SUPPORTING INFORMATION

C-terminal Tail of β-Tubulin and its Role in the Alterations of Dynein Binding Mode

Kali A. Heale, Laleh Alisaraie*

School of Pharmacy, Memorial University of Newfoundland, 300 Prince Philip Dr., A1B 3V6, St. John's, Newfoundland, Canada

Corresponding author

Email: laleh.alisaraie@mun.ca

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and MTBD-H2 respectively, (G) β-Glu447 (β-tubulin C-terminal) and MTBD Lys3384 (black) in the N-terminal, Lys3386 (red) in H1, His3387 (blue) in H1, Arg3469 (green) in H6, and Lys3472 (orange) in the H6-H7 loop, (H) β-Glu449 (β-tubulin C-terminal) and MTBD Lys3384 (black) in the N-terminal, Lys3386 (red) in H1, His3387 (blue) in H1, Arg3469 (green) in H6, Lys3472 (orange) in the H6-H7 loop and Lys3479 (magenta) in H7, (I) MTBD-H2 and α-H15, (J) Thr3399 (MTBD-H2) and α-Glu414 (H15-H16 loop), (K) MTBD-H3 and β-H8, (L) MTBD-H3 and β-H9, (M) MTBD-H3 and β-H12, (N) MTBD-H3 and β-H18, (O) MTBD-H6 and α-H16, (P) Ser3471 (MTBD-H6-H7 loop) and α-Glu415 (H16), and (Q) α-Gly416 (H16) and Arg3469 (MTBD H6), (R) Oxygen atoms (OE1-9186 and OE2-9187) of the Glu3390 (MTBD-H1) carboxyl group and the nitrogen atoms (NE-4004, NH1-4007 and NH2-4010) of the α-Arg402 (H14-H15 loop) amine group, (S) Oxygen atoms (OE1-4152 and OE2-4153) of the α-Glu415 (H16) carboxyl group and the nitrogen atoms (NE-9977, NH1-9980 and NH2-9983) of the Arg3469 (MTBD-H6) amine group, (T) Oxygen atoms (OE1-4142 and OE2-4143) of the α-Glu414 (H15-H16 loop) carboxyl group and the nitrogen atoms (NE-9977, NH1-9980 and NH2-9983) of the Arg3469 (MTBD-H6) amine group, and (U) oxygen atoms (OE1-4152 and OE2-4153) of the α-Glu415 (H16) carboxyl group and the nitrogen atoms (NE-4004, NH1-4007 and NH2-4010) of the α-Arg402 (H14-H15 loop) amine group.

Figure S7: (A) Radius of gyration (R_g/nm) *vs.* time (ps), (B) Root mean square deviation (nm)

Figure S8: Sample of conformations presenting the fluctuation of β-CTT.

Table S1*:* Salt bridge formation across the MT-MTBD interface. Interactions were identified when the distance between oxygen atoms in the carboxyl group (acidic residue side chain) and nitrogen atoms in the amine group (basic residue side chain) fell within 3.2 Å cut-off at least once during 200 ns simulation.

Figure S1: Amino acid sequences of (A) α-tubulin, (B) β-tubulin and (C) MTBD retrieved from the PDB. Root Mean Square Deviation (RMSD) data from (D) 200 ns trajectory.

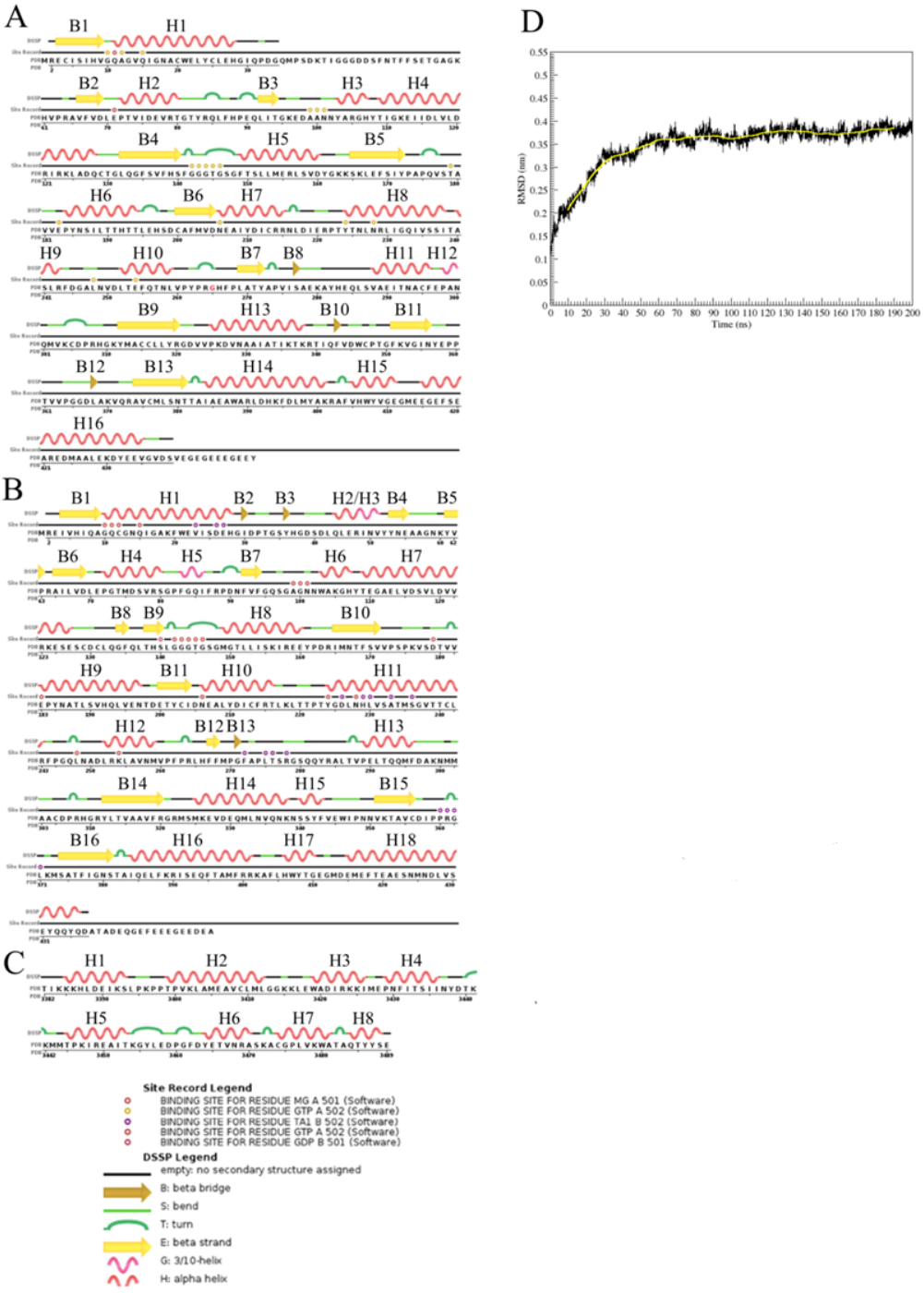


Figure S2: Sequence alignment data of (A) *D. discoideum* and *M. musculus* cytoplasmic dynein heavy chain, (B) *S. scrofa* and *S. cerevisiae* α-tubulin, and (C) *S. scrofa* and *S. cerevisiae* β-tubulin. Asterisk (*) denotes identical amino acid for both species, while a singular dot (.) denotes amino acids of different R-chain groups and a colon (:) denotes amino acids with R-chains of the same group.

Figure S3: dCOM between (A) β-H18 and MTBD, (B) β-CTT and MTBD, (C) β-H18 and MTBD-H1, and (D) β-CTT and MTBD-H1.

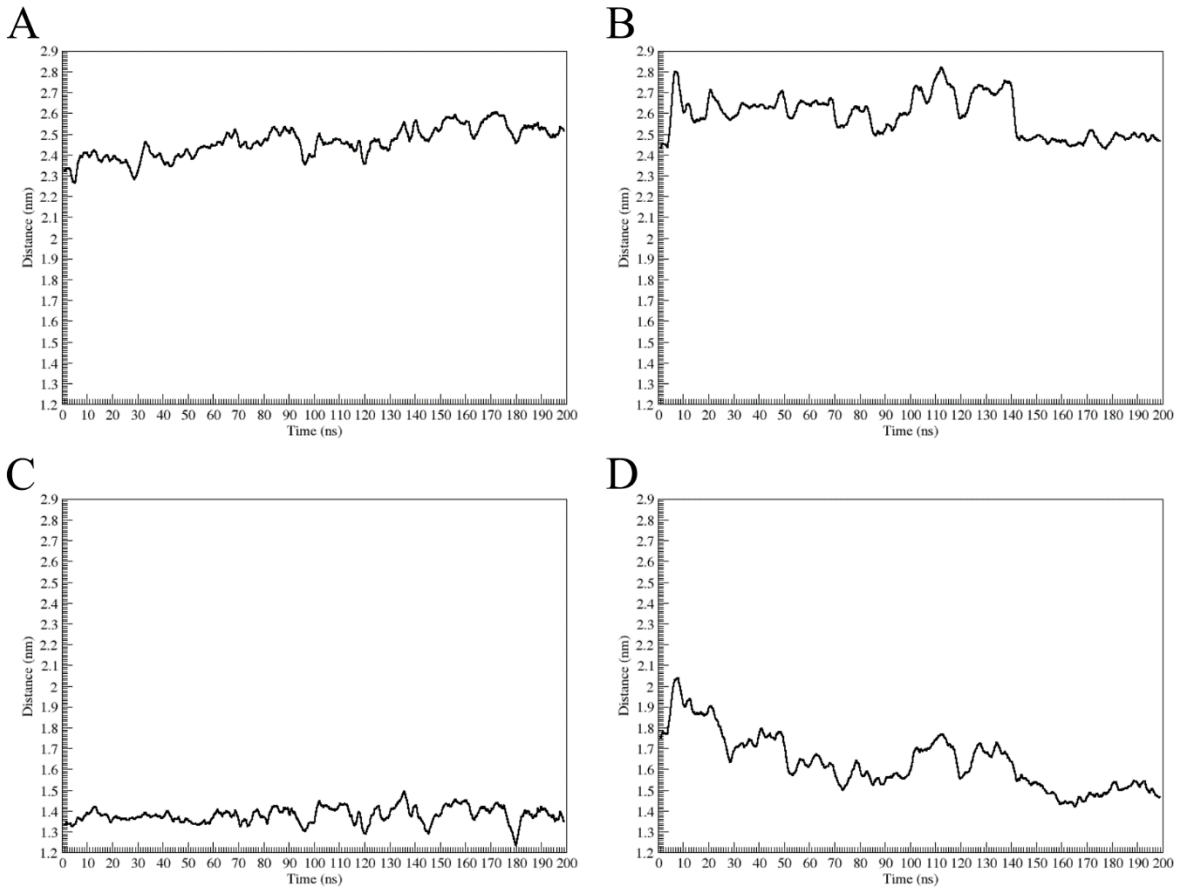


Figure S4: Number of hydrogen bonds between (A) MTBD and β-tubulin, (B) MTBD and β-H18 and (C) MTBD and β-CTT.

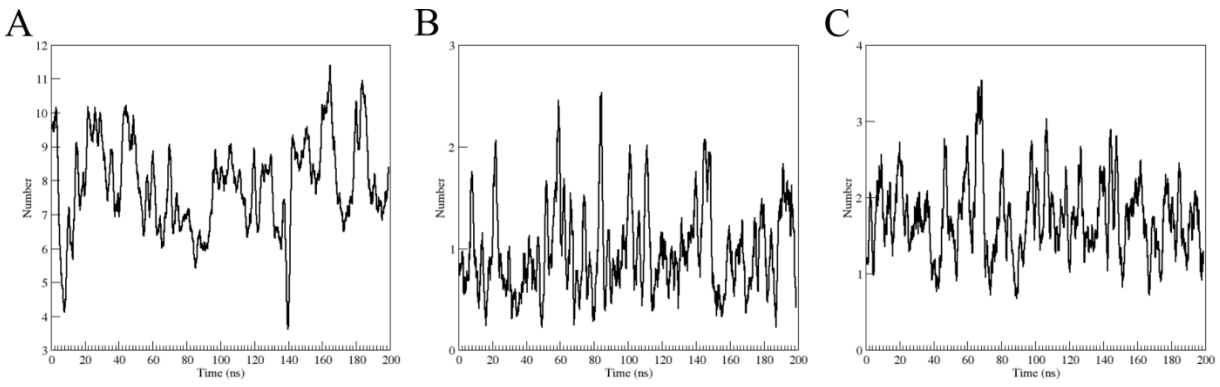


Figure S5: Percent helicity of MTBD-tubulin interface residues, (A) MTBD-H1, (Lys3385- Ser3393, 2-10), (B) MTBD-H3, (Trp3419-Ile3426, 2-9), (C) MTBD-H6, (Tyr3464-Ala3470, 2-8), (D) α-H15 (Val405-Glu411, 2-8), (E) β-H8, (Met149-Glu160, 2-12), (F) β-H9, (Glu183-Asn197, 2-16), and (G) β-H18 (Glu415-Gln436, 2-23).

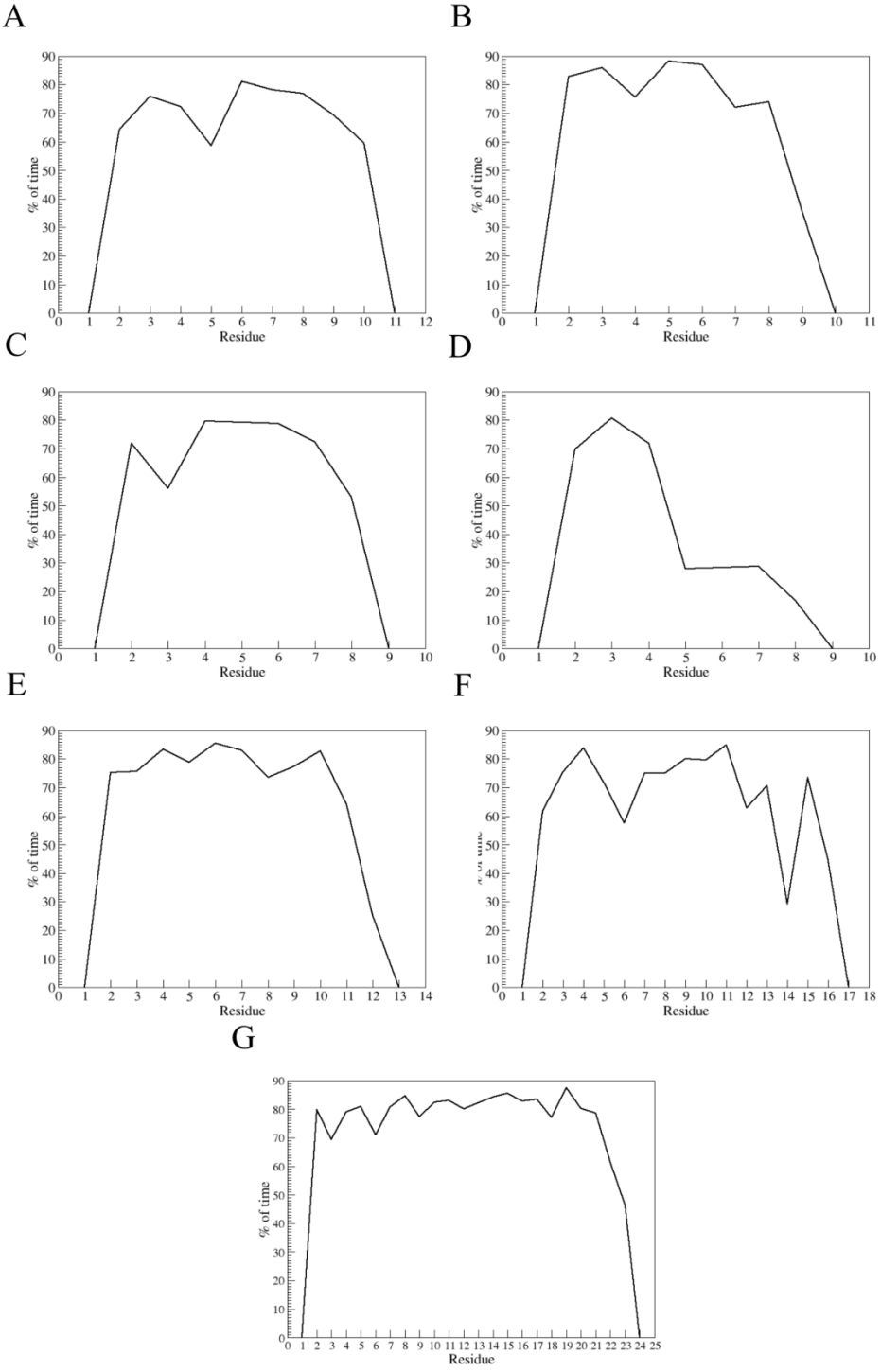
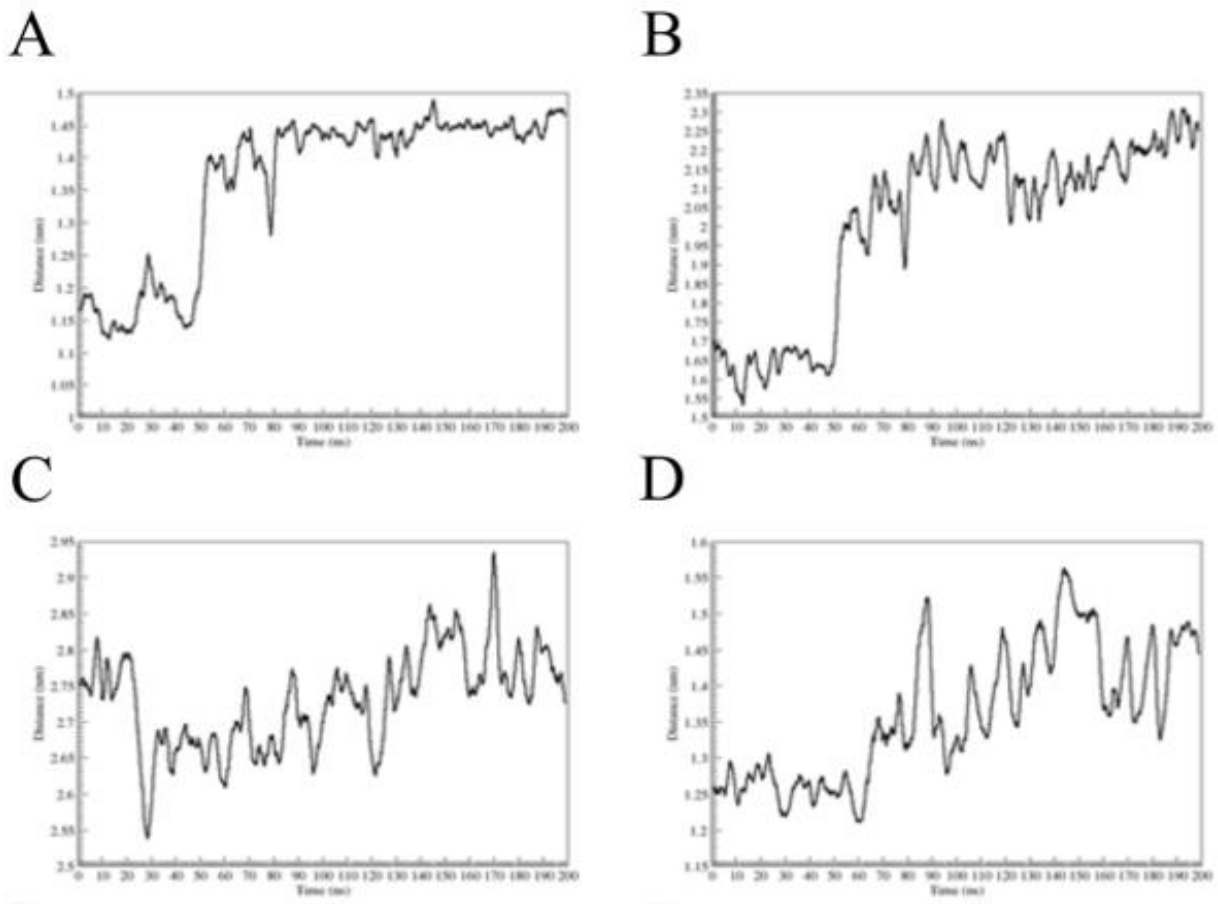


Figure S6: Distance between centers of mass (dCOM) between (A) MTBD-H1 and -H3, (B) MTBD-H1 N-terminal and -H3

N-terminal, (C) MTBD-H1 and α-H14, (D) MTBD-H1 and α-H15, (E) Ser3393 (MTBD-H1) and β-Pro263, (F) α-Glu411 (H15) and Lys3396 (black) and Lys3402 (red) in the MTBD-H1-H2 loop and MTBD-H2 respectively, (G) β-Glu447 (β-tubulin C-terminal) and MTBD Lys3384 (black) in the N-terminal, Lys3386 (red) in H1, His3387 (blue) in H1, Arg3469 (green) in H6, and Lys3472 (orange) in the H6-H7 loop, (H) β-Glu449 (β-tubulin C-terminal) and MTBD Lys3384 (black) in the N-terminal, Lys3386 (red) in H1, His3387 (blue) in H1, Arg3469 (green) in H6, Lys3472 (orange) in the H6-H7 loop and Lys3479 (magenta) in H7, (I) MTBD-H2 and α-H15, (J) Thr3399 (MTBD-H2) and α-Glu414 (H15-H16 loop), (K) MTBD-H3 and β-H8, (L) MTBD-H3 and β-H9, (M) MTBD-H3 and β-H12, (N) MTBD-H3 and β-H18, (O) MTBD-H6 and α-H16, (P) Ser3471 (MTBD-H6-H7 loop) and α-Glu415 (H16), and (Q) α-Gly416 (H16) and Arg3469 (MTBD H6), (R) Oxygen atoms (OE1-9186 and OE2-9187) of the Glu3390 (MTBD-H1) carboxyl group and the nitrogen atoms (NE-4004, NH1-4007 and NH2-4010) of the α-Arg402 (H14-H15 loop) amine group, (S) Oxygen atoms (OE1-4152 and OE2-4153) of the α-Glu415 (H16) carboxyl group and the nitrogen atoms (NE-9977, NH1-9980 and NH2-9983) of the Arg3469 (MTBD-H6) amine group, (T) Oxygen atoms (OE1-4142 and OE2-4143) of the α-Glu414 (H15-H16 loop) carboxyl group and the nitrogen atoms (NE-9977, NH1-9980 and NH2-9983) of the Arg3469 (MTBD-H6) amine group, and (U) oxygen atoms (OE1-4152 and OE2-4153) of the α-Glu415 (H16) carboxyl group and the nitrogen atoms (NE-4004, NH1-4007 and NH2-4010) of the α-Arg402 (H14-H15 loop) amine group.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B
C
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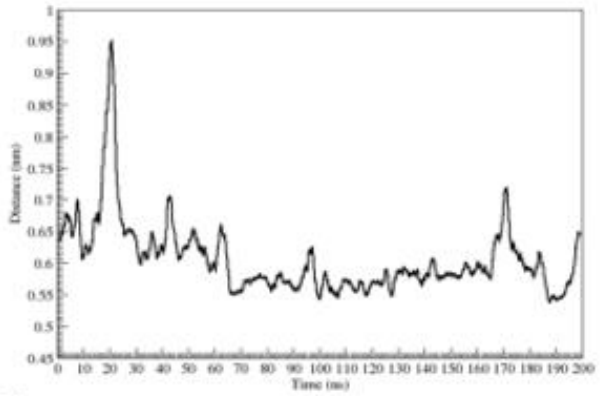

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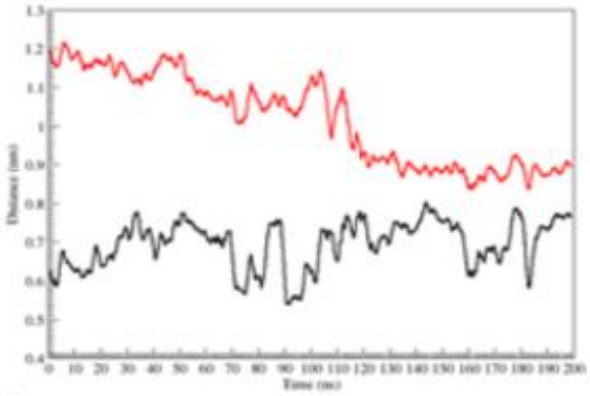

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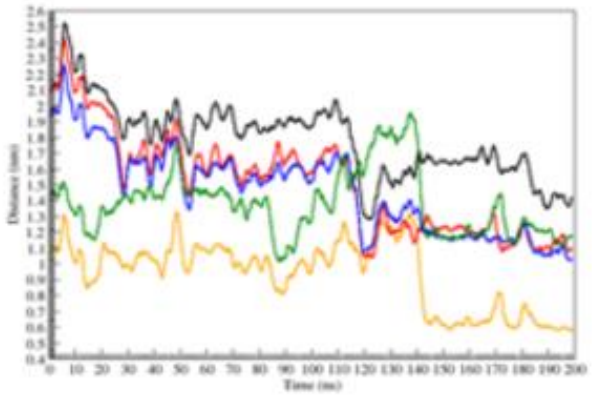

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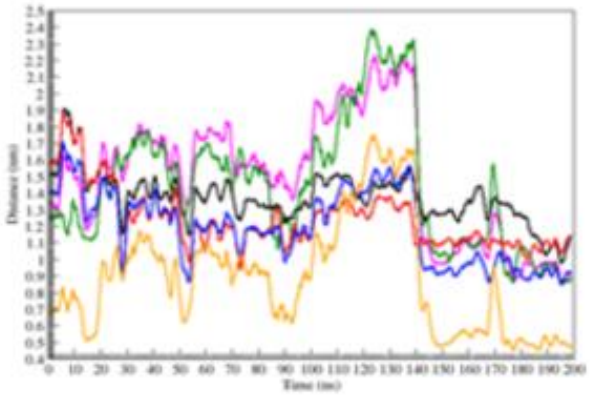

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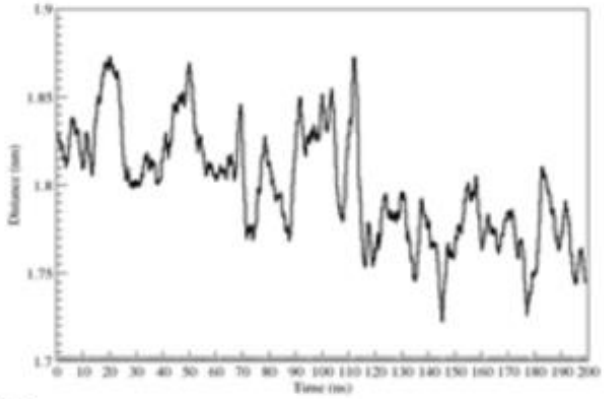
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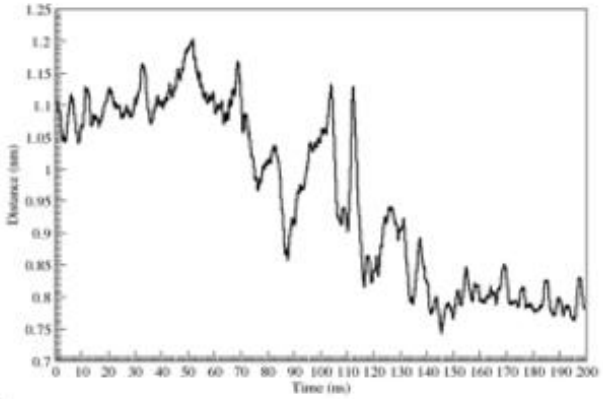
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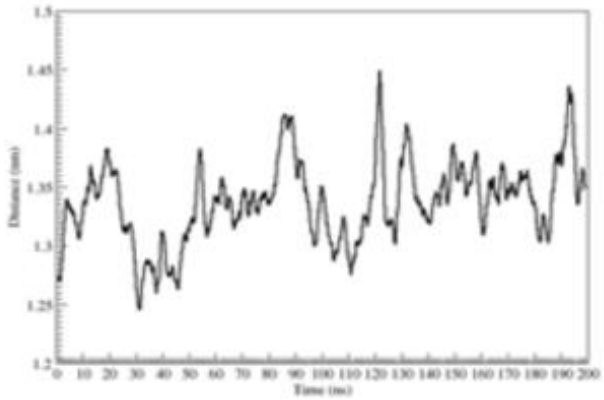
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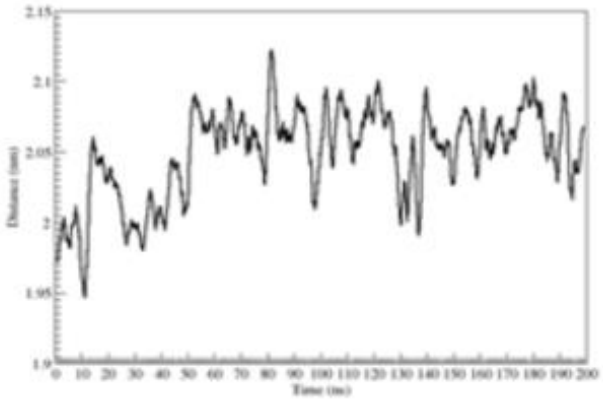
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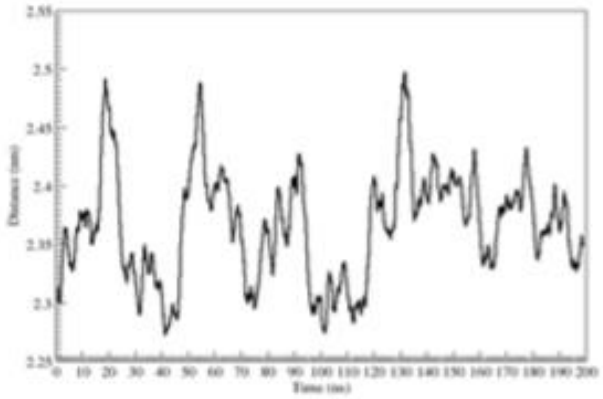

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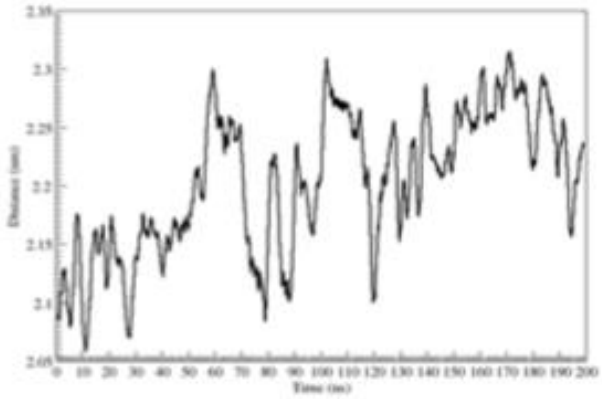

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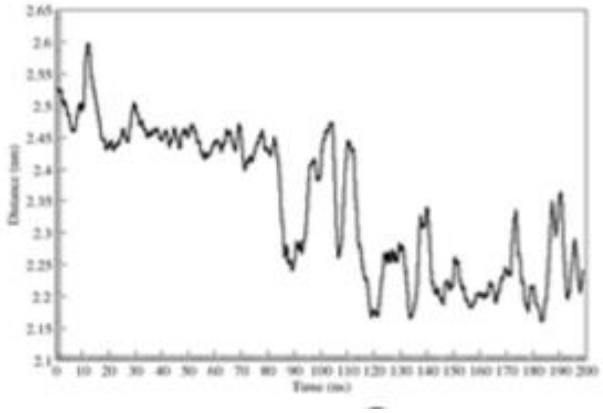

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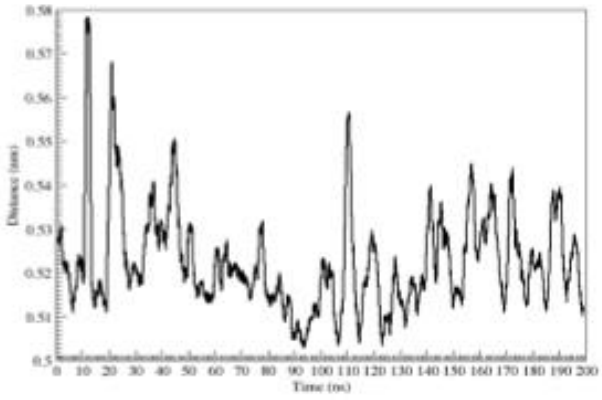

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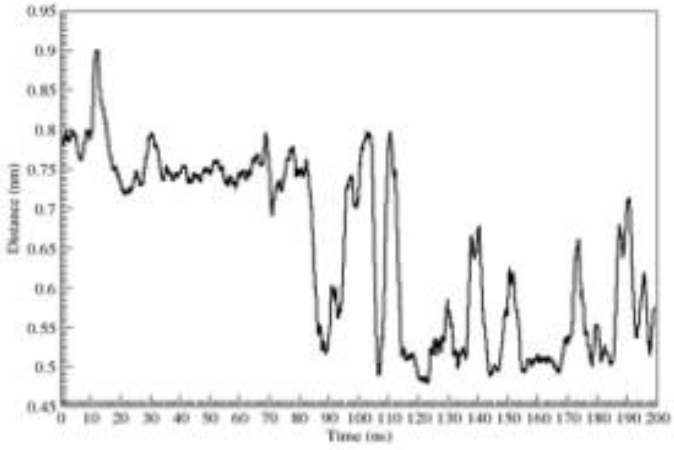

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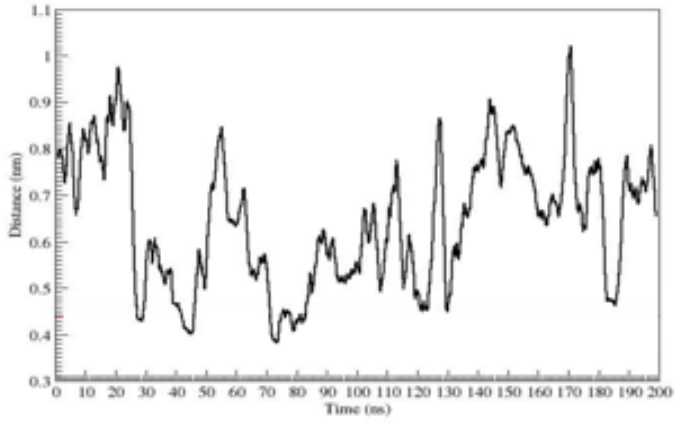
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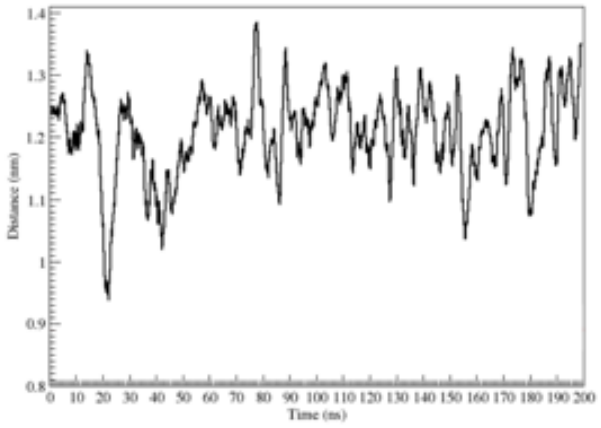
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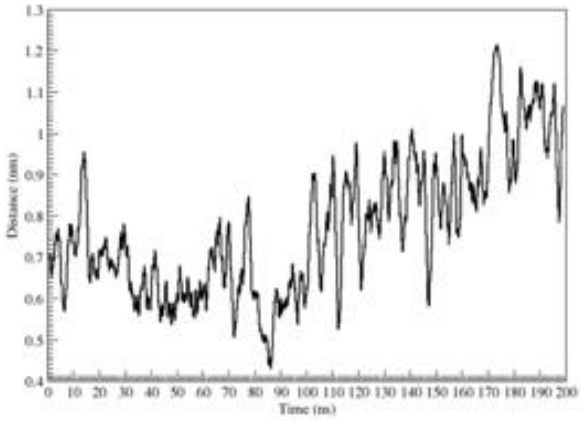
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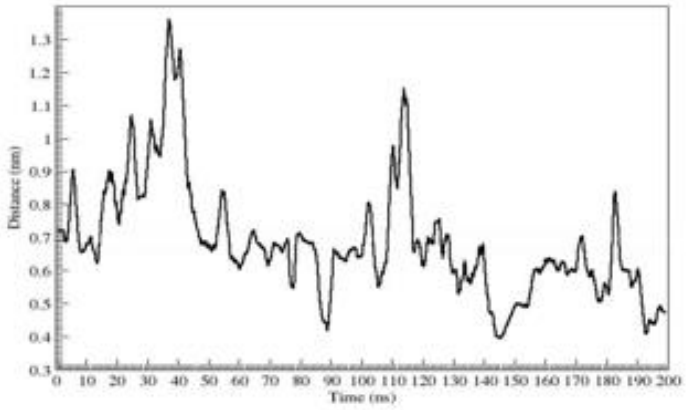
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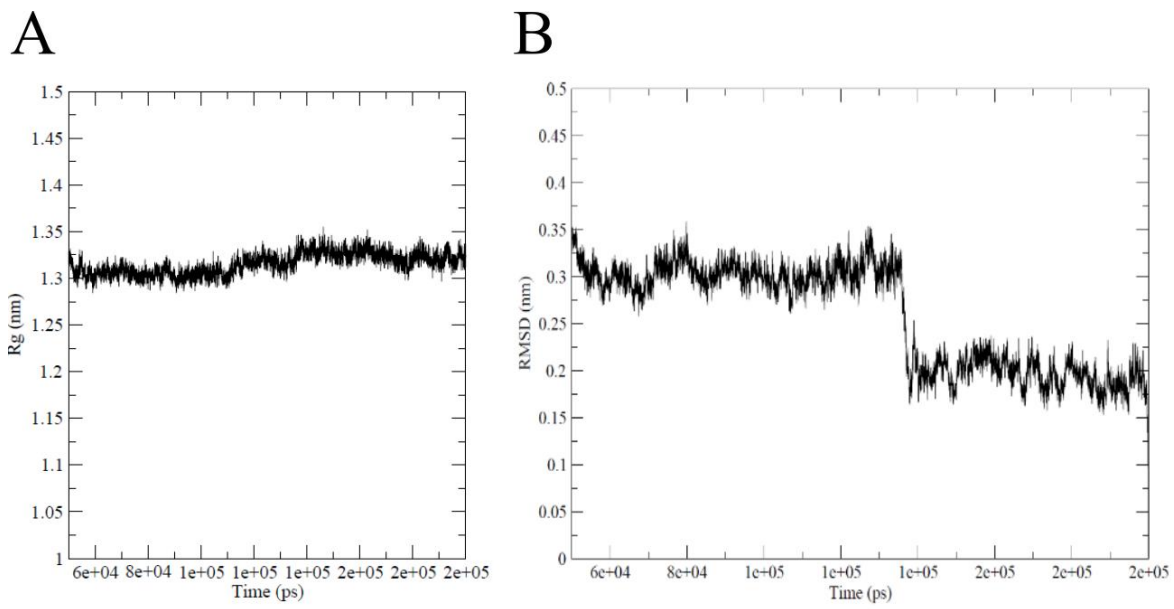

Figure S8: Sample of conformations presenting the fluctuation of β-CTT.

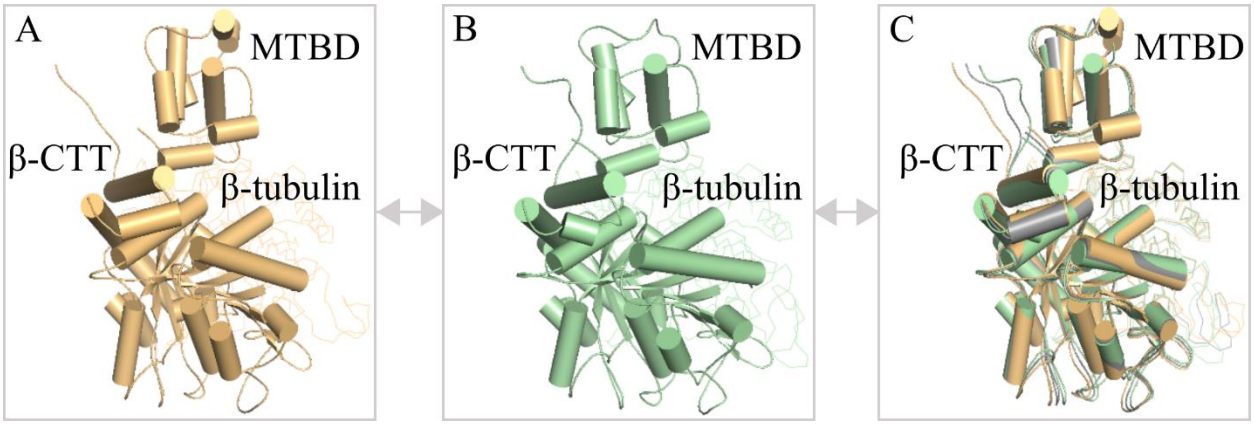

Table S1: Salt bridge formation across the MT-MTBD interface. Interactions were identified when the distance between oxygen atoms in carboxyl group (acidic residue side chain) and nitrogen atoms in amine group (basic residue side chain) fell within 3.2 Å cut-off at least once during 200 ns simulation.

Interacting Residues		
Residues of α-tubulin/ MTBD interaction	**α-tubulin**	**MTBD**
	Glu411	Lys3396
		Lys3402
	Glu414	Arg3469
	Arg402	Glu3390
Residue of β-tubulin/ MTBD interaction	**β-tubulin**	**MTBD**
	Glu159	Lys3424
		Lys3425
	Asp163	Lys3396
		Arg3423
	Glu196	Lys3385
		Lys3392
		Lys3424
	Asp199	Arg3423
	Arg264	Asp3389
	Glu420	Lys3385
		Lys3392
		Arg3469
	Asp427	Lys3385
		Lys3386
	Glu431	Lys3386
	Glu447	Lys3384
		Lys3386
		His3387

		Arg3469
		Lys3472
	Glu448	Lys3386
		Lys3472
	Glu449	His3384
		Lys3386
		Lys3387
		Arg3469
		Lys3472
		Lys3479
	Glu451	Lys3384
		Lys3385
		Lys3386
		His3387
	Glu452	Lys3384
		Lys3385
		Lys3386
		His3387
		Lys3479
	Asp453	Lys3385
		Lys3386
		His3387
	Glu454	His3387
		Lys3384