C-H... O Bonds Involving Trp Sidechain in Protein Structures

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C-H...O hydrogen bonds are increasingly recognized as significant interactions which contribute to protein folding, stability and catalytic function. They typically involve polarized C-H groups such as those within the imidazole ring of histidine. The tryptophan side chains are another candidate with the C(2)-H group the most polarized by the adjacent nitrogen.
We surveyed the Protein Data Bank, using a subset of non-redundant structures at near- atomic and atomic resolution to identify potential C-H...O bonds based on the stereochemistry of the interactions. We will present data showing the C(2)-H group acts as a donor of hydrogen bonds involving water and other molecules, occasional carbonyl groups from the main chain groups and - importantly - selected halide ions. Importantly, a number of such interactions occur within active sites of enzymes, such as haloalkane dehalogenases, suggesting an active role in the catalytic mechanisms. Our results reaffirm the importance of C-H...O interactions in proteins.