Appendix

Chapter 4

Table S1: *Details of the binding energies and quantum mechanical descriptor values for the 45 complex systems studied with B3LYP/TZVP level of theory.*

Complex	MOC	ρ	OWBO	WBI	E_I (kJ/mol)
HSH–FNF2	0.0043	0.0037	0.0011	0.0017	–0.10
ClH–FOF	0.0046	0.0070	–0.0005	0.0058	–0.19
BrH–FNF2	0.0056	0.0055	0.0023	0.0035	–0.69
H3CH–OMe2	0.0093	0.0061	0.0015	0.0023	–1.20
H3CH–NHMe2	0.0061	0.0066	–0.0020	0.0053	–1.51
MeHPH–NH3	–0.0093	0.0082	0.0164	0.0070	–1.84
HSH–BrH	0.0065	0.0051	0.0042	0.0054	–1.98
HOPh–FMe	0.0121	0.0062	0.0032	0.0018	–2.55
H2PH–OH2	–0.0008	0.0080	0.0059	0.0037	–2.64
FH–FNF2	0.0108	0.0131	0.0196	0.0092	–3.80
BrH–BrH	0.0173	0.0096	0.0377	0.0215	–4.11
FH–FOF	0.0128	0.0150	0.0142	0.0118	–4.75
FH–ClOCl	0.0294	0.0143	0.0073	0.0249	–5.55
HSH–PH2Me	0.0002	0.0096	0.0119	0.0207	–5.87
MeSH–NH2Ph	0.0109	0.0153	0.0147	0.0202	–8.00
MeOH–PH3	–0.0087	0.0125	0.0142	0.0175	–9.00
MeSH–OHMe	0.0052	0.0168	0.0174	0.0157	–9.55
MeHNH–OMe2	0.0179	0.0148	0.0106	0.0077	–10.67
MeHNH–NMe3	0.0263	0.0175	0.0155	0.0150	–10.87
MeHNH–NH3	–0.0254	0.0171	0.0202	0.0167	–12.53
ClH–SH2	0.0389	0.0187	0.0469	0.0569	–13.78
PhOH–PH2Me	0.0082	0.0160	0.0308	0.0375	–16.17
HSH–NH2Me	0.0072	0.0259	0.0676	0.0506	–16.99
MeOH–PMe3	0.0245	0.0181	0.0199	0.0464	–17.40
ClH–PH2Me	0.0363	0.0219	0.1173	0.0851	–18.52
FH–FH	0.0205	0.0263	0.0305	0.0248	–20.38
BrH–OH2	0.0137	0.0303	0.0701	0.0488	–21.67
MeOH–OH2	0.0225	0.0259	0.0364	0.0243	–21.86
HOH–OH2	0.0168	0.0256	0.0369	0.0243	–22.60
MeOH–OHMe	0.0267	0.0281	0.0400	0.0284	–22.62
FH–SH2	0.0559	0.0245	0.0491	0.0627	–22.68
HOH–OHEt	0.0224	0.0276	0.0398	0.0282	–23.17
FH–OHCl	0.0186	0.0345	0.0566	0.0393	–24.20
ClH–OH2	0.0190	0.0332	0.0621	0.0511	–26.32
HOH–NMe3	0.0454	0.0353	0.0656	0.0483	–28.34
HOH–NH3	–0.0065	0.0297	0.0550	0.0452	–28.92
MeOH–NH3	–0.0131	0.0307	0.0582	0.0476	–28.96
FH–PH2Me	0.0553	0.0277	0.0773	0.0890	–29.35
HOH–NHMe2	0.0339	0.0347	0.0655	0.0535	–29.71
HOH–NH2Me	0.0165	0.0328	0.0618	0.0525	–30.03
MeOH–NH2Me	0.0068	0.0336	0.0685	0.0543	–30.11
FH–OH2	0.0320	0.0434	0.0790	0.0612	–40.66
FH–OHMe	0.0469	0.0496	0.0945	0.0754	–44.21
ClH–NH3	0.0281	0.0540	0.1737	0.1383	–44.89
FH–OMe2	0.0536	0.0531	0.1034	0.0800	–45.03

Table S2: *Details of the binding energies and quantum mechanical descriptor values for the 45 complex systems studied with B3LYP/aug–TZVP level of theory.*

Complex	MOC	ρ	OWBO	WBI	E_I (kJ/mol)
HSH-FNF2	-0.002	0.00372	0.0031	0.0016	0.0
ClH-FOF	-0.005	0.00702	-0.0040	0.0079	0.0
BrH-FNF2	0.001	0.00551	0.0064	0.0037	-0.5
H3CH-OMe2	-0.047	0.00600	-0.0031	0.0039	-1.1
H3CH-NHMe2	-0.037	0.00649	-0.0098	0.0076	-1.3
MeHPH-NH3	-0.057	0.00784	0.0188	0.0071	-1.3
HSH-BrH	0.002	0.00511	0.0035	0.0048	-1.9
HOPh-FMe	-0.031	0.00612	0.0013	0.0025	-2.5
H2PH-OH2	-0.056	0.00774	0.0079	0.0041	-2.3
FH-FNF2	0.013	0.01307	0.0074	0.0084	-3.7
BrH-BrH	0.016	0.00966	0.0132	0.0213	-4.0
FH-FOF	0.008	0.01499	0.0092	0.0118	-4.6
FH-ClOCl	0.040	0.01436	0.0055	0.0232	-5.4
HSH-PH2Me	-0.030	0.00957	0.0079	0.0187	-5.8
MeSH-NH2Ph	-0.092	0.01518	0.0188	0.0213	-7.8
MeOH-PH3	0.014	0.01254	0.0116	0.0188	-8.9
MeSH-OHMe	-0.053	0.01664	0.0175	0.0164	-9.1
MeHNH-OMe2	-0.090	0.01477	0.0099	0.0086	-10.5
MeHNH-NMe3	-0.162	0.01747	0.0368	0.0212	-10.8
MeHNH-NH3	-0.156	0.01668	0.0189	0.0169	-11.4
ClH-SH2	0.021	0.01866	0.0756	0.0584	-13.5
PhOH-PH2Me	0.087	0.01607	0.0245	0.0390	-16.0
HSH-NH2Me	-0.098	0.02569	0.0750	0.0513	-16.4
MeOH-PMe3	0.029	0.01812	0.0871	0.0606	-17.6
ClH-PH2Me	0.026	0.02199	0.1178	0.0836	-18.7
FH-FH	-0.021	0.02606	0.0289	0.0233	-19.3
BrH-OH2	-0.089	0.03005	0.0787	0.0503	-20.0
MeOH-OH2	-0.130	0.02558	0.0346	0.0246	-20.3
HOH-OH2	-0.135	0.02530	0.0349	0.0237	-21.7
MeOH-OHMe	-0.124	0.02795	0.0407	0.0284	-21.9
FH-SH2	0.043	0.02452	0.0445	0.0632	-22.9
HOH-OHEt	-0.106	0.02753	0.0346	0.0276	-23.4
FH-OHCl	-0.128	0.03439	0.0499	0.0373	-23.9
ClH-OH2	-0.090	0.03304	0.0839	0.0522	-24.9
HOH-NMe3	-0.184	0.03527	0.0848	0.0566	-29.1
HOH-NH3	-0.150	0.02949	0.0527	0.0453	-28.5
MeOH-NH3	-0.151	0.03050	0.0614	0.0494	-27.9
FH-PH2Me	0.043	0.02782	0.0717	0.0888	-30.1
HOH-NHMe2	-0.152	0.03472	0.0569	0.0536	-30.2
HOH-NH2Me	-0.139	0.03265	0.0556	0.0521	-30.1
MeOH-NH2Me	-0.130	0.03350	0.0667	0.0551	-29.6
FH-OH2	-0.135	0.04334	0.0790	0.0606	-39.8
FH-OHMe	-0.123	0.04962	0.0896	0.0737	-44.4
ClH-NH3	-0.079	0.05415	0.1821	0.1423	-44.7
FH-OMe2	-0.112	0.05311	0.0920	0.0799	-45.9

Table S3: *Details of the binding energies and quantum mechanical descriptor values for the 45 complex systems studied with B97D/aug–TZVP level of theory.*

Complex	MOC	ρ	OWBO	WBI	E_I (kJ/mol)
HSH-FNF2	-0.002	0.00360	0.0030	0.0018	-2.2
ClH-FOF	-0.002	0.00697	-0.0039	0.0090	-2.7
BrH-FNF2	0.001	0.00540	0.0063	0.0041	-3.5
H3CH-OMe2	-0.044	0.00583	-0.0026	0.0039	-3.9
H3CH-NHMe2	-0.015	0.00639	-0.0099	0.0081	-4.8
MeHPH-NH3	-0.044	0.00779	0.0198	0.0086	-4.0
HSH-BrH	0.004	0.00502	0.0039	0.0055	-5.1
HOPh-FMe	-0.037	0.00598	0.0057	0.0030	-7.2
H2PH-OH2	-0.052	0.00761	0.0082	0.0047	-3.8
FH-FNF2	0.012	0.01313	0.0078	0.0093	-4.7
BrH-BrH	0.020	0.00967	0.0145	0.0240	-8.3
FH-FOF	0.008	0.01515	0.0097	0.0132	-4.7
FH-ClOCl	0.038	0.01449	0.0063	0.0249	-6.7
HSH-PH2Me	-0.030	0.00956	0.0085	0.0208	-9.6
MeSH-NH2Ph	-0.075	0.01523	0.0214	0.0238	-14.8
MeOH-PH3	0.002	0.01258	0.0327	0.0200	-11.7
MeSH-OHMe	-0.043	0.01671	0.0200	0.0184	-11.7
MeHNH-OMe2	-0.092	0.01470	0.0107	0.0091	-14.8
MeHNH-NMe3	-0.146	0.01753	0.0371	0.0219	-20.3
MeHNH-NH3	-0.153	0.01680	0.0189	0.0187	-13.9
ClH-SH2	0.023	0.01889	0.0776	0.0637	-16.3
PhOH-PH2Me	0.081	0.01617	0.0256	0.0411	-20.5
HSH-NH2Me	-0.075	0.02614	0.0780	0.0578	-21.6
MeOH-PMe3	0.016	0.01826	0.0869	0.0622	-22.0
ClH-PH2Me	0.021	0.02224	0.1195	0.0887	-22.5
FH-FH	-0.021	0.02648	0.0302	0.0254	-16.8
BrH-OH2	-0.078	0.03065	0.0833	0.0561	-21.3
MeOH-OH2	-0.133	0.02596	0.0357	0.0269	-20.1
HOH-OH2	-0.140	0.02568	0.0365	0.0259	-20.4
MeOH-OHMe	-0.128	0.02836	0.0423	0.0307	-23.5
FH-SH2	0.029	0.02490	0.0463	0.0661	-23.2
HOH-OHEt	-0.110	0.02795	0.0363	0.0298	-24.0
FH-OHCl	-0.135	0.03508	0.0519	0.0401	-22.6
ClH-OH2	-0.081	0.03365	0.0876	0.0575	-25.1
HOH-NMe3	-0.193	0.03581	0.0866	0.0591	-35.8
HOH-NH3	-0.154	0.03004	0.0549	0.0489	-29.2
MeOH-NH3	-0.156	0.03107	0.0631	0.0534	-30.1
FH-PH2Me	0.021	0.02815	0.0734	0.0907	-30.7
HOH-NHMe2	-0.152	0.03532	0.0597	0.0572	-35.4
HOH-NH2Me	-0.145	0.03326	0.0574	0.0560	-33.0
MeOH-NH2Me	-0.137	0.03413	0.0686	0.0592	-34.4
FH-OH2	-0.140	0.04431	0.0815	0.0646	-37.6
FH-OHMe	-0.132	0.05073	0.0922	0.0778	-43.7
ClH-NH3	-0.060	0.05528	0.1852	0.1516	-49.7
FH-OMe2	-0.131	0.05422	0.0946	0.0834	-46.5

Table S4: *Details of the binding energies and quantum mechanical descriptor values for the 45 complex systems studied with wB97XD/aug–TZVP level of theory.*

Complex	MOC	ρ	OWBO	WBI	E_I (kJ/mol)
HSH-FNF2	-0.005	0.00354	0.0025	0.0014	-1.5
ClH-FOF	-0.006	0.00682	-0.0036	0.0072	-1.3
BrH-FNF2	-0.002	0.00529	0.0057	0.0033	-2.3
H3CH-OMe2	-0.041	0.00588	-0.0034	0.0035	-3.6
H3CH-NHMe2	-0.035	0.00643	-0.0096	0.0068	-4.9
MeHPH-NH3	-0.045	0.00776	0.0185	0.0065	-4.8
HSH-BrH	0.004	0.00501	0.0030	0.0041	-4.7
HOPh-FMe	-0.031	0.00596	0.0017	0.0022	-6.9
H2PH-OH2	-0.047	0.00764	0.0080	0.0038	-4.3
FH-FNF2	0.014	0.01286	0.0065	0.0079	-4.3
BrH-BrH	0.017	0.00949	0.0291	0.0186	-6.9
FH-FOF	0.010	0.01479	0.0087	0.0111	-4.3
FH-ClOCl	0.038	0.01412	0.0049	0.0206	-5.9
HSH-PH2Me	-0.011	0.00949	0.0070	0.0167	-9.4
MeSH-NH2Ph	-0.100	0.01502	0.0160	0.0195	-15.5
MeOH-PH3	0.027	0.01242	0.0308	0.0169	-11.7
MeSH-OHMe	-0.048	0.01648	0.0136	0.0154	-13.5
MeHNH-OMe2	-0.077	0.01468	0.0091	0.0081	-16.1
MeHNH-NMe3	-0.147	0.01737	0.0363	0.0197	-20.7
MeHNH-NH3	-0.120	0.01658	0.0175	0.0160	-15.2
ClH-SH2	0.021	0.01834	0.0723	0.0531	-16.1
PhOH-PH2Me	0.103	0.01594	0.0227	0.0361	-21.0
HSH-NH2Me	-0.094	0.02537	0.0722	0.0477	-22.3
MeOH-PMe3	0.038	0.01800	0.0197	0.0457	-22.2
ClH-PH2Me	0.037	0.02175	0.1135	0.0780	-21.9
FH-FH	-0.016	0.02596	0.0281	0.0227	-18.9
BrH-OH2	-0.084	0.02968	0.0746	0.0478	-23.4
MeOH-OH2	-0.115	0.02541	0.0336	0.0238	-22.9
HOH-OH2	-0.118	0.02517	0.0341	0.0228	-23.4
MeOH-OHMe	-0.111	0.02774	0.0393	0.0272	-25.9
FH-SH2	0.046	0.02421	0.0426	0.0577	-23.5
HOH-OHEt	-0.095	0.02734	0.0337	0.0263	-26.6
FH-OHCl	-0.122	0.03420	0.0490	0.0354	-24.7
ClH-OH2	-0.081	0.03275	0.0821	0.0504	-28.0
HOH-NMe3	-0.161	0.03491	0.0579	0.0471	-36.9
HOH-NH3	-0.119	0.02930	0.0510	0.0431	-31.5
MeOH-NH3	-0.119	0.03027	0.0592	0.0473	-32.1
FH-PH2Me	0.058	0.02767	0.0690	0.0829	-31.1
HOH-NHMe2	-0.120	0.03438	0.0553	0.0509	-36.6
HOH-NH2Me	-0.107	0.03237	0.0535	0.0495	-34.6
MeOH-NH2Me	-0.097	0.03318	0.0641	0.0526	-35.6
FH-OH2	-0.126	0.04308	0.0780	0.0587	-41.0
FH-OHMe	-0.115	0.04921	0.0879	0.0711	-46.6
ClH-NH3	-0.067	0.05355	0.1800	0.1376	-49.5
FH-OMe2	-0.101	0.05257	0.0902	0.0768	-49.3

Table S5: *Details of the binding energies and quantum mechanical descriptor values for the 45 complex systems studied with MP2/aug–TZVP level of theory.*

Complex	MOC	ρ	OWBO	WBI	E_I (kJ/mol)
HSH-FNF2	-0.005	0.00368	-0.0012	0.0012	-1.1
ClH-FOF	-0.018	0.00696	-0.0024	0.0066	-0.8
BrH-FNF2	-0.002	0.00538	0.0064	0.0027	-1.8
H3CH-OMe2	-0.052	0.00601	-0.0048	0.0034	-2.6
H3CH-NHMe2	-0.052	0.00656	-0.0096	0.0065	-2.7
MeHPH-NH3	-0.079	0.00776	0.0068	0.0050	-2.0
HSH-BrH	-0.006	0.00500	0.0006	0.0030	-3.1
HOPh-FMe	-0.035	0.00610	-0.0006	0.0024	-5.2
H2PH-OH2	-0.070	0.00768	0.0096	0.0031	-2.6
FH-FNF2	0.003	0.01274	0.0032	0.0060	-2.9
BrH-BrH	0.004	0.00934	0.0254	0.0146	-4.7
FH-FOF	-0.001	0.01461	0.0044	0.0085	-3.1
FH-ClOCl	0.023	0.01385	0.0032	0.0161	-3.3
HSH-PH2Me	-0.043	0.00941	0.0062	0.0132	-6.0
MeSH-NH2Ph	-0.206	0.01513	0.0125	0.0172	-12.3
MeOH-PH3	0.004	0.01243	0.0130	0.0143	-9.1
MeSH-OHMe	-0.086	0.01643	0.0084	0.0127	-10.4
MeHNH-OMe2	-0.117	0.01468	0.0244	0.0109	-13.2
MeHNH-NMe3	-0.263	0.01757	0.0026	0.0185	-15.6
MeHNH-NH3	-0.190	0.01648	0.0201	0.0132	-11.0
ClH-SH2	-0.006	0.01804	0.0694	0.0434	-10.5
PhOH-PH2Me	0.062	0.01593	0.0283	0.0313	-17.8
HSH-NH2Me	-0.153	0.02525	0.0604	0.0404	-15.0
MeOH-PMe3	0.028	0.01793	0.0750	0.0473	-17.5
ClH-PH2Me	0.005	0.02142	0.1043	0.0660	-14.9
FH-FH	-0.033	0.02533	0.0220	0.0176	-15.8
BrH-OH2	-0.124	0.02922	0.0675	0.0406	-18.1
MeOH-OH2	-0.175	0.02519	0.0339	0.0199	-18.7
HOH-OH2	-0.175	0.02484	0.0304	0.0190	-19.2
MeOH-OHMe	-0.177	0.02762	0.0348	0.0232	-21.6
FH-SH2	0.029	0.02383	0.0408	0.0488	-18.2
HOH-OHEt	-0.162	0.02714	0.0291	0.0224	-22.1
FH-OHCl	-0.172	0.03381	0.0469	0.0302	-21.6
ClH-OH2	-0.129	0.03222	0.0736	0.0419	-21.2
HOH-NMe3	-0.317	0.03511	0.0408	0.0490	-30.1
HOH-NH3	-0.177	0.02899	0.0489	0.0370	-25.4
MeOH-NH3	-0.180	0.03008	0.0576	0.0409	-25.8
FH-PH2Me	0.037	0.02723	0.0645	0.0727	-24.2
HOH-NHMe2	-0.233	0.03438	0.0534	0.0456	-29.8
HOH-NH2Me	-0.181	0.03220	0.0523	0.0435	-27.9
MeOH-NH2Me	-0.178	0.03314	0.0639	0.0467	-28.8
FH-OH2	-0.174	0.04236	0.0721	0.0502	-34.6
FH-OHMe	-0.174	0.04867	0.0827	0.0624	-39.6
ClH-NH3	-0.132	0.05295	0.1728	0.1216	-37.8
FH-OMe2	-0.188	0.05225	0.0882	0.0684	-42.1

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.*

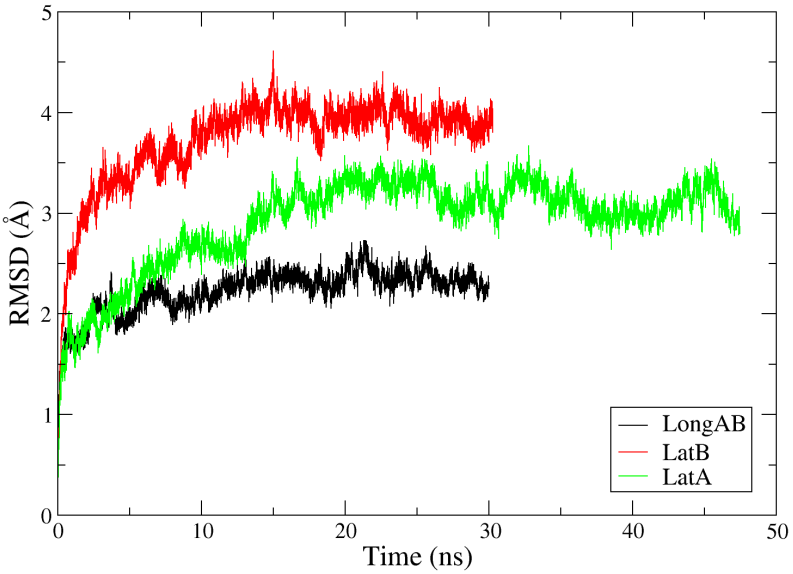

Figure S2: *An all-atom model of the LongAB system with subunit assignment.*

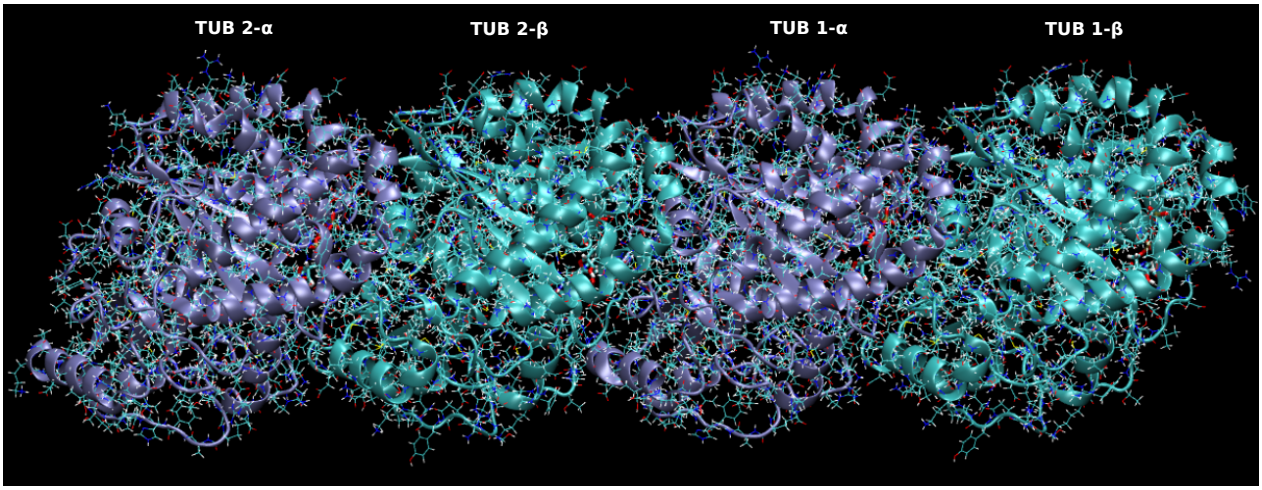

Table S6: *Energy of hydrogen bonds in the LongAB interface in kJ/mol. SS# is snapshot number.*

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.*

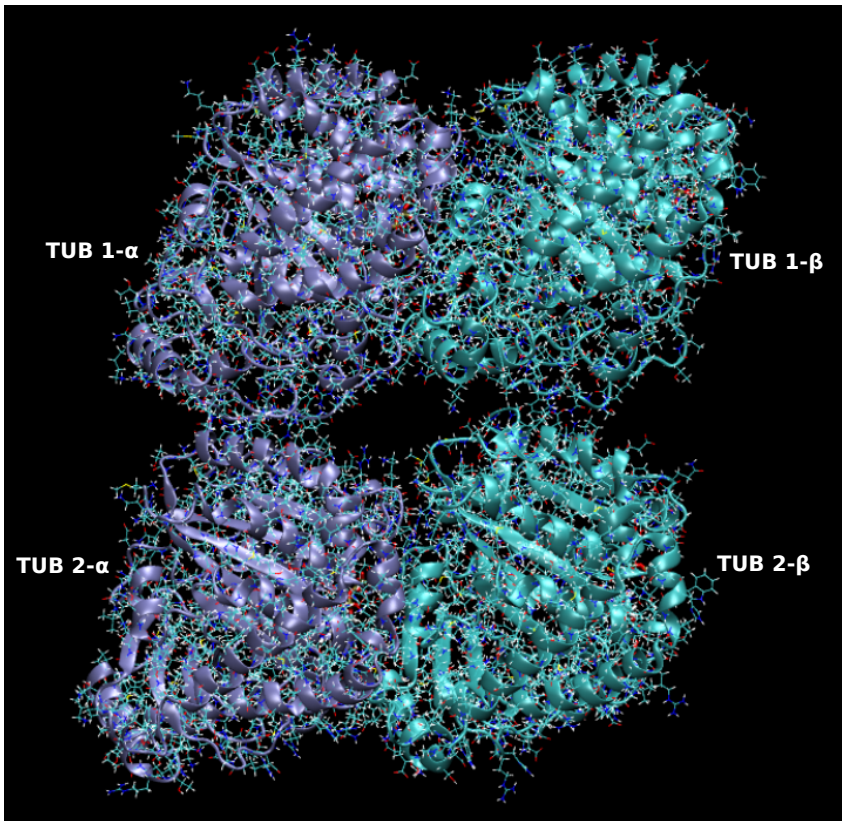

Table S7: *Energy of hydrogen bonds in the LatB interface in kJ/mol. SS# is snapshot number.*

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 S8: *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

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