

Plastic Network Model of Large Amplitude Conformational Change

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We present simple arguments that relate low energy deformations from multiple conformers to likely conformational change pathways between such conformers. We introduce the plastic network model, a minimalistic, physically motivated model that provides large amplitude conformational change pathways in biomolecular systems. We present these pathways for adenylate kinase, the single subunit of GroEL, and the F_1F_0 ATP synthase. The adenylate kinase open-to-close conformational change pathway, shown in the figure, displays a specific, experimentally verifiable order of events and closely follows a sequence of 13 experimental structures [1]. The GroEL pathway is similar to an empirical-potential targeted molecular dynamics trajectory. The F_1F_0 ATP synthase pathway naturally follows a cylindrical rotational motion. The plastic network model is also directly applicable to low-resolution macromolecular assemblies.

[1] P. Maragakis and M. Karplus, "Large Amplitude Conformational Change in Proteins Explored with a Plastic Network Model: Adenylate Kinase", *J Mol Biol* **352**, 807 (2005).

