

Highly structured water network in crystals of a deoxydinucleoside–drug complex

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[Nature](#) **volume 288**, pages129–133(1980)[Cite this article](#)

Abstract

X-ray diffraction analysis of crystals of the intercalative complex between the deoxyribonucleoside phosphate d(CpG) and the mutagen proflavine shows a highly structured arrangement of water molecules linked together by networks of hydrogen bonds to form four edge-linked pentagons per asymmetric unit. These pentagons have a general role in maximizing hydrogen bonding at 3.4-Å intervals. The conformation of the deoxyribose sugar ring at the 3' end of one strand can depend on its local aqueous environment.

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