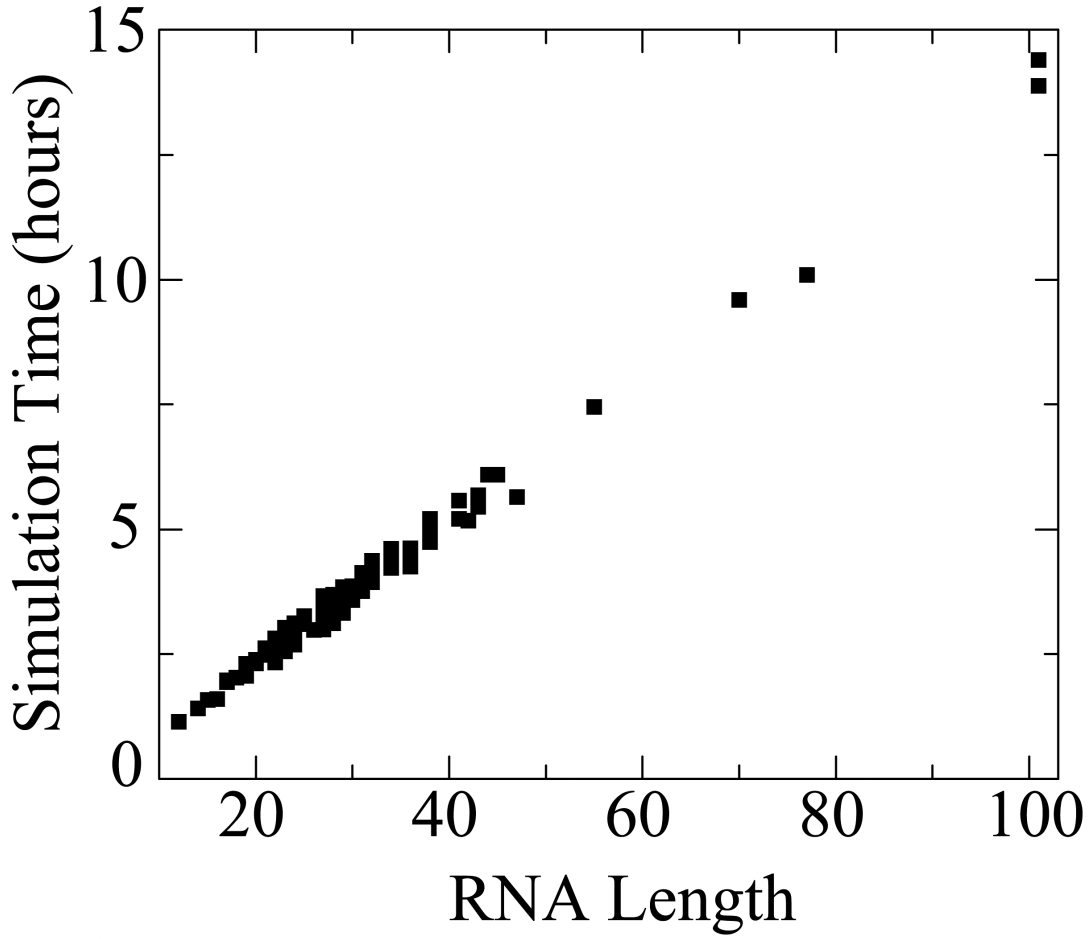
SUPPLEMENTARY DATA



Supplementary Figure 1. Linear scaling of simulation time with increasing length of RNA. Total wall-clock time spent in the simulation of 153 RNA molecules studied is plotted as a function of RNA length (total number of nucleotides). Each replica-exchange DMD simulation is performed on eight 3.6 GHz Intel Xeon compute nodes of the UNC Topsail cluster, communicating over MPI. Ten simulation runs out of 153 total simulations were temporarily suspended by the cluster and are excluded from this graph. A linear scaling in simulation time is observed with increasing size of RNA, demonstrating efficient scalability of DMD simulations for investigating dynamics of long RNA molecules.

Supplemental Table 1: List of the 153 RNA structures whose ab initio folding simulations are performed. Nucleic Acid DataBank records of corresponding RNA molecules, number of nucleotides in the corresponding RNA molecule, predicted Q values (Q_{Pred}), maximum Q value (Q_{Max}), Q value from Mfold (Q_{Mfold}), the backbone RMS deviation of predicted structure from the native structure ($RMSD_{Pred}$) and minimum RMSD, ($RMSD_{Min}$) are shown.

Nucleic Acid DataBank	Number of Nucleotides	Q_{Pred}	Q_{Max}	Q_{Mfold}	$RMSD_{Pred}$	$RMSD_{Min}$
17ra	21	1.00	1.00	1.00	2.69	1.12
1a51	41	0.88	1.00	0.92	4.27	2.18
1a60	44	1.00	1.00	0.77	4.58	2.03
1a9l	38	1.00	1.00	1.00	7.19	2.23
1anr	29	1.00	1.00	1.00	4.90	2.31
1aqo	29	0.91	1.00	0.91	3.65	1.88
1ato	19	1.00	1.00	1.00	2.35	0.95
1atv	17	1.00	1.00	1.00	1.13	0.50
1b36	38	1.00	1.00	1.00	5.17	2.13
1bgz	23	1.00	1.00	0.71	1.40	1.40
1bn0	20	1.00	1.00	1.00	1.50	0.76
1bvj	23	1.00	1.00	1.00	2.37	1.18
1cq5	43	1.00	1.00	1.00	4.90	2.23
1cql	43	1.00	1.00	1.00	5.33	2.38
1d0u	21	1.00	1.00	1.00	2.94	0.93
1e4p	24	1.00	1.00	1.00	2.44	1.46
1e95	36	1.00	1.00	0.50	3.78	2.40
1ebq	29	1.00	1.00	0.90	3.78	1.73
1ebr	30	0.78	1.00	0.90	3.66	1.70
1ebs	29	1.00	1.00	0.90	3.74	1.91
1eor	22	0.98	1.00	1.00	2.58	0.78
1esy	19	1.00	1.00	1.00	2.03	1.11
1evv	76	0.87	0.92	0.83	7.20	5.15
1f1t	38	1.00	1.00	1.00	4.93	2.91
1f6z	27	0.90	1.00	1.00	3.72	1.50
1f7f	27	0.99	1.00	1.00	3.88	1.37
1f7g	27	0.90	1.00	1.00	4.06	1.46
1f84	29	0.86	1.00	0.86	3.60	2.34
1f9l	22	0.98	1.00	1.00	2.58	0.78
1fqz	27	1.00	1.00	0.75	2.35	2.35
1fyo	27	0.88	1.00	0.89	2.46	1.00
1hlx	20	1.00	1.00	1.00	2.66	0.78
1ie1	22	0.75	1.00	0.80	3.80	1.92
1ie2	22	1.00	1.00	0.67	3.50	1.91
1ikd	22	1.00	1.00	1.00	2.18	1.06
1j4y	17	1.00	1.00	1.00	2.82	1.00
1jo7	31	0.88	1.00	1.00	3.42	1.55
1jox	21	1.00	1.00	1.00	3.53	1.57
1jp0	21	1.00	1.00	1.00	3.25	1.53
1jtj	23	1.00	1.00	1.00	3.44	1.51
1jur	22	1.00	1.00	1.00	3.02	1.13
1k2g	22	1.00	1.00	0.50	1.71	1.71
1k5i	23	1.00	1.00	1.00	2.08	0.74
1k6g	22	1.00	1.00	1.00	2.12	0.80

1k6h	22	1.00	1.00	1.00	2.20	0.83
1kaj	32	1.00	1.00	0.56	6.96	1.64
1kka	17	1.00	1.00	1.00	3.45	1.04
1kks	24	1.00	1.00	0.86	2.59	1.20
1kp7	30	1.00	1.00	1.00	3.27	1.79
1kpd	32	0.90	1.00	0.50	5.75	1.94
1kxk	70	0.78	1.00	0.74	8.40	4.69
1l1w	29	1.00	1.00	1.00	2.56	1.09
1l3d	28	1.00	1.00	0.00	3.03	1.93
1lc6	24	1.00	1.00	1.00	2.73	0.94
1ldz	30	1.00	1.00	1.00	5.29	1.50
1lvj	31	1.00	1.00	1.00	4.30	1.58
1m5l	38	1.00	1.00	1.00	3.97	1.76
1m82	25	1.00	1.00	1.00	1.60	0.66
1mfj	20	1.00	1.00	1.00	1.94	0.87
1mfk	23	1.00	1.00	1.00	2.82	1.09
1mfy	31	1.00	1.00	1.00	3.79	1.56
1mnx	42	0.86	1.00	0.00	8.77	1.88
1msy	27	0.97	1.00	0.86	3.44	2.21
1mt4	24	0.88	1.00	0.89	2.68	1.13
1n8x	36	1.00	1.00	0.79	2.61	1.04
1na2	30	1.00	1.00	1.00	3.28	1.50
1nbk	34	0.92	0.92	0.92	4.01	1.75
1nbr	29	0.91	1.00	0.92	2.82	1.26
1nc0	24	1.00	1.00	1.00	3.61	0.94
1nem	23	1.00	1.00	1.00	2.37	1.23
1oq0	15	1.00	1.00	0.83	1.61	0.91
1osw	23	1.00	1.00	1.00	2.62	1.00
1ow9	23	1.00	1.00	1.00	2.78	1.07
1p5m	55	0.00	0.35	0.94	20.07	8.49
1p5n	34	1.00	1.00	0.90	3.72	2.42
1p5o	77	0.00	0.24	0.52	24.10	10.99
1pjy	22	1.00	1.00	1.00	2.14	0.85
1q8n	38	1.00	1.00	1.00	8.37	2.93
1qc8	25	1.00	1.00	1.00	2.79	1.31
1qwa	21	1.00	1.00	1.00	2.81	1.21
1qwb	26	0.83	1.00	0.86	4.74	1.76
1r2p	34	0.98	1.00	1.00	4.22	1.52
1r7w	34	1.00	1.00	1.00	6.33	1.86
1r7z	34	1.00	1.00	1.00	7.73	1.95
1rfr	30	0.97	1.00	1.00	3.81	1.41
1rht	24	1.00	1.00	1.00	3.89	1.89
1rnk	34	0.91	1.00	0.45	4.01	2.45
1s2f	23	1.00	1.00	1.00	3.01	1.17
1s34	23	1.00	1.00	1.00	2.99	1.02
1s9s	100	0.99	1.00	0.94	10.39	5.62
1scl	29	0.71	1.00	0.75	6.04	1.91
1slo	19	1.00	1.00	1.00	2.88	0.97
1slp	19	1.00	1.00	1.00	2.99	1.04
1sy4	24	1.00	1.00	1.00	2.11	0.92
1syz	24	1.00	1.00	1.00	2.44	1.21
1szy	21	1.00	1.00	1.00	2.90	0.86
1t28	34	1.00	1.00	1.00	5.25	2.09
1tbk	17	1.00	1.00	1.00	3.28	0.87
1tjz	22	1.00	1.00	1.00	2.42	1.12
1tlr	23	1.00	1.00	1.00	2.94	1.24
1txs	38	0.97	1.00	1.00	4.88	1.77
1u2a	20	1.00	1.00	1.00	1.81	0.74
1u3k	38	1.00	1.00	1.00	6.35	2.06

1uuu	19	1.00	1.00	1.00	2.48	1.16
1wks	17	1.00	1.00	1.00	2.44	1.01
1xhp	32	1.00	1.00	1.00	2.83	1.05
1xsg	27	1.00	1.00	1.00	3.74	1.27
1xsh	27	1.00	1.00	1.00	2.42	0.97
1xst	27	1.00	1.00	1.00	3.63	1.37
1xsu	27	1.00	1.00	1.00	2.18	1.08
1xwp	15	1.00	1.00	1.00	2.24	0.84
1xwu	16	0.78	1.00	0.80	2.27	0.87
1ylg	31	0.89	1.00	0.90	3.02	1.06
1ymo	47	0.94	0.94	0.63	4.00	3.19
1yn1	17	1.00	1.00	1.00	2.84	0.95
1yn2	17	1.00	1.00	1.00	2.33	0.86
1ync	31	0.89	1.00	0.90	2.96	1.27
1yne	31	0.89	1.00	0.90	2.73	1.17
1yng	31	0.89	1.00	0.89	3.87	1.22
1ysv	27	1.00	1.00	1.00	2.17	0.83
1z2j	45	1.00	1.00	0.95	3.96	1.55
1z30	18	1.00	1.00	1.00	1.90	0.58
1z31	32	0.70	1.00	1.00	4.27	2.20
1zc5	41	1.00	1.00	0.94	3.54	1.23
28sp	28	1.00	1.00	1.00	4.26	1.33
28sr	28	1.00	1.00	1.00	3.01	1.23
2a9l	38	1.00	1.00	1.00	7.33	2.36
2aht	27	1.00	1.00	1.00	3.25	1.16
2ap0	28	0.00	0.43	0.63	7.55	3.27
2ap5	28	0.00	0.43	0.63	7.46	3.28
2au4	41	0.90	1.00	0.91	5.71	3.23
2b7g	19	1.00	1.00	1.00	1.82	0.96
2es5	23	0.89	0.89	0.90	2.72	1.11
2euy	34	0.86	1.00	0.91	4.22	1.80
2evy	14	1.00	1.00	1.00	2.32	0.76
2f87	12	1.00	1.00	1.00	1.77	0.55
2f88	34	0.98	1.00	1.00	3.14	1.51
2fdt	36	0.91	1.00	0.92	4.00	1.57
2fey	43	1.00	1.00	1.00	3.45	1.47
2frl	23	1.00	1.00	1.00	3.36	0.78
2g1g	17	1.00	1.00	1.00	2.95	0.68
2gio	29	0.88	1.00	0.89	3.25	1.34
2gv3	22	0.86	1.00	0.88	3.08	1.13
2h2x	21	1.00	1.00	1.00	3.36	1.08
2hem	24	1.00	1.00	1.00	2.59	1.19
2hns	22	1.00	1.00	1.00	2.56	0.85
2ldz	30	1.00	1.00	1.00	4.54	1.53
2tpk	36	1.00	1.00	0.58	3.75	1.74
2u2a	20	1.00	1.00	1.00	1.81	0.88
3php	23	1.00	1.00	1.00	2.52	0.90
430d	29	0.83	0.83	0.75	2.33	2.33
437d	28	1.00	1.00	0.00	3.09	1.89
480d	27	0.90	1.00	0.86	3.53	2.32

Supplemental Table 2. The averages and standard deviations of the bonded atom pairs. All the bonds, angles, and dihedrals are effectively model by a bond in the DMD simulations.

$P_i\ S_i$	4.55 ± 0.09 Å
$S_i\ P_{i+1}$	4.10 ± 0.07 Å
$S_i\ A_i$	4.85 ± 0.15 Å
$S_i\ U_i$	3.74 ± 0.08 Å
$S_i\ G_i$	4.81 ± 0.14 Å
$S_i\ C_i$	3.70 ± 0.13 Å
$P_i\ P_{i+1}$	6.25 ± 0.95 Å
$S_i\ S_{i+1}$	5.72 ± 0.45 Å
$P_i\ A_i$	7.45 ± 0.45 Å
$P_i\ U_i$	5.57 ± 0.37 Å
$P_i\ Gi$	7.43 ± 0.43 Å
$P_i\ C_i$	5.57 ± 0.37 Å
$A_i\ P_{i+1}$	7.25 ± 0.42 Å
$U_i\ P_{i+1}$	6.40 ± 0.20 Å
$G_i\ P_{i+1}$	7.20 ± 0.43 Å
$C_i\ P_{i+1}$	6.40 ± 0.20 Å
$P_{i-1}\ S_i$	9.25 ± 0.95 Å
$S_{i-1}\ P_{i+1}$	8.96 ± 0.44 Å
$A_{i-1}\ S_i$	5.68 ± 0.68 Å
$U_{i-1}\ S_i$	6.38 + 0.73 Å
$G_{i-1}\ S_i$	5.68 ± 0.68 Å
$C_{i-1}\ S_i$	6.38 ± 0.73 Å
$S_{i-1}\ A_i$	7.25 ± 0.60 Å
$S_{i-1}\ U_i$	5.66 ± 0.54 Å
$S_{i-1}\ G_i$	7.25 ± 0.60 Å
$S_{i-1}\ C_i$	5.66 ± 0.54 Å

Supplemental Table 3. The parameters for base pairing, modeled by hydrogen bonds between AU, GC and UG. The details of the DMD algorithm for the hydrogen bond can be found in (Ding et al., 2003). The hydrogen bond strengths, $\boldsymbol{E^{HB}}$**,** for AU, GC and UG are 0.5, 1.2, and 0.5 Kcal/mol, respectively.

Atom pair	d_{min}	d_0	d_1	d_{max}
C_i G_j	5.20 Å	5.46 Å	5.62 Å	5.74 Å
Si Gj	7.70 Å	8.08 Å	8.63 Å	9.00 Å
Ci Sj	9.74 Å	10.10 Å	10.53 Å	10.82 Å
Ai Uj	5.00 Å	5.25 Å	5.68 Å	5.84 Å
Si Uj	9.76 Å	9.94 Å	10.50 Å	10.76 Å
Ai Sj	7.72 Å	7.92 Å	8.82 Å	9.00 Å
Ui Gj	5.10 Å	5.65 Å	6.10 Å	6.25 Å
Si Gj	7.00 Å	7.44 Å	8.24 Å	8.70 Å
Ui Sj	9.50 Å	10.25 Å	10.80 Å	11.35 Å

Supplemental Table 4. The stacking and hydrophobic interaction strengths, expressed in kcal/mol units. The subscript indicates that the base bead is paired. For example, A_U is a base bead *A* that has been paired with a *U* bead. The cutoff distances of base stacking are 4.65 Å between purines, 4.60 Å between pyrimidines, and 3.80 Å between purine and pyrimidine. The cutoff distance for hydrophobic interactions is 6.5 Å. The hardcore distance between of all beads is set as 3.3 Å.

E^{Stack}	A_U	U_A	G_C	C_G	G_U	U_G
A_U	-0.45	-0.50	-0.75	-0.95	-0.42	-0.70
U_A	-0.50	-0.40	-0.55	-0.60	-0.35	-0.35
G_C	-0.75	-0.55	-0.81	-0.95	-0.48	-0.92
C_G	-0.95	-0.60	-0.95	-1.10	-0.47	-0.51
G_U	-0.42	-0.35	-0.48	-0.47	-0.52	+0.62
U_G	-0.70	-0.35	-0.51	-0.51	+0.62	-0.44

$E^{Hydrophobic}$	A_U	U_A	G_C	C_G	G_U	U_G
A_U	-0.25	-0.40	-0.40	-0.50	-0.25	-0.35
U_A	-0.40	-0.30	-0.25	-0.25	-0.25	-0.25
G_C	-0.40	-0.25	-0.25	-0.45	-0.25	-0.41
C_G	-0.50	-0.25	-0.45	-0.50	-0.25	-0.41
G_U	-0.25	-0.25	-0.25	-0.25	-0.30	+0.25
U_G	-0.35	-0.25	-0.41	-0.41	+0.25	-0.25

References

Ding,F., Borreguero,J.M., Buldyrey,S.V., Stanley,H.E., and Dokholyan,N.V. (2003). Mechanism for the alpha-helix to beta-hairpin transition. Proteins *53*, 220-228.