3':5'-Cyclic nucleotides: two sodium salts of cdTMP.

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Streszczenie

3':5'-Cyclic nucleotides play an outstanding role in signal transduction at the cellular level but, in spite of comprehensive knowledge of the biological role of cyclic nucleotides, their structures are not established fully. Two hydrated sodium salts of thymidine 3':5'-cyclic phosphate (cdTMP, C10H12N2O7P), namely sodium thymidine 3':5'-cyclic phosphate heptahydrate, Na(+)·C10H12N2O7P(-)·7H2O or Na(cdTMP)·7H2O, (I), and sodium thymidine 3':5'-cyclic phosphate 3.7-hydrate, Na(+)·C10H12N2O7P(-)·3.7H2O or Na(cdTMP)·3.7H2O, (II), have been obtained in crystalline form and structurally characterized, revealing one nucleotide in the asymmetric unit of (I) and eight different nucleotides in (II). All the cyclic nucleotide anions adopt a similar conformation with regard to nucleobase orientation, sugar conformation and 1,3,2-dioxaphosphorinane ring puckering. In (I), no direct inter-nucleotide hydrogen bonds are present, and adjacent nucleotide anions interact via water-mediated and Na(+)-mediated contacts. In contrast, in (II), direct thymine-phosphate N-H...O inter-nucleotide hydrogen bonds occur and these are assisted by numerous inter-nucleotide C-H...O contacts, giving rise to the self-assembly of cdTMP(-) anions into three different ribbons. Two of these three ribbons run in the same direction, while the third is antiparallel.

Słowa kluczowe

3':5'-cyclic nucleotides, thymidine 3':5'-cyclic phosphate, cdTMP, sodium salts, 1,3,2-dioxaphosphorinane, Hirshfeld surfaces, fingerprint plots