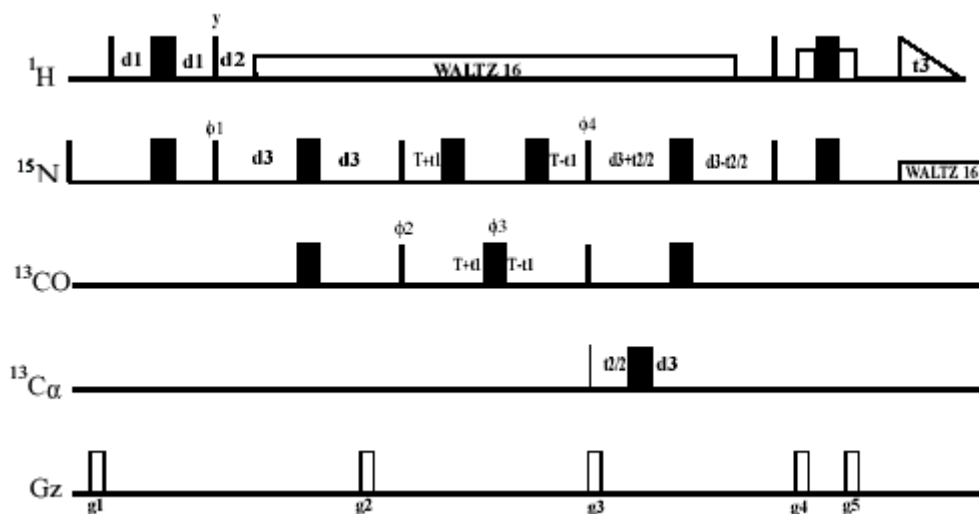


TEMPERATURE DEPENDENCE OF ANISOTROPIC PROTEIN BACKBONE

DYNAMICS

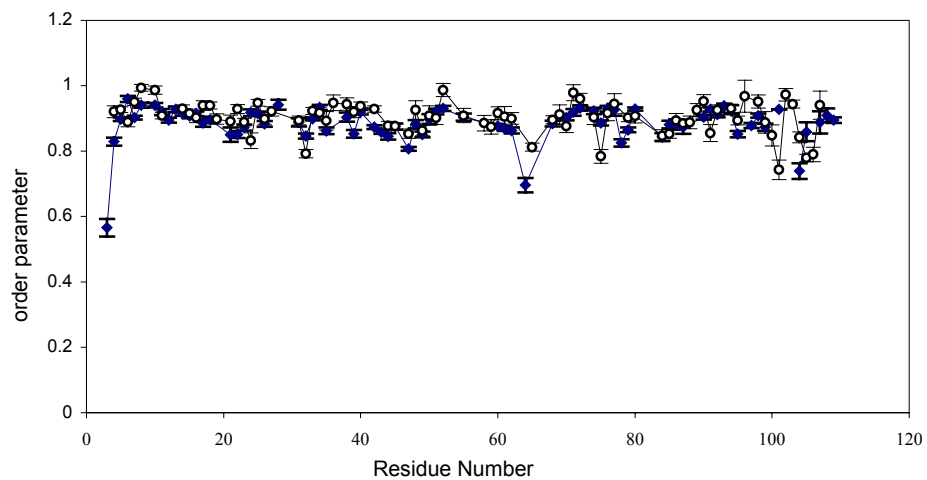
Tianzhi Wang, Sheng Cai and Erik R.P. Zuiderweg

Supplementary Material.



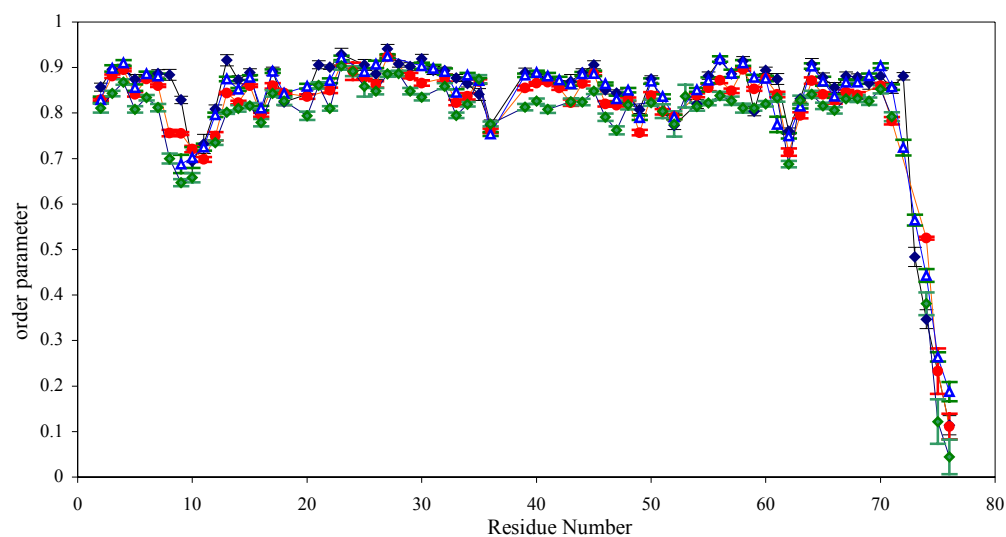
S1

Pulse sequence for the determination of ^{13}CO CSA / ^{13}CO - $^{13}\text{C}_\alpha$ DD cross-correlation rate. Narrow and wide bars denote 90° and 180° hard pulses, respectively. Pulse phases are along the x-axis unless indicated otherwise. 90° and 180° square soft pulses with duration 65 and 130 μs are used for both ^{13}CO and $^{13}\text{C}_\alpha$. The half-sine-shaped field gradient pulses of 1ms duration have strengths at the center $g_1=30\text{G/cm}$, $g_2=18\text{G/cm}$, $g_3=18\text{G/cm}$, $g_4=24\text{G/cm}$ and $g_5=24\text{G/cm}$. Constant time periods $4T$ and $2*d_3$ are used as ^{13}CO and ^{15}N chemical shift evolution periods, respectively. Delays (in milliseconds) are as follows: $d_1=2.5$, $d_2=5.55$, $d_3=14$ and $T=9$. Phase cycling is: $\phi_1=x, -x$; $\phi_2=x, x, -x, -x$; $\phi_3=4(x), 4(-x), 4(y), 4(-y)$; $\phi_4=4(x)$; receiver= $x, 2(-x), 2(x), 2(-x), x, -x, 2(x), 2(-x), 2(x), -x$. Phase ϕ_2 and ϕ_4 are incremented for States-TPPI quadrature detection. The 3D data are recorded with $36*50*1024$ complex points ($t_1*t_2*t_3$).



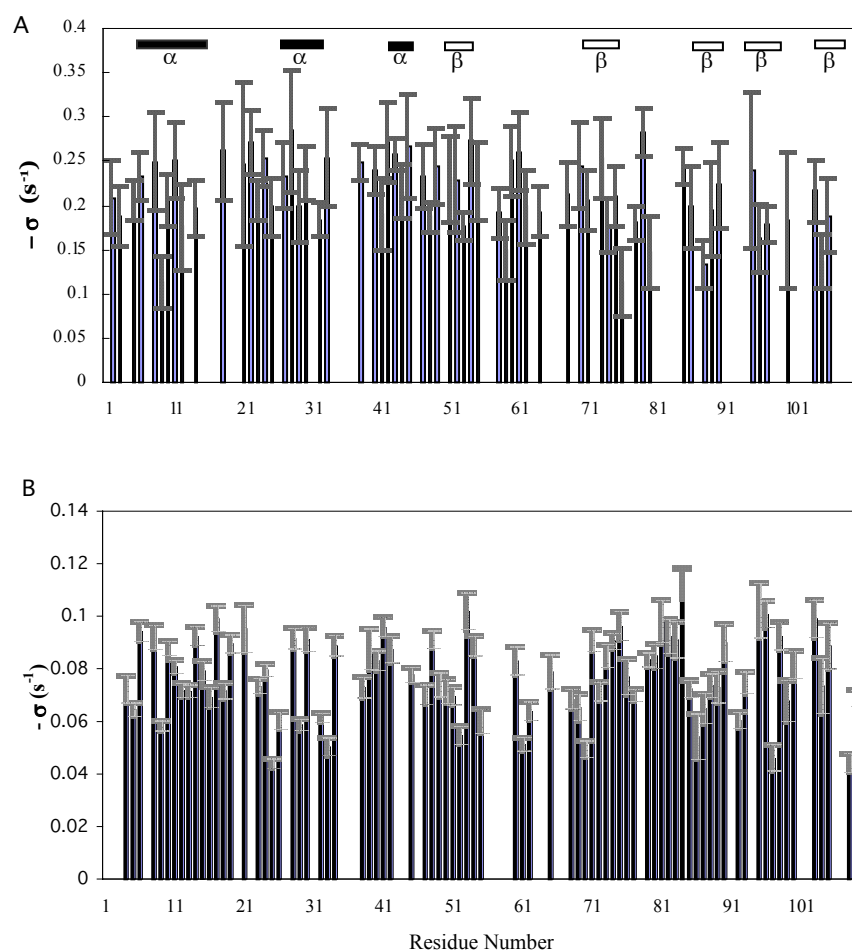
S2

The ^{15}N order parameters for $^{15}\text{N}/^{13}\text{C}$ labeled Binase (12.3 kDa), pH 7.0 in 90% $\text{H}_2\text{O}/10\text{ D}_2\text{O}$, at 278 and 303 K are presented with open circles and diamonds respectively. The data was obtained with a Bruker Avance 500 MHz spectrometer.



S 3

The ^{15}N order parameters for 1 mM $^{15}\text{N}/^{13}\text{C}$ labeled Ubiquitin in 90% $\text{H}_2\text{O}/10\text{ D}_2\text{O}$, deuterated acetic acid buffer, pH 4.7, at 278, 293, 303 and 318 K are presented with black, blue, red and green color, respectively.



S4

The ^{13}CO - $^{13}\text{C}_\alpha$ cross relaxation rates for Binase at 278 and 303 K are shown in panel A and B, respectively. The approximate locations of secondary structure elements are indicated above. The data was recorded using a 500 MHz spectrometer.