Table 1. (supplementary material) Overview of experimental parameters characterizing inter-domain motion of Pin1 bound to three peptides

Construct	Estimated correlation times				x	a / Å	$D_{\|}/D_{\perp}$	D_{axial}			
	Selected residues		τ_c / ns					LCM		Phages	
	WW	cat	WW	cat				WW	cat	WW	cat
$Pin1_{WW+L}$	12, 23, 24, 25, 32, 33 (11, 13, 14, 26)		4.0 – (5.2) av: 4.6 ± 0.6				1.39[a)]				
$Pin1_{L+CAT}$		55, 57-60, 83-85, 87, 88, 90, 91, 93, 94, 98, 104-106, 108, 110, 114-118, 121, 124, 125, 135-140, 150, 151, 158, 160, 163		9.3 ± 0.5			1.24[b)]				
$Pin1_{FL}$	12, 13, 15, 22, 24, 25, 32,	55, 57-60, 62, 83-85, 87, 88, 90, 91, 93, 94, 98, 104-106, 108, 109, 115-117, 121, 122, 124, 125, 134-136, 138, 150, 151, 156, 158-161, 163	7.6 ± 0.2	9.8 ± 0.1	0.47	2.5	1.29[c)]	2.7	9.6	3.7	12.6
$Pin1_{FL}$-WFYpSPR (Pintide peptide: MW: 934 g/mol)	11, 14, 15, 25, 26, (11, 12, 13, 26, 32)	55, 57-60, 62, 83-85, 87, 91, 92, 94, 96, 98, 105, 106, 108-110, 115, 117, 121, 122, 125, 132, 134-139, 152, 156, 158-161, 163	9.5 – (10.3) av: 9.9 ± 0.4	11.0 ± 0.1	0.79	3.3		8.3	13.1	8.9	11.9
$Pin1_{FL}$ YpSPTpSPS (CTD peptide: MW: 896 g/mol)	11, 12, 13, 14, 15, 22, 23, 24, 25, 26,	55, 56, 59, 60, 62, 82-86, 90, 93, 04, 103, 105, 107, 108, 110, 115, 116, 121, 122, 124, 125, 132, 134-137, 139, 150, 158, 160, 161, 163	8.9 ± 0.1	10.8 ± 0.1	0.68	3.1					
$Pin1_{FL}$ EQPLpTPVTDL (Cdc25 peptide: MW: 1191 g/mol)	11, 12, 13, 14, 15, 23 ,24 ,25 ,26,	55-60, 83-85, 87,88, 90, 91, 93, 94, 98, 103-105, 108-110, 114-117, 121-125, 134-139, 151, 152, 156-160	7.3 ± 0.1	9.7 ± 0.1	0.43	2.5					

MW: Molecular weight.
x: inter-domain interaction parameter.
a: hydrodynamic radius.
$D_{\|}$ / $D_{\perp}$: ratio of axial and equatorial components of the diffusion tensor.
D_{axial}: axial component of the alignment tensor.
LCM: Liquid crystalline medium.
[a)] calculated with HydroNMR from residues 10 – 38.
[b)] calculated with HydroNMR from residues 51 – 163.
[c)] calculated with HydroNMR from residues 1 – 163.

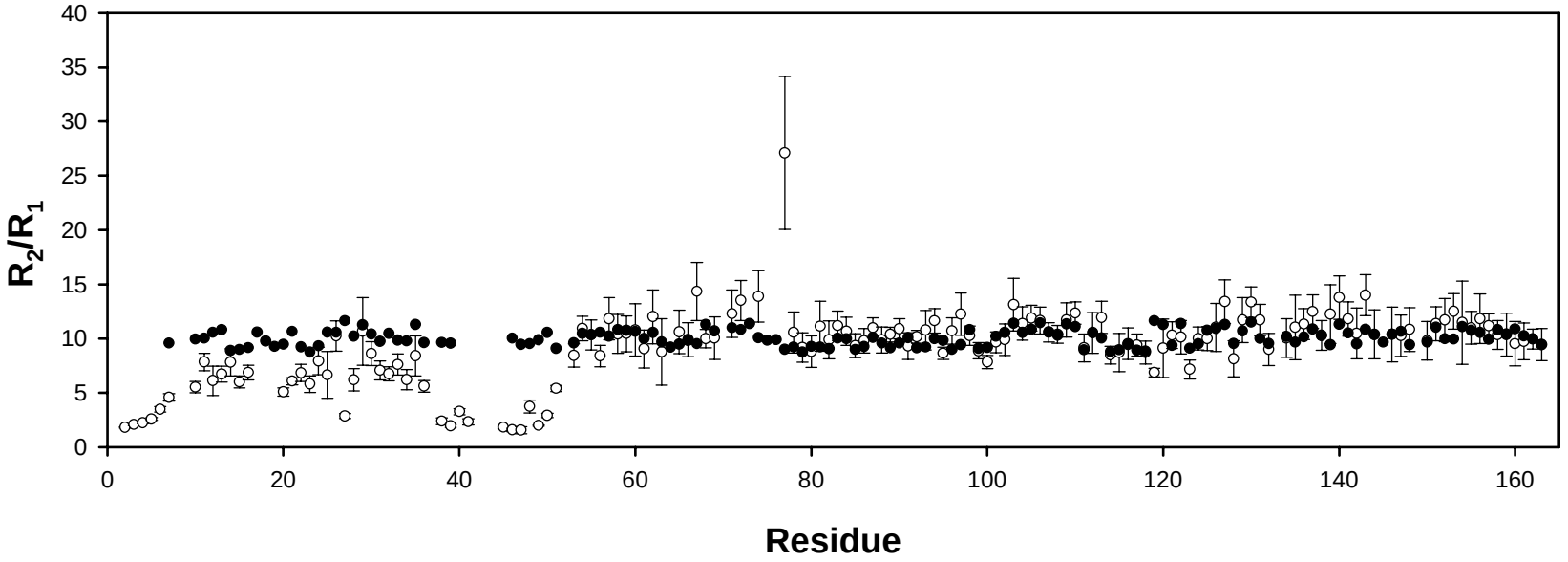

FIG. 6. (Supplementary material)