

S2 Table. Occurrences of the hydrogen bond interactions across the TMD-NBD interface in the 300-ns trajectories.

TMD	NBD	occurrence (%) ^a					
		ATP/ADP.IP		ADP.IP/ATP		ATP/ATP	
		chain A	chain C	avg ^b	stdev ^c	avg	stdev
Gln8	Trp91	48.0	29.4	59.0	34.0	34.3	35.0
Gln8	Gly121	36.5	23.1	41.1	34.2	22.6	27.1
Arg209	Leu96	40.4	13.7	29.7	14.7	26.7	13.0
Ser220	Ser79	2.1	2.6	33.4	35.3	4.2	8.6
Arg222	Met49	49.1	8.8	48.4	15.6	57.1	8.8
Gln223	Arg75	90.9	4.3	82.5	11.4	89.1	4.0
Gln223	Tyr77	92.1	1.9	92.9	2.5	89.4	3.2
Gln223	Gln143	100.0	0.0	100.0	0.0	100.0	0.0
Thr270	Ala87	36.3	18.4	29.5	21.4	40.1	19.4
chain B		occurrence (%)					
Glu1	Glu105	5.6	3.7	8.4	4.1	34.1	33.5
Leu2	Thr104	12.2	15.8	24.6	12.6	41.4	34.4
Gln8	Trp91	50.5	42.3	50.1	43.7	49.4	44.4
Gln8	Gly121	36.7	35.5	39.2	37.0	33.7	31.5
Arg209	Leu96	37.5	8.4	32.4	15.7	28.1	13.0
Asn212	His92	8.5	11.6	24.7	37.4	46.0	29.7
Ser220	Gln82	16.1	4.8	27.7	24.1	36.4	11.7
Arg222	Met49	48.2	14.0	45.4	14.8	58.9	14.9
Gln223	Arg75	87.6	2.5	85.1	5.4	84.6	4.1
Gln223	Tyr77	92.3	0.9	93.4	1.6	91.2	3.0
Gln223	Gln143	100.0	0.0	100.0	0.0	100.0	0.0
Thr270	Ala87	41.2	9.1	33.4	18.3	13.4	22.2

^a Hydrogen bond is defined the same as described in S1 Table. Only the hydrogen bond interactions with occurrence of over 30% are listed.

^b Average occurrence of hydrogen bond in five parallel 300-ns trajectories of the system.

^c Standard deviation of the occurrences of hydrogen bond in five parallel trajectories.