

Different nucleobase orientations in two cyclic 2',3'-phosphates of purine ribonucleosides: Et₃NH(2',3'-cAMP) and Et₃NH(2',3'-cGMP)·H₂O.

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The crystal structures of triethylammonium adenosine cyclic 2',3'-phosphate {systematic name: triethylammonium 4-(6-aminopurin-9-yl)-6-hydroxymethyl-2-oxido-2-oxoperhydrofurano[3,4-c][1,3,2]dioxaphosphole}, Et₃NH(2',3'-cAMP) or C(6)H(16)N(+).C(10)H(11)N(5)O(6)P(-), (I), and guanosine cyclic 2',3'-phosphate monohydrate {systematic name: triethylammonium 6-hydroxymethyl-2-oxido-2-oxo-4-(6-oxo-1,6-dihydropurin-9-yl)perhydrofurano[3,4-c][1,3,2]dioxaphosphole monohydrate}, [Et₃NH(2',3'-cGMP)].H(2)O or C(6)H(16)N(+).C(10)H(11)N(5)O(7)P(-).H(2)O, (II), reveal different nucleobase orientations, viz. anti in (I) and syn in (II). These are stabilized by different inter- and intramolecular hydrogen bonds. The structures also exhibit different ribose ring puckering [(4)E in (I) and (3)T(2) in (II)] and slightly different 1,3,2-dioxaphospholane ring conformations, viz. envelope in (I) and puckered in (II). Infinite ribbons of 2',3'-cAMP(-) and helical chains of 2',3'-cGMP(-) ions, both formed by O-H...O, N-H...X and C-H...X (X = O or N) hydrogen-bond contacts, characterize (I) and (II), respectively.

Adres publiczny

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