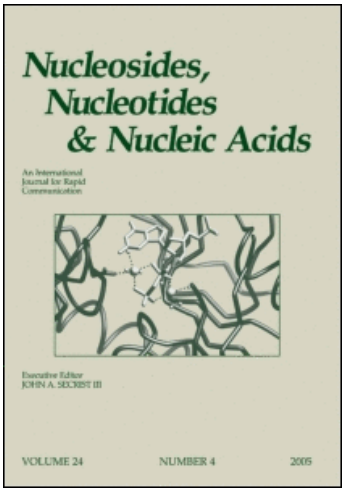

Nucleosides, Nucleotides and Nucleic Acids
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713597286

Base-Pair Mismatch in DNA at 2.3A Resolution

Tom Brown[a]; Olga Kennard[a]; Geoff Kneale[b]
[a] University Chemical Laboratory, Cambridge, U.K. [b] Dov Rabinovich, the Weizman Institute of Science, Rehovot, Israel

To cite this Article Brown, Tom , Kennard, Olga and Kneale, Geoff(1985) 'Base-Pair Mismatch in DNA at 2.3A Resolution', Nucleosides, Nucleotides and Nucleic Acids, 4: 1, 255
To link to this Article: DOI: 10.1080/07328318508077877
URL: http://dx.doi.org/10.1080/07328318508077877

NUCLEOSIDES & NUCLEOTIDES, 4(1&2), 255 (1985)

BASE-PAIR MISMATCH IN DNA AT 2.3A RESOLUTION.

Tom Brown, Olga Kennard*, Geoff Kneale, University Chemical Laboratory, Cambridge, U.K. and Dov Rabinovich, the Weizman Institute of Science, Rehovot, Israel.

Summary, X-ray single crystal analysis of the deoxyoctanucleotide $d(GGGGCTCC)_2$ has revealed, for the first time, the existence of the G.T wobble mispair in an A-DNA double helical fragment.

The G.T wobble mispair is stabilised by two hydrogen bonds and involves small rotations and translations of the bases from the standard Watson-Crick geometry. This results in minimal distortions of the neighbouring base pairs and to the backbone. G.U. wobble base pairs have previously been observed in t-RNA at around the same resolution.

The crystallographic verification, in DNA, of the existence of stable wobble pairs, with the bases in the major tautomeric forms, is of importance in the exploration of the molecular basis of mutagenesis. Point mutations can arise from the incorporation of a base pair mismatch in the DNA double helix. The nature of such mismatches has been the subject of much speculation. Theoretical predictions favouring the minor tautomeric forms, which can base pair with standard Watson-Crick geometry, and major tautomers pairing with non-standard geometry have both been proposed. The present structure gives information about the geometry of the wobble base pair, its influence on nearest neighbours and on the global conformation of the double helix.

$d(GGGGCTCC)_2$ [$P6_1$, $\underline{a}$ = 42.21, $\underline{c}$ = 43.00, Z = 6] is isomorphous with both the parent molecule $d(GGGGCCCC)_2$ and $d(GGTATACC)_2$. It was refined by CORELS starting with the coordinates of the parent compound to R = 0.197 using 1924 reflections $> 2\sigma$ at 2.25A resolution.

0732-8311/85/0401-0255$3.50/0