S3 Table. Proton chemical shifts and the vicinal coupling constants of Tat1_A4-5,8-9 in H_2O/D_2O (9:1) at 298 K.

Residue	Proton chemical shifts [ppm] HN	Hα	Hβ	Hγ	Hδ	others	$^3J_{HNH\alpha}$
Gly[1]		3.83					
Arg[2]	8.70	4.32	1.73;1.80	1.62	3.19	ε-NH 7.21	7.2
Lys[3]	8.64	4.27	1.73;1.79	1.44	1.62	Hε 2.98; ζ-NH_2 7.53	7.5
Ala[4]	8.51	4.27	1.36				
Ala[5]	8.45	4.26	1.36				
Arg[6]	8.45	4.26	1.74;1.80	1.61	3.18	ε-NH 7.21	
Gln[7]	8.57	4.29	1.96;2.06	2.36		ε-NH_2 6.95;7.64	7.7
Ala[8]	8.53	4.29	1.37				
Ala[9]	8.44	4.26	1.36				
Arg[10]	8.47	4.60	1.71;1.84	1.68	3.21	ε-NH 7.22	7.9
Pro[11]	-	4.47	1.96;2.32	2.00	3.63;3.82		-
Ser[12]	8.60	4.47	3.88;3.98				8.1
	8.67	4.45	3.92;3.99				8.8
	8.49	4.50	3.86;3.93				