

Description of Additional Supplementary Files

Supporting Movies. Related to Fig 6 and 7.

The morphs of the transitions in the coordinate system originating at the nuclease core of two Mre11 monomers from the first to the last frame of 30 nsec MD simulation for truncated WT and mutant MR complexes. The Zn ion in front, shown in a space-filling representation, is light pink. α -helices are shown as tubes; β -strands are shown as arrows. Rad50 monomers are colored in dark blue and dark green, and the Mre11 monomers are colored in orange and dark red. DNA double helix is shown in space-filling representation.

Movie S1: WT MR complex. Clockwise coaxial rotation of the coiled coils (as viewed from the Rad50 globular domain toward the Zn hook) and associated dynamic repositioning of DNA double helix in Rad50 head domain results in activating Rad50 ATPase by arranging a cutting configuration of the catalytic residues (Fig. 7B).

Movie S2: Rad50-3KA MR complex. Clockwise rotation of the coiled coils (as viewed from the Rad50 globular domain toward the Zn hook) substantially deviates from coaxiality with associated DNA dynamics in Rad50 head domain incapable of inducing the cutting configuration of the catalytic residues (Fig. 7C).

Movie S3: Rad50-3KA P168S MR complex. The P168S suppressor mutant restores the clockwise coaxial rotation of the 3KA-mutated coiled coils (as viewed from the Rad50 globular domain toward the Zn hook) with associated dynamic repositioning of DNA double helix in Rad50 head domain resulting in activation of Rad50 ATPase by restoration of a cutting configuration of the catalytic residues (Fig. 7D).