Supporting Information

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SI Text

Cleavage Assay. The 16-mer oligonucleotide (5′-TGGTAGA-C*A*TGGACGC-3′; *A*, substrate adenine) was end-labeled by incubating the substrate adenine-containing single-strand DNA with T4 polynucleotide kinase and [γ-^{32}P]ATP followed by annealing to unlabeled complementary strand (5′-AGCGTCC A °G GTCTACC-3′; °G, 8-oxoguanine) in 100 mM Tris-HCl, pH 8.0, 50 mM NaCl by heating 70 °C for 10 min and slowly cooled to 4 °C. The duplex DNA was then incubated with w.t. MutY or Glu43Gln MutY at 37 °C for various amounts of time and the reaction was quenched by adding piperidine. The mixture was heated at 90 °C for 30 min to cleave the abasic residue produced by MutY. Samples were analyzed by electrophoresis on a 20% denaturing polyacrylamide gel for 3 h at 300 V. The bands were visualized with a phosphorimaging system after exposing to a Fuji image plate.

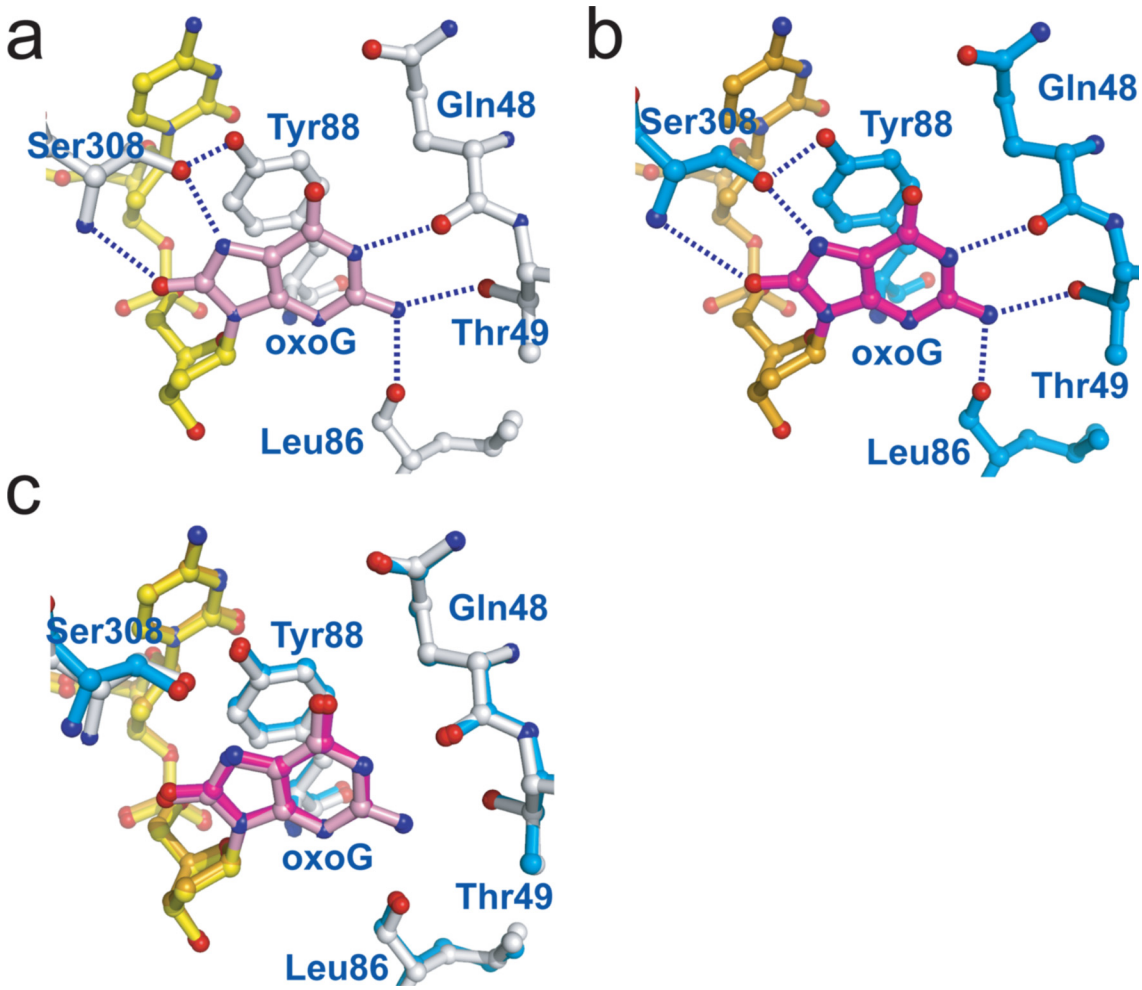

Fig. S1. Comparison of oxoG recognition by D144N MutY and *Bst* MutY. (*a*) Close-up view of oxoG recognition by D144N MutY, colored as in Fig. 3*C*. OxoG is in pink. Important hydrogen bonding interactions between oxoG lesion and the protein are denoted by dotted lines. (*b*) Close-up view of oxoG recognition by *Bst* MutY, colored as in Fig. 3*D*. OxoG is in magenta. (*c*) Heavy atom superposition of panel *A* with *B*. Color scheme as in panel *A* and *B*, respectively.

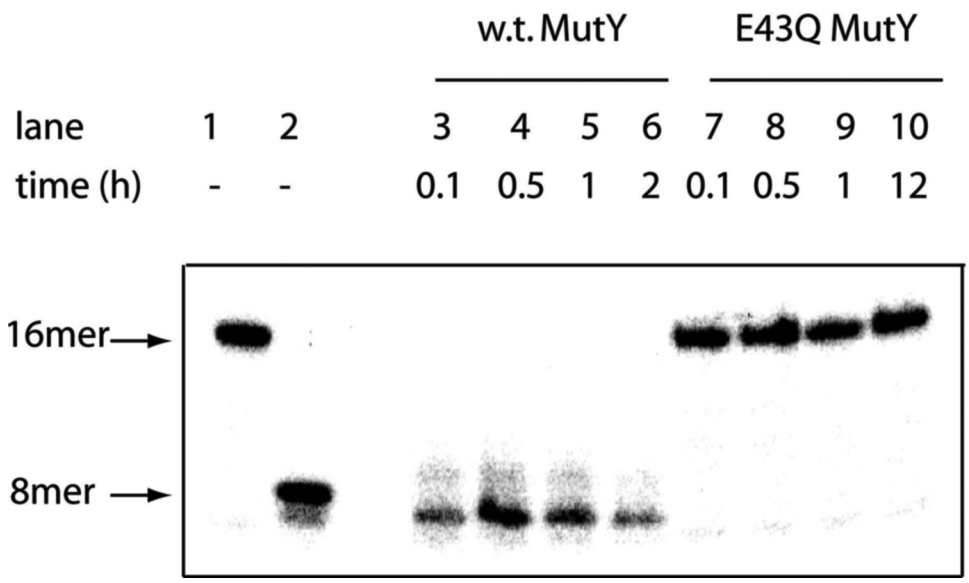

Fig. S2. Cleavage assay to detect the processing of substrate adenine-containing 16-mer DNA by w.t. MutY and Glu43Gln MutY. The appearance of the 8-mer product indicates that base-excision has taken place.

Table S1. Data Collection and Refinement Statistics

	FdA·oxoG complex
Data collection	
Space group	$P2_12_12_1$
Cell dimensions	
a, Å	37.7
b, Å	85.9
c, Å	142.1
α, °	90
β, °	90
γ, °	90
Resolution, Å	50–2.2
R_{merge}	0.075 (0.472)
$I/\sigma I$	39.8 (5.7)
Completeness, %	99.9 (100)
Redundancy	6.8 (7.2)
Refinement	
Resolution, Å	50–2.2
No. reflections	18,525
R_{work}/R_{free}, %	24.6/27.6
No. atoms	
Protein	2,766
Ligand/ion	445
Water	49
rmsds	
Bond lengths, Å	0.009
Bond angles, °	1.1
Ramanchandran plot, %*	
Most favored region	84.2
Additionally allowed region	14.5
Generously allowed region	1.3

Values in parenthesis refer to the highest resolution shell. *, calculated using PROCHECK