

P006 RNA Backbone Is Rotameric
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Despite the importance of local structural detail to a mechanistic understanding of RNA catalysis and binding functions, RNA backbone conformation has been recalcitrant to analysis. There are too many variable torsion angles per residue, and their raw empirical distributions are poorly clustered. This study applies quality-filtering techniques (using resolution, crystallographic B factor, and all-atom steric clashes) to the backbone torsion angle distributions from a selected RNA residue database. With noise levels greatly reduced, clear signal appears for the underlying angle preferences. Half-residue torsion angle distributions for $\alpha-\beta-\gamma$ and $\delta-\epsilon-\zeta$ are plotted and contoured in 3D; each shows about a dozen distinct peaks, which can then be combined in pairs to define complete RNA backbone conformers. Instead of the chemical residue, here we use a division into sugar-to-sugar "suites" to parse the RNA backbone repeats, both because most backbone steric clashes are within suites and because the relationship of successive bases is both reliably determined and conformationally important. Potential suite conformers were omitted if not represented by at least a small cluster of convincing data points after application of quality filters. The final result is a small library of RNA backbone conformers, which should provide valid conformations for nearly all RNA backbone encountered in experimental structures.