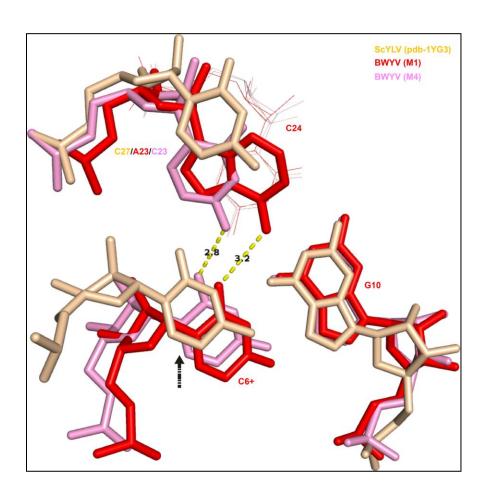
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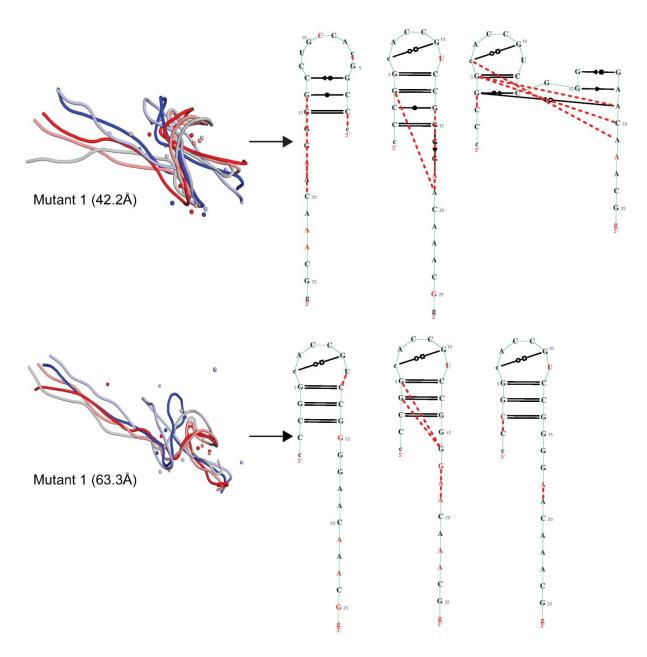
Supplementary information for "The Role of Sequence in Altering the Unfolding Pathway of an RNA Pseudoknot: A Steered Molecular Dynamics Study"

Asmita Gupta and Manju Bansal

Supplementary figure S1: Contacts between C23 (MUT2) and C6+ residue. Native structure residues were superposed on mut2 along with the structurally similar region in Sugarcane leaf yellow virus (ScYLV) containing C27 residue.

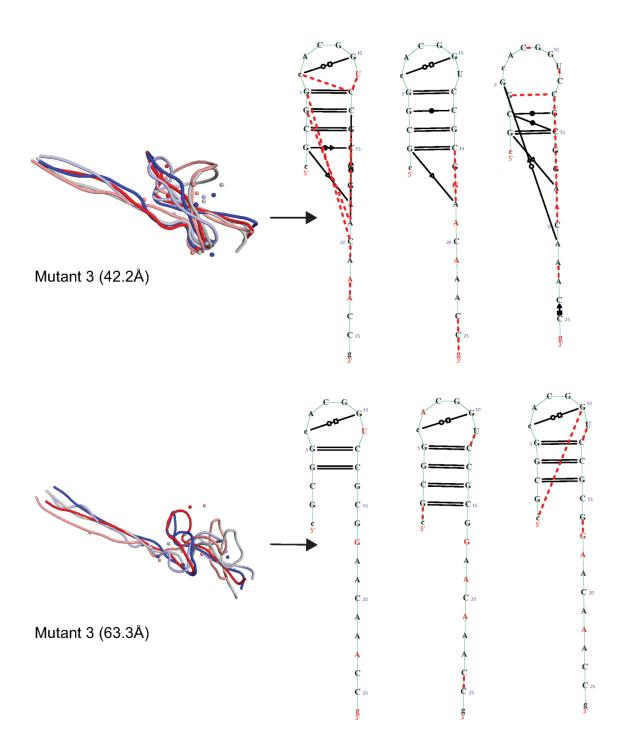


Supplementary figure S2: Snapshots extracted from mut1 simulation (C2G15) at 42 and 63Å extensions and the corresponding secondary structure representations for these intermediate structures

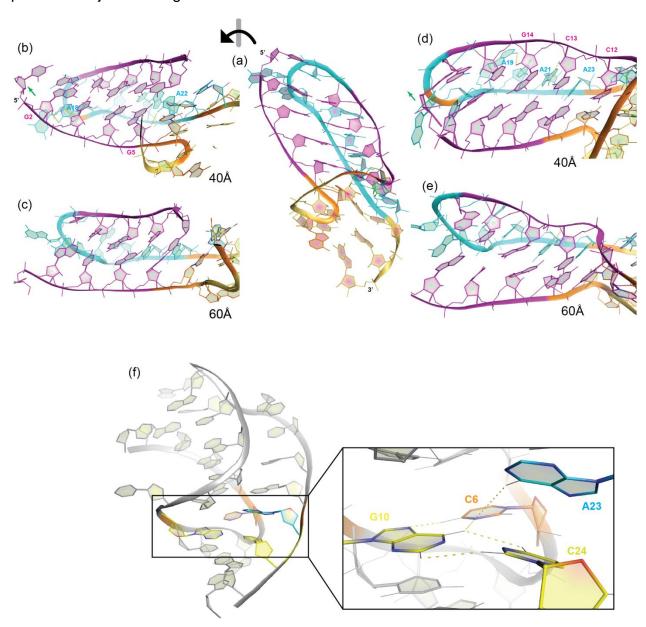


Secondary structure schematics from different pulling runs

Supplementary figure S3: Snapshots extracted from mut3 simulation (G9C25) at 42 and 63Å extensions and their corresponding secondary structure representations.



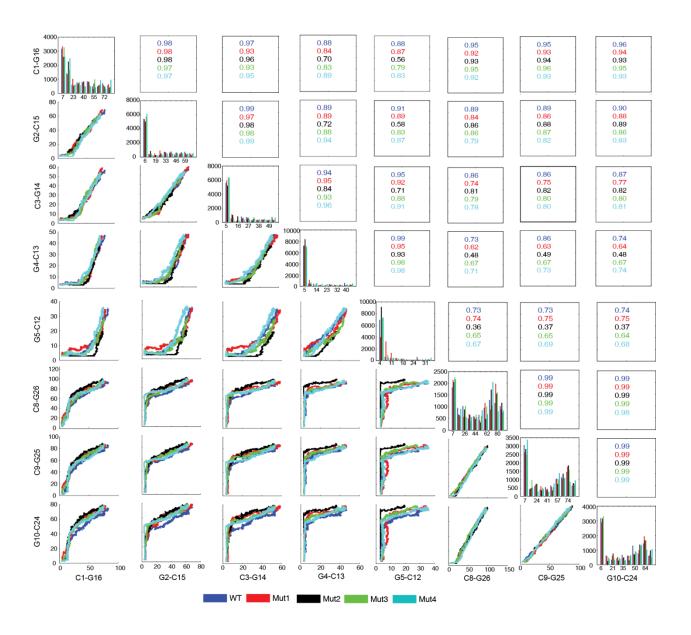
Supplementary figure S4: Disruption of strand dependent non-canonical contacts (a) tertiary structure of Beet Western Yellow Virus pseudoknot. Stem 1 is colored magenta, stem 2 is yellow, loop 1 is orange and loop 2 is cyan (b, c) hydrogen bonds formed between loop 2 residues A18, A22 and G2, G5 respectively (d, e) hydrogen bonds formed between loop 2 residues A19, A21, A23 and stem 1 residues G14, C13, C12 (f) hydrogen bonds between base quadruple formed by C6-G10-C24-A23 at the pseudoknot junction region



Supplementary figure S5: Correlation values corresponding to the matrix in figure S6

0.99 0.99 0.98 0.99	0.99 0.98 0.97 0.99 0.97	0.92 0.93 0.95 0.95 0.88	0.96 0.84 0.54 0.87 0.84	0.9 0.92 0.94 0.95 0.91	0.91 0.86 0.92 0.91 0.87
0.98	0.95	0.86	0.91	0.84	0.86
0.98	0.95	0.86	0.79	0.86	0.8
0.99	0.96	0.91	0.55	0.93	0.91
0.98	0.94	0.86	0.89	0.88	0.83
0.97	0.91	0.76	0.82	0.8	0.75
0.96	0.93	0.81	0.89	0.78	0.81
0.92	0.87	0.75	0.78	0.74	0.65
0.95	0.91	0.85	0.68	0.84	0.82
0.94	0.9	0.79	0.92	0.8	0.74
0.95	0.89	0.73	0.83	0.77	0.71
0.85	0.82	0.64	0.8	0.59	0.62
0.81	0.77	0.61	0.78	0.58	0.5
0.65	0.6	0.5	0.91	0.46	0.42
0.83	0.78	0.63	0.9	0.64	0.57
0.88	0.83	0.63	0.89	0.66	0.6
0.86	0.83	0.65	0.8	0.6	0.63
0.84	0.84	0.71	0.89	0.68	0.6
0.52	0.48	0.37	0.97	0.33	0.3
0.78	0.74	0.6	0.89	0.59	0.53
0.81	0.78	0.56	0.9	0.59	0.53
0.95 0.92 0.9 0.92 0.92	0.97 0.96 0.95 0.96 0.96	0.98 0.99 0.98 0.99 0.97	0.97 0.86 0.36 0.76 0.8	0.96 0.97 0.94 0.97 0.97	0.96 0.94 0.93 0.94
0.95 0.93 0.92 0.93 0.93	0.98 0.97 0.97 0.97 0.98	0.99 0.99 0.99 0.99	0.97 0.85 0.36 0.75	0.97 0.97 0.96 0.98 0.98	0.97 0.94 0.95 0.96 0.96
0.96	0.99	0.99	0.97	0.97	0.96
0.95	0.98	1	0.83	0.99	0.96
0.93	0.97	0.99	0.36	0.96	0.95
0.93	0.98	1	0.73	0.98	0.96
0.94	0.99	0.99	0.78	0.99	0.96

Supplementary figure S6: Correlation matrix showing base pair opening of all the WC pairs of the structure in all the simulated structures. The diagonal shows the histogram distribution of the base-pair distance. Top right triangle indicates the Spearman's correlation coefficient values. X- and Y- axes indicates the values of the distance between the corresponding base-pair.



Supplementary figure S7: Hydration and ionic densities around Mut2 structures at different stages of extension.

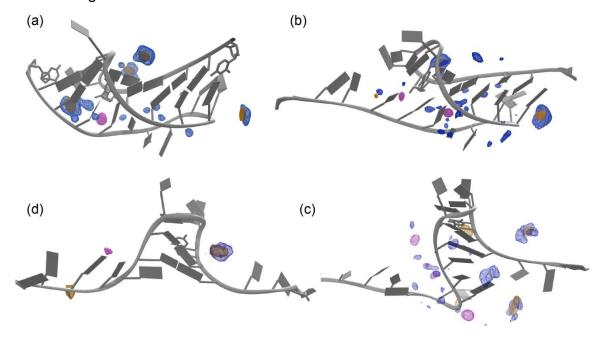
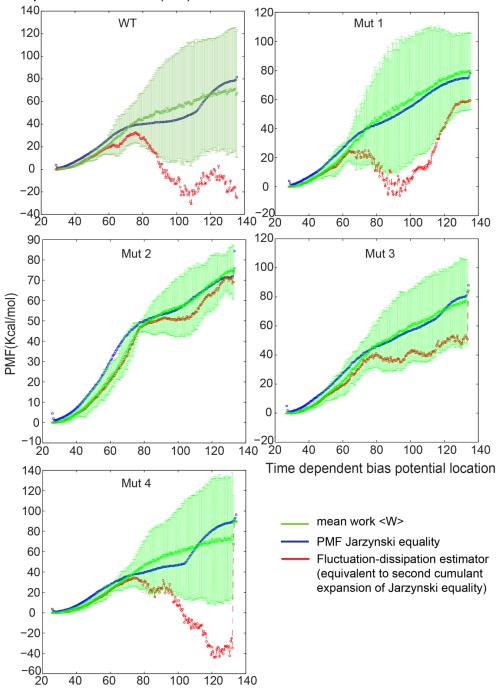


Figure S8: PMF profiles for different systems calculated using Jarzynski equality (blue) along with mean work done and its standard deviation (green) and Fluctuation – dissipation estimation (red)



Supplementary table S1: Average hydrogen bond lengths between non canonical pairs in different systems from conventional MD simulations (cMD)

pair [#]	WT		Mut1		Mut2		Mut3		Mut4		X-Ray
	mean¶	%	mean	%	mean	%	mean	%	mean	%	
G2(N2)_A18(N3) ^a	2.9	100	-	-	3.0	100	3.0	100	3.0	100	3.0
	(0.1)				(0.1)		(0.1)		(0.1)		
G2(O2')_A18(N1) ^a	2.9	85	3.1	68	2.9	75	2.9	83	2.9	89	2.7
	(0.2)		(0.3)		(0.2)		(0.2)		(0.2)		
C15(O2')_A18(O2') ^a	3.4	77	3.0	83	2.9	93	3.1	88	3.3	53	2.7
	(1.1)		(0.6)		(0.6)		(1.0)		(0.6)		
G4(N2)_A21(N1)	-	_	-	_	-	_	-	_	-	_	5.5
C13(O2')_A21(N1)	2.9	84	2.8	87	3.3	60	2.9	85	_	_	2.7
(-)_	(0.3)		(0.2)		(0.8)		(0.3)				
C13(O2)_A21(N6)	3.2	87	3.2	87	3.9	64	3.2	86	_	_	3.1
()()	(0.4)		(0.3)		(1.0)		(0.4)				
G5(N2)_A22(N1) ^b	3.1	100	3.1	100	3.0	100	3.2	95	_	_	3.0
30 (1 (2)_1 122 (1 (1)	(0.2)	100	(0.2)	100	(0.1)	100	(0.4)	,,,			2.0
G5(N2)_A22(N6) ^b	3.5	36	3.6	54	3.6	57	3.6	47	_	_	3.7
00(112)_1122(110)	(0.2)	50	(0.2)	5-	(0.2)	51	(0.2)	.,			5.7
G5(N3)_A22(N6) ^b	2.9	94	2.9	95	2.9	96	3.0	90	_	_	2.9
	(0.1)	7-1	(0.1))3	(0.1)	70	(0.2)	70			2.7
G5(O2')_A22(N6) ^b	3.0	81	3.0	78	3.0	72	3.1	77	_	_	3.0
G3(O2)_A22(110)	(0.2)	01	(0.2)	70	(0.2)	12	(0.5)	, ,			3.0
C12(O2')_A23(N1) ^{c§}	2.9	92	2.9	89	2.9	80	2.8	97	3.4	70	2.7
	(0.5))2	(0.3)	0)	(0.2)	00	(0.1)	71	(0.9)	70	2.7
C12(O2)_A23(N6) ^{c§}	3.1	88	3.0	88	3.0	66	3.0	92	3.5	64	2.8
	(0.4)	00	(0.2)	00	(0.3)	00	(0.2))2	(1.0)	04	2.0
C6(N3)_G10(O6)	2.8	98	2.8	99	2.8	96	2.8	98	2.9	97	2.7
	(0.1)	70	(0.1)	"	(0.1)	70	(0.1)	70	(0.1)	71	2.1
C6(N4)_G10(N7)	2.9	95	2.9	96	2.9	94	2.9	92	2.9	98	3.0
20(114)_010(117)	(0.1)	75	(0.1)	70	(0.1)	74	(0.1))2	(0.1)	70	3.0
C6(O2)_A23(N6) ^d	3.3	87	3.4	84	3.0	99	3.7	68	-	_	2.9
20(O2)_A23(1\0)	(0.7)	67	(0.5)	04	(0.2)	"	(0.8)	00	_	_	2.7
G14(N2)_A19(OP2)	3.5	64	(0.5)	_	3.5	58	3.2	82			2.9
314(N2)_A19(O12)	(0.9)	04	-	-	(0.9)	36	(0.7)	62	-	-	2.9
G14(O2')_A19(N6)	3.3	74			(0.5)		3.3	65			3.1
314(O2)_A19(N0)	(0.7)	74	-	-	-	-	(0.6)	03	-	-	3.1
A7(O2')_C8(OP1)	(0.7)				2.9	89	3.3	62			4.8
A7(O2)_C6(OF1)	-	-	-	-	(0.5)	09	(0.9)	02	-	-	4.0
A7(OP1)_C8(N4)					3.2	96	3.9	54			2.9
A/(UP1)_Co(N4)	-	-	-	-	(0.6)	86		34	-	-	2.9
C2(O2) A19(O2)	3.2	51	3.2	52			(1.2)	50			2.0
C3(O2)_A18(O2')	(0.5)	51		53	-	-		59	-	-	2.9
G17(N2)_G17(OP2)	(0.3)		(0.4)	6 0			(0.5)				0.4
	-	-	3.9	68	-	-	-	-	-	-	9.4
G17/000 A10/001			(2.3)	0.1	2.5	4.5	2.2	~ ~			4.5
G17(O2')_A18(OP1)	-	-	2.7	91	3.6	46	3.2	56	-	-	4.7
100/00h 100/05he	2.1	7.	(0.2)	7.	(1.0)		(0.8)	72			4.0
A22(O2')_A23(O5') ^e	3.1	74	3.1	74	3.1	65	3.1	73	-	-	4.2
	(0.2)		(0.2)		(0.2)		(0.2)				