Supporting Information

Table SI1: All the force field parameters used in this study to describe the 2'-hydroxyl torsion.

Torsion	$V_n/2$ (c27)	Multiplicity	Phase
HN5 ON5 CN7B CN7B	0.800	3	0.0
HN5 ON5 CN7B CN7B	0.000	2	0.0
HN5 ON5 CN7B CN7B	0.000	1	0.0
HN5 ON5 CN7B CN7	0.300	3	0.0
HN5 ON5 CN7B CN7	0.000	2	180.0
HN5 ON5 CN7B CN7	0.000	1	0.0

Torsion	$V_n/2$ (c27a)	Multiplicity	Phase
HN5 ON5 CN7B CN7B	1.000	3	0.0
HN5 ON5 CN7B CN7B	0.400	2	0.0
HN5 ON5 CN7B CN7B	0.800	1	0.0
HN5 ON5 CN7B CN7	0.200	3	0.0
HN5 ON5 CN7B CN7	1.200	2	180.0
HN5 ON5 CN7B CN7	2.000	1	0.0

Torsion	$V_n/2$ (c27b)	Multiplicity	Phase
HN5 ON5 CN7B CN7B	0.300	3	0.0
HN5 ON5 CN7B CN7B	0.400	2	0.0
HN5 ON5 CN7B CN7B	0.800	1	0.0
HN5 ON5 CN7B CN7	0.200	3	0.0
HN5 ON5 CN7B CN7	0.600	2	180.0
HN5 ON5 CN7B CN7	2.000	1	0.0

Torsion	$V_n/2$ (c27c)	Multiplicity	Phase
HN5 ON5 CN7B CN7B	0.400	3	0.0
HN5 ON5 CN7B CN7B	0.400	2	0.0
HN5 ON5 CN7B CN7B	0.800	1	0.0
HN5 ON5 CN7B CN7	0.200	3	0.0
HN5 ON5 CN7B CN7	0.400	2	180.0
HN5 ON5 CN7B CN7	1.800	1	0.0

Torsion	$V_n/2$ (c27d)	Multiplicity	Phase
HN5 ON5 CN7B CN7B	0.400	3	0.0
HN5 ON5 CN7B CN7B	0.400	2	0.0
HN5 ON5 CN7B CN7B	0.800	1	0.0
HN5 ON5 CN7B CN7	0.200	3	0.0
HN5 ON5 CN7B CN7	0.000	2	180.0
HN5 ON5 CN7B CN7	2.000	1	0.0

Torsion	$V_n/2$ (c27e)	Multiplicity	Phase
HN5 ON5 CN7B CN7B	0.355	3	0.0
HN5 ON5 CN7B CN7B	0.200	2	0.0
HN5 ON5 CN7B CN7B	0.400	1	0.0
HN5 ON5 CN7B CN7	0.100	3	0.0
HN5 ON5 CN7B CN7	0.600	2	180.0
HN5 ON5 CN7B CN7	1.000	1	0.0

Table SI2: Description of non-canonical RNA molecules and their simulation conditions.

	1DQH	**1EOR**	**1K5I**	**1UUU**	**1MSY**	**1L2X**	**1F7Y**	**1MME**	**1Y26**
Structure conditions	Xray	Solution NMR	Solution NMR	Solution NMR	Xray	Xray	Xray	Xray	Xray
Salt Conditions	KCl	KCl	KCl	NaCl	NaCl	KCl	NaCl	NaCl	MgCl
Simulation Time (ns)	50ns	50ns	50ns	50ns	50ns	50ns	50ns	50ns	40ns

Table SI3: Description of canonical RNA molecules and their simulation conditions.

	1SA9	**1SDR**	**1RNA**	**1YFV**	**18-mer (no PME)**	**18-mer (PME)**
Structure conditions	Xray	Xray	Xray	Solution NMR	SEQ4 model [56]	SEQ4 model [56]
Salt Conditions	KCl	KCl	NaCl	KCl	Na	Na
Simulation Time (ns)	50ns	50ns	50ns	50ns	2x100 ns	2x50 ns

Table SI4: Umbrella sampling conditions of each window of the reaction coordinate (C1'-C1' distance).

Window	End-to-end distance (Å)	Force Constant (kcal/mol/Å^2)
1	10.7	1.2
2	11.5	8.0
3	12.0	8.0
4	12.5	6.0
5	13.0	4.0
6	13.8	1.6
7	14.8	1.6
8	16.1	1.6
9	17.5	1.6
10	18.8	1.6
11	20.2	1.6
12	21.5	1.6
13	22.9	1.6
14	24.2	1.6
15	25.6	1.6
16	26.9	1.6
17	27.9	1.6
18	28.8	2.0
19	29.6	6.0
20	30.4	6.5
21	31.3	5.0
22	32.1	4.0
23	33.5	3.0
24	34.9	2.0

Table SI5: Average (standard deviation) for the non-hydrogen atom RMSD of non-canonical RNA molecules over 40-50 ns (A) canonical-region (B) non-canonical region.

(A)	**1DQH**	**1EOR**	**1K5I**	**1UUU**	**1MSY**	**1L2X**	**1F7Y**	**1MME**	**1Y26 (apo)**	**1Y26 (holo**
Charmm27	3.93 (1.00)	2.80 (0.54)	2.25 (0.59)	2.00 (0.10)	2.40 (0.10)	--	0.94 (0.29)	0.99 (0.21)	3.80 (0.20)	3.80 (0.20)
Charmm27a	2.88 (0.57)	2.24 (0.54)	1.63 (0.29)	1.91 (0.42)	1.89 (0.31)	--	0.81 (0.17)	0.75 (0.18)	2.22 (0.32)	1.81 (0.27)
Charmm27b	2.47 (0.60)	2.10 (0.44)	1.71 (0.30)	2.00 (0.40)	1.80 (0.10)	--	0.72 (0.13)	0.70 (0.10)	1.94 (0.10)	1.84 (0.11)
Charmm27c	2.63 (0.70)	2.32 (0.37)	1.76 (0.29)	--	--	--	0.72 (0.14)	0.69 (0.16)	--	--
Charmm27d	2.60 (0.42)	3.58 (1.47)	1.78 (0.30)	2.16 (0.31)	1.71 (0.20)	--	0.75 (0.16)	0.67 (0.17)	1.96 (0.11)	1.79 (0.15)
Charmm27e	2.70 (0.44)	2.10 (0.42)	1.72 (0.35)	--	--	--	0.77 (0.18)	0.71 (0.15)	--	--
(B)										
Charmm27	4.90 (3.94)	0.39 (0.12)	3.75 (0.35)	4.60 (0.10)	2.50 (0.05)	4.47 (0.60)	1.37 (0.38)	2.56 (0.61)	3.90 (0.10)	3.90 (0.10)
Charmm27a	4.29 (4.13)	0.31 (0.11)	3.47 (0.47)	5.04 (1.12)	1.44 (0.44)	1.93 (0.22)	0.94 (0.14)	1.72 (0.18)	3.40 (0.45)	3.04 (0.37)
Charmm27b	3.85 (4.26)	0.32 (0.08)	2.59 (0.63)	2.51 (0.54)	1.10 (0.10)	2.48 (0.51)	2.41 (1.56)	1.92 (0.38)	2.14 (0.50)	2.01 (0.48)
Charmm27c	4.15 (4.28)	0.31 (0.08)	2.52 (0.55)	--	--	2.66 (0.68)	3.32 (0.52)	1.72 (0.14)	--	--
Charmm27d	3.41 (3.53)	0.40 (0.15)	2.93 (0.68)	4.72 (0.51)	0.96 (0.15)	2.80 (0.64)	3.82 (0.94)	1.69 (0.20)	2.30 (0.45)	1.97 (0.50)
Charmm27e	2.65 (1.82)	0.31 (0.09)	2.72 (0.61)	--	--	2.82 (0.50)	3.89 (0.94)	3.39 (0.90)	--	--

Table SI6: Average for the non-hydrogen atom RMSD of canonical RNA (standard deviation).

	1SA9	**1SDR**	**1RNA**	**1YFV**
Charmm27	1.64 (0.66)	3.41 (0.59)	7.54 (1.79)	1.05 (0.22)
Charmm27a	1.19 (0.24)	2.57 (0.49)	--	1.09 (0.20)
Charmm27b	1.14 (0.21)	2.51 (0.51)	2.24 (0.64)	1.08 (0.20)
Charmm27c	1.13 (0.20)	2.41 (0.45)	--	1.11 (0.21)
Charmm27d	1.15 (0.21)	1.81 (0.43)	2.23 (0.62)	1.09 (0.22)
Charmm27e	1.18 (0.22)	3.21 (0.71)	--	1.03 (0.20)

Table SI7: Quasiharmonic entropies (kcal/mol/K) for 14 central basepairs. Results based on the 40 to 100 ns regions of the trajectories using time frames saved every 5 ps.

Simulation	**S_{conf}**
c27 No PME	3.065
c27d No PME	2.784
c27 PME	3.017
c27d PME	2.763

Figure SI1: Secondary structure representation of non-canonical RNA molecules. Solid line between two nucleic acid bases represent Watson-Crick (WC) type interactions, whereas the dotted lines represent non-canonical interactions involving hydrogen bonds between the corresponding nucleotides. The shaded regions represent the non-canonical regions, and the 5'-ends are denoted by arrows.

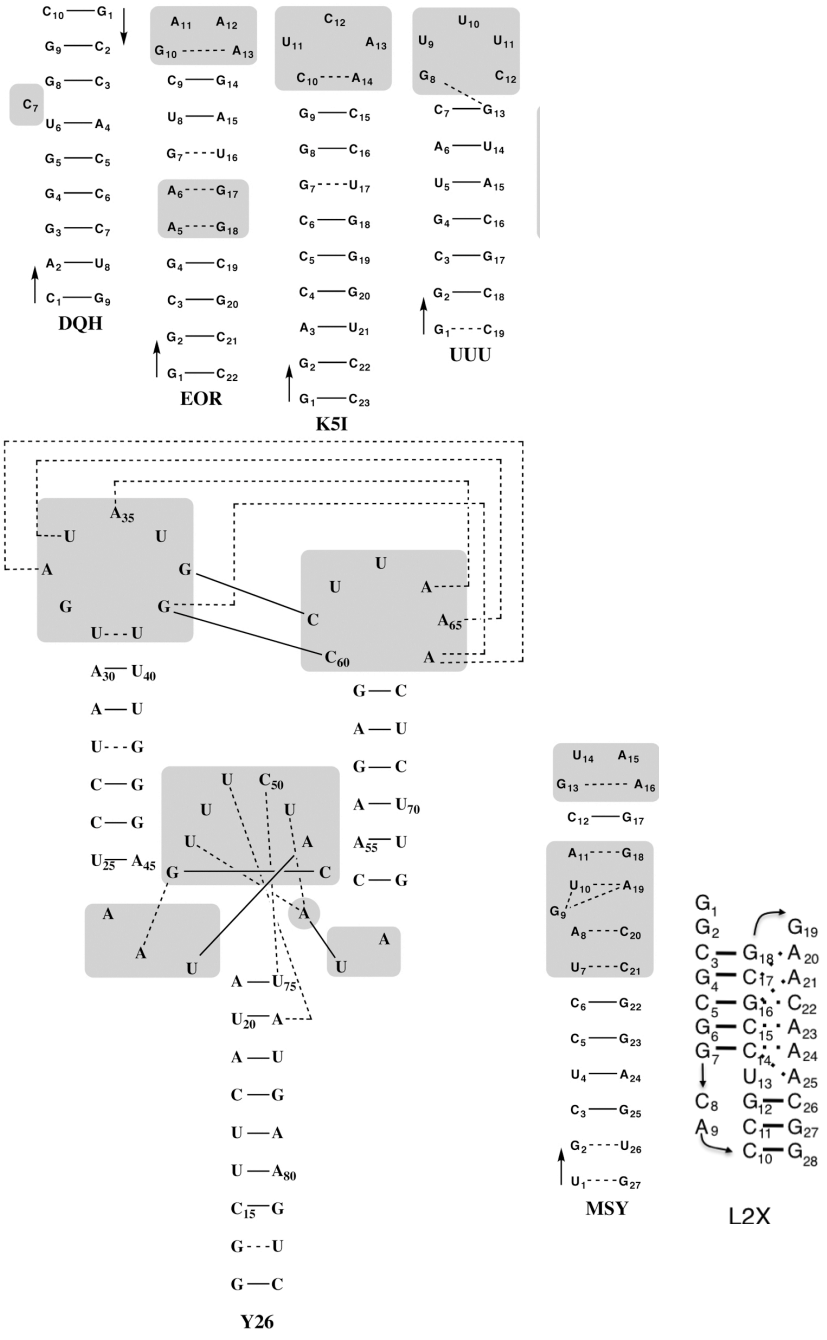


Figure SI2: Experimental structures some of the non-canonical RNAs.

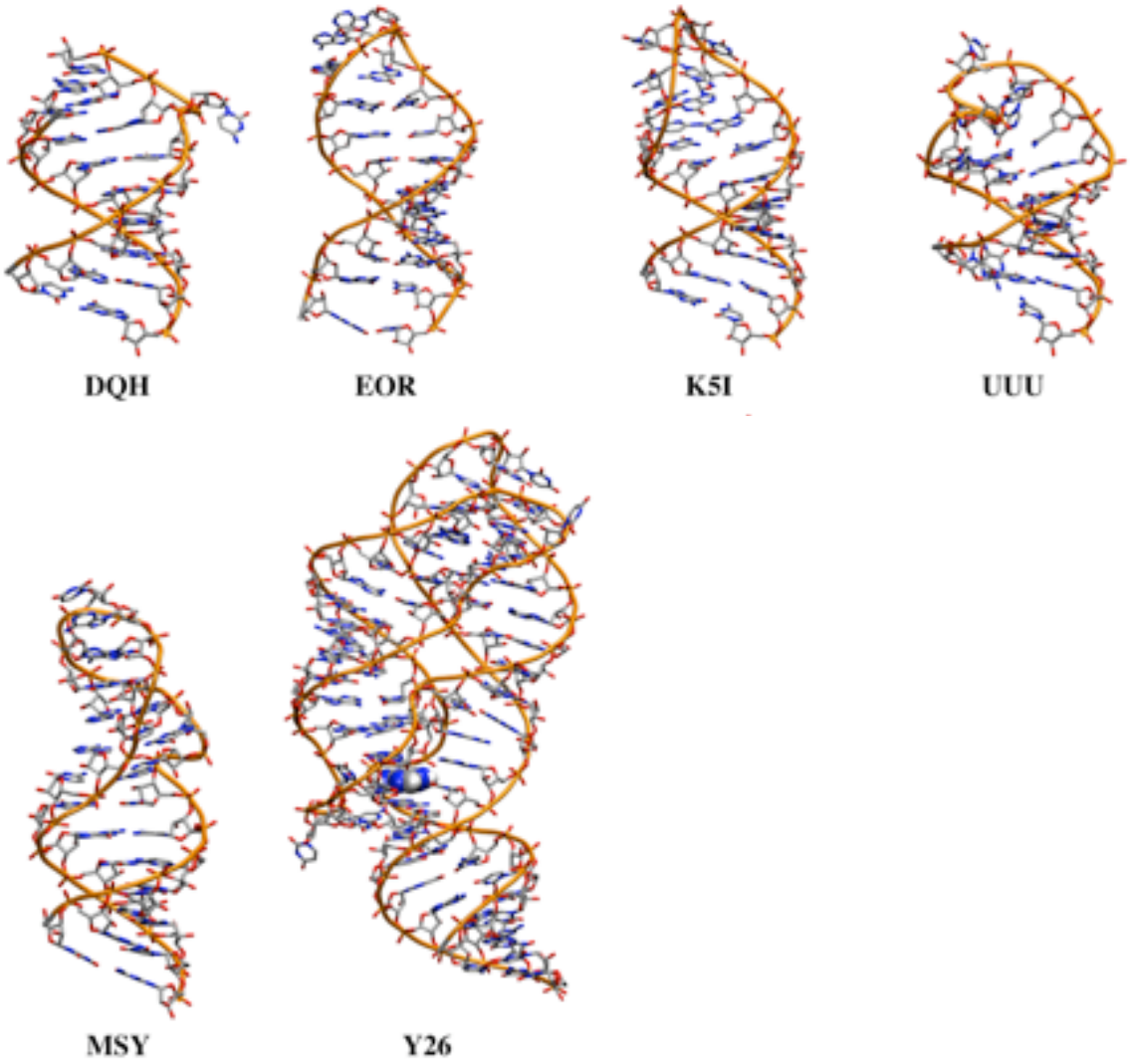


Figure SI3: Individual pseudorotation angles of the ribose for the **(A)** 1K5I canonical, **(B)** 1K5I non-canonical, **(C)** 1UUU canonical, and **(D)** 1UUU non-canonical regions to evaluate each of the force field parameter sets. [Solid-blue line represents the original CHARMM27 parameters; Dash-dot lines represent variants of CHARMM27 parameters -- Red: CHARMM27a, yellow: CHARMM27b, magenta: CHARMM27c, green: CHARMM27d, black: CHARMM27e; Solid horizontal-cyan line indicates the region of C3'-endo ribose conformation and the dashed horizontal-cyan lines indicate the region of the C2'-endo ribose conformation].

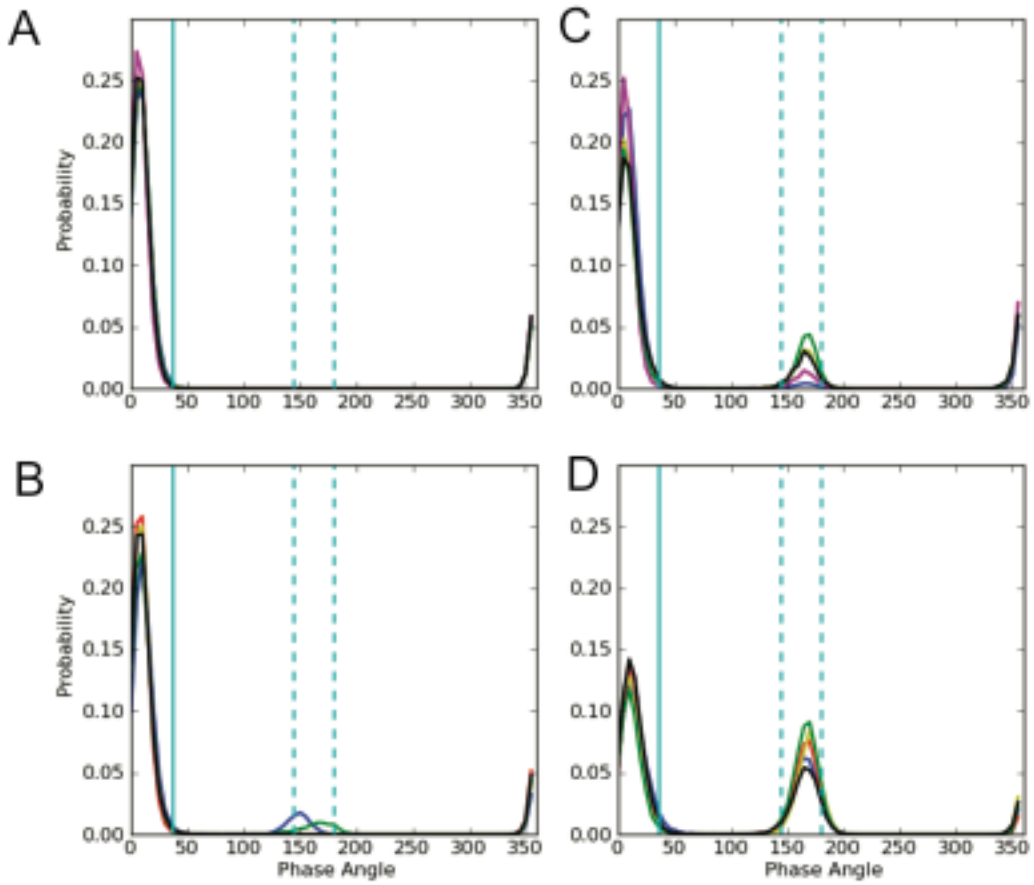
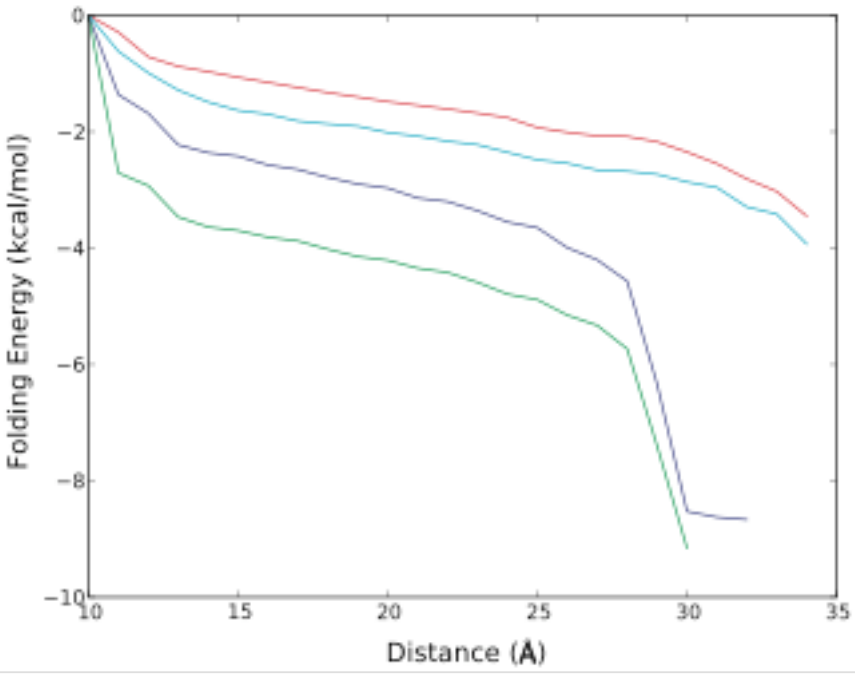


Figure SI4: Free energy of folding as a function of the cutoff end-to-end distance used to define the folded and unfolded states of **(A)** 1F7Y **(B)**1MME. [Blue: CHARMM27, Red: CHARMM27a, Cyan: CHARMM27b, Green: CHARMM27d.]

(A)



(B)

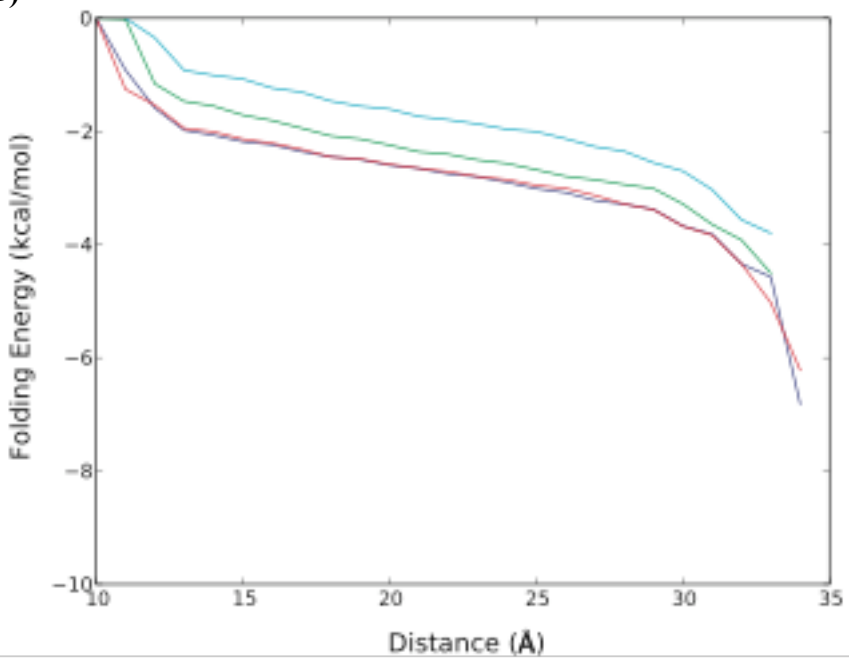
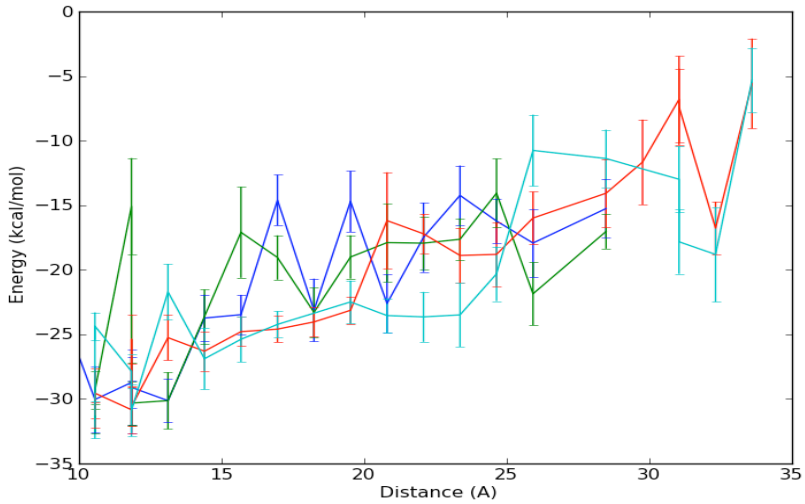


Figure SI5: Base-stacking interaction energy for each PMF window which is based on the end-to-end distance values. [Blue: CHARMM27, Red: CHARMM27a, Cyan: CHARMM27b, Green: CHARMM27d.] **(A)** 1F7Y **(B)**1MME.

(A)



(B)

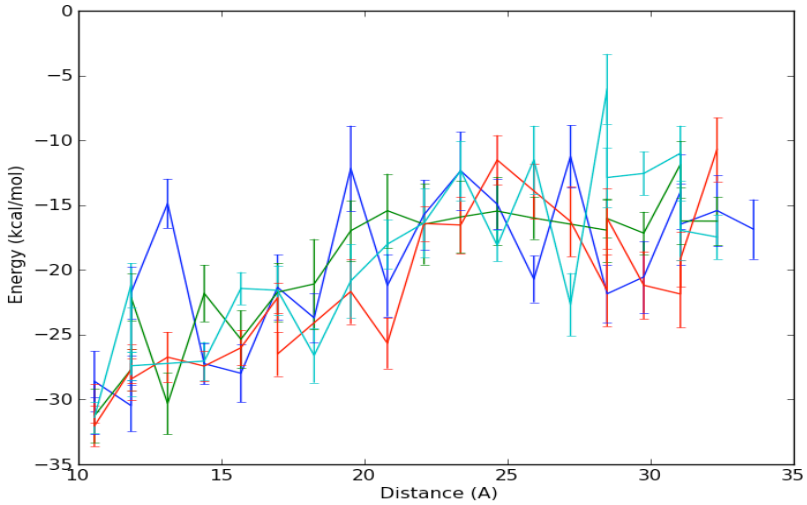


Figure SI6: Evaluation of force field parameters based on the probability distribution for selected helicodial parameters. [Solid-blue line represents the original CHARMM27 parameters; Dash-dot lines represent variants of CHARMM27 parameters -- Red: CHARMM27a, yellow: CHARMM27b, magenta: CHARMM27c, green: CHARMM27d, black: CHARMM27e; Solid cyan line indicates survey-analysis data].

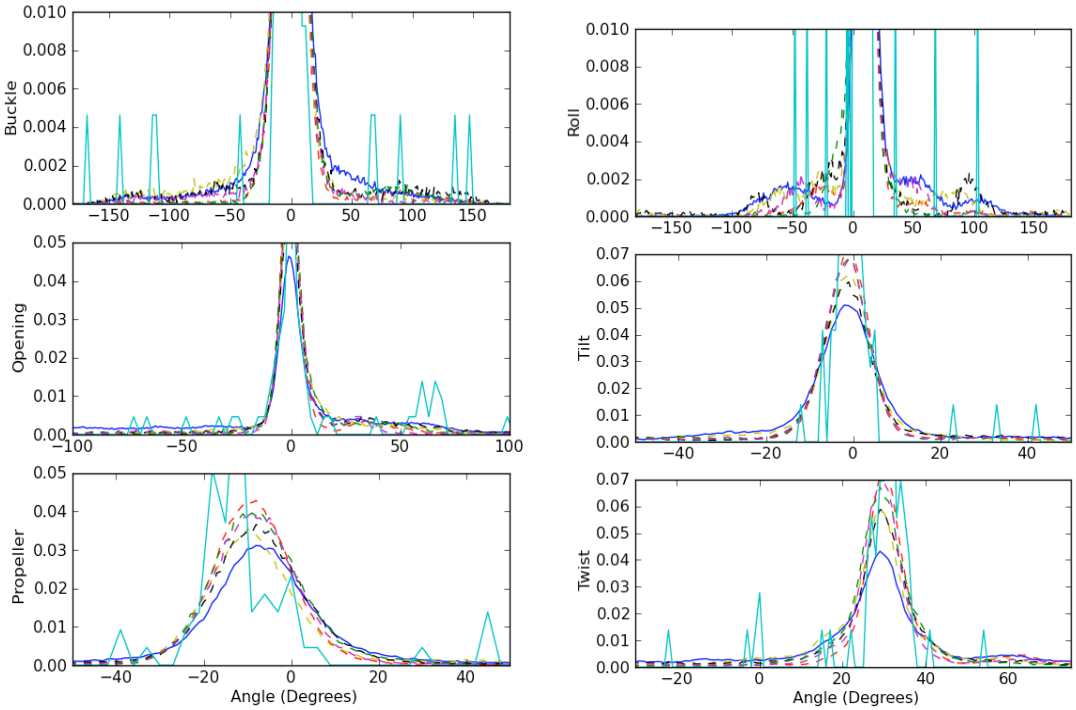


Figure SI7: The root mean square fluctuations (RMSF) averaged over each nucleotide based on a backbone alignment for the following force field parameter sets: CHARMM27 (blue), CHARMM27b (yellow), and CHARMM27d (green).

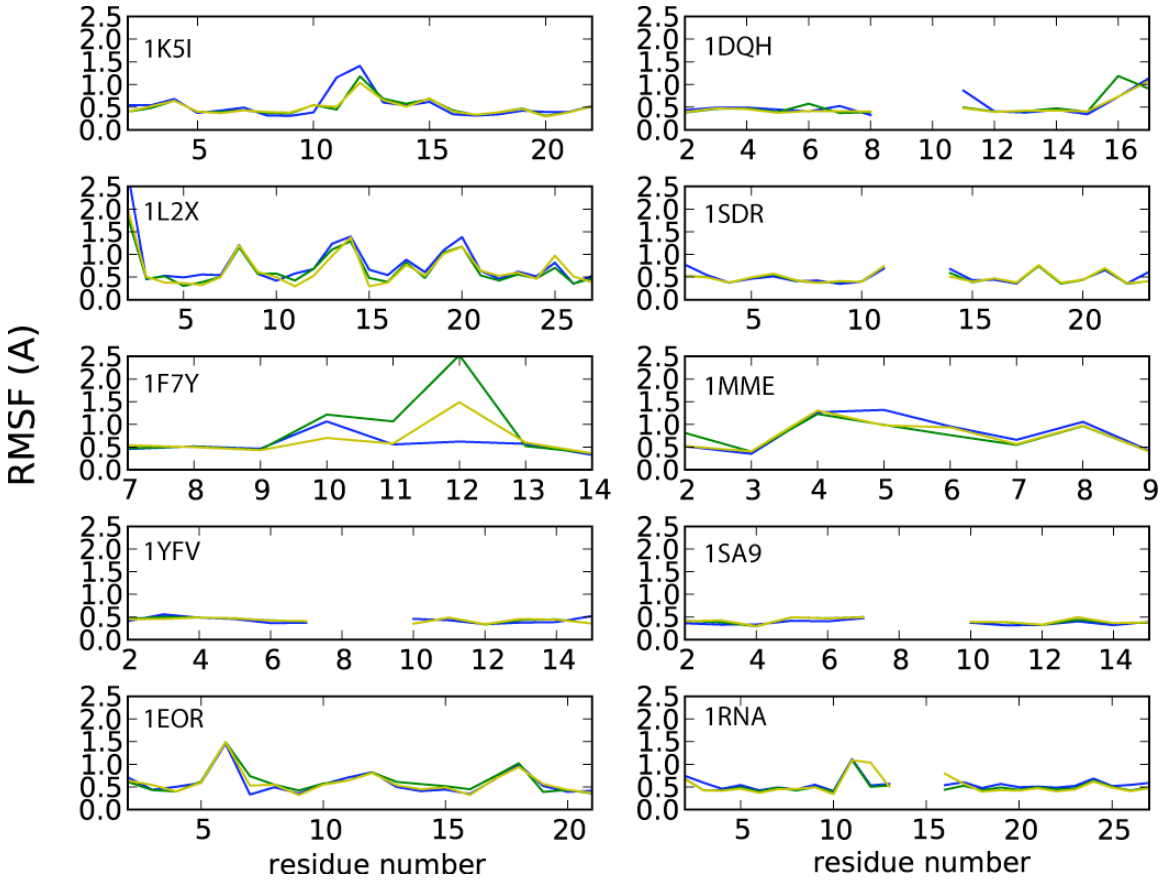


Figure SI8: The nucleic acid root mean square fluctuations (RMSF) averaged over each nucleotide base based on a backbone alignment for the following force field parameter sets: CHARMM27 (blue), CHARMM27b (yellow), and CHARMM27d (green).

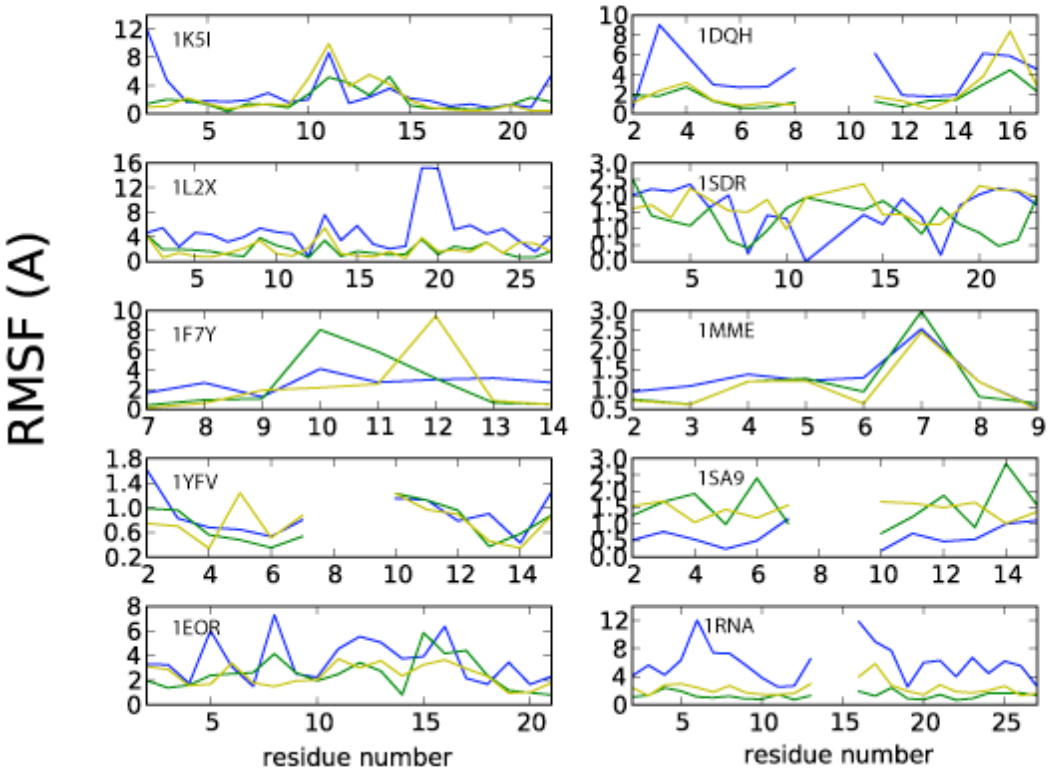


Figure SI9: Results from 18mer RNA. N1-N3 distance distributions for 14 central basepairs distributions. [Blue: Original CHARMM; Green: CHARMM27d] **(A)** No PME **(B)** PME.

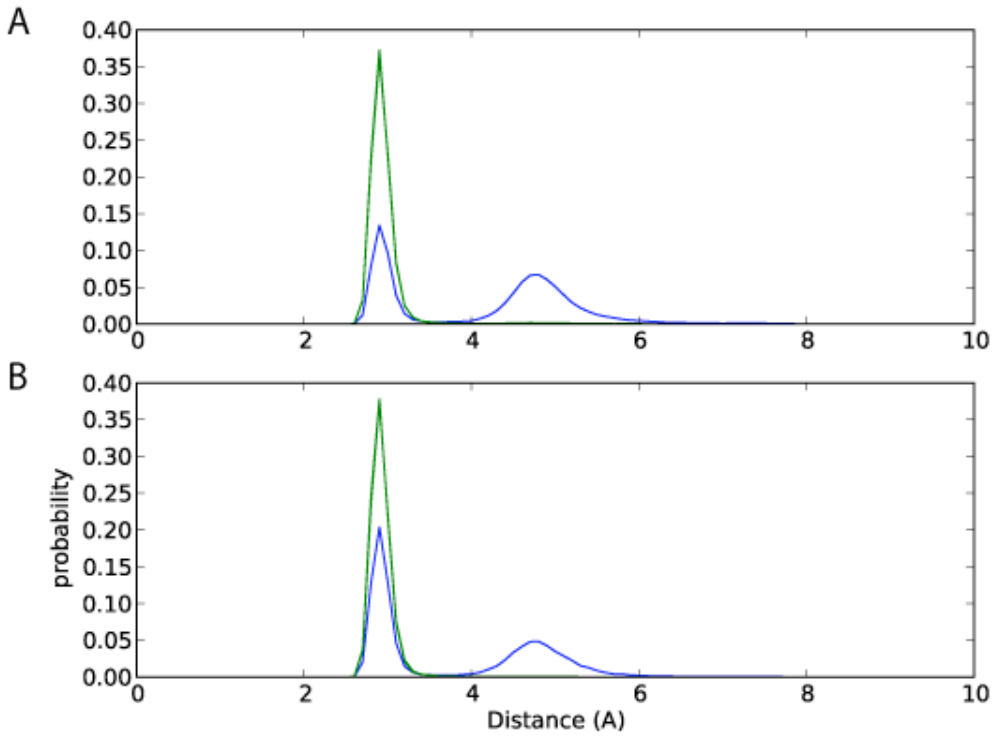


Figure SI10: Results from 18mer RNA. 2'hydroxyl distributions for 14 central basepairs distributions. [Blue: Original CHARMM; Green: CHARMM27d] **(A)** No PME **(B)** PME.