SUPPORTING INFORMATION

Temperature dependence of internal motions of protein side-chain NH_3^+ groups: Insight into energy barriers for transient breakage of hydrogen bonds

Levani Zandarashvili and Junji Iwahara

^{15}N relaxation parameters measured for the HoxD9 homeodomain – DNA complex at four distinct temperatures.

Lys 3 NH_3^+		15 ˚C	22 ˚C	28 ˚C	35 ˚C
600 MHz	^{15}N R_1 [s^{-1}]	0.440 ± 0.001	0.365 ± 0.001	0.295 ± 0.002	0.27 ± 0.01
	{^{1}H-}^{15}N NOE	-3.22 ± 0.01	-3.01 ± 0.01	-2.99 ± 0.04	-3.07 ± 0.06
800 MHz	^{15}N R_1 [s^{-1}]	0.385 ± 0.001	0.324 ± 0.001	0.280 ± 0.01	0.25 ± 0.01
	^{15}N $R_{2,ini}$ [s^{-1}]	1.76 ± 0.01	1.45 ± 0.02	1.06 ± 0.04	0.98 ± 0.05
	{^{1}H-}^{15}N NOE	-2.57 ± 0.01	-2.49 ± 0.02	-2.39 ± 0.03	-2.40 ± 0.03
	$R(4N_zH_zH_z)$ [s^{-1}]	21.3 ± 0.1	37.0 ± 0.2	53.7 ± 0.2	104 ± 2

Lys 55 NH_3^+		15 ˚C	22 ˚C	28 ˚C	35 ˚C
600 MHz	^{15}N R_1 [s^{-1}]	0.689 ± 0.003	0.607 ± 0.005	0.510 ± 0.011	0.59 ± 0.04
	{^{1}H-}^{15}N NOE	-3.06 ± 0.02	-2.92 ± 0.04	-2.94 ± 0.11	-2.94 ± 0.17
800 MHz	^{15}N R_1 [s^{-1}]	0.584 ± 0.002	0.506 ± 0.004	0.429 ± 0.018	0.42 ± 0.02
	^{15}N $R_{2,ini}$ [s^{-1}]	3.12 ± 0.04	2.54 ± 0.07	2.39 ± 0.20	1.98 ± 0.21
	{^{1}H-}^{15}N NOE	-2.93 ± 0.02	-2.75 ± 0.06	-2.70 ± 0.10	-2.72 ± 0.08
	$R(4N_zH_zH_z)$ [s^{-1}]	34.9 ± 0.4	60.6 ± 1.1	87.1 ± 1.5	154 ± 14

Lys 57 NH_3^+		15 ˚C	22 ˚C	28 ˚C	35 ˚C
600 MHz	^{15}N R_1 [s^{-1}]	1.282 ± 0.004	1.130 ± 0.004	0.941 ± 0.005	0.80 ± 0.02
	{^{1}H-}^{15}N NOE	-2.56 ± 0.02	-2.93 ± 0.03	-3.00 ± 0.04	-3.17 ± 0.04
800 MHz	^{15}N R_1 [s^{-1}]	1.055 ± 0.003	0.915 ± 0.003	0.765 ± 0.004	0.74 ± 0.01
	^{15}N $R_{2,ini}$ [s^{-1}]	3.57 ± 0.03	3.13 ± 0.03	2.58 ± 0.04	2.27 ± 0.04
	{^{1}H-}^{15}N NOE	-2.17 ± 0.01	-2.53 ± 0.03	-2.89 ± 0.03	-3.00 ± 0.03
	$R(4N_zH_zH_z)$ [s^{-1}]	14.7 ± 0.1	23.7 ± 0.2	32.6 ± 0.2	63.4 ± 0.4