

**P005** Improving the Accuracy of Backbone Conformations in Large RNA Structures

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For the somewhat error-prone backbone fitting in experimental structures of large RNAs, problem areas can be diagnosed both by our library of RNA backbone conformers and, even more sensitively, by our all-atom steric contact analysis (including hydrogens). These new criteria often show what model corrections are needed. A related protocol is successful for proteins in lowering  $R$  and  $R_{\text{free}}$  while greatly improving sterics, sidechain rotamericity, and Ramachandran criteria. As a demanding test case in the RNA world, we are making corrections to problem backbone residues in the RNA of the *Haloarcula marismortui* large ribosomal subunit (PDB code 1S72). Changes include sugar puckers, movement of C5' and its H atoms away from serious steric clashes, and concerted changes of nearby dihedral angles (e.g.,  $\alpha$  and  $\gamma$ ) by close to  $120^\circ$ . A partial set of such corrections, plus a partial set of corrections to the ribosomal proteins, will be tried out to aid in an upcoming refinement of somewhat higher-resolution ribosome data by Schmeing and Steitz at Yale. We are also refining such backbone corrections in examples of mid-size RNAs to determine what level of increased accuracy and electron-density-map improvement is attainable.