High resolution crystal structures of \([d(CGCAATTCGCG)]_2\) co-crystallized with polynuclear platinum(II) complexes: Non-covalent interactions between DNA and potential anticancer drugs.

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Polynuclear Pt(II) complexes as potential anticancer drugs, \([[\text{cis-Pt(NH}_3]_2(\mu\text{-pyrazolato})(\mu\text{-hydroxo})]^{2+}\) (AMPZ) and \([[\text{trans-Pt(NH}_3]_2(\text{hexanediamine})_2(\mu\text{-trans-Pt(NH}_3]_2(\text{hexanediamine})_2)]^{6+}\) (AH78), experience intense non-covalent association with DNA, probably due to their high positive charges. In order to elucidate the significance of such non-covalent interactions in their cytotoxic mechanism, the two complexes were co-crystallized with the double-stranded DNA, \([d(CGCAATTCGCG)]_2\), and their crystal structures were solved and anisotropically refined. In the high resolution DNA structures with AMPZ (1.25 Å) and AH78 (1.11 Å), the former non-covalently binds to the minor-groove, and the latter is arranged like a chain along the helix backbone. The structures and their significance will be presented.

![AMPZ](image1)

![AH78](image2)

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