Analysis and Visualization of TLS Motion in Proteins using the mmLib Toolkit

Ethan A. Merritt, Jay Painter, *Biomolecular Structure Center and Dept of Biochemistry, University of Washington, Seattle.* E-mail: merritt@u.washington.edu

We have developed a programming library, mmLib [1], which provides a rich set of tools for the import, manipulation, and export of macromolecular structural models described in CIF and mmCIF. Using this toolkit, we are developing higher level tools for visualization and structural/functional analysis. We are in particular working to infer and model functionally important modes of protein flexibility directly from single crystal structures.

TLS (Translation/Libration/Screw) models describe rigid-body vibrational motions of arbitrary objects. A single-group TLS model can be used to 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. We are developing a web-based analysis tool, **TLSMD**, that generates optimal multi-segment 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 interactive graphics program **TLSVIEW** [2] allows visualization of these and other models for rigid-body motion in proteins, using animation and a variety of static representations.

Both tools are applicable to protein structures at any resolution.

[1] Painter J., Merritt E.A., *J. Appl. Cryst.,* 2004, **37**, 174-178. [2] Painter J., Merritt E.A., *Acta Cryst.,* 2005, **D61**, 465-471.

Keywords: graphics, dynamics, docking computation