

**Table S3. Details of NMR experiments and samples for the 51Z2 structure determination.**

Experiment	Data points, NS ( $t_{\text{mix}}$ )	Sample / Solvent
$^1\text{H}$ - $^{15}\text{N}$ ]-HSQC	2048/256, 4	1.13 mM in H <sub>2</sub> O
HNCACB	2048/64/160, 32	1.13 mM in H <sub>2</sub> O
CC(CO)NH	2048/96/168, 16	1.13 mM in H <sub>2</sub> O
H(CCCO)NH	2048/64/128, 32	1.13 mM in H <sub>2</sub> O
HNCO	2048/64/128, 8	1.13 mM in H <sub>2</sub> O
HNHA	2048/128/96, 16	1.13 mM in H <sub>2</sub> O
HN(CA)CO	2048/64/128, 32	1.13 mM in H <sub>2</sub> O
$^1\text{H}$ - $^{15}\text{N}$ ]-NOESY-HSQC	2048/96/280, 16 (180 ms)	1.13 mM in H <sub>2</sub> O
$^1\text{H}$ - $^{13}\text{C}$ ]-HSQC (ali)	1024/128, 16	1.13 mM in H <sub>2</sub> O
$^1\text{H}$ - $^{13}\text{C}$ ]-HSQC (ali)	1024/128, 16	0.90 mM in D <sub>2</sub> O
H(C)CH-TOCSY	2048/128/144, 8 (12 ms)	0.90 mM in D <sub>2</sub> O
H(C)CH-COSY	2048/128/128, 16	0.90 mM in D <sub>2</sub> O
$^1\text{H}$ - $^{13}\text{C}$ ]-NOESY-HSQC (ali)	2048/192/256, 8 (120 ms)	0.90 mM in D <sub>2</sub> O
$^1\text{H}$ - $^{13}\text{C}$ ]-HSQC (aro)	1024/256, 4	0.90 mM in D <sub>2</sub> O
(HB)CB(CGCD)HD	1024/128, 448	0.90 mM in D <sub>2</sub> O
(HB)CB(CGCDCE)HE	1024/128, 512	0.90 mM in D <sub>2</sub> O
H(CC)H-COSY aro.	2048/608, 64	1.00 mM in D <sub>2</sub> O
$^1\text{H}$ - $^{13}\text{C}$ ]-NOESY-HSQC (aro)	2048/80/1024, 8 (120 ms)	1.00 mM in D <sub>2</sub> O

Bruker AvanceIII NMR spectrometers with  $^1\text{H}$  resonance frequencies of 750 MHz or 600 MHz were utilized. All experiments were performed with  $^{13}\text{C}$  and  $^{15}\text{N}$ -labeled 51Z2 and the respective implementations of pulse programs in the TOPSPIN v. 2.1 software bundle. Resolution, number of scans (NS) and, where appropriate, mixing times ( $t_{\text{mix}}$ ) are given. Protein concentration was determined spectrophotometrically using a molar extinction coefficient of  $13980 \text{ M}^{-1} \text{ cm}^{-1}$  as calculated from the amino acid sequence by the Protparam tool [1] at [www.expasy.org/protparam/](http://www.expasy.org/protparam/). Spectra were recorded at 283 K. 51Z2 buffer conditions were 90 mM NaCl, 45 mM L-arginine, 45 mM L-glutamate, 9 mM DTT, 0.05 % (w/v) NaN<sub>3</sub>, pH 7.4 in 90% H<sub>2</sub>O/10% D<sub>2</sub>O or in 100% D<sub>2</sub>O.