

Table S2: **Base pairing**

		simulation									
base pairs ↓		G1491A		G1491U		U1495C		U1406C/U1495A		NON_MUT ¹	
1406: ²	1495 ³	99.53	97.81	97.85	98.99	80.62	84.16	89.40	89.63	96.38	97.01
A1408:	A1492	5.56	0.76	3.70	1.85	—	14.99	1.73	—	—	8.98
	A1493	48.68	35.73	47.28	25.44	6.11	23.96	—	—	49.75	24.99
C1409:	1491 ⁴	28.60	34.47	15.94	20.65	not applicable					
	A1492	32.70	15.96	18.32	9.65	not applicable					

Percentage of simulation time when base pairs were formed (i.e., at least one hydrogen bond was present). Two values are shown for each simulation corresponding to two A-sites.

¹ data from our previous study (Romanowska J., Setny P., Trylska J., *J. Phys. Chem. B* **2008**);

² this base is U in G1491A, G1491U, NON_MUT and U1495C; and C in U1406C/U1495A simulation;

³ this base is U in G1491A, G1491U and NON_MUT; C in U1495C; and A in U1406C/U1495A simulation;

⁴ this base is A in G1491A, and U in G1491U.