Supplementary material:

Table. SI: Mean and standard deviations (within parenthesis) of intra basepair parameters from crystal structure database analysis. We have tabulated only frequent basepairs in the non-redundant dataset (frequency greater than 10).

No	Basepair (Frequency /frequency in triad) for the first 32 basepairs)	Buckle (^{O})	Open (^{O})	Propeller (^{O})	Stagger (Å)	Shear (Å)	Stretch (Å)
1	G:C W:W C (5676/264)	-5.39(9.3)	0.49(3.8)	-6.51(7.9)	-0.14(0.4)	-0.07(0.4)	2.86(0.1)
2	A:U W:W C (1711/81)	-1.96(8.3)	3.27(4.5)	-6.56(8.3)	-0.04(0.4)	0.11(0.3)	2.79(0.1)
3	G:U W:W C (825/28)	-1.51(8.5)	-0.61(5.8)	-6.55(7.3)	-0.17(0.4)	-2.22(0.4)	2.81(0.2)
4	A:G H:S T (531/36)	-2.12(14.0)	13.11(5.7)	1.07(13.1)	0.14(0.5)	2.24(0.4)	3.31(0.2)
5	A:U H:W T (401/36)	-1.41(13.6)	-0.39(6.6)	-1.17(9.8)	-0.04(0.5)	0.17(0.5)	2.82(0.2)
6	A:G W:W C (142/0)	-10.77(14.2)	1.27(5.8)	-8.55(12.0)	-0.41(0.4)	0.07(0.5)	2.8(0.2)
7	A:A H:H T (106/3)	-9.63(15.2)	-4.66(3.3)	5.81(13.2)	-0.35(0.3)	2.51(0.4)	2.86(0.2)
8	G:A S:W T (86/7)	13.04(19.0)	13.62(7.0)	0.27(16.6)	0.16(0.6)	1.85(0.4)	3.32(0.2)
9	A:A H:W T (80/24)	1.84(12.8)	5.7(5.2)	-2.88(19.6)	0.04(0.5)	2.31(0.4)	2.92(0.2)
10	A:U H:W C (77/14)	-3.59(18.1)	2.93(6.8)	-4.53(12.4)	0.15(0.6)	-0.22(0.4)	2.8(0.2)
11	U:U W:W C (76/0)	-10.11(8.6)	-2.33(5.3)	-12.64(8.0)	-0.15(0.4)	-2.36(0.4)	2.86(0.2)
12	A:C H:W T (75/3)	-1.26(20.5)	4.3(6.4)	-5.68(15.6)	-0.18(0.5)	2.37(0.4)	2.91(0.2)
13	G:C W:W T (63/1)	-4.35(15.4)	7.34(7.3)	-6.67(10.7)	-0.09(0.4)	-2.27(0.5)	2.88(0.2)
14	A:A W:W T (59/25)	7.87(11.3)	-7.58(7.5)	-2.04(30.2)	-0.14(0.7)	2.19(0.5)	2.87(0.2)

15	A:U W:W T (59/3)	0.05(12.7)	-1.9(7.4)	0.13(13.3)	0.03(0.6)	-0.24(0.4)	2.83(0.2)
16	G:G H:W C (48/2)	6.43(12.6)	-3.86(6.2)	-0.31(12.1)	0.08(0.6)	-2.94(0.4)	2.88(0.2)
17	G:G H:W T (39/0)	9.29(12.9)	1.77(6.6)	-0.64(8.4)	-0.13(0.3)	-0.02(0.6)	2.89(0.2)
18	G:G S:S T (32/4)	4.64(22.1)	-4.54(3.6)	13.25(18.5)	-0.66(0.5)	1.27(0.3)	3.46(0.2)
19	U:U W:W T (20/0)	-6.22(16.0)	-4.52(3.2)	-4.36(10.2)	0.11(0.4)	-2.35(0.4)	2.79(0.2)
20	A:G s:s T (285/30)	15.84(26.9)	27.99(7.2)	-7.44(13.6)	0.22(0.9)	1.71(0.3)	3.02(0.2)
21	G:U s:h C (53/0)	-11.75(18.2)	-1.22(5.5)	0.15(7.4)	-0.1(0.6)	0.99(0.4)	3.44(0.1)
22	A:A h:s T (49/0)	-5.65(13.5)	-1.39(6.0)	1.66(9.4)	-0.13(0.5)	2.38(0.3)	2.75(0.2)
23	A:G w:s C (48/6)	-19.31(28.9)	45.49(12.6)	-6.41(24.2)	-0.1(0.9)	2.07(0.4)	2.84(0.2)
24	A:U s:w C (18/2)	-21.67(10.6)	-3.7(4.2)	11.59(12.3)	0.14(0.3)	0.15(0.3)	2.95(0.2)
25	U:U w:h T (17/0)	15.73(18.7)	-13.61(6.9)	-9.00(15.1)	-0.18(0.7)	2.59(0.3)	2.91(0.2)
26	A:C w:w C (14/0)	-10.02(12.4)	14.26(10.4)	-8.08(6.6)	0.05(0.9)	2.45(0.4)	2.44(0.4)
27	A:A w:w C (12/0)	-16.84(15.7)	21.66(13.2)	-15.44(12.8)	-0.77(0.2)	-2.14(0.9)	2.48(0.2)
28	A:A W:S C (86/0)	-4.49(13.8)	-29.14(10.1)	-12.72(12.2)	-0.38(0.4)	-2.51(0.5)	3.52(0.3)
29	A:U w:s T (69/1)	-1.57(21.0)	-58.71(12.1)	-18.61(14.6)	-0.33(0.9)	-0.4(0.5)	4.06(0.3)
30	A:C W:S C (61/0)	-4.44(22.8)	-34.74(10.3)	-21.29(14.5)	-0.47(0.6)	0.3(0.6)	4.23(0.4)
31	A:G S:S C (35/5)	1.6(23.2)	-15.89(20.7)	-8.36(30.3)	-0.13(1.0)	2.36(0.4)	3.82(0.5)
32	A:U W:S C (18/0)	-17.64(37.2)	-31.48(8.3)	-1.47(13.4)	-0.59(0.5)	0.44(0.4)	4.26(0.3)

33	A:C +:W C (29)	-2.59(18.0)	6.92(9.8)	-9.51(7.4)	0.04(0.4)	-2.44(0.7)	2.78(0.2)
34	C:U W:W C (22)	7.01(22.3)	-5.14(9.0)	-16.44(14.2)	0.14(0.7)	0.59(0.8)	2.94(0.3)
35	G:C S:S C (22)	0.42(21.9)	-22.19(7.1)	-13.71(22.0)	-0.63(1.0)	0.77(0.5)	4.16(0.4)
36	A:C S:W C (21)	0.96(21.6)	-27.6(5.6)	-17.53(22.0)	-0.55(0.6)	2.58(0.3)	3.48(0.1)
37	G:U S:S C (20)	21.75(7.0)	-21.75(4.2)	-14.57(12.5)	-1.00(0.6)	0.82(0.5)	4.19(0.2)
38	A:U h:s T (19)	-2.23(12.9)	-54.33(11.2)	10.28(14.2)	-0.89(0.8)	0.8(0.7)	3.65(0.4)
39	A:A s:s C (18)	-27.28(22.0)	-32.16(5.2)	-3.25(21.7)	-0.76(1.0)	-2.56(0.4)	2.92(0.3)
40	G:C S:W T (16)	0.88(25.3)	14.28(8.6)	-10.51(20.8)	-0.10(0.7)	1.77(0.5)	3.24(0.2)
41	G:C h:h T (12)	5.92(15.4)	-6.33(7.5)	1.19(6.5)	0.12(0.6)	3.35(0.7)	2.94(0.1)
42	G:U S:W C (11)	-15.28(4.7)	9.72(4.4)	21.46(9.3)	0.87(0.4)	0.51(0.3)	2.97(0.2)
43	G:C W:+ C (11)	0.42(9.1)	-2.44(11.2)	-7.48(10.0)	-0.08(0.5)	-2.3(0.5)	3.04(0.3)
44	A:C W:W T (10)	3.64(8.6)	8.63(12.9)	-27.68(8.8)	-0.3(0.8)	2.44(0.5)	2.81(0.2)

Table. SII: The co-ordinates of the final geometries of the basepairs after optimized through B3LYP/6-31G** method, along with the intra basepair parameters values, interaction energies associated with them and the source of initial structure for optimization.

```
HEADER   System 1: G:C W:W C Basepair optimized from PDB ID 1DFU:
HEADER   97(M)-79(N). Interaction energy -24.18Kcal/mole obtained from
HEADER   B3LYP/6-31G(2d,2p). Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-0.30, Open=-3.43,
HEADER   Propeller=2.21, Stagger=0.12 Shear=0.17 Stretch=2.92
ATOM      1  C4    G     1       3.244   0.411   0.014
ATOM      2  C5    G     1       2.804  -0.915  -0.006
ATOM      3  N7    G     1       3.872  -1.791   0.039
ATOM      4  C8    G     1       4.922  -1.015   0.084
ATOM      5  N9    G     1       4.613   0.337   0.070
ATOM      6  N3    G     1       2.517   1.546  -0.016
ATOM      7  C2    G     1       1.216   1.314  -0.073
ATOM      8  N1    G     1       0.674   0.054  -0.084
ATOM      9  C6    G     1       1.397  -1.151  -0.053
ATOM     10  C1'   G     1       5.534   1.453   0.137
ATOM     11  O6    G     1       0.799  -2.232  -0.064
ATOM     12  N2    G     1       0.350   2.350  -0.155
ATOM     13  H8    G     1       5.948  -1.351   0.125
ATOM     14  H1    G     1      -0.354  -0.041  -0.094
ATOM     15  HN21  G     1       0.748   3.260  -0.002
ATOM     16  HN22  G     1      -0.656   2.222  -0.036
ATOM     17  H1'A  G     1       4.963   2.374   0.022
ATOM     18  H1'B  G     1       6.052   1.475   1.100
ATOM     19  H1'C  G     1       6.276   1.390  -0.663
ATOM     20  O2    C     2      -2.557   2.011   0.066
ATOM     21  C2    C     2      -3.006   0.865   0.027
ATOM     22  N1    C     2      -4.412   0.705   0.043
ATOM     23  C6    C     2      -4.963  -0.538   0.020
ATOM     24  C5    C     2      -4.197  -1.655  -0.026
ATOM     25  C4    C     2      -2.773  -1.470  -0.047
ATOM     26  N3    C     2      -2.234  -0.248  -0.028
ATOM     27  C1'   C     2      -5.226   1.913   0.122
ATOM     28  N4    C     2      -1.953  -2.524  -0.090
ATOM     29  H6    C     2      -6.045  -0.578   0.040
ATOM     30  H5    C     2      -4.643  -2.639  -0.045
ATOM     31  HN41  C     2      -0.922  -2.405  -0.089
ATOM     32  HN42  C     2      -2.344  -3.449  -0.098
ATOM     33  H1'A  C     2      -6.278   1.642   0.031
ATOM     34  H1'B  C     2      -5.058   2.422   1.073
ATOM     35  H1'C  C     2      -4.949   2.600  -0.679
ENDMODEL

HEADER   System 2: A:U W:W C Basepair optimized from PDB ID 1ASY:
HEADER   607(S)-666(S). Interaction energy is -11.64Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p). Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-0.98, Open=0.03,
HEADER   Propeller=0.35, Stagger=0.0, Shear=0.09, Stretch=2.86
ATOM      1  N1    A     1       0.626   0.112   0.023
ATOM      2  C6    A     1       1.433  -0.973   0.013
```

```
ATOM      3  C5    A     1       2.826  -0.750   0.006
ATOM      4  C4    A     1       3.241   0.581   0.007
ATOM      5  N3    A     1       2.459   1.671   0.017
ATOM      6  C2    A     1       1.170   1.342   0.025
ATOM      7  N9    A     1       4.617   0.529  -0.004
ATOM      8  C8    A     1       4.943  -0.811  -0.013
ATOM      9  N7    A     1       3.906  -1.613  -0.006
ATOM     10  C1'   A     1       5.521   1.662  -0.042
ATOM     11  N6    A     1       0.897  -2.201   0.009
ATOM     12  H8    A     1       5.975  -1.134  -0.022
ATOM     13  H2    A     1       0.450   2.156   0.034
ATOM     14  HN61  A     1       1.522  -2.989  -0.003
ATOM     15  HN62  A     1      -0.117  -2.330   0.008
ATOM     16  H1'A  A     1       4.930   2.570   0.086
ATOM     17  H1'B  A     1       6.256   1.596   0.763
ATOM     18  H1'C  A     1       6.043   1.712  -1.001
ATOM     19  C6    U     2      -4.905  -0.403  -0.011
ATOM     20  C5    U     2      -4.163  -1.530  -0.007
ATOM     21  C4    U     2      -2.717  -1.432   0.004
ATOM     22  N3    U     2      -2.224  -0.133   0.017
ATOM     23  C2    U     2      -2.961   1.030   0.009
ATOM     24  N1    U     2      -4.352   0.851   0.001
ATOM     25  C1'   U     2      -5.165   2.062  -0.045
ATOM     26  O2    U     2      -2.468   2.143   0.008
ATOM     27  O4    U     2      -1.959  -2.401   0.002
ATOM     28  H6    U     2      -5.988  -0.427  -0.022
ATOM     29  H5    U     2      -4.614  -2.510  -0.013
ATOM     30  H3    U     2      -1.184  -0.017   0.022
ATOM     31  H1'A  U     2      -6.214   1.788   0.066
ATOM     32  H1'B  U     2      -4.873   2.738   0.759
ATOM     33  H1'C  U     2      -5.022   2.583  -0.994
ENDMODEL

HEADER   System 3: G:U W:W C Basepair optimized from PDB ID 1ASY:
HEADER   610(S)-625(S). Interaction energy is -12.20Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p). Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=3.94, Open = 4.11,
HEADER   Propeller=-1.30, Stagger=-0.15, Shear=-2.42, Stretch=2.84
ATOM      1  N7    G     1       8.120   0.179   3.234
ATOM      2  C5    G     1       7.509   0.085   2.000
ATOM      3  C4    G     1       8.461   0.087   0.977
ATOM      4  N9    G     1       9.675   0.182   1.604
ATOM      5  C8    G     1       9.397   0.235   2.961
ATOM      6  N3    G     1       8.276   0.019  -0.364
ATOM      7  C2    G     1       7.005  -0.071  -0.680
ATOM      8  N1    G     1       5.992  -0.080   0.231
ATOM      9  C6    G     1       6.126   0.009   1.633
ATOM     10  O6    G     1       5.114   0.017   2.332
ATOM     11  N2    G     1       6.631  -0.214  -1.993
ATOM     12  C1'   G     1      10.963   0.247   0.963
ATOM     13  H8    G     1      10.194   0.311   3.687
ATOM     14  H1    G     1       5.023  -0.115  -0.108
ATOM     15  HN21  G     1       7.337   0.067  -2.656
ATOM     16  HN22  G     1       5.687   0.061  -2.226
ATOM     17  H1'A  G     1      11.742   0.318   1.720
ATOM     18  H1'B  G     1      11.117  -0.651   0.366
ATOM     19  H1'C  G     1      11.002   1.123   0.317
```

```
ATOM     20  C6    U     2       0.000   0.000   0.000
ATOM     21  C5    U     2       0.000   0.000   1.346
ATOM     22  C4    U     2       1.259   0.000   2.080
ATOM     23  N3    U     2       2.401  -0.002   1.245
ATOM     24  C2    U     2       2.405   0.000  -0.119
ATOM     25  N1    U     2       1.163  -0.004  -0.739
ATOM     26  C1    U     2       1.154   0.028  -2.198
ATOM     27  O2    U     2       3.426   0.004  -0.811
ATOM     28  O4    U     2       1.372   0.002   3.287
ATOM     29  H6    U     2      -0.911   0.001  -0.585
ATOM     30  H5    U     2      -0.918  -0.001   1.913
ATOM     31  H3    U     2       3.324   0.001   1.713
ATOM     32  H1'A  U     2       0.130  -0.097  -2.550
ATOM     33  H1'B  U     2       1.548   0.978  -2.565
ATOM     34  H1'C  U     2       1.775  -0.776  -2.593
ENDMODEL

HEADER   System 4: A:G H:S T Basepair optimized from PDB ID 1MZP :
HEADER   21(B)-44(B). Interaction energy is -8.06Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p). Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=6.42, Open =-20.30,
HEADER   Propeller=-40.90, Stagger=0.05, Shear=1.95, Stretch=3.24
ATOM      1  C4    A     1       4.039   0.006  -0.041
ATOM      2  C5    A     1       2.659   0.015   0.176
ATOM      3  N7    A     1       2.112   1.220  -0.237
ATOM      4  C8    A     1       3.138   1.903  -0.691
ATOM      5  N9    A     1       4.330   1.229  -0.609
ATOM      6  N3    A     1       4.893  -0.981   0.243
ATOM      7  C2    A     1       4.258  -2.020   0.790
ATOM      8  N1    A     1       2.952  -2.167   1.048
ATOM      9  C6    A     1       2.114  -1.159   0.741
ATOM     10  C1'   A     1       5.651   1.698  -0.989
ATOM     11  N6    A     1       0.799  -1.310   1.011
ATOM     28  H8    A     1       3.085   2.900  -1.104
ATOM     29  H2    A     1       4.882  -2.868   1.059
ATOM     30  HN61  A     1       0.095  -0.715   0.577
ATOM     31  HN62  A     1       0.519  -2.224   1.330
ATOM     32  H1'A  A     1       6.282   0.827  -1.164
ATOM     33  H1'B  A     1       5.585   2.290  -1.903
ATOM     34  H1'C  A     1       6.099   2.305  -0.197
ATOM     12  N2    A     2      -0.646   2.307   0.183
ATOM     13  C2    A     2      -1.711   1.465   0.141
ATOM     14  N1    A     2      -2.937   1.979   0.468
ATOM     15  C6    A     2      -4.202   1.297   0.444
ATOM     16  C5    A     2      -4.009  -0.053  -0.009
ATOM     17  C4    A     2      -2.720  -0.474  -0.328
ATOM     18  N3    A     2      -1.549   0.213  -0.248
ATOM     19  N9    G     2      -2.853  -1.771  -0.753
ATOM     20  C8    G     2      -4.204  -2.063  -0.663
ATOM     21  N7    G     2      -4.923  -1.064  -0.224
ATOM     22  C1'   G     2      -1.796  -2.647  -1.223
ATOM     23  O6    G     2      -5.202   1.901   0.770
ATOM     24  H8    G     2      -4.580  -3.036  -0.942
ATOM     25  H1    G     2      -3.021   2.957   0.713
ATOM     26  HN21  G     2       0.283   1.892   0.045
ATOM     27  HN22  G     2      -0.691   3.088   0.818
ATOM     35  H1'A  G     2      -0.916  -2.044  -1.444
```

```
ATOM     36  H1'B  G     2      -1.531  -3.395  -0.469
ATOM     37  H1'C  G     2      -2.113  -3.161  -2.132
ENDMODEL

HEADER   System 5: A:U H:W T Basepair optimized from PDB ID 1ASY:
HEADER   614(S)-608(S. Interaction energy is -11.39 Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p). Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-3.2O, Open =-7.49,
HEADER   Propeller=1.52, Stagger=0.00, Shear=0.15, Stretch=2.79
ATOM      1  N3    U     1       1.929   0.381   0.052
ATOM      2  C2    U     1       2.595  -0.811   0.001
ATOM      3  N1    U     1       3.987  -0.713  -0.034
ATOM      4  C6    U     1       4.602   0.517  -0.033
ATOM      5  C5    U     1       3.927   1.683   0.009
ATOM      6  C4    U     1       2.474   1.669   0.049
ATOM      7  O2    U     1       2.035  -1.902  -0.013
ATOM      8  C1'   U     1       4.746  -1.958  -0.113
ATOM      9  O4    U     1       1.750   2.654   0.076
ATOM     21  H6    U     1       5.685   0.484  -0.066
ATOM     22  H5    U     1       4.439   2.634   0.011
ATOM     23  H3    U     1       0.885   0.329   0.067
ATOM     31  H1'A  U     1       5.804  -1.723  -0.011
ATOM     32  H1'B  U     1       4.438  -2.634   0.684
ATOM     33  H1'C  U     1       4.572  -2.456  -1.070
ATOM     10  N7    A     2      -0.859   0.497   0.052
ATOM     11  C8    A     2      -1.367   1.708   0.017
ATOM     12  N9    A     2      -2.738   1.711  -0.024
ATOM     13  C4    A     2      -3.132   0.386  -0.018
ATOM     14  C5    A     2      -1.948  -0.350   0.029
ATOM     15  C6    A     2      -2.080  -1.755   0.042
ATOM     16  N1    A     2      -3.321  -2.275   0.011
ATOM     17  C2    A     2      -4.367  -1.438  -0.028
ATOM     18  N3    A     2      -4.375  -0.101  -0.048
ATOM     19  C1'   A     2      -3.613   2.868  -0.100
ATOM     20  N6    A     2      -1.020  -2.586   0.091
ATOM     24  H8    A     2      -0.765   2.605   0.022
ATOM     25  H2    A     2      -5.342  -1.916  -0.049
ATOM     26  HN61  A     2      -0.064  -2.251   0.050
ATOM     27  HN62  A     2      -1.200  -3.575   0.046
ATOM     28  H1'A  A     2      -4.640   2.523   0.018
ATOM     29  H1'B  A     2      -3.377   3.577   0.696
ATOM     30  H1'C  A     2      -3.514   3.367  -1.067
ENDMODEL

HEADER   System 6: A:G W:W C Basepair optimized from PDB ID 1QVG:
HEADER   2596(O)-2582(O).Interaction energy is -13.60Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=6.14, Open =-2.93,
HEADER   Propeller=-12.80, Stagger=-0.21, Shear=-0.01,  Stretch=2.94
ATOM      1  C4    A     1       4.172  -0.482   0.066
ATOM      2  N9    A     1       5.524  -0.266  -0.068
ATOM      3  C8    A     1       5.669   1.094  -0.250
ATOM      4  N7    A     1       4.536   1.755  -0.244
ATOM      5  C5    A     1       3.584   0.776  -0.050
ATOM      6  N3    A     1       3.540  -1.649   0.267
ATOM      7  C2    A     1       2.226  -1.472   0.334
ATOM      8  N1    A     1       1.514  -0.336   0.219
```

```
ATOM      9  C6    A     1       2.174   0.834   0.029
ATOM     10  C1'   A     1       6.557  -1.285  -0.045
ATOM     11  N6    A     1       1.493   1.977  -0.086
ATOM     12  H8    A     1       6.646   1.537  -0.380
ATOM     13  H2    A     1       1.637  -2.369   0.508
ATOM     14  HN61  A     1       2.020   2.824  -0.223
ATOM     15  HN62  A     1       0.473   2.015   0.029
ATOM     16  H1'A  A     1       6.067  -2.249   0.089
ATOM     17  H1'B  A     1       7.113  -1.291  -0.985
ATOM     18  H1'C  A     1       7.252  -1.117   0.782
ATOM     19  N1    G     2      -1.427  -0.274   0.048
ATOM     20  C6    G     2      -2.025   1.005   0.113
ATOM     21  C5    G     2      -3.453   0.903   0.057
ATOM     22  C4    G     2      -4.022  -0.365  -0.053
ATOM     23  N3    G     2      -3.404  -1.566  -0.146
ATOM     24  C2    G     2      -2.097  -1.454  -0.090
ATOM     25  N9    G     2      -5.378  -0.160  -0.079
ATOM     26  C8    G     2      -5.554   1.209   0.017
ATOM     27  N7    G     2      -4.432   1.876   0.096
ATOM     28  C1'   G     2      -6.397  -1.193  -0.140
ATOM     29  O6    G     2      -1.322   2.008   0.207
ATOM     30  N2    G     2      -1.319  -2.592  -0.125
ATOM     31  H8    G     2      -6.545   1.639   0.022
ATOM     32  H1    G     2      -0.394  -0.297   0.143
ATOM     33  HN21  G     2      -1.840  -3.399  -0.438
ATOM     34  HN22  G     2      -0.424  -2.492  -0.582
ATOM     35  H1'A  G     2      -5.895  -2.138  -0.344
ATOM     36  H1'B  G     2      -6.934  -1.272   0.808
ATOM     37  H1'C  G     2      -7.112  -0.981  -0.938
ENDMODEL

HEADER   System 7: A:A H:H T Basepair optimized from PDB ID 1ASY:
HEADER   609(R)-623(R).Interaction energy is -8.49 Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p). Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-0.06, Open=-0.06,
HEADER   Propeller=-32.10, Stagger=0.01, Shear=2.67, Stretch= 2.88
ATOM      1  C4    A     1      -3.863   0.122   0.120
ATOM      2  C5    A     1      -2.511  -0.182  -0.060
ATOM      3  N7    A     1      -1.727   0.930   0.202
ATOM      4  C8    A     1      -2.588   1.866   0.530
ATOM      5  N9    A     1      -3.895   1.446   0.505
ATOM      6  N3    A     1      -4.904  -0.697  -0.049
ATOM      7  C2    A     1      -4.499  -1.910  -0.431
ATOM      8  N1    A     1      -3.255  -2.358  -0.635
ATOM      9  C6    A     1      -2.221  -1.510  -0.450
ATOM     10  C1'   A     1      -5.096   2.216   0.779
ATOM     11  N6    A     1      -0.974  -1.966  -0.667
ATOM     12  H8    A     1      -2.329   2.878   0.804
ATOM     13  H2    A     1      -5.288  -2.640  -0.598
ATOM     14  HN61  A     1      -0.144  -1.458  -0.359
ATOM     15  HN62  A     1      -0.893  -2.952  -0.857
ATOM     16  H1'A  A     1      -5.933   1.518   0.780
ATOM     17  H1'B  A     1      -5.030   2.704   1.753
ATOM     18  H1'C  A     1      -5.262   2.972   0.006
ATOM     19  N7    A     2       1.725  -0.931   0.200
ATOM     20  C8    A     2       2.583  -1.872   0.520
ATOM     21  N9    A     2       3.891  -1.454   0.508
```

```
ATOM     22  C4    A     2       3.862  -0.124   0.141
ATOM     23  C5    A     2       2.512   0.184  -0.041
ATOM     24  N3    A     2       4.905   0.696  -0.011
ATOM     25  C2    A     2       4.503   1.914  -0.379
ATOM     26  N1    A     2       3.261   2.366  -0.583
ATOM     27  C6    A     2       2.225   1.517  -0.416
ATOM     28  C1'   A     2       5.089  -2.228   0.780
ATOM     29  N6    A     2       0.979   1.977  -0.632
ATOM     30  H8    A     2       2.321  -2.888   0.779
ATOM     31  H2    A     2       5.293   2.645  -0.532
ATOM     32  HN61  A     2       0.147   1.465  -0.337
ATOM     33  HN62  A     2       0.899   2.965  -0.809
ATOM     34  H1'A  A     2       5.928  -1.533   0.780
ATOM     35  H1'B  A     2       5.023  -2.717   1.754
ATOM     36  H1'C  A     2       5.251  -2.984   0.006
ENDMODEL

HEADER   System 8: G:A S:W T Basepair optimized from PDB ID 1FFK:
HEADER   166(O)-924(O).Interaction energy is -8.98Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p). Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=6.74, Open=-18.40,
HEADER   Propeller=-17.40, Stagger=-0.07, Shear=1.82, Stretch=3.32
ATOM      1  C4    G     1       2.999   0.631  -0.023
ATOM      2  C5    G     1       4.315   0.179  -0.093
ATOM      3  N7    G     1       5.189   1.235  -0.250
ATOM      4  C8    G     1       4.421   2.291  -0.275
ATOM      5  N9    G     1       3.074   1.995  -0.145
ATOM      6  N3    G     1       1.854  -0.086   0.120
ATOM      7  C2    G     1       2.061  -1.389   0.193
ATOM      8  N1    G     1       3.316  -1.932   0.132
ATOM      9  C6    G     1       4.564  -1.234  -0.008
ATOM     10  C1'   G     1       1.969   2.932  -0.113
ATOM     11  O6    G     1       5.596  -1.871  -0.037
ATOM     12  N2    G     1       1.014  -2.233   0.375
ATOM     13  H8    G     1       4.757   3.312  -0.385
ATOM     14  H1    G     1       3.430  -2.933   0.222
ATOM     15  HN21  G     1       0.068  -1.867   0.203
ATOM     16  HN22  G     1       1.155  -3.208   0.167
ATOM     17  H1'A  G     1       1.153   2.568  -0.740
ATOM     18  H1'B  G     1       1.600   3.072   0.908
ATOM     19  H1'C  A     2       2.308   3.894  -0.499
ATOM     20  N1    A     2      -1.760  -1.201  -0.045
ATOM     21  C6    A     2      -1.985   0.111   0.197
ATOM     22  C5    A     2      -3.318   0.569   0.164
ATOM     23  C4    A     2      -4.296  -0.386  -0.118
ATOM     24  N3    A     2      -4.100  -1.688  -0.362
ATOM     25  C2    A     2      -2.809  -2.000  -0.305
ATOM     26  N9    A     2      -5.488   0.302  -0.104
ATOM     27  C8    A     2      -5.163   1.610   0.185
ATOM     28  N7    A     2      -3.880   1.818   0.352
ATOM     29  C1'   A     2      -6.806  -0.262  -0.336
ATOM     30  N6    A     2      -0.949   0.922   0.464
ATOM     31  H8    A     2      -5.929   2.371   0.255
ATOM     32  H2    A     2      -2.561  -3.041  -0.492
ATOM     33  HN61  A     2      -1.142   1.896   0.626
ATOM     34  HN62  A     2       0.016   0.589   0.396
```

```
ATOM     35  H1'A  A     2      -6.673  -1.253  -0.769
ATOM     36  H1'B  A     2      -7.367  -0.356   0.598
ATOM     37  H1'C  A     2      -7.368   0.364  -1.032
ENDMODEL

HEADER   System 9: A:A H:W T Basepair optimized from PDB ID 1FFK:
HEADER   460(O)-455(O).Interaction energy -9.61Kcal/mole obtained from
HEADER   B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-1.40, Open=0.95,
HEADER   Propeller=17.58, Stagger=0.0, Shear= 2.50, Stretch= 2.94
ATOM      1  C4    A     1      -4.144   0.207  -0.060
ATOM      2  C5    A     1      -2.795  -0.139   0.049
ATOM      3  N7    A     1      -2.000   0.995  -0.018
ATOM      4  C8    A     1      -2.852   1.983  -0.165
ATOM      5  N9    A     1      -4.162   1.581  -0.200
ATOM      6  N3    A     1      -5.196  -0.614  -0.029
ATOM      7  C2    A     1      -4.805  -1.881   0.128
ATOM      8  N1    A     1      -3.567  -2.373   0.237
ATOM      9  C6    A     1      -2.521  -1.521   0.197
ATOM     10  C1'   A     1      -5.351   2.401  -0.353
ATOM     11  N6    A     1      -1.281  -2.024   0.314
ATOM     12  H8    A     1      -2.580   3.026  -0.255
ATOM     13  H2    A     1      -5.602  -2.620   0.169
ATOM     14  HN21  A     1      -0.434  -1.469   0.167
ATOM     15  HN22  A     1      -1.209  -3.028   0.355
ATOM     16  H1'A  A     1      -6.213   1.738  -0.281
ATOM     17  H1'B  A     1      -5.407   3.153   0.437
ATOM     18  H1'C  A     1      -5.361   2.897  -1.326
ATOM     19  N6    A     2       0.928   1.451   0.378
ATOM     20  C6    A     2       1.836   0.493   0.140
ATOM     21  C5    A     2       3.225   0.749   0.125
ATOM     22  C4    A     2       4.058  -0.341  -0.122
ATOM     23  N3    A     2       3.679  -1.606  -0.348
ATOM     24  C2    A     2       2.355  -1.723  -0.308
ATOM     25  N1    A     2       1.428  -0.776  -0.082
ATOM     26  N9    A     2       5.338   0.163  -0.079
ATOM     27  C8    A     2       5.202   1.512   0.183
ATOM     28  N7    A     2       3.957   1.905   0.313
ATOM     29  C1'   A     2       6.559  -0.595  -0.281
ATOM     30  H8    A     2       6.070   2.150   0.270
ATOM     31  H2    A     2       1.961  -2.721  -0.483
ATOM     32  HN61  A     2       1.265   2.394   0.481
ATOM     33  HN62  A     2      -0.073   1.272   0.258
ATOM     34  H1'A  A     2       6.303  -1.653  -0.233
ATOM     35  H1'B  A     2       7.004  -0.381  -1.256
ATOM     36  H1'C  A     2       7.283  -0.363   0.503
ENDMODEL

HEADER   System 10: A:U H:W C Basepair optimized from PDB ID 1FFZ:
HEADER   2470(A)-2277(A). Interaction energy -12.06Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p). Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-0.24, Open=2.23,
HEADER   Propeller=-2.63, Stagger=-0.01, Shear=-0.13, Stretch=2.79
ATOM      1  C4    A     1       3.054  -0.683   0.008
ATOM      2  N9    A     1       2.457  -1.930   0.029
ATOM      3  C8    A     1       1.104  -1.708   0.028
ATOM      4  N7    A     1       0.793  -0.432   0.007
```

```
ATOM      5  C5    A     1       2.004   0.235  -0.006
ATOM      6  N3    A     1       4.361  -0.406  -0.004
ATOM      7  C2    A     1       4.565   0.914  -0.032
ATOM      8  N1    A     1       3.672   1.910  -0.046
ATOM      9  C6    A     1       2.357   1.603  -0.033
ATOM     10  C1'   A     1       3.161  -3.201   0.069
ATOM     11  N6    A     1       1.463   2.606  -0.050
ATOM     12  H8    A     1       0.380  -2.509   0.038
ATOM     13  H2    A     1       5.606   1.228  -0.045
ATOM     14  HN61  A     1       0.457   2.462  -0.011
ATOM     15  HN62  A     1       1.832   3.543  -0.054
ATOM     16  H1'A  A     1       4.222  -2.984  -0.046
ATOM     17  H1'B  A     1       2.999  -3.708   1.023
ATOM     18  H1'C  A     1       2.831  -3.849  -0.746
ATOM     19  N3    U     2      -1.921   0.246   0.013
ATOM     20  C2    U     2      -2.715  -0.872  -0.019
ATOM     21  N1    U     2      -4.092  -0.622  -0.007
ATOM     22  C6    U     2      -4.579   0.660   0.027
ATOM     23  C5    U     2      -3.776   1.747   0.056
ATOM     24  C4    U     2      -2.335   1.572   0.045
ATOM     25  C1'   U     2      -4.966  -1.788  -0.080
ATOM     26  O2    U     2      -2.281  -2.012  -0.055
ATOM     27  O4    U     2      -1.517   2.488   0.060
ATOM     28  H6    U     2      -5.659   0.740   0.030
ATOM     29  H5    U     2      -4.177   2.748   0.086
ATOM     30  H3    U     2      -0.892   0.059   0.007
ATOM     31  H1'A  U     2      -6.000  -1.471   0.059
ATOM     32  H1'B  U     2      -4.865  -2.281  -1.050
ATOM     33  H1'C  U     2      -4.694  -2.505   0.694
ENDMODEL

HEADER   System 11: U:U W:W C Basepair optimized from PDB ID 2QAO:
HEADER   1856(B)-1886(B).Interaction energy is -9.64Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=2.27, Open=-0.66,
HEADER   Propeller=-6.57, Stagger=0.03, Shear=2.55, Stretch= 2.85
ATOM      1  C6    U     1      32.460 213.440 -81.410
ATOM      2  N1    U     1      31.652 214.547 -81.299
ATOM      3  C2    U     1      31.802 215.629 -82.160
ATOM      4  N3    U     1      32.791 215.513 -83.095
ATOM      5  C4    U     1      33.661 214.419 -83.281
ATOM      6  C5    U     1      33.429 213.332 -82.339
ATOM      7  C1'   U     1      30.605 214.648 -80.286
ATOM      8  O2    U     1      31.068 216.608 -82.052
ATOM      9  O4    U     1      34.502 214.435 -84.156
ATOM     22  H6    U     1      32.257 212.655 -80.692
ATOM     23  H5    U     1      34.051 212.453 -82.411
ATOM     24  H3    U     1      32.906 216.325 -83.720
ATOM     25  H1'A  U     1      30.602 213.732 -79.697
ATOM     26  H1'B  U     1      30.788 215.503 -79.634
ATOM     27  H1'C  U     1      29.631 214.785 -80.759
ATOM     10  N3    U     2      31.086 218.868 -83.796
ATOM     11  C2    U     2      30.120 219.850 -83.702
ATOM     12  N1    U     2      30.263 220.900 -84.619
ATOM     13  C6    U     2      31.294 220.922 -85.521
ATOM     14  C5    U     2      32.226 219.949 -85.594
ATOM     15  C4    U     2      32.152 218.820 -84.689
```

```
ATOM     16  C1'   U     2      29.258 221.956 -84.555
ATOM     17  O2    U     2      29.209 219.830 -82.901
ATOM     18  O4    U     2      32.945 217.881 -84.681
ATOM     19  H6    U     2      31.309 221.782 -86.179
ATOM     20  H5    U     2      33.031 219.982 -86.313
ATOM     21  H3    U     2      31.007 218.089 -83.128
ATOM     28  H1'A  U     2      29.492 222.708 -85.308
ATOM     29  H1'B  U     2      28.265 221.545 -84.741
ATOM     30  H1'C  U     2      29.253 222.414 -83.565
ENDMODEL

HEADER   System 12: A:C H:W T  Basepair optimized from PDB ID 1JSE:
HEADER   1055(A)-1200(A).Interaction energy is -12.71Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-0.35, Open=-2.73,
HEADER   Propeller=0.09, Stagger=0.0,  Shear=2.41, Stretch= 2.93
ATOM     12  C1'   C     1       5.588   0.873   0.684
ATOM     13  N1    C     1       4.490   0.142   0.066
ATOM     14  C2    C     1       3.169   0.555   0.409
ATOM     15  O2    C     1       3.037   1.485   1.190
ATOM     16  N3    C     1       2.130  -0.119  -0.161
ATOM     17  C4    C     1       2.335  -1.122  -1.005
ATOM     18  N4    C     1       1.256  -1.733  -1.521
ATOM     19  C5    C     1       3.657  -1.553  -1.363
ATOM     20  C6    C     1       4.692  -0.883  -0.796
ATOM     27  H1'A  C     1       5.529   1.930   0.422
ATOM     28  H1'B  C     1       5.525   0.796   1.770
ATOM     29  H1'C  C     1       6.534   0.456   0.336
ATOM     30  HN41  C     1       0.311  -1.424  -1.264
ATOM     31  H5    C     1       3.829  -2.370  -2.049
ATOM     32  H6    C     1       5.726  -1.135  -1.005
ATOM     33  HN42  C     1       1.373  -2.497  -2.164
ATOM      1  C1'   A     2      -5.104  -1.444  -1.260
ATOM      2  N9    A     2      -3.767  -1.011  -0.898
ATOM      3  C8    A     2      -2.567  -1.515  -1.329
ATOM      4  N7    A     2      -1.525  -0.902  -0.816
ATOM      5  C5    A     2      -2.067   0.074   0.009
ATOM      6  C6    A     2      -1.507   1.072   0.849
ATOM      7  N6    A     2      -0.194   1.260   1.002
ATOM      8  N1    A     2      -2.361   1.872   1.528
ATOM      9  C2    A     2      -3.675   1.690   1.380
ATOM     10  N3    A     2      -4.324   0.795   0.629
ATOM     11  C4    A     2      -3.461   0.018  -0.031
ATOM     21  H1'A  A     2      -5.807  -0.820  -0.709
ATOM     22  H1'B  A     2      -5.262  -2.490  -0.988
ATOM     23  H1'C  A     2      -5.279  -1.320  -2.331
ATOM     24  H8    A     2      -2.523  -2.340  -2.025
ATOM     25  HN61  A     2       0.114   1.993   1.620
ATOM     26  H2    A     2      -4.304   2.366   1.954
ATOM     34  HN62  A     2       0.520   0.702   0.530
ENDMODEL

HEADER   System 13: G:C W:W T Basepair optimized from PDB ID 1H4S:
HEADER   15(T)-48(T).Interaction energy is -11.83Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p). Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-17.61, Open=13.42,
HEADER   Propeller=-37.98, Stagger=0.06, Shear=-2.54,Stretch=3.02
```

```
ATOM      1  C6    G     1       0.076   0.300  -0.043
ATOM      2  C5    G     1       0.048   0.374   1.394
ATOM      3  C4    G     1       1.175  -0.032   2.105
ATOM      4  N3    G     1       2.360  -0.494   1.640
ATOM      5  C2    G     1       2.381  -0.571   0.325
ATOM      6  N1    G     1       1.336  -0.217  -0.476
ATOM      7  N9    G     1       0.858   0.146   3.430
ATOM      8  C8    G     1      -0.433   0.643   3.447
ATOM      9  N7    G     1      -0.948   0.794   2.255
ATOM     10  C1'   G     1       1.715  -0.149   4.560
ATOM     11  N2    G     1       3.493  -1.074  -0.301
ATOM     12  O6    G     1      -0.770   0.596  -0.866
ATOM     26  H8    G     1      -0.928   0.872   4.379
ATOM     27  H1    G     1       1.431  -0.355  -1.484
ATOM     28  HN21  G     1       4.287  -1.132   0.317
ATOM     29  HN22  G     1       3.697  -0.727  -1.235
ATOM     30  H1'A  G     1       2.675  -0.484   4.170
ATOM     31  H1'B  G     1       1.869   0.742   5.174
ATOM     32  H1'C  G     1       1.288  -0.939   5.182
ATOM     13  O2    C     2       1.963  -0.694  -3.296
ATOM     14  C2    C     2       2.948  -0.238  -3.865
ATOM     15  N1    C     2       2.843   0.040  -5.251
ATOM     16  C6    C     2       3.895   0.545  -5.935
ATOM     17  C5    C     2       5.082   0.803  -5.325
ATOM     18  C4    C     2       5.154   0.516  -3.927
ATOM     19  N3    C     2       4.135   0.019  -3.244
ATOM     20  C1'   C     2       1.553  -0.228  -5.883
ATOM     21  N4    C     2       6.314   0.725  -3.254
ATOM     22  HN41  C     2       6.279   0.670  -2.249
ATOM     23  HN42  C     2       7.037   1.290  -3.664
ATOM     24  H5    C     2       5.920   1.202  -5.877
ATOM     25  H6    C     2       3.734   0.731  -6.990
ATOM     33  H1'A  C     2       0.769   0.334  -5.373
ATOM     34  H1'B  C     2       1.605   0.066  -6.931
ATOM     35  H1'C  C     2       1.312  -1.289  -5.803
ENDMODEL


HEADER   System 14: A:A W:W T Basepair optimized from PDB ID 1QVG:
HEADER   2566(O)-2699(O).Interaction energy is -10.27Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=4.40, Open =0.0,
HEADER   Propeller=-12.10, Stagger=0.0, Shear=2.27, Stretch= 2.98
ATOM      1  N9    A     1      -5.610   0.097  -0.100
ATOM      2  C8    A     1      -5.490   1.466   0.035
ATOM      3  N7    A     1      -4.250   1.881   0.147
ATOM      4  C5    A     1      -3.506   0.720   0.082
ATOM      5  C4    A     1      -4.325  -0.396  -0.073
ATOM      6  N3    A     1      -3.934  -1.675  -0.172
ATOM      7  C2    A     1      -2.610  -1.777  -0.103
ATOM      8  N1    A     1      -1.695  -0.803   0.044
ATOM      9  C6    A     1      -2.115   0.480   0.138
ATOM     10  N6    A     1      -1.216   1.463   0.291
ATOM     11  C1'   A     1      -6.822  -0.685  -0.255
ATOM     12  H2    A     1      -2.205  -2.783  -0.175
ATOM     13  H8    A     1      -6.364   2.100   0.046
ATOM     14  HN61  A     1      -1.559   2.409   0.304
```

```
ATOM     15  HN62  A     1      -0.210   1.273   0.219
ATOM     16  H1'A  A     1      -6.549  -1.738  -0.181
ATOM     17  H1'B  A     1      -7.538  -0.443   0.533
ATOM     18  H1'C  A     1      -7.286  -0.506  -1.229
ATOM     19  N6    A     2       1.216  -1.461   0.292
ATOM     20  C6    A     2       2.115  -0.479   0.136
ATOM     21  C5    A     2       3.506  -0.720   0.078
ATOM     22  C4    A     2       4.325   0.396  -0.080
ATOM     23  N3    A     2       3.934   1.674  -0.181
ATOM     24  C2    A     2       2.610   1.777  -0.111
ATOM     25  N1    A     2       1.696   0.803   0.039
ATOM     26  N9    A     2       5.610  -0.098  -0.106
ATOM     27  C8    A     2       5.490  -1.466   0.032
ATOM     28  N7    A     2       4.250  -1.881   0.146
ATOM     29  C1'   A     2       6.822   0.684  -0.264
ATOM     30  H2    A     2       2.205   2.783  -0.185
ATOM     31  H8    A     2       6.364  -2.101   0.044
ATOM     32  HN61  A     2       1.558  -2.407   0.308
ATOM     33  HN62  A     2       0.210  -1.272   0.221
ATOM     34  H1'A  A     2       6.550   1.737  -0.190
ATOM     35  H1'B  A     2       7.538   0.442   0.525
ATOM     36  H1'C  A     2       7.285   0.505  -1.238
ENDMODEL

HEADER   System 15: A:U W:W T Basepair optimized from PDB ID 1ASZ:
HEADER   615(R)-648(R). Interaction energy -10.51Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-0.67, Open=-7.96,
HEADER   Propeller=-0.57, Stagger=0.03, Shear=-0.06, Stretch= 2.81
ATOM      1  N7    A     1      -3.743  -1.798  -0.013
ATOM      2  C5    A     1      -2.732  -0.858   0.004
ATOM      3  C4    A     1      -3.250   0.439   0.012
ATOM      4  N9    A     1      -4.617   0.283   0.001
ATOM      5  C8    A     1      -4.841  -1.079  -0.016
ATOM      6  N3    A     1      -2.560   1.588   0.027
ATOM      7  C2    A     1      -1.250   1.366   0.033
ATOM      8  N1    A     1      -0.615   0.179   0.025
ATOM      9  C6    A     1      -1.326  -0.967   0.010
ATOM     10  N6    A     1      -0.667  -2.138   0.001
ATOM     11  C1'   A     1      -5.595   1.356  -0.032
ATOM     21  H8    U     2      -5.846  -1.474  -0.028
ATOM     22  H2    U     2      -0.592   2.229   0.043
ATOM     23  HN61  U     2      -1.193  -2.995  -0.017
ATOM     24  HN62  U     2       0.350  -2.158   0.001
ATOM     28  H1'A  U     2      -5.057   2.296   0.090
ATOM     29  H1'B  U     2      -6.125   1.371  -0.988
ATOM     30  H1'C  U     2      -6.318   1.245   0.778
ATOM     12  N3    A     1       2.185   0.376  -0.008
ATOM     13  C2    A     1       2.907  -0.783  -0.007
ATOM     14  N1    A     1       4.293  -0.627  -0.018
ATOM     15  C6    A     1       4.860   0.626  -0.018
ATOM     16  C5    A     1       4.133   1.761  -0.015
ATOM     17  C4    A     1       2.680   1.685  -0.007
ATOM     18  C1'   A     1       5.100  -1.843   0.018
ATOM     19  O2    U     2       2.399  -1.901   0.004
ATOM     20  O4    U     2       1.920   2.640   0.001
ATOM     25  H6    U     2       5.944   0.637  -0.021
```

```
ATOM     26  H5    U     2       4.600   2.734  -0.017
ATOM     27  H3    U     2       1.141   0.275   0.004
ATOM     31  H1'A  U     2       6.149  -1.574  -0.100
ATOM     32  H1'B  U     2       4.962  -2.367   0.966
ATOM     33  H1'C  U     2       4.801  -2.516  -0.787
ENDMODEL

HEADER   System 16: G:G H:W C Basepair optimized from PDB ID 2QAL:
HEADER   1053(A)-1057(A).Interaction energy is -11.33Kcal/mole
HEADER   obtained from B3LYP/6-31G(2d,2p).Basepair parameters value
HEADER   obtained by B3LYP/6-31G(2d,2p) method are: Buckle=-49.94,
HEADER   Open =-15.61, Propeller=-14.42,Stagger=0.08,
HEADER   Shear=-2.44, Stretch=2.98
ATOM      1  C4    G     1     127.854  15.590 -16.928
ATOM      2  N9    G     1     128.805  16.579 -16.922
ATOM      3  C8    G     1     128.615  17.284 -15.751
ATOM      4  N7    G     1     127.633  16.819 -15.021
ATOM      5  C5    G     1     127.141  15.753 -15.745
ATOM      6  N3    G     1     127.682  14.659 -17.895
ATOM      7  C2    G     1     126.681  13.848 -17.647
ATOM      8  N1    G     1     125.913  13.919 -16.515
ATOM      9  C6    G     1     126.059  14.862 -15.462
ATOM     10  C1'   G     1     129.787  16.833 -17.962
ATOM     11  O6    G     1     125.302  14.819 -14.505
ATOM     12  N2    G     1     126.331  12.902 -18.575
ATOM     29  H8    G     1     129.239  18.129 -15.499
ATOM     30  H1    G     1     125.099  13.325 -16.415
ATOM     31  HN21  G     1     127.029  12.770 -19.291
ATOM     32  HN22  G     1     125.917  12.046 -18.237
ATOM     33  H1'A  G     1     129.710  16.034 -18.698
ATOM     34  H1'B  G     1     129.594  17.790 -18.453
ATOM     35  H1'C  G     1     130.795  16.840 -17.542
ATOM     13  N2    G     2     125.854  18.027 -12.6962
ATOM     14  C2    G     2     124.586  18.310 -13.137
ATOM     15  N1    G     2     123.978  17.357 -13.903
ATOM     16  C6    G     2     122.670  17.433 -14.471
ATOM     17  C5    G     2     122.037  18.663 -14.073
ATOM     18  C4    G     2     122.748  19.545 -13.261
ATOM     19  N3    G     2     124.010  19.439 -12.782
ATOM     20  N9    G     2     121.905  20.607 -13.047
ATOM     21  C8    G     2     120.740  20.311 -13.732
ATOM     22  N7    G     2     120.782  19.164 -14.357
ATOM     23  C1'   G     2     122.194  21.778 -12.245
ATOM     24  O6    G     2     122.262  16.524 -15.169
ATOM     25  H8    G     2     119.903  20.994 -13.726
ATOM     26  H1    G     2     124.459  16.470 -14.064
ATOM     27  HN21  G     2     126.299  18.839 -12.294
ATOM     28  HN22  G     2     126.453  17.508 -13.335
ATOM     36  H1'A  G     2     123.240  21.727 -11.946
ATOM     37  H1'B  G     2     122.029  22.692 -12.821
ATOM     38  H1'C  G     2     121.570  21.807 -11.347
ENDMODEL

HEADER   System 17: G:G H:W T Basepair optimized from PDB ID 1QVG:
HEADER   868(O)-775(O). Interaction energy -15.25Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p). Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=10.26, Open=-9.91,
```

```
HEADER   Propeller=3.48, Stagger=0.03, Shear=0.17, Stretch= 2.85
ATOM      1  C4    G     1      -3.531   0.803   0.010
ATOM      2  C5    G     1      -2.489  -0.112  -0.090
ATOM      3  N7    G     1      -1.286   0.543  -0.193
ATOM      4  C8    G     1      -1.582   1.818  -0.155
ATOM      5  N9    G     1      -2.938   2.041  -0.033
ATOM      6  N3    G     1      -4.858   0.551   0.123
ATOM      7  C2    G     1      -5.127  -0.730   0.166
ATOM      8  N1    G     1      -4.173  -1.714   0.092
ATOM      9  C6    G     1      -2.769  -1.511  -0.033
ATOM     10  C1'   G     1      -3.620   3.324   0.035
ATOM     11  O6    G     1      -2.014  -2.472  -0.061
ATOM     12  N2    G     1      -6.425  -1.151   0.353
ATOM     13  H8    G     1      -0.848   2.611  -0.203
ATOM     14  H1    G     1      -4.440  -2.684   0.206
ATOM     15  HN21  G     1      -7.095  -0.406   0.222
ATOM     16  HN22  G     1      -6.693  -2.008  -0.108
ATOM     17  H1'A  G     1      -4.676   3.130   0.214
ATOM     18  H1'B  G     1      -3.218   3.926   0.852
ATOM     19  H1'C  G     1      -3.507   3.871  -0.903
ATOM     20  N1    G     2       1.502  -0.047  -0.211
ATOM     21  C6    G     2       2.238   1.160  -0.101
ATOM     22  C5    G     2       3.640   0.878   0.022
ATOM     23  C4    G     2       4.046  -0.458   0.031
ATOM     24  N3    G     2       3.299  -1.580  -0.069
ATOM     25  C2    G     2       2.012  -1.312  -0.196
ATOM     26  N9    G     2       5.412  -0.421   0.167
ATOM     27  C8    G     2       5.753   0.918   0.234
ATOM     28  N7    G     2       4.727   1.723   0.151
ATOM     29  C1'   G     2       6.301  -1.562   0.239
ATOM     30  O6    G     2       1.647   2.234  -0.118
ATOM     31  N2    G     2       1.129  -2.338  -0.371
ATOM     32  H8    G     2       6.784   1.227   0.342
ATOM     33  H1    G     2       0.483   0.084  -0.274
ATOM     34  HN21  G     2       1.504  -3.246  -0.148
ATOM     35  HN22  G     2       0.138  -2.206  -0.200
ATOM     36  H1'A  G     2       5.705  -2.467   0.120
ATOM     37  H1'B  G     2       7.049  -1.524  -0.558
ATOM     38  H1'C  G     2       6.813  -1.599   1.204
ENDMODEL

HEADER   System 18: G:G S:S T Basepair optimized from PDB ID 1FFK:
HEADER   315(O)-336(O). Interaction energy -6.50Kcal/mole obtained from
HEADER   B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-13.00, Open=0.08,
HEADER   Propeller=30.85, Stagger=0.0, Shear=1.17, Stretch= 3.53
ATOM      1  C4    G     1       3.099   0.597   0.117
ATOM      2  C5    G     1       4.295  -0.116   0.160
ATOM      3  N7    G     1       5.337   0.698   0.553
ATOM      4  C8    G     1       4.785   1.865   0.743
ATOM      5  N9    G     1       3.421   1.874   0.499
ATOM      6  N3    G     1       1.853   0.162  -0.210
ATOM      7  C2    G     1       1.819  -1.123  -0.516
ATOM      8  N1    G     1       2.937  -1.909  -0.508
ATOM      9  C6    G     1       4.281  -1.512  -0.182
ATOM     10  C1'   G     1       2.522   3.006   0.593
ATOM     11  O6    G     1       5.166  -2.338  -0.229
```

```
ATOM     12  N2    G     1       0.645  -1.694  -0.894
ATOM     13  H8    G     1       5.296   2.762   1.063
ATOM     14  H1    G     1       2.867  -2.882  -0.772
ATOM     15  HN21  G     1       0.218  -1.190  -0.662
ATOM     16  HN22  G     1       0.586  -2.699  -0.887
ATOM     17  H1'A  G     1       1.577   2.692   1.042
ATOM     18  H1'B  G     1       2.975   3.770   1.226
ATOM     19  H1'C  G     1       2.322   3.439  -0.392
ATOM     20  N3    G     2      -1.854  -0.164  -0.212
ATOM     21  C2    G     2      -1.818   1.120  -0.519
ATOM     22  N1    G     2      -2.935   1.908  -0.510
ATOM     23  C6    G     2      -4.279   1.513  -0.182
ATOM     24  C5    G     2      -4.294   0.117   0.160
ATOM     25  C4    G     2      -3.099  -0.598   0.117
ATOM     26  N9    G     2      -3.423  -1.874   0.499
ATOM     27  C8    G     2      -4.786  -1.863   0.745
ATOM     28  N7    G     2      -5.338  -0.695   0.555
ATOM     29  C1'   G     2      -2.526  -3.007   0.589
ATOM     30  O6    G     2      -5.163   2.340  -0.229
ATOM     31  N2    G     2      -0.643   1.690  -0.899
ATOM     32  H8    G     2      -5.298  -2.758   1.065
ATOM     33  H1    G     2      -2.864   2.881  -0.775
ATOM     34  HN21  G     2       0.219   1.186  -0.666
ATOM     35  HN22  G     2      -0.584   2.695  -0.892
ATOM     36  H1'A  G     2      -1.581  -2.697   1.039
ATOM     37  H1'B  G     2      -2.980  -3.773   1.219
ATOM     38  H1'C  G     2      -2.327  -3.437  -0.398
ENDMODEL


HEADER   System 19: U:U W:W T  Basepair optimized from PDB ID 2J02:
HEADER   956(A)-960(A).Interaction energy is -9.00Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-0.34, Open =0.02,
HEADER   Propeller=-0.89, Stagger=0.0, Shear=-2.58, Stretch= 2.89
ATOM      1  C6    U     1    -139.689   8.498 -13.133
ATOM      2  N1    U     1    -139.511   7.137 -13.225
ATOM      3  C2    U     1    -138.799   6.580 -14.281
ATOM      4  N3    U     1    -138.304   7.468 -15.196
ATOM      5  C4    U     1    -138.437   8.870 -15.181
ATOM      6  C5    U     1    -139.196   9.363 -14.040
ATOM      7  C1'   U     1    -140.053   6.212 -12.233
ATOM      8  O2    U     1    -138.647   5.364 -14.350
ATOM      9  O4    U     1    -137.945   9.550 -16.059
ATOM     22  H6    U     1    -140.258   8.826 -12.272
ATOM     23  H5    U     1    -139.347  10.428 -13.948
ATOM     24  H3    U     1    -137.779   7.050 -15.976
ATOM     25  H1'A  U     1    -140.575   6.788 -11.470
ATOM     26  H1'B  U     1    -140.745   5.513 -12.704
ATOM     27  H1'C  U     1    -139.250   5.636 -11.773
ATOM     10  O2    U     2    -136.892   6.054 -17.259
ATOM     11  C2    U     2    -136.725   4.840 -17.318
ATOM     12  N1    U     2    -136.006   4.283 -18.371
ATOM     13  C6    U     2    -135.810   2.925 -18.451
ATOM     14  C5    U     2    -136.289   2.060 -17.536
ATOM     15  C4    U     2    -137.054   2.552 -16.399
ATOM     16  N3    U     2    -137.207   3.953 -16.396
```

```
ATOM     17  C1'   U     2    -135.480   5.207 -19.372
ATOM     18  O4    U     2    -137.536   1.873 -15.515
ATOM     19  H6    U     2    -135.237   2.598 -19.310
ATOM     20  H5    U     2    -136.123   0.997 -17.619
ATOM     21  H3    U     2    -137.740   4.369 -15.621
ATOM     28  H1'A  U     2    -134.935   4.634 -20.121
ATOM     29  H1'B  U     2    -136.294   5.754 -19.850
ATOM     30  H1'C  U     2    -134.812   5.932 -18.906
ENDMODEL


HEADER   System 20: A:G s:s T Basepair optimized from PDB ID 1FFK:
HEADER   243(O)-274(O). Interaction energy is -4.56 Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=1.52, Open =23.45,
HEADER   Propeller=-33.60, Stagger=-0.90, Shear=1.38, Stretch= 3.20
ATOM      1  C2    A     1      -1.701   0.916   0.819
ATOM      2  N1    A     1      -2.598   1.905   0.885
ATOM      3  C6    A     1      -3.854   1.658   0.473
ATOM      4  C5    A     1      -4.175   0.373  -0.005
ATOM      5  C4    A     1      -3.134  -0.558  -0.013
ATOM      6  N3    A     1      -1.878  -0.340   0.394
ATOM      7  N9    A     1      -3.680  -1.710  -0.528
ATOM      8  C8    A     1      -5.004  -1.413  -0.788
ATOM      9  N7    A     1      -5.343  -0.182  -0.494
ATOM     10  C1'   A     1      -3.001  -2.978  -0.727
ATOM     11  N6    A     1      -4.757   2.667   0.505
ATOM     12  H8    A     1      -5.664  -2.159  -1.207
ATOM     13  H2    A     1      -0.693   1.160   1.142
ATOM     14  HN61  A     1      -5.732   2.447   0.384
ATOM     15  HN62  A     1      -4.509   3.494   1.022
ATOM     16  H1'A  A     1      -1.952  -2.788  -0.957
ATOM     17  H1'B  A     1      -3.060  -3.604   0.167
ATOM     18  H1'C  A     1      -3.458  -3.508  -1.564
ATOM     19  C4    G     2       2.956   0.610  -0.204
ATOM     20  C5    G     2       4.219   0.041  -0.042
ATOM     21  N7    G     2       5.210   0.969  -0.291
ATOM     22  C8    G     2       4.561   2.063  -0.591
ATOM     23  N9    G     2       3.185   1.915  -0.559
ATOM     24  N3    G     2       1.732   0.045  -0.053
ATOM     25  C2    G     2       1.797  -1.227   0.270
ATOM     26  N1    G     2       2.984  -1.887   0.453
ATOM     27  C6    G     2       4.307  -1.347   0.321
ATOM     28  C1'   G     2       2.175   2.926  -0.810
ATOM     29  O6    G     2       5.262  -2.073   0.508
ATOM     30  N2    G     2       0.649  -1.967   0.389
ATOM     31  H8    G     2       5.009   3.011  -0.851
ATOM     32  H1    G     2       2.978  -2.880   0.647
ATOM     33  HN21  G     2      -0.213  -1.412   0.423
ATOM     34  HN22  G     2       0.680  -2.719   1.062
ATOM     35  H1'A  G     2       1.231   2.423  -1.019
ATOM     36  H1'B  G     2       2.042   3.578   0.058
ATOM     37  H1'C  G     2       2.459   3.532  -1.672
ENDMODEL

HEADER   System 21: G:U s:h C Basepair optimized from PDB ID 3CME:
```

```
HEADER   1917(O)-1918(O).Interaction energy is -6.01 Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=3.61, Open=4.60,
HEADER   Propeller=25.57, Stagger=0.47, Shear=0.63, Stretch=3.39
ATOM      1  N7    G     1     118.517  99.367  95.510
ATOM      2  C5    G     1     117.450 100.142  95.101
ATOM      3  C4    G     1     117.320 101.274  95.904
ATOM      4  N9    G     1     118.331 101.182  96.827
ATOM      5  C8    G     1     119.014 100.014  96.529
ATOM      6  N3    G     1     116.405 102.273  95.844
ATOM      7  C2    G     1     115.530 102.105  94.873
ATOM      8  N1    G     1     115.567 101.028  94.025
ATOM      9  C6    G     1     116.510  99.947  94.032
ATOM     10  N2    G     1     114.570 103.041  94.647
ATOM     11  O6    G     1     116.408  99.069  93.200
ATOM     12  C1'   G     1     118.629 102.133  97.876
ATOM     22  H8    G     1     119.865  99.705  97.118
ATOM     23  H1    G     1     114.896 100.961  93.272
ATOM     24  HN21  G     1     114.389 103.713  95.395
ATOM     25  HN22  G     1     113.751 102.753  94.135
ATOM     32  H1'A  G     1     119.215 101.638  98.652
ATOM     33  H1'B  G     1     119.200 102.984  97.493
ATOM     34  H1'C  G     1     117.699 102.501  98.310
ATOM     13  O4    U     2     113.868 105.111  96.579
ATOM     14  C4    U     2     114.713 105.734  97.212
ATOM     15  N3    U     2     114.342 106.889  97.904
ATOM     16  C2    U     2     115.145 107.729  98.655
ATOM     17  N1    U     2     116.483 107.337  98.709
ATOM     18  C6    U     2     116.921 106.208  98.063
ATOM     19  C5    U     2     116.116 105.403  97.336
ATOM     20  C1'   U     2     117.379 108.192  99.485
ATOM     21  O2    U     2     114.734 108.721  99.219
ATOM     26  H6    U     2     117.978 106.002  98.179
ATOM     27  H5    U     2     116.478 104.509  96.845
ATOM     28  H3    U     2     113.369 107.160  97.847
ATOM     29  H1'A  U     2     118.383 107.773  99.442
ATOM     30  H1'B  U     2     117.383 109.203  99.076
ATOM     31  H1'C  U     2     117.045 108.245 100.522
ENDMODEL

HEADER   System 22: A:A h:s T Basepair optimized from PDB ID 1GTR:
HEADER   13(B)-22(B).Interaction energy is -4.01Kcal/mole obtained from
HEADER   B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle= 4.32, Open=-1.05,
HEADER   Propeller=18.61, Stagger=-0.44, Shear=2.29, Stretch=2.92
ATOM      1  N9    A     1      -7.078  -3.285  -0.135
ATOM      2  C4    A     1      -5.810  -3.819  -0.210
ATOM      3  C5    A     1      -4.960  -2.824   0.281
ATOM      4  N7    A     1      -5.681  -1.703   0.654
ATOM      5  C8    A     1      -6.925  -2.022   0.390
ATOM      6  N3    A     1      -5.463  -5.033  -0.649
ATOM      7  C2    A     1      -4.144  -5.213  -0.561
ATOM      8  N1    A     1      -3.206  -4.367  -0.119
ATOM      9  C6    A     1      -3.585  -3.146   0.308
ATOM     10  N6    A     1      -2.626  -2.293   0.723
ATOM     11  C1'   A     1      -8.304  -3.947  -0.538
ATOM     27  H8    A     1      -7.779  -1.380   0.557
```

```
ATOM     28  H2    A     1      -3.776  -6.181  -0.893
ATOM     29  HN61  A     1      -2.839  -1.400   1.167
ATOM     30  HN62  A     1      -1.705  -2.685   0.826
ATOM     31  H1'A  A     1      -8.041  -4.950  -0.873
ATOM     32  H1'B  A     1      -9.001  -4.020   0.300
ATOM     33  H1'C  A     1      -8.787  -3.411  -1.360
ATOM     12  N3    A     2      -2.946   0.450   2.016
ATOM     13  C4    A     2      -2.013   1.363   2.307
ATOM     14  C5    A     2      -2.213   2.558   3.001
ATOM     15  C6    A     2      -3.529   2.810   3.428
ATOM     16  N1    A     2      -4.491   1.920   3.136
ATOM     17  C2    A     2      -4.156   0.813   2.461
ATOM     18  N7    A     2      -1.036   3.276   3.110
ATOM     19  C8    A     2      -0.156   2.525   2.496
ATOM     20  N9    A     2      -0.675   1.354   1.983
ATOM     21  C1'   A     2       0.034   0.311   1.266
ATOM     22  N6    A     2      -3.859   3.911   4.151
ATOM     23  H8    A     2       0.890   2.765   2.372
ATOM     24  H2    A     2      -4.959   0.122   2.226
ATOM     25  HN61  A     2      -3.202   4.673   4.178
ATOM     26  HN62  A     2      -4.840   4.124   4.233
ATOM     34  H1'A  A     2       0.950   0.724   0.844
ATOM     35  H1'B  A     2       0.291  -0.520   1.929
ATOM     36  H1'C  A     2      -0.593  -0.065   0.457
ENDMODEL

HEADER   System 23: A:G w:s C Basepair optimized from PDB ID 1SM1:
HEADER   991(O)-2020(O). Interaction energy is -4.61 Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-4.35, Open=34.47,
HEADER   Propeller=-16.40, Stagger=0.04, Shear=2.23, Stretch= 3.07
ATOM      1  C2    A     1      -1.588   0.240   0.110
ATOM      2  N1    A     1      -1.731  -1.078  -0.139
ATOM      3  C6    A     1      -2.970  -1.584  -0.259
ATOM      4  C5    A     1      -4.066  -0.714  -0.131
ATOM      5  C4    A     1      -3.761   0.625   0.122
ATOM      6  N3    A     1      -2.541   1.157   0.253
ATOM      7  N9    A     1      -4.977   1.263   0.201
ATOM      8  C8    A     1      -5.929   0.286  -0.009
ATOM      9  N7    A     1      -5.430  -0.910  -0.211
ATOM     10  C1'   A     1      -5.187   2.680   0.442
ATOM     11  N6    A     1      -3.131  -2.918  -0.466
ATOM     12  H8    A     1      -6.982   0.526   0.004
ATOM     13  H2    A     1      -0.558   0.572   0.200
ATOM     14  HN61  A     1      -4.043  -3.229  -0.760
ATOM     15  HN62  A     1      -2.336  -3.436  -0.805
ATOM     16  H1'A  A     1      -4.215   3.129   0.642
ATOM     17  H1'B  A     1      -5.631   3.163  -0.431
ATOM     18  H1'C  A     1      -5.838   2.829   1.307
ATOM     19  C4    G     2       3.061   0.693  -0.069
ATOM     20  C5    G     2       4.382   0.247  -0.007
ATOM     21  N7    G     2       5.264   1.302  -0.119
ATOM     22  C8    G     2       4.497   2.352  -0.246
ATOM     23  N9    G     2       3.146   2.054  -0.224
ATOM     24  N3    G     2       1.912  -0.022   0.002
ATOM     25  C2    G     2       2.120  -1.312   0.160
ATOM     26  N1    G     2       3.377  -1.858   0.224
```

```
ATOM     27  C6    G     2       4.628  -1.159   0.160
ATOM     28  C1'   G     2       2.047   2.992  -0.353
ATOM     29  O6    G     2       5.663  -1.788   0.251
ATOM     30  N2    G     2       1.066  -2.162   0.318
ATOM     31  H8    G     2       4.842   3.370  -0.359
ATOM     32  H1    G     2       3.485  -2.849   0.389
ATOM     33  HN21  G     2       0.137  -1.806   0.081
ATOM     34  HN22  G     2       1.217  -3.138   0.117
ATOM     35  H1'A  G     2       1.108   2.449  -0.255
ATOM     36  H1'B  G     2       2.097   3.754   0.429
ATOM     37  H1'C  G     2       2.070   3.482  -1.330
ENDMODEL

HEADER   System 24: A:U s:w C  Basepair optimized from PDB ID 1M1K:
HEADER   329(A)-346(O). Interaction energy is -6.89Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p).  Basepair parameters value obtained
HEADER   by B3LYP/6-31G(2d,2p) method are: Buckle=2.34,Open =-6.63,
HEADER   Propeller=2.83, Stagger=0.03, Shear=0.16, Stretch=2.98
ATOM      1  C6    U     1      -4.665  -0.710  -0.012
ATOM      2  C5    U     1      -3.901  -1.820   0.032
ATOM      3  C4    U     1      -2.453  -1.702   0.054
ATOM      4  N3    U     1      -1.988  -0.379   0.031
ATOM      5  C2    U     1      -2.752   0.762  -0.020
ATOM      6  N1    U     1      -4.134   0.557  -0.034
ATOM      7  C1'   U     1      -4.972   1.748  -0.118
ATOM      8  O2    U     1      -2.285   1.890  -0.053
ATOM      9  O4    U     1      -1.677  -2.643   0.088
ATOM     10  H6    U     1      -5.747  -0.754  -0.032
ATOM     11  H5    U     1      -4.334  -2.808   0.051
ATOM     12  H3    U     1      -0.963  -0.240   0.043
ATOM     13  H1'A  U     1      -6.016   1.454  -0.016
ATOM     14  H1'B  U     1      -4.709   2.448   0.676
ATOM     15  H1'C  U     1      -4.828   2.253  -1.075
ATOM     16  N3    A     2       0.991  -0.305   0.042
ATOM     17  C2    A     2       1.366  -1.592   0.002
ATOM     18  N1    A     2       2.606  -2.091  -0.044
ATOM     19  C6    A     2       3.640  -1.236  -0.049
ATOM     20  C5    A     2       3.385   0.147  -0.020
ATOM     21  C4    A     2       2.040   0.529   0.027
ATOM     22  N9    A     2       2.058   1.906   0.046
ATOM     23  C8    A     2       3.389   2.263   0.009
ATOM     24  N7    A     2       4.219   1.249  -0.033
ATOM     25  C1'   A     2       0.927   2.818   0.134
ATOM     26  N6    A     2       4.901  -1.736  -0.050
ATOM     27  H8    A     2       3.684   3.303   0.013
ATOM     28  H2    A     2       0.553  -2.312   0.008
ATOM     29  HN61  A     2       5.659  -1.109  -0.266
ATOM     30  HN62  A     2       5.007  -2.712  -0.274
ATOM     31  H1'A  A     2      -0.007   2.270   0.018
ATOM     32  H1'B  A     2       0.919   3.323   1.103
ATOM     33  H1'C  A     2       0.992   3.568  -0.657
ENDMODEL

HEADER   System 25: U:U w:h T Basepair optimized from PDB ID 1W2B:
HEADER   2781(O)-2791(O). Interaction energy is -6.85Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p). Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-2.05, Open=9.07,
```

```
HEADER   Propeller=2.52, Stagger=0.01, Shear= 2.70, Stretch= 3.04
ATOM      1  C6    U     1      -3.145  -1.391   0.016
ATOM      2  C5    U     1      -1.877  -0.923  -0.025
ATOM      3  C4    U     1      -1.656   0.507  -0.057
ATOM      4  N3    U     1      -2.828   1.268  -0.045
ATOM      5  C2    U     1      -4.133   0.815   0.003
ATOM      6  N1    U     1      -4.252  -0.575   0.025
ATOM      7  C1'   U     1      -5.612  -1.100   0.103
ATOM      8  O2    U     1      -5.099   1.550   0.024
ATOM      9  O4    U     1      -0.575   1.085  -0.091
ATOM     10  H6    U     1      -3.364  -2.450   0.042
ATOM     11  H5    U     1      -1.010  -1.570  -0.035
ATOM     12  H3    U     1      -2.714   2.272  -0.062
ATOM     13  H1'A  U     1      -5.582  -2.185   0.004
ATOM     14  H1'B  U     1      -6.070  -0.834   1.058
ATOM     15  H1'C  U     1      -6.220  -0.675  -0.695
ATOM     16  N3    U     2       2.081   0.003  -0.033
ATOM     17  C2    U     2       3.128   0.900   0.001
ATOM     18  N1    U     2       4.403   0.314   0.024
ATOM     19  C6    U     2       4.563  -1.047   0.026
ATOM     20  C5    U     2       3.522  -1.905  -0.002
ATOM     21  C4    U     2       2.163  -1.391  -0.032
ATOM     22  C1'   U     2       5.533   1.234   0.092
ATOM     23  O2    U     2       2.992   2.106   0.013
ATOM     24  O4    U     2       1.156  -2.086  -0.053
ATOM     25  H6    U     2       5.591  -1.388   0.051
ATOM     26  H5    U     2       3.666  -2.974  -0.003
ATOM     27  H3    U     2       1.137   0.412  -0.054
ATOM     28  H1'A  U     2       6.460   0.668  -0.004
ATOM     29  H1'B  U     2       5.465   1.968  -0.711
ATOM     30  H1'C  U     2       5.531   1.773   1.042
ENDMODEL

HEADER   System 26: A:C w:w C Basepair optimized from PDB ID 1M5K:
HEADER   20(B)-63(B). Interaction energy is -5.34Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=4.42, Open=13.55,
HEADER   Propeller=-4.84, Stagger=0.01 Shear=-2.60 Stretch=2.7
ATOM      1  N1    A     1       1.084  -0.916   0.064
ATOM      2  C6    A     1       2.295  -1.490   0.072
ATOM      3  C5    A     1       3.432  -0.668   0.029
ATOM      4  C4    A     1       3.186   0.706  -0.025
ATOM      5  N3    A     1       1.993   1.308  -0.037
ATOM      6  C2    A     1       0.993   0.431   0.011
ATOM      7  N9    A     1       4.431   1.293  -0.049
ATOM      8  C8    A     1       5.338   0.254  -0.007
ATOM      9  N7    A     1       4.787  -0.936   0.043
ATOM     10  C1'   A     1       4.709   2.715  -0.129
ATOM     11  N6    A     1       2.395  -2.851   0.086
ATOM     12  H8    A     1       6.402   0.444  -0.013
ATOM     13  H2    A     1      -0.021   0.822   0.012
ATOM     14  HN61  A     1       3.298  -3.228   0.329
ATOM     15  HN62  A     1       1.592  -3.362   0.418
ATOM     16  H1'A  A     1       3.764   3.248  -0.016
ATOM     17  H1'B  A     1       5.389   3.018   0.670
ATOM     18  H1'C  A     1       5.149   2.973  -1.095
ATOM     19  C6    C     2      -5.106  -0.790  -0.106
```

```
ATOM     20  C5    C     2      -4.086  -1.684  -0.145
ATOM     21  C4    C     2      -2.756  -1.147  -0.067
ATOM     22  N3    C     2      -2.512   0.152   0.024
ATOM     23  C2    C     2      -3.536   1.053   0.059
ATOM     24  N1    C     2      -4.874   0.540  -0.008
ATOM     25  C1'   C     2      -5.954   1.514   0.064
ATOM     26  O2    C     2      -3.401   2.262   0.145
ATOM     27  N4    C     2      -1.705  -1.994  -0.075
ATOM     28  H6    C     2      -6.146  -1.094  -0.150
ATOM     29  H5    C     2      -4.274  -2.745  -0.224
ATOM     30  HN41  C     2      -0.746  -1.638  -0.044
ATOM     31  HN42  C     2      -1.865  -2.975  -0.217
ATOM     32  H1'A  C     2      -6.910   1.000  -0.046
ATOM     33  H1'B  C     2      -5.925   2.038   1.022
ATOM     34  H1'C  C     2      -5.838   2.261  -0.722
ENDMODEL

HEADER   System 27: A:A w:w C Basepair optimized from PDB ID 1FFK:
HEADER   635(O)-620(O).Interaction energy is -4.34Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=8.96, Open=14.47,
HEADER   Propeller=-0.22, Stagger=0.09, Shear=2.50, Stretch=2.75
ATOM      1  C4    A     1      -3.978  -0.625   0.028
ATOM      2  C5    A     1      -4.006   0.773   0.029
ATOM      3  N7    A     1      -5.303   1.248   0.098
ATOM      4  C8    A     1      -6.030   0.158   0.140
ATOM      5  N9    A     1      -5.299  -1.010   0.102
ATOM      6  N3    A     1      -2.897  -1.406  -0.042
ATOM      7  C2    A     1      -1.777  -0.688  -0.119
ATOM      8  N1    A     1      -1.652   0.653  -0.129
ATOM      9  C6    A     1      -2.757   1.413  -0.053
ATOM     10  C1'   A     1      -5.789  -2.377   0.142
ATOM     11  N6    A     1      -2.631   2.767  -0.023
ATOM     12  H8    A     1      -7.110   0.137   0.198
ATOM     13  H2    A     1      -0.837  -1.229  -0.183
ATOM     14  HN61  A     1      -3.463   3.311  -0.191
ATOM     15  HN62  A     1      -1.761   3.151  -0.353
ATOM     16  H1'A  A     1      -4.933  -3.037   0.007
ATOM     17  H1'B  A     1      -6.260  -2.594   1.104
ATOM     18  H1'C  A     1      -6.509  -2.552  -0.660
ATOM     19  N6    A     2       1.310   1.389  -0.186
ATOM     20  C6    A     2       2.183   0.365  -0.136
ATOM     21  C5    A     2       3.574   0.570  -0.016
ATOM     22  C4    A     2       4.366  -0.578   0.006
ATOM     23  N3    A     2       3.945  -1.846  -0.076
ATOM     24  C2    A     2       2.616  -1.905  -0.185
ATOM     25  N1    A     2       1.728  -0.901  -0.218
ATOM     26  N9    A     2       5.660  -0.122   0.134
ATOM     27  C8    A     2       5.571   1.254   0.184
ATOM     28  N7    A     2       4.345   1.712   0.097
ATOM     29  C1'   A     2       6.854  -0.940   0.217
ATOM     30  H8    A     2       6.458   1.865   0.283
ATOM     31  H2    A     2       2.191  -2.903  -0.255
ATOM     32  HN61  A     2       1.668   2.308   0.014
ATOM     33  HN62  A     2       0.307   1.204  -0.141
ATOM     34  H1'A  A     2       6.556  -1.981   0.085
ATOM     35  H1'B  A     2       7.565  -0.670  -0.568
```

```
ATOM     36  H1'C  A     2       7.337  -0.830   1.191
ENDMODEL

HEADER   System 28: A:A W:S C Basepair optimized from PDB ID 1N78:
HEADER   89(D)-96(D).Interaction energy is –14.76 Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-18.29,Open=-26.14,
HEADER   Propeller=-46.70, Stagger=-0.21, Shear=-2.49, Stretch=3.40
ATOM      1  C1'   A     1       4.284  -0.346  -3.476
ATOM      2  N9    A     1       3.440   0.256  -2.460
ATOM      3  C8    A     1       3.551   1.509  -1.894
ATOM      4  N7    A     1       2.635   1.769  -0.993
ATOM      5  C5    A     1       1.868   0.621  -0.961
ATOM      6  C6    A     1       0.743   0.257  -0.195
ATOM      7  N6    A     1       0.180   1.093   0.699
ATOM      8  N1    A     1       0.218  -0.971  -0.403
ATOM      9  C2    A     1       0.792  -1.784  -1.310
ATOM     10  N3    A     1       1.852  -1.555  -2.074
ATOM     11  C4    A     1       2.350  -0.330  -1.860
ATOM     31  H8    A     1       4.338   2.186  -2.194
ATOM     32  H2    A     1       0.311  -2.751  -1.423
ATOM     33  HN61  A     1       0.673   1.955   0.870
ATOM     34  HN62  A     1      -0.410   0.741   1.456
ATOM     47  H1'A  A     1       5.317  -0.420  -3.129
ATOM     48  H1'B  A     1       3.900  -1.347  -3.673
ATOM     49  H1'C  A     1       4.255   0.237  -4.400
ATOM     12  O5'   A     2      -6.354  -3.210   2.881
ATOM     13  C5'   A     2      -6.343  -2.963   1.479
ATOM     14  C4'   A     2      -5.032  -2.383   0.970
ATOM     15  O4'   A     2      -4.829  -1.086   1.556
ATOM     16  C3'   A     2      -3.761  -3.186   1.301
ATOM     17  O3'   A     2      -3.503  -4.237   0.409
ATOM     18  C2'   A     2      -2.686  -2.082   1.273
ATOM     19  O2'   A     2      -2.341  -1.901  -0.077
ATOM     20  C1'   A     2      -3.465  -0.865   1.821
ATOM     21  N9    A     2      -3.293  -0.684   3.266
ATOM     22  C8    A     2      -4.145  -1.082   4.282
ATOM     23  N7    A     2      -3.703  -0.783   5.482
ATOM     24  C5    A     2      -2.496  -0.155   5.249
ATOM     25  C6    A     2      -1.533   0.406   6.106
ATOM     26  N6    A     2      -1.659   0.373   7.455
ATOM     27  N1    A     2      -0.433   0.967   5.574
ATOM     28  C2    A     2      -0.299   0.959   4.245
ATOM     29  N3    A     2      -1.131   0.463   3.323
ATOM     30  C4    A     2      -2.222  -0.083   3.881
ATOM     35  H8    A     2      -5.068  -1.592   4.052
ATOM     36  H2    A     2       0.610   1.416   3.864
ATOM     37  HN61  A     2      -1.043   0.963   7.991
ATOM     38  HN62  A     2      -2.560   0.143   7.841
ATOM     39  H1'   A     2      -3.125   0.053   1.336
ATOM     40  H2'   A     2      -1.814  -2.308   1.893
ATOM     41  HO2'  A     2      -1.433  -1.503  -0.132
ATOM     42  H3'   A     2      -3.836  -3.604   2.310
ATOM     43  HO3'  A     2      -3.017  -3.820  -0.320
ATOM     44  H4'   A     2      -5.099  -2.282  -0.121
ATOM     45  H5'A  A     2      -6.561  -3.874   0.909
ATOM     46  H5'B  A     2      -7.146  -2.247   1.290
```

```
ATOM     50  HO5'  A     2      -5.951  -4.069   3.042
ENDMODEL
HEADER   System 29: A:U w:s T Basepair optimized from PDB ID
HEADER   4TNA: 8-21. Interaction energy is -10.64 Kcal/mole obtained
HEADER   from B3LYP/6-31G(2d,2p). Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=31.63, Open=-34.60,
HEADER   Propeller=2.77, Stagger=-1.20, Shear=0.79, Stretch= 3.66
ATOM     18  N1    A     1       2.180   0.110  -0.670
ATOM     19  C2    A     1       2.478  -1.193  -0.842
ATOM     20  N3    A     1       3.632  -1.801  -0.590
ATOM     21  C4    A     1       4.543  -0.952  -0.102
ATOM     22  C5    A     1       4.374   0.413   0.143
ATOM     23  C6    A     1       3.111   0.944  -0.168
ATOM     24  N7    A     1       5.523   0.972   0.667
ATOM     25  C8    A     1       6.360  -0.035   0.728
ATOM     26  N9    A     1       5.835  -1.229   0.279
ATOM     27  C1'   A     1       6.486  -2.526   0.216
ATOM     28  N6    A     1       2.801   2.252  -0.008
ATOM     40  H8    A     1       7.375   0.023   1.092
ATOM     41  H2    A     1       1.665  -1.805  -1.214
ATOM     42  HN61  A     1       3.436   2.826   0.521
ATOM     43  HN62  A     1       1.829   2.520  -0.062
ATOM     45  H1'A  A     1       5.763  -3.238  -0.181
ATOM     46  H1'B  A     1       7.355  -2.492  -0.444
ATOM     47  H1'C  A     1       6.800  -2.851   1.210
ATOM      1  C6    U     2      -3.785  -0.637   0.750
ATOM      2  N1    U     2      -2.449  -0.707   0.430
ATOM      3  C2    U     2      -1.846  -1.911   0.077
ATOM      4  N3    U     2      -2.686  -3.000   0.112
ATOM      5  C4    U     2      -4.062  -3.032   0.427
ATOM      6  C5    U     2      -4.589  -1.722   0.757
ATOM      7  C1'   U     2      -1.554   0.478   0.446
ATOM      8  C2'   U     2      -1.283   1.031  -0.969
ATOM      9  C3'   U     2      -2.316   2.165  -1.078
ATOM     10  C4'   U     2      -2.367   2.674   0.373
ATOM     11  O4'   U     2      -2.158   1.508   1.189
ATOM     12  O2'   U     2      -0.016   1.641  -1.062
ATOM     13  O3'   U     2      -1.981   3.152  -2.018
ATOM     14  C5'   U     2      -3.652   3.365   0.800
ATOM     15  O5'   U     2      -4.818   2.573   0.602
ATOM     16  O2    U     2      -0.669  -1.982  -0.240
ATOM     17  O4    U     2      -4.668  -4.085   0.397
ATOM     44  HO5'  U     2      -5.113   2.685  -0.307
ATOM     29  H5'A  U     2      -3.720   4.323   0.270
ATOM     30  H5'B  U     2      -3.605   3.577   1.871
ATOM     31  H4'   U     2      -1.535   3.375   0.522
ATOM     32  H3'   U     2      -3.289   1.748  -1.356
ATOM     33  H2'   U     2      -1.407   0.255  -1.729
ATOM     34  H1'   U     2      -0.624   0.157   0.914
ATOM     35  HO2'  U     2       0.701   0.947  -1.043
ATOM     36  H6    U     2      -4.141   0.357   0.988
ATOM     37  H5    U     2      -5.636  -1.642   1.011
ATOM     38  H3    U     2      -2.264  -3.883  -0.141
ATOM     39  HO3'  U     2      -1.012   3.145  -2.055
ENDMODEL

HEADER   System 30: A:C W:S  C Basepair optimized from PDB ID 1HNX:
```

```
HEADER   1280(A)-1149(A). Interaction energy is -10.00 Kcal/mole
HEADER   obtained from B3LYP/6-31G(2d,2p). Basepair parameters value
HEADER   obtained by B3LYP/6-31G(2d,2p) method are: Buckle=42.14,
HEADER   Open=-35.20, Propeller=-13.10,
HEADER   Stagger=-1.23, Shear=-0.76, Stretch=4.21
ATOM     12  O2'   C     1       0.152  -1.795   0.863
ATOM     13  C2'   C     1       1.177  -1.167   0.135
ATOM     14  C1'   C     1       2.200  -0.488   1.075
ATOM     15  O4'   C     1       3.242  -1.406   1.306
ATOM     16  C4'   C     1       3.006  -2.636   0.604
ATOM     17  C3'   C     1       2.021  -2.280  -0.522
ATOM     18  N1    C     1       2.770   0.752   0.495
ATOM     19  C6    C     1       3.987   0.783  -0.097
ATOM     20  C5    C     1       4.478   1.946  -0.605
ATOM     21  C4    C     1       3.657   3.104  -0.462
ATOM     22  N3    C     1       2.466   3.084   0.115
ATOM     23  C2    C     1       1.970   1.918   0.596
ATOM     24  O2    C     1       0.866   1.807   1.132
ATOM     25  N4    C     1       4.075   4.300  -0.965
ATOM     26  C5'   C     1       4.340  -3.224   0.171
ATOM     27  O5'   C     1       5.049  -2.406  -0.756
ATOM     28  O3'   C     1       1.253  -3.365  -0.966
ATOM     33  H5'A  C     1       4.162  -4.228  -0.233
ATOM     34  H5'B  C     1       4.989  -3.323   1.045
ATOM     35  H4'   C     1       2.514  -3.352   1.277
ATOM     36  H3'   C     1       2.568  -1.872  -1.379
ATOM     37  H2'   C     1       0.770  -0.456  -0.588
ATOM     38  H1'   C     1       1.716  -0.199   2.006
ATOM     39  HO2'  C     1      -0.672  -1.248   0.770
ATOM     40  H6    C     1       4.520  -0.159  -0.139
ATOM     41  H5    C     1       5.445   1.979  -1.086
ATOM     42  HN41  C     1       3.547   5.107  -0.669
ATOM     43  HN42  C     1       5.054   4.439  -1.147
ATOM     44  HO3'  C     1       0.484  -3.365  -0.371
ATOM     48  H05'  C     1       4.699  -2.578  -1.636
ATOM      1  N7    A     2      -4.913   1.996   0.142
ATOM      2  C5    A     2      -4.096   0.882   0.137
ATOM      3  C4    A     2      -4.805  -0.259  -0.232
ATOM      4  N9    A     2      -6.093   0.170  -0.457
ATOM      5  C8    A     2      -6.084   1.528  -0.214
ATOM      6  N3    A     2      -4.321  -1.504  -0.346
ATOM      7  C2    A     2      -3.028  -1.543  -0.052
ATOM      8  N1    A     2      -2.216  -0.536   0.320
ATOM      9  C6    A     2      -2.723   0.716   0.424
ATOM     10  N6    A     2      -1.942   1.738   0.789
ATOM     11  C1'   A     2      -7.212  -0.661  -0.862
ATOM     29  H8    A     2      -6.984   2.117  -0.320
ATOM     30  H2    A     2      -2.546  -2.514  -0.115
ATOM     31  HN61  A     2      -2.355   2.656   0.810
ATOM     32  HN62  A     2      -0.934   1.654   0.912
ATOM     45  H1'A  A     2      -6.840  -1.678  -0.985
ATOM     46  H1'B  A     2      -7.995  -0.657  -0.101
ATOM     47  H1'C  A     2      -7.629  -0.315  -1.810
ENDMODEL

HEADER   System 31: A:G S:S C  Basepair optimized from PDB ID: 3CME:
HEADER   1797(O)-2483(O). Interaction energy is -7.78Kcal/mole obtained
```

```
HEADER   from B3LYP/6-31G(2d,2p).Basepair parameters value obtained by
HEADER   B3LYP/6-31G(2d,2p) method are: Buckle=-15.40, Open=-8.22,
HEADER   Propeller=-53.8, Stagger=-0.20, Shear=-1.87, Stretch=3.73
ATOM      1  N9    G     1      -3.863   1.286   1.180
ATOM      2  C4    G     1      -3.678   0.190   0.379
ATOM      3  C5    G     1      -4.957  -0.285   0.095
ATOM      4  N7    G     1      -5.917   0.493   0.706
ATOM      5  C8    G     1      -5.233   1.408   1.339
ATOM      6  C6    G     1      -5.098  -1.445  -0.739
ATOM      7  N1    G     1      -3.796  -1.917  -1.126
ATOM      8  C2    G     1      -2.586  -1.374  -0.800
ATOM      9  N3    G     1      -2.476  -0.301  -0.038
ATOM     10  N2    G     1      -1.473  -1.952  -1.326
ATOM     11  O6    G     1      -6.078  -2.043  -1.129
ATOM     12  C1'   G     1      -2.846   2.119   1.801
ATOM     44  H8    G     1      -5.648   2.206   1.935
ATOM     45  H1    G     1      -3.837  -2.738  -1.715
ATOM     46  HN61  G     1      -0.576  -1.820  -0.847
ATOM     47  HN62  G     1      -1.579  -2.858  -1.753
ATOM     48  H1'A  G     1      -3.329   3.014   2.195
ATOM     49  H1'B  G     1      -2.365   1.587   2.628
ATOM     50  H1'C  G     1      -2.086   2.408   1.075
ATOM     13  N3    A     2       1.247  -2.182  -0.128
ATOM     14  C4    A     2       2.392  -1.481  -0.086
ATOM     15  C5    A     2       3.624  -1.951   0.375
ATOM     16  C6    A     2       3.651  -3.281   0.830
ATOM     17  N1    A     2       2.520  -4.008   0.793
ATOM     18  C2    A     2       1.411  -3.427   0.330
ATOM     19  N9    A     2       2.619  -0.181  -0.466
ATOM     20  C8    A     2       3.959   0.060  -0.218
ATOM     21  N7    A     2       4.593  -0.974   0.284
ATOM     22  N6    A     2       4.772  -3.849   1.335
ATOM     23  C1'   A     2       1.616   0.740  -1.015
ATOM     24  C2'   A     2       0.663   1.317   0.061
ATOM     25  C3'   A     2       1.426   2.600   0.451
ATOM     26  C4'   A     2       1.960   3.053  -0.910
ATOM     27  O4'   A     2       2.272   1.834  -1.609
ATOM     28  O2'   A     2      -0.560   1.669  -0.523
ATOM     29  O3'   A     2       0.650   3.629   1.025
ATOM     30  C5'   A     2       3.179   3.950  -0.871
ATOM     31  O5'   A     2       4.194   3.330  -0.091
ATOM     32  H5'A  A     2       2.869   4.908  -0.432
ATOM     33  H5'B  A     2       3.522   4.132  -1.897
ATOM     34  H4'   A     2       1.157   3.581  -1.438
ATOM     35  H3'   A     2       2.274   2.336   1.091
ATOM     36  H2'   A     2       0.539   0.616   0.894
ATOM     37  H1'   A     2       1.044   0.191  -1.767
ATOM     38  HO2'  A     2      -1.186   0.916  -0.418
ATOM     39  H8    A     2       4.382   1.031  -0.422
ATOM     40  H2    A     2       0.522  -4.053   0.326
ATOM     41  HN61  A     2       5.652  -3.382   1.190
ATOM     42  HN62  A     2       4.770  -4.847   1.467
ATOM     43  H03'  A     2       0.581   3.463   1.970
ATOM     51  HO5'  A     2       4.973   3.893  -0.098
ENDMODEL

HEADER   System 32: A:U W:S C  Basepair optimized from PDB ID
```

```
HEADER   1F1T: 11(A)-26(A). Interaction energy is -14.55 Kcal/mole
HEADER   obtained from B3LYP/6-31G(2d,2p). Basepair parameters value
HEADER   obtained by B3LYP/6-31G(2d,2p) method are: Buckle=-45.50,
HEADER   Open =-30.70, Propeller=-20.70,
HEADER   Stagger=-1.29, Shear=0.56, Stretch=4.20
ATOM      1  N7    A     1       4.959   2.031  -0.301
ATOM      2  C5    A     1       4.155   0.912  -0.212
ATOM      3  C4    A     1       4.872  -0.188   0.259
ATOM      4  N9    A     1       6.152   0.273   0.459
ATOM      5  C8    A     1       6.131   1.607   0.108
ATOM      6  N3    A     1       4.400  -1.424   0.470
ATOM      7  C2    A     1       3.111  -1.505   0.168
ATOM      8  N1    A     1       2.293  -0.538  -0.292
ATOM      9  C6    A     1       2.789   0.702  -0.497
ATOM     10  N6    A     1       1.996   1.677  -0.967
ATOM     11  C1'   A     1       7.271  -0.500   0.968
ATOM     12  H8    A     1       7.023   2.214   0.174
ATOM     13  H2    A     1       2.639  -2.474   0.305
ATOM     14  HN61  A     1       2.380   2.606  -1.024
ATOM     15  HN62  A     1       0.989   1.569  -1.019
ATOM     16  H1'A  A     1       7.015  -1.556   0.890
ATOM     17  H1'B  A     1       8.166  -0.299   0.376
ATOM     18  H1'C  A     1       7.472  -0.261   2.016
ATOM     19  O2'   U     2      -0.061  -1.805  -0.886
ATOM     20  C2'   U     2      -1.096  -1.226  -0.128
ATOM     21  C1'   U     2      -2.091  -0.474  -1.043
ATOM     22  O4'   U     2      -3.113  -1.374  -1.389
ATOM     23  C4'   U     2      -2.899  -2.654  -0.767
ATOM     24  C3'   U     2      -1.958  -2.383   0.422
ATOM     25  N1    U     2      -2.701   0.718  -0.393
ATOM     26  C6    U     2      -3.925   0.662   0.239
ATOM     27  C5    U     2      -4.492   1.738   0.826
ATOM     28  C4    U     2      -3.825   3.025   0.807
ATOM     29  N3    U     2      -2.583   2.978   0.132
ATOM     30  C2    U     2      -1.978   1.897  -0.459
ATOM     31  O2    U     2      -0.884   1.975  -1.008
ATOM     32  O4    U     2      -4.214   4.070   1.290
ATOM     33  O3'   U     2      -1.199  -3.499   0.803
ATOM     34  C5'   U     2      -4.234  -3.278  -0.417
ATOM     35  O5'   U     2      -4.878  -2.475   0.568
ATOM     36  HO2'  U     2       0.763  -1.265  -0.761
ATOM     37  H05'  U     2      -5.731  -2.867   0.774
ATOM     38  H5    U     2      -5.452   1.668   1.316
ATOM     39  H6    U     2      -4.396  -0.312   0.223
ATOM     40  H4'   U     2      -2.385  -3.319  -1.473
ATOM     41  H1'   U     2      -1.576  -0.107  -1.930
ATOM     42  HO3'  U     2      -0.422  -3.469   0.222
ATOM     43  H3'   U     2      -2.546  -2.056   1.283
ATOM     44  H3    U     2      -2.065   3.846   0.091
ATOM     45  H2'   U     2      -0.700  -0.573   0.655
ATOM     46  H5'A  U     2      -4.847  -3.359  -1.323
ATOM     47  H5'B  U     2      -4.035  -4.290  -0.038
END
```

Table SIII: Sugar-pucker pseudorotation amplitude and phase of the involved sugars in the sugar mediated basepair systems along with crystallographic average and standard deviation.

		(System 28)	(System 29)	(System 30)	(System 31)	(System 32)
	Method	A:A W:S C	A:U w:s T	A:C W:S C	A:G S:S C	A:U W:S C
Amplitude	MP2/6-31G**	39.3	39.4	38.2	42.1	39.2
Phase		9.1	13.2	16.5	8	15.6
Amplitude	B3LYP/6-31G**	35.2	35.1	33.8	38.7	34.1
Phase		12.1	14.5	18.8	8.6	17.2
Amplitude	HF/cc-pVDZ	36.9	36.6	36.4	39.1	40.1
Phase		13.7	18.2	18.6	11.8	17.1
Amplitude	GGA:PW91/DZP	40.6	39.4	40.3	44.1	43.4
Phase		12.1	11	11.3	17.7	10.1
Amplitude	AM1	8.7	18.1	9.5	9.7	18.5
Phase		-48.4	-16.1	-30.9	-70.9	3.3
Amplitude	PM3	5.2	14.1	8.7	8.8	26
Phase		78.5	38.9	11.5	104.7	33.1
Amplitude	AMBER	45.3	37.8	36.6	39	41.7
Phase		22.1	22.7	16.1	30.1	11.2
Amplitude	Crystal Data Set	38.1 (3.6)	39.4 (5.2)	38.4 (2.7)	36.9 (3.8)	39.2 (3.3)
Phase	Avg. (Std.)	13.9 (10.4)	20.2 (28.3)	14.5 (4.9)	41.4 (55.4)	18.5 (7.5)

Table. SIV: Pyramidalization and bond order values of the bases and basepairs obtained through various quantum chemical methods

	Base/basepair	MP2/6-31G**		HF/cc-pVDZ		B3LYP/6-31G**		GGA: PW91/ DZP[#]
		Bond Order	Pyr (^{O})	Bond Order	Pyr (^{O})	Bond Order	Pyr (^{O})	Pyr (^{O})
	Adenine (isolated)	1.066	32.28	1.337	29.02	1.213	28.54	23.25
	Guanine (isolated)	1.032	45.87	1.235	40.28	1.143	42.7	42.51
	Cytosine (isolated)	1.066	34.23	1.292	28.17	1.199	30.38	27.59
1	G:C W:WC	1.107	30.91	1.337	19.35	1.250	16.27	0.02
		1.191	8.88	1.436	3.54	1.354	0.99	0.02
2	A:U W:W C	1.129	14.69	1.427	0.05	1.315	0.66	2.36
3	G:U W:W C[$]	1.049	39.96	1.257	35.30	1.158	36.86	35.58
4	A:G H: S T	1.107	28.52	1.378	22.84	1.279	18.40	0.71
		1.099	38.67	1.300	32.41	1.230	32.17	27.51
5	A:U H:W T	1.105	16.46	1.401	10.99	1.272	3.46	4.29
6	A:G W:W C	1.151	22.34	1.437	20.36	1.338	5.93	8.54
	[$]	1.033	44.89	1.244	40.88	1.151	42.03	43.03
7	A:A H:H T	1.112	29.45	1.382	24.66	1.285	17.31	7.11
		1.113	29.54	1.382	24.75	1.285	17.31	5.90
8	G:A S:W T	1.101	36.97	1.307	31.42	1.240	28.37	28.35
		1.123	17.87	1.412	14.86	1.298	6.28	16.11
9	A:A H: W T	1.118	24.16	1.401	18.31	1.305	11.25	14.52
		1.133	24.44	1.414	18.43	1.299	11.34	6.95
10	A:U H:W C	1.113	11.78	1.412	0.33	1.295	2.76	3.19
12	A:C H:W T	1.146	9.40	1.450	0.01	1.329	0.11	1.00
		1.144	16.32	1.407	0.04	1.301	0.07	10.19
13	G:C W:W T	1.095	50.87	1.300	29.80	1.189	38.63	31.67
	[$]	1.080	40.41	1.321	22.09	1.220	22.71	18.44
14	A:A W:W T	1.138	16.06	1.434	1.69	1.310	9.94	1.85
		1.138	15.95	1.434	13.65	1.310	9.83	1.41
15	A:U W:W T	1.120	18.16	1.420	0.99	1.283	0.64	6.95
16	G:G H:W C	1.080[$]	35.60	1.295[$]	28.35	1.165[$]	41.64 [$]	27.44
		1.080[$]	0.44	1.296[$]	28.29	1.186	37.71	38.02[$]
17	G:G H:W T	1.076	33.81	1.299	26.61	1.201	28.90	28.49
	[$]	1.039	44.60	1.244	39.39	1.153	41.23	40.78
18	G:G S:S T	1.093	35.91	1.302	26.69	1.225	29.21	26.96
		1.093	35.89	1.303	26.76	1.225	29.07	32.18
20	A:G s:s T [$]	1.059	35.60	1.356[$]	24.76	1.225	22.80	9.21
		1.041	44.42	1.274	37.09	1.194	38.82	38.41
21	G:U s:h C	1.089	38.11	1.302	32.35	1.226	31.90	27.15
22	A:A h:s T	1.102	23.92	1.385	19.28	1.275	15.16	5.61

	[$]	1.071	30.67	1.346	27.01	1.218	26.15	18.87
23	A:G w:s C [$]	1.065	26.09	1.344	26.22	1.212	28.35	26.85
		1.072	41.70	1.278	35.78	1.212	30.41	32.08
24	A:U s:w C [$]	1.072	30.44	1.344	27.95	1.217	28.02	19.78
26	A:C w:w C [$]	1.053	37.66	1.317	34.73	1.198	32.24	31.08
		1.117	29.01	1.349	21.15	1.279	5.96	17.63
27	A:A w:w C	1.119	19.24	1.400	19.64	1.283	16.21	9.25
	[$]	1.061	33.99	1.332	31.34	1.205	26.90	28.17
28	A:A W:S C	1.126	28.57	1.407	25.02	1.288	23.71	12.52
	[$]	1.071	28.85	1.354	25.93	1.223	28.94	18.48
29	A:U w:s T[$]	1.118	32.05	1.350	25.56	1.227	22.35	20.07
30	A:C W:S C	1.144	19.66	1.453	14.83	1.326	7.73	5.70
	[$]	1.075	32.17	1.310	29.94	1.210	28.44	23.44
31	A:G S:S C [$]	1.079	28.40	1.361	24.20	1.226	23.00	14.50
		1.080	30.81	1.307	31.07	1.221	30.34	22.01
32	A:U W:S C	1.130	21.53	1.410	22.71	1.297	14.48	11.91

[$] Represents the free amino groups

[#] Bond order values could not be calculated by this method

Table. SV: Intra Basepair Parameters of the Basepairs in the optimized geometries obtained by different methods and the average and standard deviations of the basepair parameters in the crystal dataset.

Serial No.	Basepair	Method	Buckle (^{O})	Open Angle(^{O})	Propeller(^{O})	Stagger (Å)	Shear (Å)	Stretch (Å)
1	G:C W:W C	MP2/6-31G**	-4.92	-3.08	-7.88	-0.14	0.12	2.93
		HF/cc-pVDZ	-4.2	-3.04	-3.63	-0.09	0.21	3.04
		B3LYP/6-31G**	-0.3	-3.43	2.21	0.12	0.17	2.92
		PW91/DZP	-1.5	0.48	-2.37	-0.37	0.29	2.85
		AM1	51.24	0.47	1.66	-0.69	0.2	2.98
		AMBER	-3.28	-2.21	2.54	0	0.34	2.91
		AMBER_WATER	18.13	6.29	19.8	0.74	-0.64	2.75
		PM3	-3.98	-0.22	-1.81	-0.48	0.06	2.77
		CRYSTAL_AVG	-5.39	0.49	-6.51	-0.14	-0.07	2.86
		CRYSTAL_STDV	9.31	3.77	7.88	0.37	0.38	0.13
2	A:U W:W C	MP2/6-31G**	-4.42	3.12	-2.24	0.08	0.08	2.83
		HF/cc-pVDZ	0.03	2.03	0.03	0	0.13	2.99
		B3LYP/6-31G**	-0.98	0.03	0.35	0	0.09	2.86
		PW91/DZP	4.11	1.23	-1.73	-0.03	0.03	2.78
		AM1	13.22	-8.76	3.35	0.1	0.06	3.44
		AMBER	6.2	-1.65	-3.98	-0.11	0.21	2.93
		AMBER_WATER	71.64	-36.6	-30.18	-0.2	0.46	4.1
		PM3	-5.17	-1.03	-3.66	0.21	0.05	2.81
		CRYSTAL_AVG	-1.96	3.27	-6.56	-0.04	0.11	2.79
		CRYSTAL_STDV	8.3	4.5	8.27	0.36	0.29	0.12
3	G:U W:W C	MP2/6-31G**	-4.03	0.66	-0.09	0.13	-2.4	2.86
		HF/cc-pVDZ	-0.52	1.71	-1.94	-0.08	-2.54	2.94
		B3LYP/6-31G**	3.94	4.11	-1.3	-0.15	-2.42	2.84
		PW91/DZP	-0.87	0.29	-5.78	-0.04	-2.33	2.79
		AM1	-16.78	6.12	3.76	-0.47	2.23	2.99
		AMBER	0.85	0.18	-1.91	0.02	-2.54	2.86
		AMBER_WATER	18.72	0.35	7.6	-0.11	-2.55	2.86
		PM3	-0.03	3.26	-3.57	-0.21	-2.52	2.74
		CRYSTAL_AVG	-1.51	-0.61	-6.55	-0.17	-2.22	2.81
		CRYSTAL_STDV	8.48	5.8	7.32	0.41	0.43	0.15
4	A:G H:S T	MP2/6-31G**	13.55	-24.57	-47.02	0.19	1.79	3.13
		HF/cc-pVDZ	4.49	-21.1	-46.7	0.15	1.9	3.39
		B3LYP/6-31G**	6.42	-20.3	-40.9	0.05	1.95	3.24
		PW91/DZP	-13	-18.15	-24.78	0.23	2.09	3.21
		AM1	-48.92	11.42	17.95	0.91	2.7	3.23
		AMBER	-17.57	-25.05	-49.97	0.11	1.9	3.18
		AMBER_WATER	-38.3	-11.5	-13.68	-0.48	2.09	3.43
		PM3	32.89	-16.04	-29.79	0.56	1.98	3.24
		CRYSTAL_AVG	-2.12	-13.1	1.07	-0.14	2.24	3.31
		CRYSTAL_STDV	14.1	5.7	13.1	0.5	0.36	0.17
5	A:U H:W T	MP2/6-31G**	6.24	-5.41	-1.93	-0.09	0.11	2.79
		HF/cc-pVDZ	4.21	-3.28	-1.63	-0.06	0.07	2.95
		B3LYP/6-31G**	-3.2	-7.49	1.52	0	0.15	2.79
		PW91/DZP	4.9	-2.93	-0.91	-0.03	0.11	2.77
		AM1	16.81	11.36	-2.99	0.02	0.14	3.46
		AMBER	6.97	1.46	-0.46	0	0.02	2.93
		AMBER_WATER	52.24	-4.58	28.68	-1.35	0.18	2.66
		PM3	-6.11	5.63	8.66	0.22	0.16	2.79

		CRYSTAL_AVG	-1.41	-0.39	-1.17	-0.04	0.17	2.82
		CRYSTAL_STDV	13.6	6.63	9.75	0.46	0.49	0.19
6	A:G W:W C	MP2/6-31G**	-0.24	-1.6	-21.9	-0.13	-0.1	2.89
		HF/cc-pVDZ	-3.85	-2.85	-21	-0.2	0.01	3.06
		B3LYP/6-31G**	6.14	-2.93	-12.8	-0.21	-0.01	2.94
		PW91/DZP	3.72	-1.84	-19.01	-0.31	-0.08	2.82
		AM1	11.18	-8.26	1.19	0.27	-0.36	3.39
		AMBER	4.56	-2.6	-6.64	-0.15	-0.08	2.95
		AMBER_WATER	-18.3	-7.92	20.25	0.07	0.31	3.02
		PM3	-12.7	0.06	-5.09	-0.03	0.03	2.8
		CRYSTAL_AVG	-10.8	1.27	-8.55	-0.41	0.07	2.8
		CRYSTAL_STDV	14.2	5.84	12.05	0.41	0.5	0.19
7	A:A H:H T	MP2/6-31G**	15.21	0	-45.8	0	2.48	2.75
		HF/cc-pVDZ	11.2	-0.01	-37.5	0	2.6	3.01
		B3LYP/6-31G**	-0.06	-0.06	-32.1	0.01	2.67	2.88
		PW91/DZP	2.3	-0.01	-10.44	-0.02	2.72	2.9
		AM1	16.84	-0.26	-7.71	-0.07	3.57	3.28
		AMBER	0.62	0.23	-10.65	-0.01	2.65	2.94
		AMBER_WATER	37.77	3.16	3.16	0.36	2.83	2.84
		PM3	-0.03	-0.01	0.05	-0.53	3.03	2.69
		CRYSTAL_AVG	-9.63	-4.66	5.81	-0.35	2.51	2.86
		CRYSTAL_STDV	15.8	3.28	13.25	0.29	0.35	0.17
8	G:A S:W T	MP2/6-31G**	10.55	-17.39	-24.4	-0.03	1.74	3.28
		HF/cc-pVDZ	11.35	-16	-19.5	-0.05	1.76	3.48
		B3LYP/6-31G**	6.74	-18.4	-17.4	-0.07	1.82	3.32
		PW91/DZP	4.05	-39.08	-34.67	0.01	2.24	2.81
		AM1	59.36	8.72	-2.08	-0.86	2.49	3.35
		AMBER	-14.84	-19.73	-25.88	0.1	1.79	3.28
		AMBER_WATER	8.9	-16.1	22.67	0.58	1.72	3.26
		PM3	21.81	-17.95	-4.62	0	1.86	3.15
		CRYSTAL_AVG	13.04	-13.6	0.27	-0.16	1.85	3.32
		CRYSTAL_STDV	19	7.02	16.55	0.58	0.37	0.2
9	A:A H:W T	MP2/6-31G**	-10.37	1.87	28.94	0.01	2.45	2.89
		HF/cc-pVDZ	-7.74	1.11	21.05	0.01	2.51	3.11
		B3LYP/6-31G**	-1.4	0.95	17.58	0	2.5	2.94
		PW91/DZP	-0.13	2.91	22.63	0.14	2.51	2.83
		AM1	-10.41	5.65	31.66	-0.61	8.5	-2.3
		AMBER	10.64	1.05	9.17	-0.07	2.55	2.94
		AMBER_WATER	60.6	-7.48	59.44	-0.72	2.38	2.63
		PM3	-2.3	0.32	0.68	0.44	2.73	2.72
		CRYSTAL_AVG	1.84	5.7	-2.88	0.04	2.31	2.92
		CRYSTAL_STDV	12.8	5.23	19.57	0.5	0.36	0.19
10	A:U H:W C	MP2/6-31G**	-4.51	2.42	-1.76	0.04	-0.1	2.8
		HF/cc-pVDZ	0.12	1.24	0.06	0	-0.06	2.96
		B3LYP/6-31G**	-0.24	2.23	-2.63	-0.01	-0.13	2.79
		PW91/DZP	0.49	-0.17	-3.62	0	-0.11	2.79
		AM1	12.59	-11.03	2.72	-0.02	-0.22	3.47
		AMBER	2.47	-4.48	-3.77	-0.2	0.06	2.92
		AMBER_WATER	117.8	-39.5	-7.38	0.97	0.69	3.23
		PM3	-6.61	-2.96	-4.11	0.21	-0.24	2.78
		CRYSTAL_AVG	-3.59	2.93	-4.53	0.15	-0.22	2.8
		CRYSTAL_STDV	18.1	6.78	12.38	0.6	0.43	0.16
11	U:U W:W C	MP2/6-31G**	-1.5	-1.17	2.86	0	2.54	2.89
		HF/cc-pVDZ	-0.01	-0.22	0	0	2.74	2.95
		B3LYP/6-31G**	2.27	-0.66	-6.57	0.03	2.55	2.85

		PW91/DZP	0.07	-0.57	-2.82	-0.02	2.48	2.82
		AM1	0.95	1.47	-1.05	0.00	2.97	2.97
		AMBER	-2.55	-1.75	-0.95	0	-2.8	2.83
		AMBER_WATER	2.77	-0.16	9.64	0.14	-2.89	2.82
		PM3	-2.12	2.73	-4.3	0.09	2.6	2.74
		CRYSTAL_AVG	-10.1	-2.33	-12.6	-0.15	-2.36	2.86
		CRYSTAL_STDV	8.56	5.29	8.02	0.4	0.37	0.16
12	A:C H:W T	MP2/6-31G**	2.39	-3.64	1.28	-0.23	2.33	2.92
		HF/cc-pVDZ	0.01	-3.59	0	0	2.37	3.09
		B3LYP/6-31G**	-0.35	-2.73	0.09	0	2.41	2.93
		PW91/DZP	15.61	-2.05	0.19	0	2.41	2.86
		AM1	62.03	-30.34	13.82	0.73	2.35	3.67
		AMBER	1.95	-3.35	3.53	0.02	2.25	2.92
		AMBER_WATER	2.47	-7.19	-10.61	0.39	2.26	2.9
		PM3	17.29	-0.69	-14.6	-0.03	2.61	2.74
		CRYSTAL_AVG	-1.26	-4.3	-5.68	0.18	2.37	2.91
		CRYSTAL_STDV	20.5	6.37	15.61	0.48	0.36	0.18
13	G:C W:W T	MP2/6-31G**	-164.44	5.65	-63.64	0.13	-0.97	2.87
		HF/cc-pVDZ	-30.58	68.21	-43.03	0.15	-3.56	3.19
		B3LYP/6-31G**	-17.61	13.42	-37.98	0.06	-2.54	3.02
		PW91/DZP	-16.06	10.64	-11.47	0.2	-2.65	3.02
		AM1	-14.33	82.47	-25.94	-0.64	-4.05	2.74
		AMBER	-1.85	-16.16	-3.18	0.01	-3.24	2.90
		AMBER_WATER	-38.25	17.63	59.91	1.09	-1.35	2.64
		PM3	16.6	1.37	16.07	-0.31	-2.59	2.79
		CRYSTAL_AVG	-4.35	7.34	-6.67	-0.09	-2.27	2.88
		CRYSTAL_STDV	15.35	7.3	10.69	0.42	0.48	0.16
14	A:A W:W T	MP2/6-31G**	0.1	-0.02	0.22	0.33	2.33	2.98
		HF/cc-pVDZ	-0.84	0.03	1.24	0	2.34	3.16
		B3LYP/6-31G**	4.4	0	-12.1	0	2.27	2.98
		PW91/DZP	-1.18	-0.18	0.07	-0.08	2.33	2.88
		AM1	-0.23	0	0.35	-0.01	2.86	3.53
		AMBER	12.35	0.17	8	0.02	2.33	2.96
		AMBER_WATER	28.87	23.3	76.09	1.01	1.93	2.68
		PM3	-0.75	-0.04	-0.02	-0.43	2.36	2.78
		CRYSTAL_AVG	7.87	-7.58	-2.04	-0.53	2.19	2.87
		CRYSTAL_STDV	11.3	7.53	30.17	0.49	0.47	0.23
15	A:U W:W T	MP2/6-31G**	-5.73	-5.62	2.77	0.1	-0.1	2.83
		HF/cc-pVDZ	0.28	-3.58	-0.3	-0.01	-0.13	2.99
		B3LYP/6-31G**	-0.67	-7.96	-0.57	0.03	-0.06	2.81
		PW91/DZP	-4.69	-3.74	2.62	0.04	-0.05	2.78
		AM1	-0.75	-10.25	1.68	-0.01	-0.14	3.47
		AMBER	-4.74	-1.02	-1.37	0.03	-0.16	2.93
		AMBER_WATER	-23.8	-5.81	6.23	-0.07	-0.29	2.9
		PM3	-6.16	3.85	7.75	0.22	-0.14	2.8
		CRYSTAL_AVG	0.05	-1.9	0.13	0.03	-0.24	2.83
		CRYSTAL_STDV	12.7	7.42	13.34	0.55	0.41	0.19
16	G:G H:W C	MP2/6-31G**	-51.38	-86.65	-18.78	-0.75	-4.07	3.82
			-49.34#	0.35#	25.86#	0.06#	1.88#	2.72#
		HF/cc-pVDZ	-14.52	-94.54	-8.67	-0.32	-4.25	4.18
			-16.19#	0.04#	4.87#	0.01#	2.17#	2.87#
		B3LYP/6-31G**	-49.98	-15.60	-41.41	0.08	-2.44	2.98
		PW91/DZP	13.27	-4.84	1.75	0.16	-2.99	3.06
		AM1	64.95	6.80	35.59	0.21	-3.73	2.64
		AMBER	7.54	-6.09	-0.59	-0.14	-3.81	2.90

		AMBER_WATER	41.76	1.43	7.79	0.85	3.55	2.73
		PM3	22.52	0.11	32.7	0.08	-2.79	2.71
		CRYSTAL_AVG	6.43	-3.86	-0.31	0.08	-2.94	2.88
		CRYSTAL_STDV	12.62	6.2	12.13	0.61	0.41	0.18
17	G:G H:W T	MP2/6-31G**	-10.94	-11.38	-5.16	-0.11	0.15	2.83
		HF/cc-pVDZ	7.49	-10.4	4.94	0.08	0.14	2.96
		B3LYP/6-31G**	10.26	-9.91	3.48	0.03	0.17	2.85
		PW91/DZP	20.52	-7.64	2.86	-0.01	0.2	2.83
		AM1	29.14	-10.73	-2.39	-0.78	-0.38	3.22
		AMBER	28.84	-3.69	0.8	-0.54	0.08	2.87
		AMBER_WATER	-0.77	-32.2	-49.07	1.78	-2.21	2.52
		PM3	-12.89	-1.76	-12.01	0.05	0.24	2.81
		CRYSTAL_AVG	9.29	1.77	-0.64	-0.13	-0.02	2.89
		CRYSTAL_STDV	12.9	6.59	8.36	0.28	0.65	0.17
18	G:G S:S T	MP2/6-31G**	-11.51	-0.1	41.89	-0.02	1.05	3.45
		HF/cc-pVDZ	-7.71	0.09	40.71	0	1.09	3.67
		B3LYP/6-31G**	-13	0.08	30.85	0	1.17	3.53
		PW91/DZP	0.96	-4.17	36.56	-0.43	1.19	3.43
		AM1	-67.72	-18.84	-15.13	-0.66	1.92	3.63
		AMBER	24.24	-0.8	53.1	-0.05	1.13	3.47
		AMBER_WATER	-123	18.67	2.05	2.25	2.55	2.36
		PM3	-44.78	5.06	8.71	-0.63	1.28	1.28
		CRYSTAL_AVG	4.64	-4.54	13.3	-0.66	1.27	3.46
		CRYSTAL_STDV	22.1	3.6	18.48	0.46	0.29	0.24
19	U:U W:W T	MP2/6-31G**	0.31	-0.01	0.38	0	-2.6	2.93
		HF/cc-pVDZ	-0.31	0.14	-0.66	-0.01	-2.75	2.97
		B3LYP/6-31G**	-0.34	0.02	-0.89	0	-2.58	2.89
		PW91/DZP	-11.5	0.1	-6.55	0.02	-2.49	2.86
		AM1	-0.29	-0.02	-0.07	0.00	-3.05	2.94
		AMBER	-11.02	-0.13	-8.5	0.02	-2.73	2.88
		AMBER_WATER	16.27	1.81	20.85	0.26	-2.51	2.93
		PM3	0.79	0.01	1.26	0.28	-2.69	2.67
		CRYSTAL_AVG	-6.22	-4.52	-4.36	0.11	-2.35	2.79
		CRYSTAL_STDV	16	3.25	10.24	0.45	0.45	0.16
20	A:G s:s T	MP2/6-31G**	97.13	47.17	-61.45	-2.56	-0.1	1.64
		HF/cc-pVDZ	-9.47	19.51	-14.3	-0.55	1.6	3.46
		B3LYP/6-31G**	1.52	23.45	-33.6	-0.9	1.38	3.2
		PW91/DZP	-10.6	24.27	-20.69	-0.56	1.55	3.15
		AM1	-22.03	23.91	-2.91	-1.01	2.30	3.42
		AMBER	-102.7	49.3	80.69	2.75	-0.4	1.58
		AMBER_WATER	-7.42	-7.42	34.68	-0.13	1.2	3.42
		PM3	-9.31	30.88	-2.52	-0.23	1.72	2.93
		CRYSTAL_AVG	-15.8	27.99	-7.44	0.22	1.71	3.02
		CRYSTAL_STDV	26.9	7.23	13.6	0.88	0.29	0.21
21	G:U s:h C	MP2/6-31G**	3.12	7.74	27.12	0.48	0.63	3.27
		HF/cc-pVDZ	4.18	0.19	26.19	0.46	0.74	3.65
		B3LYP/6-31G**	3.61	4.6	25.57	0.47	0.63	3.39
		PW91/DZP	-5.65	6.24	-1.47	0.14	0.61	3.30
		AM1	-151.35	12.53	83.67	5.50	-0.67	-0.33
		AMBER	-1.75	-0.73	0.09	-0.06	0.99	3.54
		AMBER_WATER	-19.4	-3.27	9.42	-0.76	0.96	3.47
		PM3	-13.95	-0.67	-6.7	0.19	0.71	3.48
		CRYSTAL_AVG	-11.8	-1.22	0.15	-0.1	0.99	3.44
		CRYSTAL_STDV	18.2	5.48	7.45	0.56	0.37	0.14
22	A:A h:s T	MP2/6-31G**	-13.38	0.45	12.11	0.18	2.25	2.91

		HF/cc-pVDZ	-9.97	-2.23	-2.79	0.28	2.39	3.09
		B3LYP/6-31G**	4.32	-1.05	18.61	-0.44	2.29	2.92
		PW91/DZP	-6.49	-0.95	2.42	0.01	2.36	2.85
		AM1	-19.09	-9.09	7.28	0.39	3.08	3.17
		AMBER	-99.06	-36.54	84.24	-2.59	0.78	1.33
		AMBER_WATER	43.61	33.02	61.18	-0.15	1.7	3.62
		PM3	-21.65	7.69	6.33	0.24	2.53	2.91
		CRYSTAL_AVG	-5.65	-1.39	1.66	-0.13	2.38	2.75
		CRYSTAL_STDV	13.5	6.01	9.41	0.52	0.3	0.2
23	A:G w:s C	MP2/6-31G**	15.39	40.75	10.49	0.4	2.1	2.97
		HF/cc-pVDZ	13.41	37.95	7.47	0.49	2.19	3.18
		B3LYP/6-31G**	-4.35	34.47	-16.4	0.04	2.23	3.07
		PW91/DZP	12.78	45.91	-42.34	-0.73	1.84	2.81
		AM1	-63.96	18.13	-2.31	1.04	-3.02	2.85
		AMBER	89.19	46.9	-50.66	-2.23	0.59	2.02
		AMBER_WATER	31.8	40.84	-22.56	-1.46	1.94	2.79
		PM3	23.58	58.14	-16.57	0.78	2.32	2.8
		CRYSTAL_AVG	-19.3	45.49	-6.41	-0.1	2.07	2.84
		CRYSTAL_STDV	28.9	12.6	24.19	0.92	0.43	0.25
24	A:U s:w C	MP2/6-31G**	-14.57	-3.24	17.21	0.24	0.18	2.94
		HF/cc-pVDZ	-9.3	-3.84	11.43	0.17	0.21	3.12
		B3LYP/6-31G**	2.34	-6.63	2.83	0.03	0.16	2.98
		PW91/DZP	-19.9	-4.37	9.29	0.22	0.14	2.9
		AM1	6.60	-5.34	1.90	0.03	-0.33	3.05
		AMBER	-25	-1.85	-1.3	0.62	0.21	2.94
		AMBER_WATER	-11.6	-5.87	-65.02	-0.6	0.19	3.04
		PM3	-8.6	1.69	23.38	-0.09	0.23	2.83
		CRYSTAL_AVG	-21.7	-3.7	11.6	0.14	0.15	2.95
		CRYSTAL_STDV	10.6	4.23	12.27	0.32	0.26	0.17
25	U:U w:h T	MP2/6-31G**	0.72	7.7	-1.09	0.01	2.54	3.07
		HF/cc-pVDZ	0.07	8.13	-0.07	0	2.74	3.16
		B3LYP/6-31G**	-2.05	9.07	2.52	0.01	2.7	3.04
		PW91/DZP	3.9	8.77	1.01	0	2.54	3.01
		AM1	0.56	3.99	1.38	0.01	2.67	3.18
		AMBER	6.39	15.07	1.91	-0.14	3.03	3.09
		AMBER_WATER	-7.91	4.58	-15.64	1.37	2.9	2.74
		PM3	-7.46	16.05	-10.77	0.09	2.63	3.15
		CRYSTAL_AVG	15.73	13.61	-9	0.18	2.59	2.91
		CRYSTAL_STDV	18.7	6.89	15.07	0.67	0.3	0.22
26	A:C w:w C	MP2/6-31G**	21.14	18.68	-6.29	-0.22	-2.4	2.66
		HF/cc-pVDZ	18.18	18.57	-4.92	-0.09	-2.49	2.81
		B3LYP/6-31G**	4.42	13.55	-4.84	0.01	-2.6	2.7
		PW91/DZP	17.17	15.25	-8.41	-0.06	-2.44	2.63
		AM1	71.17	1.69	6.98	-1.01	-3.38	2.54
		AMBER	12.31	10.95	-5.11	0.18	-2.51	2.75
		AMBER_WATER	-16.1	-1.02	-31.03	-1.81	-2.45	2.73
		PM3	13.99	5.78	-2.44	-0.35	-2.51	2.71
		CRYSTAL_AVG	10.02	14.26	-8.08	0.05	-2.45	2.44
		CRYSTAL_STDV	12.4	10.4	6.61	0.94	0.45	0.38
27	A:A w:w C	MP2/6-31G**	0.17	17.78	-11.53	0.15	2.61	2.64
		HF/cc-pVDZ	2.21	17.69	-8.78	0.14	2.67	2.82
		B3LYP/6-31G**	8.96	14.47	-0.22	0.09	2.5	2.75
		PW91/DZP	6.63	15.95	-8.07	0.07	2.56	2.58
		AM1	6.61	23.24	-12.85	0.42	3.20	2.89
		AMBER	-7.39	15.03	-24.01	-0.72	-2.53	2.66

		AMBER_WATER	30.68	6.1	-18.36	0.03	-2.86	2.9
		PM3	-15.26	4.06	-1.01	-0.38	2.58	2.73
		CRYSTAL_AVG	-16.8	21.66	-15.4	-0.77	-2.14	2.48
		CRYSTAL_STDV	15.7	13.2	12.76	0.21	0.91	0.19
28	A:A W:S C	MP2/6-31G**	36.53	-10.99	-3.97	-0.33	-2.60	3.21
		HF/cc-pVDZ	-13.34	-26.85	-46.15	0.00	-2.40	3.53
		B3LYP/6-31G**	-18.29	-26.14	-46.70	-0.21	-2.49	3.40
		PW91/DZP	28.33	-19.49	-27.51	-0.24	-2.75	3.25
		AM1	-85.49	-35.53	-44.98	-0.95	-2.98	3.50
		AMBER	-29.78	-19.76	34.35	-0.87	-2.35	3.01
		AMBER_WATER	-34.75	-37.75	41.92	-1.96	-2.02	2.57
		PM3	19.74	-15.04	-5.63	-0.54	-2.88	3.01
		CRYSTAL_AVG	-4.49	-29.14	-12.72	-0.38	-2.51	3.52
		CRYSTAL_STDV	13.85	10.12	12.24	0.40	0.46	0.26
29	A:U w:s T	MP2/6-31G**	74.76	-56.77	36.37	-2.97	2.9	2.14
		HF/cc-pVDZ	-22.88	-49.46	-22.95	-0.71	0.33	4.3
		B3LYP/6-31G**	31.63	-34.6	2.77	-1.2	0.79	3.66
		PW91/DZP	31.47	-36.06	-16.15	-1.1	0.26	3.66
		AM1	13.26	-34.82	-13.83	-0.90	0.44	3.63
		AMBER	-11.21	-149.7	-105.9	3.57	0.37	-0.88
		AMBER_WATER	21.71	-31.7	-28.68	-0.1	0.39	3.93
		PM3	-65.03	-37.98	-28.52	-1.62	-0.58	3.75
		CRYSTAL_AVG	-1.57	-58.7	-18.6	-0.33	-0.4	4.06
		CRYSTAL_STDV	21	12.1	14.55	0.88	0.51	0.31
30	A:C W:S C	MP2/6-31G**	46.82	-32.19	-16.43	-1.1	-0.9	4.15
		HF/cc-pVDZ	26.99	-34.5	-19.8	-0.93	-0.9	4.35
		B3LYP/6-31G**	42.14	-35.2	-13.1	-1.23	-0.76	4.21
		PW91/DZP	-19.5	-24.35	-25.65	-0.99	-0.36	3.83
		AM1	47.39	-43.82	-8.24	-1.67	-1.52	4.20
		AMBER	5.24	-28.33	-10.61	-0.69	-0.95	3.97
		AMBER_WATER	-54.7	-14.3	-43.43	-1.33	-0.2	3.42
		PM3	37.64	-42.97	-7.5	-1.76	-0.73	4.16
		CRYSTAL_AVG	-4.44	-34.7	-21.3	-0.47	0.3	4.23
		CRYSTAL_STDV	22.8	10.3	14.47	0.62	0.64	0.37
31	A:G S:S C	MP2/6-31G**	-9.51	-3.2	-48.48	-0.65	-1.8	3.74
		HF/cc-pVDZ	-3.21	-9.3	-59.4	-0.02	-1.83	3.84
		B3LYP/6-31G**	-15.4	-8.22	-53.8	-0.2	-1.87	3.73
		PW91/DZP	20.34	-1.13	-59.39	-0.62	-2.16	3.58
		AM1	53.08	-2.15	-14.86	-1.06	-3.03	3.37
		AMBER	107.02	20.68	-63.88	-0.87	-2.05	3.27
		AMBER_WATER	-48	-6.39	0.97	0.56	-2	3.67
		PM3	34.06	0.63	-40.04	-0.28	-2.3	3.52
		CRYSTAL_AVG	-1.6	-15.8	-8.36	-0.13	-2.36	3.82
		CRYSTAL_STDV	23.2	20.7	30.3	0.95	0.39	0.46
32	A:U W:S C	MP2/6-31G**	-83.93	-35.11	-18.25	-0.77	-0.6	4.57
		HF/cc-pVDZ	-42.61	-29.2	-23.8	-1.01	0.8	4.3
		B3LYP/6-31G**	-45.45	-30.7	-20.7	-1.29	0.56	4.2
		PW91/DZP	6.59	-24.65	-9.28	-0.74	0.54	3.98
		AM1	71.92	-28.53	-25.99	-1.78	-0.52	4.25
		AMBER	1.76	-13.47	20.28	0.68	0.84	3.42
		AMBER_WATER	-80.5	-1.48	-45.97	-2.99	1.18	2.59
		PM3	-45.88	-32.03	-15.68	-2.2	0.4	3.78
		CRYSTAL_AVG	-17.6	-31.5	-1.47	-0.59	0.44	4.26
		CRYSTAL_STDV	37.2	8.33	13.42	0.5	0.45	0.28

[#] Represents the basepair parameters when it is in W:W T conformations.