

Global DNA dynamics of 8-oxoguanine repair by human OGG1 revealed by stopped-flow kinetics and molecular dynamic simulation

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SUPPLEMENTARY MATERIALS

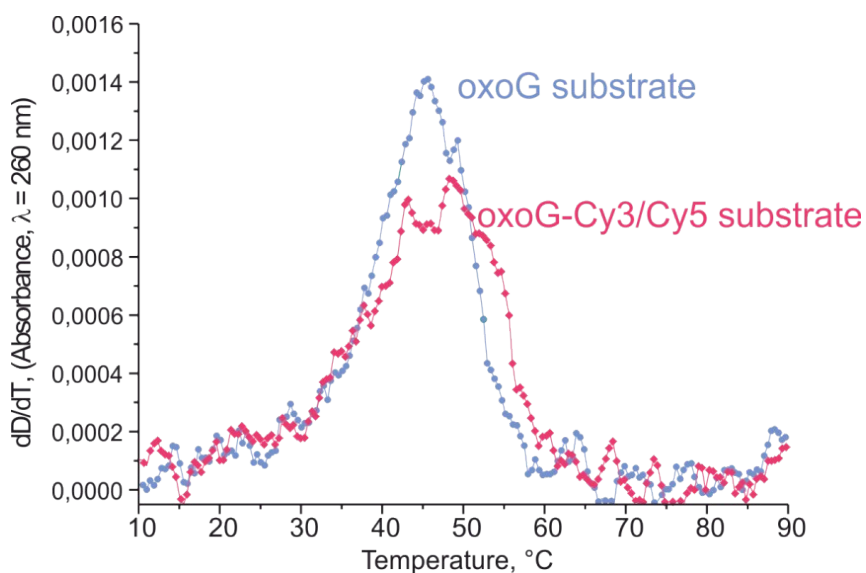


Figure S1. The thermodynamic melting curves for the **oxoG** and **oxoG-Cy3/Cy5** DNA duplexes

A

B

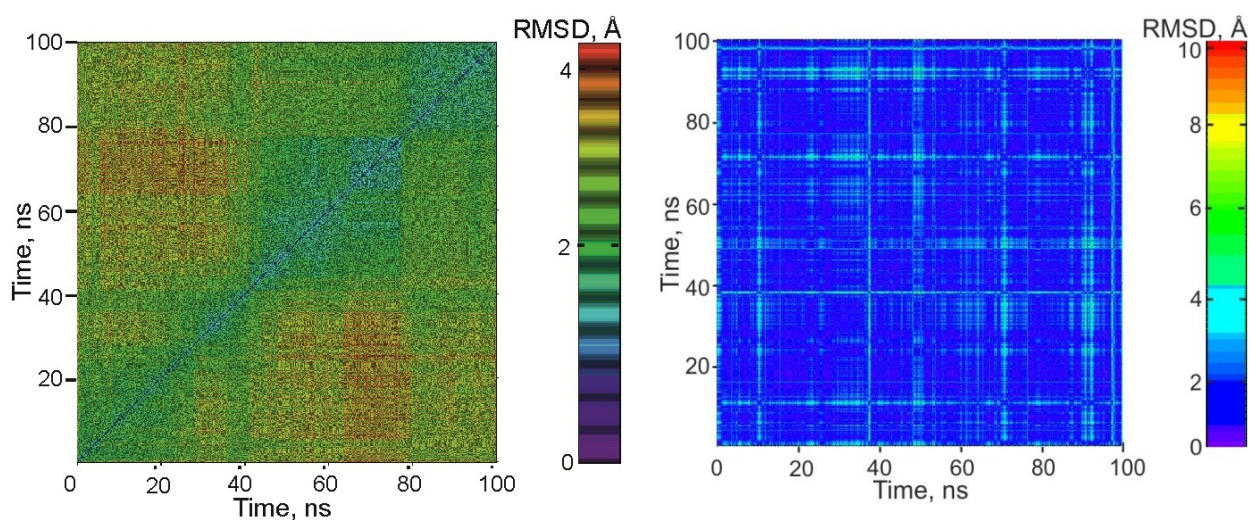
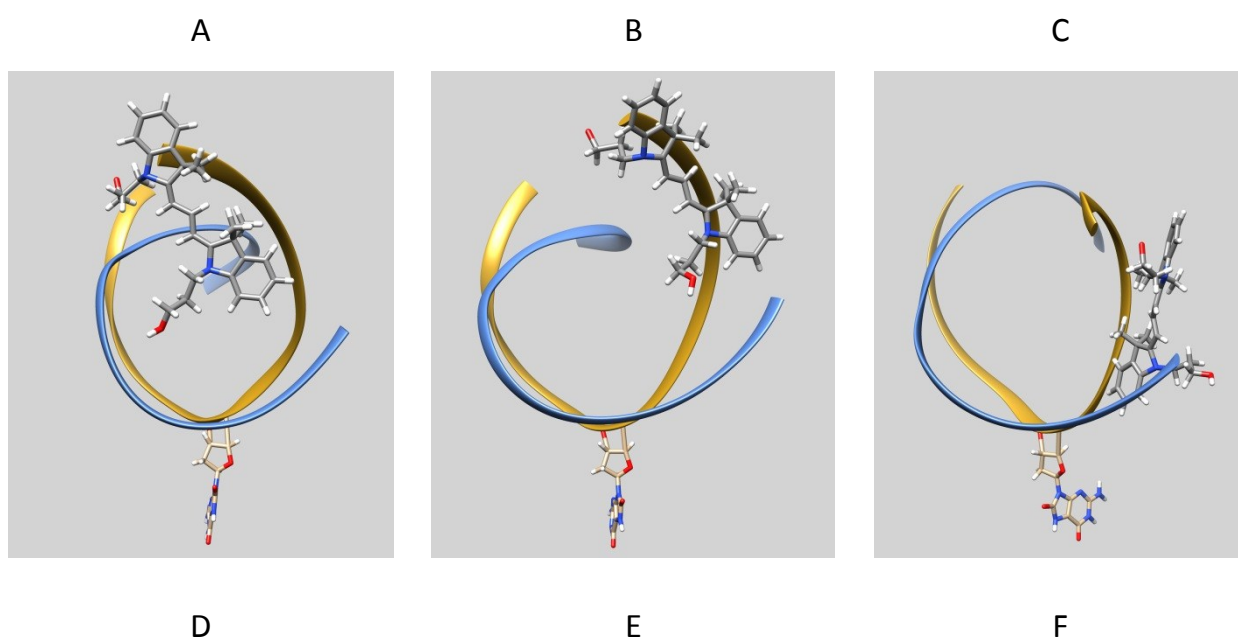


Figure S2. Two-dimensional RMSD plot of values calculated along a 100 ns trajectory for 8-oxoG and Cy3/Cy5 containing DNA in a complex with hOGG1 (A) and free DNA duplex (B). The x- and y-axes represent the MD simulation time in ns.

Figure S3. The MD movie for hOGG1 complex with DNA duplex containing Cy3/Cy5 FRET pair was captured during 100 ns trajectory playback



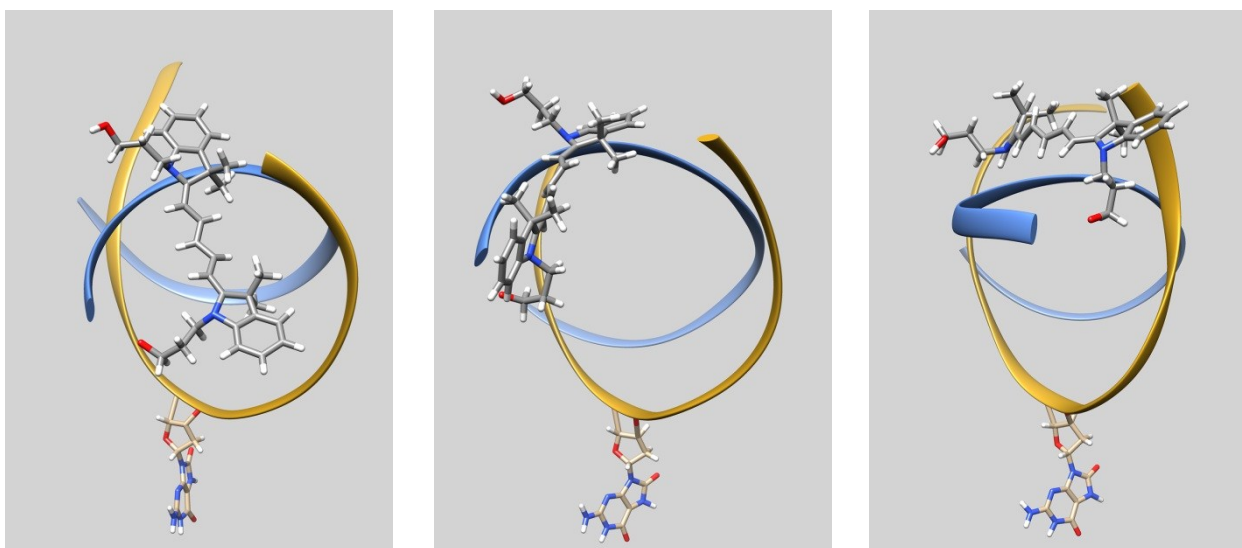


FIGURE S4. Typical snapshots of Cy3 (**A - C**) attached to 5' terminal T and Cy5 (**D - F**) attached to 5' terminal G on the duplex (8-oxoG displayed at the bottom of the DNA helix) in the complex with hOGG1 (not displayed): (**A, D**) primary base-stacked configuration, (**B, E**) unstacked configuration, (**C, F**) wandering dye.

FIGURE S5. The MD movie for DNA duplex containing Cy3/Cy5 FRET pair was captured during 100 ns trajectory playback.

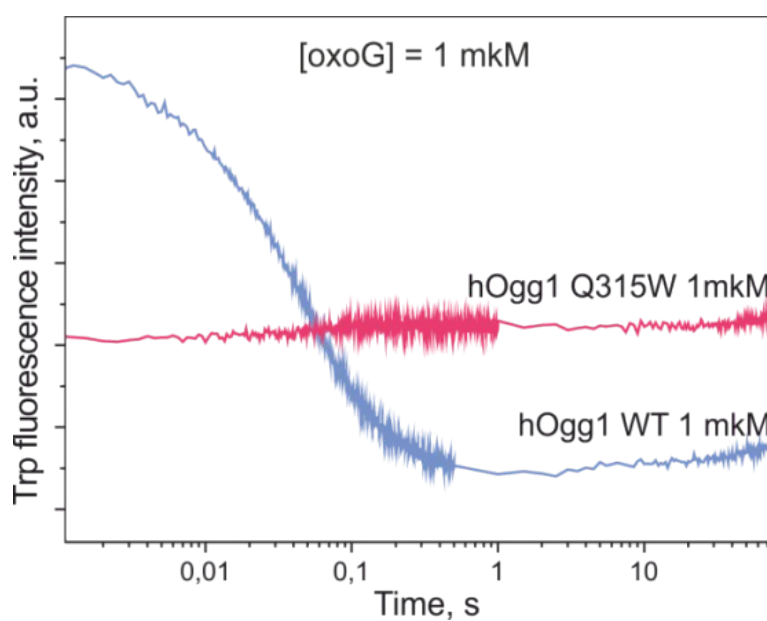


FIGURE S6. Comparison of the Trp fluorescence traces of interaction between 1 μ M oxoG DNA duplex and 1 μ M hOGG1 WT (blue line) or hOGG1 Q315 (pink line).

FIGURE S7. Active site amino acids dynamics for Q315W hOGG1 was captured during 100 ns MD trajectory playback.

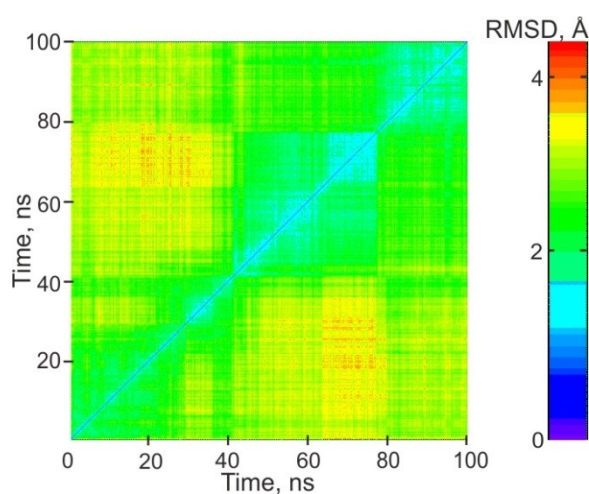


FIGURE S8. Two-dimensional RMSD plot of values calculated along a 100 ns trajectory for Q315W hOGG1 with 8-oxoG and Cy3/Cy5 containing DNA complex. The x- and y-axes represent the MD simulation time in ns.

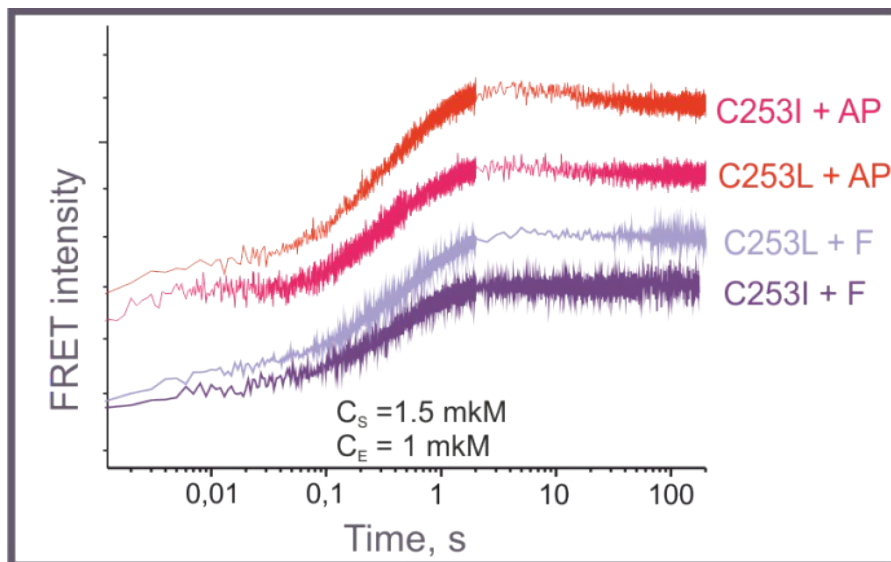


FIGURE S9. FRET traces of the time course of interaction between hOGG1 C253I and C253L with DNA contained natural AP-site or its synthetic analogue.