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
**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 μM oxoG DNA duplex and 1 μM 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.