The Amounts of Thermal Vibrations and Static Disorder in Protein X-ray Crystallographic B-factors

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Abstract

Crystallographic B-factors provide direct dynamical information on the internal mobility of proteins that is closely linked to function, and are also widely used as a benchmark in assessing elastic network models. A significant question in the field is: what is the exact amount of thermal vibrations in protein crystallographic B-factors? This work sets out to answer this question. First, we carry out a thorough, statistically sound analysis of crystallographic B-factors of over 10,000 structures. Second, by employing a highly accurate all-atom model with the well-known CHARMM force field, we obtain computationally the magnitudes of thermal vibrations of nearly 1,000 structures. Our key findings are: (i) the magnitude of thermal vibrations, surprisingly, is nearly protein-independent, as a corollary to the universality in vibrational spectra of globular proteins established earlier; (ii) the magnitude of thermal vibrations is small, less than 0.1 ^{2} at 100 K; (iii) the percentage of thermal vibrations in B-factors is the lowest at low resolution and low temperature (<10%) but increases to as high as 60% for structures determined at high resolution and at room temperature. The significance of this work is that it provides for the first time, using an extremely large dataset, a thorough analysis of B-factors and their thermal and static disorder components. The results clearly demonstrate that structures determined at high resolution and at room temperature have the richest dynamics information. Since such structures are relatively rare in the PDB database, the work naturally calls for more such structures to be determined experimentally.

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