

## Supplementary Material

**Figure S1.** (a) Amber 4.1 atom types and atomic charges for 2'-deoxyribose and ribose sugars. (b) CFF95 atom types and atomic charges for 2'-deoxyribose and ribose sugars.

### MSCFF Parameters (Tables S1-S5)

The potential forms are described in the Methods section and discussed in detail in reference 63.

**Table S1.** MSCFF Exponential-6 Van Der Waals Parameters.

Atom Type	$R_0$ (Å)	$D_0$ (kcal/mol)	$\zeta$
H_	3.1950	0.0152	12.382
H__A	3.1950	0.0001	12.000
C_3	3.8983	0.0951	14.034
C_S	3.8983	0.0951	14.034
C_R	3.8983	0.0951	14.034
N_R	3.6621	0.0774	13.843
O_3	3.4046	0.0957	13.483
O_S	3.4046	0.0957	13.483
O_3:::H__A <sup>a</sup>	2.7500	0.2000	9.000

<sup>a</sup>A specific off-diagonal non-bond Morse potential for hydrogen bonding.<sup>63</sup>

**Table S2.** MSCFF Harmonic Bond Parameters.

Bond ( <i>ij</i> )	$K$ (kcal/mol)	$R_0$ (Å)
C_3 -H_	659.8	1.111
C_3 -C_3	699.6	1.514
C_S -H_	659.8	1.111
C_S -C_3	699.6	1.514
C_R -H_	712.3	1.083
C_R -C_R	951.8	1.407
N_R -C_3	1046.5	1.456
N_R -C_R	1359.3	1.373
O_3 -H__A	1128.4	0.988
O_3 -C_3	1030.8	1.415
O_3 -C_S	1030.8	1.415
O_S -C_3	1030.8	1.415

Table S3. MSCFF Angle Parameters.

Angle ( <i>ijk</i> )			K (kcal/mol)	$\theta_0$ (°)
H_	-C_3	-H_	75.6	109.5
C_3	-C_3	-H_	117.4	109.5
C_S	-C_3	-H_	117.4	109.5
C_S	-C_3	-C_3	214.2	109.5
N_R	-C_3	-H_	170.1	109.5
N_R	-C_3	-C_3	303.6	109.5
O_3	-C_3	-H_	165.9	109.5
O_3	-C_3	-C_3	290.0	109.5
O_3	-C_3	-C_S	290.0	109.5
O_S	-C_3	-H_	165.9	109.5
O_S	-C_3	-C_3	290.0	109.5
O_S	-C_3	-C_S	290.0	109.5
O_S	-C_3	-N_R	413.5	109.5
C_3	-C_S	-H_	117.4	109.5
C_3	-C_S	-C_3	214.2	109.5
O_3	-C_S	-H_	165.9	109.5
O_3	-C_S	-C_3	290.0	109.5
C_R	-C_R	-H_	117.1	120.0
C_R	-C_R	-C_R	229.3	120.0
N_R	-C_R	-H_	162.4	120.0
N_R	-C_R	-C_R	314.5	120.0
C_R	-N_R	-C_3	216.8	120.0
C_R	-N_R	-C_R	247.2	120.0
C_3	-O_3	-H__A	174.3	109.5
C_S	-O_3	-H__A	174.3	109.5
C_3	-O_S	-C_3	297.8	112.0

**Table S4.** MSCFF Torsion Parameters.

Torsion ( <i>ijkl</i> )				v0	v2	v3	v4	v6
X	-C_3	-C_3	-X	1.059		1.059		
X	-C_S	-C_3	-X	1.059		1.059		
X	-O_3	-C_3	-X	1.000		1.000		
X	-O_S	-C_3	-X	1.000		1.000		
X	-O_3	-C_S	-X	1.000		1.000		
X	-C_R	-C_R	-X	15.000	-15.000			
X	-N_R	-C_R	-X	15.000	-15.000			
X	-N_R	-C_3	-X	0.500				-0.500
H__A	-O_3	-C_3	-H_	4.000	3.000	1.000		
H__A	-O_3	-C_S	-H_	4.000	3.000	1.000		
C_3	-C_S	-C_3	-O_S	9.159	8.100	1.059		
O_3	-C_S	-C_3	-O_3	11.559	1.500	1.059	-9.000	
O_3	-C_S	-C_3	-O_S	11.559	1.500	1.059	-9.000	
O_3	-C_3	-C_3	-N_R	11.559	1.500	1.059	-9.000	
O_S	-C_3	-C_3	-O_3	11.559	1.500	1.059	-9.000	

**Table S5.** MSCFF Inversion Parameters.

Inversion ( <i>cijk</i> )				K (kcal/mol)
N_R	-X	-X	-X	6.000
C_R	-X	-X	-X	6.000

Figure S1.

