SUPPORTING INFORMATION

Key players of I-DmoI endonuclease catalysis revealed from structure and dynamics

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Additional details on the MD simulations.

The three crystallographic structures were minimized and solvated using the SPC water model in an octahedral box (a minimum distance of 1.1 nm between the proteins and the box was imposed). The neutrality of the three systems was reached by adding Mg^{+2} ions in order to better reproduce the experimental conditions. The systems were then equilibrated by heating slowly the temperature up to reach the working temperature of these enzymes (343 K). The first 10 ns at 343 K were considered as equilibration and all the analysis of this work refer to the remaining 200 ns (productive runs). The convergence of the trajectories was checked by the RMSD behavior and from the block analysis of the RMSF (data not shown). In the case of RMSD, the fluctuations are all within 0.03-0.04 nm, whereas for the RMSF we divided each trajectories in four blocks of 50 ns and for each block we calculated the per-residue RMSF, which resulted in differences between MD blocks all below two standard deviations. The essential dynamics analysis was executed on the C-alpha atoms using the 200 ns long MD trajectories. The comparison of the first ten eigenvectors was executed by calculating the Root Mean Square Inner Product (RMSIP)[1]. Eigenvectors showing values of RMSIP greater than 0.5 (as occurring when the principal eigenvectors of both the E117A and Q42A/K120M mutants are compared to the wild-type ones) are considered very similar[1].

Figure S1. Root mean square deviations of the WT (black line), Q42A/K120M (green line) and E117A (red line) I-DmoI along the MD trajectories.
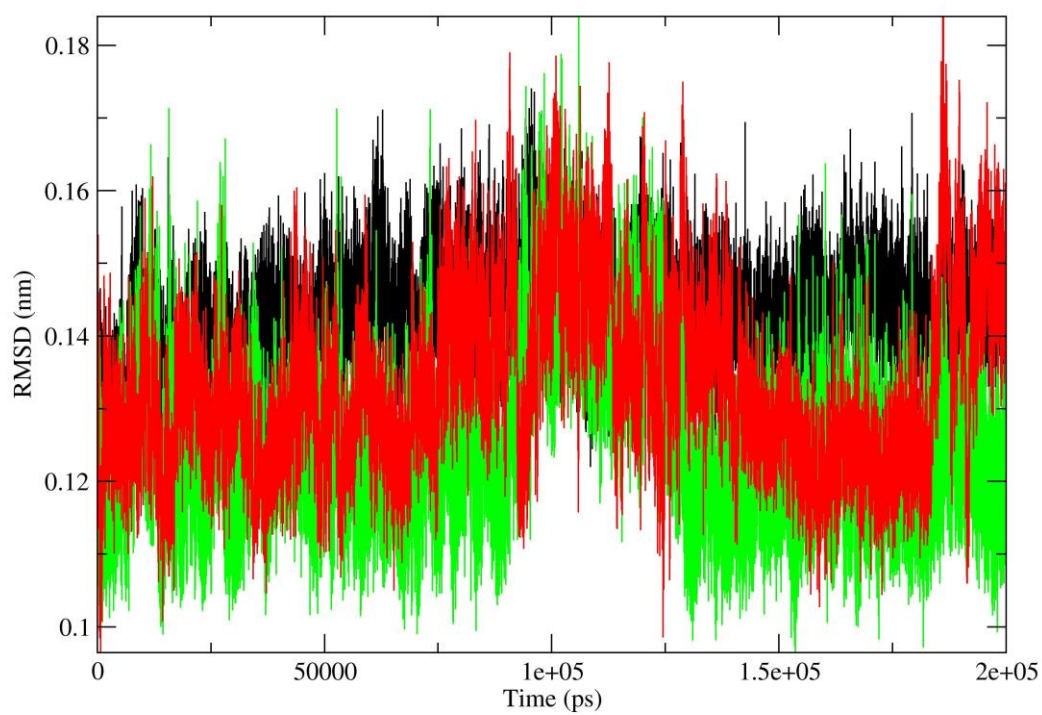
Figure S2.- Root mean square fluctuations per residue for the three proteins (WT=black line, E117A=red line and Q42A/K120M=green line). Small circles represent the mutations.
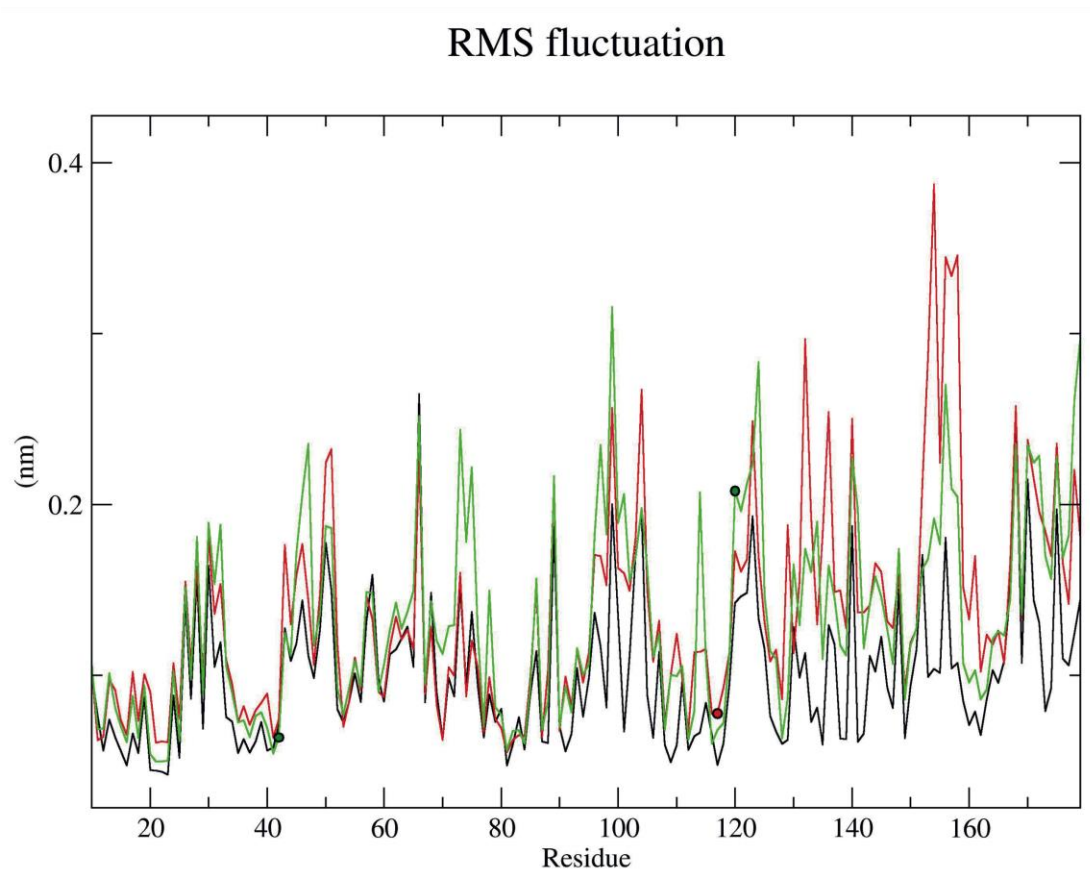
RMS fluctuation

Figure S3. Components of the first three eigenvectors (WT=black lines, E117A=red lines and Q42A/K120M=green lines).
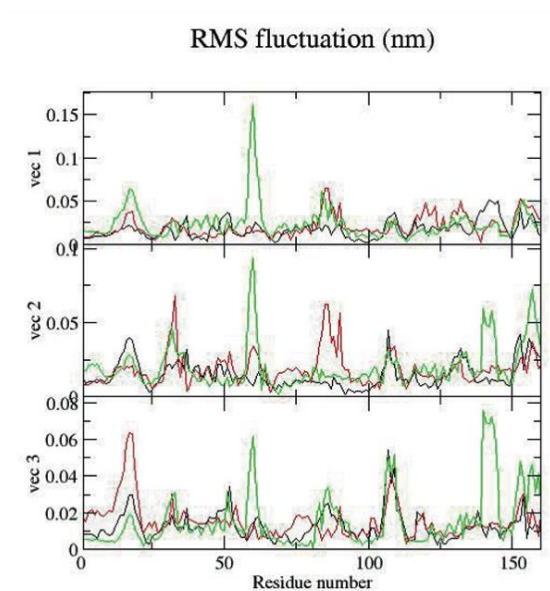
Figure S4. Top: the wt (left), E117A (center) and Q42A/K120M (right) extreme of the projections along the first eigenvector represented by tube representation in different colors (cyan and green). The DNA is represented by "trace" and "lines".Bottom: the projection of the trajectories on their essential subspace (wt, left,; E117A, center; Q42A/K120M, right).
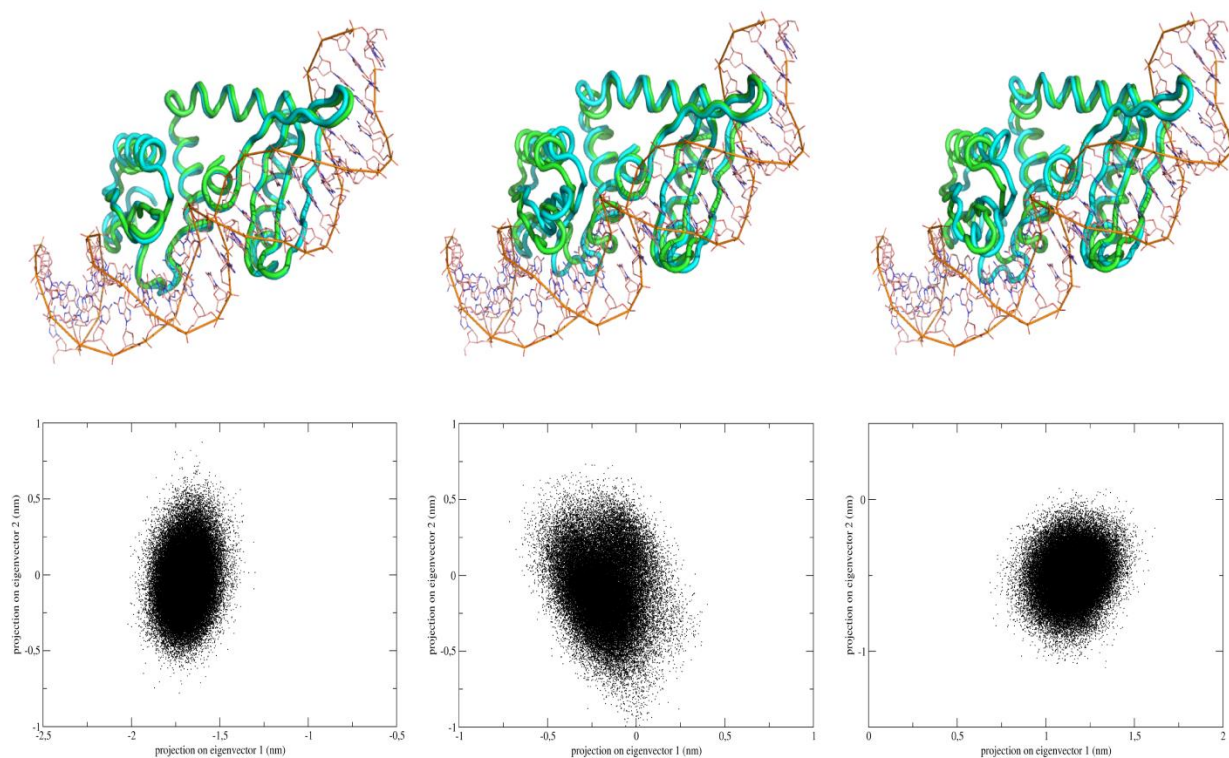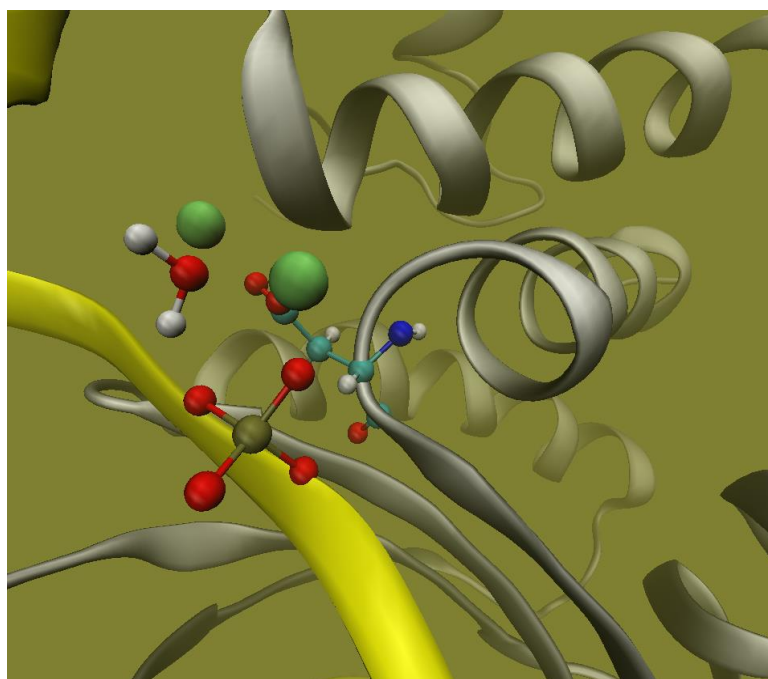
Figure S5. Representative snapshot of the active centre as sampled by MD trajectory of the I-DmoI WT (the Mn ions, the phosphorous group and water are in ball and stick and the rest of the system in cartoon representation).

References:
1) Laberge M, Yonetani T., Molecular dynamics simulations of hemoglobin A in different states and bound to DPG: effector-linked perturbation of tertiary conformations and HbA concerted dynamics. Biophys J. 2008, 1;94(7):2737-51