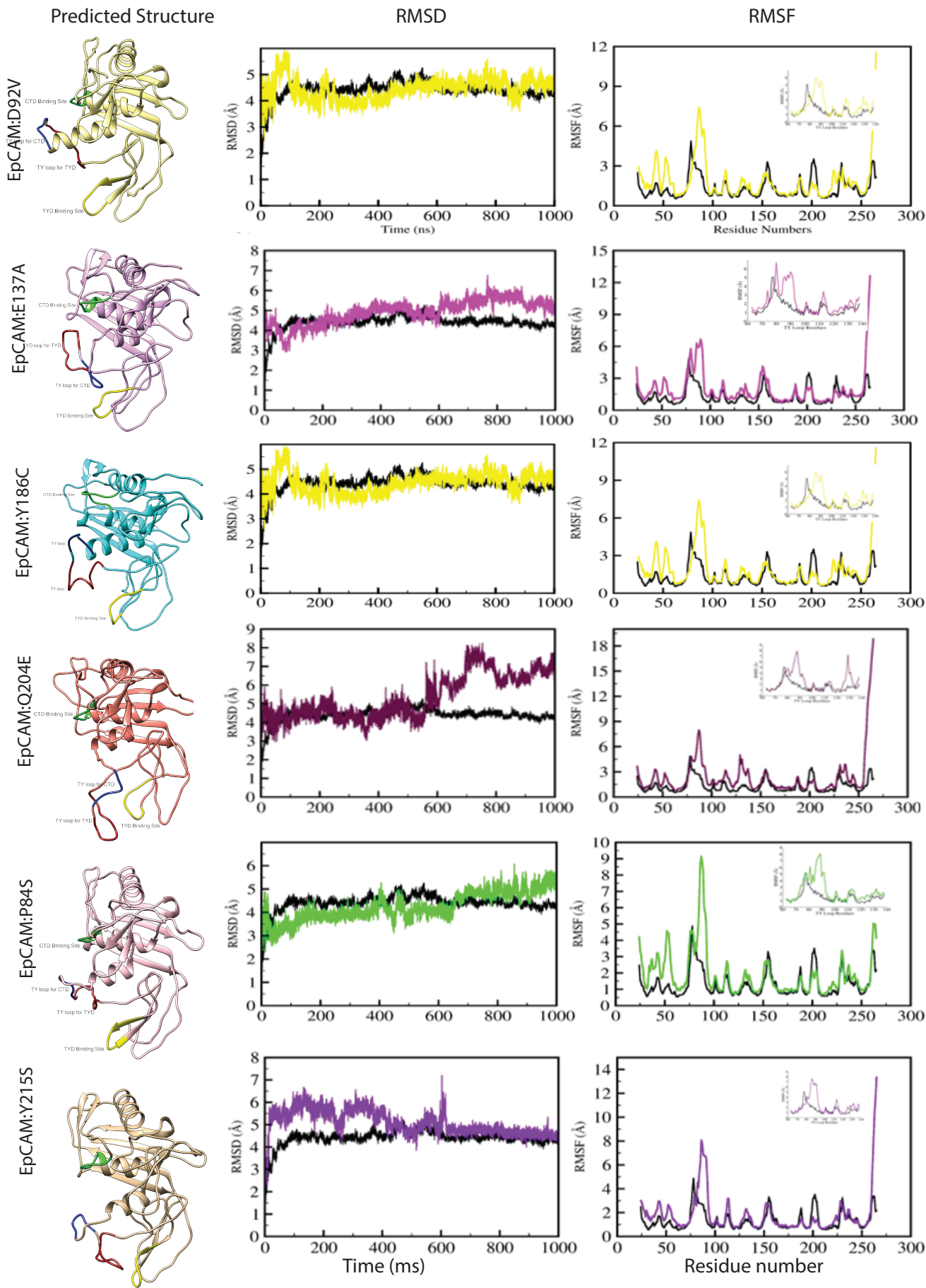
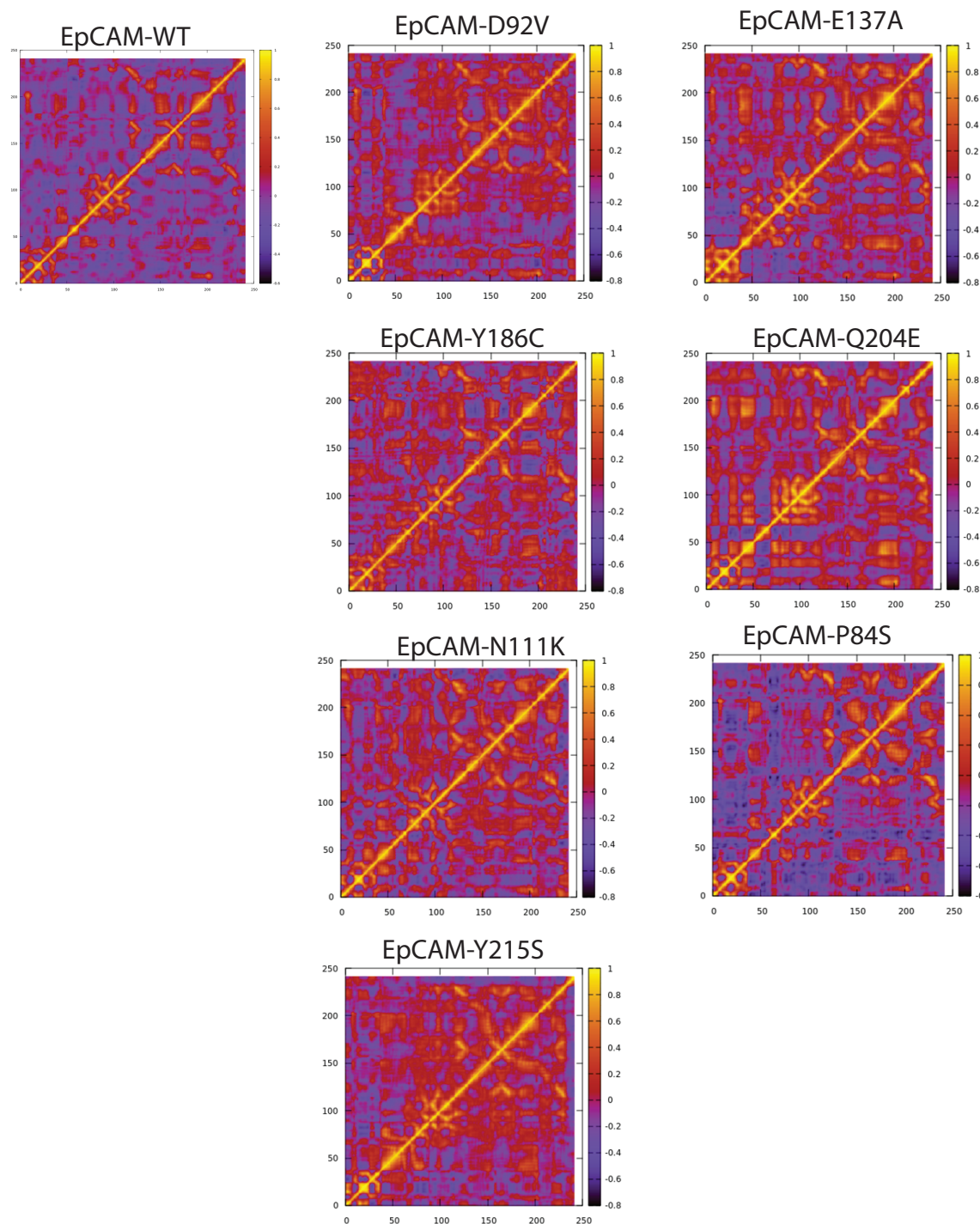


Supplementary Figure 4 A.



Supplementary Figure 4B.



Supplementary Figure 4. (A) Structural analysis graphs for the backbone of EpCAM mutants. EpCAM-WT data shown in Figure 4. Cross correlation matrix of C-alpha atoms during 1ms simulation for wild type EpCAM and mutants, D92V, E137A, Y186C, Q204E, N111K, P84S and Y215S. The range of motion is indicated by various colors in the panel. The strongest negative correlation (anti-correlation) given in value minus (blue) whereas the strongest positive correlation is given in value plus (yellow) and red indicates no apparent correlated motion between the two residues. **(B)** Dynamic cross correlation matrices map of modeled wild type EpCAM and mutant systems. Structural changes during MD simulation for D92V, E137A, Y186C, Q204E, P84S, and Y215S mutants, shown through RMSD and RMSF analyses. The results demonstrate significant conformational changes in EpCAM-WT and its mutants, emphasizing the structural impact of cancer-associated mutations.