Bridging of anions by hydrogen bonds in nest motifs and its significance for Schellman loops and other larger motifs within proteins

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Abstract

The nest is a protein motif of three consecutive amino acid residues with dihedral angles 1,2-(RL) (RL nests) or 1,2-(LR) (LR nests). Many nests form a depression in which an anion or -negative acceptor atom is bound by hydrogen bonds from the main chain NH groups. We have determined the extent and nature of this bridging in a database of protein structures using a computer program written for the purpose. Acceptor anions are bound by a pair of bridging hydrogen bonds in 40% of RL nests and 20% of LR nests. Two thirds of the bridges are between the NH groups at Positions 1 and 3 of the motif (N1N3-bridging)which confers a concavity to the nest; one third are of the N2N3 typewhich does not. In bridged LR nests N2N3-bridging predominates (14% N1N3: 75% N2N3), whereas in bridged RL nests the reverse is true (69% N1N3: 25% N2N3). Most bridged nests occur within larger motifs: 45% in (hexapeptide) Schellman loops with an additional 4 0 hydrogen bond (N1N3), 11% in Schellman loops with an additional 5 1 hydrogen bond (N2N3), 12% in a composite structure including a type1-bulge loop and an asx- or ST- motif (N1N3)remarkably homologous to the N1N3-bridged Schellman loopand 3% in a composite structure including a type2-bulge loop and an asx-motif (N2N3). A third hydrogen bond is a previously unrecognized feature of Schellman loops as those lacking bridged nests have an additional 4 0 hydrogen bond. Proteins 2014; 82:3023-3031. (c) 2014 Wiley Periodicals, Inc.

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