

Electronic Supplementary Information

Physico-chemical profiles of the wobble $\leftrightarrow$ Watson-Crick $G^* \cdot 2AP(w) \leftrightarrow G \cdot 2AP(WC)$ and $A \cdot 2AP(w) \leftrightarrow A^* \cdot 2AP(WC)$ tautomerisations: A QM/QTAIM comprehensive survey

Ol'ha O. Brovarets^{a,b,✉}, Ivan S. Voiteshenko^b & Dmytro M. Hovorun^{a,b}

^aDepartment of Molecular and Quantum Biophysics, Institute of Molecular Biology and Genetics, National Academy of Sciences of Ukraine, 150 Akademika Zabolotnoho Str., 03680 Kyiv, Ukraine

^bDepartment of Molecular Biotechnology and Bioinformatics, Institute of High Technologies, Taras Shevchenko National University of Kyiv, 2-h Akademika Hlushkova Ave., 03022 Kyiv, Ukraine

✉ Corresponding author. E-mail: o.o.brovarets@imbg.org.ua

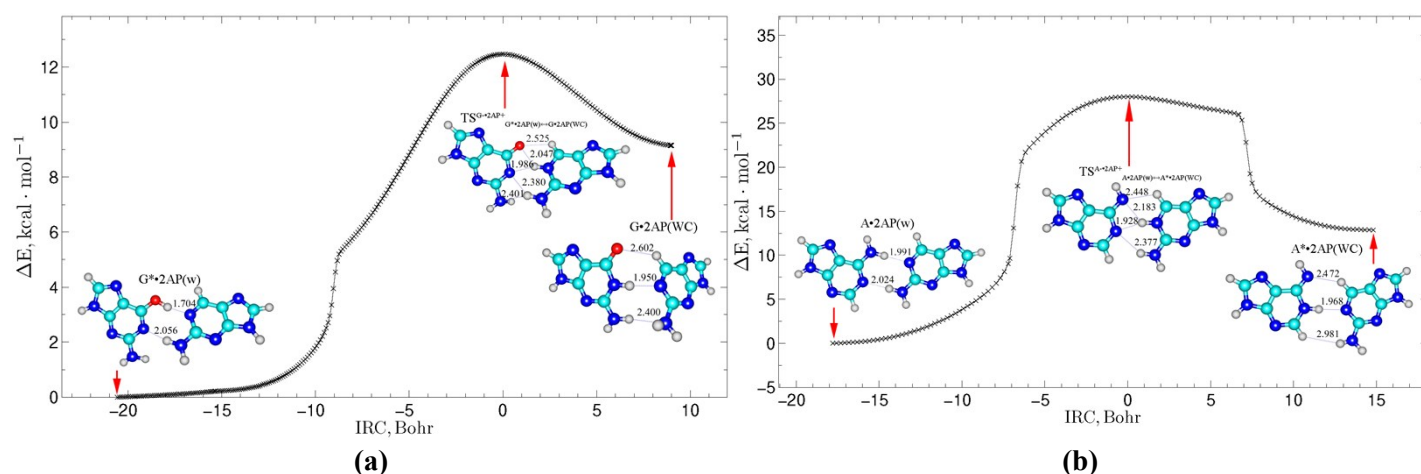


Fig. S1. Profiles of the relative electronic energy ΔE along the IRC of the (a) $G^* \cdot 2AP(w) \leftrightarrow G \cdot 2AP(WC)$ and (b) $A \cdot 2AP(w) \leftrightarrow A^* \cdot 2AP(WC)$ wobble $\leftrightarrow$ Watson-Crick tautomerisations *via* the sequential single proton transfer obtained at the B3LYP/6-311++G(d,p) level of theory in the continuum with $\epsilon=4$, characteristic for the active center of the DNA-polymerase.