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Non watson-crick base pairs in RNA double Helices: PDB database analysis

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RNA macromolecules perform various enzymatic and gene regulatory functions, which requires their specific stable three-dimensional structures. Specific structures of RNA is always stabilized by base pairing and stacking interactions and RNA showed various types of base pairing in addition to canonical Watson-Crick or wobble GU types. Analysis of all available RNA structures by detecting all types of base pairs, stabilized by two or more hydrogen bonds, show there are huge variations of non canonical base pairs appearing frequently, such as A:A, A:G, etc, through their Hoogsteen or Sugar edge interactions as well. These base pairs are often seen within double helices, stacked on top of another base pair with good stacking geometry. These data have been organized in a database (<http://hdrnas.saha.ac.in/rnabpdb>) along with their orientation parameters. The data now can be used for generation of structures of various functional RNA, such as miRNA, using our RNAHelix software, which can lead to better predictions of their functions. Further analysis using ab initio quantum chemical calculations indicate possibility of double helix formation by some of the non-canonical base pairs. Some of the base pairs show bimodal distributions in their structural parameters, which appears to have great implication. Structural data analysis augmented by stacking energy analysis, using dispersion corrected DFT and MP2 methods, and all-atom molecular dynamics simulations further indicate possibility of Intrinsically Disordered Structure of RNA for certain sequence. This indicates that perhaps all types of base pairing modes may not give stable double helical structures.