Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information for

Liquid Crystal Ordering of Nucleic Acids

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Section 1: System Details

The PMF calculation on RNA reported in the manuscript is done for 4 different reaction coordinates. The following table contains the details of the simulated systems,

Table S1.1: Details of the Simulated Systems with RNA for PMF Calculation

System Configuration	**Box dimension [Å ×Å× Å]**	**Total number of atoms**	**Number of Na^+ added for net neutralization**
Following helix configuration	[66.2×66.1×74.8]	26359	12
Same helix configuration	[66.2×62.0×77.1]	25237	12
Side-by-side configuration	[93.8×59.9×58.9]	26815	12
Shifted-end Configuration	[65.4×68.1×76.9]	27622	12

Table S1.2: Details of the Simulated Systems with RNA for Liquid Crystal Calculation

System configuration		Volume fraction of the solute (%)	Box dimension [Å ×Å× Å]	Total number of atoms	Number of Na+ added for net neutralization	Volume fraction DNA system with same amount of water buffer as RNA system (%)
Following helix configuration		47	[101.0×141.8×86.1]	95070	540	52
		36	[111.4×152.0×95.9]	130944	540	40
		23	[131.3×171.8×116.0]	223320	540	31
		18	[140.8×182.0×125.4]	279453	540	20
Same helix configuration		47	[100.9×140.7×86.1]	91788	540	52
		36	[111.0×150.5×95.9]	126633	540	40
		23	[130.5×170.5×116.0]	217749	540	31
		18	[140.6×180.7×125.5]	274140	540	20
Shifted-end Configuration		48	[101.0×141.5×92.0]	102312	540	54
		37	[111.4×151.8×101.3]	137934	540	44
		23	[131.0×171.8×121.7]	233376	540	34
		19	[140.8×181.8×131.5]	292287	540	21
Following helix configuration	**75mM of NaCl**	47	[101.0×141.8×86.1]	95078	540 Na^+ and 34 NaCl molecules	52
	150mM of NaCl	47	[101.0×141.8×86.1]	95128	540 Na^+ and 68 NaCl molecules	52

Section 2: Restraints Used for Umbrella Sampling

Section 2.1: Following Helix and Same Helix Configuration

In Figure S1 we have represented the schematic of PMF calculation between two RNA in following helix and same helix configuration. The number specifies the residue index. The distance between the center of mass of residue 4,5 and 9,16 is defined as reaction coordinate (RC). Addition restraint with a harmonic constant 0.18 kcal/mol/degree^2 between the dihedral angle by 4,5,16,9 residue is applied to keep the two fragments in their following helix or same helix configuration. Also, to keep the fragments axially aligned we applied an addition axial restraint with force constant 0.18 kcal/mol/degree^2 between the two vector defined by joining the COM of 1,8 and 4,5,9,16 residue and 4,5,9,16 and 12,13 residues.

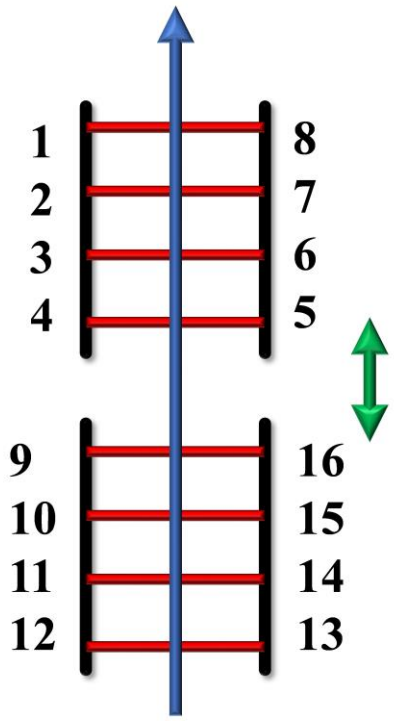

Fig S1. Schematic representation of the two RNA fragments used for PMF calculation in following helix and same helix configuration. The number represents residue index. Green arrow represents the RC

coordinate used for umbrella sampling. Blue arrow is the axial restraint applied to keep the fragments axially aligned.

Section 2.2: Side-by-side Configuration

In side-by-side configuration the two RNAs are placed parallel to each other [Fig S2]. The distance between the center of mass of the fragments are defined as the reaction coordinate (green arrow). Additional restraints with a force constant 0.18 kcal/mol/deg^2 are applied to keep the fragments aligned along their helical axis (to the arrow direction). More precisely we have used two more angle restraints. One is defined by joining the COM of 1-8, 4-5, 12-13 base pair and another by joining the COM 4-5, 12-13, 9-16 base pair.

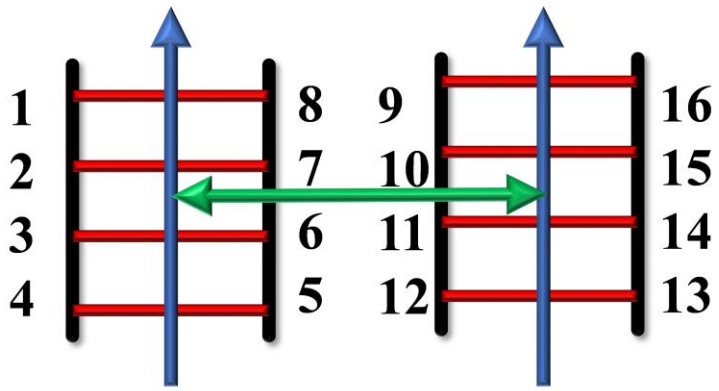

Fig S2. Schematic representation of the two RNA fragments used for PMF calculation in side-by-side configuration. The number represents residue index. Green arrow represents the RC coordinate used for umbrella sampling. Blue arrow is the axial restraint applied to keep the fragments aligned to their helical axis.

Section 2.3: Shifted-end Configuration

In Figure S3 we have shown schematic representation of two RNA fragments for PMF calculation. The center of mass distance between the hanging base pairs is defined as the RC. Addition distant restraint between 1 and 13 residues with a fore constant 1 kcal/mol/Å^2 is applied to keep them aligned.

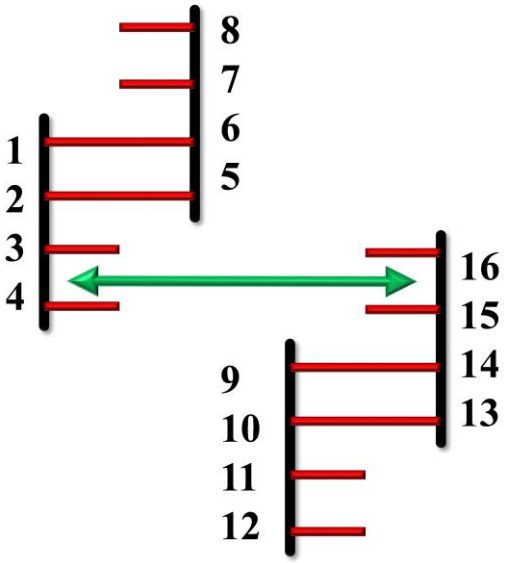

Fig S3. Schematic representation of the two RNA fragments used for PMF calculation in shifted-end configuration. The number represents residue index. Green arrow represents the RC coordinate used for umbrella sampling.

Section 3: Details of the Simulated 12bp DNA and RNA Systems

To calculate the average rise, helical rise and other helicoidal parameters of NAs we have simulated a 12bp dsDNA having sequence $d(cgcgatatcgcg)_2$ and a 12bp dsRNA having sequence $d(cgcgauaucgcg)_2$ in water environment. We performed MD simulation for 100ns in NVT ensemble with same protocol given in methods section of the main manuscript. RMSD of the non-hydrogen atoms are calculated with respect to the initially energy minimized structure given in figure S4(a). Then we calculate all the helicoidal quantities averaged over last 20ns. In figure S4(b), (c), (d) we have plotted the average helical rise, X-displacement and slide of the DNA and RNA respectively. The average radius (defined as the COM distance of two bases in the middle of the NA) of the DNA or RNA is given in figure S5.

Section 3.1 RMSD and Helical parameters of the 12bp nucleic acids

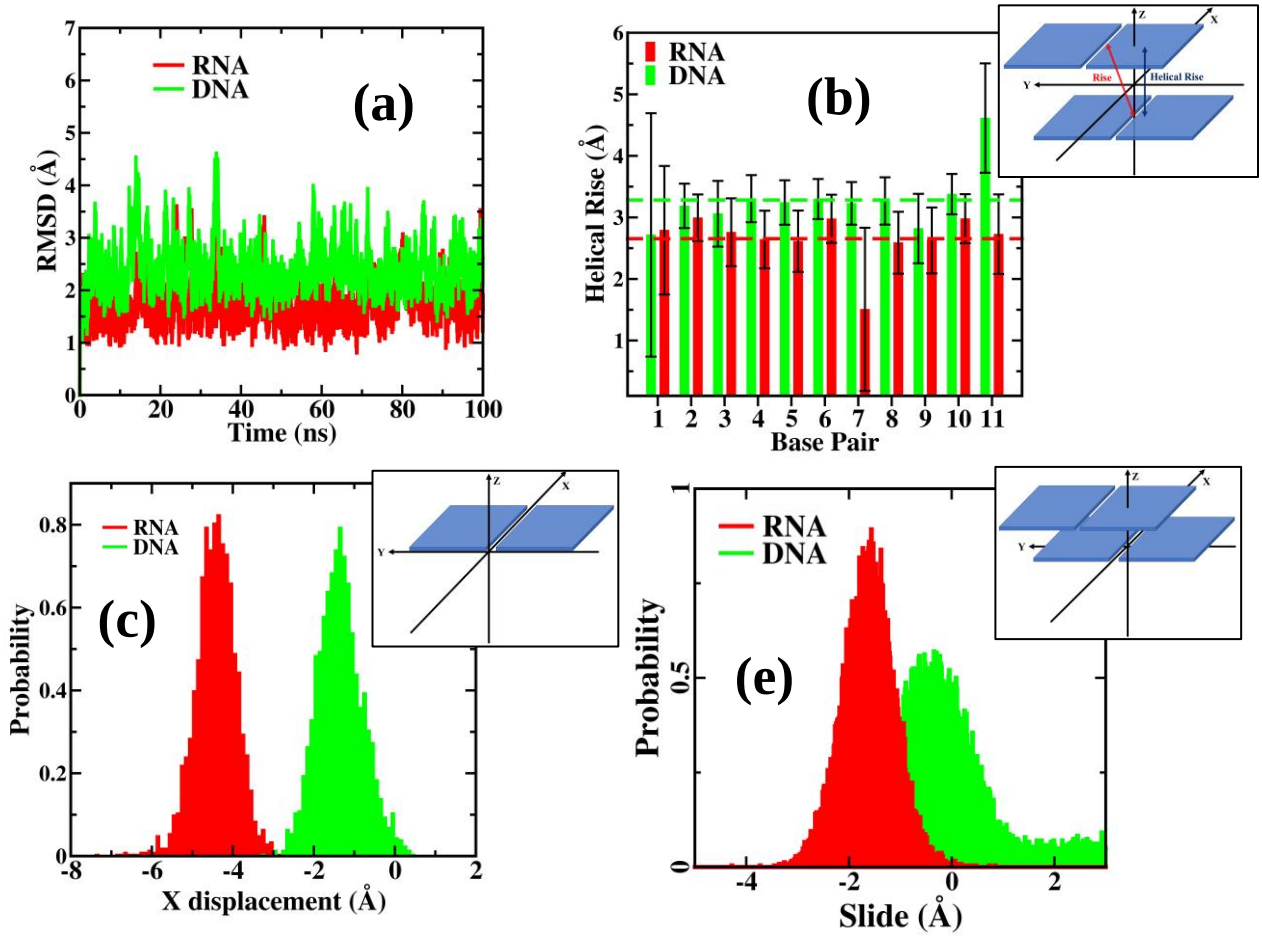

Fig S4. (a) Root mean square deviation of the 12bp dsDNA and dsRNA. (b) Average helical rise (average over last 20 ns) between consecutive base pairs. The helical rise of dsDNA is higher than dsRNA. The definition of rise vs helical rise (Assuming Z is the direction of Helical axis) is given in the inset of the graph. Histogram plot of average X-displacement (c) and slide (d) (average over last 20 ns). The definition is given is the inset of the graph. In both cases RNA has higher average x-displacement and slide value than dsRNA.

Section 3.1 Radius of the 12bp nucleic acids

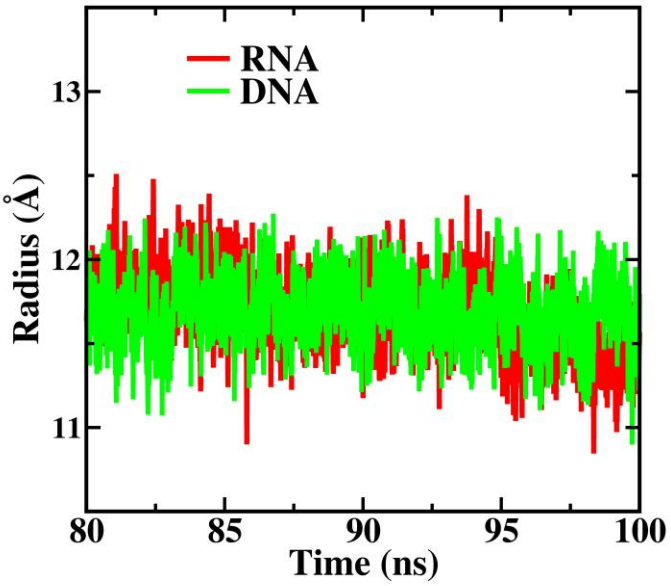

Fig S5. Average radius of dsDNA and dsRNA.

Section 4: PMF in Side-by-side Configuration with Different Initial Configuration

We have calculated PMF in side-by-side configuration with different initial configuration and no axial restraint. We have rotated one nucleic acid fragment such that it makes either 0°, 90°, -90°,180° angle with the other [Fig S6 (a), (b), (c), (d)]. Since there are no axial restraint as in the case of side-by-side configuration in the main-text, they are free to topple to minimize the electrostatic repulsion. Still we found that the PMFs are repulsive in nature though it is reduced than the case (side-by-side configuration of main-text) where axial restraint is present. Also, there are several local minima in the PMF, because the NAs are free to topple and aligned such that the bases become interfacial.

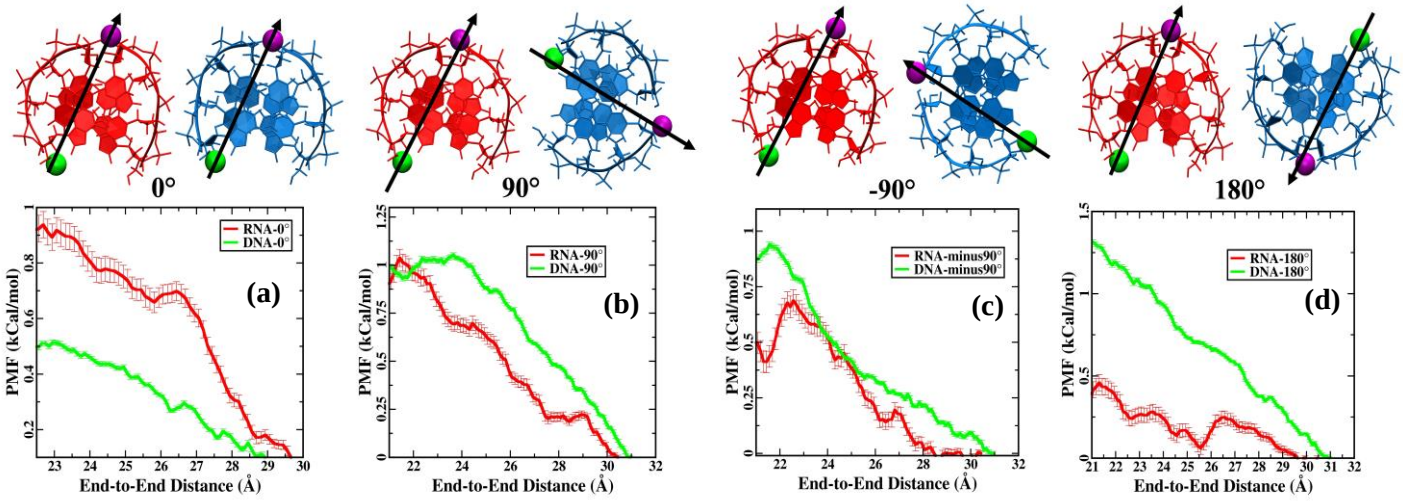

Fig S6. PMF between two dsRNA in side-by-side configuration with only distance between center of mass restraint. One of RNA is rotated such a way it makes an angle (a) 0°, (b) 90°, (c) -90°, (d) 180°.

Section 5: Temperature Dependence of the PMF in Shifted-end Configuration

To understand the temperature dependence of the PMF in shifted end configuration we have performed PMF calculation for different temperature 280K, 293K, 300K, 310K using the procedure explained in S2.3. In figure S7 (a), (b), (c), (d) the PMF profiles for both DNA and RNA are given.

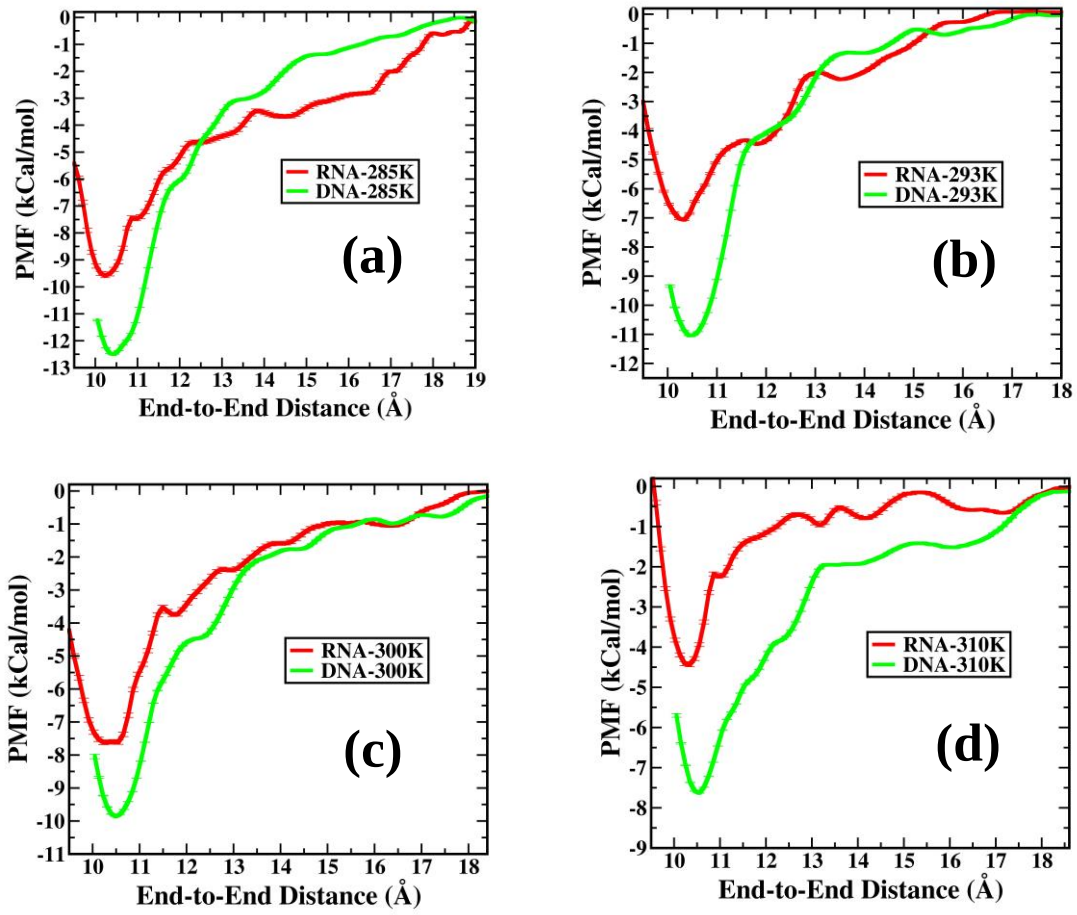

Fig S7. PMF profiles of dsDNA and dsRNA in shifted-end configuration at temperature (a) 280K, (b) 293K, (c) 300K, (d) 310K.

Section 6: Time Evolution of the Nematic Order Parameter

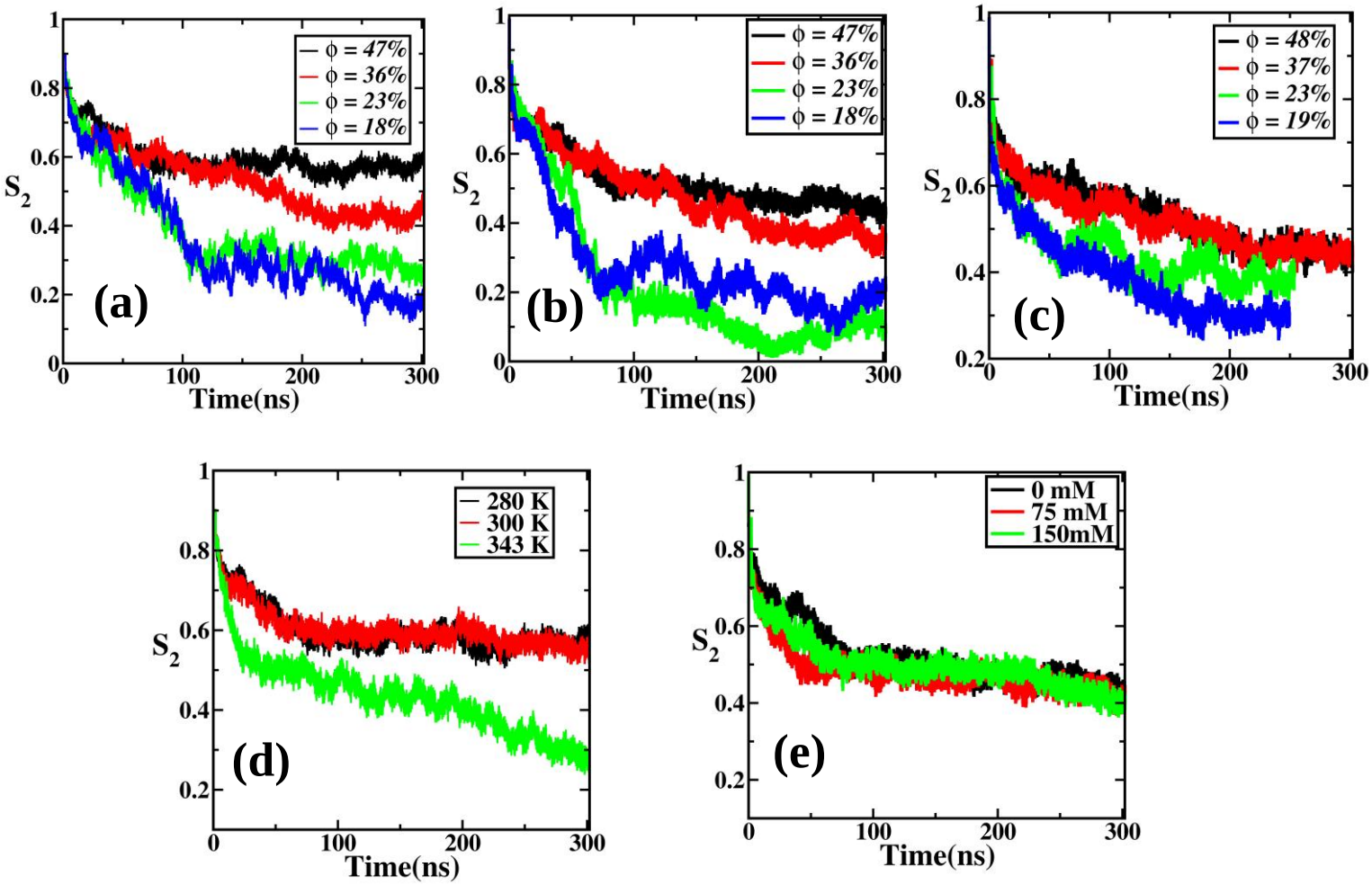

Fig S8. Time evolution of the nematic order parameter, S_2 for dsRNA in (a) FH configuration, (b) SH configuration, (c) shifted-end configuration. (d) Time evolution of S_2 for different temperature in SH configuration with highest volume fraction. (e) Time evolution of S_2 for different molarity in SH configuration with highest volume fraction.

Section 7: PMF Calculation and LC Order Parameter for RNA with Different Sequence

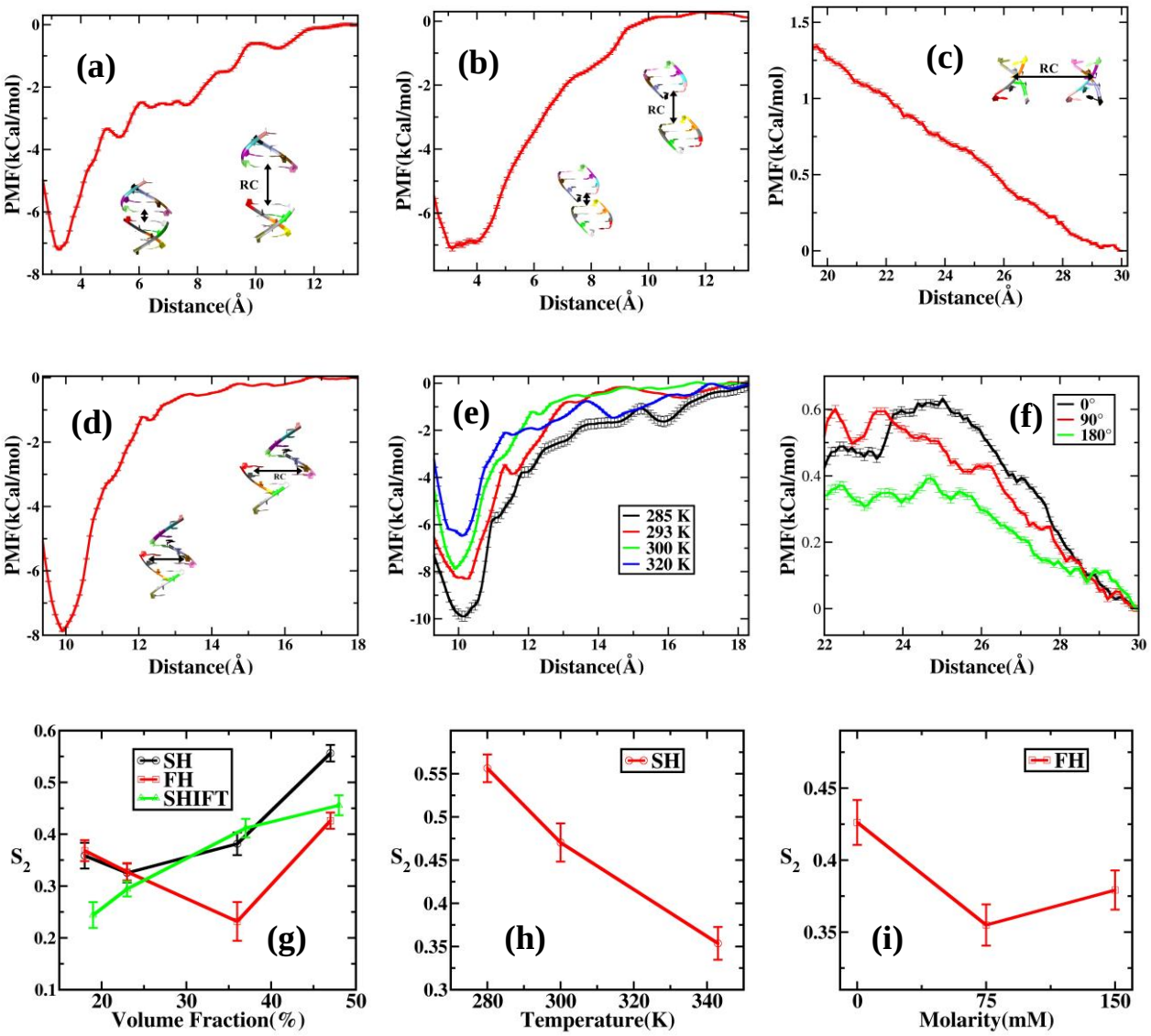

Fig S9. PMF between two dsRNA with different sequence. (a) FH configuration with sequence d(uacg)$_2$. (b) SH configuration with sequence d(gauc)$_2$. (c) Side-by-side configuration with sequence d(gauc)$_2$. (d) Shifted-end configuration with sequence d(aucg)$_2$ and (e) in different temperature. As we have already described in the section 5, the PMF here is also decreasing with increasing temperature. (e) Side-by-side configuration with only COM distance between the NAs as reaction coordinate and with no axial restraint. Since, here the NA fragments are free to rotate in any direction, they rotate in a way such that two bases become interfacial. Due to this multiple minimum in the PMF is arises. The protocol for PMF calculation is same as explained in the previous chapters.(g)-(i) LC Order Parameter for RNA with different sequence. (g) LC order parameter in different configuration with RNA sequence d(augc)$_2$. (h) Order parameter in different temperature in SH configuration with highest volume fraction. (i) Order parameter in different molarity in FH configuration with highest volume fraction.

Section 8: Structure of the RNA column

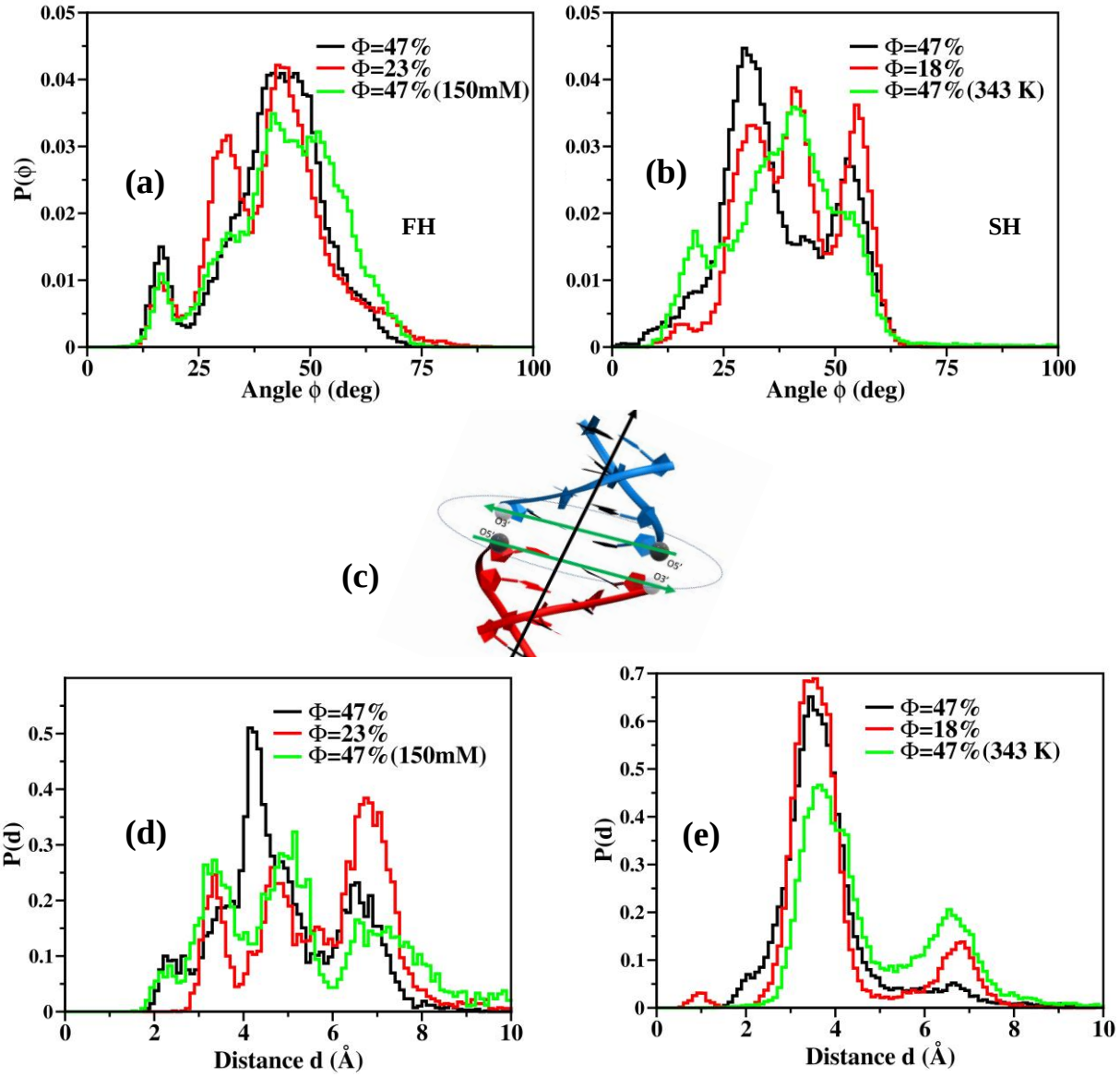

Fig S10. Structure of the RNA columns. Azimuthal angle distribution of the neighboring RNA fragments starting from (a) FH configuration and (b) SH configuration. (c) Definition of the azimuthal angle. The projection of the vectors joining 05' and 03' atoms are taken on the plane perpendicular to the common helical axis. The angle between the projected vector is the azimuthal angle (φ). The common helical axis is drawn by joining the com of faraway base pairs. The base pair fraying of the terminal bases sometimes leads to the marginally different helical axis than the actual one, which attributed to a slightly different azimuthal angle around 45°. Distance distribution of the neighboring NA fragments starting from (d) FH configuration and (e) SH configuration.