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Study on the stability of the DNA hairpin d(ATCCAT-GTTA-TAGGAT) employing molecular dynamics simulation SANGWOOK WU, Department of Physics, Pukyong National University,Busan 608-737, Korea, HONGGU CHUN COLLABORATION¹ — DNA hairpin plays a critical role in the regulation of gene expression and DNA recombination. We studied the conformation of the DNA hairpin, d(ATCCAT-GTTA-TAGGAT) (PDB id:1AC7), employing molecular dynamics (MD) simulation. Despite the non-canonical Watson-Crick base pair (G:A) in the tetraloop (GTTA), MD simulation reveals that the conformation of the DNA hairpin is remarkably stable. In this study, we discuss about the physical/chemical origin of the stability of the DNA hairpin.

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