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Table 1: ^1H Chemical Shifts for $\mu\text{-Aga-I}$ at 298K, pH=2.6^a

Supplementary page 1 of 1

	NH ^b	α	β	γ	other	$^3J_{\text{NH,H } \alpha}$
E1	-	4.14	2.17	2.60		
C2	8.63	4.90	2.96, 3.24			6.2
V3	8.85**	4.18	1.83	0.86, 0.92		7.4
P4	-	4.13	1.92, 2.06	1.62, 1.92	$\delta=3.64, 3.82$	
E5	7.41	2.83	1.16, 1.46	2.06, 2.22		< 5
N6	9.21	4.14	2.87, 3.20		$\delta\text{NH}_2=(7.58, 6.87)$	7.0
G7	8.45*	3.33, 4.06	-			
H8	8.50	5.02	3.18		$\delta=27.37, \epsilon_1 8.65$	
C9	7.81*	5.01	2.94, 3.18			9.4
R10	8.48	4.31	1.50	1.50	$\delta=2.98, \text{NH}\epsilon=7.04$	
D11	8.76	4.26	2.46, 2.67			4.1
W12	7.94	4.44	3.20, 3.38		$\delta_1=7.01, \epsilon_3=7.52, \zeta^3=7.13, n^2=7.21, \zeta^2=7.46, \text{NH}=10.1$	
Y13	7.69	4.46	2.64, 2.86		$\delta_1 = 6.96, E = 6.78$	
D14	8.38	4.75	2.68, 2.91			
E15	8.46	4.46	1.98, 2.30	2.36		4.1
C16	8.59	5.04	2.67, 3.01			
C17	9.14**	4.48	2.50, 3.48			4.1
E18	8.42	4.11	1.99, 2.08	2.49		< 5
G19	8.82	3.38, 3.98	-			
F20	8.04**	5.12	2.73, 3.02		$\epsilon=7.21, \delta=6.74, \zeta=7.26$	10.4
Y21	9.41**	4.94	2.85, 3.02		$\delta=7.02, \epsilon=6.71$	9.3
C22	8.90	4.45	3.00			7.4
S23	8.72*	4.65	3.48, 3.88			9.3
C24	9.16	5.22	2.93			10.3
R25	7.75	4.12	1.76, 1.85	1.66, 2.76	$\delta=3.19, \text{NH}\epsilon=7.17$	6.0
Q26	8.26	4.82	1.94, 2.01	2.22 2.30	$\delta\text{NH}_2=7.55, 6.86$	9.3
P27	-	4.32	1.88, 2.32	2.00	$\delta=3.64$	
P28	-	4.62	2.20, 2.38	1.68, 2.02	$\delta=3.54$	
K29	8.31	4.42	1.80	1.26	$\delta=1.57, \epsilon=2.87$	7.4
C30	8.28	5.29	2.74, 3.56			9.2
I31	8.55**	5.25	1.43	1.03, 1.28	$\delta\text{CH}_3=0.76, \gamma\text{CH}_3=0.64$	9.4
C32	8.15**	5.01	2.46, 2.84			5.8
R33	9.34**	4.92	1.39, 1.90	1.66	$\delta=3.20, \text{NH}\epsilon=7.12$	10.1
N34	8.84	4.39	2.75		$\delta\text{NH}_2=7.45, 6.88$	5.5
N35	8.43	4.63	2.56, 2.70		$\delta\text{NH}_2=7.33, 6.65$	
N36	8.49	4.60	2.64, 2.76		$\delta\text{NH}_2=7.39, 7.08$	

a- Chemical shifts relative to internal TSP.

b- Very slowly and slowly exchanging NH's are indicated by * and **, respectively. NH resonances for residues 3, 17, 20, 21, 31, 32 and 33 persisted even after 60 hours in D₂O at room temperature.