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Tools for visualization and analysis of TLS motion in proteins. E.A. Merritt, J. Painter, Biomolecular Structure Center and Dept of Biochemistry, Univ. of Washington, Seattle, WA 98195.

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 a crystal lattice. More complex TLS models are broadly applicable to describing inter-domain and other internal vibrational modes of proteins. However, the use of multi-segment TLS models in crystallographic structure analysis has been relatively limited, partly because the physical meaning of the refined TLS parameters is not intuitive.

We introduce here an interactive visualization tool, TLSView, for the display and interpretation of inter-domain or other motions in protein structural models. A separate web-based analysis tool, TLSMD, is being developed to generate optimal multi-segment TLS models. TLSView and TLSMD may be used to prepare TLS models for crystallographic refinement, and to analyze the physical significance of TLS motion in refined structures. The tools are applicable to structures at any resolution.

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