



ID de Contribution: 70

Type: Non spécifié

X-ray Crystal Structures of Extensively Simplified BPTI Variants Determined Using the KEK Photon Factory Facility

Abstract

Protein stabilization is very difficult to rationalize as it often results from multiple mutations, whose effects are intertwined. Rather, it is worth investigating the 3-D structures of proteins differed by a single and/or a few amino acid substitutions, followed by their thermodynamic studies to elucidate the stabilization mechanism. Here, we report the X-ray crystal structures of several BPTI variants containing 19 to 23 alanines (out of 58 residues) that were determined using the Photon Factory synchrotron radiation source at KEK. All extensively simplified BPTI variants retained almost perfectly the wild-type BPTI structure. However, pair wise RMS deviations at C α atoms indicated that small local structural fluctuations, found in the wild-type structure (7PTI), were significantly reduced in the simplified BPTI structures. The temperature factors (main chain, side chain and average temperature factors) were also significantly reduced at and/or around the alanine substitution sites. Moreover, new hydration structures (protein water interaction) were observed at/around the substitution sites that could contribute to rigidify the native structure.

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