

The phosphoryl transfer reaction in the bacterial PTS. Model of the HPr~P~IIANtr protein complex

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The histidine-containing protein HPr plays a central role in the phosphotransfer reaction that, in the bacterial phosphoenolpyruvate:sugar phosphotransferase system, leads to the phosphorylation of specific carbohydrates at the time of their translocation across the bacterial membrane. In *Escherichia coli* HPr is also able to phosphorylate the protein IIANtr, which is encoded by the *rpoN* operon and is involved in nitrogen regulation in bacteria. As the phosphoryl transfer reaction occurs concomitantly with the formation of a transient complex between HPr and IIANtr, the model of the P~HPr in complex with IIANtr (HPr~P~IIANtr) was built by *in silico* analysis. The model obtained is fully compatible with data describing the NMR chemical shifts relative to the interaction between HPr and IIAMtl, a protein which is structurally similar to IIANtr. The model shows that, due to good surface complementarity of the two proteins, intermolecular hydrogen bonds are formed by the invariant amino acids Arg17 of HPr and Arg57 of IIANtr. Other intermolecular interactions have hydrophobic character.