Supplementary Information for

Understanding the role of the CB1 toggle switch in interaction networks using molecular dynamics simulation

Sangho Ji[1, †] , Wonjin Yang[1, †], Wookyung Yu[1, 2, *]

1 Department of Brain and Cognitive Sciences, DGIST, 333 Techno jungang-daero, Daegu, 42988, Republic of Korea

2 Core Protein Resources Center, DGIST, 42988, 333 Techno jungang-daero, Daegu, Republic of Korea

† These authors contributed equally to this work.

* Author to whom correspondence should be addressed.

Wookyung Yu : wkyu@dgist.ac.kr

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Table S1. Residues of secondary structure in CB1

Secondary Structure	Active state	Inactive state
N-terminal	1-16	1-16
Transmembrane helix 1	17-48	17-48
Intracellular loop 1	49-54	49-54
Transmembrane helix 2	55-80	55-80
Extracellular loop 1	81-87	81-88
Transmembrane helix 3	88-121	89-122
Intracellular loop 2	122-131	123-131
Transmembrane helix 4	132-155	132-155
Extracellular loop 2	156-175	156-174
Transmembrane helix 5	176-202	175-211
Intracellular loop 3	203-239	212-232
Transmembrane helix 6	240-271	233-271
Extracellular loop 3	272-274	272-303
Transmembrane helix 7	275-313	304-313
C-term	314-316	314-316

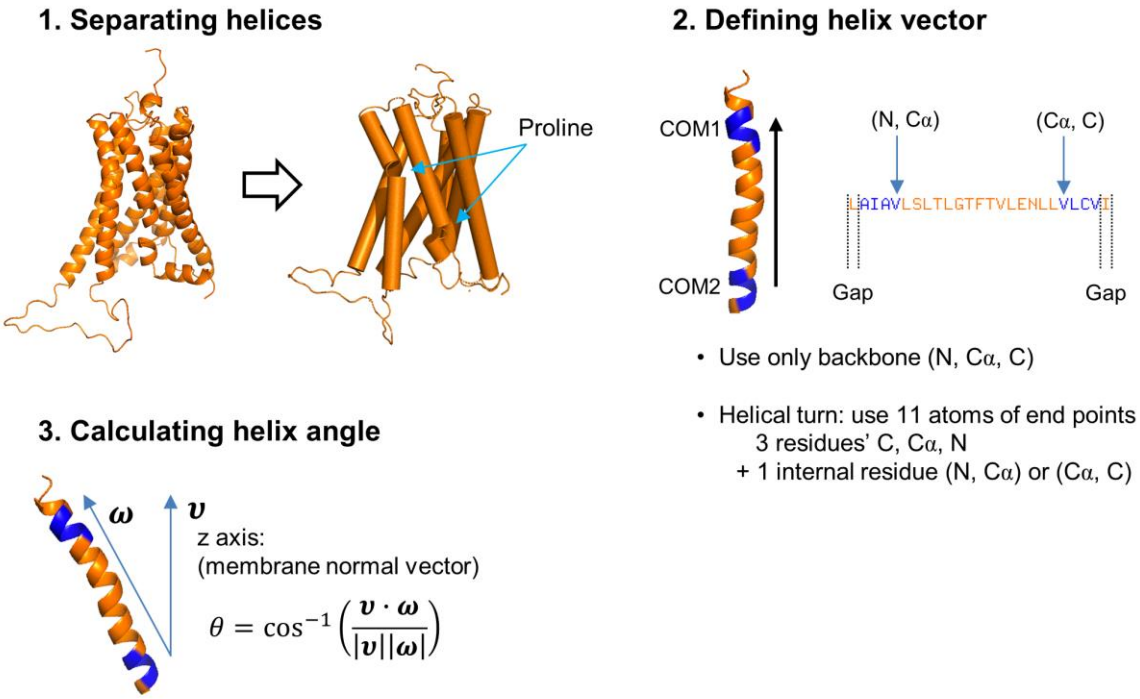

Fig. S1. The process of calculating helix angle. All trajectories are aligned to its X-ray crystal structure.

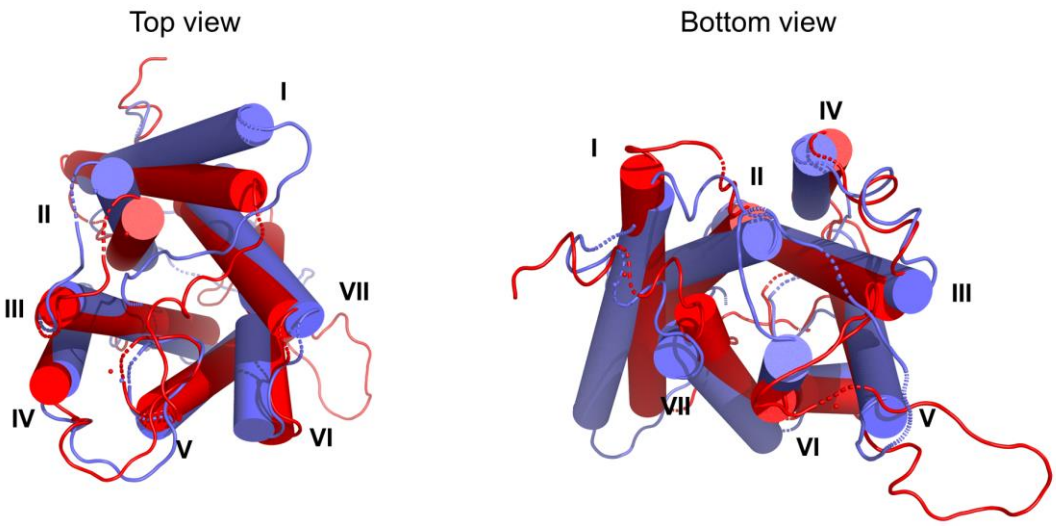

Fig. S2. The comparison of averaged structure between active and inactive state of CB1. The active and inactive states of CB1 are shown in red and blue color, respectively.

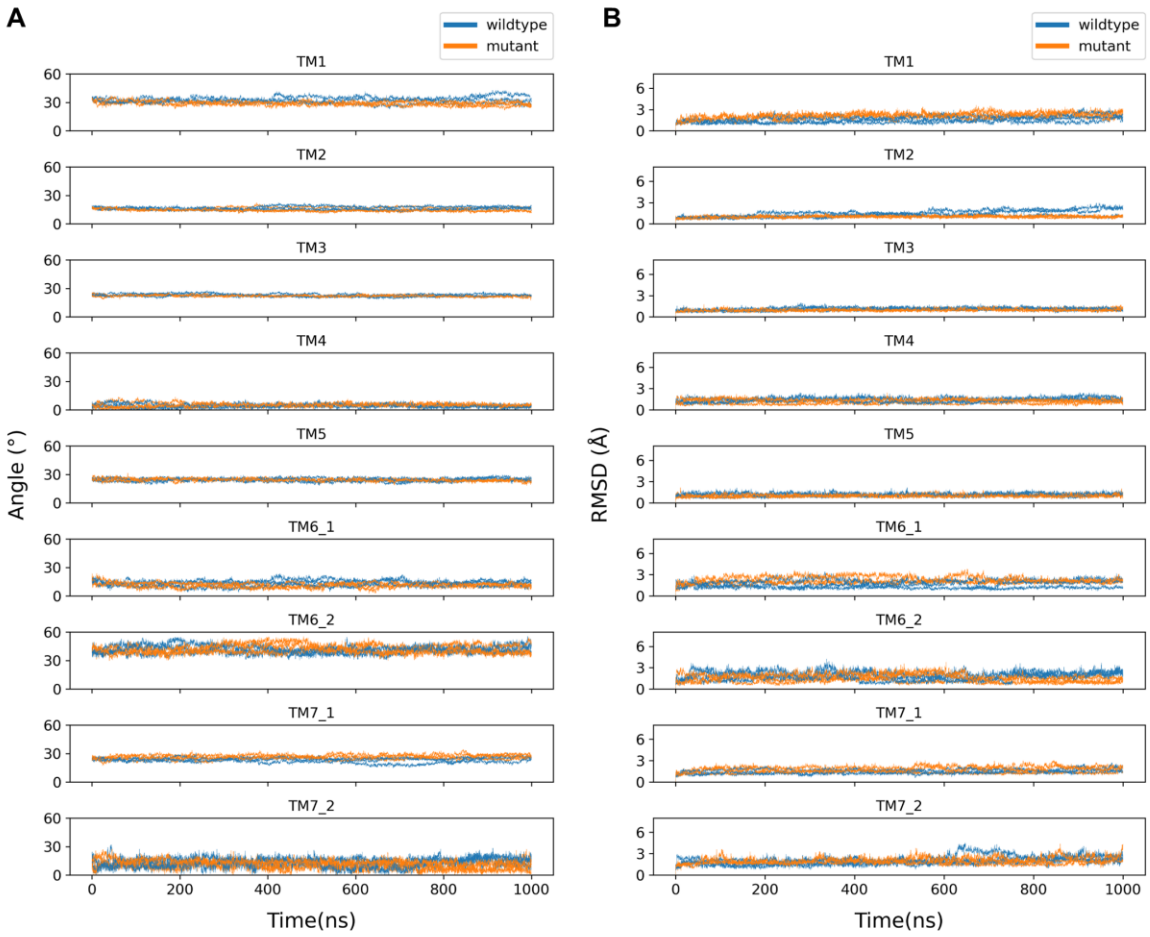

Fig. S3. Time evolution of (A) angle and (B) RMSD for each helix in active state. The wildtype and mutant systems are colored as blue and orange, respectively. The angle and RMSD of three replications are overlayed in the plot.

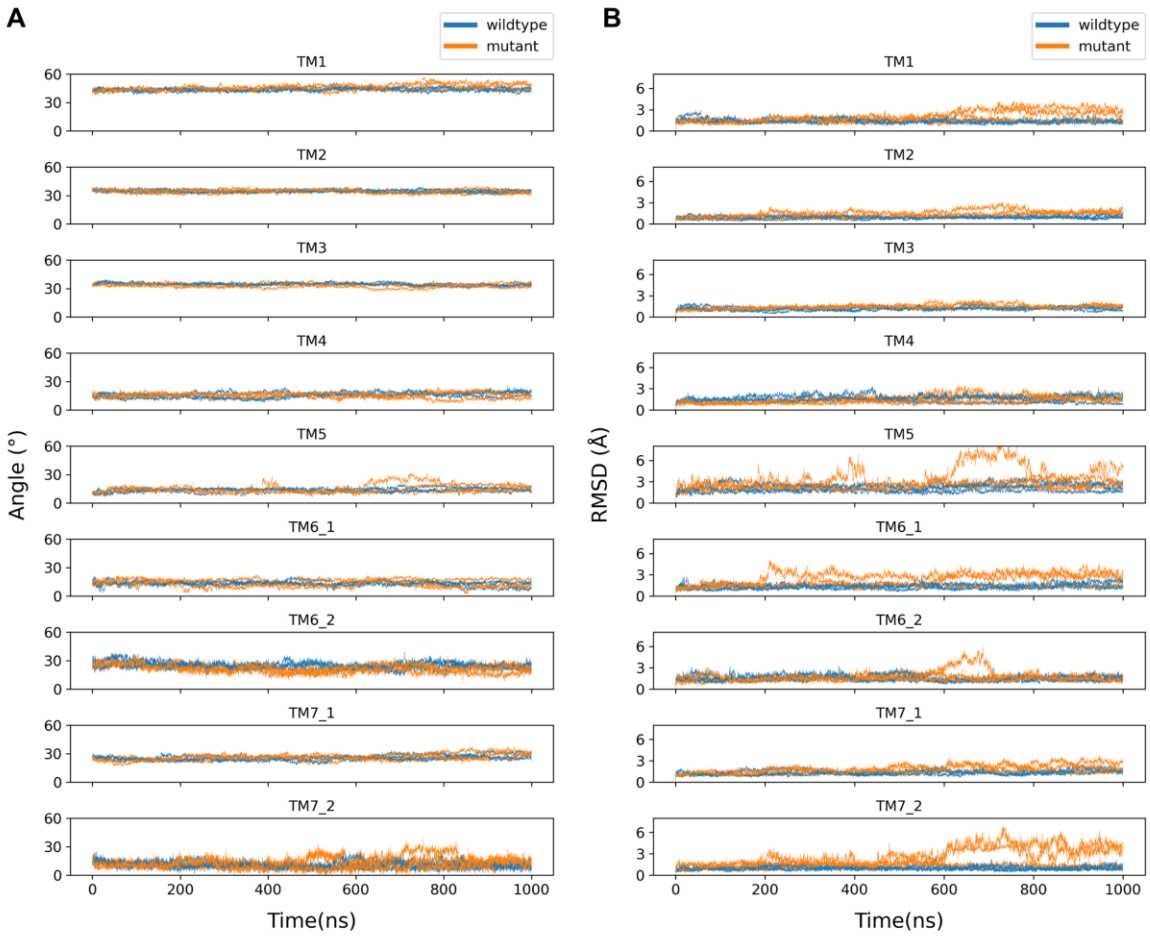

Fig. S4. Time evolution of (A) angle and (B) RMSD for each helix in inactive state. The wildtype and mutant systems are colored as blue and orange, respectively. The angle and RMSD of three replications are overlayed in the plot.

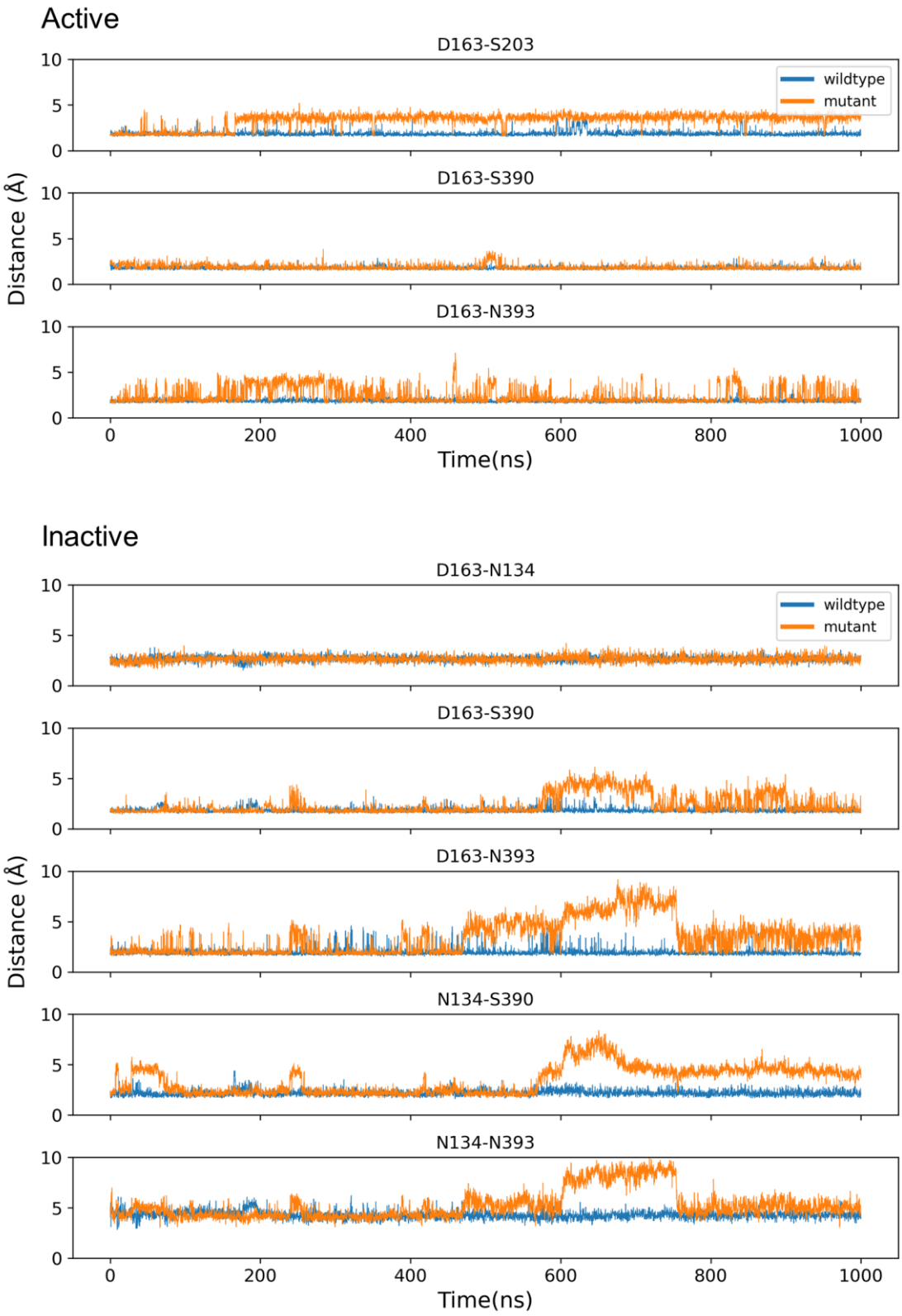

Fig. S5. The hydrogen bond distances in Na+ pocket. The wildtype and mutant CB1 are colored as blue and orange, respectively.

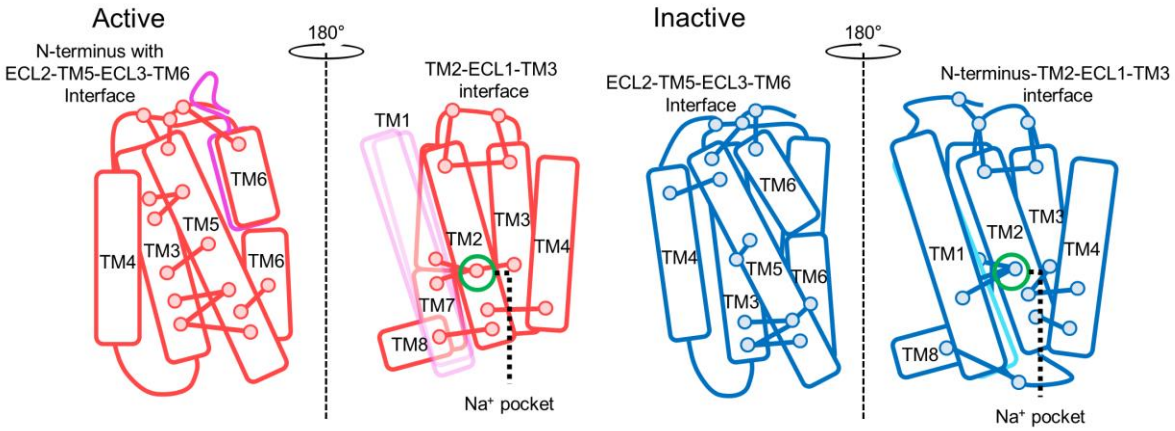

Fig. S6. Schematic inter-helical interaction with relative helical position. The active and inactive of wildtype CB1 structures are colored as red and blue and of mutant CB1 are magenta and cyan, respectively. Pairwise interactions are presented as solid lines, which are decreased after the mutation. Especially, the position of Na^+ pocket is marked as green circle.