

Supporting information for Stanger *et al.* (October 2, 2001) *Proc. Natl. Acad. Sci. USA*, 10.1073/pnas.211536998.

Table 8. Proton resonances (ppm) for $^D\text{P-TT}_2$ in 9:1 H₂O/D₂O (4°C)

Residue	N-H	α H	β H	Others
Thr	—	3.97	4.16	γ CH ₃ 1.30
Thr	9.02	4.78	4.12	γ CH ₃ 1.18
Thr	8.71	4.51	4.14	γ CH ₃ 1.17
Thr	8.46	4.72	3.95	γ CH ₃ 1.06
Arg	8.59	4.51	1.79, 1.71	γ CH ₂ 1.48 δ CH ₂ 3.11 ϵ NH 7.15 NH ₂ ⁺ 6.92, 6.50
Tyr	8.65	5.15	2.77, 2.72	2,6 H 6.93 3,5 H 6.77
Val	9.08	4.40	1.99	γ CH ₃ 0.84
Glu	8.64		1.97, 1.87	γ CH ₂ 2.23
Val	9.00	4.61	1.96	γ CH ₃ 0.92
D Pro	—	4.36	2.37, 1.99	γ CH ₂ 2.12, 2.06 δ CH ₂ 3.87
Gly	8.73	4.03, 3.76	—	—
Orn	7.93	4.61	1.80	γ CH ₂ 1.68 δ CH ₂ 3.00 δ NH ₃ ⁺ 7.68
Lys	8.59	4.65	1.62, 1.53	γ CH ₂ 1.14 δ CH ₂ 1.33 ϵ CH ₂ 2.57 ϵ NH ₃ ⁺ 7.41
Ile	9.20	4.54	1.90	γ CH ₃ 0.89 γ CH ₂ 1.38, 1.20 δ CH ₃ 0.80
Leu	8.66	4.16	1.53, 1.39	γ CH 1.30 δ CH ₃ 0.62, 0.53
Gln	8.92	4.53	2.01, 1.82	γ CH ₂ 2.24, 2.19

				δ NH 7.45, 6.99
Thr [†]	8.69	4.72	4.10	γ CH ₃ 1.14
Thr [†]	8.63	4.54	4.15	γ CH ₃ 1.16
Thr	8.62	4.68	4.17	γ CH ₃ 1.18
Thr	8.35	4.36	4.25	γ CH ₃ 1.18
-NH₂	7.76, 7.28			

[†] The proton spin systems for the Thr-17 and Thr-18 residues could not be distinguished. The resonances in this table reflect one of two assignment possibilities.