Supporting Information for publication

Exploring the molecular basis of dsRNA recognition by Mss116p using molecular dynamics simulations and free energy calculations

Qiao Xue, Ji-Long Zhang, Qing-Chuan Zheng, Ying-Lu Cui, Lin Chen, Wen-Ting Chu and Hong-Xing Zhang**

State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, Changchun 130023, China

Table S1. Residues give more than 2 kcal/mol binding affinity. (kcal/mol)

Residue	ΔE_{vdw}	ΔE_{ele}	ΔG_{GB}	ΔG_{SA}	ΔG_{pol}[a]	ΔG_{nonpol}[b]	ΔG[c]
Thr382	-2.14 +/- 1.93	-15.88 +/- 2.61	11.44 +/- 1.47	-0.15 +/- 0.02	-4.44	-2.29	-6.73 +/- 2.95
Val383	-1.17 +/- 1.94	-13.98 +/- 2.71	9.55 +/- 1.38	-0.10 +/- 0.07	-4.43	-1.26	-5.70 +/- 3.16
Hie407	-1.11 +/- 1.51	0.26 +/- 3.76	-3.41 +/- 2.92	-0.00 +/- 0.06	-3.15	-1.11	-4.26 +/- 2.29
Gly408	-1.27 +/- 0.90	-6.62 +/- 1.61	3.50 +/- 1.40	-0.29 +/- 0.04	-3.12	-1.56	-4.68 +/- 3.33
Lys409	-1.71 +/- 1.73	-342.77 +/- 9.76	336.01 +/- 8.26	-0.41 +/- 0.10	-6.76	-2.12	-8.88 +/- 3.78
Gln412	-3.90 +/- 1.64	-8.10 +/- 3.85	9.89 +/- 2.12	-0.82 +/- 0.07	1.79	-4.73	-2.93 +/- 1.65
Lys414	-2.81 +/- 1.91	-304.28 +/- 9.62	305.03 +/- 9.15	-0.86 +/- 0.13	0.74	-3.67	-2.92 +/- 1.15
Arg415	-0.56 +/- 2.16	-313.97 +/- 7.78	298.45 +/- 6.09	-0.26 +/- 0.06	-15.52	-0.82	-16.34 +/- 2.62
Thr433	-0.26 +/- 2.01	-17.69 +/- 2.58	13.95 +/- 1.75	-0.12 +/- 0.02	-3.74	-0.37	-4.11 +/- 2.09
Val435	-2.40 +/- 1.89	-12.63 +/- 2.41	7.80 +/- 1.79	-0.08 +/- 0.03	-4.83	-2.47	-7.31 +/- 5.09
Gly436	-0.64 +/- 1.03	-2.94 +/- 5.52	1.03 +/- 4.12	-0.10 +/- 0.07	-1.92	-0.73	-2.65 +/- 1.39
Arg438	-0.53 +/- 1.98	-275.47 +/- 7.49	263.08 +/- 6.43	-0.51 +/- 0.10	-12.39	-1.04	-13.43 +/- 2.58
Arg538	-4.63 +/- 1.95	-249.01 +/- 11.85	249.87 +/- 10.12	-0.75 +/- 0.12	0.86	-5.38	-4.52 +/- 1.72
Lys542	-1.09 +/- 1.96	-243.75 +/- 12.74	240.70 +/- 12.42	-0.44 +/- 0.24	-3.05	-1.52	-4.57 +/- 3.25
Lys579	-2.28 +/- 1.78	-231.68 +/- 12.07	232.52 +/- 12.40	-0.62 +/- 0.19	0.83	-2.90	-2.06 +/- 2.55

[a] $\Delta G_{pol} = \Delta E_{ele} + \Delta G_{GB,}$ [b] $\Delta G_{nonpol} = \Delta E_{vdw} + \Delta G_{SA}$ [c] $\Delta G = \Delta E_{ele} + \Delta G_{GB} + \Delta E_{vdw} + \Delta G_{SA}$

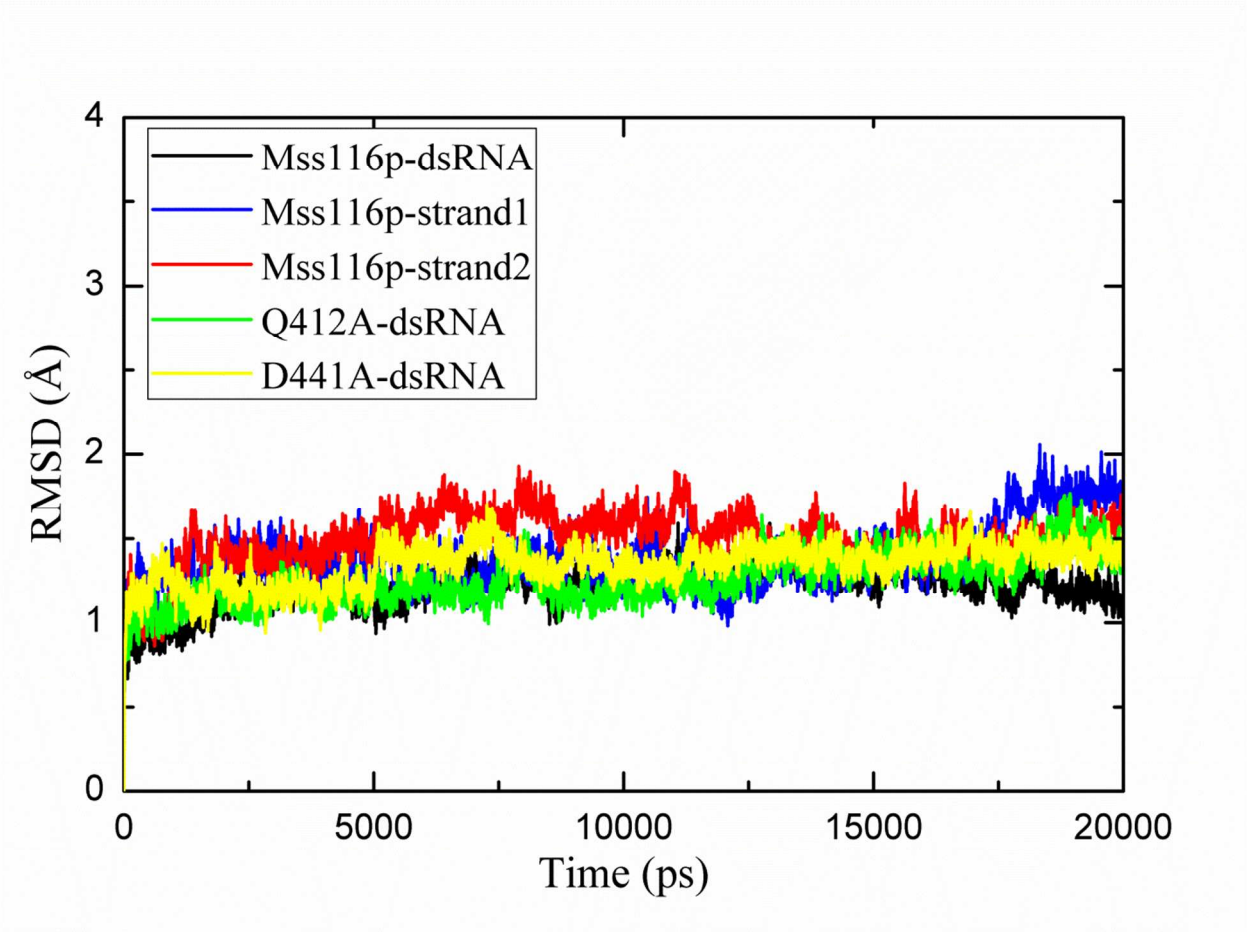

Figure S1. Time-dependent rms deviation values from the starting structures along the simulation trajectory for Mss116p-dsRNA, Mss116p-strand 1, Mss116p-strand 2, Q412A-dsRNA, D441A-dsRNA complexes.

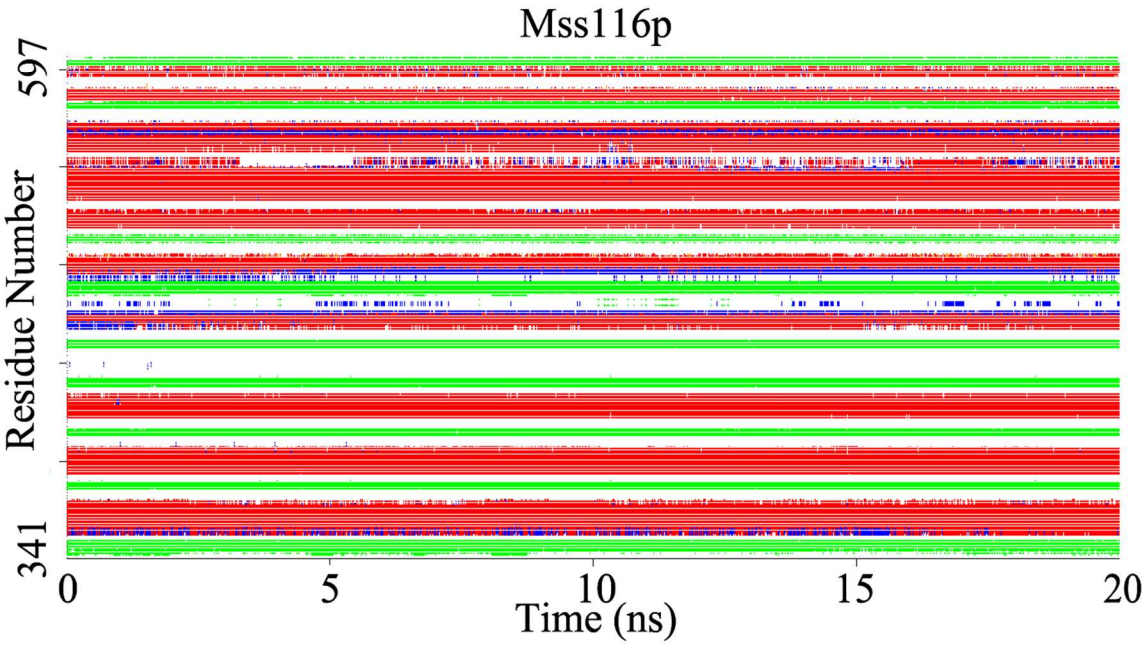

Figure S2. Second structure variation along MD simulations for Mss116p in Mss116p-dsRNA complex. Residues in β-sheet are shown in green; α-helix, red; 310-helix, blue; π-helix, orange; nonregular or other secondary structure, white.

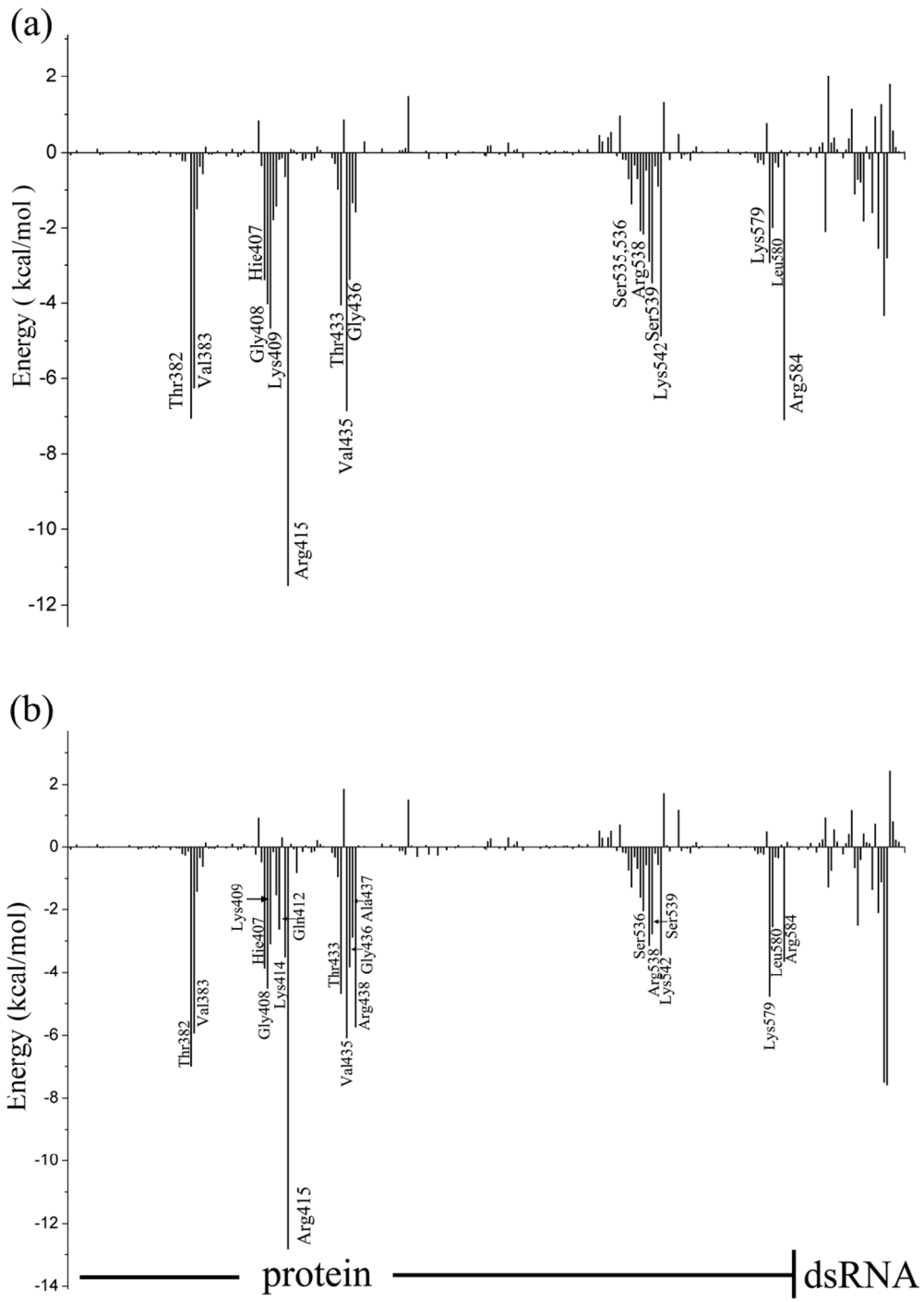

Figure S3. The contribution of each residue and ribonucleotide to Q412A-dsRNA, D441A-dsRNA complexes.

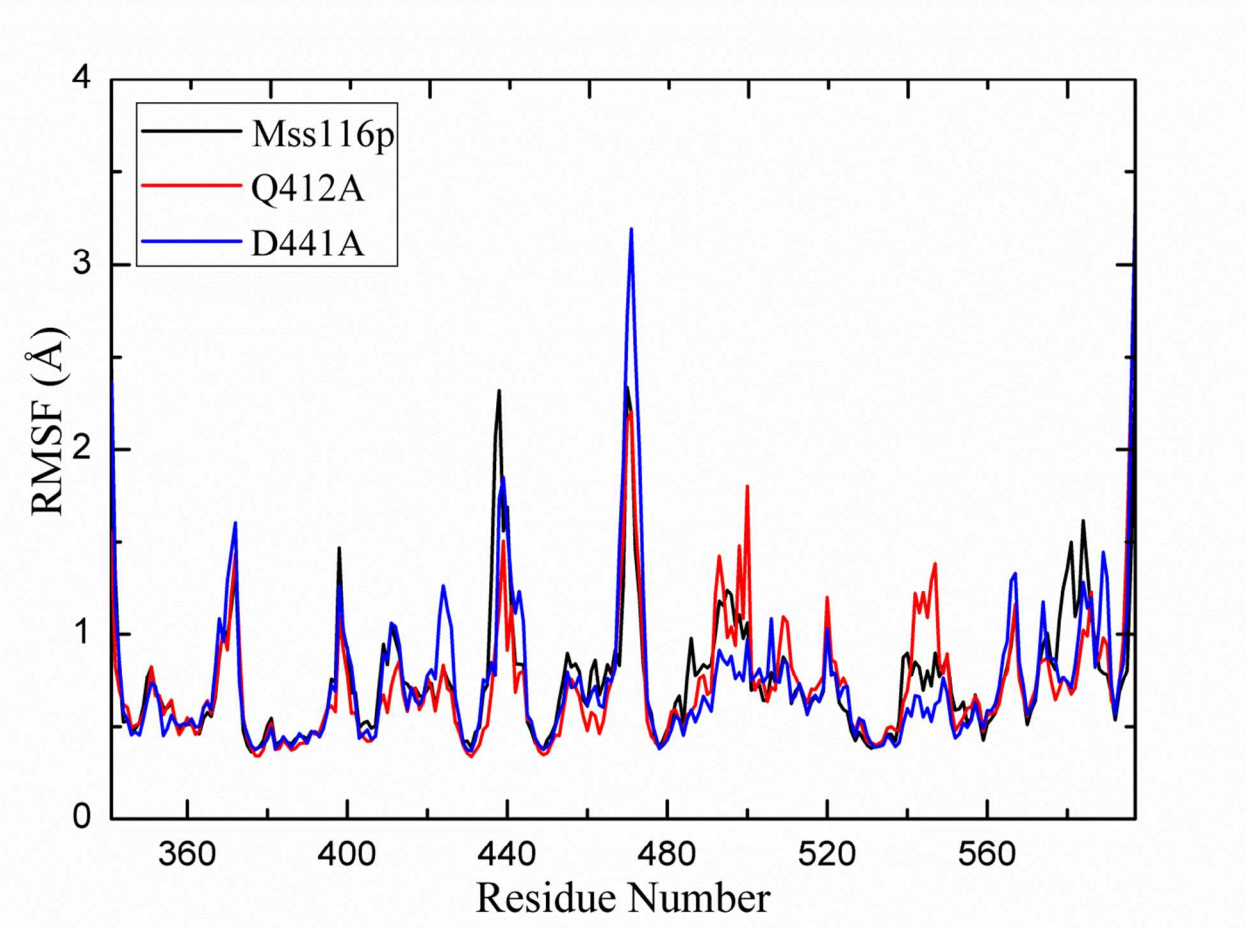

Figure S4. RMSF relative to initial structure for backbone atoms of Mss116p-dsRNA, Q412A-dsRNA, D441A-dsRNA complexes.