Configurational Entropy Elucidates the Role of Salt-Bridge Networks in Protein Thermostability

John H. Missimer, Michel O. Steinmetz, Riccardo Baron, Fritz K. Winkler,
Richard A. Kammerer, Xavier Daura, and Wilfred F. van Gunsteren

Figure S1. The X-ray crystallographic structure of the three-stranded ccβ-p coiled coil showing the single salt bridge between Arg8 and Glu13' and crystal-packing contacts: (1) the NH1 atom of Arg3' forms hydrogen bonds with the O atoms of Leu14* and Arg15* in a neighboring trimer; (2) the OE1 and OE2 atoms of Glu4' and Glu11' make salt bridges with sodium and zinc ions, respectively; (3) the Arg8** of a neighboring trimer restricts the conformation of the Arg10' side chain, which influences the conformation of the Glu6' side chain via a water mediated hydrogen bond.
Figure S2. Selected hydrogen bonds (left) and salt bridges (right) of ccβ-p trimer at 330K. Green denotes i, i-4 interactions between backbone atoms; yellow i,i-3 interactions; cyan interactions between backbone and side-chain atoms; and violet interactions between side-chain atoms. Maroon denotes interhelical interactions.
Figure S3. Secondary structure of ccβ-p trimer at 370K. Green denotes α-helix, red H-bonded turn, yellow 3_10-helix, orange bend, cyan β-bridge, violet extended-strand, and blue π-helix.
Figure S4. Hydrogen bonds of the ccβ-p monomer at 278K (left) and 330K (right). The color coding for the bonds is the same as in Figure S2.
Figure S5. Salt bridges of ccβ-p monomer at 278K (left) and 330K (right). Green denotes i, i-4 bridges and blue, i,i+5 bridges. The star denotes the two possible hydrogen atoms, indicated by overlapping shades of green or blue.
Figure S6. Convergence of configurational entropies computed for all residues of the monomer and the three helices of the trimer at 278K and 330K.