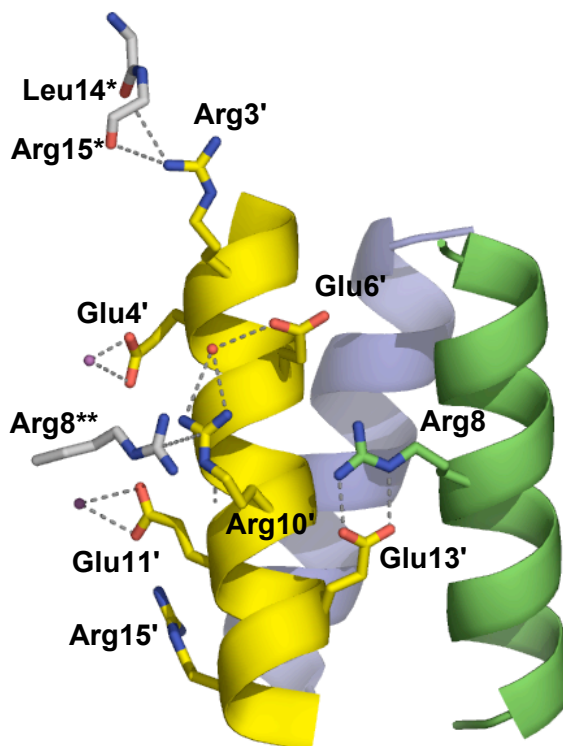


## Configurational Entropy Elucidates the Role of Salt-Bridge Networks in Protein Thermostability

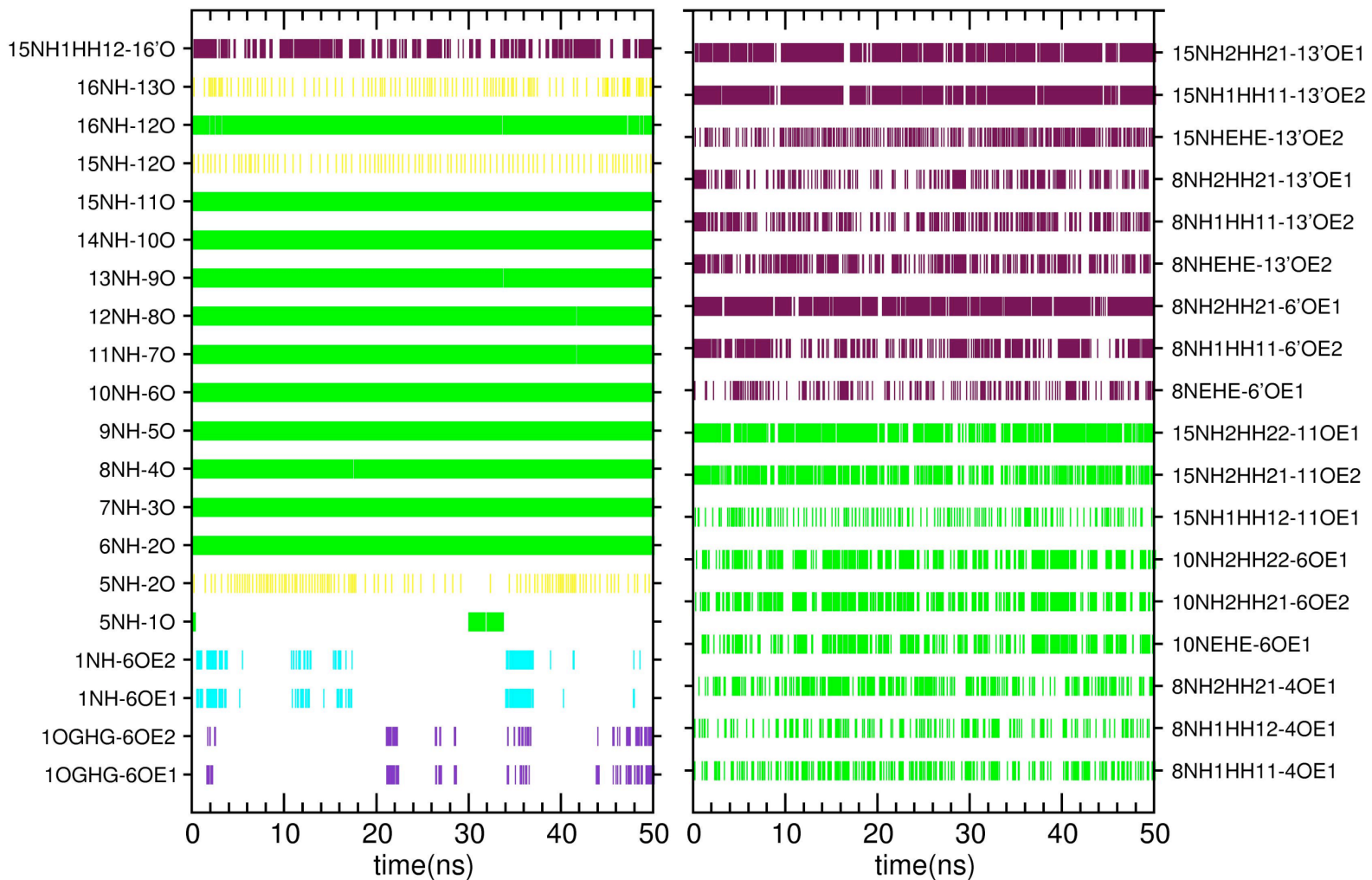
John H. Missimer, Michel O. Steinmetz, Riccardo Baron, Fritz K. Winkler,

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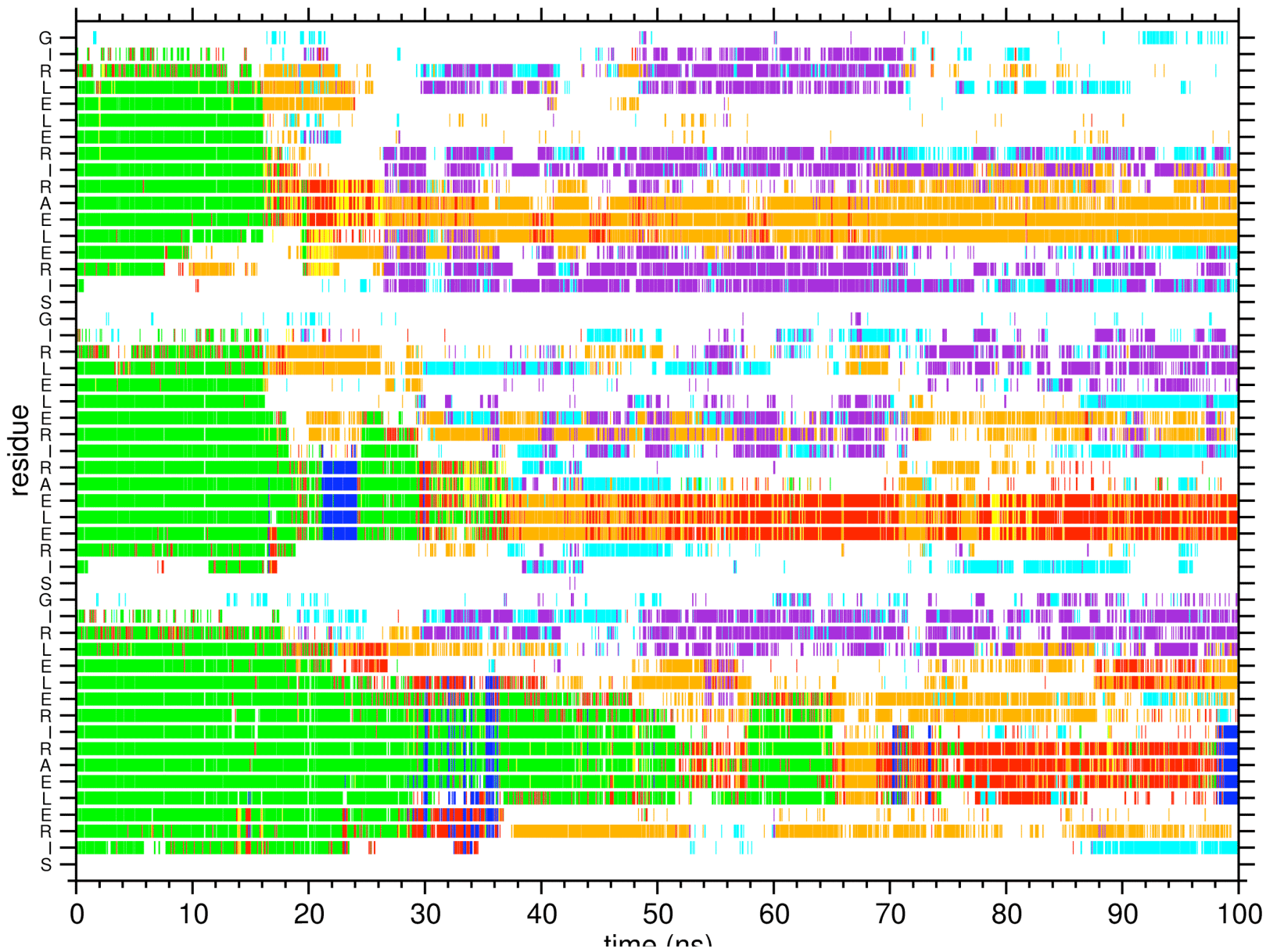
**Figure S1.** The X-ray crystallographic structure of the three-stranded cc $\beta$ -p coiled coil showing the single salt bridge between Arg8 and Glu13' and crystal-packing contacts: (1) the NH1 atom of Arg3' forms hydrogen bonds with the O atoms of Leu14\* and Arg15\* in a neighboring trimer; (2) 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 cc $\beta$ -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.

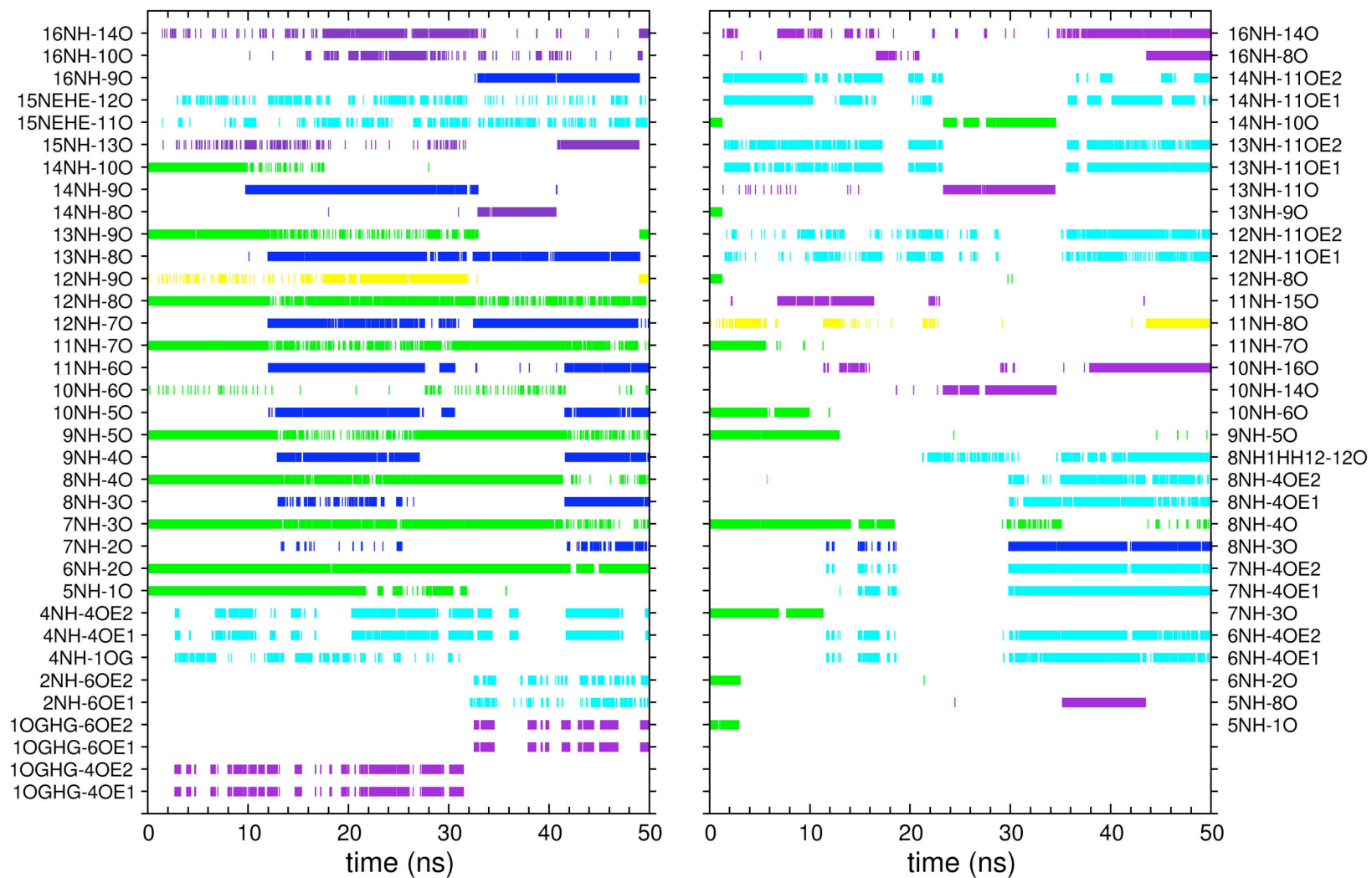


**Figure S3.** Secondary structure of cc $\beta$ -p trimer at 370K. Green denotes  $\alpha$ -helix, red H-bonded turn, yellow  $3_{10}$ -helix, orange bend, cyan  $\beta$ -bridge, violet extended-strand, and blue  $\pi$ -helix.

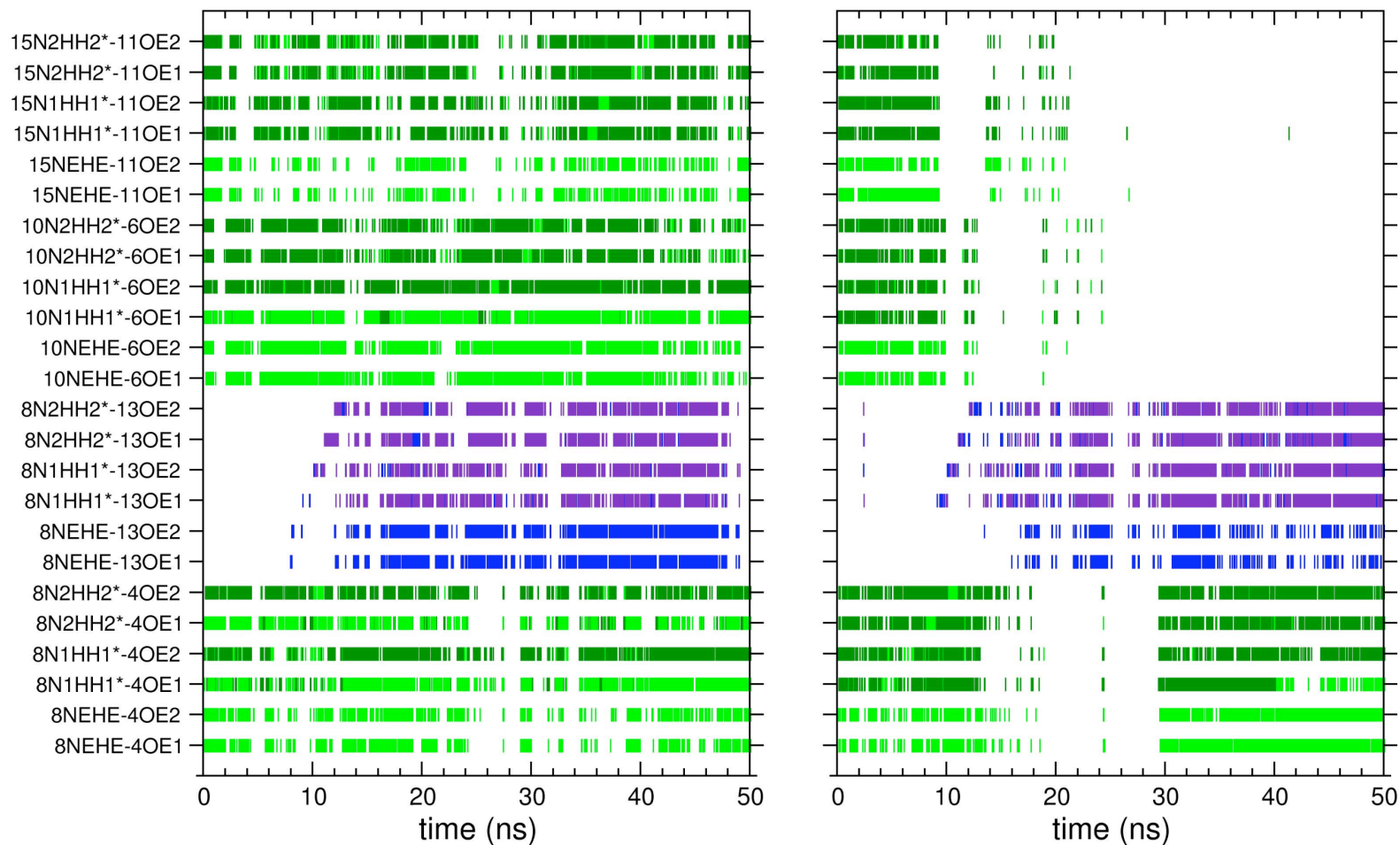


**Figure S4.** Hydrogen bonds of the cc $\beta$ -p monomer at 278K (left) and 330K (right). The color coding for the bonds is the same as in

Figure S2.



**Figure S5.** Salt bridges of cc $\beta$ -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.

