Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

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

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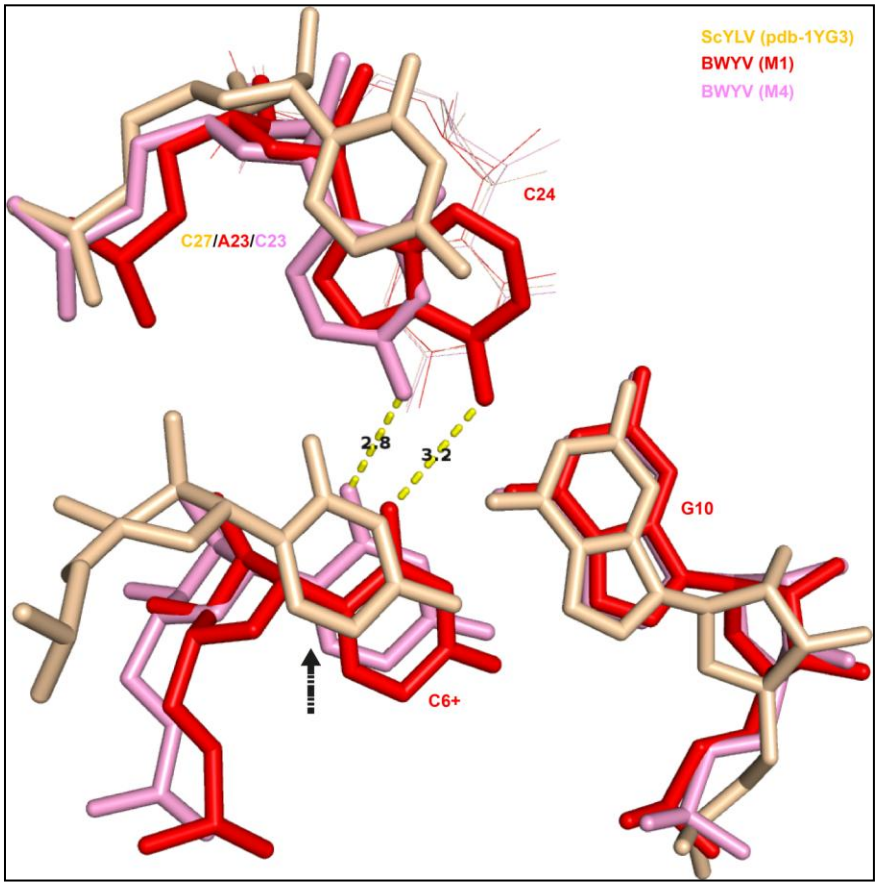
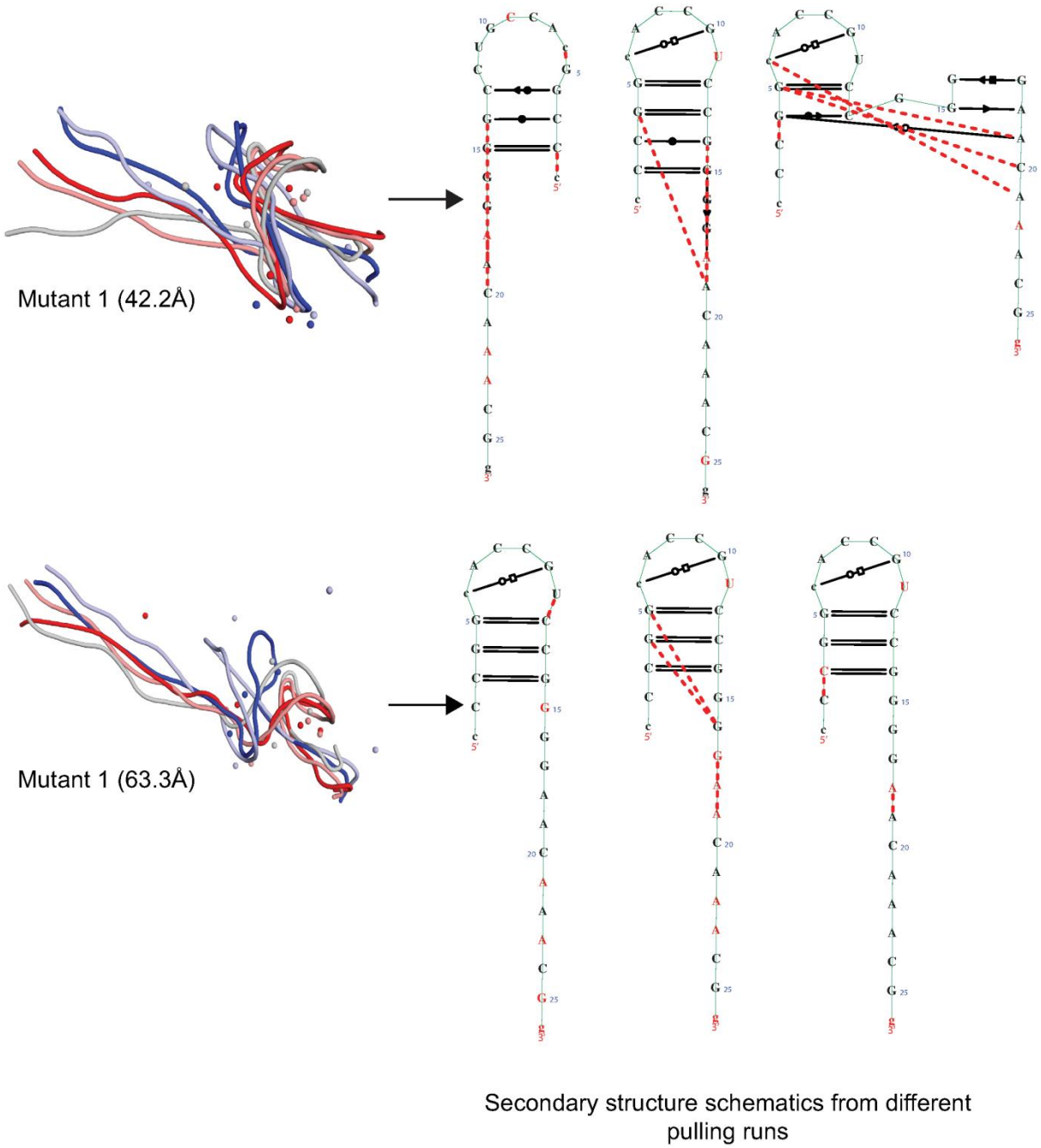
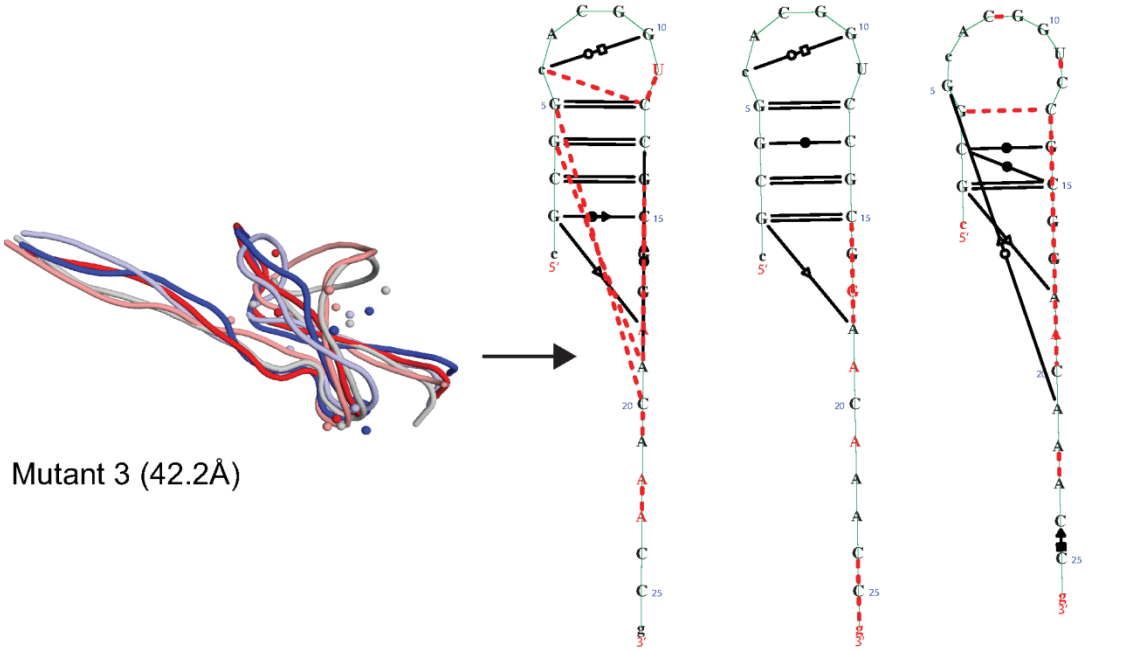
Supplementary figure S1: Contacts between C23 (MUT2) and C6+ residue. Native structure residues were superposed on mut2 along with the structurally similar region in Sugarcane leaf yellow virus (ScYLV) containing C27 residue.



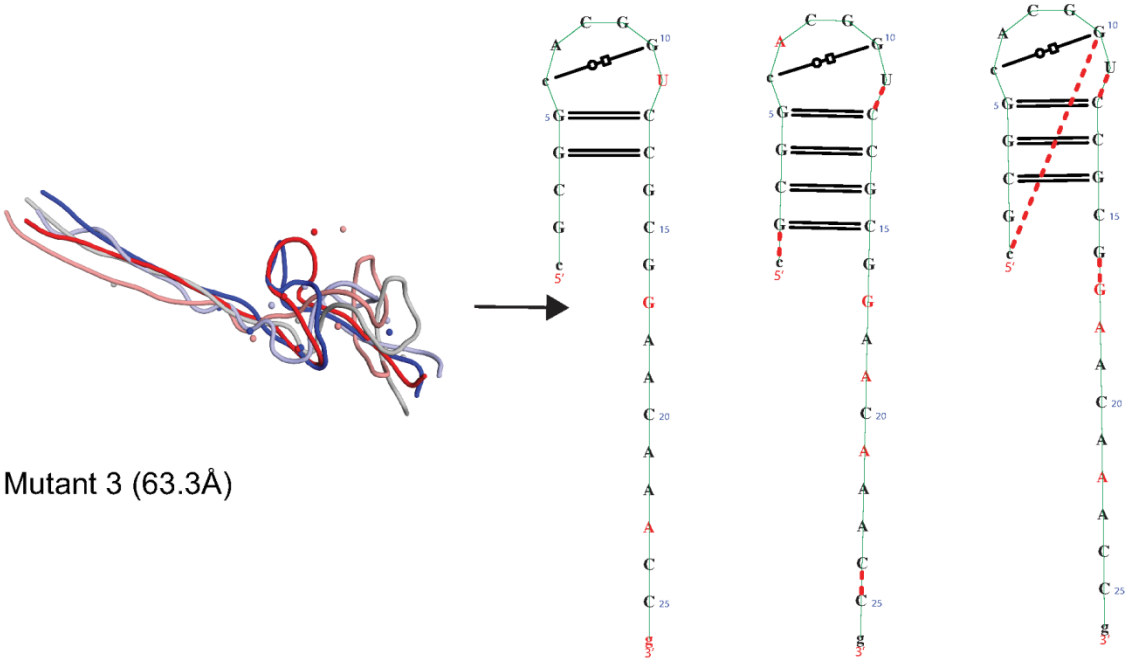
Supplementary figure S2: Snapshots extracted from mut1 simulation (C2G15) at 42 and 63Å extensions and the corresponding secondary structure representations for these intermediate structures



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

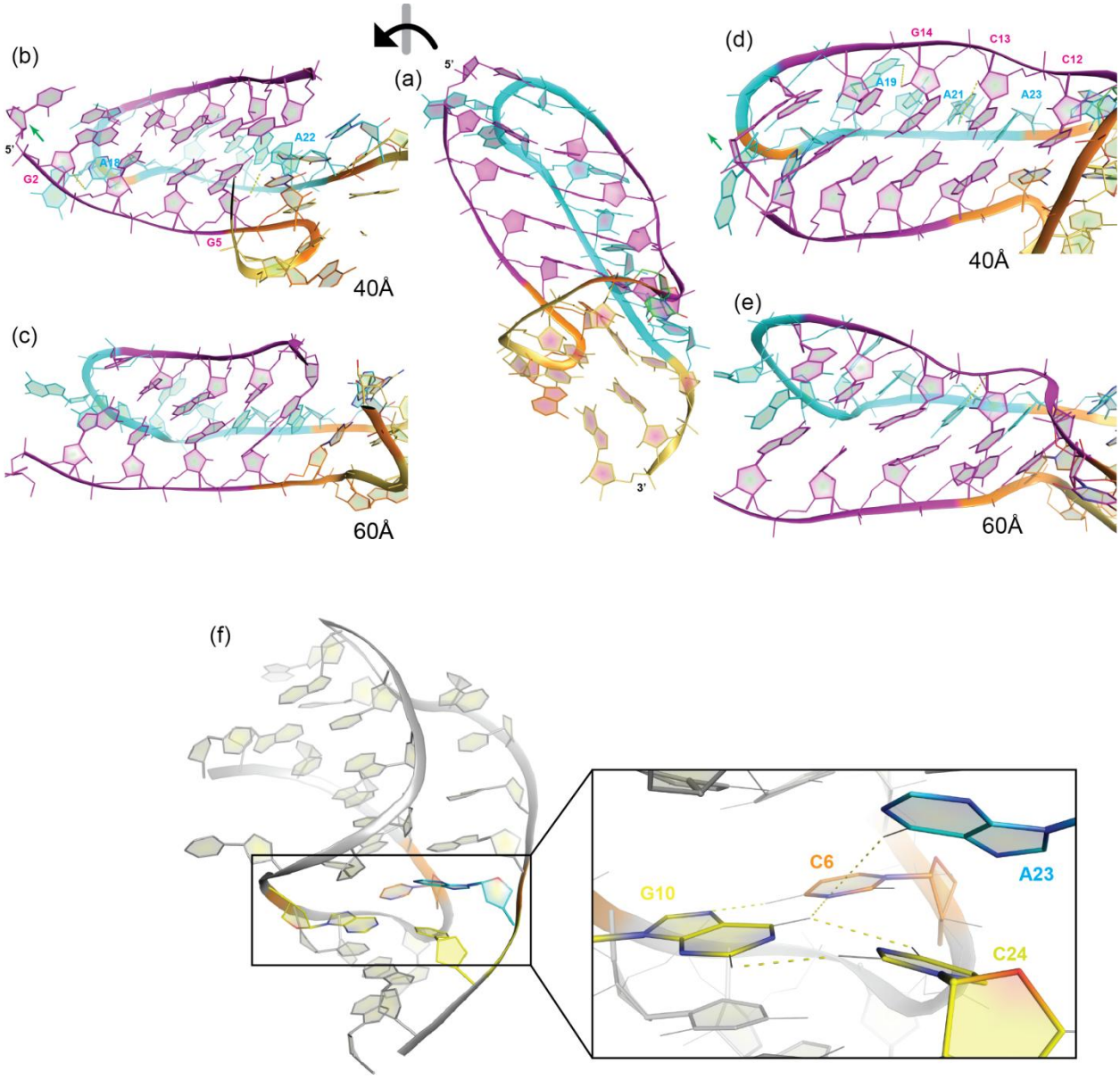


Mutant 3 (42.2Å)



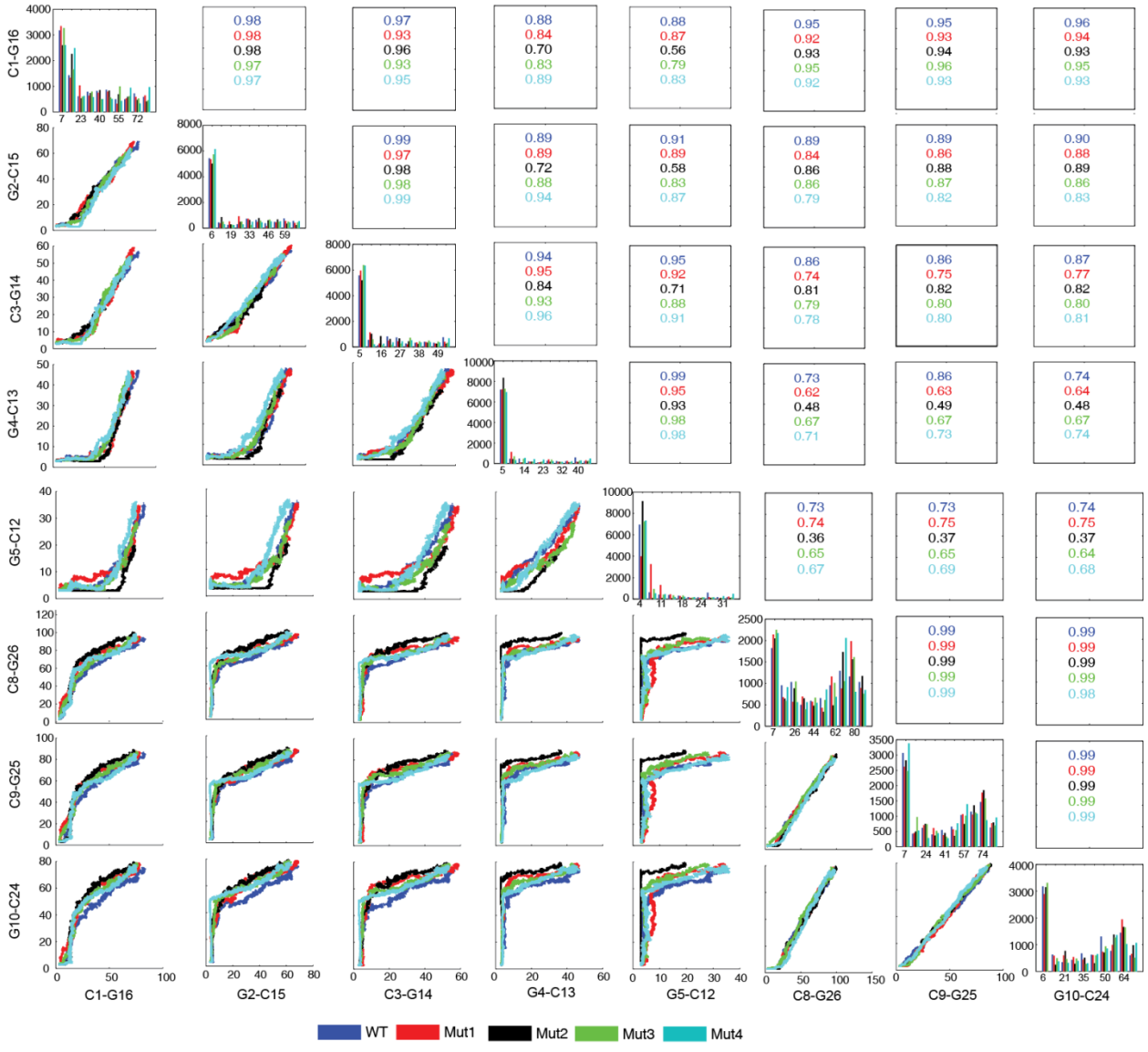
Mutant 3 (63.3Å)

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

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.

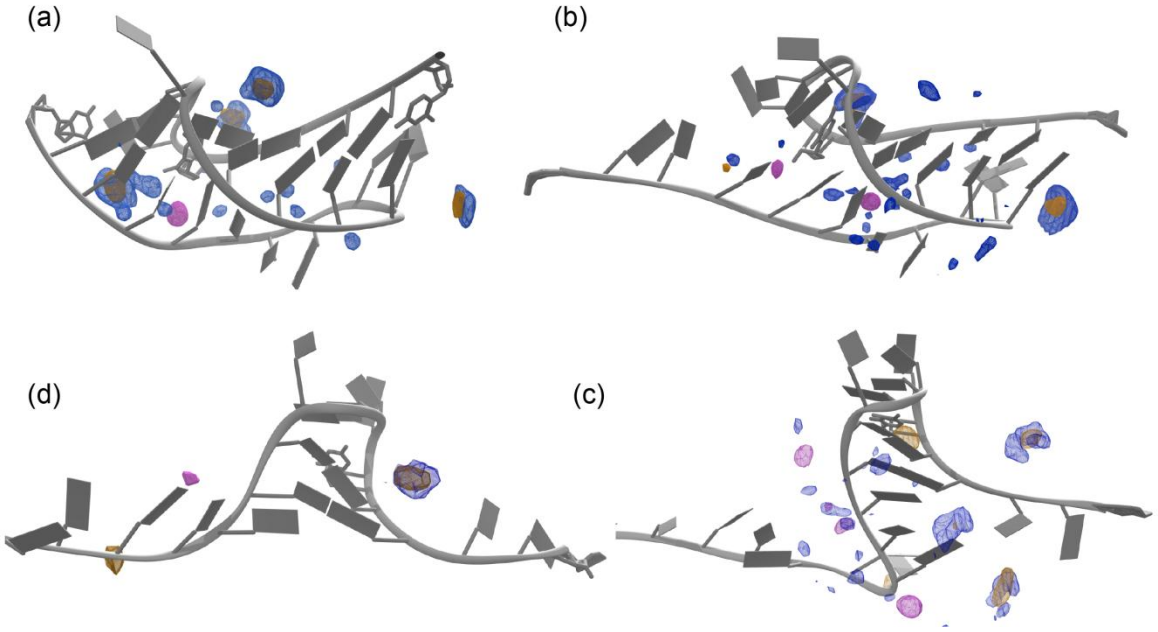
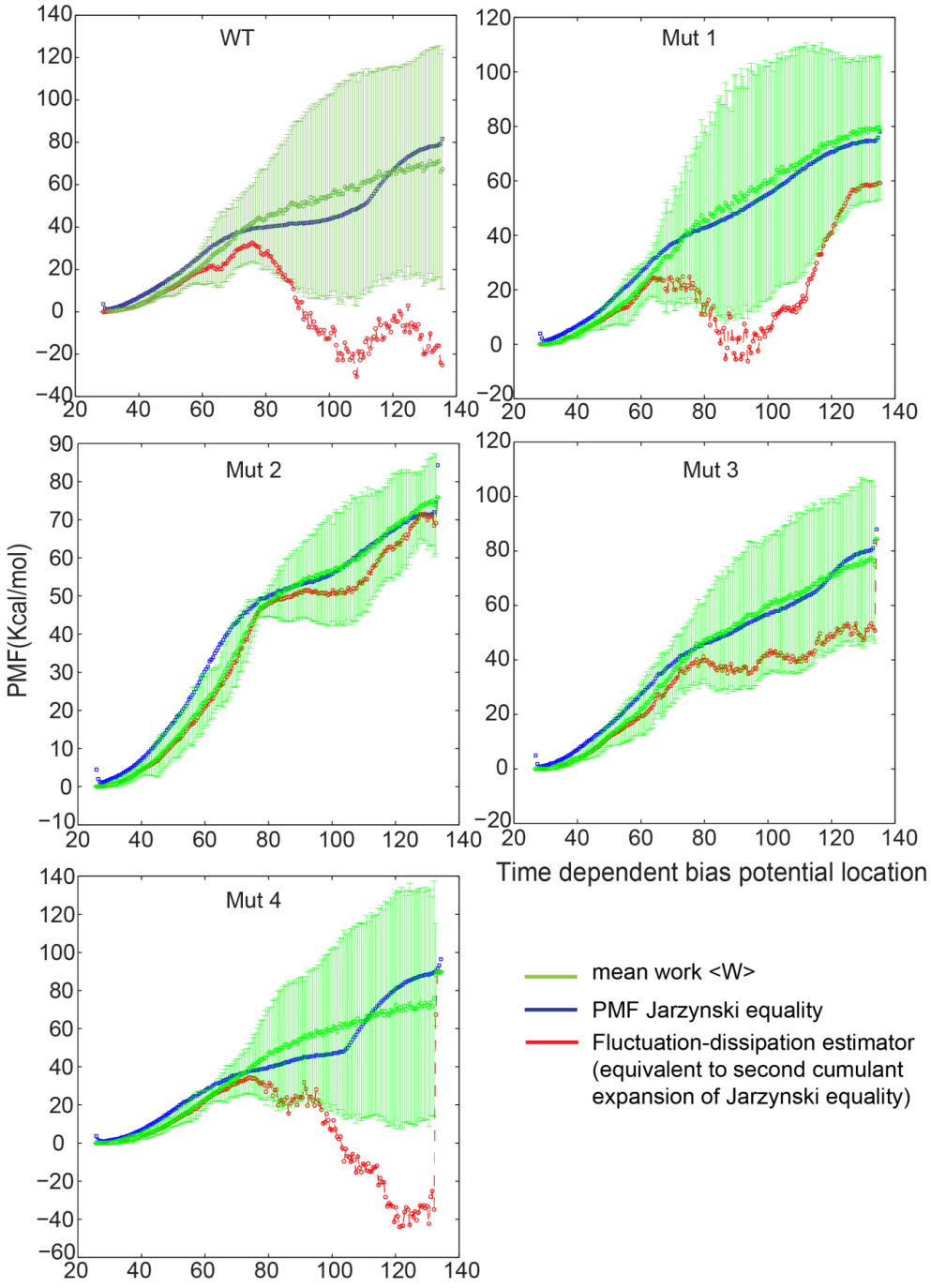


Figure S8: PMF profiles for different systems calculated using Jarzynski equality (blue) along with mean work done and its standard deviation (green) and Fluctuation – dissipation estimation (red)



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 (0.1)	100	-	-	3.0 (0.1)	100	3.0 (0.1)	100	3.0 (0.1)	100	3.0
G2(O2')_A18(N1)[a]	2.9 (0.2)	85	3.1 (0.3)	68	2.9 (0.2)	75	2.9 (0.2)	83	2.9 (0.2)	89	2.7
C15(O2')_A18(O2')[a]	3.4 (1.1)	77	3.0 (0.6)	83	2.9 (0.6)	93	3.1 (1.0)	88	3.3 (0.6)	53	2.7
G4(N2)_A21(N1)	-	-	-	-	-	-	-	-	-	-	5.5
C13(O2')_A21(N1)	2.9 (0.3)	84	2.8 (0.2)	87	3.3 (0.8)	60	2.9 (0.3)	85	-	-	2.7
C13(O2)_A21(N6)	3.2 (0.4)	87	3.2 (0.3)	87	3.9 (1.0)	64	3.2 (0.4)	86	-	-	3.1
G5(N2)_A22(N1)[b]	3.1 (0.2)	100	3.1 (0.2)	100	3.0 (0.1)	100	3.2 (0.4)	95	-	-	3.0
G5(N2)_A22(N6)[b]	3.5 (0.2)	36	3.6 (0.2)	54	3.6 (0.2)	57	3.6 (0.2)	47	-	-	3.7
G5(N3)_A22(N6)[b]	2.9 (0.1)	94	2.9 (0.1)	95	2.9 (0.1)	96	3.0 (0.2)	90	-	-	2.9
G5(O2')_A22(N6)[b]	3.0 (0.2)	81	3.0 (0.2)	78	3.0 (0.2)	72	3.1 (0.5)	77	-	-	3.0
C12(O2')_A23(N1)[c§]	2.9 (0.5)	92	2.9 (0.3)	89	2.9 (0.2)	80	2.8 (0.1)	97	3.4 (0.9)	70	2.7
C12(O2)_A23(N6)[c§]	3.1 (0.4)	88	3.0 (0.2)	88	3.0 (0.3)	66	3.0 (0.2)	92	3.5 (1.0)	64	2.8
C6(N3)_G10(O6)	2.8 (0.1)	98	2.8 (0.1)	99	2.8 (0.1)	96	2.8 (0.1)	98	2.9 (0.1)	97	2.7
C6(N4)_G10(N7)	2.9 (0.1)	95	2.9 (0.1)	96	2.9 (0.1)	94	2.9 (0.1)	92	2.9 (0.1)	98	3.0
C6(O2)_A23(N6)[d]	3.3 (0.7)	87	3.4 (0.5)	84	3.0 (0.2)	99	3.7 (0.8)	68	-	-	2.9
G14(N2)_A19(OP2)	3.5 (0.9)	64	-	-	3.5 (0.9)	58	3.2 (0.7)	82	-	-	2.9
G14(O2')_A19(N6)	3.3 (0.7)	74	-	-	-	-	3.3 (0.6)	65	-	-	3.1
A7(O2')_C8(OP1)	-	-	-	-	2.9 (0.5)	89	3.3 (0.9)	62	-	-	4.8
A7(OP1)_C8(N4)	-	-	-	-	3.2 (0.6)	86	3.9 (1.2)	54	-	-	2.9
C3(O2)_A18(O2')	3.2 (0.5)	51	3.2 (0.4)	53	-	-	3.2 (0.5)	59	-	-	2.9
G17(N2)_G17(OP2)	-	-	3.9 (2.3)	68	-	-	-	-	-	-	9.4
G17(O2')_A18(OP1)	-	-	2.7 (0.2)	91	3.6 (1.0)	46	3.2 (0.8)	56	-	-	4.7
A22(O2')_A23(O5')[e]	3.1 (0.2)	74	3.1 (0.2)	74	3.1 (0.2)	65	3.1 (0.2)	73	-	-	4.2