X-Ray Analyses of DNA Dodecamers Containing 2'-Deoxy-5-formyluridine

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It is known that formylation of thymine base induces purine transition in DNA replication. In order to establish the structural basis for such mutagenesis, crystal structures of two kinds of DNA dodecamers $d(CGCGRATf^5UCGCG)$ with $f^5U=2$ '-deoxy-5-formyluridine and R=A or G have been determined. The f^5U residues form a Watson-Crick-type pair with A[1,2] and two types of pairs

(wobble and reversed wobble) with G[3] (*see* figure), the latter being the first example. Structural modeling suggests that the DNA polymerase can accept the reversed wobble pair with G, as well as the Watson-Crick pair with A.

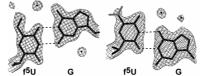


Figure 2|Fo|-|Fc| maps around the f⁶U residues found in crystals of f⁶U:G.

[1] Tsunoda M., Karino N., et al., *Acta. Cryst.*, 2001, **D57**, 345. [2] Tsunoda M., Kondo J., et al., *Biophys. Chem.*, 2002, **95**, 227. [3] Tsunoda M., Sakaue T., et al., *Nucleic Acids Res. Suppl.*, 2001, **1**, 279.

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