Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

SUPPORTING INFORMATION

Properties of water in the region between a tubulin dimer and a single motor head of kinesin.

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Definition of the hydrogen bond: the hydrogen bond between two water molecules is formed if the oxygen-oxygen distance fulfills the relation (Wernet, Ph. *et al. Science* 2004,**304**, 995):

$$d_{OO} \leq -0.000044 \cdot \beta_{OOH}^2 + 0.33[\text{nm}] \qquad \text{(E1)}$$

where β_{OOH} is the O-O-H angle (in degrees), while d_{OO} is the oxygen-oxygen distance. We additionally demanded the total interaction energy between two hydrogen-bonded molecules to be negative – it is roughly equivalent to demanding the force acting between these molecules to be attractive.

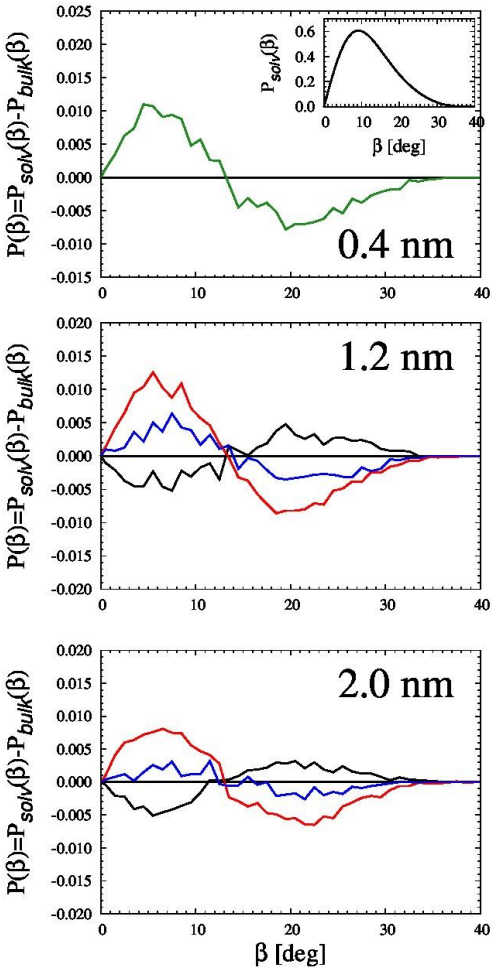

Figure S1. The probability distribution, $\Delta P(\beta)$, of values of β angle (eq. E1) for water in solvation layer between the kinesin catalytic domain and the tubulin dimer for the systems with the kinesin in distances 0.4, 1.2 and 2.0 nm away from the tubulin dimer. Red line represents results for the first solvation shell of kinesin, blue line corresponds to the first solvation shell of tubulin, while black line describes results for the intermediate region (*i.e.* obtained for water molecules farther than 0.4 nm from the proteins). The green line (for the distance 0.4 nm) depicts the results obtained for all water molecules in the region between the proteins. This Figure represents results obtained for *real dynamics*. The probability distribution $P(\beta)$ is presented in inset.

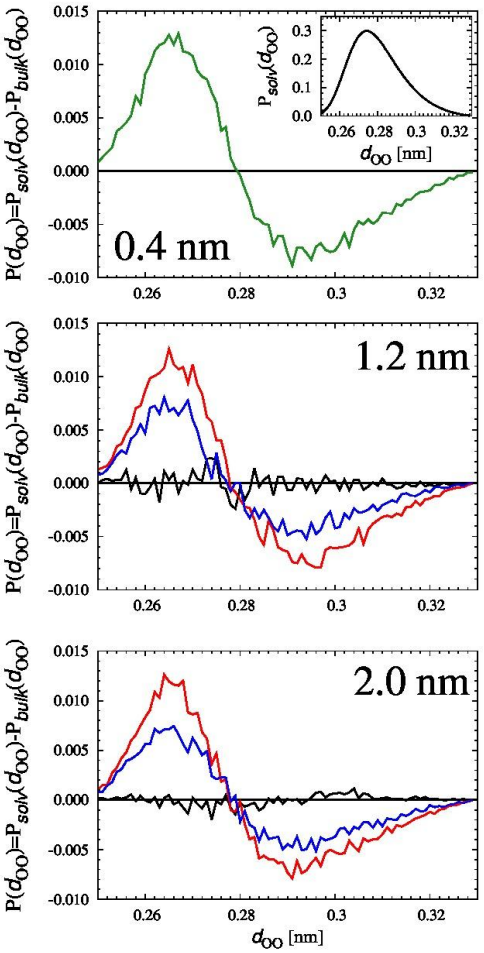

Figure S2. The probability distribution, $\Delta P(d_{OO})$, of values of d_{OO} distance (eq. E1) for water in solvation layer between the kinesin catalytic domain and the tubulin dimer for the systems with the kinesin in distances 0.4, 1.2 and 2.0 nm away from the tubulin dimer. Red line represents results for the first solvation shell of kinesin, blue line corresponds to the first solvation shell of tubulin, while black line describes results for the intermediate region (*i.e.* obtained for water molecules farther than 0.4 nm from the proteins). The green line (for the distance 0.4 nm) depicts the results obtained for all water molecules in the region between the proteins. This Figure represents results obtained for *real dynamics*. The probability distribution $P(d_{OO})$ is presented in inset.

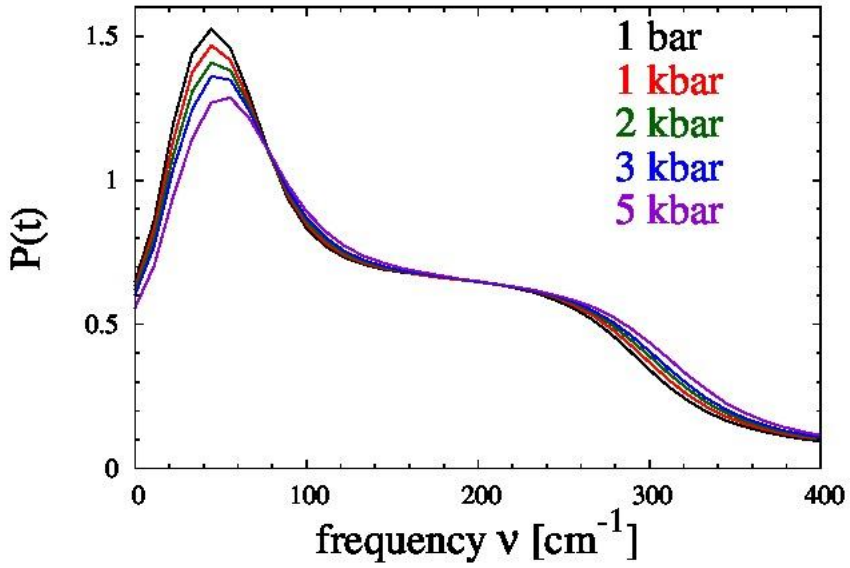

Figure S3. The spectra of the translational velocity autocorrelation function of water under various pressures up to 5 kbar. This pressure interval corresponds to the change of water density from 0.9981 g/cm^3 to 1.1579 g/cm^3.

Table T1. Results of Gaussian decomposition of the translational spectra of water under various pressures – the location of the maximum of the main band.

Pressure [kbar]	$\bar{\nu}_{max}$ [cm^{-1}]
0.001	41.0
1.0	42.2
2.0	43.2
3.0	44.4
5.0	46.9