SUPPORTING INFORMATION AVAILABLE

Table 2: Proton Chemical Shift Assignments for the Pdht sequence[a]

residue	HN	Hα	Hβ	Hγ	others
Arg-1	8.82	4.05	1.90	1.63	$CH_2\delta$ 3.22
Lys-2	na	4.41	1.81	1.45	$CH_2\delta$ 1.71; $CH_2\varepsilon$ 2.97
Ser-3	8.59	4.51	3.79		
Ile-4	8.39	4.23	1.83	1.43, 1.15	$CH_3\gamma$ 0.88 ; $CH_3\delta$ 0.84
Arg-5	8.47	4.45	1.75, 1.69	1.60	$CH_2\delta$ 3.14
Ile-6	8.44	4.18	1.78	1.44, 1.14	$CH_3\gamma$ 0.87 ; $CH_3\delta$ 0.83
Gln-7	8.62	4.27	2.01, 1.89	2.25	$NH_2\delta$ 7.53, 6.89
Arg-8	8.57	4.37	1.82, 1.72	1.60	$CH_2\delta$ 3.16
Gly-9 trans	8.44	4.17			
cis	8.43	4.08, 3.95			
Dht-10 trans		4.87	3.38, 3.19		$CH_2\delta$ 4.62
cis		4.99	3.43, 3.35		$CH_2\delta$ 4.70
Gly-11	8.67	3.92			
Arg-12	8.05	4.28	1.78, 1.68	1.54	$CH_2\delta$ 3.16
Ala-13	8.31	4.27	1.28		
Phe-14	8.25	4.68	3.02, 2.97		Hδ 7.18; Hε7.29; Hη7.26
Val-15	8.22	4.21	1.99	0.88	
Thr-16	8.36	4.42	4.11	1.16	
Ile-17	8.37	4.23	1.85	1.45, 1.16	$CH_3\gamma$ 0.88 ; $CH_3\delta$ 0.83
Gly-18	8.16	3.75			

[a] Proton assignments are in H_2O at 15 °C, pH 5.7 (at 500 MHz). [na] Not assigned

Table 3: Proton Chemical Shift Assignments for the P1053 sequence[a]

residue	HN	Hα	Hβ	Hγ	others
Arg-1	8.70	4.00	1.88	1.64	CH_2δ 3.17
Lys-2	8.42	4.40	1.84	1.44	CH_2δ 1.71 ; CH_2ε 2.98
Ser-3	8.58	4.52	3.82		
Ile-4	8.38	4.24	1.84	1.45, 1.17	CH_3γ 0.89 ; CH_3δ 0.86
Arg-5	8.46	4.49	1.83, 1.71	1.59	CH_2δ 3.12
Ile-6	8.47	4.24	1.80	1.46, 1.16	CH_3γ 0.89 ; CH_3δ 0.86
Gln-7	8.62	4.22	2.02, 1.90	2.26	NH_2δ 7.54, 6.91
Arg-8	8.58	4.39	1.85, 1.73	1.61	CH_2δ 3.15
Gly-9	8.33	4.05, 4.14			
Pro-10		4.42	2.21, 2.00	1.96	CH_2δ 3.60
Gly-11	8.58	3.93			
Arg-12	8.16	4.29	1.80, 1.70	1.56	CH_2δ 3.15
Ala-13	8.27	4.28	1.30		
Phe-14	8.24	4.68	3.05, 3.00		Hδ 7.18 ; Hε 7.30 ; Hη7.25
Val-15	8.23	4.22	2.01	0.90	
Thr-16	8.37	4.44	4.13	1.19	
Ile-17	8.38	4.25	1.85	1.44, 1.18	CH_3γ 0.94; CH_3δ 0.86
Gly-18	8.14	3.75			

[a] Proton assignments are in H_2O at 15 °C, pH 5.7 (at 500 MHz).

Table 4 : Geometric statistics and experimental restraints of the 10 refined structures

experimental data	
distance restraints	137
dihedral restraints	19
pairwise RMSD (Å)	
All backbone atoms	0.93-0.54
backbone atoms of residues 5-13	0.50-0.33
backbone atoms of residues 8-11	0.21-0.13
IRMA R-factor	0.47-051