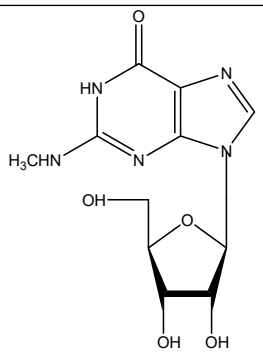
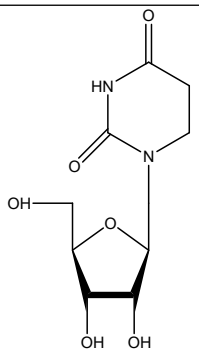
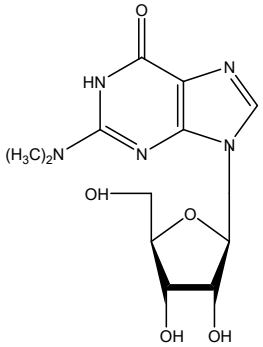
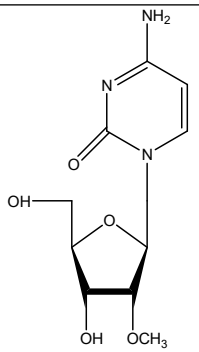
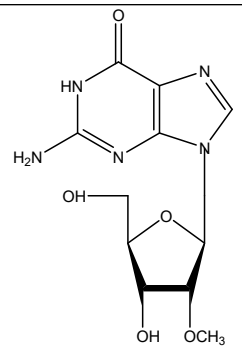
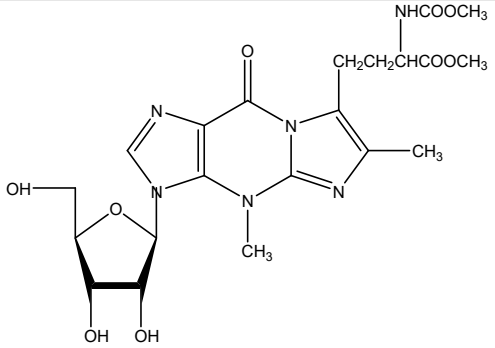
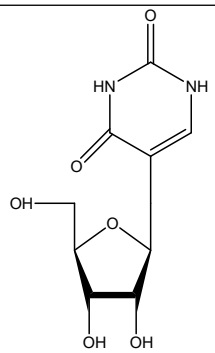
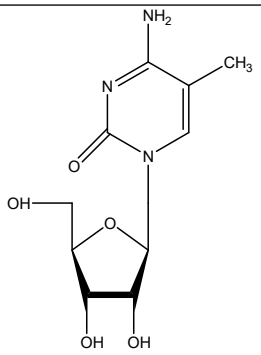
Table S1. Eleven modified nucleotides that exist in the yeast $tRNA^{Phe}$, and their corresponding three-letter codes and chemical structures.

Modified nucleotide	Three-letter code	Chemical structure
m^2G	2MG	
D	DHU	
$m^2{}_2G$	DMG	
C_m	MRC	

G_m	MRG	
Y	WBG	
Ψ	PSU	
m^5C	5MC	

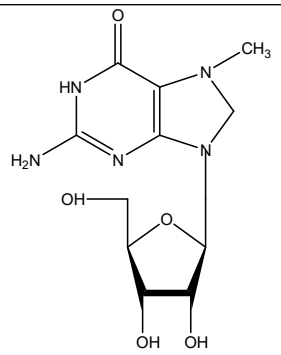
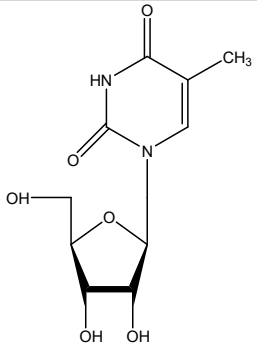
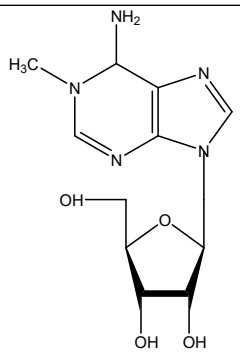
m^7G	7MG	
T	5MU	
m^1A	1MA	

Table S2. The selected atoms on DAU and the $tRNA^{Phe}$ for the five poses in the adaptive steered MD simulations.

Poses	DAU		RNA	
	Atom ID	Atom name	Residue ID	Atom name
1	18	C9	G_{15}	C4
2	12	C5	m^5C_{49}	C5
3	24	C12	G_{15}	C5
4	24	C12	G_{18}	C4
5	18	C9	A_{23}	C4

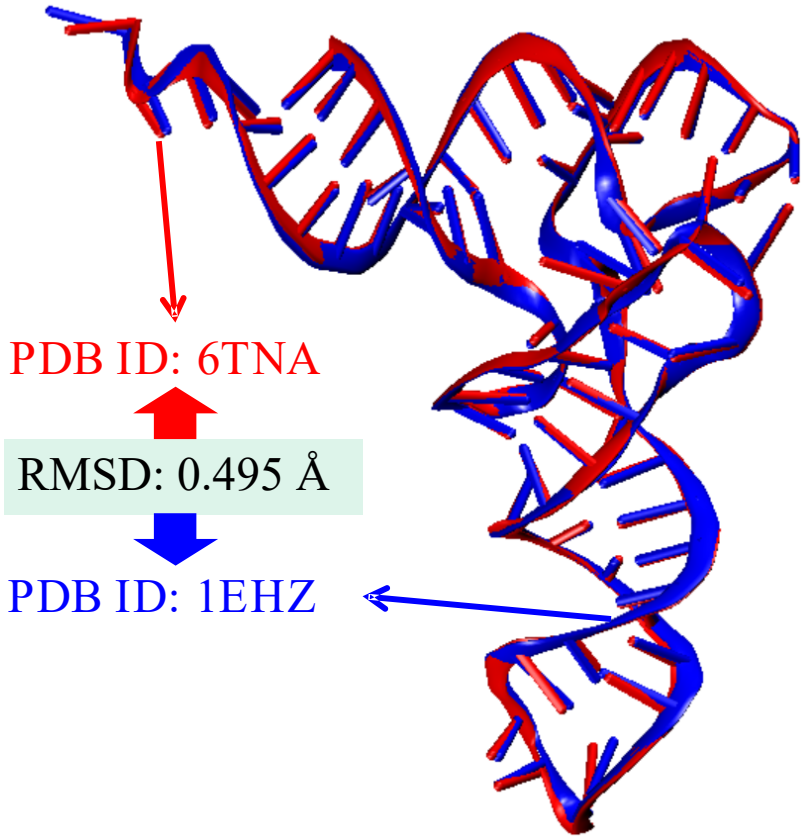


Figure S1. Calculation of backbone RMSD to compare the two crystal $tRNA^{Phe}$ structures.

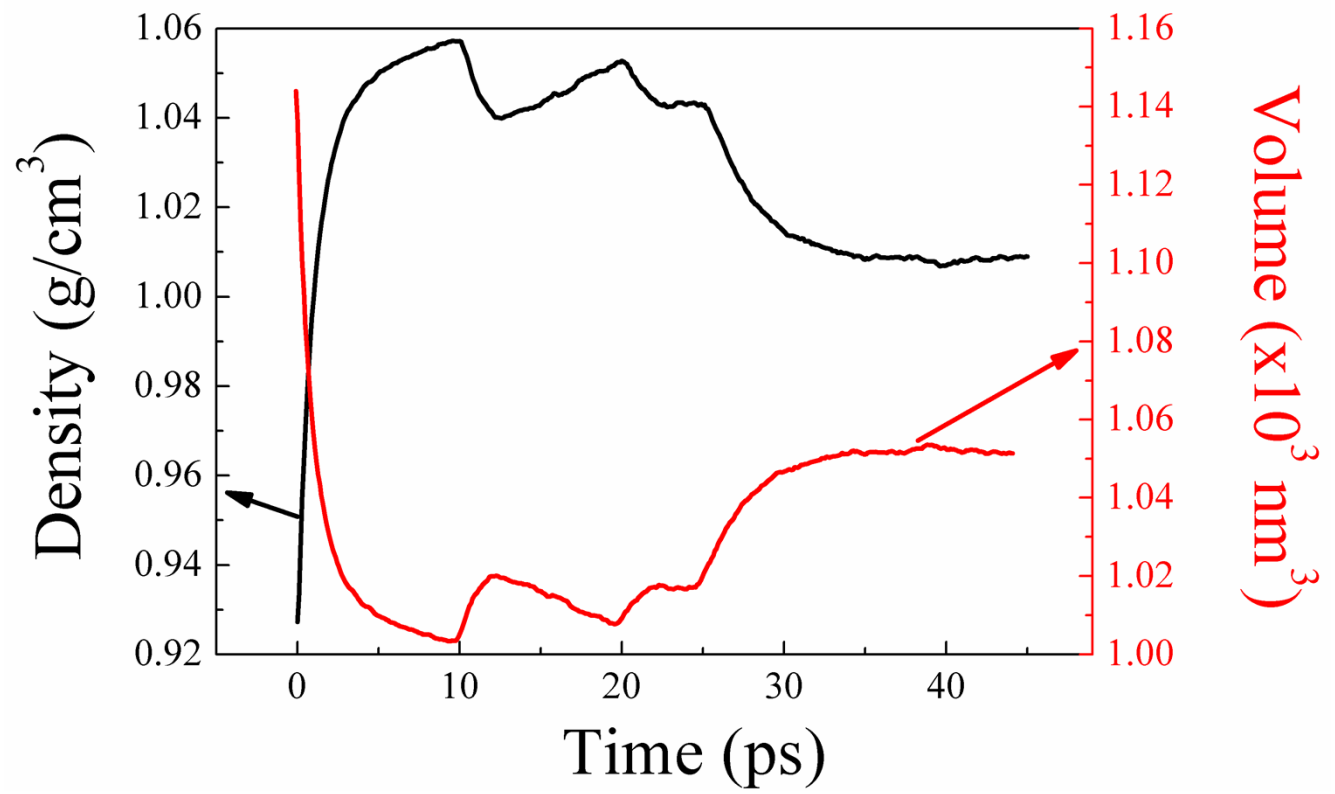


Figure S2. The changes of density (black) and volume (red) are monitored in the 45-ps NPT ensemble MD simulation to ensure that our simulation system reaches stable box sizes.

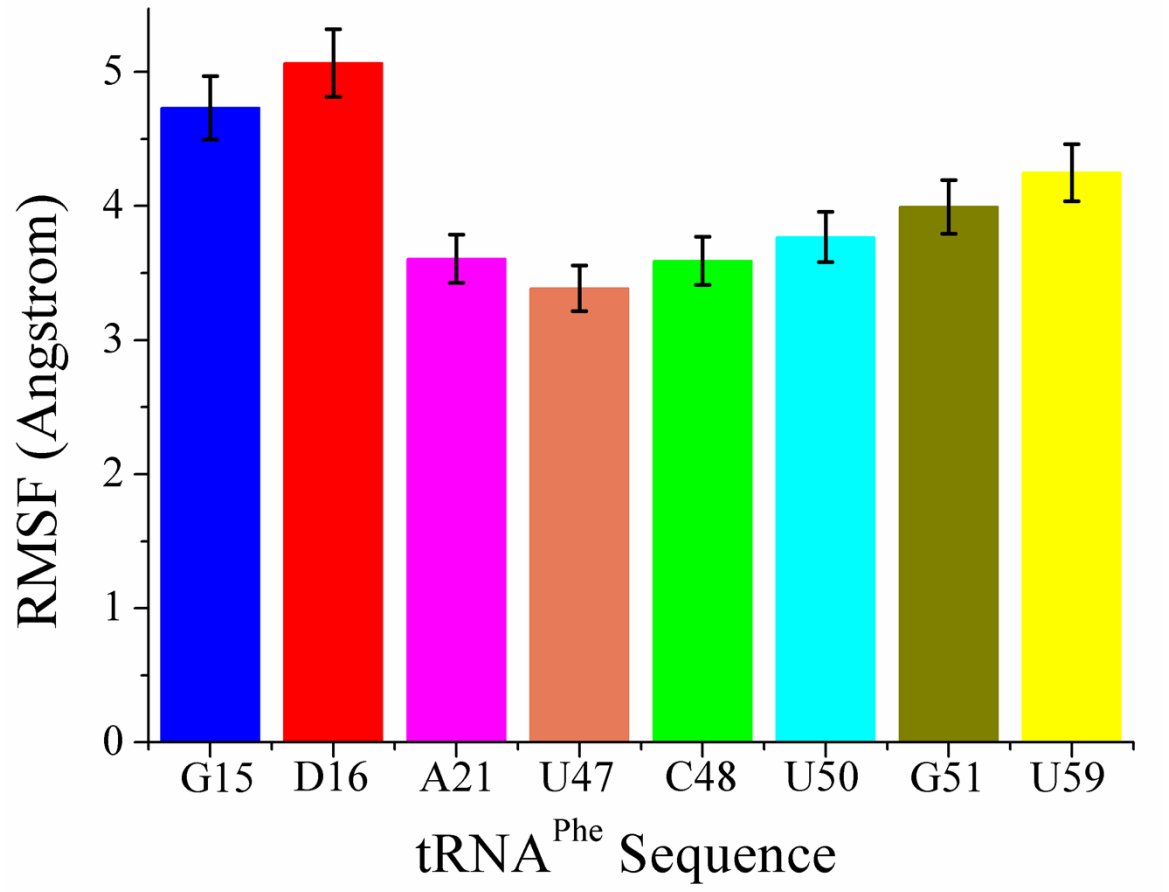


Figure S3. The RMSF values of the eight key nucleotides, *viz*. G_{15}, D_{16}, A_{21}, U_{47}, C_{48}, U_{50}, G_{51} and U_{59}, on the last 5-ns simulation trajectories of Pose 3. Small displacement deviations of the eight nucleotides indicate that our simulations have reached an equilibrated state after 150-ns conventional MD simulations.

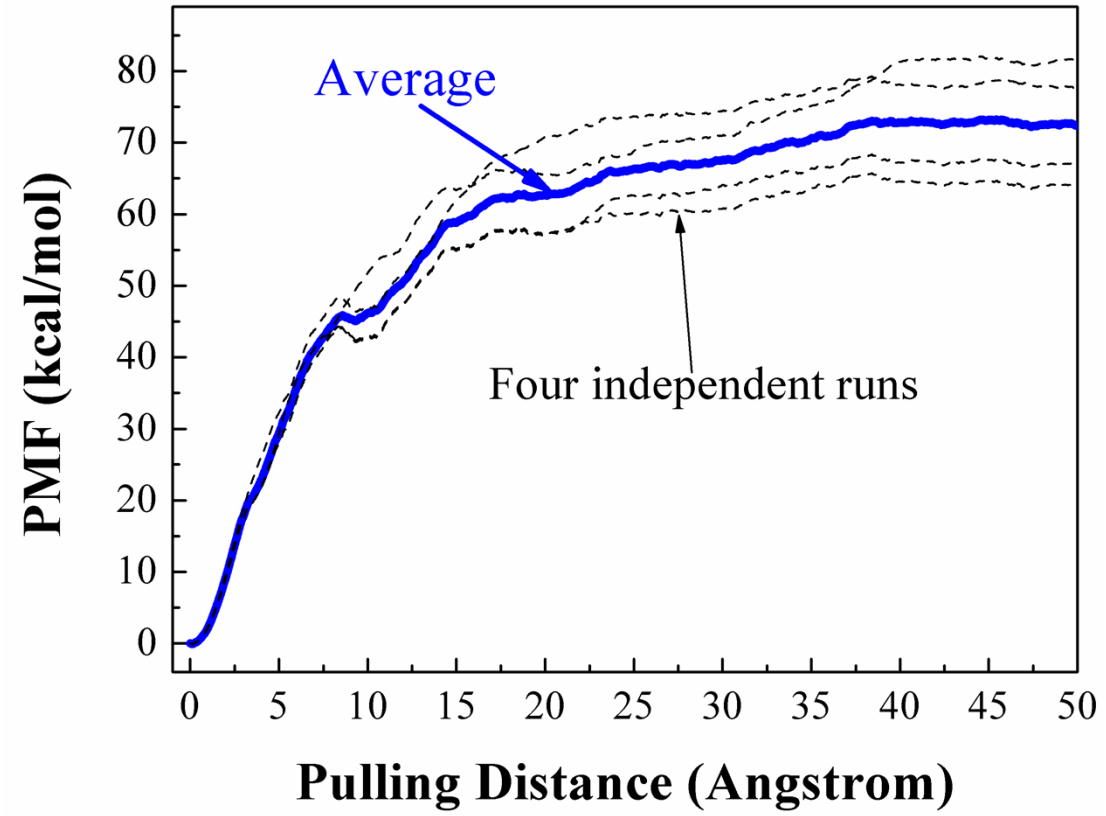


Figure S4. PMF profile of Pose 3 obtained by averaging four independent adaptive steered MD simulation runs.