

Table 1. Alignment parameters obtained from fits of D_{NH}^{A} , D_{NH}^{B} and D_{NH}

Data	α	β	γ	$A_a (\times 10^{-4})$	R
D_{NH}^{A}	64.9±0.5	73.3±0.5	242.7±0.5	-3.31±0.04	0.13±0.01
D_{NH}^{B}	61.3±2.5	77.6±2.5	189.4±2.5	-6.4±0.3	0.38±0.07
D_{NH}	60.5±0.5	75.9±0.5	195.6±0.5	-7.35±0.05	0.36±0.01

D_{NH}^{A} , D_{NH}^{B} and D_{NH} correspond to dipolar couplings of the apo form (measured directly on the 6.8% sample), the invisible bound form (measured via relaxation dispersion, 6.8% sample) and the completely bound state (measured directly on a fully bound sample). Values of (α, β, γ) correspond to the Euler angles of an active rotation of the protein from the PDB frame to the alignment frame. As discussed in the text the net charge of the apo SH3 domain is -12, and not surprisingly, the degree of alignment in Pf1 phage (negatively charged) is smaller than for the bound form of the domain for which the net charge is -6. The ~15% increase in the value of A_a calculated from D_{NH} relative to D_{NH}^{B} reflects the fact that more phage was used in the fully bound sample than for the 6.8% bound complex. Note the excellent agreement between the orientations of the alignment frames of the bound state that are obtained from dipolar couplings of the ‘invisible bound conformation’ that is in equilibrium with the predominant apo form (D_{NH}^{B}) and from the 100% bound conformation that can be observed directly (D_{NH}). Order tensor parameters that were based on dipolar couplings measured directly using the IPAP approach [Ottiger, M., Delaglio, F. & Bax, A. (1998) *J. Magn. Reson.* **131**, 373-8] were calculated from all experimentally measured couplings (*i.e.*, including residues for which ΔD_{NH} could not be measured via relaxation dispersion).