

SUPPLEMENTARY TABLE S3. NUCLEAR MAGNETIC RESONANCE EXPERIMENTS AND RELATED ACQUISITION PARAMETERS FOR THE DETERMINATION OF STRUCTURE AND FAST TIMESCALE DYNAMICS OF  $\Delta 76$  Tb1-C-Grx1

Experiments	Time domain dimensions (nucleus)			Spectral width (ppm)				
	$t_1$	$t_2$	$t_3$	F1	F2	F3	NS	Refs.
[ $^1\text{H}$ - $^{15}\text{N}$ ] TROSY <sup>a</sup>	512( $^{15}\text{N}$ )	1536( $^1\text{H}$ )	-	50	15	-	2	(11, 14)
HNCO <sup>a</sup>	128( $^{13}\text{C}$ )	192( $^{15}\text{N}$ )	1024( $^1\text{H}$ )	12	27	11	2	(11, 14)
HN(CA)CO <sup>a</sup>	128( $^{13}\text{C}$ )	192( $^{15}\text{N}$ )	1024( $^1\text{H}$ )	12	27	11	4	(11, 14)
HNCACB <sup>a</sup>	200( $^{13}\text{C}$ )	192( $^{15}\text{N}$ )	1024( $^1\text{H}$ )	61	27	11	4	(11, 14)
HBHA(CBCACO)NH <sup>b</sup>	102( $^1\text{H}$ )	192( $^{15}\text{N}$ )	1024( $^1\text{H}$ )	5	27	11	8	(16)
HN(CO)CACB <sup>a</sup>	200( $^{13}\text{C}$ )	192( $^{15}\text{N}$ )	1024( $^1\text{H}$ )	61	27	11	4	(16)
H(CCCO)NH-TOCSY <sup>b</sup>	180( $^1\text{H}$ )	192( $^{15}\text{N}$ )	1024( $^1\text{H}$ )	6	27	11	8	(16)
(H)C(CCO)NH-TOCSY <sup>b</sup>	182( $^{13}\text{C}$ )	192( $^{15}\text{N}$ )	1024( $^1\text{H}$ )	65	27	11	8	(16)
HCCH TOCSY <sup>c</sup>	196( $^1\text{H}$ )	232( $^{13}\text{C}$ )	1024( $^1\text{H}$ )	6	67	11	8	(9)
[ $^1\text{H}$ - $^{13}\text{C}$ ] CT TROSY (aromatics) <sup>d</sup>	144( $^{13}\text{C}$ )	640( $^1\text{H}$ )		40	9		32	(12)
(H)CB(CGCD)HD <sup>d</sup>	62( $^{13}\text{C}$ )	512( $^1\text{H}$ )		29	8		512	(12)
(H)CB(CGCC)H-TOCSY (Tyr-optimized) <sup>d</sup>	62( $^{13}\text{C}$ )	512( $^1\text{H}$ )		29	8		256	(12)
(H)CB(CGCC)H-TOCSY (Phe-optimized) <sup>d</sup>	62( $^{13}\text{C}$ )	512( $^1\text{H}$ )		29	8		384	(12)
(H)CCH-TOCSY (arom) <sup>d</sup>	254( $^{13}\text{C}$ )	200( $^{13}\text{C}$ )	640( $^1\text{H}$ )	121	121	10	16	(12)
NOESY-[ $^{13}\text{C}$ - $^1\text{H}$ ] HSQC <sup>e</sup>	320( $^1\text{H}$ )	320( $^{13}\text{C}$ )	1280( $^1\text{H}$ )	11	67	11	4	(13)
[ $^{13}\text{C}$ - $^1\text{H}$ ] HSQC <sup>e</sup>	400( $^{13}\text{C}$ )	1536( $^1\text{H}$ )		70	12		4	
[ $^{15}\text{N}$ - $^1\text{H}$ ] FHSQC <sup>e</sup>	640( $^{15}\text{N}$ )	1280( $^1\text{H}$ )		50	12		4	
NOESY [ $^{15}\text{N}$ - $^1\text{H}$ ] FHSQC <sup>e</sup>	352( $^1\text{H}$ )	236( $^{15}\text{N}$ )	1280( $^1\text{H}$ )	11	27	11	4	(13)
NOESY-[ $^{13}\text{C}$ - $^1\text{H}$ ]-HMQC (arom.) <sup>e</sup>	352( $^1\text{H}$ )	88( $^{13}\text{C}$ )	832( $^1\text{H}$ )	11	26	7	8	
$^{15}\text{N}$ R1 <sup>f</sup>	128( $^{15}\text{N}$ )	2048( $^1\text{H}$ )		28	12		40	(7)
$^{15}\text{N}$ R2 <sup>f</sup>	128( $^{15}\text{N}$ )	1024( $^1\text{H}$ )		28	12		32	(7)
$^{15}\text{N}$ { $^1\text{H}$ } NOE <sup>f</sup>	256( $^{15}\text{N}$ )	2048( $^1\text{H}$ )		28	12		48	(7)

Spectra marked as "a," "b," "c," and "d" were processed with Bruker software TOPSPIN 1.3 and analyzed through CARA (10), whereas those marked as "e" were processed and analyzed using NMRPIPE (4).

<sup>a</sup>Spectra acquired as their TROSY (14) and BEST (11) implementations on a 800-MHz spectrometer equipped with a triple-resonance cryoprobe at 298K in the Shigemitsu tube.

<sup>b</sup>Spectra acquired as their TROSY (14) implementations on a 800-MHz instrument equipped with a triple-resonance cryoprobe at 298K in the Shigemitsu tube.

<sup>c</sup>Spectra acquired on a 800-MHz instrument equipped with a triple-resonance cryoprobe at 298K in the Shigemitsu tube.

<sup>d</sup>Spectra acquired on a 500-MHz spectrometer equipped with a triple-resonance cryoprobe at 298K in the Shigemitsu tube.

<sup>e</sup>Spectra acquired on a 900-MHz spectrometer equipped with a triple-resonance cryoprobe at 298K exploiting a shaped tube (17).

<sup>f</sup>Spectra acquired on a 600-MHz spectrometer at 298K with sample in the Shigemitsu tube. Delay times for R1 were 10, 50, 100, 200, 400, 700, 1000, 1300, 1600, and 1000 ms. For R2 measurements, the following delays were exploited: 16.31, 32.64, 48.96, 65.28, 97.92, 146.89, 179.52, and 228.5 ms.

HSQC, heteronuclear single-quantum coherence.