

Supporting Information

Correlation Between Charge Transport and Base Excision

Repair in the MutY DNA Glycosylase

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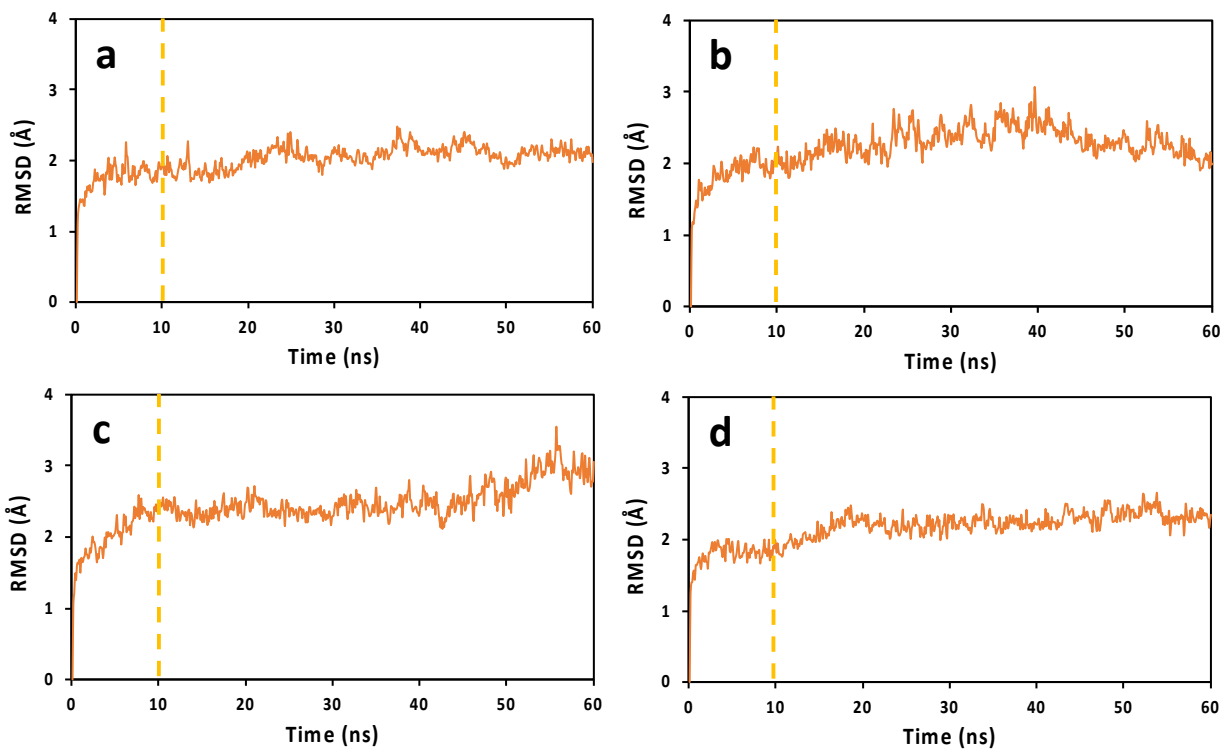


Figure S1. RMSD of the MutY-DNA complex during the MD production run for (a, c) the WT protein and (b, d) the R153L mutant, using either (a, b) the A₃₊ FF or (c, d) the A₂₊ FF to describe the [Fe₄S₄] cluster.

Table S1. Mean value and standard deviation of the center-to-center distance (in Å) for the indicated redox pairs obtained from MD simulations of the WT-DNA and R153L-DNA complexes using the A_{3+} FF to describe the $[Fe_4S_4]$.

Redox pair	WT protein complex	R153L protein complex
$[Fe_4S_4]$ -DA18	19.25 ± 0.33	19.49 ± 1.18
$[Fe_4S_4]$ -W20	10.69 ± 0.22	10.88 ± 0.26
$[Fe_4S_4]$ -DA17	21.96 ± 0.43	23.06 ± 0.67
$[Fe_4S_4]$ -DA10	25.48 ± 0.94	25.97 ± 1.90
DA18-DA17	11.86 ± 0.30	12.29 ± 0.46
DA18-DA10	21.82 ± 0.50	21.65 ± 0.75
W20-DA18	15.79 ± 0.40	15.88 ± 0.54
W20-DA10	27.43 ± 0.78	27.81 ± 1.46

Table S2. Mean value and standard deviation of the center-to-center distance (in Å) for the indicated redox pairs obtained from MD simulations of the WT-DNA and R153L-DNA complexes using the A_{2+} FF to describe the $[Fe_4S_4]$.

Redox pair	WT protein complex	R153L protein complex
$[Fe_4S_4]$ -DA18	18.79 ± 1.34	20.44 ± 0.37
$[Fe_4S_4]$ -W20	10.76 ± 0.24	11.03 ± 0.27
$[Fe_4S_4]$ -DA17	21.99 ± 0.65	22.20 ± 0.41
$[Fe_4S_4]$ -DA10	22.26 ± 0.88	21.64 ± 0.64
DA18-DA17	11.81 ± 0.62	12.04 ± 0.41
DA18-DA10	19.28 ± 1.02	19.83 ± 0.52
W20-DA18	15.04 ± 1.37	15.95 ± 0.45
W20-DA10	24.50 ± 1.06	23.73 ± 0.91