Supporting Material

Analysis of the strength of interfacial hydrogen bonds between tubulin dimers using quantum theory of atoms in molecules

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Figure S1: RMSD equilibration of the backbone atoms of the interfacial residues relative to the starting structure in the three systems; LongAB, LatB and LatA.

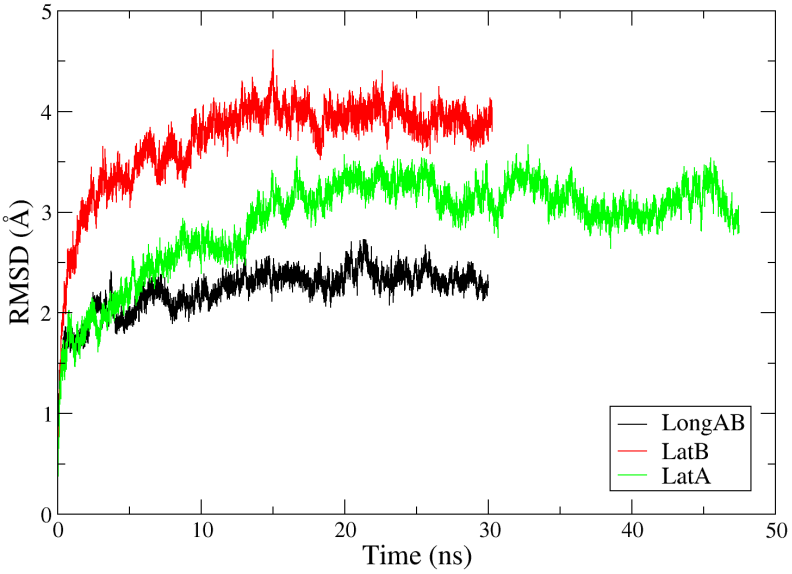

Figure S2: An all-atom model of the LongAB system with subunit assignment.

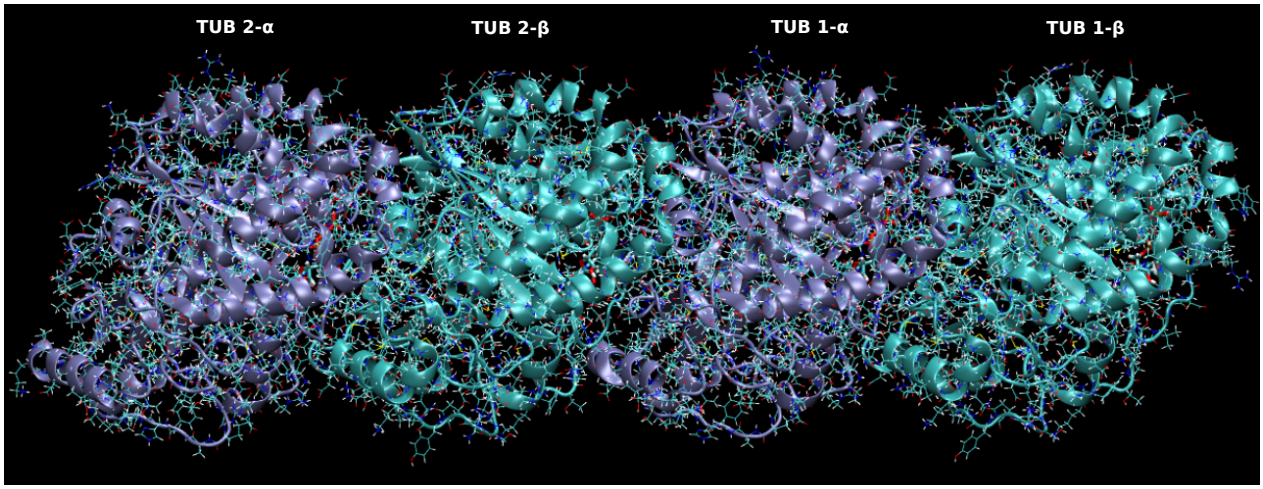

Table S1: Energy of hydrogen bonds in the LongAB interface in kJ/mol. SS# is snapshot number.

TUB 1–α	TUB 2–β	SS1	SS2	SS3	SS4	SS5	SS6	SS7	SS8	$E_{average}$	SD
Arg2	Glu71	-62.5	-33.4	-42.6	-42.3	-38.3	-20.1	-58.7	-23.2	-40.1	15
Glu434	Arg401	-30.0	-17.5	-39.3	-59.0	-32.4	-44.3	-38.1	0.0	-32.6	18
Tyr262	Arg401	-46.7	-45.0	-32.7	-45.5	0.0	-13.3	-25.6	-47.6	-32.0	18
Arg243	Asp76	-37.3	-17.3	-39.4	-35.7	0.0	-24.4	-42.8	-42.1	-29.9	15
Thr349	Val181	-44.6	-34.6	-13.8	-14.3	-43.6	-21.5	-21.0	-13.0	-25.8	13
Asp438	Arg401	-26.3	-55.1	-57.1	0.0	0.0	0.0	0.0	-52.7	-23.9	27
Val260	His406	-31.7	-34.1	-12.9	-8.8	-12.1	-41.6	-15.5	-20.0	-22.1	12
Gln133	Gly98	-16.8	-39.1	-20.7	-22.8	-21.2	-28.2	-10.7	-16.0	-21.9	9
Thr257	Gly100	-22.7	-35.5	-17.6	-27.2	-16.3	-13.2	-14.3	-24.2	-21.4	8
Lys352	Thr180	-18.5	-16.8	-22.1	0.0	-30.4	-16.3	-32.1	-12.9	-18.7	10
Asn249	Gln11	-22.6	-20.8	-27.5	-23.1	0.0	-28.6	0.0	-26.3	-18.6	12
Asn329	Lys176	-26.4	-18.2	-26.1	-19.4	-24.4	0.0	0.0	-7.6	-15.3	11
Lys163	Glu411	-34.2	0.0	-40.1	0.0	0.0	-43.7	0.0	0.0	-14.8	21
Asn258	Val181	0.0	-14.8	-15.6	-29.7	-8.8	-9.4	-22.4	-10.2	-13.9	9
Lys352	Asp179	0.0	0.0	0.0	-20.0	-12.2	-33.7	-12.9	0.0	-9.9	12
Asn249	Glu71	0.0	0.0	-31.3	0.0	0.0	-22.8	0.0	0.0	-6.8	13
Asp345	Arg400	0.0	0.0	0.0	0.0	0.0	-28.0	-23.6	0.0	-6.4	12
Asn258	Asn101	0.0	-20.6	0.0	0.0	-14.3	0.0	-12.9	0.0	-6.0	9
Arg2	Gln96	-3.5	0.0	0.0	-15.2	0.0	0.0	0.0	-23.8	-5.3	9
Val260	Trp407	0.0	-9.5	0.0	-4.3	-17.7	-6.7	0.0	0.0	-4.8	6
Gln133	Ser97	0.0	0.0	-4.7	0.0	0.0	0.0	0.0	-30.4	-4.4	11
Leu132	Gln96	0.0	0.0	0.0	0.0	0.0	-18.5	-14.8	0.0	-4.2	8
Asn258	Val182	0.0	-13.8	-13.5	0.0	0.0	0.0	0.0	0.0	-3.4	6
Lys326	Tyr210	0.0	0.0	0.0	0.0	0.0	-17.9	0.0	0.0	-2.2	6
Thr130	Gln96	0	0	0	0	-17	0	0	0	-2.1	6
Asn258	Thr180	0.0	0.0	0.0	-16.1	0.0	0.0	0.0	0.0	-2.0	6
Val437	Arg401	0.0	0.0	0.0	0.0	0.0	-11.6	0.0	0.0	-1.4	4
Val353	Asp179	0.0	-5.0	-4.4	0.0	0.0	0.0	0.0	0.0	-1.2	2
Lys336	Lys176	0.0	0.0	-2.3	0.0	0.0	0.0	0.0	-4.2	-0.8	2
Glu254	Asn101	0.0	0.0	0.0	0.0	0.0	0.0	-3.5	0.0	-0.4	1
Total Energy		-424	-431	-464	-384	-289	-444	-349	-354	-392	59

Figure S3: An all-atom model of the LatB system with subunit assignment.

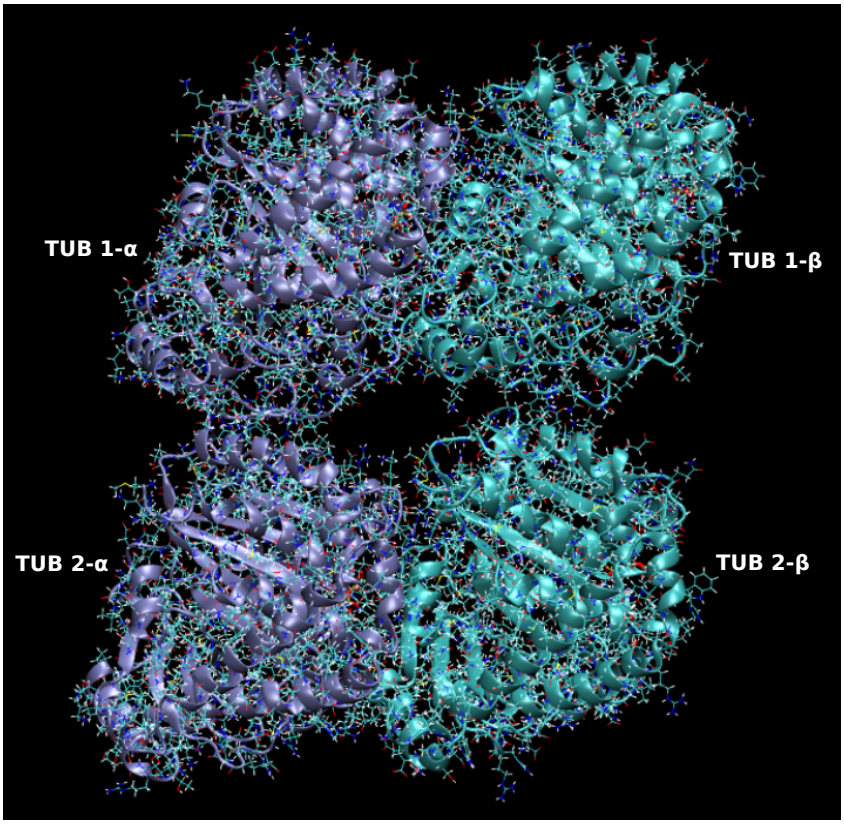

Figure S4: An all-atom model of the LatA system with subunit assignment.

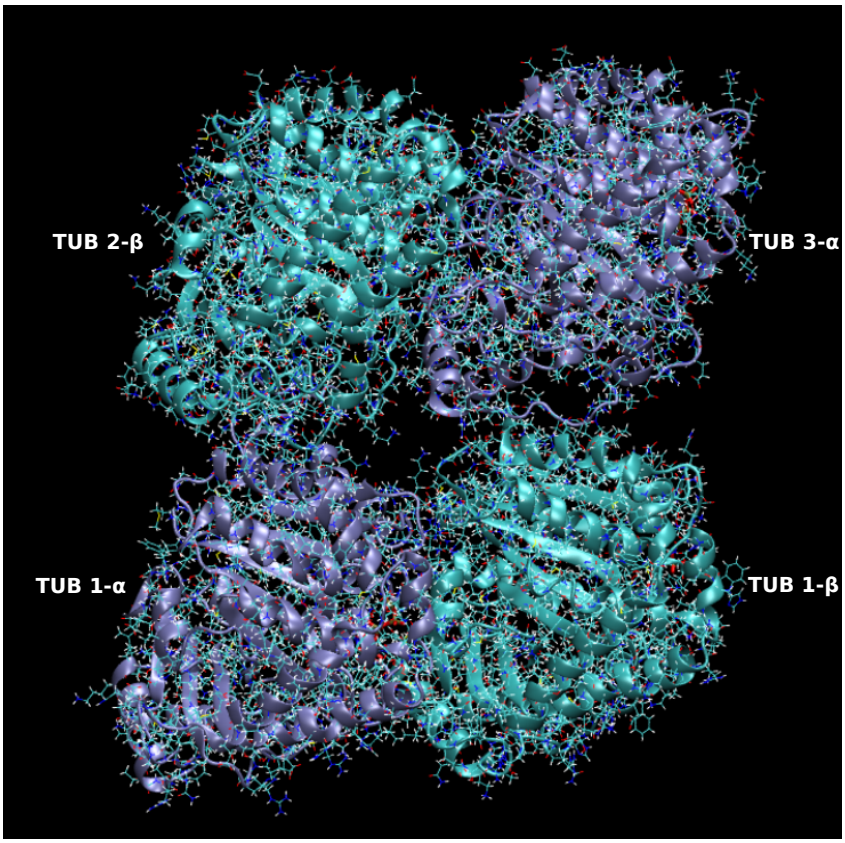

Table S2: Energy of hydrogen bonds in the LatB interface in kJ/mol. SS# is snapshot number.

α–α **Interactions**											
TUB 1–α	TUB 2–α	SS1	SS2	SS3	SS4	SS5	SS6	SS7	SS8	$E_{average}$	SD
Arg215	Glu90	0.0	-44.0	-36.7	-49.3	-64.7	-51.4	-40.6	-55.3	-42.7	19
Lys338	Asp127	-24.5	-13.8	-33.6	-34.1	-26.2	-41.9	-28.9	-24.7	-28.5	8
Glu297	Arg121	-26.1	-21.9	-40.0	0.0	-62.8	0.0	-23.6	-22.2	-24.6	20
Glu297	Lys124	-20.0	-29.2	-15.9	-38.3	0.0	-32.1	-35.8	-17.1	-23.5	13
Glu284	Ser54	0.0	-32.6	-24.3	0.0	-33.4	-24.5	-38.7	-24.8	-22.3	15
Gln372	Glu55	-28.0	0.0	-13.7	-28.0	-15.9	-20.9	-16.9	-24.2	-18.4	9
Tyr282	Ser48	0.0	-31.8	-19.3	-20.9	-8.1	0.0	0.0	-13.2	-11.7	12
His283	Phe49	-7.5	-8.8	-28.2	0.0	-12.8	-5.8	-7.9	-13.5	-10.5	8
Ala278	Asn50	-20.3	0.0	0.0	-10.0	-14.9	0.0	0.0	0.0	-5.7	8
Arg373	Ser54	-8.1	0.0	-25.4	0.0	0.0	0.0	0.0	0.0	-4.2	9
Glu284	Lys60	0.0	0.0	0.0	0.0	0.0	-8.5	-23.6	0.0	-4.0	8
Leu286	Ser54	0.0	-2.9	-7.6	0.0	-9.3	-4.7	0.0	-6.1	-3.8	4
Gln285	Gly57	-15.1	0.0	0.0	0.0	0.0	0.0	-11.9	0.0	-3.4	6
Gln372	Thr56	0.0	0.0	0.0	0.0	0.0	-24.6	0.0	0.0	-3.1	9
His283	Asn50	0.0	-11.3	0.0	0.0	0.0	0.0	0.0	0.0	-1.4	4
Glu290	Gln128	0	0	0	0	-9	0	0	0	-1.1	3
Lys370	Thr51	0.0	0.0	0.0	0.0	0.0	0.0	-7.1	0.0	-0.9	3
Total Subunit Energy		-149	-196	-245	-180	-257	-214	-235	-201	-210	35
β–β **Interactions**											
TUB 1–β	TUB 2–β	SS1	SS2	SS3	SS4	SS5	SS6	SS7	SS8	$E_{average}$	SD
Arg308	Asp116	-46.7	-58.9	0.0	-37.5	-69.8	-57.4	-54.3	-33.7	-44.8	22
Glu290	Arg88	-51.6	-35.3	-32.2	-55.4	-22.6	-30.3	-30.3	-53.9	-38.9	13
Arg308	Asp120	-29.2	-26.9	-27.3	-25.6	-37.7	-27.6	-61.5	-58.2	-36.7	15
Lys299	Asp90	-11.0	-37.8	-25.5	-34.6	-31.0	-34.7	-31.3	-55.0	-32.6	12
Asp297	Lys124	-31.8	0.0	-31.3	0.0	-32.1	0.0	-29.0	-54.4	-22.3	20
Tyr342	Asp120	0.0	-9.9	0.0	-10.8	-25.1	-8.1	-41.7	-51.8	-18.4	19
Ser280	Arg88	-14.5	-21.7	-6.3	-22.9	0.0	-51.6	0.0	-16.1	-16.6	17
Lys338	Lys124	-6.4	-20.8	-15.5	-24.9	-25.2	0.0	0.0	-25.4	-14.8	11
Lys338	Ser126	-24.0	-23.6	-7.2	0.0	-14.0	0.0	0.0	-27.5	-12.0	12
Lys338	Arg123	0.0	0.0	0.0	0.0	0.0	-35.9	-19.9	-4.1	-7.5	13
Asn334	Glu127	0.0	-19.0	0.0	-32.7	0.0	0.0	0.0	0.0	-6.5	12
Asn335	Glu128	0.0	-6.8	0.0	0.0	0.0	0.0	0.0	0.0	-0.9	2
Total Subunit Energy		-215	-261	-145	-244	-257	-246	-268	-380	-252	65
Total Energy		-365	-457	-390	-425	-514	-460	-503	-581	-462	70

Table S3: Energy of hydrogen bonds in the LatA interface in kJ/mol. SS# is snapshot number.

α–β **Interactions**											
TUB 1–α	TUB 2–β	SS1	SS2	SS3	SS4	SS5	SS6	SS7	SS8	$E_{average}$	SD
Asp47	Arg284	-44.6	-17.9	-41.5	-40.4	-32.1	-54.1	-71.1	-36.0	-42.2	15.7
Lys124	Asp297	-24.7	-19.4	-39.2	-42.9	-29.9	-25.5	-27.4	-44.8	-31.7	9.4
Gln85	Ser280	-31.4	-23.8	0.0	-29.4	-34.9	-23.1	-22.4	-23.4	-23.6	10.6
Asp46	Arg278	-26.7	-10.3	-39.2	-39.6	-14.3	-19.8	-33.9	0.0	-23.0	14.4
Asp127	Asn334	-25.0	-24.3	-27.9	-16.4	-21.9	-21.8	-28.5	-15.0	-22.6	4.9
Asp120	Lys338	-39.2	0.0	-20.4	-36.6	-26.5	0.0	-25.3	-31.4	-22.4	15.1
Gln128	Gln293	-6.5	-20.3	-27.8	-36.5	-10.6	-28.8	-18.1	0.0	-18.6	12.3
Asp47	Gln282	-32.0	-8.2	-17.8	0.0	-29.7	0.0	-8.6	-36.0	-16.5	14.5
Glu55	Arg284	-39.8	0.0	-45.9	0.0	0.0	-19.8	-13.0	0.0	-14.8	18.9
Arg121	Asp297	0.0	-69.3	0.0	0.0	-35.3	0.0	0.0	0.0	-13.1	25.9
Asp47	Arg278	0.0	-18.5	0.0	0.0	0.0	-34.0	-16.8	-25.5	-11.9	13.7
Ser54	Lys372	0.0	0.0	0.0	0.0	-21.1	-18.6	-13.5	-24.3	-9.7	10.8
Lys124	Gln293	0.0	-12.8	-17.0	0.0	-15.6	0.0	0.0	-9.9	-6.9	7.7
His88	Gln281	0.0	-9.3	-19.8	-16.2	0.0	0.0	0.0	0.0	-5.7	8.3
Ser54	Arg284	-11.1	0.0	0.0	0.0	-32.0	0.0	0.0	0.0	-5.4	11.4
Arg123	Asn334	0.0	-15.8	0.0	-5.3	0.0	-1.9	-16.1	0.0	-4.9	7.1
Thr56	Gly370	-7.7	-16.7	-4.4	-7.5	0.0	0.0	0.0	0.0	-4.5	6.0
Gly59	Arg284	0.0	0.0	-19.2	-16.3	0.0	0.0	0.0	0.0	-4.4	8.2
Phe53	Ser374	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-31.1	-3.9	11.0
Asn50	Gln282	0.0	0.0	0.0	-9.6	0.0	-20.4	0.0	0.0	-3.8	7.5
Phe87	Ser280	0.0	0.0	-24.5	0.0	0.0	0.0	0.0	0.0	-3.1	8.7
Gln128	Thr287	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-18.8	-2.4	6.7
Ser54	Met373	0.0	0.0	0.0	0.0	0.0	-15.1	0.0	0.0	-1.9	5.3
Gln128	Glu290	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-14.6	-1.8	5.2
Total Subunit Energy		-289	-267	-344	-297	-304	-283	-295	-311	-299	23
β–α **Interactions**											
TUB 1–β	TUB 3–α	SS1	SS2	SS3	SS4	SS5	SS6	SS7	SS8	$E_{average}$	SD
Arg88	Glu279	-45.6	-26.5	-36.3	-47.6	-40.4	-40.1	-45.3	0.0	-35.2	15.7
Lys124	Glu284	-25.6	0.0	-36.6	-32.4	-30.2	-38.7	-35.2	-17.2	-27.0	12.9
Ile86	Tyr282	-7.5	-29.9	0.0	-31.9	-38.9	-23.1	-25.2	-27.1	-22.9	12.9
Asp90	Lys280	-36.6	0.0	-27.4	-19.7	-39.1	-25.8	0.0	0.0	-18.6	16.5
Asn54	Glu284	-37.0	0.0	-24.6	0.0	0.0	-19.8	-14.5	-19.5	-14.4	13.6
Glu127	Thr334	0.0	-34.3	0.0	-33.4	-43.0	0.0	0.0	0.0	-13.8	19.3
Asp90	Ala281	-17.4	-14.8	0.0	0.0	-22.6	-17.9	-30.9	0.0	-12.9	11.7
Glu127	Thr337	0.0	-22.9	0.0	-39.0	0.0	0.0	0.0	-20.4	-10.3	15.2
Glu55	Gln285	-5.4	-13.1	-11.9	-9.3	-6.7	-20.2	-9.1	0.0	-9.5	6.0
Thr33	His283	0.0	0.0	-18.3	-5.2	0.0	0.0	0.0	-11.6	-4.4	7.0
Asp120	Lys338	-18.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-2.3	6.5
Arg88	Ala281	0.0	0.0	0.0	-8.4	0.0	-5.0	0.0	0.0	-1.7	3.2
Total Subunit Energy		-193	-141	-155	-227	-221	-191	-160	-96	-173	44
Total Energy		-482	-408	-499	-523	-525	-474	-455	-406	-472	46