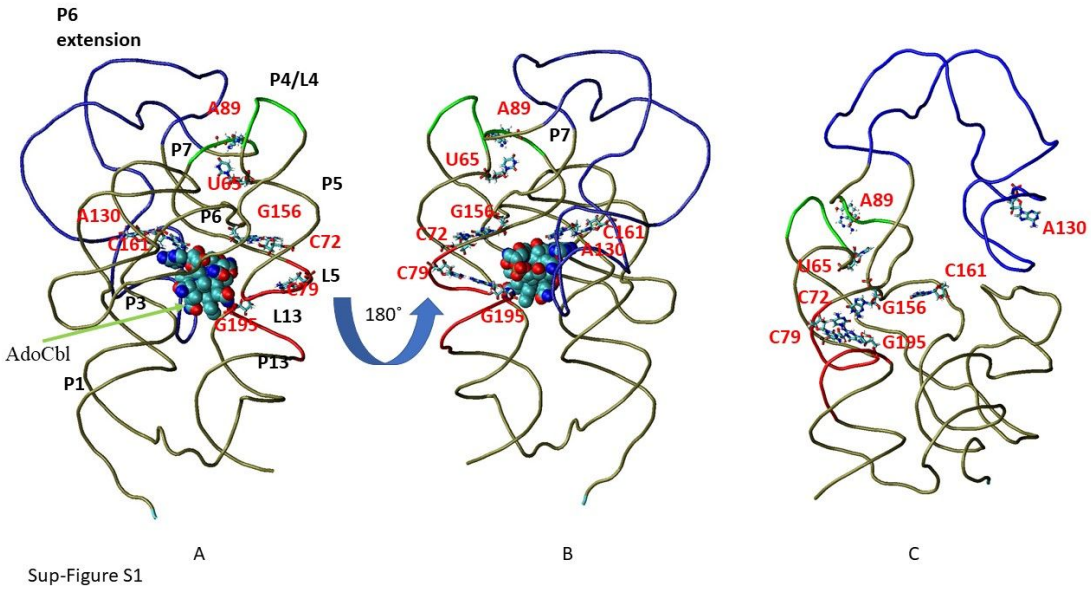

Sup-Figure S1

Figure S1: Illustration of fold architecture of *Tte*AdoCbl riboswitch. (A) and (B) are two views of *Tte*AdoCbl riboswitch crystal structure. (C) A snapshot from Replica-Exchange Molecular Dynamics (REMD) simulation with P6-extension open for AdoCbl binding. The key nucleotide base pairs defined the global fold are labeled in red. The AdoCbl is represented as vdw spheres.

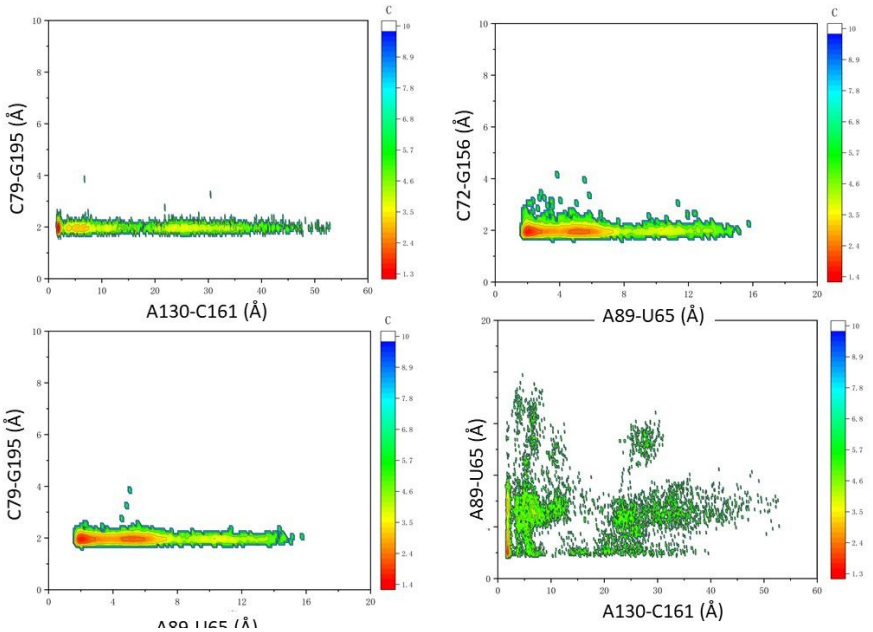

Figure S2: Two-dimensional density distributions of four hydrogen bonds in the TteAdoCbl riboswitch at the 320-330K region.

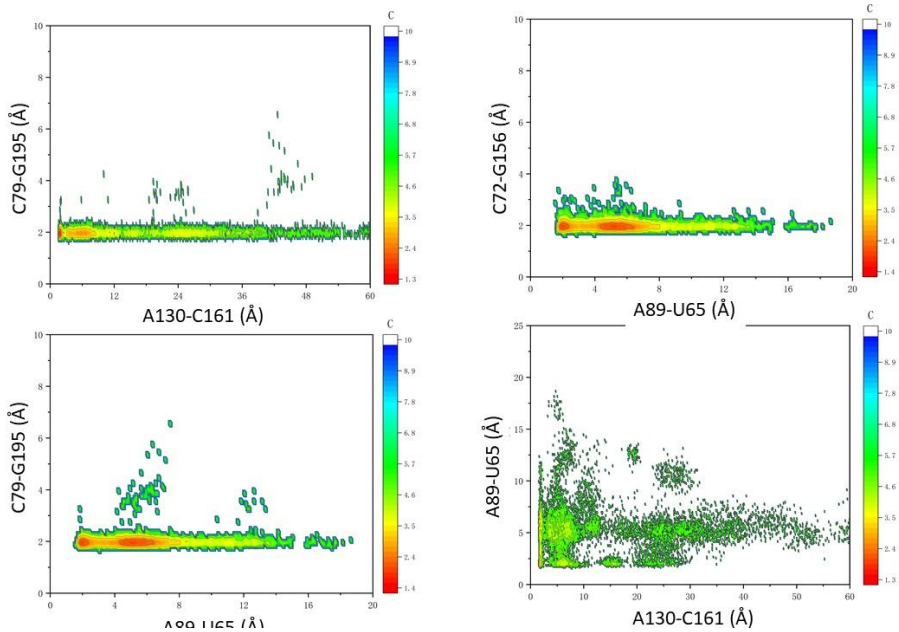

Figure S3: Two-dimensional density distributions of four hydrogen bonds in the TteAdoCbl riboswitch at the 340-350K region.

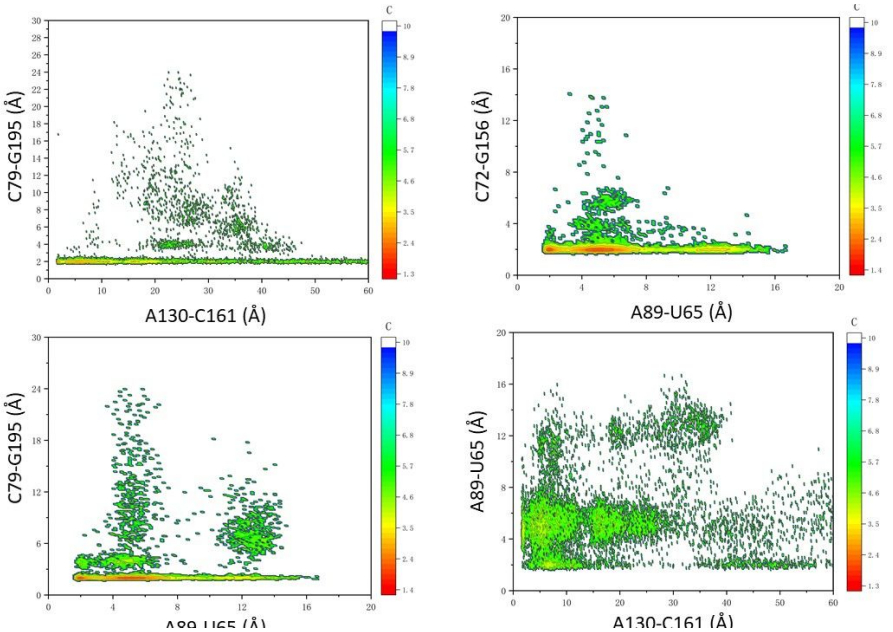

Figure S4: Two-dimensional density distributions of four hydrogen bonds in the TteAdoCbl riboswitch at the 390-400K region.

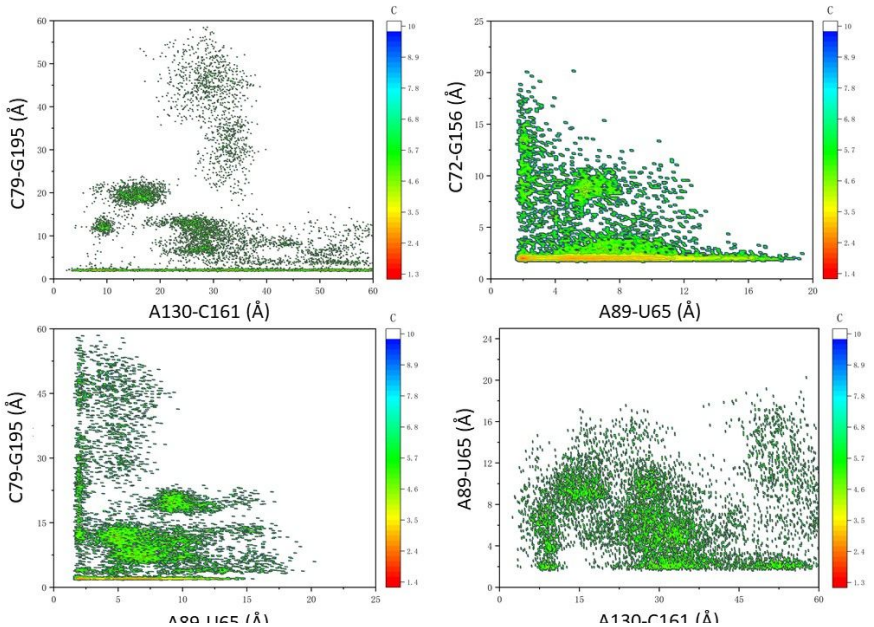

Figure S5: Two-dimensional density distributions of four hydrogen bonds in the TteAdoCbl riboswitch at the 440-450K region.