

Supporting Information

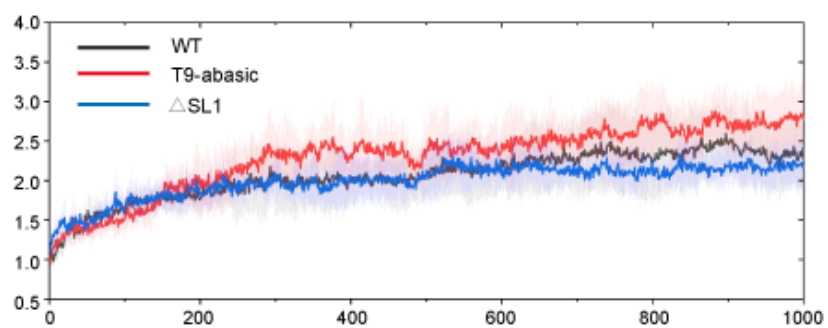


Figure S1. Time evolution of the root-mean-square deviation (RMSD) of Ago2 backbone atoms with respect to the initial structure

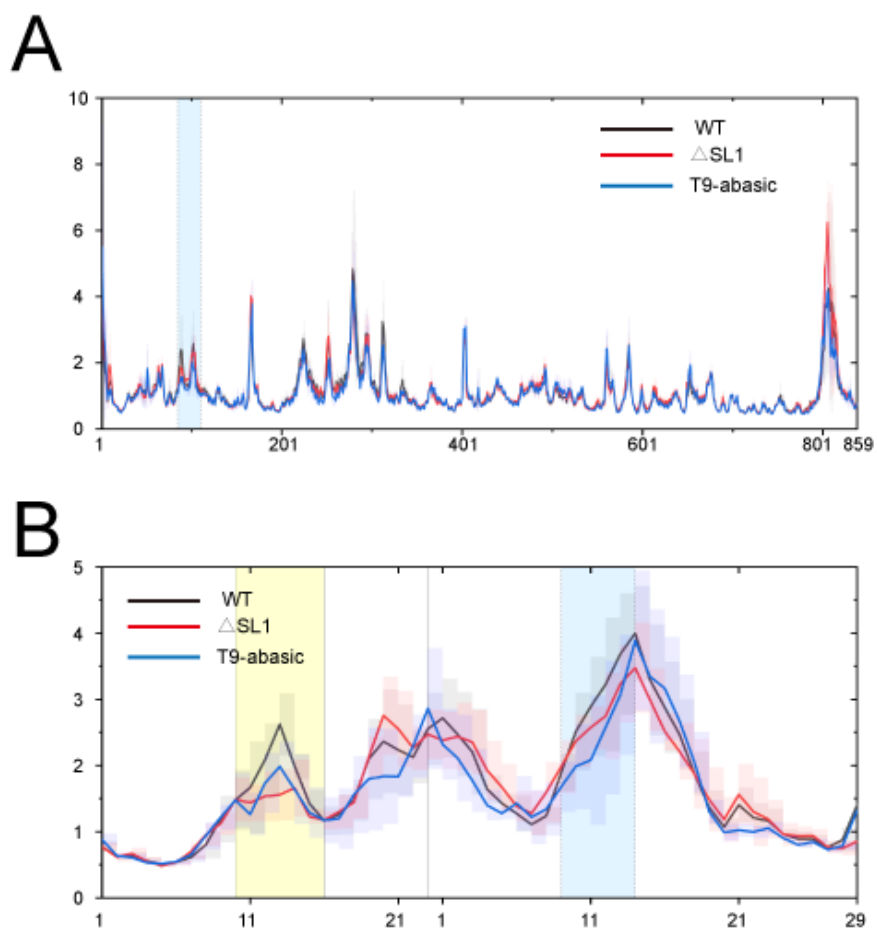


Figure S2. (A) Root-mean-square fluctuations (RMSF) of Ago2 C α atoms averaged over 5 independent runs in the three systems. The significant fluctuation differences are marked with blue backgrounds. (B) RMSF of RNA P atoms averaged over 5 independent runs in the three systems. The significant fluctuation differences are marked with yellow and blue (represents the SL1 region) backgrounds.

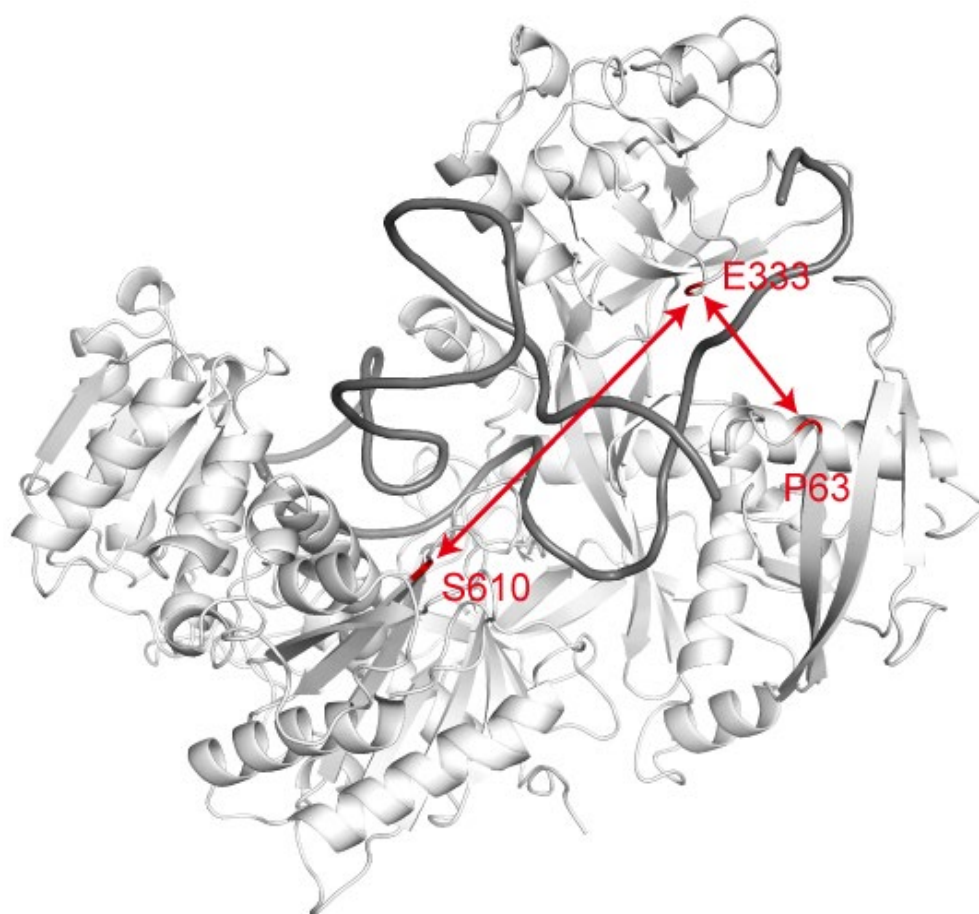


Figure S3. $d_{E333-V610}$ represents the distance between the PAZ and PIWI domains while $d_{E333-P63}$ represents the distance between PAZ and N domains.

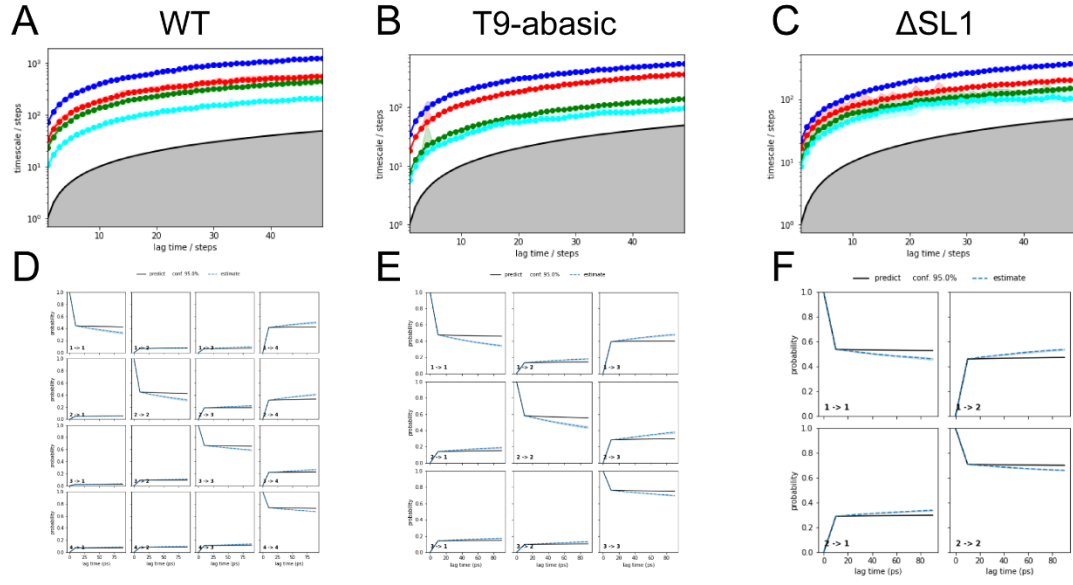


Figure S4. The MSM timescale test in the WT system (A), the T9-abasic system (B) and the Δ SL1 system (C). The MSM Chapman–Kolmogorov test in the WT system (D), the T9-abasic system (E) and the Δ SL1 system (F).

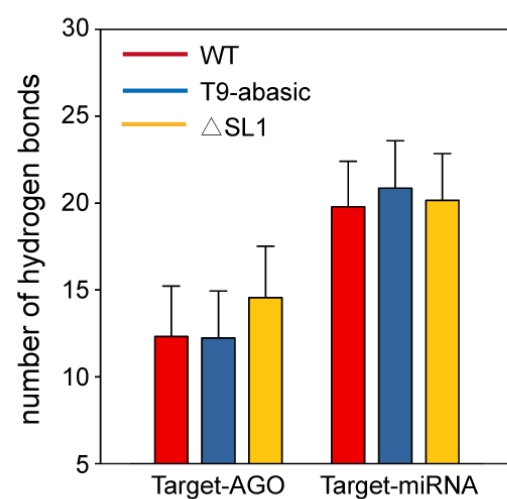


Figure S5. The number of hydrogen bonds of the target RNA with the Ago2 protein and miRNA.