

W0182

Protein Structure as a Blurred Snapshot – Dynamic Information from a Static Experiment. Ethan A Merritt, Dept of Biochemistry, Univ. of Washington, Seattle, WA 98195 USA.

A crystal structure is usually thought of as static information, i.e. it is a snapshot of a protein at rest. But the distribution of thermal parameters in a well-refined structure can be strongly indicative of dynamic motions and allowed flexibility. This distribution of B_{iso} or U^{ij} terms can be modeled as arising from TLS (Translation/Libration/Screw) rigid-body vibrational motion. A one-group TLS model can approximate the vibration of an entire protein molecule within the crystal lattice. More complex TLS models are broadly applicable to describe inter-domain and other internal vibrational modes of proteins. Use of multi-group TLS models in crystallographic refinement can improve R and R_{free} significantly compared to conventional models. This is a strong hint that the flexibility described by the model is truly present in the protein.

We have developed an analysis tool, TLSMD, that generates optimal multi-group TLS models. These may be used to analyze the presence and physical significance of TLS motion in existing structures, to guide additional crystallographic refinement, or to generate target models of protein flexibility for use in computational protein-protein or protein-ligand docking. The analysis is applicable to protein structures at any resolution.

<http://skuld.bmsc.washington.edu/~tlsmd>