The table below shows the rate constants used for the analysis in the paper expect when explicitly stated otherwise. The columns provide the transition name, the rate used, the range from literature when applicable, the references for that range, and finally if needed a reason explaining why this rate is used. The table is color coded to show the method for obtaining the rate constant, as described in the following text. Uncolored rows represent rates which were obtained from publication. In some cases we chose one particular publication over another (that reference is shown in bold), or we adjusted the rate constant within the published range. Unfortunately this was early in our research project, and we do not have information stating our particular reason for choosing the rate constant, other than it being within the published range.

The orange bands designate when the rate is calculated using Hanggi's rate equation for escaping an energy barrier with a cusp as described in the manuscript. This equation is seen below:

$$k_{cusp} = \frac{DU''(x_0)}{2\pi k_B T}\sqrt{\frac{\pi E_b}{k_B T}}e^{\frac{E_b}{k_B T}} \qquad \text{Equation 1}$$

In the previous equation is the escape rate to get over the barrier, D is the diffusion constant, is the second spatial derivative of the energy landscape evaluated at the energy minimum, and is the cusp barrier height. In this case is the energy of the WLC extended from the equilibrium position to the binding site. All of these rates are for an unbound head stepping and binding to an adjacent binding site. In these rows the contour length, L_0, and distance to the binding site, d, are specified. The WLC parameters are given in the manuscript.

The rows are colored yellow when we used Bell's equation to calculate the unbinding rate.

$$k = k_0 e^{\int_{l-\delta}^{l} F(x)dx} \qquad \text{Equation 2}$$

where is the unbinding rate with no force applied, l is the distance from the unbound equilibrium position to the position at its binding site (i.e. the neck linker is significantly extended when the head is bound), and is the distance from the binding site to the transition state. For this work we used a δ of 2.5 nm (see main text for references). In each of these cases the neck linker tension accelerates unbinding above the rate of unbinding under no tension, k_0. The extension of the neck linker is labeled in the table as s. The rates for k_0 are obtained from the literature (blank color coding).

The green rows indicate the two rate constants for which we could not find published rates and which were not produced by our modeling. In these two cases we could only find a similar transition but for a bound head not an unbound head. So for both of these rates we used the published bound head rate constant. These two rates come from a rare state and thus do not impact the results regardless of their particular values.

When our chemical gating model changed the rate constants we colored these rows purple. There are two different configurations in which we felt that the neck would not dock to the kinesin head: when a

bound docked head is in front of a bound undocked head and when both bound heads are docked. We did not note when the rate is affected by chemical gating and the Bell equation simultaneously. Those rows were left yellow. However because we specify the contour length and distance the docking configuration could be deduced using Figure 1.

The blue rows are the inorganic phosphate release rows. We could not keep these rates within the published range and observe correct run time and run length (similar to Shastry et al as noted in the main text). We decided to raise the inorganic phosphate release to 250 /s except for when ADP-P_i was in front of an undocked state. Then we lowered the value to 25 /s which is within range but different from the other rates for no reason other than it lowered the run length and run time too much if set to 250 s^{-1}.

These rate constants can be loaded into our software using the file "Rate Constants used.dat" at https://sourceforge.net/project/admin/explorer.php?group_id=362373.

Table S1. Transitions rates used in the Paper

Transition	Rate	Range	Reference	Reason
Unbound ADP Release ADP	2.000E-3	.002-.1	[1-4]	
Unbound ADP Capture P	2.000E+1	25	[1]	
Unbound Empty Bind ADP	6.000E+0	6	[4]	
Unbound Empty Bind ATP	4.000E+0	4	[1]	
Unbound ADP Stepping with Empty Forward	3.675E+1			Equation 1: L_0=9.88 nm d=8.2 nm
Unbound ADP Stepping with Empty Backward	3.675E+1			Equation 1: L_0=9.88 nm d=8.2 nm
Unbound ATP Hydrolyze to ADP-P	1.000E+1	6-10	[1,4,**5**]	
Unbound ATP Release ATP	5.000E+1	150		Could not find this value so used the value from the bound case
Unbound ADP-P Release P	2.500E+2	20-250	[1,2,6]	
Unbound ADP-P Form ATP	2.500E+1			Could not find this value so used the bound ATP synthesis rate
Unbound Empty Stepping with Empty Forward	3.675E+1			Equation 1: L_0=9.88 nm d=8.2 nm
Unbound Empty Stepping with Empty Backward	3.675E+1			Equation 1: L_0=9.88 nm d=8.2 nm
Unbound ADP Stepping with ADP-P Forward	4.900E+5			Equation 1: L_0=6.08 nm d=4.4 nm
Unbound ADP Stepping with ADP-P Backward	0.000E+0			Equation 1: L_0=6.08 nm d=12 nm
Unbound ADP Stepping with ADP Forward	3.675E+1			Equation 1: L_0=9.88 nm d=8.2 nm
Unbound ADP Stepping with	3.675E+1			Equation 1: L_0=9.88 nm

ADP Backward				d=8.2 nm
Unbound ADP Stepping with ATP Forward	4.900E+5			Equation 1: L_0=6.08 nm d=4.4 nm
Unbound ADP Stepping with ATP Backward	0.000E+0			Equation 1: L_0=6.08 nm d=12 nm
Unbound Empty Stepping with ADP-P Forward	4.900E+5			Equation 1: L_0=6.08 nm d=4.4 nm
Unbound Empty Stepping with ADP-P Backward	0.000E+0			Equation 1: L_0=6.08 nm d=12 nm
Unbound Empty Stepping with ADP Forward	3.675E+1			Equation 1: L_0=9.88 nm d=8.2 nm
Unbound Empty Stepping with ADP Backward	3.675E+1			Equation 1: L_0=9.88 nm d=8.2 nm
Unbound Empty Stepping with ATP Forward	4.900E+5			Equation 1: L_0=6.08 nm d=4.4 nm
Unbound Empty Stepping with ATP Backward	0.000E+0			Equation 1: L_0=6.08 nm d=12 nm
Unbound ATP Stepping with ADP-P Forward	0.000E+0			Equation 1: L_0=2.28 nm d=8.2 nm
Unbound ATP Stepping with ADP-P Backward	0.000E+0			Equation 1: L_0=2.28 nm d=8.2 nm
Unbound ATP Stepping with ADP Forward	0.000E+0			Equation 1: L_0=6.08 nm d=12 nm
Unbound ATP Stepping with ADP Backward	4.900E+5			Equation 1: L_0=6.08 nm d=4.4 nm
Unbound ATP Stepping with ATP Forward	0.000E+0			Equation 1: L_0=2.28 nm d=8.2 nm
Unbound ATP Stepping with ATP Backward	0.000E+0			Equation 1: L_0=2.28 nm d=8.2 nm
Unbound ATP Stepping with Empty Forward	0.000E+0			Equation 1: L_0=6.08 nm d=12 nm
Unbound ATP Stepping with Empty Backward	4.900E+5			Equation 1: L_0=6.08 nm d=4.4 nm
Unbound ADP-P Stepping with ADP-P Forward	0.000E+0			Equation 1: L_0=2.28 nm d=8.2 nm
Unbound ADP-P Stepping with ADP-P Backward	0.000E+0			Equation 1: L_0=2.28 nm d=8.2 nm
Unbound ADP-P Stepping with ADP Forward	0.000E+0			Equation 1: L_0=6.08 nm d=12 nm
Unbound ADP-P Stepping with ADP Backward	4.900E+5			Equation 1: L_0=6.08 nm d=4.4 nm
Unbound ADP-P Stepping with ATP Forward	0.000E+0			Equation 1: L_0=2.28 nm d=8.2 nm
Unbound ADP-P Stepping with ATP Backward	0.000E+0			Equation 1: L_0=2.28 nm d=8.2 nm
Unbound ADP-P Stepping with Empty Forward	0.000E+0			Equation 1: L_0=6.08 nm d=4.4 nm

Unbound ADP-P Stepping with Empty Backward	4.900E+5			Equation 1: L_0=6.08 nm d=4.4 nm
Bound Empty in front of Bound ATP Binding ATP	3.000E+0	1-3.8	[2,4,6-12]	
Bound Empty in front of Bound ATP Binding ADP	2.500E-1	.25	[13]	
Bound Empty in front of Bound ATP Unbinding	7.661E-1			Equation 2: L_0=6.08 nm s=4.4 nm
Bound Empty in back of Bound ATP Binding ATP	3.000E-1	.3-3.8	[2,4,6-12]	
Bound Empty in back of Bound ATP Binding ADP	2.500E-1	.25	[13]	
Bound Empty in back of Bound ATP Unbinding	2.460E+2			Equation 2: L_0=9.88 nm s=8.2 nm
Bound Empty in front of Bound ADP-P Binding ATP	3.000E+0	1-3.8	[2,4,6-12]	
Bound Empty in front of Bound ADP-P Binding ADP	2.500E-1	.25	[13]	
Bound Empty in front of Bound ADP-P Unbinding	7.661E-1			Equation 2: L_0=6.08 nm s=4.4 nm
Bound Empty in back of Bound ADP-P Binding ATP	3.000E-1	.3-3.8	[2,4,6-12]	
Bound Empty in back of Bound ADP-P Binding ADP	2.500E-1	.25	[13]	
Bound Empty in back of Bound ADP-P Unbinding	2.460E+2			Equation 2: L_0=9.88 nm s=8.2 nm
Bound Empty in front of Bound ADP Binding ATP	3.000E+0	1-3.8	[2,4,6-12]	
Bound Empty in front of Bound ADP Binding ADP	2.500E-1	.25	[13]	
Bound Empty in front of Bound ADP Unbinding	2.460E+2			Equation 2: L_0=9.88 nm s=8.2 nm
Bound Empty in back of Bound ADP Binding ATP	3.000E-1	.3-3.8	[2,4,6-12]	
Bound Empty in back of Bound ADP Binding ADP	2.500E-1	.25	[13]	
Bound Empty in back of Bound ADP Unbinding	2.460E+2			Equation 2: L_0=9.88 nm s=8.2 nm
Bound Empty in front of Bound Empty Binding ATP	3.000E+0	1-3.8	[2,4,6-12]	
Bound Empty in front of Bound Empty Binding ADP	2.500E-1	.25	[13]	
Bound Empty in front of Bound Empty Unbinding	2.460E+2			Equation 2: L_0=9.88 nm s=8.2 nm
Bound Empty in back of Bound Empty Binding ATP	3.000E-1	.3-3.8	[2,4,6-12]	
Bound Empty in back of Bound	2.500E-1	.25	[13]	

Empty Binding ADP				
Bound Empty in back of Bound Empty Unbinding	2.460E+2			Equation 2: L_0=9.88 nm s=8.2 nm
Bound Empty with Unbound Anything Binding ATP	2.000E+1	20	[14]	
Bound Empty with Unbound Anything Binding ADP	1.500E+0	1.5	[15]	
Bound Empty with Unbound Anything Unbinding	7.000E-3	.0009-.2	[3,6]	
Bound ATP in front of Bound ATP Becoming ADP-P	8.000E+0	8-300	[2,6,8-10,16,17]	
Bound ATP in front of Bound ATP Releasing ATP	5.000E+2	30-600	[2-4,6,8,9,11,12,16,18]	In our chemical gating theory this acts like ADP bound head
Bound ATP in front of Bound ATP Unbinding	7.661E-1			Equation 2: L_0=6.08 nm s=4.4 nm
Bound ATP in back of Bound ATP Becoming ADP-P	8.000E+2	100-800	[2,6,8-10,16,17]	
Bound ATP in back of Bound ATP Releasing ATP	5.000E+1	30-200	[2,4,6-8,12,15]	
Bound ATP in back of Bound ATP Unbinding	7.661E-1			Equation 2: L_0=6.08 nm s=4.4 nm
Bound ATP in front of Bound ADP-P Becoming ADP-P	8.000E+0	8-300	[2,6,8-10,16,17]	
Bound ATP in front of Bound ADP-P Releasing ATP	5.000E+2	30-600	[2-4,6,8,9,11,12,16,18]	In our chemical gating theory this acts like ADP bound head
Bound ATP in front of Bound ADP-P Unbinding	7.661E-1			Equation 2: L_0=6.08 nm s=4.4 nm
Bound ATP in back of Bound ADP-P Becoming ADP-P	8.000E+2	100-800	[2,6,8-10,16,17]	
Bound ATP in back of Bound ADP-P Releasing ATP	5.000E+1	30-200	[2,4,6-8,12,15]	
Bound ATP in back of Bound ADP-P Unbinding	7.661E-1			Equation 2: L_0=6.08 nm s=4.4 nm
Bound ATP in front of Bound ADP Becoming ADP-P	8.000E+0	8-800	[2,6,8-10,16,17]	
Bound ATP in front of Bound ADP Releasing ATP	5.000E+0	.01-300	[2-4,6,8,9,12,15]	In our chemical gating theory this acts like ADP bound head
Bound ATP in front of Bound ADP Unbinding	2.460E+2			Equation 2: L_0=9.88 nm s=8.2 nm
Bound ATP in back of Bound ADP Becoming ADP-P	8.000E+2	100-800	[2,6,8-10,16,17]	
Bound ATP in back of Bound ADP Releasing ATP	5.000E+1	30-200	[2,4,6-8,12,15]	
Bound ATP in back of Bound	7.661E-1			Equation 2: L_0=6.08 nm

ADP Unbinding				s=4.4 nm
Bound ATP in front of Bound Empty Becoming ADP-P	8.000E+0	8-800	[2,6,8-10,16,17]	
Bound ATP in front of Bound Empty Releasing ATP	5.000E+0	.01-300	[2-4,6,8,9,12,15]	In our chemical gating theory this acts like ADP bound head
Bound ATP in front of Bound Empty Unbinding	2.460E+2			Equation 2: L_0=9.88 nm s=8.2 nm
Bound ATP in back of Bound Empty Becoming ADP-P	8.000E+2	100-800	[2,6,8-10,16,17]	
Bound ATP in back of Bound Empty Releasing ATP	5.000E+1	30-200	[2,4,6-8,12,15]	
Bound ATP in back of Bound Empty Unbinding	7.661E-1			Equation 2: L_0=6.08 nm s=4.4 nm
Bound ATP with anything unbound Becoming ADP-P	4.000E+2	200->300	[14,19]	
Bound ATP with anything unbound Releasing ATP	2.000E+2	200	[14]	
Bound ATP with anything unbound Unbinding	7.000E-3	.007-.9	[6]	
Bound ADP-P in front of Bound ATP Releasing P	2.500E+2	13- >100	[4,8,11,12]	Adjusted rate constant
Bound ADP-P in front of Bound ATP Forming ATP	2.500E+1	18-25	[1,6]	
Bound ADP-P in front of Bound ATP Unbinding	7.661E-1			Equation 2: L_0=6.08 nm s=4.4 nm
Bound ADP-P in back of Bound ATP Releasing P	2.500E+2	13- >100	[4,8,11,12]	Adjusted rate constant
Bound ADP-P in back of Bound ATP Forming ATP	2.500E+1	18-25	[1,6]	
Bound ADP-P in back of Bound ATP Unbinding	7.661E-1			Equation 2: L_0=6.08 nm s=4.4 nm
Bound ADP-P in front of Bound ADP-P Releasing P	2.500E+2	13- >100	[4,8,11,12]	Adjusted rate constant
Bound ADP-P in front of Bound ADP-P Forming ATP	2.500E+1	18-25	[1,6]	
Bound ADP-P in front of Bound ADP-P Unbinding	7.661E-1			Equation 2: L_0=6.08 nm s=4.4 nm
Bound ADP-P in back of Bound ADP-P Releasing P	2.500E+2	13- >100	[4,8,11,12]	Adjusted rate constant
Bound ADP-P in back of Bound ADP-P Forming ATP	2.500E+1	18-25	[1,6]	
Bound ADP-P in back of Bound ADP-P Unbinding	7.661E-1			Equation 2: L_0=6.08 nm s=4.4 nm
Bound ADP-P in front of Bound ADP Releasing P	2.500E+2	13- >100	[4,8,11,12]	Adjusted rate constant
Bound ADP-P in front of Bound	2.500E+1	18-25	[1,6]	

ADP Forming ATP				
Bound ADP-P in front of Bound ADP Unbinding	2.460E+2			Equation 2: L_0=9.88 nm s=8.2 nm
Bound ADP-P in back of Bound ADP Releasing P	2.500E+1	13- >100	[4,8,11,12]	
Bound ADP-P in back of Bound ADP Forming ATP	2.500E+1	18-25	[1,6]	
Bound ADP-P in back of Bound ADP Unbinding	7.661E-1			Equation 2: L_0=6.08 nm s=4.4 nm
Bound ADP-P in front of Bound Empty Releasing P	2.500E+2	13- >100	[4,8,11,12]	Adjusted rate constant
Bound ADP-P in front of Bound Empty Forming ATP	2.500E+1	18-25	[1,6]	
Bound ADP-P in front of Bound Empty Unbinding	2.460E+2			Equation 2: L_0=9.88 nm s=8.2 nm
Bound ADP-P in back of Bound Empty Releasing P	2.500E+1	13- >100	[4,8,11,12]	
Bound ADP-P in back of Bound Empty Forming ATP	2.500E+1	18-25	[1,6]	
Bound ADP-P in back of Bound Empty Unbinding	7.661E-1			Equation 2: L_0=6.08 nm s=4.4 nm
Bound ADP-P with Anything Unbound Releasing P	8.100E+1	81	[14]	
Bound ADP-P with Anything Unbound Forming ATP	2.500E+1	18-25	[1,6]	
Bound ADP-P with Anything Unbound Unbinding	7.000E-3	1.67-20	[2,3]	It is generally accepted that this off rate is similar ATP and empty unbinding so it was adjusted.
Bound ADP in front of Bound ATP Capture P	2.000E+1	25	[1]	
Bound ADP in front of Bound ATP Release ADP	5.000E+2	30-600	[2-4,6,8,9,11,12,16,18]	
Bound ADP in front of Bound ATP Unbinding	2.736E+3			Equation 2: L_0=6.08 nm s=4.4 nm
Bound ADP in back of Bound ATP Capture P	2.000E+1	25	[1]	
Bound ADP in back of Bound ATP Release ADP	5.000E+2	30-600	[2-4,6,8,9,11,12,16,18]	
Bound ADP in back of Bound ATP Unbinding	8.787E+5			Equation 2: L_0=9.88 nm s=8.2 nm
Bound ADP in front of Bound ADP-P Capture P	2.000E+1	25	[1]	
Bound ADP in front of Bound ADP-P Release ADP	5.000E+2	30-600	[2-4,6,8,9,11,12,16,18]	
Bound ADP in front of Bound ADP-P Unbinding	2.736E+3			Equation 2: L_0=6.08 nm s=4.4 nm

Bound ADP in back of Bound ADP-P Capture P	2.000E+1	25	[1]	
Bound ADP in back of Bound ADP-P Release ADP	5.000E+2	30-600	[2-4,6,8,9,11,12,16,18]	
Bound ADP in back of Bound ADP-P Unbinding	8.787E+5			Equation 2: L_0=9.88 nm s=8.2 nm
Bound ADP in front of Bound ADP Capture P	2.000E+1	25	[1]	
Bound ADP in front of Bound ADP Release ADP	5.000E+0	.01-300	[2-4,6,8,9,12,15]	
Bound ADP in front of Bound ADP Unbinding	8.787E+5			Equation 2: L_0=9.88 nm s=8.2 nm
Bound ADP in back of Bound ADP Capture P	2.000E+1	25	[1]	
Bound ADP in back of Bound ADP Release ADP	5.000E+0	.01-300	[2-4,6,8,9,12,15]	
Bound ADP in back of Bound ADP Unbinding	8.787E+5			Equation 2: L_0=9.88 nm s=8.2 nm
Bound ADP in front of Bound Empty Capture P	2.000E+1	25	[1]	
Bound ADP in front of Bound Empty Release ADP	5.000E+0	.01-300	[2-4,6,8,9,12,15]	
Bound ADP in front of Bound Empty Unbinding	8.787E+5			Equation 2: L_0=9.88 nm s=8.2 nm
Bound ADP in back of Bound Empty Capture P	2.000E+1	25	[1]	
Bound ADP in back of Bound Empty Release ADP	5.000E+0	.01-300	[2-4,6,8,9,12,15]	
Bound ADP in back of Bound Empty Unbinding	8.787E+5			Equation 2: L_0=9.88 nm s=8.2 nm
Bound ADP with Anything Unbound Capture P	2.000E+1	25	[1]	
Bound ADP with Anything Unbound Release ADP	1.100E+2	110	[15]	
Bound ADP with Anything Unbound Unbinding	2.500E+1	1-25	[6]	

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