Supplementary Material

**Allosteric** **mechanism for SL RNA recognition by polypyrimidine tract binding protein RRM1: an atomistic MD simulation and network-based study**

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The authors state no conflict of interest.

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Fig. S1 Time evolutions of the root mean square deviations (RMSDs) of PTB-WT, complex-WT and complex-L151G systems (A), those of protein parts in PTB-WT, complex-WT and complex-L151G systems (B), and those of RNA parts in complex-WT and complex-L151G systems (C) during 1000 ns MD simulations. Here, Ca atoms in protein and P atoms in RNA are considered in RMSD calculation.

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Fig. S2 Comparison of nucleotide RMSFs for RNA parts in complex-WT and complex-L151G systems.

FigureS3

Fig. S3 The superimposed low-energy conformations of complex-WT and complex-L151G systems sampled from the individual free energy landscape along PC1 and PC2.