H-bonds in Crambin: Coherence in an α-helix

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We applied coherence analysis, which engineers use to identify linear interactions in stochastic systems, to molecular dynamics simulations of crambin, a thionin storage protein found in Abyssinian cabbage. For frequencies between 0.391 GHz and 5.08 GHz (corresponding reciprocally to times of 2.56 ns and 0.197 ns), the displacement of oxygen and nitrogen atoms across the H-bonds in the α-helices are strongly correlated, with a coherence greater than 0.9; the secondary structure causes the H-bonds to effectively act as a spring. Similar coherence behavior is observed for covalent bonds and other noncovalent interactions including H-bonds in β-sheets and salt bridges. In contrast, arbitrary pairs of atoms that are physically distant have uncorrelated motions and negligible coherence. Strong coherence is also observed between the average position of adjacent leaves (groups of atoms) in an α-helix, suggesting that the harmonic analysis of classical molecular dynamics can successfully describe the propagation of allosteric interactions through the structure.