Supporting Information

Refinement of the Cornell *et al.* Nucleic Acids Force Field based on Reference Quantum Chemical Calculations of Glycosidic Torsion Profiles

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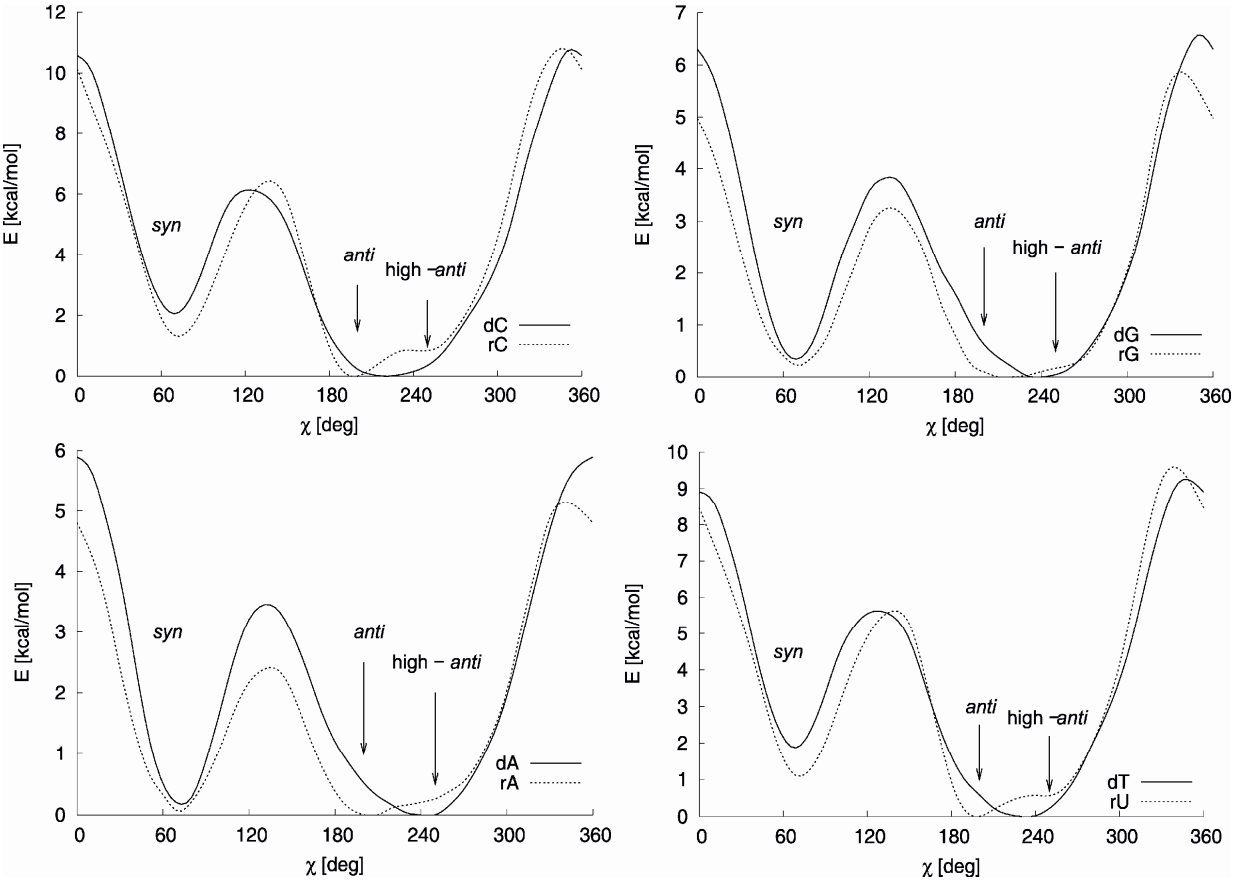
Figure S1. χ torsion profile for rX (full line) and dX (dotted line). The typical average X-ray values for A-RNA, B-DNA and Z-DNA are marked. PBE/LP data with inclusion of solvent effects.



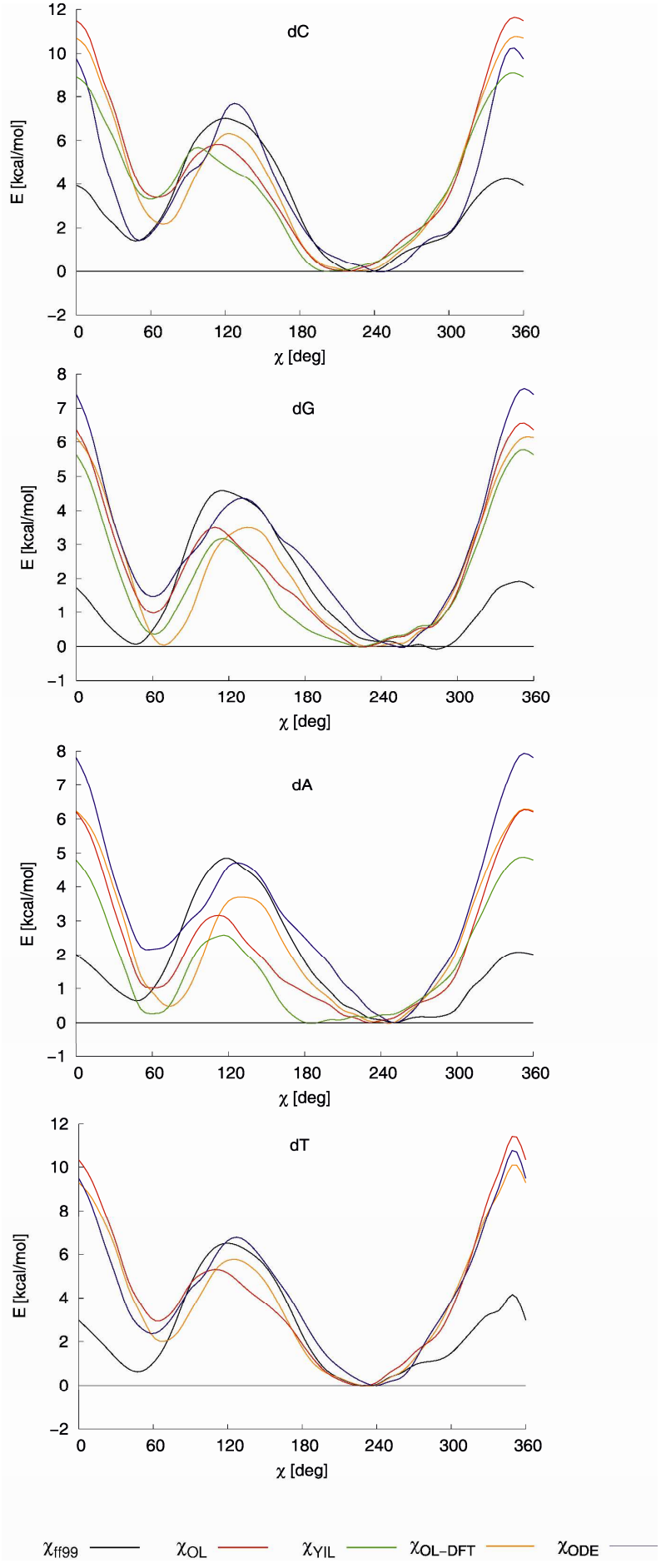


Figure S2. Torsion profiles in solvent (full force field energies) for χ angle for ff99 (black), Ode *et al.* (blue), Yildirim *et al.* (green) and parameters derived herein ($\chi_{OL\text{-}DFT}$ orange, χ_{OL} red) for deoxyribonucleosides. Compare this figure with Fig. 6 in the article.

Figure S3. QM torsion profiles calculated in vacuum and with COSMO solvent model (PBE/LP-1.06-23), MM torsion profiles in vacuum and with PB solvent model and the χ dihedral term contribution to the torsion derived from the continuum solvent data of 2-deoxyribonucleoside with C2'-endo (full line) and C3'-endo (dotted line) sugar puckers and ribonucleoside with C3'-endo sugar pucker (dashed line). All data are given in one high-resolution picture which can be enlarged to simplify comparison.

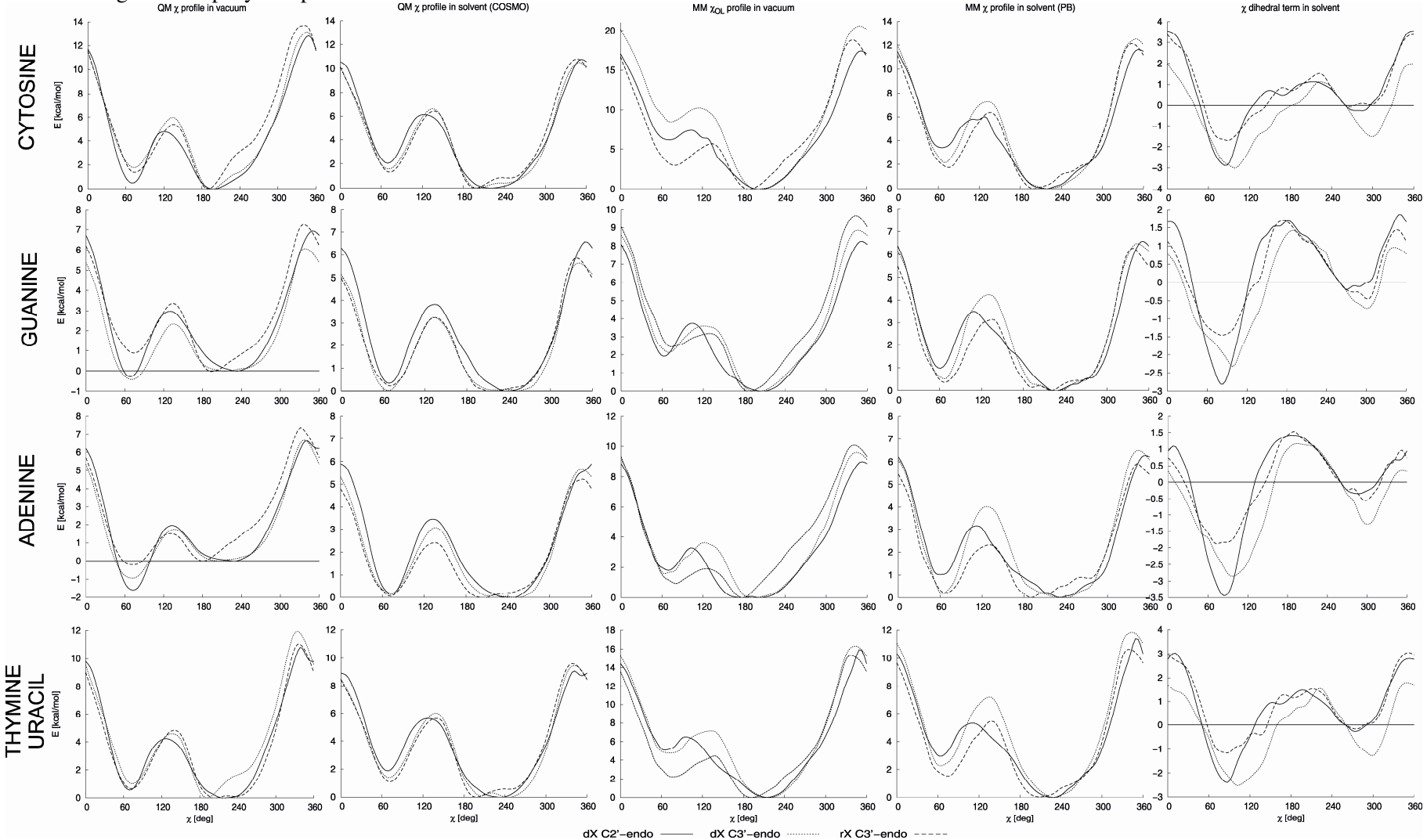


Table S1. The dihedral parameters for $\chi_{OL\text{-}DFT}$ parameterization. CJ is a new atom type introduced to distinguish C from U (T).

Nucleoside	Torsion (atom type)	n	$V_n/2$	ϕ
A,G	C8-N9-C1'-H1' (CK-N*-CT-H2)	3	0.5138	0.0
	C8-N9-C1'-C2' (CK-N*-CT-CT)	1	11.5732	180.0
	C8-N9-C1'-O4' (CK-N*-CT-OS)	1	12.0348	115.4514
		2	1.4803	355.4794
		3	0.9597	194.7709
		4	0.1558	100.2963
C	C6-N1-C1'-H1' (CJ-N*-CT-H2)	3	1.44805	0.0
	C6-N1-C1'-C2' (CJ-N*-CT-CT)	1	6.50527	180.0
	C6-N1-C1'-O4' (CJ-N*-CT-OS)	1	7.32714	120.0722
		2	1.71364	1.4610
		3	2.32071	185.4723
		4	0.31543	92.78265
T,U	C6-N1-C1'-H1' (CM-N*-CT-H2)	3	0.71700	0.0
	C6-N1-C1'-C2' (CM-N*-CT-CT)	1	5.1551	180.0
	C6-N1-C1'-O4' (CM-N*-CT-OS)	1	5.7949	120.1382
		2	1.6720	3.0939
		3	1.2674	189.7034
		4	0.2813	111.2030

Table S2. Average structural parameters (last 20 ns of 100 ns simulations) for the A-RNA duplex 2R20' obtained using the ff99bsc0 force field combined with various χ corrections (values with ff99 force field in italics). Standard deviations are shown for the unmodified force fields for orientation and they are very similar for the other force fields. RMSD is mass-weighted, for all atoms.

Parameter	X-ray	No χ correction	χ_{YIL}	$\chi_{OL\text{-}DFT}$*	χ_{OL}
χ/°	197.1 ± 4.4	202.8 ± 9.3 *204.8 ± 13.6*	196.7 *194.6*	198.3 *196.1*	200.4 *197.7*
P/°	14.1 ± 6.0	18.1 ± 13.1 *24.8 ± 23.2*	16.2 *13.1*	19.6 *15.8*	16.9 *14.8*
Minor gr. width/Å	15.4 ± 0.1	16.0 ± 0.6 *15.5 ± 0.8*	15.7 *15.4*	16.0 *15.7*	16.0 *15.6*
Major gr. width /Å	14.7 ± 1.5	16.1 ± 2.4 *18.4 ± 3.0*	18.1 *20.2*	17.0 *19.6*	16.7 *19.4*
Slide/Å	-1.70 ± 0.25	-1.56 ± 0.51 *-1.60 ± 0.57*	-1.98 *-2.14*	-1.83 *-1.97*	-1.73 *-1.98*
Roll/°	8.14 ± 4.09	7.82 ± 6.35 *7.46 ± 6.46*	4.75 *4.01*	6.90 *5.61*	6.97 *4.93*
Propeller/°	-12.5 ± 4.5	-14.6 ± 8.7 *-15.5 ± 8.9*	-7.0 *-5.7*	-11.5 *-10.2*	-11.6 *-10.1*
X-displ./Å	-4.45 ± 1.18	-4.37 ± 1.81 *-4.46 ± 2.28*	-4.76 *-4.88*	-4.87 *-4.87*	-4.64 *-5.29*
Inclination/°	12.3 ± 8.3	14.9 ± 12.0 *14.5 ± 13.1*	9.1 *7.7*	13.3 *10.8*	13.4 *10.0*
Helical twist/°	32.3 ± 3.6	31.2 ± 4.5 *31.7 ± 5.7*	30.2 *30.5*	30.6 *30.3*	31.1 *29.4*
RMSD/Å		1.40 *1.62*	1.37 *1.57*	1.31 *1.41*	1.36 *1.64*

* results for $\chi_{OL\text{-}DFT}$ are average of last 20 ns of a 50 ns trajectory

Table S3. Average structural parameters (last 20 ns of 100 ns simulations) for the A-RNA duplex 1RNA obtained using the ff99bsc0 force field combined with various χ corrections (values with ff99 force field in italics). Standard deviations are shown for the unmodified force fields for orientation and they are very similar for the other force fields. RMSD is mass-weighted, for all atoms.

Parameter	X-ray	No χ correction	χ_{YIL}	$\chi_{OL\text{-}DFT}$	χ_{OL}
χ/°	199.3 ± 9.0	213.3 ± 14.0 *211.2 ± 12.0*	199.3 *197.2*	203.0 *205.5*	205.6 *207.5*
P/°	18.4 ± 1.6	24.1 ± 17.2 *25.0 ± 19.3*	15.8 *14.4*	23.0 *32.5*	19.7 *21.9*
Minor gr. width/Å	16.1 ± 0.4	16.2 ± 0.8 *15.9 ± 0.8*	15.5 *15.2*	15.8 *15.2*	15.9 *15.8*
Major gr. width /Å	12.3 ± 1.5	15.3 ± 2.4 *17.1 ± 2.5*	15.9 *18.1*	15.2 *16.7*	14.8 *16.9*
Slide/Å	-1.29 ± 0.1	-1.06 ± 0.59 *-1.29 ± 0.51*	-1.70 *-1.92*	-1.49 *-1.59*	-1.40 *-1.40*
Roll/°	9.96 ± 5.10	14.10 ± 8.12 *12.07 ± 6.81*	7.47 *5.69*	10.69 *8.89*	11.05 *10.40*
Propeller/°	-18.8 ± 2.3	-11.5 ± 10.6 *-14.5 ± 9.4*	-13.4 *-11.5*	-15.7 *-15.1*	-15.1 *-9.8*
X-displ./Å	-4.07 ± 1.47	-4.18 ± 1.83 *-4.19 ± 1.71*	-4.31 *-4.62*	-4.27 *-4.35*	-4.15 *-4.32*
Inclination/°	18.8 ± 10.8	25.8 ± 14.1 *21.4 ± 12.0*	13.2 *10.3*	18.6 *16.1*	19.4 *19.1*
Helical twist/°	32.7 ± 4.1	32.3 ± 6.0 *32.7 ± 4.7*	32.0 *31.3*	33.1 *32.2*	32.8 *31.6*
RMSD/Å		2.03 *1.96*	1.96 *2.44*	1.77 *2.32*	1.70 *2.12*