



The first 3':5'-cyclic nucleotide-amino acid complex: L-His-cIMP.

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Streszczenie

In the crystal structure of the L -His-cIMP complex, *i.e.* L -histidinium inosine 3':5'-cyclic phosphate [systematic name: 5-(2-amino-2-carboxyethyl)-1*H*-imidazol-3-ium 7-hydroxy-2-oxo-6-(6-oxo-6,9-dihydro-1*H*-purin-9-yl)-4*a*,6,7,7*a*-tetrahydro-4*H*-1,3,5,2λ⁵-furo[3,2-*d*][1,3,2λ⁵]dioxaphosphinin-2-olate], C₆H₁₀N₃O₂⁺·C₁₀H₁₀N₄O₇P⁻, the Hoogsteen edge of the hypoxanthine (Hyp) base of cIMP and the Hyp face are engaged in specific amino acid-nucleotide (His...cIMP) recognition, *i.e.* by abutting edge-to-edge and by π-π stacking, respectively. The Watson-Crick edge of Hyp and the cIMP phosphate group play a role in nonspecific His...cIMP contacts. The interactions between the cIMP anions (*anti*/C3'-*endo*/*trans-gauche*/chair conformers) are realized mainly between riboses and phosphate groups. The results for this L -His-cIMP complex, compared with those for the previously reported solvated L -His-IMP crystal structure, indicate a different nature of amino acid-nucleotide recognition and interactions upon the 3':5'-cyclization of the nucleotide phosphate group.

Adres publiczny

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