Supplementary Material

DPT tautomerisation of the G·A\textsubscript{syn} and A\textsuperscript{*}·G\textsuperscript{*}_\textsubscript{syn} DNA mismatches: A QM/QTAIM combined atomistic investigation

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Fig. S1 Profiles of: (a) the electronic energy $E$ of the base mispair and (b) the first derivative of the electronic energy $E$ with respect to the IRC - $dE/d$IRC - along the IRC of the $A^*\cdot G^*_{\text{syn}} \leftrightarrow A\cdot G^*_{\text{syn}}$ tautomerisation via the DPT obtained at the B3LYP/6-311++G(d,p) level of theory in vacuo. The position of the TS$_{A^*\cdot G^*_{\text{syn}} \leftrightarrow A\cdot G^*_{\text{syn}}}$ corresponds to IRC=0.00 Bohr.

Fig. S2 Profile of the dipole moment $\mu$ of the base mispair along the IRC of the $A^*\cdot G^*_{\text{syn}} \leftrightarrow A\cdot G^*_{\text{syn}}$ tautomerisation via the DPT obtained at the B3LYP/6-311++G(d,p) level of theory in vacuo.
Fig. S3 Profiles of: (a) the electron density $\rho$; (b) the Laplacian of the electron density $\Delta \rho$; (c) the ellipticity $\varepsilon$ and (d) the energy of the H-bond $E_{HB}$, estimated by the EML formula [1,2], at the (3,-1) BCPs of the covalent and hydrogen bonds along the IRC of the $A^\ast G^\ast_{\text{syn}} \leftrightarrow A \cdot G^\ast_{\text{syn}}$ tautomerisation via the DPT obtained at the B3LYP/6-311++G(d,p) level of theory in vacuo.
**Fig. S4** Profiles of: (a) the distance $d_{A-B}$ between the electronegative A and B atoms; (b) the distance $d_{AH/BB}$ between the hydrogen and electronegative A or B atoms and (c) the angle $\angle AH\cdots B$ of the AH···B H-bonds along the IRC of the A*·G*$_{syn}$$\leftrightarrow$A·G*$_{syn}$ tautomerisation via the DPT obtained at the B3LYP/6-311++G(d,p) level of theory in vacuo.
Fig. S5 Profiles of the NBO charges of the hydrogen atoms involved in the O6H₁⋯N6/N6H₁⋯O6 and N1H₁⋯N7/N7H₁⋯N1 H-bonds along the IRC of the Aᵦ·G*ₚ₀ ↔ A·G*₀ tautomeration via the DPT obtained at the B3LYP/6-311++G(d,p) level of theory in vacuo.

Fig. S6 Profiles of: (a) the distance R(H-H) between the glycosidic hydrogens and (b) the α₁ (⧹N9H(A)H(Gₚ₀)) and α₂ (⧹N9H(Gₚ₀)H(A)) glycosidic angles along the IRC of the Aᵦ·G*ₚ₀ ↔ A·G*₀ tautomeration via the DPT obtained at the B3LYP/6-311++G(d,p) level of theory in vacuo.

References.