Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Conformational Modifications Induced by Internal Tandem Duplications on the FLT3 Kinase and Juxtamembrane Domains

Supporting Information

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Supporting Information Available

The Supporting Information contain a superposition of the 5 starting models of the wt FLT3 (1), the potential energy, RMSD, SASA, and radius of gyration calculated from the equilibration of all systems (2-8), the PCA of the entire protein (9), contact map between the ITDs and the αC-helix (10), the contact map difference between the FLT3-ITD and the native protein of the distances between the JM-B motif and the activation loop and the catalytic loop (11), the contact map difference between the FLT3-ITD and the native protein of the distances between the JM-S and two portions (residues 805-810 and 862-867) of the C-lobe (12).

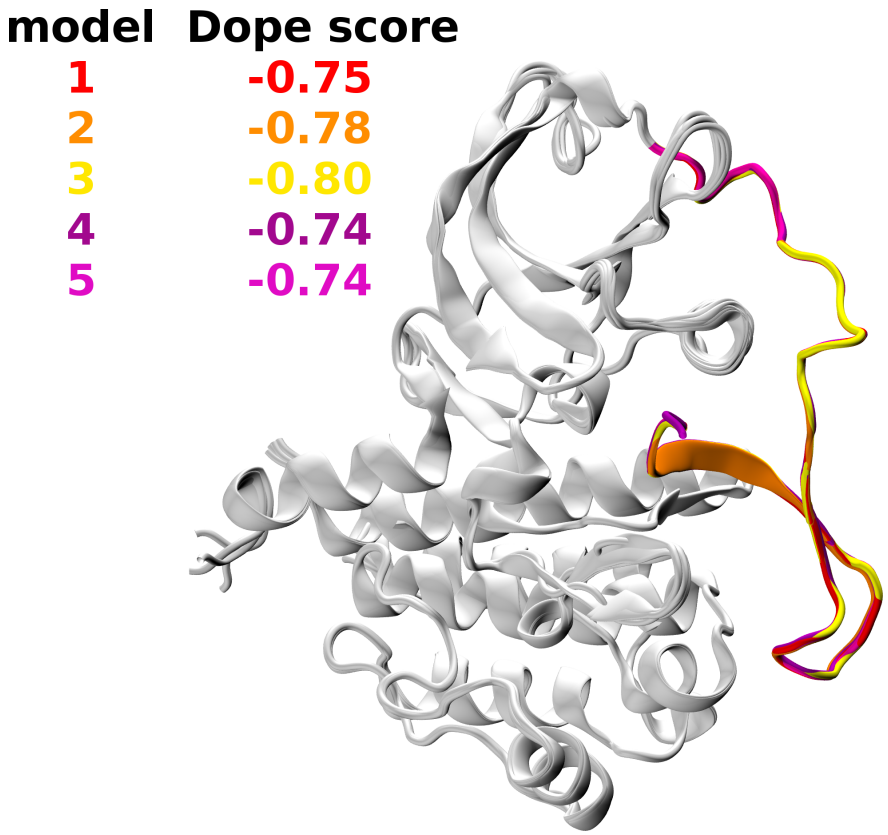

Figure 1: Superposition of the 5 models generated from the PDB entries 4XUF, 4RT7, and 4RJB. The DOPE score obtained for the different models are also reported.

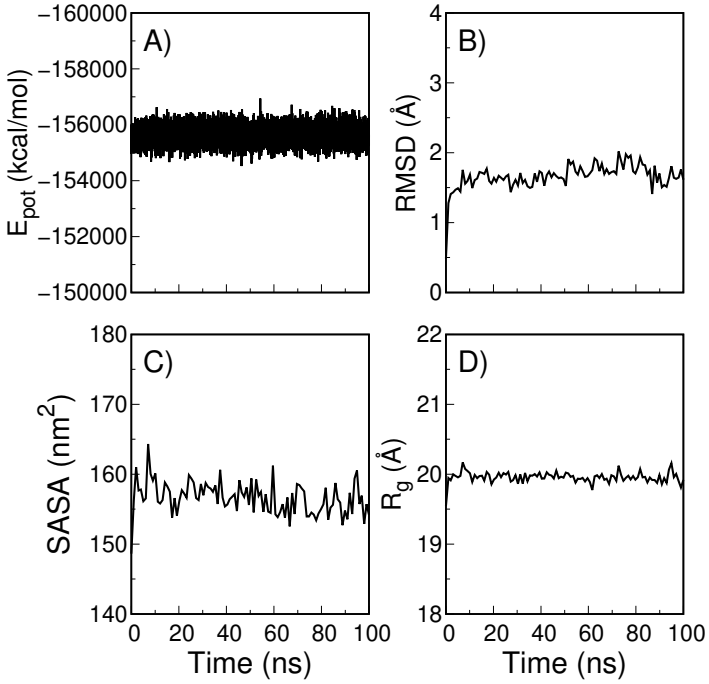

Figure 2: Parameters variation calculated from the equilibration simulations of the wt FLT3. A) Potential energy, B) Cα RMSD, C) SASA, D) Radius of gyration. All properties have stabilised well before the 100 ns time point.

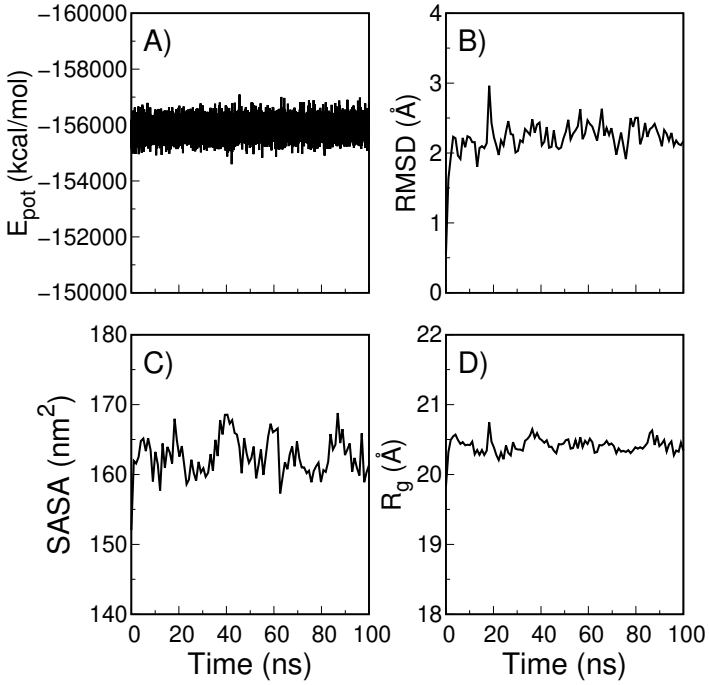

Figure 3: Parameters variation calculated from the equilibration simulations of the LDN-ITD. A) Potential energy, B) Cα RMSD, C) SASA, D) Radius of gyration. All properties have stabilised well before the 100 ns time point.

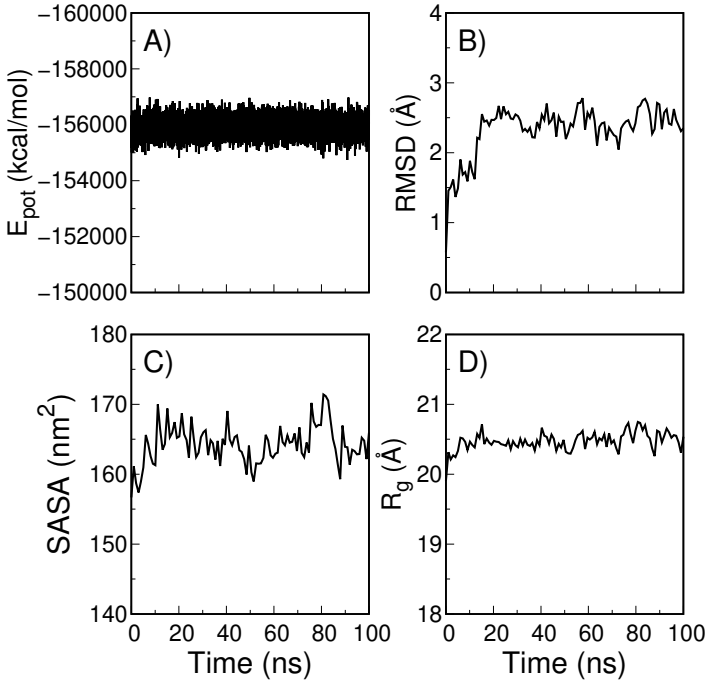

Figure 4: Parameters variation calculated from the equilibration simulations of the DQN-ITD. A) Potential energy, B) Cα RMSD, C) SASA, D) Radius of gyration. All properties have stabilised well before the 100 ns time point.

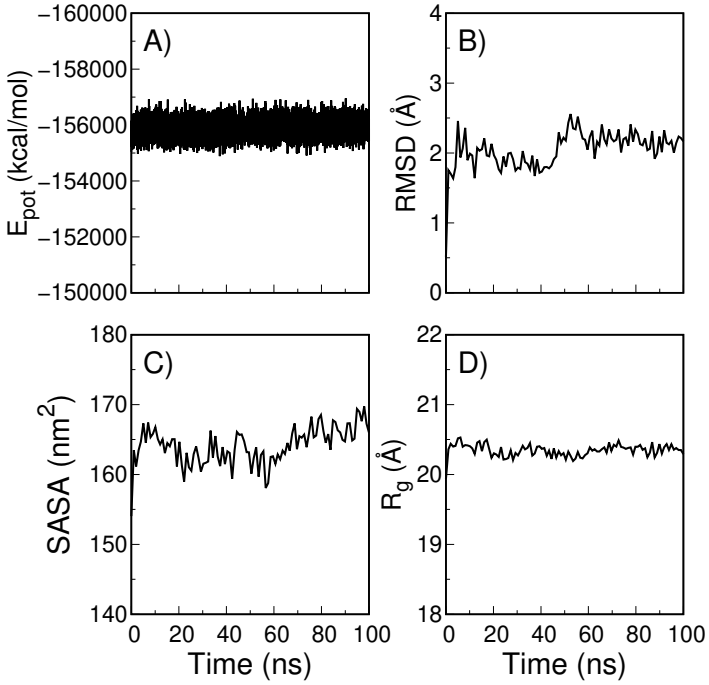

Figure 5: Parameters variation calculated from the equilibration simulations of the DYV-ITD. A) Potential energy, B) Cα RMSD, C) SASA, D) Radius of gyration. All properties have stabilised well before the 100 ns time point.

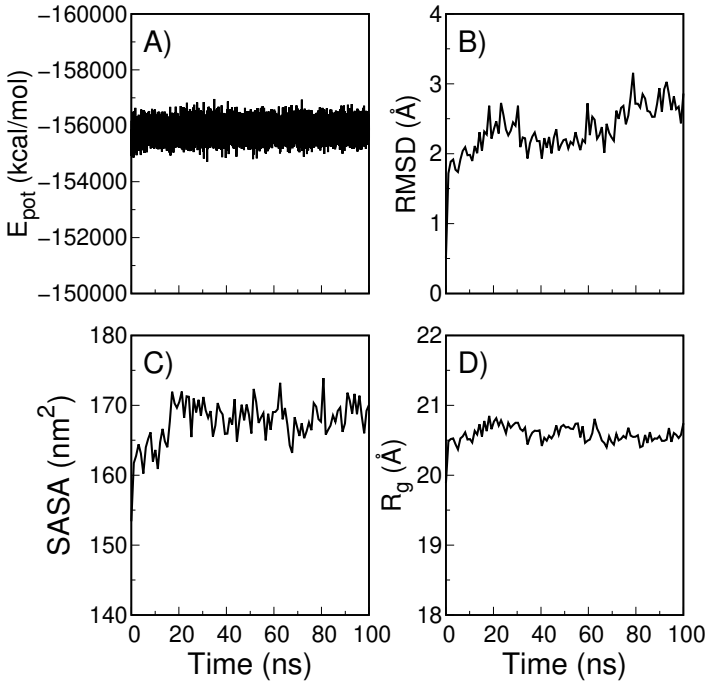

Figure 6: Parameters variation calculated from the equilibration simulations of the EYE-ITD. A) Potential energy, B) Cα RMSD, C) SASA, D) Radius of gyration. All properties have stabilised well before the 100 ns time point.

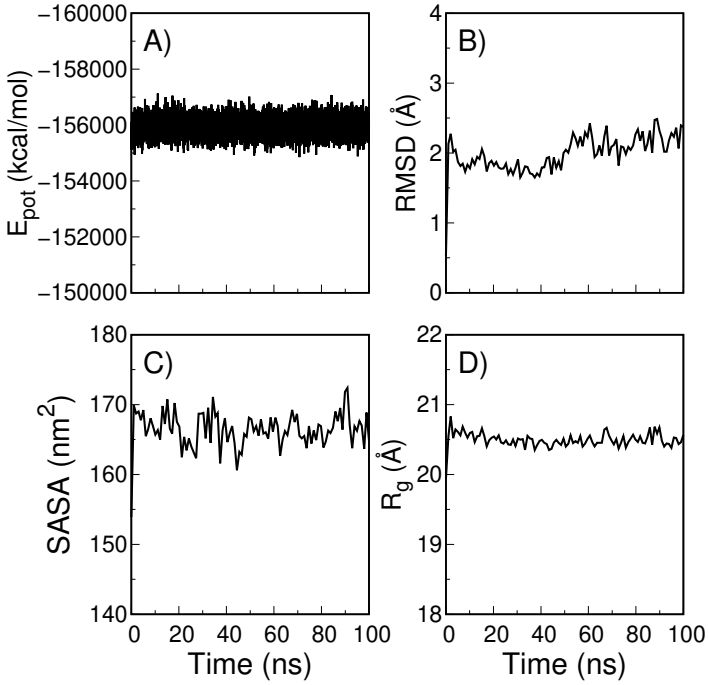

Figure 7: Parameters variation calculated from the equilibration simulations of the FRE-ITD. A) Potential energy, B) Cα RMSD, C) SASA, D) Radius of gyration. All properties have stabilised well before the 100 ns time point.

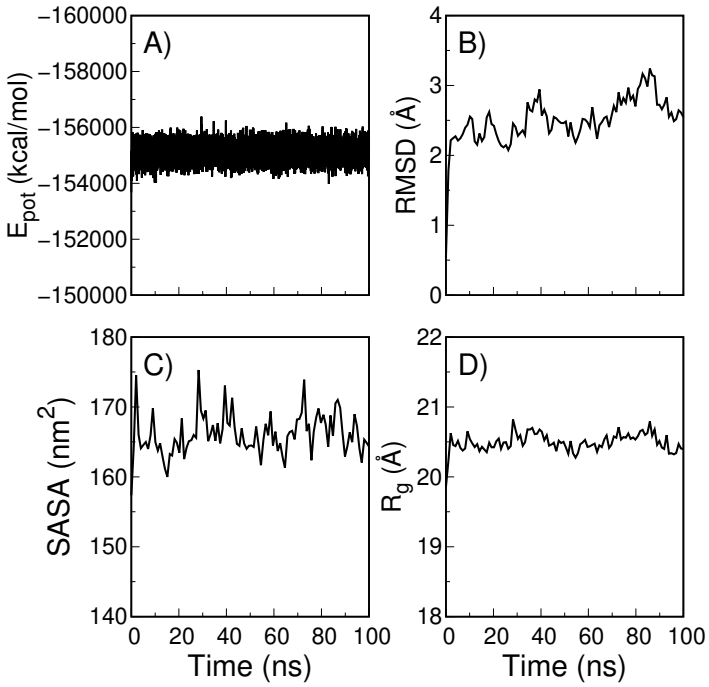

Figure 8: Parameters variation calculated from the equilibration simulations of the FEI-ITD. A) Potential energy, B) Cα RMSD, C) SASA, D) Radius of gyration. All properties have stabilised well before the 100 ns time point.

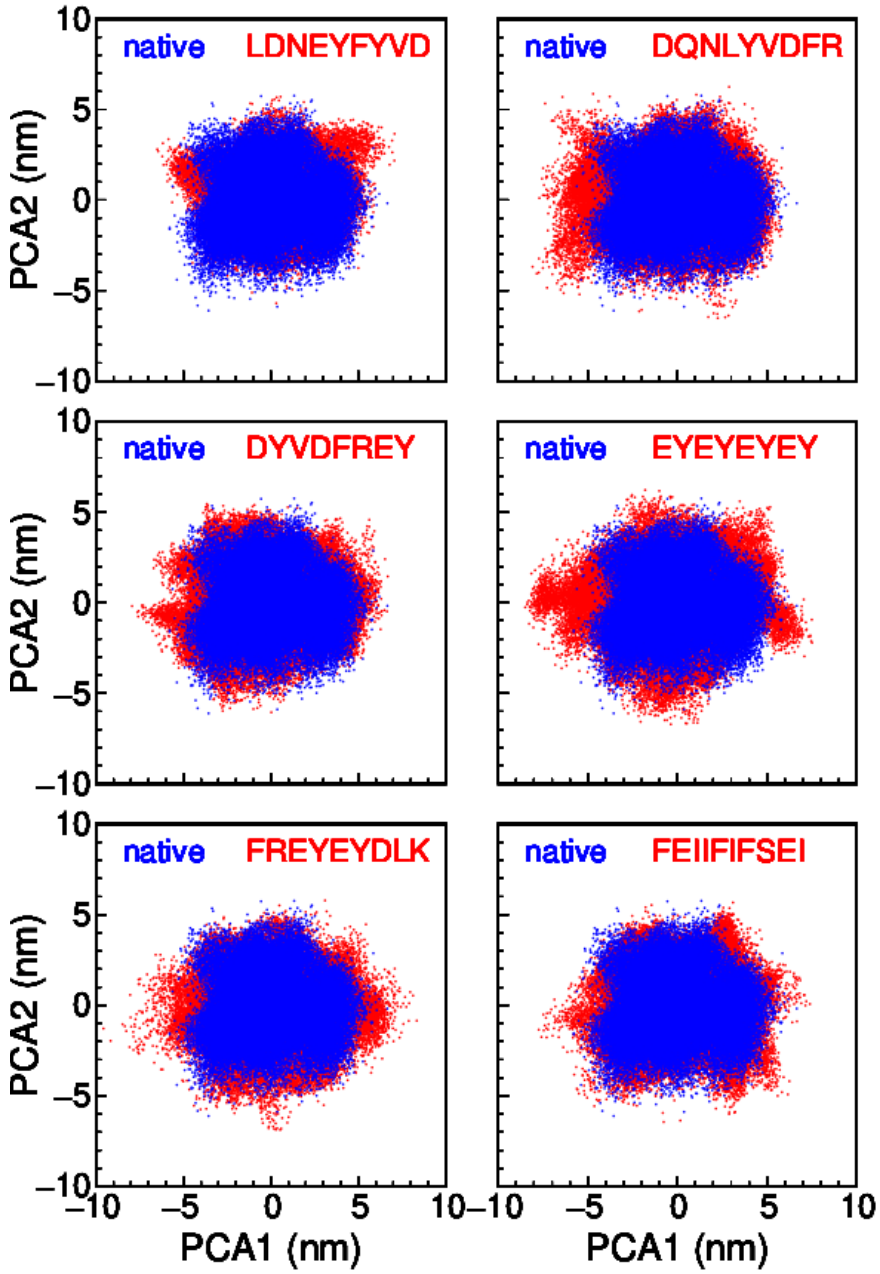

Figure 9: Projection of all protein heavy atoms (non hydrogen atoms) in phase space along the first two principal eigenvectors. The native protein is shown in blue while the FLT3-ITD are shown in red.

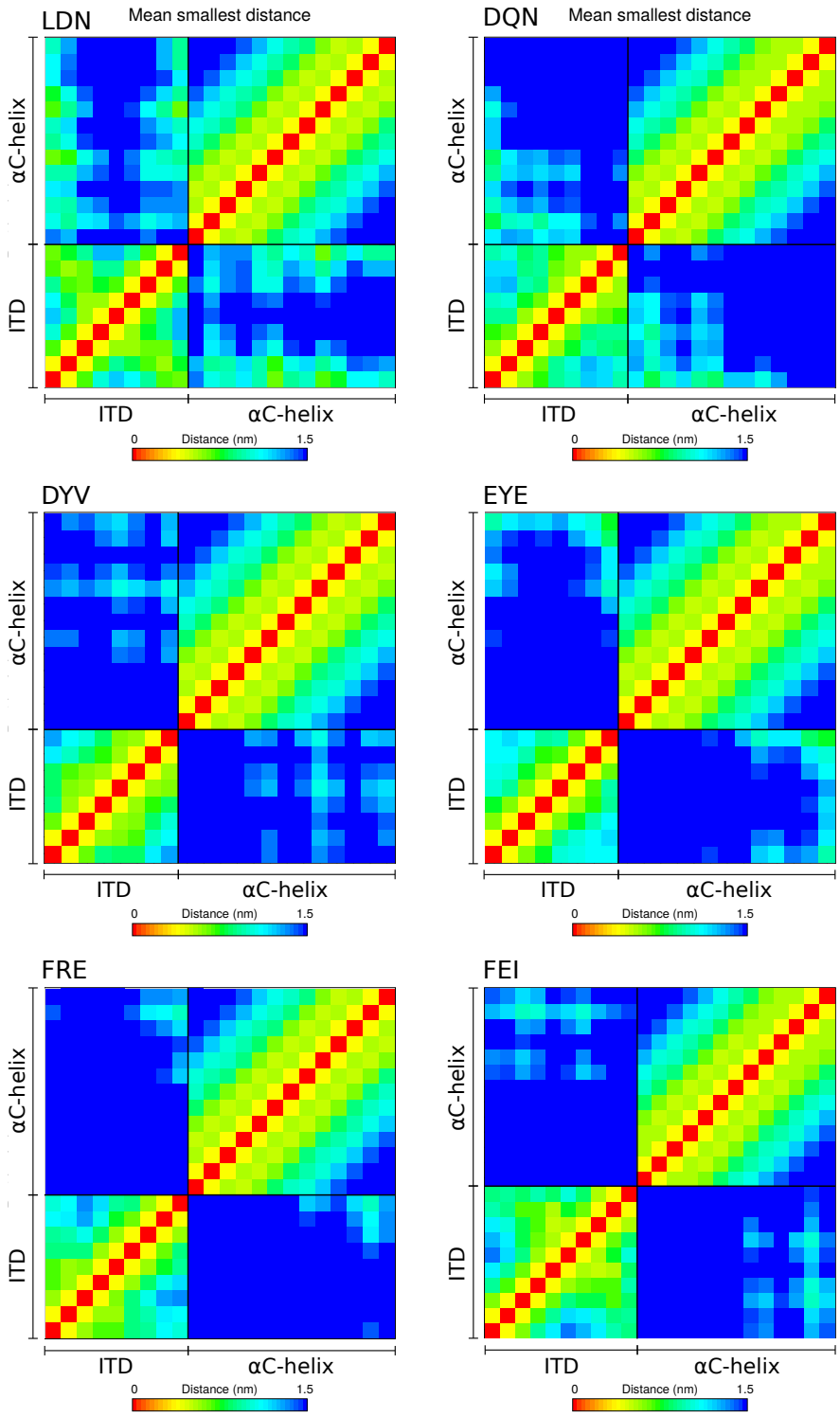

Figure 10: Contacts map calculated between the ITD sequences and the αC-helix. Distances are calculated using the Cα atoms.

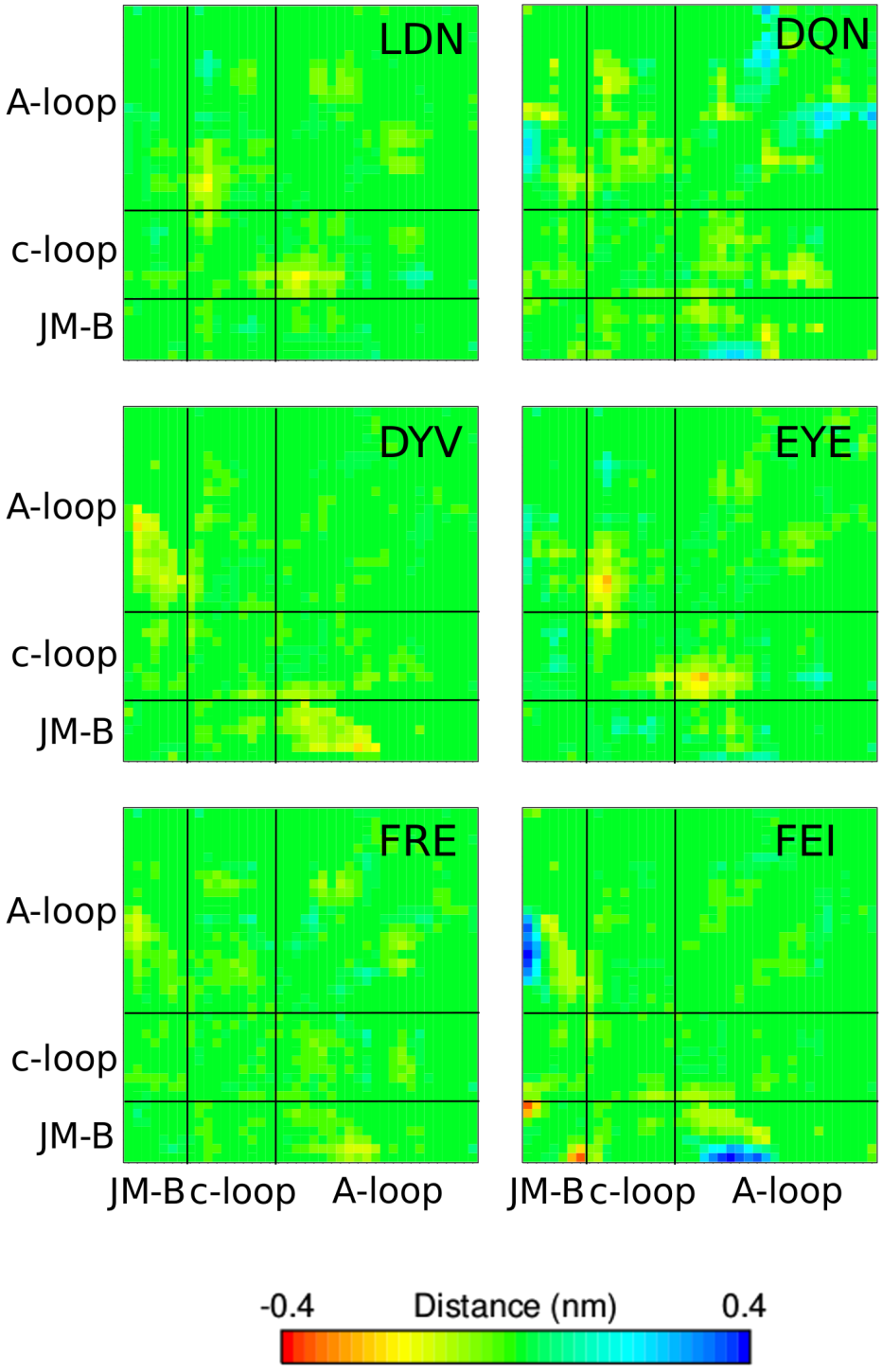

Figure 11: Contacts map difference calculated between the FLT3-ITD and the native protein. Distances are calculated using the Cα atoms.

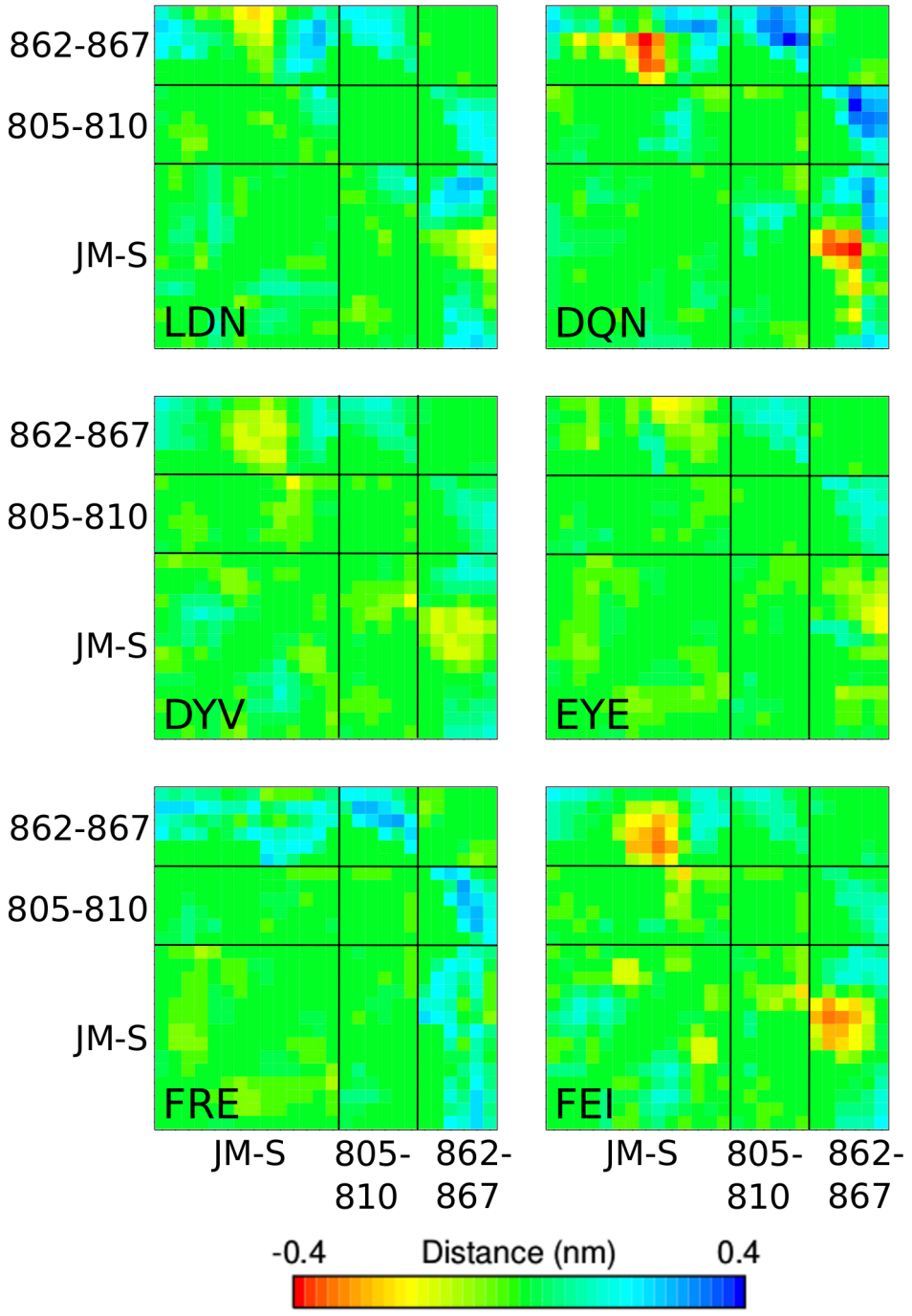

Figure 12: Contacts map difference calculated between the FLT3-ITD and the native protein. Distances are calculated using the Cα atoms.

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