5    C1    B   15  14  12    1.36    121.00    180.00      -0.5215
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  18   H5     HA     E    17   15   14     1.09     120.00     180.00        0.1928
  19   C4     CA     B    17   15   14     1.43     116.90       0.00        0.8185
  20   N4     N2     B    19   17   15     1.32     120.10     180.00       -0.9530
  21   H41    H      E    20   19   17     1.01     117.70     180.00        0.4234
  22   H42    H      E    20   19   17     1.01     120.27       0.00        0.4234
  23   N3     NC     S    19   17   15     1.33     121.70       0.00       -0.7584
  24   C2     C      S    23   19   17     1.36     120.50       0.00        0.7538
  25   O2     O      E    24   23   19     1.24     122.40     180.00       -0.6252
  26   C3'    C3     M     9    6    5     1.53     115.78    -329.11        0.2022
  27   H3'    H1     E    26    9    6     1.09     109.50      30.00        0.0615
  28   C2'    CT     B    26    9    6     1.53     102.80     -86.30        0.0670
  29   H2'1   H1     E    28   26    9     1.09     109.50     120.00        0.0972
  30   O2'    OH     S    28   26    9     1.43     109.50     240.00       -0.6139
  31   HO'2   HO     E    30   28   26     0.96     107.00     180.00        0.4186
  32   O3'    OR     M    26    9    6     1.42     116.52    -203.47       -0.5246

CHARGE RC5E
  0.4295 -0.6223  0.0558  0.0679  0.0679
  0.1065  0.1174 -0.3548  0.0066  0.2029
 -0.0484  0.0053  0.1958 -0.5215  0.1928
  0.8185 -0.9530  0.4234  0.4234 -0.7584
  0.7538 -0.6252  0.2022  0.0615  0.0670
  0.0972 -0.6139  0.4186 -0.5246

IMPROPER
 C6   C2   N1   C1'
 N1   N3   C2   O2
 C4   H41  N4   H42
 N1   C5   C6   H6
 C6   C4   C5   H5
 N3   C5   C4   N4

LOOP CLOSING EXPLICIT
 C1'  C2'
 C2   N1

DONE
R-CYTOSINE - with 5' - phosphate group and 3' - O(minus) group

 RC   INT     1
 CORRECT OMIT DU   BEG
   0.0
   1   DUMM   DU     M     0   -1   -2     0.00       0.00       0.00        0.0000
   2   DUMM   DU     M     1    0   -1     1.00       0.00       0.00        0.0000
   3   DUMM   DU     M     2    1    0     1.00      90.00       0.00        0.0000
   4   P      P      M     3    2    1     1.60     119.04     200.00        1.1662
   5   O1P    OP     E     4    3    2     1.48     109.61     150.00       -0.7760
   6   O2P    OP     E     4    3    2     1.48     109.58      20.00       -0.7760
   7   O5'    OR     M     4    3    2     1.60     101.43     -98.89       -0.4989
   8   C5'    CI     M     7    4    3     1.44     119.00     -39.22        0.0558
   9   H5'1   H1     E     8    7    4     1.09     109.50      60.00        0.0679
  10   H5'2   H1     E     8    7    4     1.09     109.50     -60.00        0.0679
  11   C4'    CT     M     8    7    4     1.52     110.00     180.00        0.1065
  12   H4'    H1     E    11    8    7     1.09     109.50    -200.00        0.1174
  13   O4'    OS     S    11    8    7     1.46     108.86     -86.31       -0.3548
  14   C1'    CT     B    13   11    8     1.42     110.04     105.60        0.0066
  15   H1'    H2     E    14   13   11     1.09     109.50    -240.00        0.2029
  16   N1     N*     S    14   13   11     1.49     108.10    -127.70       -0.0484
  17   C6     C1     B    16   14   13     1.36     121.10      81.59        0.0053
  18   H6     H4     E    17   16   14     1.08     120.00       0.00        0.1958
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  19   C5    C1    B   17  16  14    1.36    121.00    180.00      -0.5215
  20   H5    HA    E   19  17  16    1.09    120.00    180.00       0.1928
  21   C4    CA    B   19  17  16    1.43    116.90      0.00       0.8185
  22   N4    N2    B   21  19  17    1.32    120.10    180.00      -0.9530
  23   H41   H     E   22  21  19    1.01    117.70    180.00       0.4234
  24   H42   H     E   22  21  19    1.01    120.27      0.00       0.4234
  25   N3    NC    S   21  19  17    1.33    121.70      0.00      -0.7584
  26   C2    C     S   25  21  19    1.36    120.50      0.00       0.7538
  27   O2    O     E   26  25  21    1.24    122.40    180.00      -0.6252
  28   C3'   C3    M   11   8   7    1.53    115.78   -329.11       0.2022
  29   H3'   H1    E   28  11   8    1.09    109.50     30.00       0.0615
  30   C2'   CT    B   28  11   8    1.53    102.80    -86.30       0.0670
  31   H2'1  H1    E   30  28  11    1.09    109.50    120.00       0.0972
  32   O2'   OH    S   30  28  11    1.43    109.50    240.00      -0.6139
  33   HO'2  HO    E   32  30  28    0.96    107.00    180.00       0.4186
  34   O3'   OR    M   28  11   8    1.42    116.52   -203.47      -0.5246

CHARGE RC
  1.1662 -0.7760 -0.7760 -0.4989  0.0558
  0.0679  0.0679  0.1065  0.1174 -0.3548
  0.0066  0.2029 -0.0484  0.0053  0.1958
 -0.5215  0.1928  0.8185 -0.9530  0.4234
  0.4234 -0.7584  0.7538 -0.6252  0.2022
  0.0615  0.0670  0.0972 -0.6139  0.4186
 -0.5246

IMPROPER
 C6   C2   N1   C1'
 N1   N3   C2   O2
 C4   H41  N4   H42
 N1   C5   C6   H6
 C6   C4   C5   H5
 N3   C5   C4   N4

LOOP CLOSING EXPLICIT
 C1'  C2'
 C2   N1

DONE
R-CYTOSINE - with 5' - phosphate group and 3' - OH group

 RC3  INT     1
 CORRECT OMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00      0.00      0.00       0.0000
   2   DUMM  DU    M    1   0  -1    1.00      0.00      0.00       0.0000
   3   DUMM  DU    M    2   1   0    1.00     90.00      0.00       0.0000
   4   P     P     M    3   2   1    1.60    119.04    200.00       1.1662
   5   O1P   OP    E    4   3   2    1.48    109.61    150.00      -0.7760
   6   O2P   OP    E    4   3   2    1.48    109.58     20.00      -0.7760
   7   O5'   OR    M    4   3   2    1.60    101.43    -98.89      -0.4989
   8   C5'   CI    M    7   4   3    1.44    119.00    -39.22       0.0558
   9   H5'1  H1    E    8   7   4    1.09    109.50     60.00       0.0679
  10   H5'2  H1    E    8   7   4    1.09    109.50    -60.00       0.0679
  11   C4'   CT    M    8   7   4    1.52    110.00    180.00       0.1065
  12   H4'   H1    E   11   8   7    1.09    109.50   -200.00       0.1174
  13   O4'   OS    S   11   8   7    1.46    108.86    -86.31      -0.3548
  14   C1'   CT    B   13  11   8    1.42    110.04    105.60       0.0066
  15   H1'   H2    E   14  13  11    1.09    109.50   -240.00       0.2029
  16   N1    N*    S   14  13  11    1.49    108.10   -127.70      -0.0484
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  17   C6    C1    B   16  14  13    1.36    121.10     81.59       0.0053
  18   H6    H4    E   17  16  14    1.08    120.00      0.00       0.1958
  19   C5    C1    B   17  16  14    1.36    121.00    180.00      -0.5215
  20   H5    HA    E   19  17  16    1.09    120.00    180.00       0.1928
  21   C4    CA    B   19  17  16    1.43    116.90      0.00       0.8185
  22   N4    N2    B   21  19  17    1.32    120.10    180.00      -0.9530
  23   H41   H     E   22  21  19    1.01    117.70    180.00       0.4234
  24   H42   H     E   22  21  19    1.01    120.27      0.00       0.4234
  25   N3    NC    S   21  19  17    1.33    121.70      0.00      -0.7584
  26   C2    C     S   25  21  19    1.36    120.50      0.00       0.7538
  27   O2    O     E   26  25  21    1.24    122.40    180.00      -0.6252
  28   C3'   C3    M   11   8   7    1.53    115.78   -329.11       0.2022
  29   H3'   H1    E   28  11   8    1.09    109.50     30.00       0.0615
  30   C2'   CT    B   28  11   8    1.53    102.80    -86.30       0.0670
  31   H2'1  H1    E   30  28  11    1.09    109.50    120.00       0.0972
  32   O2'   OH    S   30  28  11    1.43    109.50    240.00      -0.6139
  33   HO'2  HO    E   32  30  28    0.96    107.00    180.00       0.4186
  34   O3'   OH    M   28  11   8    1.42    116.52   -203.47      -0.6541
  35   H3T   HO    M   34  28  11    0.96    114.97    180.00       0.4376

CHARGE RC3E
  1.1662 -0.7760 -0.7760 -0.4989  0.0558
  0.0679  0.0679  0.1065  0.1174 -0.3548
  0.0066  0.2029 -0.0484  0.0053  0.1958
 -0.5215  0.1928  0.8185 -0.9530  0.4234
  0.4234 -0.7584  0.7538 -0.6252  0.2022
  0.0615  0.0670  0.0972 -0.6139  0.4186
 -0.6541  0.4376

IMPROPER
 C6   C2   N1   C1'
 N1   N3   C2   O2
 C4   H41  N4   H42
 N1   C5   C6   H6
 C6   C4   C5   H5
 N3   C5   C4   N4

LOOP CLOSING EXPLICIT
 C1'  C2'
 C2   N1

DONE
R-CYTOSINE - with 5' - OH group and 3' - OH group

 RCN  INT     1
 CORRECT NOMIT DU   BEG
   0.0
   1   DUMM  DU    M    0  -1  -2    0.00      0.00      0.00       0.0000
   2   DUMM  DU    M    1   0  -1    1.00      0.00      0.00       0.0000
   3   DUMM  DU    M    2   1   0    1.00     90.00      0.00       0.0000
   4   H5T   HO    M    3   2   1    1.00    120.00    180.00       0.4295
   5   O5'   OH    M    4   3   2    0.96    101.43    -98.89      -0.6223
   6   C5'   CI    M    5   4   3    1.44    119.00    -39.22       0.0558
   7   H5'1  H1    E    6   5   4    1.09    109.50     60.00       0.0679
   8   H5'2  H1    E    6   5   4    1.09    109.50    -60.00       0.0679
   9   C4'   CT    M    6   5   4    1.52    110.00   -180.00       0.1065
  10   H4'   H1    E    9   6   5    1.09    109.50   -200.00       0.1174
  11   O4'   OS    S    9   6   5    1.46    108.86    -86.31      -0.3548
  12   C1'   CT    B   11   9   5    1.42    110.04    105.60       0.0066
  13   H1'   H2    E   12  11   9    1.09    109.50   -240.00       0.2029
```

```
  14   N1    N*    S   12  11   9    1.49    108.10   -127.70      -0.0484
  15   C6    C1    B   14  12  11    1.36    121.10     81.59       0.0053
  16   H6    H4    E   15  14  12    1.08    120.00      0.00       0.1958
  17   C5    C1    B   15  14  12    1.36    121.00    180.00      -0.5215
  18   H5    HA    E   17  15  14    1.09    120.00    180.00       0.1928
  19   C4    CA    B   17  15  14    1.43    116.90      0.00       0.8185
  20   N4    N2    B   19  17  15    1.32    120.10    180.00      -0.9530
  21   H41   H     E   20  19  17    1.01    117.70    180.00       0.4234
  22   H42   H     E   20  19  17    1.01    120.27      0.00       0.4234
  23   N3    NC    S   19  17  15    1.33    121.70      0.00      -0.7584
  24   C2    C     S   23  19  17    1.36    120.50      0.00       0.7538
  25   O2    O     E   24  23  19    1.24    122.40    180.00      -0.6252
  26   C3'   C3    M    9   6   5    1.53    115.78   -329.11       0.2022
  27   H3'   H1    E   26   9   6    1.09    109.50     30.00       0.0615
  28   C2'   CT    B   26   9   6    1.53    102.80    -86.30       0.0670
  29   H2'1  H1    E   28  26   9    1.09    109.50    120.00       0.0972
  30   O2'   OH    S   28  26   9    1.43    109.50    240.00      -0.6139
  31   HO'2  HO    E   30  28  26    0.96    107.00    180.00       0.4186
  32   O3'   OH    M   26   9   6    1.42    116.52   -203.47      -0.6541
  33   H3T   HO    M   32  26   9    0.96    114.97    180.00       0.4376

CHARGE  resp RCYT
  0.4295 -0.6223  0.0558  0.0679  0.0679
  0.1065  0.1174 -0.3548  0.0066  0.2029
 -0.0484  0.0053  0.1958 -0.5215  0.1928
  0.8185 -0.9530  0.4234  0.4234 -0.7584
  0.7538 -0.6252  0.2022  0.0615  0.0670
  0.0972 -0.6139  0.4186 -0.6541  0.4376

IMPROPER
 C6   C2   N1   C1'
 N1   N3   C2   O2
 C4   H41  N4   H42
 N1   C5   C6   H6
 C6   C4   C5   H5
 N3   C5   C4   N4

LOOP CLOSING EXPLICIT
 C1'  C2'
 C2   N1

DONE
STOP
```

frcmod.parmbsc0

```
modifies parm99 for nucleic acids: see http://mmb.pcb.ub.es/PARMBSC0/
MASS
CI  12.001

BOND
CI-H1  340.0    1.090
CI-CT  310.0    1.526
OS-CI  320.0    1.410
OH-CI  320.0    1.410

ANGLE
H1-CI-CT    50.0      109.50
H1-CI-H1    35.0      109.50
CI-CT-H1    50.0      109.50
CI-CT-OS    50.0      109.50
CI-CT-CT    40.0      109.50
OS-CI-H1    50.0      109.50
OS-CI-CT    50.0      109.50
P -OS-CI   100.0      120.50
OH-CI-H1    50.0      109.50
OH-CI-CT    50.0      109.50
HO-OH-CI    55.0      108.50

DIHE
X -CI-OS-X     3       1.150       0.0         3.0
X -CI-OH-X     3       0.500       0.0         3.0
X -CI-CT-X     9       1.400       0.0         3.0
CT-OS-CT-CI    1       0.383       0.0        -3.0
CT-OS-CT-CI    1       0.100     180.0         2.0
H1-CI-CT-OS    1       0.250       0.0         1.0
H1-CI-CT-OH    1       0.250       0.0         1.0
H1-CT-CI-OS    1       0.250       0.0         1.0
H1-CT-CI-OH    1       0.250       0.0         1.0
CI-CT-CT-CT    1       0.180       0.0        -3.0
CI-CT-CT-CT    1       0.250     180.0        -2.0
CI-CT-CT-CT    1       0.200     180.0         1.0
OS-P -OS-CI    1       0.185181   31.79508    -1.0  alfa
OS-P -OS-CI    1       1.256531  351.95960    -2.0  alfa
OS-P -OS-CI    1       0.354858  357.24748     3.0  alfa
OH-P -OS-CI    1       0.185181   31.79508    -1.0  alfa
OH-P -OS-CI    1       1.256531  351.95960    -2.0  alfa
OH-P -OS-CI    1       0.354858  357.24748     3.0  alfa
CT-CT-CI-OS    1       1.178040  190.97653    -1.0  gamma
CT-CT-CI-OS    1       0.092102  295.63279    -2.0  gamma
CT-CT-CI-OS    1       0.962830  348.09535     3.0  gamma
CT-CT-CI-OH    1       1.178040  190.97653    -1.0  gamma
CT-CT-CI-OH    1       0.092102  295.63279    -2.0  gamma
CT-CT-CI-OH    1       0.962830  348.09535     3.0  gamma

NONB
CI          1.9080  0.1094
```

frcmod.OL3.chi

```
Original parameter file
MASS
C2 12.01         0.360              sp2 C 5 memb.ring in purines
C1 12.01         0.360              sp2 C  pyrimidines in pos. 5 & 6

BOND
C2-H5  367.0    1.080       changed from 340. bsd on C6H6 nmodes; ADE,GUA
C2-N*  440.0    1.371       JCC,7,(1986),230; ADE,GUA
C2-NB  529.0    1.304       JCC,7,(1986),230; ADE,GUA
C -C1  410.0    1.444       JCC,7,(1986),230; THY,URA
CA-C1  427.0    1.433       JCC,7,(1986),230; CYT
C1-C1  549.0    1.350       JCC,7,(1986),230; CYT,THY,URA
C1-CT  317.0    1.510       JCC,7,(1986),230; THY
C1-HA  367.0    1.080       changed from 340. bsd on C6H6 nmodes; CYT,URA
C1-H4  367.0    1.080       changed from 340. bsd on C6H6 nmodes; CYT,URA
C1-N*  448.0    1.365       JCC,7,(1986),230; CYT,THY,URA

ANGLE
H5-C2-N*    50.0      123.05
H5-C2-NB    50.0      123.05
N*-C2-NB    70.0      113.90
CB-N*-C2    70.0      105.40
C2-N*-CT    70.0      128.80
CB-NB-C2    70.0      103.80
C1-C -NA    70.0      114.10
C1-C -O     80.0      125.30
C1-CA-N2    70.0      120.10
C1-CA-NC    70.0      121.50
C -C1-C1    63.0      120.70    changed from 85.0  bsd on C6H6 nmodes; NA thy
C -C1-CT    70.0      119.70
C -C1-HA    50.0      119.70
C -C1-H4    50.0      119.70
CA-C1-C1    63.0      117.00    changed from 85.0  bsd on C6H6 nmodes; NA cyt
CA-C1-HA    50.0      123.30
CA-C1-H4    50.0      123.30
C1-C1-CT    70.0      119.70
C1-C1-HA    50.0      119.70
C1-C1-H4    50.0      119.70
C1-C1-N*    70.0      121.20
H4-C1-N*    50.0      119.10
H1-CT-C1    50.0      109.50    Junmei et al, 1999
HC-CT-C1    50.0      109.50    changed based on NMA nmodes
C -N*-C1    70.0      121.60
C1-N*-CT    70.0      121.20

DIHEDRAL
X -C2-N*-X    4    6.80        180.0            2.         JCC,7,(1986),230
X -C2-NB-X    2   20.00        180.0            2.         JCC,7,(1986),230
X -C -C1-X    4    8.70        180.0            2.         intrpol.bsd.on C6H6
X -CA-C1-X    4   10.20        180.0            2.         intrpol.bsd.on C6H6
X -C1-C1-X    4   26.60        180.0            2.         intrpol.bsd.on C6H6
X -C1-CT-X    6    0.00          0.0            3.         JCC,7,(1986),230
X -C1-N*-X    4    7.40        180.0            2.         JCC,7,(1986),230
HC-CT-C1-C1   1    0.38        180.0           -3.         Junmei et al, 1999
HC-CT-C1-C1   1    1.15          0.0            1.         Junmei et al, 1999
C1-C1-C -O    1    2.175       180.0           -2.         Junmei et al, 1999
C1-C1-C -O    1    0.30          0.0            3.         Junmei et al, 1999
OS-CT-N*-C2   1    0.96561      68.7902        -1.         ol3 chi ade
OS-CT-N*-C2   1    1.07403      15.6360        -2.         ol3 chi ade
```

```
OS-CT-N*-C2   1    0.45754     171.5787          -3.          ol3 chi ade
OS-CT-N*-C2   1    0.30917      19.0921           4.          ol3 chi ade
OS-CT-N*-CK   1    0.70510      74.7558          -1.          ol3 chi gua
OS-CT-N*-CK   1    1.06546       6.2286          -2.          ol3 chi gua
OS-CT-N*-CK   1    0.44273     168.6503          -3.          ol3 chi gua
OS-CT-N*-CK   1    0.25602       3.9746           4.          ol3 chi gua
OS-CT-N*-C1   1    1.22506     146.9892          -1.          ol3 chi cyt
OS-CT-N*-C1   1    1.63459      16.4766          -2.          ol3 chi cyt
OS-CT-N*-C1   1    0.93747     185.8774          -3.          ol3 chi cyt
OS-CT-N*-C1   1    0.31033      32.1590           4.          ol3 chi cyt
OS-CT-N*-CM   1    1.02514     149.8583          -1.          ol3 chi ura,thy
OS-CT-N*-CM   1    1.74876      16.7648          -2.          ol3 chi ura,thy
OS-CT-N*-CM   1    0.58150     179.3474          -3.          ol3 chi ura,thy
OS-CT-N*-CM   1    0.35148      16.0016           4.          ol3 chi ura,thy

IMPROPER
X -X -C2-H5          1.1          180.          2.
CB-C2-N*-CT          1.0          180.          2.
X -X -C1-H4          1.1          180.          2.
X -X -C1-HA          1.1          180.          2.
C -C1-N*-CT          1.0          180.          2.          dac guess, 9/94
C -C1-C1-CT          1.1          180.          2.          dac guess, 9/94
C1-N2-CA-NC          1.1          180.          2.          dac guess, 9/94

NONBOND
C2          1.9080  0.0860             Spellmeyer
C1          1.9080  0.0860             Spellmeyer
```

frcmod.99bsc0-chiol3-CaseP

```
# force field modification for O2 (->OP) and OS (->OR) according to
Steinbrecher, Latzer, and Case, JCTC 2012 including corrected 1-4 VdW parameters
for delta, tau2, zeta, alpha, and gamma dihedrals.
MASS
OP 16.00         0.434              carboxyl and phosphate group oxygen (O2)
OR 16.00         0.465              ether and ester oxygen (OS)

BOND
C -OP  656.0    1.250       JCC,7,(1986),230; GLU,ASP
OP-P   525.0    1.480       JCC,7,(1986),230; NA PHOSPHATES
C -OR  450.0    1.323       Junmei et al, 1999
CM-OR  480.0    1.240       Junmei et al, 1999
CT-OR  320.0    1.410       JCC,7,(1986),230; NUCLEIC ACIDS
OR-P   230.0    1.610       JCC,7,(1986),230; NA PHOSPHATES
HO-OR  553.0    0.960       JCC,7,(1986),230; NUCLEOTIDE ENDS
OR-CI  320.0    1.410
C3-OR  320.0    1.410       JCC,7,(1986),230; NUCLEIC ACIDS

ANGLE
CT-C -OP    70.0      117.00
OP-C -OP    80.0      126.00    AA GLU            (SCH JPC 79,2379)
OP-C -O2    80.0      126.00    AA GLU            (SCH JPC 79,2379)
O2-C -OP    80.0      126.00    AA GLU            (SCH JPC 79,2379)
OP-P -OH    45.0      108.23
OP-P -OP   140.0      119.90
OP-P -O2   140.0      119.90
O2-P -OP   140.0      119.90
OP-P -OR   100.0      108.23
CT-C -OR    80.0      115.00    Junmei et al, 1999
O -C -OR    80.0      125.00    Junmei et al, 1999
H5-C -OR    50.0      107.00    Junmei et al, 1999
CM-CM-OR    80.0      125.00    Junmei et al, 1999
H4-CM-OR    50.0      113.00    Junmei et al, 1999
H1-CT-OR    50.0      109.50    changed based on NMA nmodes
H2-CT-OR    50.0      109.50    changed based on NMA nmodes
C -CT-OR    60.0      109.50    Junmei et al, 1999
CM-CT-OR    50.0      109.50    Junmei et al, 1999
CT-CT-OR    50.0      109.50
OR-CT-OR   160.0      101.00    Junmei et al, 1999
OS-CT-OR   160.0      101.00    Junmei et al, 1999
OR-CT-OS   160.0      101.00    Junmei et al, 1999
OR-CT-CY    50.0      110.00    Junmei et al, 1999
OR-CT-CZ    50.0      110.00    Junmei et al, 1999
OR-CT-N*    50.0      109.50
C -OR-CT    60.0      117.00    Junmei et al, 1999
CM-OR-CT    60.0      117.00    Junmei et al, 1999
CT-OR-CT    60.0      109.50
CT-OR-P    100.0      120.50
P -OR-P    100.0      120.50
OH-P -OR    45.0      102.60
OR-P -OR    45.0      102.60
OS-P -OR    45.0      102.60
OR-P -OS    45.0      102.60
CI-CT-OR    50.0      109.50
OR-CI-H1    50.0      109.50
OR-CI-CT    50.0      109.50
P -OR-CI   100.0      120.50
H1-C3-OR    50.0      109.50    changed based on NMA nmodes
CT-C3-OR    50.0      109.50
```

```
C3-CT-OR    50.0       109.50
C3-OR-P    100.0       120.50

DIHE
X -OP-C -OP         10.5         180.0              2.          JCC,7,(1986),230
X -O2-C -OP         10.5         180.0              2.          JCC,7,(1986),230
X -OP-C -O2         10.5         180.0              2.          JCC,7,(1986),230
X -C -OR-X     2    5.40         180.0              2.          Junmei et al, 1999
X -CM-OR-X     2    2.10         180.0              2.          Junmei et al, 1999
X -CT-OR-X     3    1.15           0.0              3.          JCC,7,(1986),230
X -OR-P -X     3    0.75           0.0              3.          JCC,7,(1986),230
OH-P -OR-CT    1    0.25           0.0             -3.          JCC,7,(1986),230
OH-P -OR-CT    1    1.20           0.0              2.          gg&gt ene.631g*/mp2
OR-P -OR-C3    1    0.374954       0.660088        -3.          zeta corrected for
1-4 VdW
OR-P -OR-C3    1    1.196555       0.421469        -2.          zeta corrected for
1-4 VdW
OR-P -OR-C3    1    0.062735     193.362            1.          zeta corrected for
1-4 VdW
OH-P -OR-C3    1    0.374954       0.660088        -3.          zeta corrected for
1-4 VdW
OH-P -OR-C3    1    1.196555       0.421469        -2.          zeta corrected for
1-4 VdW
OH-P -OR-C3    1    0.062735     193.362            1.          zeta corrected for
1-4 VdW
OS-P -OR-CT    1    0.25           0.0             -3.          JCC,7,(1986),230
OS-P -OR-CT    1    1.20           0.0              2.          gg&gt ene.631g*/mp2
OR-P -OS-CT    1    0.25           0.0             -3.          JCC,7,(1986),230
OR-P -OS-CT    1    1.20           0.0              2.          gg&gt ene.631g*/mp2
CT-CT-OR-CT    1    0.383          0.0             -3.
CT-CT-OR-CT    1    0.1          180.0              2.
CT-CT-OR-C     1    0.383          0.0             -3.          Junmei et al, 1999
CT-CT-OR-C     1    0.80         180.0              1.          Junmei et al, 1999
CT-OR-CT-OR    1    0.10           0.0             -3.          Junmei et al, 1999
CT-OR-CT-OR    1    0.85         180.0             -2.          Junmei et al, 1999
CT-OR-CT-OR    1    1.35         180.0              1.          Junmei et al, 1999
CT-OS-CT-OR    1    0.10           0.0             -3.          Junmei et al, 1999
CT-OS-CT-OR    1    0.85         180.0             -2.          Junmei et al, 1999
CT-OS-CT-OR    1    1.35         180.0              1.          Junmei et al, 1999
CT-OR-CT-OS    1    0.10           0.0             -3.          Junmei et al, 1999
CT-OR-CT-OS    1    0.85         180.0             -2.          Junmei et al, 1999
CT-OR-CT-OS    1    1.35         180.0              1.          Junmei et al, 1999
CT-OR-CT-N*    1    0.383          0.0             -3.          parm98.dat,
TC,PC,PAK
CT-OR-CT-N*    1    0.65           0.0              2.          Piotr et al.
O -C -OR-CT    1    2.70         180.0             -2.          Junmei et al, 1999
O -C -OR-CT    1    1.40         180.0              1.          Junmei et al, 1999
OR-CT-N*-CK    1    0.00         000.0             -2.          parm98, TC,PC,PAK
OR-CT-N*-CK    1    2.50           0.0              1.          parm98, TC,PC,PAK
OR-CT-N*-CM    1    0.00         000.0             -2.          parm98, TC,PC,PAK
OR-CT-N*-CM    1    2.50           0.0              1.          parm98, TC,PC,PAK
OR-CT-CT-OR    1    0.144          0.0             -3.          parm98, TC,PC,PAK
OR-CT-CT-OR    1    1.175          0.0              2.          Piotr et al.
OS-CT-CT-OR    1    0.144          0.0             -3.          parm98, TC,PC,PAK
OS-CT-CT-OR    1    1.175          0.0              2.          Piotr et al.
OR-C3-CT-OS    1    0.098221      52.691           -3.          delta corrected for
1-4 VdW
OR-C3-CT-OS    1    1.199546      10.01992          2.          delta corrected for
1-4 VdW
```

```
OR-C3-CT-OH   1    0.033754      0.0            -3.         tau2(mirror)
corrected for 1-4 VdW
OR-C3-CT-OH   1    1.094752      0.0             2.         tau2(mirror)
corrected for 1-4 VdW
H1-C3-CT-OR   1    0.025904    146.58           -3.         delta corrected for
1-4 VdW
H1-C3-CT-OR   1    0.200389    353.98061         1.         delta corrected for
1-4 VdW
H1-CT-C3-OR   1    0.025904    146.58           -3.         tau corrected for 1-
4 VdW
H1-CT-C3-OR   1    0.200389    353.98061         1.         tau corrected for 1-
4 VdW
HC-CT-CT-OR   1    0.000         0.0            -3.         JCC,7,(1986),230
HC-CT-CT-OR   1    0.25          0.0             1.         Junmei et al, 1999
X -CI-OR-X    3    1.150         0.0             3.0
CT-OR-CT-CI   1    0.383         0.0            -3.0
CT-OR-CT-CI   1    0.100       180.0             2.0
H1-CI-CT-OR   1    0.250         0.0             1.0
H1-CT-CI-OR   1    0.85333     359.85087         1.0  gamma corrected for 1-4
VdW
OR-P -OR-CI   1    0.125609     41.051          -1.0  alpha corrected for 1-4
VdW
OR-P -OR-CI   1    1.251237    352.34289        -2.0  alpha corrected for 1-4
VdW
OR-P -OR-CI   1    0.478513    358.47366         3.0  alpha corrected for 1-4
VdW
C3-CT-CI-OR   1    0.988048    171.1526         -1.0  gamma corrected for 1-4
VdW
C3-CT-CI-OR   1    0.027335    183.6548         -2.0  gamma corrected for 1-4
VdW
C3-CT-CI-OR   1    0.827287    346.2412          3.0  gamma corrected for 1-4
VdW
OR-CT-N*-C2   1    0.96561      68.7902         -1.         ol3 chi ade
OR-CT-N*-C2   1    1.07403      15.6360         -2.         ol3 chi ade
OR-CT-N*-C2   1    0.45754     171.5787         -3.         ol3 chi ade
OR-CT-N*-C2   1    0.30917      19.0921          4.         ol3 chi ade
OR-CT-N*-CK   1    0.70510      74.7558         -1.         ol3 chi gua
OR-CT-N*-CK   1    1.06546       6.2286         -2.         ol3 chi gua
OR-CT-N*-CK   1    0.44273     168.6503         -3.         ol3 chi gua
OR-CT-N*-CK   1    0.25602       3.9746          4.         ol3 chi gua
OR-CT-N*-C1   1    1.22506     146.9892         -1.         ol3 chi cyt
OR-CT-N*-C1   1    1.63459      16.4766         -2.         ol3 chi cyt
OR-CT-N*-C1   1    0.93747     185.8774         -3.         ol3 chi cyt
OR-CT-N*-C1   1    0.31033      32.1590          4.         ol3 chi cyt
OR-CT-N*-CM   1    1.02514     149.8583         -1.         ol3 chi ura,thy
OR-CT-N*-CM   1    1.74876      16.7648         -2.         ol3 chi ura,thy
OR-CT-N*-CM   1    0.58150     179.3474         -3.         ol3 chi ura,thy
OR-CT-N*-CM   1    0.35148      16.0016          4.         ol3 chi ura,thy
X -C3-OR-X    3    1.15          0.0             3.         JCC,7,(1986),230
C3-CT-OR-CT   1    0.383         0.0            -3.
C3-CT-OR-CT   1    0.1         180.0             2.
OR-C3-CT-OR   1    0.144         0.0            -3.         parm98, TC,PC,PAK
OR-C3-CT-OR   1    1.175         0.0             2.         Piotr et al.
OS-C3-CT-OR   1    0.144         0.0            -3.         parm98, TC,PC,PAK
OS-C3-CT-OR   1    1.175         0.0             2.         Piotr et al.
OR-C3-CT-OS   1    0.144         0.0            -3.         parm98, TC,PC,PAK
OR-C3-CT-OS   1    1.175         0.0             2.         Piotr et al.
OR-C3-CT-OH   1    0.144         0.0            -3.         parm98, TC,PC,PAK
OR-C3-CT-OH   1    1.175         0.0             2.         Piotr et al.
OR-CT-C3-OH   1    0.144         0.0            -3.         parm98, TC,PC,PAK
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OR-CT-C3-OH   1    1.175         0.0             2.         Piotr et al.
H1-C3-CT-OR   1    0.000         0.0            -3.         JCC,7,(1986),230
H1-C3-CT-OR   1    0.25          0.0             1.         Junmei et al, 1999
H1-CT-C3-OR   1    0.000         0.0            -3.         JCC,7,(1986),230
H1-CT-C3-OR   1    0.25          0.0             1.         Junmei et al, 1999
HC-CT-C3-OR   1    0.000         0.0            -3.         JCC,7,(1986),230
HC-CT-C3-OR   1    0.25          0.0             1.         Junmei et al, 1999
OR-C3-CT-CI   1    0.182735      6.319592        3.0        delta corrected for
1-4 VdW
OR-C3-CT-CT   1    0.24569      12.31214         3.0        tau2(mirror)
corrected for 1-4 VdW
C3-OR-P -OP   1    0.12716       0.052366        3.0        zeta corrected for
1-4 VdW
CI-OR-P -OP   1    0.12716       0.052366        3.0        alpha corrected for
1-4 VdW
OR-CI-CT-OS   1    0.15377       0.485128        3.0        gammma corrected for
1-4 VdW


NONBON
OP          1.7493  0.2100            Case et al., JCTC 2012
OR          1.7718  0.1700            Case et al., JCTC 2012
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