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PAPER

Sequential Myosin Phosphorylation Activates Tarantula Thick Filament via a Disorder-Order Transition

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SUPPORTING MATERIAL

SUPPLEMENTARY TABLES

Table S1 Summary of the characteristics and conditions of the systems studied

Peptide	Number of atoms	Number of water molecules	Temperature (°K)	Ensemble used	Simulation length (µs)
FH NTE	77,360	25.386	310	NPT	1.2
BH NTE	72,610	23,806	310	NPT	1.2
BH NTE pSer45	55,512	18,117	310	NPT	1.15
FH NTE pSer35	62,175	20,334	310	NPT	2.18
FH NTE pSer35/pSer45	55,732	18,190	310	NPT	2.15

SUPPLEMENTARY FIGURE LEGENDS

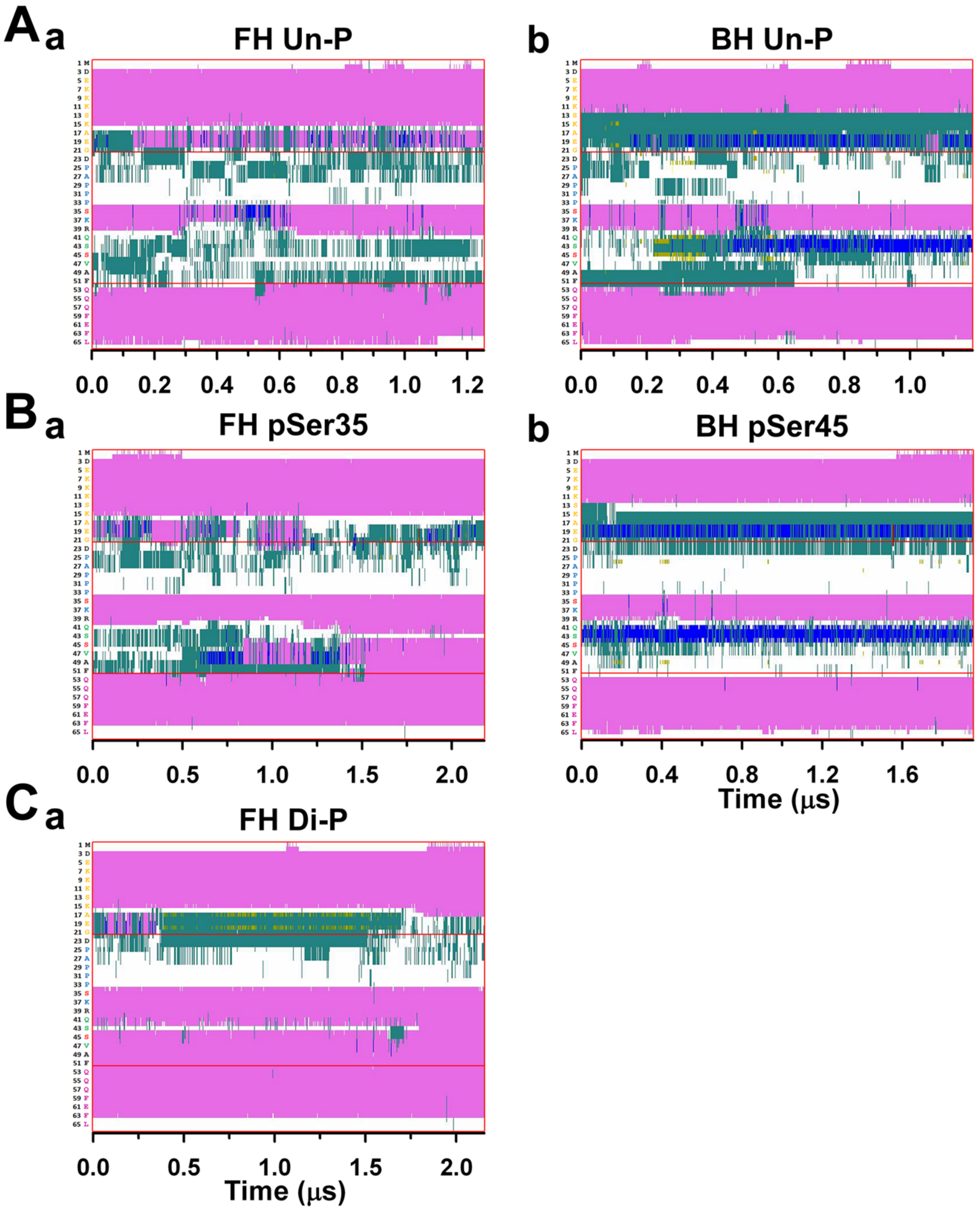

Fig. S1 Evolution of the secondary structure of the complete NTE plus helix A peptides of the free (a) and blocked (b) heads in different phosphorylation conditions: unphosphorylated (A), monophosphorylated (B) and diphosphorylated (C). Secondary structure colour key: 3-10 helix (blue), α-helix (pink), turn (cyan), coil (white), β-sheet (yellow).

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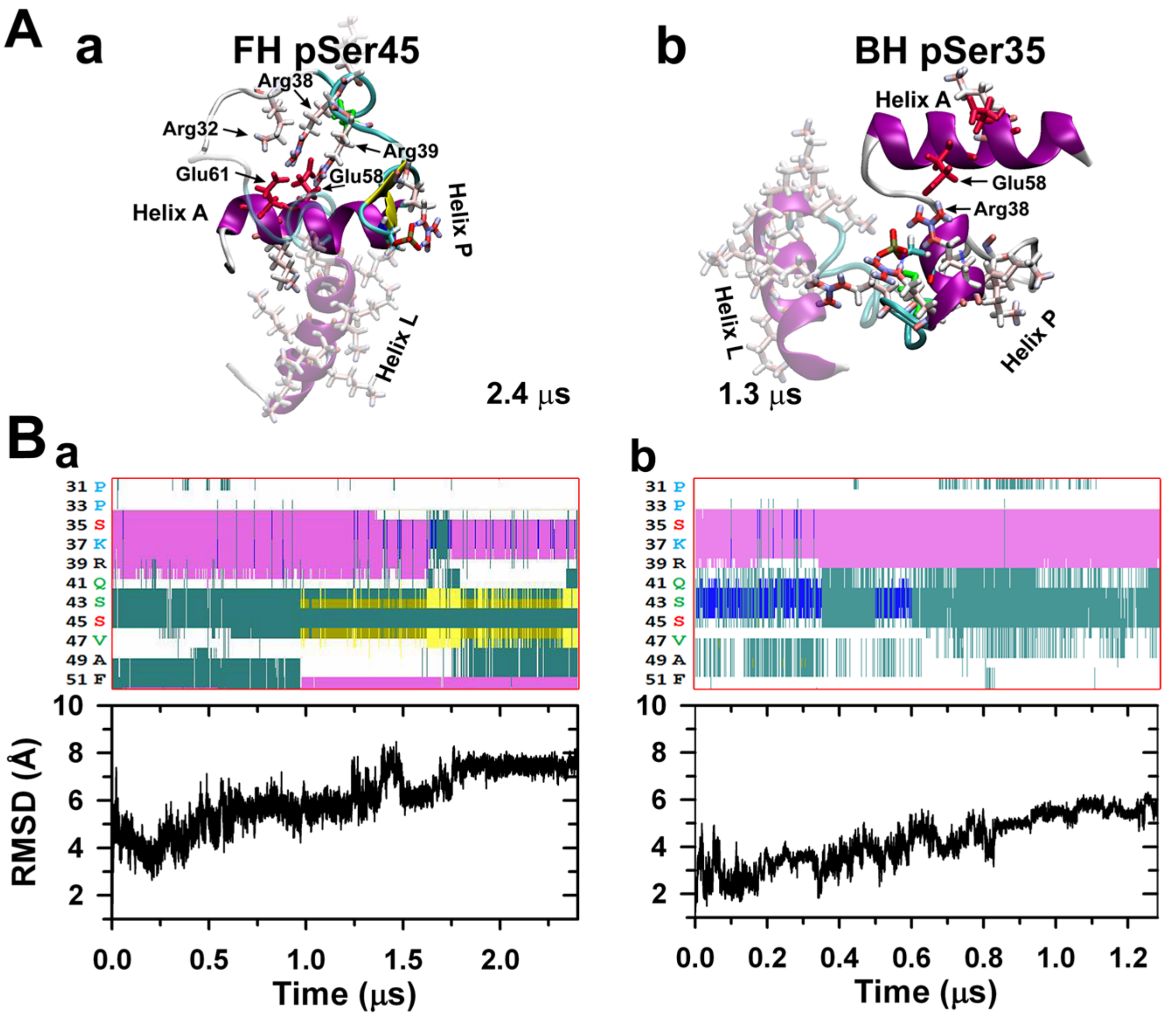
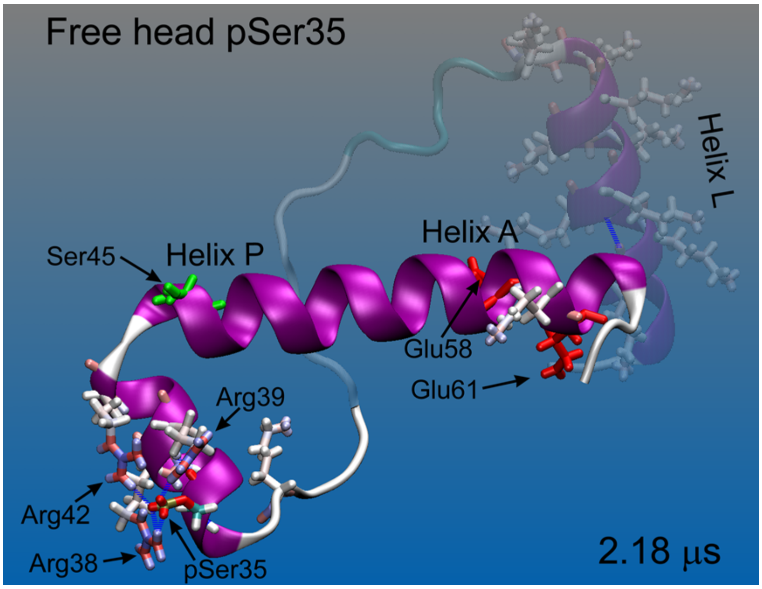
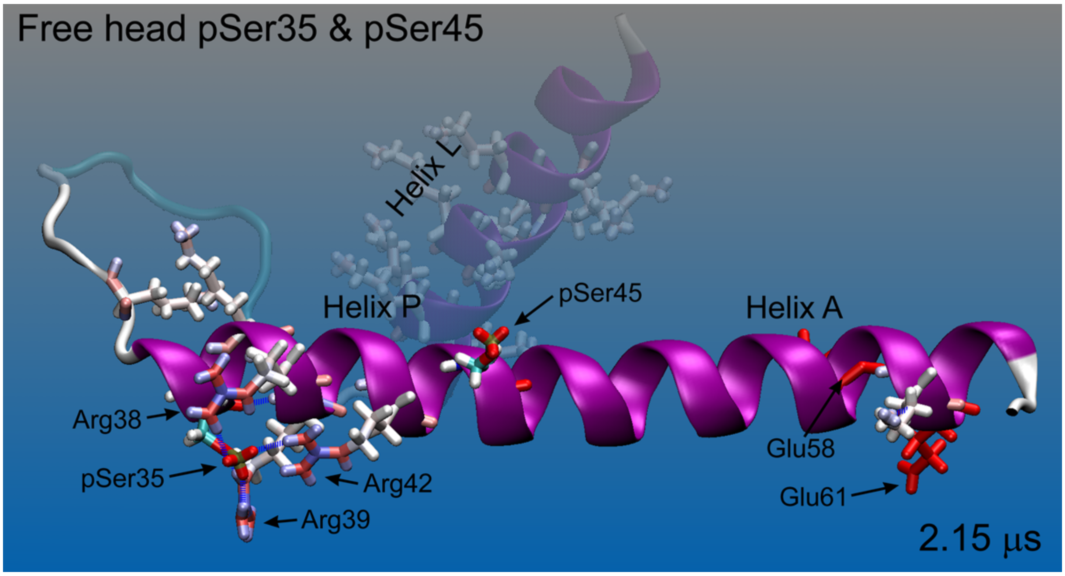


Fig. S2. (A) The stabilized FH and BH un-P compact peptides (Fig. 2Ba,b) were phosphorylated at Ser45 and Ser35 respectively (A), stabilizing after 2.4 (a) and 1.3 μs (b) to compact conformations. (B) Evolution of the secondary structure of both NTE helices P_{PKC} (Ser32-Arg38) and P_{MLCK} (Ala40-Phe48) regions along each peptide trajectories. Secondary structure colour key: 3-10 helix (blue), α-helix (pink), turn (cyan), coil (white), β-sheet (yellow).

SUPPLEMENTARY MOVIES LEGENDS



Movie S1. 2.18 µs evolution of the trajectories of the secondary structure of the un-P 3DTP NTE free head peptide plus helix A (static at right) after Ser35 monophosphorylation.



Movie S2 2.15 µs evolution of the trajectories of the secondary structure of the pSer35 monophosphorylated 3DTP NTE free head peptide plus helix A (static at right) after diphosphorylation at Ser45.