

(C) ADP+Pi

HB Broken	domain	t(ns)	occ
R190-D231	sw-l- β 7	947.28	0.99
H191-R203	sw-l-sw-l	971.52	0.90
T195-N198	sw-l-sw-l	972.00	0.94
N198-H200	sw-l-sw-l	1011.12	0.87
A193-S201	sw-l-sw-l	1042.80	0.98
E36-V51	β 1a/b- β 2	1350.96	0.86
E136-H191	β 4-sw-l	1354.08	0.93
E236-N255	sw-ll- α 4	1480.56	0.96
N216-Q221	β 6-L10	2002.56	0.95
Q214-L223	β 6- β 7	2632.80	0.87
R203-E236	sw-l-sw-ll	5343.84	0.91
HB Formed	domain	t(ns)	occ
E157-R278	β 5a-L12	169.44	0.99
E136-R190	β 4-sw-l	1691.52	0.97
V73-G225	α 1b- β 7	2112.96	0.85
E199-R203	sw-l-sw-l	3814.80	0.85
D147-R171	L8a- β 5c	5136.96	0.89

NP Broken	domain	t(ns)	occ
V194-E199	sw-l-sw-l	977.04	0.97
A193-R203	sw-l-sw-l	1019.76	0.96
T195-S201	sw-l-sw-l	1024.32	0.93
V192-S202	sw-l-sw-l	1345.92	0.82
H191-S204	sw-l-sw-l	1346.40	0.84
E215-K222	β 6- β 7	2020.08	0.98
N198-S201	sw-l-sw-l	3717.12	0.87
NP Formed	domain	t(ns)	occ
G76-S224	L3a- β 7	2109.84	0.83

(D) ADP_{pre}

HB Broken	domain	t(ns)	occ
N216-Q221	β 6-L10	390.00	0.93
H200-S204	sw-l-sw-l	1042.32	0.81
N198-S202	sw-l-sw-l	1054.56	0.80
N196-H200	sw-l-sw-l	1078.32	0.95
M197-S201	sw-l-sw-l	1091.76	0.97
D37-T38	β 1a/b- β 1b	2039.52	0.83
HB Formed	domain	t(ns)	occ
Q86-S235	P-loop-sw-ll	151.44	0.89
E6-K68	CS- α 1b	386.16	0.96
K91-D231	P-loop- β 7	717.60	0.86
N78-S224	L3a- β 7	2367.36	0.92

NP Broken	None.		
NP Formed	domain	t(ns)	occ
R16-G90	β 1-P-loop	440.64	0.85
L223-N293	β 7-L13	2388.00	0.92
N78-L223	L3a- β 7	2397.60	0.89
V162-K222	β 5b- β 7	2420.16	0.91

(E) APO _{α}

HB Broken	domain	t(ns)	occ
Q86-S303	P-loop- β 8	416.64	0.84
HB Formed	domain	t(ns)	occ
Q214-N216	β 6- β 6	723.36	0.87

NP Broken	domain	t(ns)	occ
V238-A243	L11-L11	182.88	0.87
E215-K222	β 6- β 7	613.92	0.87
L126-N216	β 4- β 6	646.56	0.83
NP Formed	domain	t(ns)	occ
V238-K252	L11- α 4	191.28	0.94
F128-L223	β 4- β 7	702.72	0.81
L126-T219	β 4-L10	736.08	0.88
V70-Y118	α 1b- α 2b	762.48	0.93

(F) APO

HB Broken	None.		
HB Formed	domain	t(ns)	occ
D49-K323	β 1c/ β 2- α 6	1206.00	0.94
K237-A243	L11-L11	3672.48	0.86

NP Broken	None.		
NP Formed	domain	t(ns)	occ
V11-K323	β 1- α 6	1221.84	0.94
Q320-I325	α 6- α 6	1680.96	0.85
S239-E244	L11-L11	3793.68	0.87

(A) ATP

Hbond	Domain	Occ. (time)
S259- α E415	$\alpha 4$	0.95
K237- α E414	L11	0.80
R161- β D427	L8b	0.99
R278- β D427	L12	0.97
E157- β E420	$\beta 5a$	0.89
R278- β E420	L12	0.99 (1886.88)
Nonpolar	Domain	Occ. (time)
K252- α G412	$\alpha 4$	0.97
K256- α V409	$\alpha 4$	0.93
S259- α V409	$\alpha 4$	0.88
S239- α Y108	L11	0.85
Y274- β E431	L12	0.91
Y274- β Q434	L12	0.88
H156- β E420	$\beta 5a$	0.85
Y274- β D427	L12	0.84
Y274- β S430	L12	0.83
H156- β M416	$\beta 5a$	0.81
E157- β E420	$\beta 5a$	0.90 (795.60)

(B) ADP+Pi

Hbond	Domain	Occ. (time)
S259- α E415	$\alpha 4$	0.97
N263- α R402	$\alpha 4$	0.97
K237- α E414	L11	0.96
K237- α E417	L11	0.91
K313- α E423	$\alpha 6$	0.84
R161- β D427	L8b	1.00
R278- β E420	L12	0.97
E157- β E420	$\beta 5a$	0.96
R278- β D427	L12	0.90
Y274- β E431	L12	0.81 (1497.12)
Nonpolar	Domain	Occ. (time)
S259- α V409	$\alpha 4$	0.99
K256- α V409	$\alpha 4$	0.98
K256- α G410	$\alpha 4$	0.87
S239- α Y108	L11	0.84
K252- α G412	$\alpha 4$	0.84
K256- α G410	$\alpha 4$	0.90 (183.60)
H156- β E420	$\beta 5a$	0.99
Y274- β D427	L12	0.94
H156- β M416	$\beta 5a$	0.92
E157- β E420	$\beta 5a$	0.92
Y274- β Q434	L12	0.91
Y274- β E431	L12	0.91
E157- β S423	$\beta 5a$	0.90
R278- β D427	L12	0.86
Y274- β S430	L12	0.84
K159- β T419	$\beta 5a$	0.82

(C) ADP_{pre}

Hbond	Domain	Occ. (time)
K237- α E417	L11	0.81
R278- β E420	L12	0.98 (728.40)
R284- β E420	$\alpha 5$	0.97 (716.88)
R278- β D427	L12	0.98 {879.60}
Nonpolar	Domain	Occ. (time)
K256- α V409	$\alpha 4$	0.95
S259- α V409	$\alpha 4$	0.83
V329- α R422	NL	0.94 (1851.84)
V329- α E423	NL	0.92 (1857.84)
L317- α G416	$\alpha 6$	0.85 (388.32)
Y274- β E431	L12	0.89
Y274- β Q434	L12	0.88
Y274- β S430	L12	0.87
Y274- β D427	L12	0.82

(D) APO _{α}

Hbond	Domain	Occ. (time)
S259- α E415	$\alpha 4$	0.94
E270- α R402	$\alpha 4$	0.91
K44- α E423	L2	0.90
R321- α E415	$\alpha 6$	0.87
K44- α E420	L2	0.87 (307.44)
S235- α E414	sw-II	0.83 {159.60}
R161- β D427	L8b	1.00
Nonpolar	Domain	Occ. (time)
L317- α G416	$\alpha 6$	0.88
Y274- β D427	L12	0.97
Y274- β Q434	L12	0.95
Y274- β E431	L12	0.94
Y274- β S430	L12	0.88

(E) APO

Hbond	Domain	Occ. (time)
K237- α E414	L11	0.89
K44- α E423	L2	0.89
D279- β R264	L12	0.99
R161- β D427	L8b	0.99
R278- β N424	L12	0.96
R278- β E196	L12	0.83
R284- β E420	$\alpha 5$	0.90 (2399.76)
Nonpolar	Domain	Occ. (time)
K256- α V409	$\alpha 4$	0.95
S259- α V409	$\alpha 4$	0.94
L248- α Y108	$\alpha 4$	0.90
K252- α G412	$\alpha 4$	0.89
L317- α G416	$\alpha 6$	0.85
Y274- β Q434	L12	0.96
Y274- β E431	L12	0.95
Y274- β S430	L12	0.87

Supplementary File 3. Kinesin-MT contacts. For a residue pair in the first column, α and β in front of the second residue denote the tubulin type. Domain: domain name to which the kinesin residue belongs (Figure Supplement 1). Contacts with α - or β -tubulin are ordered based on occupancy. Contacts whose occupancy after breakage or formation is greater than 80% have the transition time (nanoseconds) in parentheses (formation) or in curly brackets (breakage).