Allosteric Control of Kinesin's Motor Domain by Tubulin: A Molecular Dynamics Study - Electronic Supplementary Information (ESI)

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Appendix: Choice of coordinate system

In order to visualize how the molecular structure of kinesin depends on its nucleotide state, we have compared the dominant conformations of the *ATP* and *ADP* states as well as those of the *ATP* and *Empty* states. For a given pair of states, this comparison was performed by superimposing their β sheet cores and identifying the rotations of the $\alpha 4$ and $\alpha 6$ helices. In order to describe these rotations in an unambiguous way, we used a Cartesian coordinate system (x, y, z) that was defined with respect to the dominant conformation of the *ATP* state, both in solution and attached to tubulin.

The y-axis of this coordinate system was taken to be parallel to the long principal axis of the $\alpha 4$ helix, which contains residues 272 to 287, and to point from residue 287 to residue 272. Furthermore, the z-axis was taken to be parallel to the straight line that goes through the C_α atoms of residues 272 and 217 and to point from residue 272 to residue 217. The latter residue belongs to the $\beta 6$ strand. The x-axis then follows from the requirement that the three axes form a right-handed triad.

This choice of the coordinate axes applies both to kinesin in solution and attached to tubulin. In the latter case, the choice has the useful property that the long principal axis of tubulin is perpendicular to the z-axis and, thus, parallel to the (x, y)-plane, see Fig. S1 and Fig. S2. In these figures, the long principal axis of tubulin is parallel to the X-axis. The angle θ between the x-axis and the X-axis was found to be $\theta = 23°$, see Fig. S2.

Figure S1:

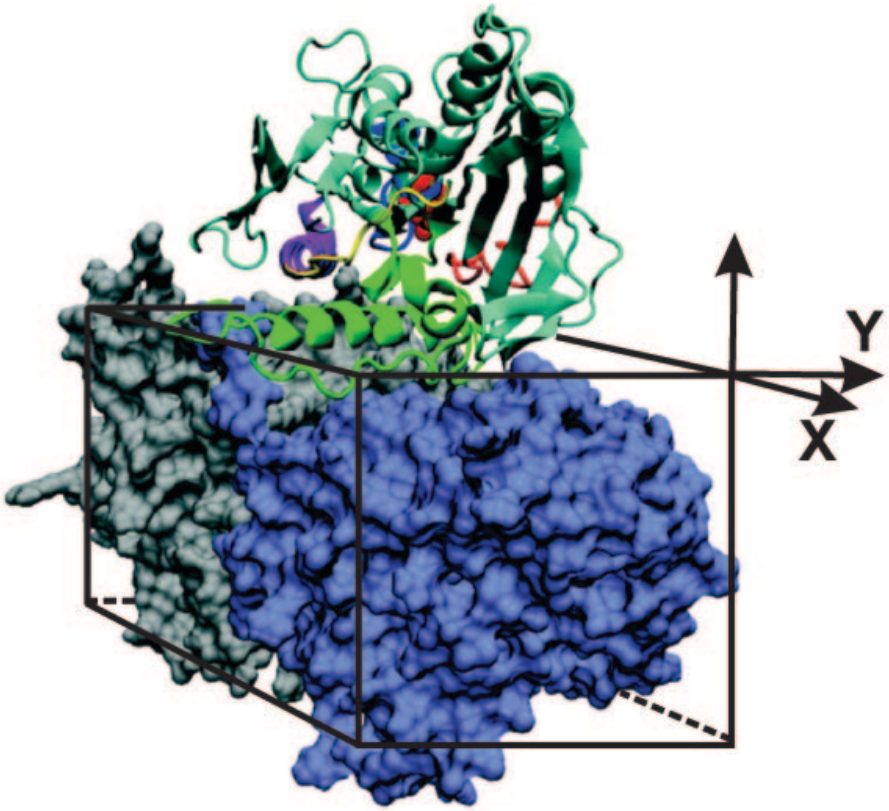

Figure S1: Configuration of the kinesin motor domain attached to a tubulin dimer. Kinesin is shown in ribbon representation with the same color coding as in Fig. 1. The tubulin dimer is depicted in surface representation; the colors distinguish between α-tubulin (gray) and β-tubulin (blue). The X-axis is parallel to the long principal axis of tubulin and points from the α- to the β-tubulin, i.e., from the minus to the plus end of the filament.

Figure S2:

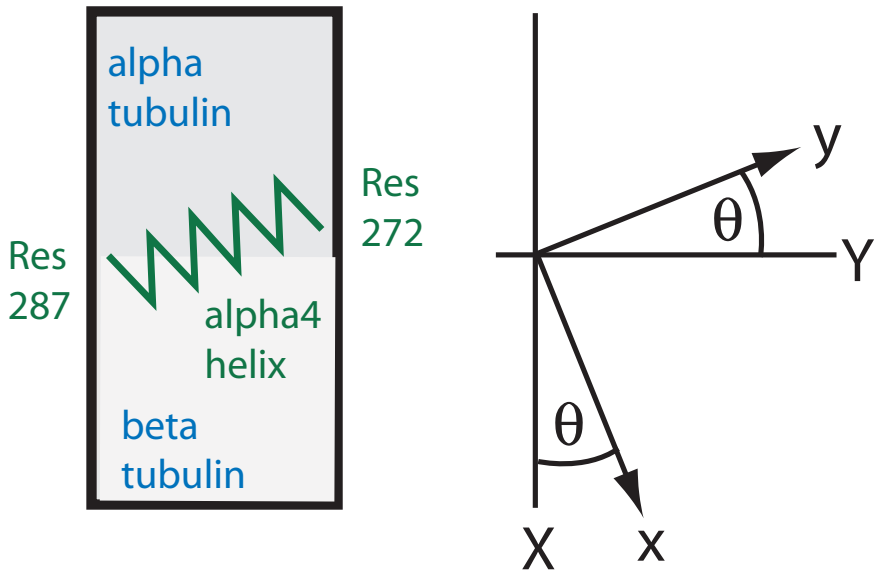

Figure S2: The orientation of the $\alpha 4$ helix relative to the tubulin dimer when viewed from above, i.e., from positive values of z. The coordinates x and y are chosen as explained in Text S1 with the y-axis being parallel to the $\alpha 4$ helix. The X-axis is parallel to the long principal axis of tubulin; the angle θ between the x- and X-axis is $\theta = 23°$.

Table S1: Displacements of neck linker

ATP binding			Phosphate release		
N-terminus of neck linker:					
Comp.	Average	SD	Comp.	Average	SD
x_T-x_E	-0.196	0.216	x_D-x_T	0.109	0.238
y_T-y_E	0.051	0.117	y_D-y_T	-0.073	0.098
z_T-z_E	0.169	0.212	z_D-z_T	-0.049	0.189
Center-of-mass of neck linker:					
Comp.	Average	SD	Comp.	Average	SD
x_T-x_E	-0.09	0.204	x_D-x_T	0.157	0.186
y_T-y_E	-0.019	0.122	y_D-y_T	0.132	0.164
z_T-z_E	0.093	0.194	z_D-z_T	-0.455	0.261
C-terminus of neck linker:					
Comp.	Average	SD	Comp.	Average	SD
x_T-x_E	-0.003	0.307	x_D-x_T	-0.026	0.4
y_T-y_E	-0.181	0.395	y_D-y_T	0.386	0.652
z_T-z_E	0.061	0.401	z_D-z_T	-0.793	0.59

Table S1: Average value and standard deviation (SD) of the neck linker's displacements in units of nm for the motor domain attached to tubulin. The three components of the displacement and SD vectors are given with respect to the coordinates x, y, and z as defined in Text S1; the subscripts E, T, and D refer to the *Empty, ATP, and ADP* state of the motor domain, respectively. The first three columns on the left correspond to ATP binding, i.e., to the transition from the *Empty* to the *ATP* nucleotide state; the last three columns on the right to phosphate release, i.e., to the transition from the *ATP* to the *ADP* nucleotide state.