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Toward non-crystalline protein structure determination by bayesian RMC

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High-resolution protein structures, obtained by X-ray crystallography or NMR spectroscopy, are available for only a small fraction of known proteins. The structural solutions of membrane proteins are particularly limited by the difficulty of crystallization. In this work we describe a reverse Monte Carlo algorithm that utilizes the pair distribution function in the fitting procedure. The tendency of RMC to fit nonrealistic solutions is supplemented by prior statistics from the Ramachandran distributions of dihedral angles and in predicted distributions from chemical shift data. This de novo Bayesian algorithm works with prior information that is accessible without crystallization or time consuming NMR experiments. These coarse structural solutions are suitable starting configurations for further refinement by molecular dynamics or other methods. The comparative utility of different experimental inputs is discussed, and a set of known test structures is modeled to demonstrate the accuracy of the approach.