(A) *ATP*

HB Broken	domain	t(ns)	occ
K240-Y307	L11-L14	229.44	0.83
K240-E311	L11-α6	634.80	0.81
D147-S149	L8a-L8a	894.24	0.85
S224-N332	β7-NL	918.24	0.81
G76-N332	L3a-NL	920.40	0.91
R190-D231	sw-I-β7	1042.56	0.99
T92-D231	α2a-β7	1340.16	0.97
E96-R190	α2a-sw-I	1584.00	0.93
E136-H191	β4-sw-I	1677.12	0.81
T195-N198	sw-I-sw-I	1825.68	0.97
A193-S201	sw-I-sw-I	1826.16	0.93
N216-Q221	β6-L10	2016.72	0.96
R203-E250	sw-I-α4	3593.28	0.86

HB Formed	domain	t(ns)	occ
A83-L232	β3-β7	1332.00	0.87
E136-R190	β4-sw-I	1584.96	0.99
E157-R278	β5a-L12	1890.48	0.93
H205-S257	β6-α4	2664.00	0.87
I137-N253	β4-α4	2758.08	0.81
R190-E250	sw-I-α4	2948.64	0.90
S202-R203	sw-I-sw-I	3900.72	0.84

NP Broken	domain	t(ns)	occ
K213-L335	β6-NL	716.16	0.82
N8-K326	CS-NL	910.32	0.97
Y77-V329	L3a-NL	916.08	0.90
L99-I183	L5-α3	1251.36	0.92
V230-L232	β7-β7	1341.84	0.94
H191-S204	sw-I-sw-I	1676.88	0.85
T195-S201	sw-I-sw-I	1820.40	0.91
V194-E199	sw-I-sw-I	1825.20	0.98
A193-R203	sw-I-sw-I	1833.84	0.98
E215-K222	β6-β7	2004.96	0.99
E136-S204	β4-sw-I	2673.84	0.96
L139-E250	β4-α4	2675.76	0.96
Y138-S204	β4-sw-I	2688.00	0.99
E250-I254	α4-α4	2883.12	0.80

NP Formed	domain	t(ns)	occ
K91-A233	P-loop-β7	1118.64	0.99
I183-K187	α3-α3	1142.88	0.89
K91-D231	P-loop-β7	1323.60	0.93
E215-Q218	β6-L10	2143.68	0.83
L232-I254	β7-α4	2809.92	0.83

(B) *Kin-only*

HB Broken	domain	t(ns)	occ
A5-V329	CS-NL	571.20	0.86
S289-N327	α5-NL	579.36	0.92
G291-N327	L13-NL	579.84	0.91
S289-T296	α5-β8	591.36	0.81
D288-N293	α5-L13	619.20	0.86
E136-H191	β4-sw-I	1284.72	0.90
R190-D231	sw-I-β7	1299.36	0.99
A193-S201	sw-I-sw-I	1302.72	0.95
T195-N198	sw-I-sw-I	1348.80	0.95
D158-R161	β5a-L8b	1355.76	0.91
N216-Q221	β6-L10	2125.20	0.93
G245-D249	L11-α4	2318.64	0.84
A246-E250	α4-α4	2348.16	0.90
V247-A251	α4-α4	2743.92	0.82

HB Formed	domain	t(ns)	occ
R203-E250	sw-I-α4	544.80	0.96
D288-S289	α5-α5	660.24	0.95
E6-K10	CS-β1	930.48	0.93
R190-S206	sw-I-β6	1333.68	0.83
R278-A337	L12-NL	1780.08	0.83
M1-D49	CS-β1c/β2	2441.28	0.97
D3-R50	CS-β2	2443.44	0.99

NP Broken	domain	t(ns)	occ
D288-G292	α5-L13	628.56	0.97
E6-T328	CS-NL	770.88	0.83
K150-L153	L8a-L8a	801.12	0.84
E6-K326	CS-NL	915.60	0.81
T195-S201	sw-I-sw-I	1317.84	0.85
E215-K222	β6-β7	2191.92	0.86
A243-V247	L11-α4	2307.84	0.86
A246-D249	α4-α4	2341.92	0.89
R50-D64	β2-α1a	2448.48	0.94
V247-E250	α4-α4	2754.48	0.84
L248-K252	α4-α4	2898.96	0.81

NP Formed	domain	t(ns)	occ
Y228-L286	β7-α5	634.56	0.85
Y228-S289	β7-α5	649.68	0.98
N78-S289	L3a-α5	663.36	0.96
R143-K150	β5-L8a	864.96	0.89
Y277-T336	L12-NL	2778.48	0.84
Y277-L335	L12-NL	2782.80	0.90
V275-L335	L12-NL	2790.96	0.95
L268-L335	α4-NL	2799.60	0.84

Supplementary File 2. Intra-kinesin hydrogen bonds (HB) and nonpolar (NP) contacts that break or form during each simulation. The corresponding domain names, transition time, and average occupancy (occ) before breakage or after formation of a contact are shown. Only clear transitions were considered where the average occupancy before breakage or after formation is greater than 80%. **(A)** *ATP*, **(B)** *Kin-only*. **Next page: (C)** *ADP+Pi*, **(D)** ADP_{pre}, **(E)** APO_{α}, and **(F)** *APO*.