Supporting Information

Insights into the Dynamics and Dissociation Mechanism of a Protein Redox Complex Using Molecular Dynamics

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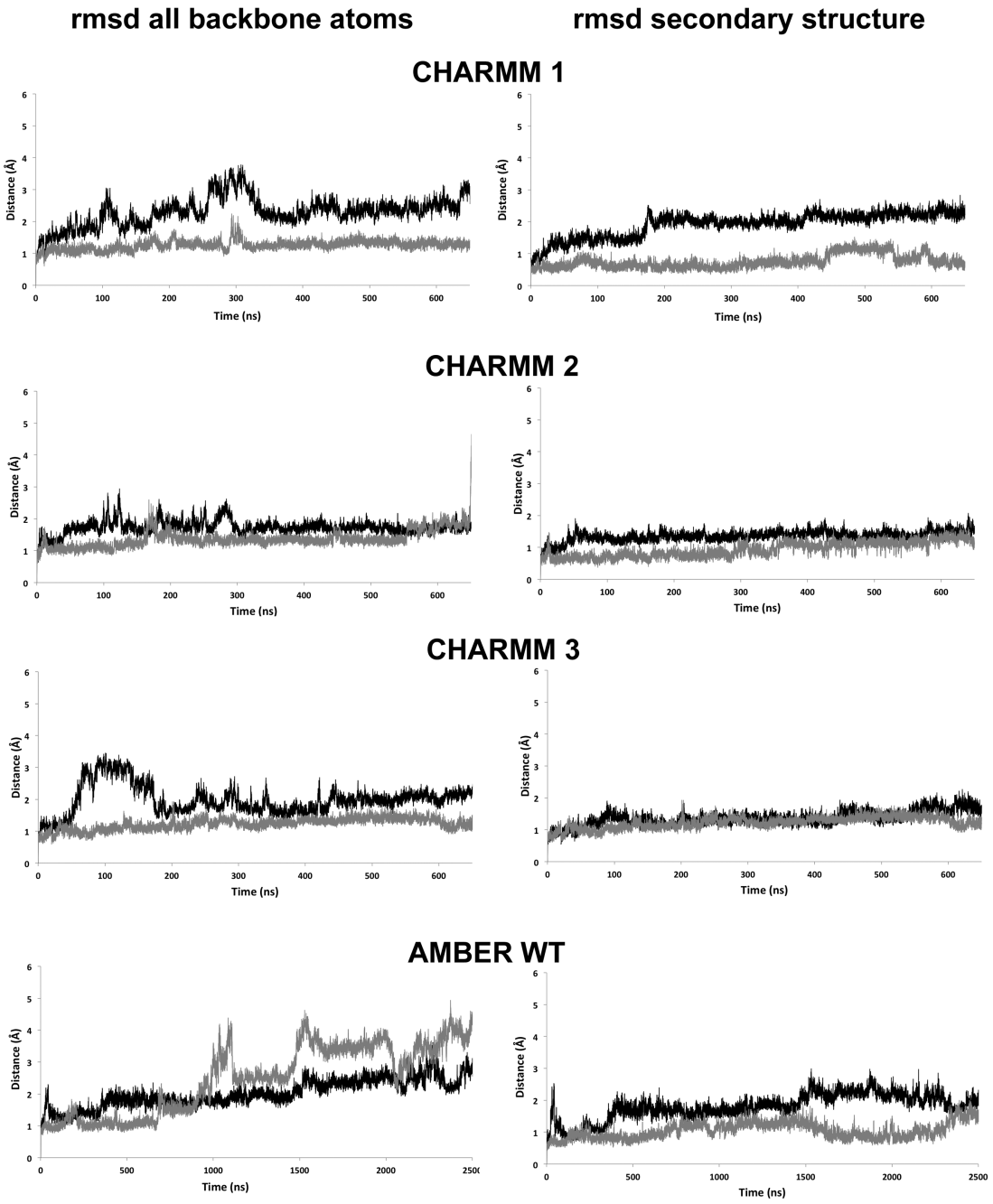

Figure S1. Root mean square deviation of all backbone atoms (CA, C, N) relative to the first frame for all 4 wild type MD trajectories. Panels on the left are for the entire protein while on the right only residues in regular secondary structure (helices and sheets) are included. Black lines correspond to LmCytc while gray lines correspond to LmP.

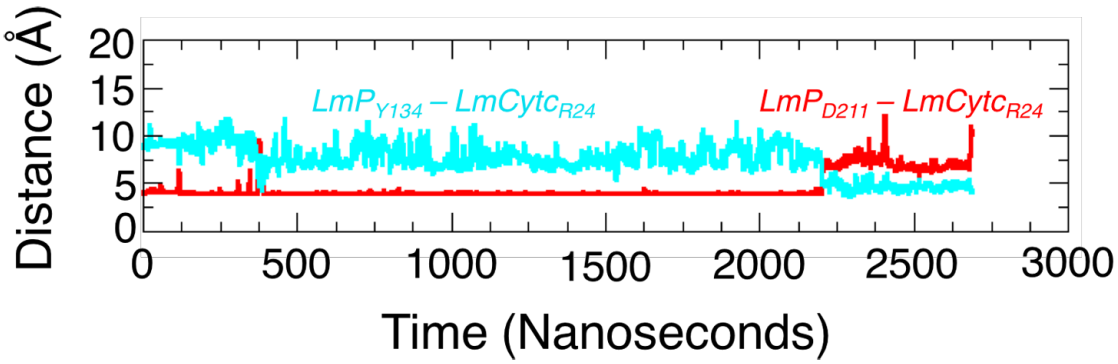

Figure S2. The distances between LmP Y134 and LmCytc R24 (cyan) and the electron transfer (ET) active ion-pair of LmP D211 and LmCytc R24 (red) are displayed for the multi-microsecond Amber simulation. Breakage of the ET ion-pair is followed by formation of the intermediate LmP Y134-LmCytc R24 interaction, identical to that observed in CHARMM replicate 1 and Amber mutant simulations.

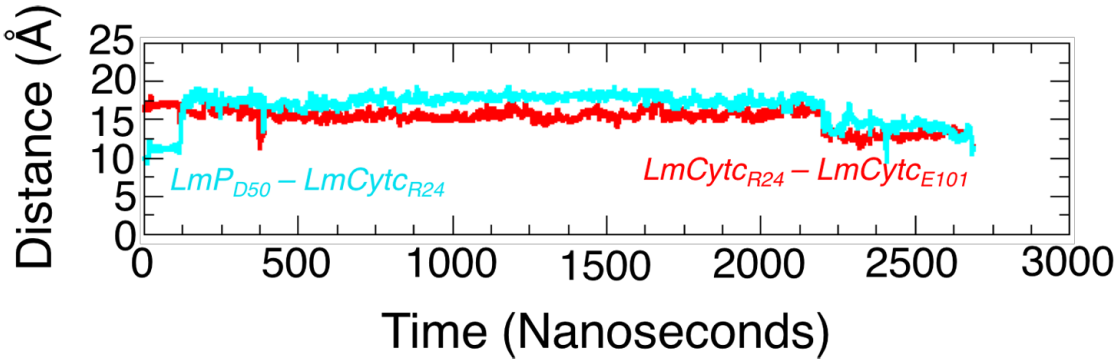

Figure S3. The distances between LmP D50 and LmCytc R24 (cyan) and LmCytcR24 and LmCytcE101 (red) for the multi-microsecond Amber simulation replicate.

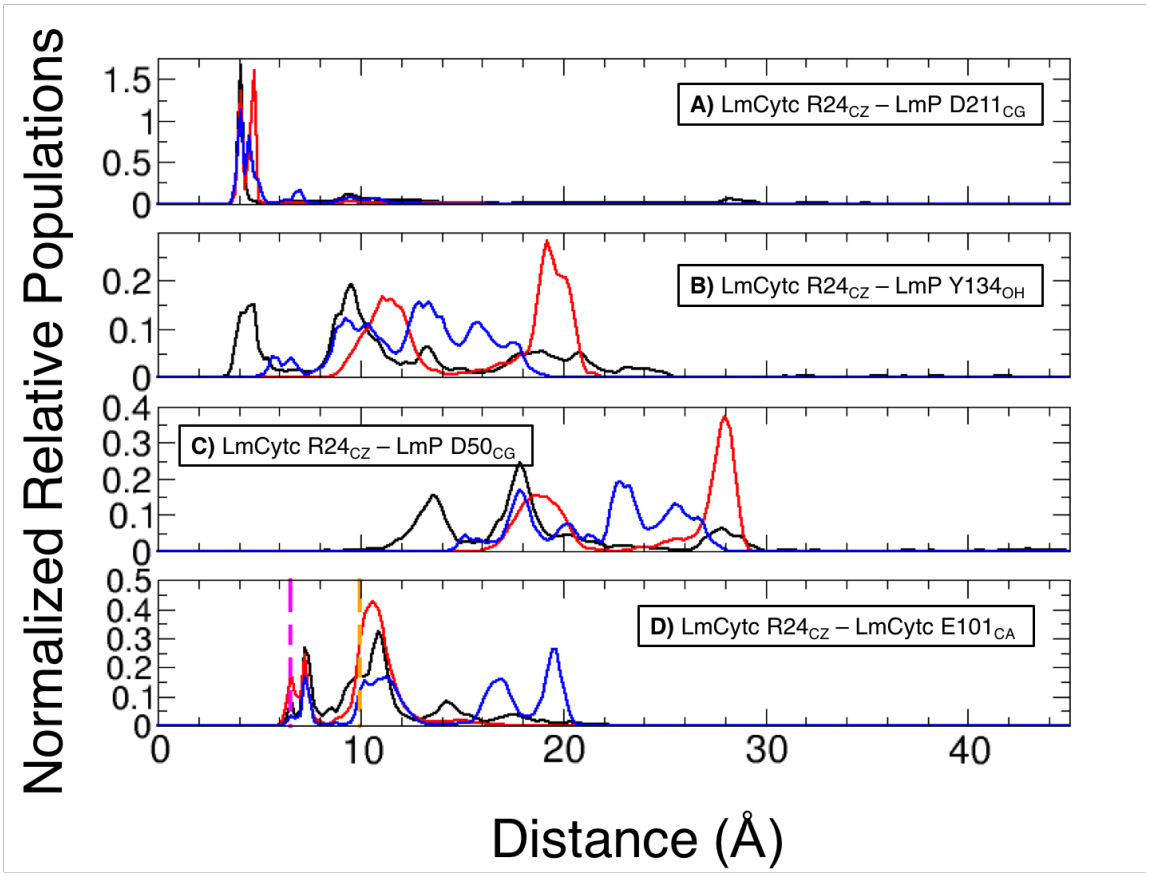

Figure S4. Interpolations of the normalized distance distributions between interacting residues are highlighted in A through D where CHARMM replicate 1 is shown in black, CHARMM replicate 2 in red and CHARMM replicate 3 in blue. The highlighted interactions are as follows; A) The electron transfer active interprotein ion-pair of LmCytc R24(CZ) and LmP D211(CG), B) the transient interaction between LmCytc R24(NE) and LmP Y134(OH), C) the distances between LmCytc R24(CZ) and D50 of LmP helix A and, D) the intramolecular ion pair between LmCytc R24(CZ) and LmCytc E101(CA). In D, the experimentally observed distance for the intramolecular ion pair in the individual structure (PDBID 4DY9) is shown in pink and the equivalent distance in the co-crystal structure (PDBID 4GED) in orange. Evolutions of these distaces are shown in Figure 4.

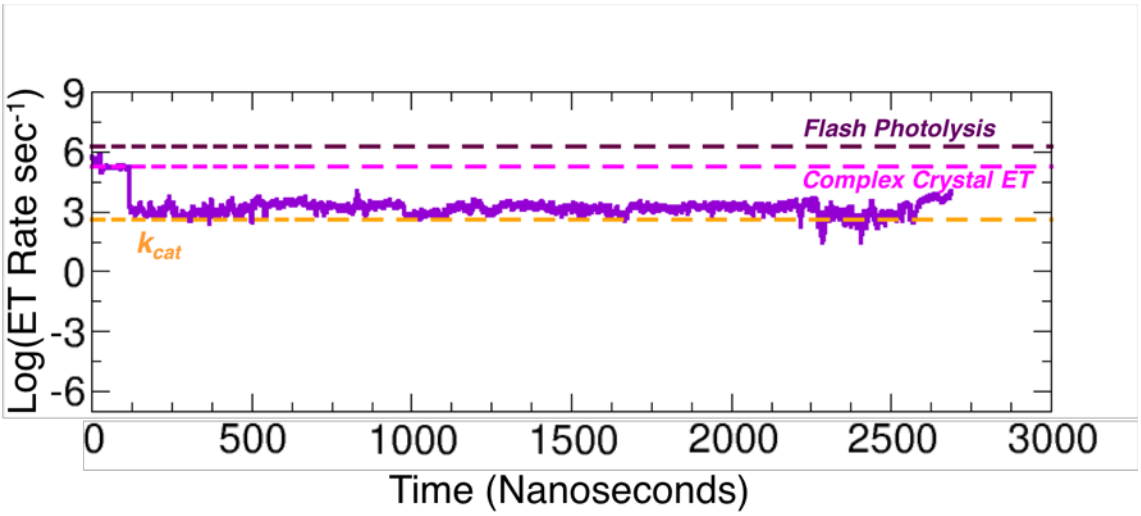

Figure S5. The calculated electron transfer (ET) rate from the multi-microsecond Amber simulation replicate is displayed in purple, similar to Figure 7. For reference, the known flash photolysis, complex crystal structure ET rate and kcat are displayed in dark violet, pink and orange respectively.