SUPPLEMENTARY DATA

Consisting of two Tables and one Figure.

Table S1: ^{1}H chemical shifts, $^{3}J_{HNHA}$ coupling constants and backbone amide temperature coefficients of R1 in 95% H_2O/5% $^{2}H_2O$ with 10mM acetate at pH 4.5 and 278 K.

Residue	**NH**	**$C^{\alpha}H$**	**$C^{\beta}H$**	Others	$^{3}J_{HNHA}$ Hz	$\Delta\delta/\Delta T$ (ppb/°C)
Val 1	----	3.76	2.18	$C^{\gamma}H_3$ 1.00,0.86		
Phe 2	8.83	4.65	3.08	C(2,6)H 7.27 C(3,5)H 7.35	6.7	8.2
Ala 3	8.40	4.20	1.26		6.9	6.2
Glu 4	8.24	4.11	1.85	$C^{\gamma}H_2$ 2.21,2.13	7.0	
Phe 5	8.38	4.63	3.10,3.00	C(2,6)H 7.23 C(3,5)H 7.32	7.3	
Leu 6	8.20	4.59	1.55	$C^{\gamma}H$ 1.51 $C^{\delta}H_3$ 0.89	7.5	8.3
Pro 7	----	4.30	2.23,1.77	$C^{\gamma}H_2$ 1.97 $C^{\delta}H_2$ 3.69,3.58		
Leu 8	8.35	4.20	1.56	$C^{\gamma}H$ 1.41 $C^{\delta}H_3$ 0.89,0.83	7.2	
Phe 9	8.25	4.62	3.11,3.04	C(2,6)H 7.21	7.9	
Ser 10	8.24	4.38	3.85,3.75		6.6	
Lys 11	8.43	4.16	1.62	$C^{\gamma}H_2$ 1.18 $C^{\delta}H_2$ 1.60 $C^{\varepsilon}H_2$ 2.90 $N^{\varepsilon}H_3^{+}$ 7.61	6.8	
Phe 12	8.29	4.62	3.21,2.96	C(2,6)H 7.25 C(3,5)H 7.36	7.0	
Gly 13	8.31	3.98,3.85				
Ser 14	8.30	4.43	3.91,3.86		5.9	
Arg 15	8.51	4.31	1.86,1.75	$C^{\gamma}H_2$ 1.61 $C^{\delta}H_2$ 3.15 NH 7.23	10.3	
Met 16	8.32	4.39	1.94	$C^{\gamma}H_2$ 2.51,2.44	7.1	
His 17	8.63	4.71	3.21,3.12	C(2)H 8.59, C(4)H 7.25	7.5	7.2
Ile 18	8.34	4.11	1.81	$C^{\gamma}H_2$ 1.43,1.15 $C^{\gamma}H_3$ 0.87 $C^{\delta}H_3$ 0.83	8.4	
Leu 19	8.53	4.38	1.62	$C^{\delta}H_3$ 0.85,0.93		8.7
Lys 20	8.03	4.14	1.79,1.71	$C^{\gamma}H_2$ 1.38 $C^{\delta}H_2$ 1.66 $C^{\varepsilon}H_2$ 2.97 $N^{\varepsilon}H_3^{+}$ 7.60	7.4	8.2

Table S2: Summary of Experimental Constraints and Structural Statistics for R1

	R1
No. of distance restraints	204
intraresidue (*i =j)*	96
sequential (|*i-j*| = 1)	98
medium-range (1 < |*i-j*| < 5)	10
long-range (|*i-j*| > 4)	0
hydrogen bond restraints	0
No. of dihedral restraints	16
Energies[a]	
E_{NOE} (kcal mol^{-1})	7.8±1.3
RMS deviations from experimental data	
NOEs (Å)	0.028±0.002
Dihedrals (deg)	0.267±0.228
Deviations from ideal[b]	
angles (deg)	0.63±0.03
bonds (Å)	0.0044±0.0003
impropers (deg)	0.41±0.02
RMS deviations[c]	
backbone atoms (global)	>2
backbone atoms (residues 5-10, 13-17)	1.43, 1.16
Ramachandran plot[d] (%)	
most favored	45.9
allowed	52.2
additionally allowed	1.9
disallowed	0

[a] The values for E_{NOE} are calculated from a square-well potential with force constants of 50 kcal mol^{-1} $Å^2$. [b] The values for the bonds, angles, and impropers show the deviations from ideal values based on perfect stereochemistry. [c] The r.m.s.d. (in Å) over the backbone heavy atoms (N, C^{α}, C) for the indicated residues. [d] As determined by the program PROCHECK-NMR (Laskowski et al., 1996) except for Pro and Gly.

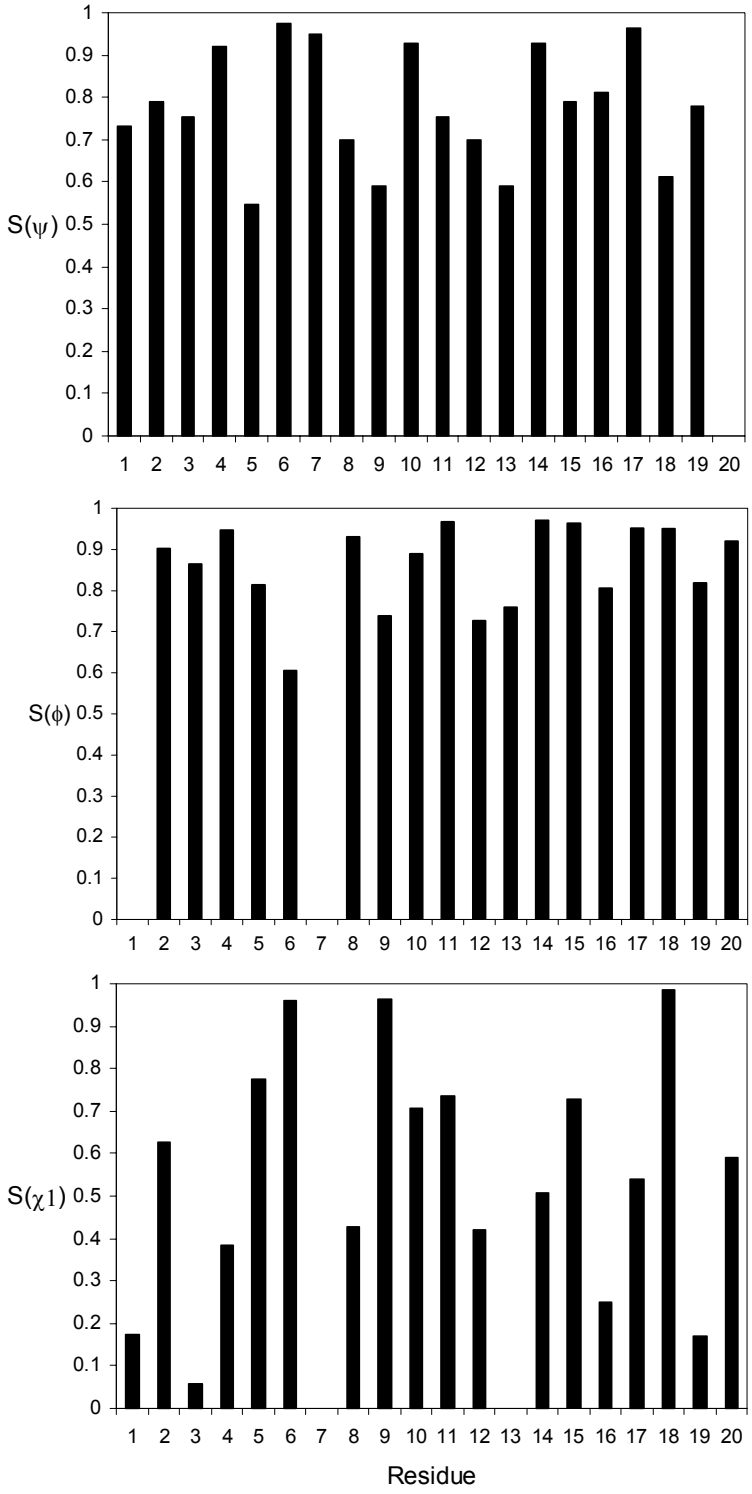

Figure S1. Angular order parameters as a function of residue number for R1. Angular parameters were calculated using the program MOLMOL (Koradi et al., 1996).