

Supplementary Information

Structural dynamic analysis of apo and ATP-bound IRAK4 kinase

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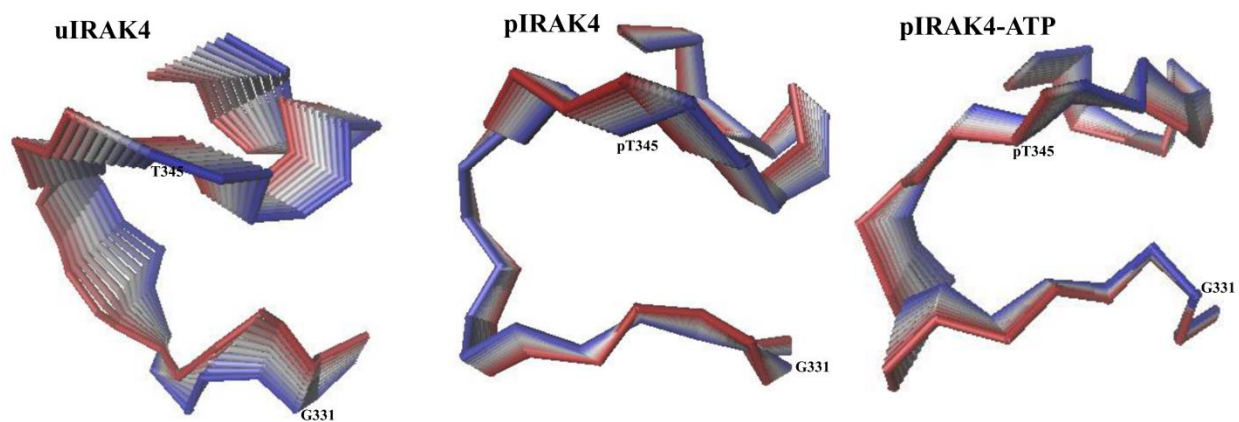


Figure S1: Superimposition of the IRAK4 KD activation segment. The principal motion of the first eigenvector is superimposed sequentially with 10 frames of the trajectory to show the structural variation within the activation segment. Red and blue colors represent from minimum to maximum, respectively. $C\alpha$ atoms of G331 and T345 are highlighted. The protein is represented in the trace model.

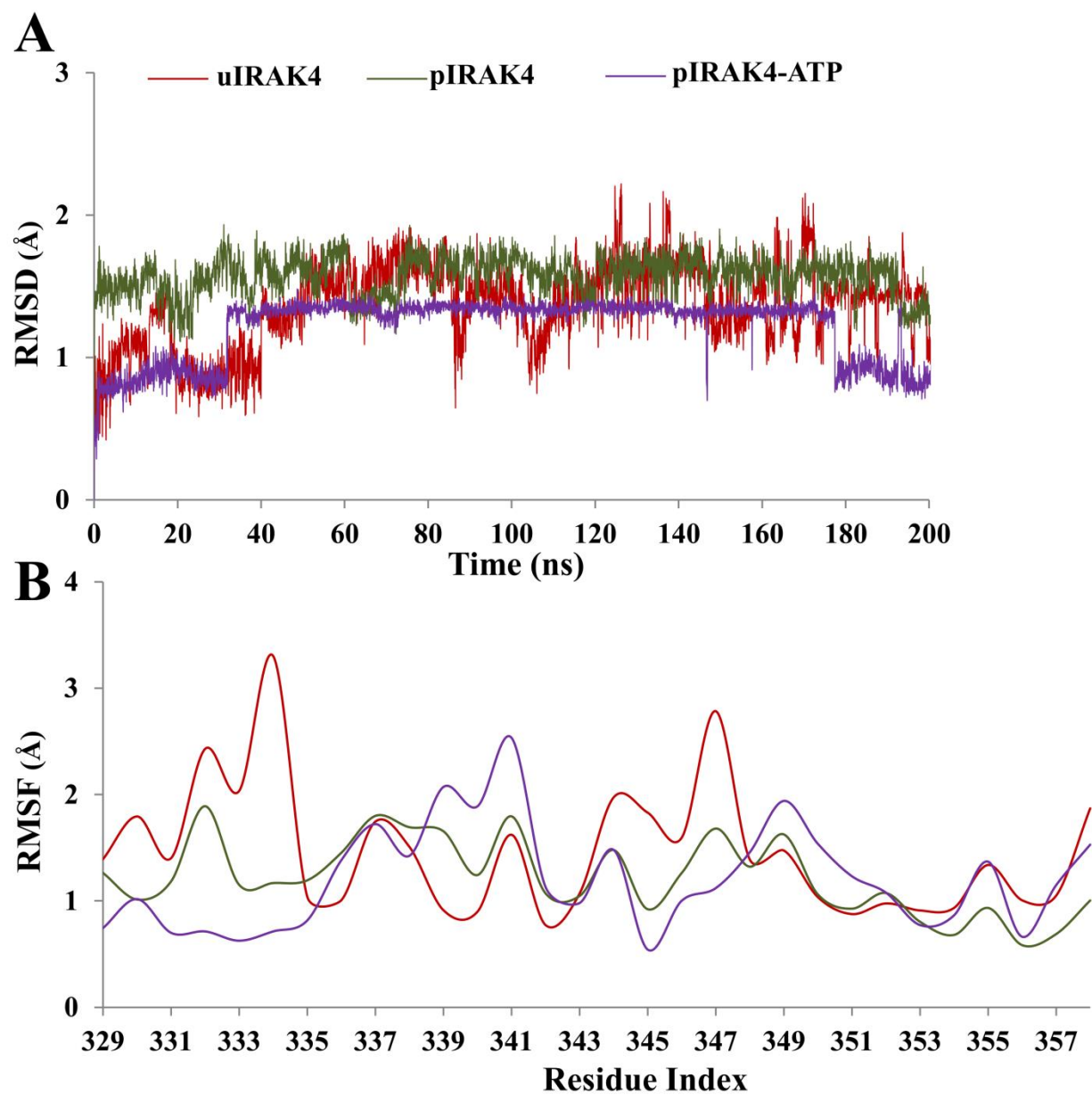


Figure S2: RMSD and RMSF calculations of the DFG motif and activation segment, respectively. (A) RMSD plot of the residues for the DFG motif with respect to the initial structure. (B) RMSF plot of the residue fluctuations obtained for the activation segment.

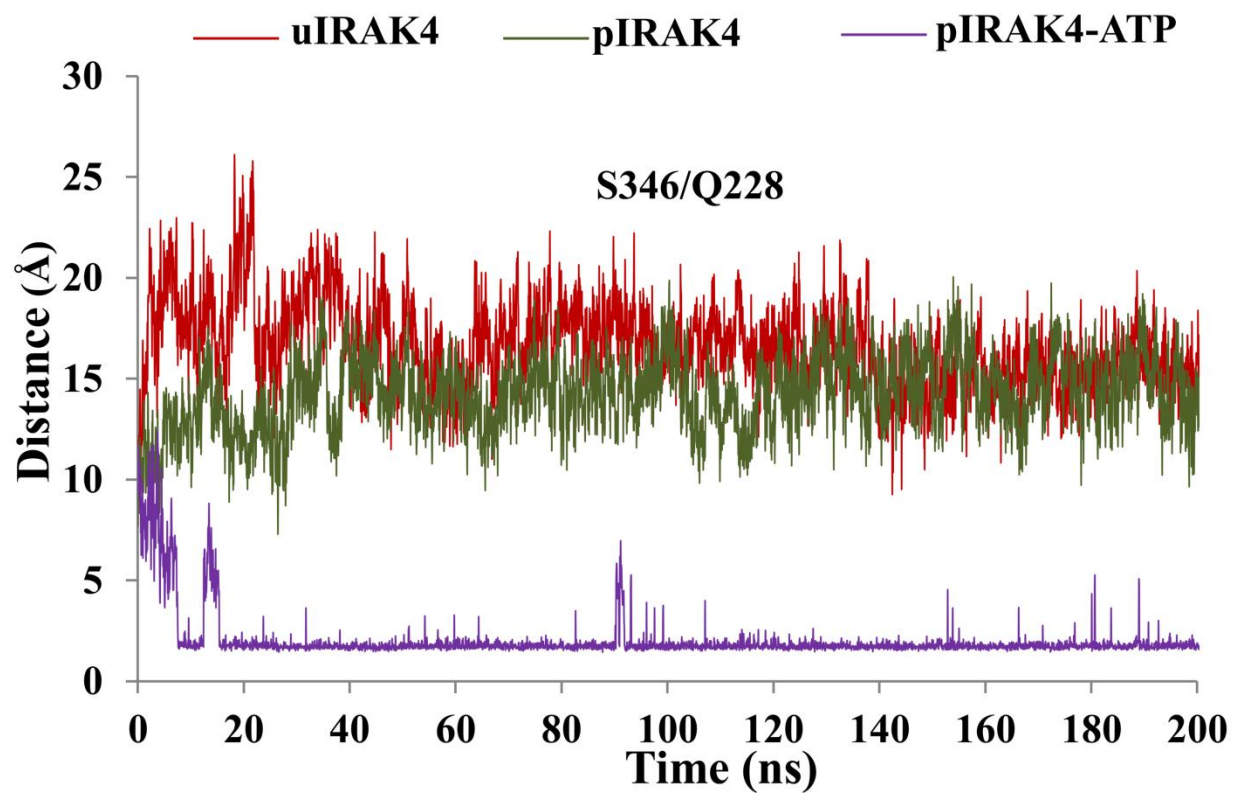


Figure S3: S346/Q228 residue minimum distance. Minimum distance between S346 from the activation loop and Q228 from helix α C as a function of time were calculated for both apo and ATP-bound trajectory.

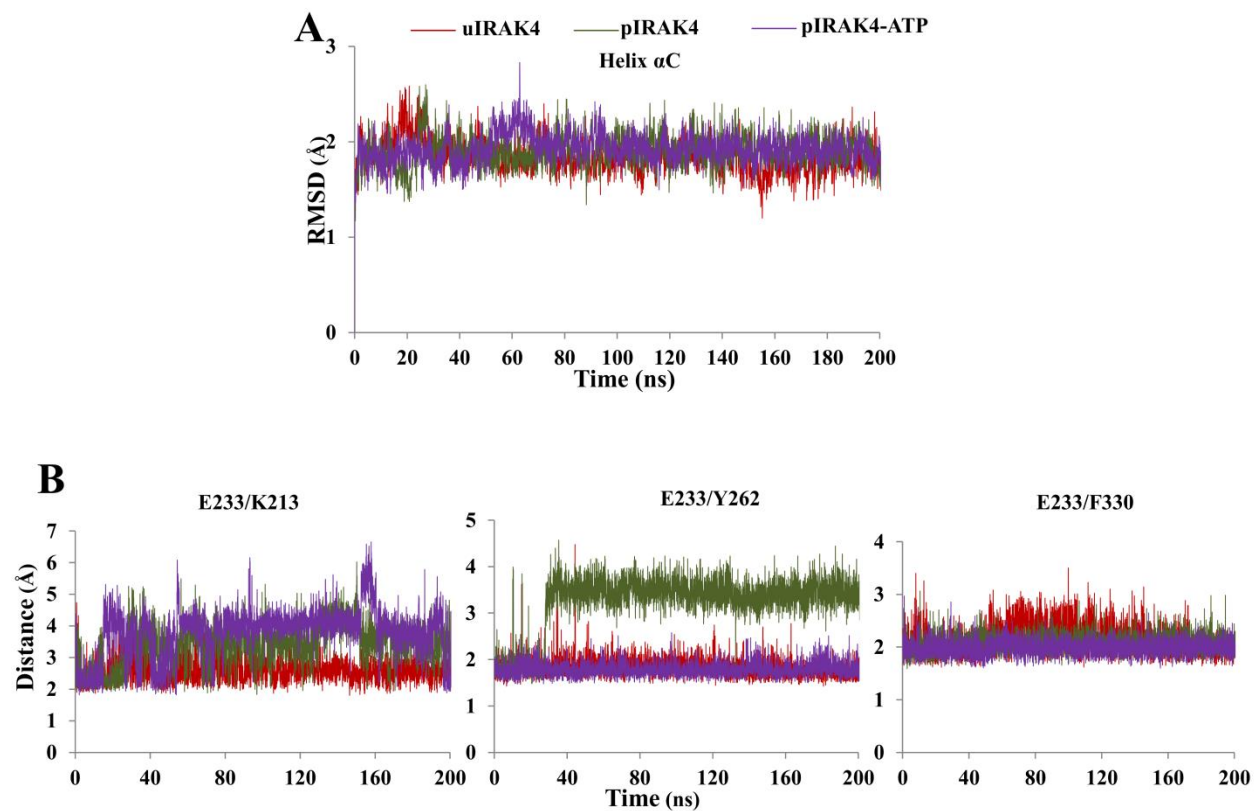


Figure S4: RMSD and minimum distance calculations. (A) RMSD plot of the residues for the helix αC with respect to the initial structure. (B) Residue minimum distances of E213/K233, E233/Y262, and E233/F330 were calculated as a function of time.

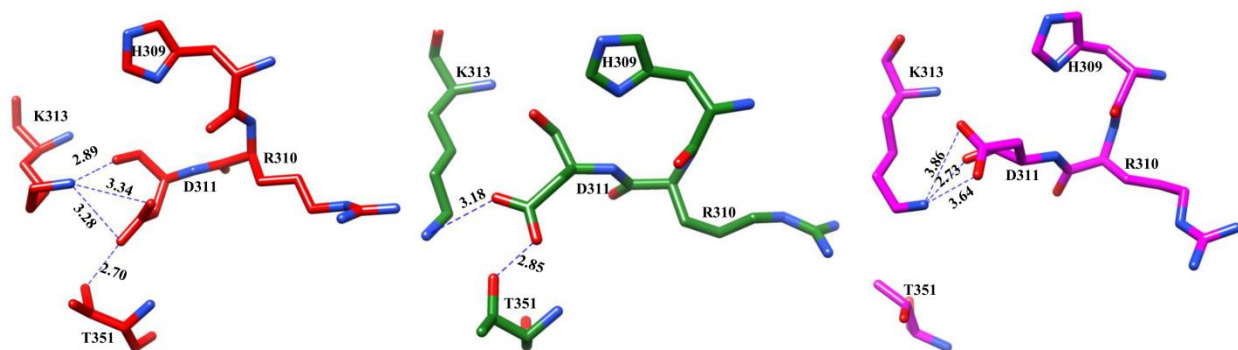


Figure S5: Structural representation of HRD motif. Color codes are given in the Figure 2 legend

Movie. S1-S3: Animation movie of first principal motion of apo unphosphorylated IRAK4 KD (uIRAK4), apo phosphorylated IRAK4 KD (pIRAK4) and ATP bound phosphorylated IRAK4 (pIRAK4-ATP) respectively. All the movies were generated using chimera with 100 snapshots of the whole trajectory. Structural parts were shown in various color and color codes are given according to the Figure.1. Average structure (slate gray color) is superimposed on to the frames to show the collective motions projected along eigenvector 1.

Movie. S4-S6: Animation movie of second principal motion of apo unphosphorylated IRAK4 KD (uIRAK4), apo phosphorylated IRAK4 KD (pIRAK4) and ATP bound phosphorylated IRAK4 (pIRAK4-ATP) respectively. All the movies were generated using chimera with 100 snapshots of the whole trajectory. Color codes are given according to the Figure.1. Average structure (slate gray color) is superimposed on to the frames to show the collective motions projected along eigenvector 2.