Table SI1. Experimental values of longitudinal (R_1) and transverse (R_2) relaxation rates and *NOE*s for the backbone amide ^{15}N nuclei in *apo*-S100A1-βME protein at 9.4 and 11.7 T (experimental uncertainties are given in parantheses).

Residue	9.4 T			11.7 T		
	R_1 (s^{-1})	R_2 (s^{-1})	*NOE*	R_1 (s^{-1})	R_2 (s^{-1})	*NOE*
Ser2				1.63 (0.10)	6.1 (0.4)	0.35 (0.12)
Glu3	2.98 (0.27)	10.9 (3.3)	0.48 (0.14)	2.09 (0.07)	9.5 (0.4)	0.87 (0.07)
Leu4	2.59 (0.06)	9.6 (0.6)	0.61 (0.07)	1.81 (0.03)	10.6 (0.2)	0.82 (0.04)
Glu5	2.55 (0.08)	10.4 (0.2)	0.79 (0.06)	1.91 (0.02)	10.6 (0.2)	0.79 (0.04)
Thr6	2.52 (0.08)	9.5 (0.4)	0.85 (0.10)	1.90 (0.04)	10.7 (0.2)	0.88 (0.03)
Ala7	2.62 (0.05)	9.7 (0.3)	0.81 (0.05)	1.89 (0.03)	10.5 (0.3)	0.82 (0.03)
Met8	2.46 (0.04)	10.1 (0.2)	0.78 (0.05)	1.84 (0.03)	10.5 (0.1)	0.80 (0.02)
Glu9	2.57 (0.08)	10.5 (0.3)	0.43 (0.03)	1.84 (0.02)	10.9 (0.1)	0.83 (0.02)
Thr10	2.50 (0.04)	10.5 (0.2)	0.68 (0.04)	1.85 (0.02)	10.8 (0.1)	0.83 (0.02)
Leu11	2.50 (0.06)	10.2 (0.5)	0.66 (0.05)	1.85 (0.02)	11.1 (0.1)	0.84 (0.03)
Ile12	2.64 (0.03)	9.4 (0.2)	0.56 (0.04)	1.86 (0.02)	9.7 (0.1)	0.84 (0.03)
Asn13	2.57 (0.11)	10.2 (0.3)	0.85 (0.07)	1.85 (0.02)	11.0 (0.1)	0.86 (0.03)
Val14	2.61 (0.07)	10.0 (0.2)	0.77 (0.06)	1.85 (0.02)	11.2 (0.1)	0.86 (0.02)
Phe15	2.54 (0.10)	11.0 (0.2)	0.89 (0.08)	1.82 (0.02)	11.4 (0.1)	0.88 (0.02)
His16	2.55 (0.12)	10.9 (0.2)	0.70 (0.07)	1.87 (0.04)	11.2 (0.1)	0.84 (0.05)
Ala17	2.54 (0.09)	9.8 (0.3)	0.59 (0.05)	1.87 (0.02)	10.6 (0.1)	0.80 (0.02)
His18	2.74 (0.07)	9.7 (0.4)	0.66 (0.07)	1.91 (0.03)	10.4 (0.1)	0.84 (0.02)
Ser19	2.52 (0.20)	11.6 (0.3)	0.61 (0.10)	1.86 (0.05)	13.2 (0.3)	0.78 (0.05)
Gly20	2.61 (0.11)	8.6 (0.5)	0.68 (0.09)	1.98 (0.05)	10.3 (0.1)	0.74 (0.05)
Lys21	2.49 (0.08)	7.2 (0.3)	0.55 (0.10)	1.92 (0.07)	9.1 (0.1)	0.68 (0.03)
Glu22	2.73 (0.06)	9.0 (0.1)	0.78 (0.07)	1.89 (0.04)	15.1 (1.4)	0.69 (0.06)
Gly23				2.22 (0.14)	12.8 (0.2)	0.75 (0.08)
Asp24	2.31 (0.13)	8.2 (1.0)	0.56 (0.09)	2.02 (0.10)	8.8 (0.2)	0.72 (0.05)
Lys25	2.27 (0.19)	9.4 (0.3)	0.49 (0.07)	1.96 (0.04)	13.3 (0.2)	0.67 (0.04)
Tyr26	2.58 (0.14)	9.1 (0.1)	0.77 (0.10)	1.96 (0.03)	10.0 (0.1)	0.75 (0.02)
Lys27				1.87 (0.03)	6.6 (0.2)	0.73 (0.02)
Leu28	3.07 (0.22)	11.0 (0.7)	0.39 (0.09)	1.82 (0.04)	11.3 (0.1)	0.77 (0.02)

Ser29	2.69 (0.10)	8.8 (0.4)	0.57 (0.08)	1.91 (0.03)	9.0 (0.1)	0.78 (0.02)
Lys30	2.87 (0.24)	10.4 (0.9)	0.65 (0.11)	2.02 (0.02)	9.8 (0.1)	0.75 (0.07)
Lys31	2.70 (0.09)	9.7 (0.3)	0.98 (0.09)	1.87 (0.02)	10.2 (0.1)	0.78 (0.03)
Glu32	2.20 (0.13)	9.6 (0.4)	0.80 (0.10)	1.89 (0.02)	10.2 (0.1)	0.77 (0.03)
Leu33	2.71 (0.13)	9.3 (0.5)	0.90 (0.13)	1.91 (0.03)	10.1 (0.2)	0.75 (0.04)
Lys34	2.52 (0.13)	10.0 (0.1)	0.72 (0.11)	1.89 (0.02)	10.2 (0.1)	0.77 (0.04)
Glu35	2.65 (0.08)	9.7 (0.3)	0.76 (0.06)	1.87 (0.02)	10.2 (0.1)	0.78 (0.04)
Leu36	2.46 (0.11)	8.9 (0.2)	0.87 (0.09)	1.90 (0.02)	9.6 (0.1)	0.73 (0.02)
Leu37	2.68 (0.03)	9.6 (0.1)	0.67 (0.05)	1.91 (0.04)	10.9 (0.1)	0.82 (0.03)
Gln38	2.65 (0.15)	9.2 (0.1)	0.84 (0.11)	1.88 (0.04)	10.1 (0.1)	0.84 (0.02)
Thr39	2.58 (0.06)	8.8 (0.2)	0.66 (0.06)	1.85 (0.02)	9.4 (0.1)	0.79 (0.02)
Glu40				1.90 (0.03)	9.8 (0.1)	0.80 (0.03)
Leu41	2.76 (0.05)	9.2 (0.4)	0.57 (0.10)	1.86 (0.03)	9.7 (0.2)	0.75 (0.02)
Ser42	2.37 (0.06)	8.7 (0.1)	0.71 (0.05)	1.75 (0.02)	9.1 (0.1)	0.77 (0.02)
Gly43	2.70 (0.09)	9.0 (0.6)	0.85 (0.11)	2.11 (0.07)	10.0 (0.2)	0.80 (0.02)
Phe44	2.30 (0.02)	7.7 (0.3)	0.75 (0.08)	1.78 (0.02)	9.3 (0.1)	0.77 (0.04)
Leu45	2.57 (0.07)	9.7 (0.1)	0.65 (0.05)	1.92 (0.03)	10.3 (0.1)	0.80 (0.02)
Asp46	2.51 (0.11)	8.9 (0.3)	0.63 (0.06)	1.78 (0.02)	9.4 (0.1)	0.73 (0.02)
Ala47	2.39 (0.03)	8.7 (0.4)	0.56 (0.04)	1.78 (0.02)	9.2 (0.1)	0.71 (0.02)
Gln48	2.52 (0.03)	8.3 (0.2)	0.69 (0.05)	1.84 (0.03)	8.9 (0.1)	0.75 (0.02)
Lys49	2.54 (0.09)	7.5 (0.3)	0.68 (0.05)	1.98 (0.02)	7.9 (0.1)	0.62 (0.02)
Asp50	2.48 (0.07)	8.3 (0.2)	0.56 (0.04)	1.96 (0.02)	8.7 (0.1)	0.66 (0.03)
Ala51	2.43 (0.03)	7.3 (0.2)	0.53 (0.03)	1.89 (0.02)	7.8 (0.1)	0.69 (0.01)
Asp52	2.76 (0.28)	9.1 (0.5)	0.50 (0.07)	2.07 (0.08)	10.3 (0.2)	0.79 (0.02)
Ala53	2.52 (0.03)	9.3 (0.4)	0.67 (0.05)	2.02 (0.03)	10.1 (0.1)	0.78 (0.02)
Val54	2.43 (0.06)	8.4 (0.4)	0.60 (0.05)	1.75 (0.02)	8.9 (0.1)	0.70 (0.02)
Asp55	2.48 (0.03)	9.3 (0.4)	0.59 (0.05)	1.83 (0.02)	10.0 (0.1)	0.73 (0.04)
Lys56	2.57 (0.05)	9.7 (0.2)	0.77 (0.04)	1.78 (0.01)	10.2 (0.1)	0.74 (0.02)
Val57	2.53 (0.08)	9.2 (0.5)	0.50 (0.10)	1.75 (0.02)	9.5 (0.1)	0.72 (0.02)
Met58	2.59 (0.09)	10.6 (0.2)	0.65 (0.08)	1.79 (0.02)	10.3 (0.1)	0.81 (0.02)
Lys59	2.48 (0.04)	9.8 (0.2)	0.62 (0.05)	1.82 (0.01)	10.4 (0.1)	0.81 (0.03)
Glu60	2.42 (0.06)	9.0 (0.2)	0.61 (0.06)	1.76 (0.02)	10.0 (0.1)	0.72 (0.02)
Leu61	2.50 (0.10)	9.9 (0.2)	0.82 (0.11)	1.78 (0.02)	9.8 (0.1)	0.75 (0.04)

Asp62	2.39 (0.10)	9.3 (0.3)	0.64 (0.07)	1.73 (0.01)	9.3 (0.1)	0.74 (0.03)
Glu63	2.31 (0.06)	8.9 (0.4)	0.73 (0.09)	1.68 (0.02)	8.8 (0.1)	0.63 (0.02)
Asp64	2.52 (0.03)	9.9 (0.2)	0.70 (0.04)	1.92 (0.02)	9.1 (0.1)	0.71 (0.01)
Gly65	2.52 (0.07)	7.3 (0.2)	0.42 (0.07)	2.01 (0.05)	8.0 (0.1)	0.65 (0.04)
Asp66	2.74 (0.08)	8.1 (0.4)	0.59 (0.07)	2.09 (0.03)	8.7 (0.1)	0.78 (0.01)
Gly67	2.44 (0.07)	7.2 (0.4)	0.57 (0.09)	2.02 (0.04)	8.5 (0.2)	0.66 (0.04)
Glu68	2.50 (0.06)	8.8 (0.4)	0.52 (0.05)	1.93 (0.02)	8.9 (0.1)	0.78 (0.01)
Val69	2.50 (0.57)	10.1 (1.1)	0.70 (0.13)	1.86 (0.03)	9.6 (0.1)	0.74 (0.02)
Asp70	2.40 (0.06)	9.0 (0.3)	0.67 (0.06)	1.84 (0.02)	10.0 (0.1)	0.82 (0.01)
Phe71	2.65 (0.25)	9.6 (0.6)	0.65 (0.08)	1.89 (0.02)	10.2 (0.2)	0.79 (0.03)
Gln72	2.48 (0.05)	9.4 (0.1)	0.68 (0.05)	1.81 (0.02)	10.0 (0.1)	0.77 (0.03)
Glu73				1.83 (0.02)	10.0 (0.1)	0.79 (0.01)
Tyr74	2.56 (0.07)	8.3 (0.4)	0.63 (0.11)	1.85 (0.02)	10.1 (0.1)	0.79 (0.05)
Val75	2.71 (0.09)	9.9 (0.4)	0.71 0.05)	1.90 (0.02)	10.8 (0.1)	0.81 (0.03)
Val76	2.47 (0.05)	9.6 (0.3)	0.73 (0.05)	1.82 (0.01)	10.6 (0.1)	0.84 (0.02)
Leu77	2.52 (0.06)	11.2 (0.4)	0.63 (0.08)	1.86 (0.01)	11.5 (0.1)	0.82 (0.03)
Val78				1.86 (0.01)	9.4 (0.1)	0.78 (0.01)
Ala79	2.97 (0.06)	9.6 (0.3)	0.74 (0.07)	1.93 (0.03)	10.2 (0.2)	0.83 (0.03)
Ala80	2.41 (0.03)	8.6 (0.3)	0.70 (0.05)	1.82 (0.02)	9.2 (0.2)	0.68 (0.02)
Leu81	2.53 (0.08)	9.9 (0.4)	0.65 (0.05)	1.89 (0.02)	10.8 (0.1)	0.83 (0.02)
Thr82	2.58 (0.03)	10.5 (0.5)	0.72 (0.06)	1.85 (0.02)	10.7 (0.1)	0.80 (0.02)
Val83	2.72 (0.05)	9.6 (0.3)	0.70 (0.08)	1.88 (0.03)	10.7 (0.2)	0.83 (0.02)
Ala84	2.53 (0.07)	9.44 (0.3)	0.79 (0.07)	1.87 (0.02)	10.8 (0.1)	0.81 (0.01)
Cys85	2.68 (0.09)	9.9 (0.3)	0.75 (0.06)	1.89 (0.01)	11.1 (0.1)	0.87 (0.02)
Asn86	2.53 (0.06)	10.7 (0.2)	0.83 (0.06)	1.94 (0.03)	10.5 (0.1)	0.82 (0.03)
Asn87	2.55 (0.09)	10.7 (0.1)	0.69 (0.06)	1.88 (0.01)	11.1 (0.1)	0.82 (0.03)
Phe88	2.52 (0.07)	9.7 (0.4)	0.66 (0.05)	1.79 (0.01)	10.3 (0.1)	0.79 (0.03)
Phe89	2.54 (0.09)	9.6 (0.2)	0.68 (0.08)	1.83 (0.02)	10.5 (0.1)	0.79 (0.03)
Trp90	2.54 (0.09)	9.6 (0.5)	0.55 (0.06)	1.84 (0.02)	9.8 (0.1)	0.76 (0.03)
Glu91	2.44 (0.04)	7.6 (0.1)	0.45 (0.04)	1.88 (0.02)	8.0 (0.1)	0.62 (0.02)
Asn92	2.41 (0.05)	7.1 (0.6)	0.33 (0.02)	1.98 (0.06)	5.9 (0.2)	0.44 (0.02)
Ser93	1.35 (0.02)	2.32 (0.05)	-0.49 (0.02)	1.24 (0.01)	2.64 (0.03)	-0.81 (0.02)

Table SI2. Experimental values of longitudinal (R_1) and transverse (R_2) relaxation rates and *NOE*s for the backbone amide ^{15}N nuclei in *apo*-S100A1 protein at 9.4 and 11.7 T (experimental uncertainties are given in parantheses).

Residue	9.4 T			11.7 T		
	R_1 (s^{-1})	R_2 (s^{-1})	*NOE*	R_1 (s^{-1})	R_2 (s^{-1})	*NOE*
Ser2						
Glu3	3.21 (0.74)	12.7 (2.8)	0.84 (0.13)	2.07 (0.09)	9.6 (0.3)	0.77 (0.05)
Leu4	2.74 (0.16)	9.8 (0.4)	0.91 (0.06)	1.96 (0.11)	10.8 (0.4)	0.80 (0.07)
Glu5	3.05 (0.16)	9.5 (0.7)	1.02 (0.09)	2.03 (0.04)	10.4 (0.2)	0.81 (0.03)
Thr6	2.78 (0.25)	10.1 (0.7)	0.67 (0.05)	2.00 (0.03)	9.9 (0.4)	0.79 (0.04)
Ala7	2.68 (0.20)	9.9 (1.2)	0.65 (0.05)	1.95 (0.02)	10.4 (0.2)	0.81 (0.05)
Met8	2.42 (0.21)	8.9 (0.5)	0.83 (0.06)	1.93 (0.04)	9.8 (0.2)	0.71 (0.07)
Glu9						
Thr10	2.54 (0.29)	9.7 (0.5)	0.70 (0.06)	1.92 (0.04)	10.3 (0.2)	0.81 (0.08)
Leu11						
Ile12	3.13 (0.12)	9.7 (0.8)	0.68 (0.07)	1.96 (0.05)	10.0 (0.2)	0.80 (0.08)
Asn13						
Val14						
Phe15	2.77 (0.17)	10.2 (0.3)	0.95 (0.06)	1.97 (0.02)	10.1 (0.1)	0.78 (0.02)
His16	2.63 (0.22)	10.5 (0.6)	0.85 (0.07)	1.96 (0.02)	10.1 (0.2)	0.72 (0.05)
Ala17	2.74 (0.15)	9.9 (0.7)	1.20 (0.07)	1.94 (0.04)	11.0 (0.1)	0.81 (0.04)
His18						
Ser19	3.16 (0.68)	9.0 (3.7)	1.27 (0.19)	1.76 (0.10)	15.3 (0.8)	0.59 (0.02)
Gly20	2.77 (0.16)	8.4 (0.5)	0.85 (0.08)	2.05 (0.05)	9.8 (0.1)	0.88 (0.11)
Lys21						
Glu22	2.62 (0.26)	11.4 (2.8)	0.99 (0.10)	1.88 (0.05)	15.8 (0.8)	0.64 (0.08)
Gly23	2.58 (0.22)	6.3 (1.1)	0.60 (0.05)	1.95 (0.05)	10.0 (0.2)	0.72 (0.03)
Asp24	2.50 (0.24)	11.4 (3.6)	0.74 (0.11)	1.98 (0.08)	9.3 (0.3)	0.74 (0.03)
Lys25	2.45 (0.44)	8.0 (1.1)	0.63 (0.07)	1.94 (0.06)	11.8 (0.4)	0.73 (0.04)
Tyr26	2.57 (0.18)	10.1 (0.5)	0.72 (0.06)	1.97 (0.02)	10.5 (0.2)	0.78 (0.03)
Lys27						
Leu28						

Ser29						
Lys30	2.27 (0.16)	8.5 (0.8)	1.08 (0.13)	2.02 (0.03)	9.2 (0.3)	0.86 (0.06)
Lys31	2.72 (0.11)	9.6 (0.4)	0.87 (0.06)	2.00 (0.02)	9.6 (0.2)	0.73 (0.08)
Glu32				1.97 (0.02)	9.0 (0.1)	0.83 (0.07)
Leu33						
Lys34						
Glu35				1.93 (0.03)	9.7 (0.1)	0.72 (0.04)
Leu36	2.75 (0.22)	8.2 (0.2)	0.34 (0.03)	2.05 (0.04)	9.5 (0.1)	0.79 (0.06)
Leu37	2.84 (0.17)	9.6 (0.2)	0.83 (0.04)	2.03 (0.09)	10.5 (0.5)	0.78 (0.07)
Gln38	2.73 (0.20)	8.4 (0.5)	0.61 (0.05)	1.93 (0.01)	9.6 (0.2)	0.80 (0.05)
Thr39	2.68 (0.15)	8.5 (0.4)	0.91 (0.06)	1.92 (0.03)	8.9 (0.2)	0.85 (0.05)
Glu40	2.58 (0.32)	9.1 (0.5)	0.45 (0.04)	2.01 (0.03)	9.3 (0.1)	0.78 (0.01)
Leu41	2.62 (0.32)	9.3 (0.6)	0.67 (0.06)	1.93 (0.03)	9.5 (0.2)	0.82 (0.05)
Ser42	2.54 (0.09)	9.0 (0.2)	0.73 (0.05)	1.89 (0.03)	8.9 (0.1)	0.73 (0.04)
Gly43	2.39 (0.29)	8.5 (0.4)	1.38 (0.13)	2.03 (0.05)	9.3 (0.1)	0.69 (0.06)
Phe44	2.10 (0.12)	8.7 (0.6)	0.72 (0.07)	1.77 (0.05)	9.1 (0.3)	0.81 (0.02)
Leu45	2.54 (0.27)	8.8 (0.9)	0.56 (0.06)	1.91 (0.05)	9.7 (0.3)	0.74 (0.01)
Asp46	2.60 (0.11)	8.7 (0.3)	0.58 (0.04)	1.93 (0.02)	9.1 (0.1)	0.69 (0.01)
Ala47	2.62 (0.13)	8.8 (0.2)	0.75 (0.05)	1.80 (0.03)	8.7 (0.1)	0.73 (0.06)
Gln48	2.59 (0.10)	7.8 (0.2)	0.73 (0.04)	1.88 (0.02)	7.3 (0.1)	0.60 (0.03)
Lys49	2.55 (0.36)	7.7 (0.8)	0.33 (0.04)	1.88 (0.03)	8.6 (0.2)	0.63 (0.05)
Asp50						
Ala51	2.38 (0.18)	8.0 (0.3)	0.59 (0.05)	1.76 (0.02)	8.7 (0.2)	0.70 (0.02)
Asp52	2.56 (0.08)	9.3 (0.5)	0.84 (0.04)	1.84 (0.02)	9.5 (0.1)	0.82 (0.03)
Ala53	2.71 (0.08)	9.4 (0.3)	1.05 (0.06)	1.84 (0.01)	9.3 (0.1)	0.79 (0.02)
Val54				1.87 (0.02)	9.5 (0.1)	0.74 (0.04)
Asp55	2.69 (0.09)	10.0 (0.2)	0.69 (0.03)	1.87 (0.02)	10.1 (0.2)	0.76 (0.01)
Lys56						
Val57	2.56 (0.11)	8.7 (0.4)	0.76 (0.05)	1.85 (0.01)	9.2 (0.1)	0.76 (0.05)
Met58	2.58 (0.12)	9.5 (0.4)	0.81 (0.06)	1.90 (0.02)	9.9 (0.2)	0.79 (0.04)
Lys59	2.45 (0.09)	10.3 (0.3)	0.86 (0.05)	1.87 (0.02)	10.0 (0.1)	0.78 (0.04)
Glu60	2.49 (0.13)	9.5 (0.2)	0.89 (0.05)	1.87 (0.02)	9.6 (0.1)	0.74 (0.04)
Leu61	2.49 (0.11)	9.6 (0.4)	0.76 (0.06)	1.90 (0.03)	9.7 (0.2)	0.70 (0.06)

Asp62	2.23 (0.06)	9.1 (0.4)	0.70 (0.05)	1.78 (0.02)	9.2 (0.1)	0.76 (0.04)
Glu63	2.41 (0.17)	8.7 (0.4)	0.72 (0.06)	1.76 (0.02)	9.2 (0.1)	0.65 (0.01)
Asp64	2.39 (0.14)	9.3 (0.4)	0.69 (0.04)	1.84 (0.03)	8.5 (0.1)	0.68 (0.05)
Gly65	2.40 (0.10)	8.0 (0.4)	0.76 (0.06)	1.83 (0.02)	8.2 (0.1)	0.65 (0.06)
Asp66	2.51 (0.20)	8.4 (0.3)	0.59 (0.04)	1.96 (0.03)	8.5 (0.1)	0.62 (0.03)
Gly67	2.38 (0.25)	9.2 (0.3)	0.70 (0.07)	1.94 (0.04)	9.0 (0.2)	0.78 (0.04)
Glu68	2.60 (0.25)	8.6 (0.7)	0.65 (0.05)	1.78 (0.03)	8.1 (0.1)	0.67 (0.03)
Val69	2.42 (0.28)	9.2 (0.6)	1.01 (0.12)	1.84 (0.04)	9.1 (0.2)	0.65 (0.07)
Asp70	2.31 (0.11)	8.1 (0.5)	0.83 (0.07)	1.87 (0.03)	9.3 (0.2)	0.74 (0.08)
Phe71	3.80 (0.47)	9.8 (1.5)	0.60 (0.09)	1.90 (0.02)	9.9 (0.1)	0.87 (0.06)
Gln72	2.33 (0.16)	8.9 (0.4)	0.64 (0.04)	1.88 (0.02)	9.2 (0.2)	0.75 (0.02)
Glu73	2.55 (0.15)	9.0 (0.2)	0.75 (0.06)	1.82 (0.02)	9.7 (0.1)	0.73 (0.02)
Tyr74	2.23 (0.18)	8.6 (0.3)	0.81 (0.07)	1.93 (0.03)	10.0 (0.1)	0.77 (0.05)
Val75	2.82 (0.20)	9.9 (0.2)	0.60 (0.05)	1.96 (0.03)	10.1 (0.2)	0.76 (0.02)
Val76	2.81 (0.19)	10.2 (0.4)	0.72 (0.06)	1.93 (0.03)	9.9 (0.2)	0.75 (0.06)
Leu77				1.85 (0.03)	7.6 (0.2)	0.64 (0.03)
Val78				1.90 (0.02)	9.8 (0.1)	0.77 (0.03)
Ala79	2.96 (0.18)	10.0 (0.5)	0.86 (0.06)	1.99 (0.02)	9.8 (0.2)	0.80 (0.11)
Ala80						
Leu81	2.62 (0.14)	10.5 (0.5)	0.81 (0.09)	1.89 (0.02)	10.0 (0.1)	0.75 (0.10)
Thr82	3.21 (0.36)	10.7 (0.5)	0.73 (0.06)	1.89 (0.03)	10.1 (0.1)	0.72 (0.03)
Val83	2.42 (0.21)	8.4 (0.4)	0.58 (0.05)	1.96 (0.04)	9.9 (0.1)	0.67 (0.02)
Ala84	2.64 (0.31)	10.7 (0.5)	0.77 (0.07)	1.91 (0.03)	10.4 (0.1)	0.74 (0.04)
Cys85						
Asn86	2.78 (0.32)	8.5 (0.2)	0.67 (0.04)	1.81 (0.04)	8.6 (0.2)	0.67 (0.06)
Asn87						
Phe88						
Phe89	2.94 (0.34)	9.4 (0.9)	0.75 (0.06)	1.98 (0.03)	10.8 (0.2)	0.88 (0.04)
Trp90						
Glu91	2.21 (0.08)	5.5 (0.1)	0.35 (0.02)	1.87 (0.04)	4.9 (0.1)	0.36 (0.02)
Asn92						
Ser93	1.13 (0.09)	2.4 (0.1)	-1.19 (0.03)	1.06 (0.04)	1.9 (0.1)	-0.92 (0.11)

Table SI3.Order parameters (S^2) and chemical exchange terms (R_{ex}) at 9.4 T for the backbone amide ^{15}N nuclei in *apo*-S100A1-βME and *apo*-S100A1 proteins. Monte Carlo derived uncertainties are given in parantheses. Correlation times for internal motions τ_{int} are not given because their uncertainties often approach their values and, therefore, they cannot be used in the analysis of molecular dynamics. Optimization of model-free parameters was carried out using $\Delta\sigma$ = -160 ppm and r_{NH} = 1.05 Å.

Residue	*apo*-S100A1-βME		*apo*-S100A1	
	S^2	R_{ex} (s^{-1})	S^2	R_{ex} (s^{-1})
Ser2	0.58 (0.07) [a]	0.0 (0.1) [a]		
Glu3	0.69 (0.09)	0.8 (0.4)	0.77 (0.12)	0.8 (0.5)
Leu4	0.97 (0.03)	0.7 (0.3)	0.79 (0.19) [b]	1.6 (0.9) [b]
Glu5	0.90 (0.04)	1.0 (0.1)	0.81 (0.07)	1.2 (0.3)
Thr6	0.92 (0.06)	0.9 (0.2)	0.85 (0.5)	0.9 (0.3)
Ala7	0.90 (0.05)	0.8 (0.2)	0.88 (0.05)	1.1 (0.3)
Met8	0.97 (0.03)	0.7 (0.2)	0.91 (0.06)	0.6 (0.3)
Glu9	0.93 (0.05)	1.2 (0.2)		
Thr10	0.95 (0.03)	1.0 (0.1)	0.91 (0.06)	0.9 (0.3)
Leu11	0.96 (0.03)	1.1 (0.2)		
Ile12	0.91(0.05)	0.4 (0.2)	0.83 (0.07)	0.8 (0.2)
Asn13	0.96 (0.03)	1.0 (0.1)		
Val14	0.95 (0.03)	1.1 (0.2)		
Phe15	0.98 (0.02)	1.3 (0.3)	0.88 (0.05)	0.8 (0.2)
His16	0.95 (0.04)	1.2 (0.3)	0.90 (0.05)	0.8 (0.3)
Ala17	0.93 (0.04)	0.9 (0.2)	0.91 (0.06)	1.3 (0.3)
His18	0.87 (0.05)	0.9 (0.2)		
Ser19	0.92 (0.07)	2.7 (0.4)	0.85 (0.06)	4.5 (0.6)
Gly20	0.78 (0.09)	1.2 (0.4)	0.79 (0.07)	0.9 (0.2)
Lys21	0.66 (0.10)	1.0 (0.4)		
Glu22	0.86 (0.05)	0.4 (0.3)	0.90 (0.09)	4.5 (0.6)
Gly23	0.53 (0.20) [c]	3.6 (0.8) [c]	0.83 (0.08)	1.1 (0.3)
Asp24	0.75 (0.14)	0.6 (0.6)	0.86 (0.10)	0.5 (0.4)
Lys25	0.60 (0.08)	3.8 (0.4)	0.85 (0.10)	2.1 (0.5)

Tyr26	0.83 (0.05)	0.8 (0.3)	0.89 (0.04)	1.1 (0.2)
Lys27	0.70 (0.04) [c]	0.0 (0.0) [c]		
Leu28	0.96 (0.04)	1.3 (0.3)		
Ser29	0.89 (0.05)	0.3 (0.1)		
Lys30	0.78 (0.06)	0.9 (0.3)	0.85 (0.08)	0.6 (0.4)
Lys31	0.95 (0.04)	0.5 (0.1)	0.87 (0.04)	0.6 (0.2)
Glu32	0.91 (0.06)	0.7 (0.3)	0.85 (0.09) [c]	0.4 (0.4) [c]
Leu33	0.90 (0.06)	0.7 (0.3)		
Lys34	0.94 (0.04)	0.7 (0.2)		
Glu35	0.95 (0.03)	0.6 (0.2)	0.88 (0.09) [c]	0.8 (0.4) [c]
Leu36	0.88 (0.09)	0.6 (0.2)	0.57 (0.07)	1.9 (0.3)
Leu37	0.81 (0.09)	1.4 (0.2)	0.76 (0.19) [b]	1.7 (0.7) [b]
Gln38	0.92 (0.06)	0.6 (0.2)	0.89 (0.05)	0.6 (0.3)
Thr39	0.95 (0.03)	0.1 (0.2)	0.92 (0.04)	0.0 (0.1)
Glu40	0.92 (0.05) [c]	0.5 (0.2) [c]	0.87 (0.05)	0.5 (0.2)
Leu41	0.92 (0.05)	0.4 (0.2)	0.94 (0.05)	0.5 (0.3)
Ser42	0.93 (0.02)	0.0 (0.1)	0.96 (0.04)	0.0 (0.1)
Gly43	0.69 (0.09)	1.1 (0.3)	0.78 (0.10)	0.8 (0.4)
Phe44	0.87 (0.08)	0.4 (0.4)	0.91 (0.02)	0.3 (0.3)
Leu45	0.94 (0.05)	0.6 (0.2)	0.91 (0.06)	0.7 (0.3)
Asp46	0.94 (0.03)	0.2 (0.2)	0.86 (0.04)	0.5 (0.2)
Ala47	0.93 (0.03)	0.9 (0.2)	0.93 (0.02)	0.0 (0.0)
Gln48	0.88 (0.03)	0.0 (0.1)	0.71 (0.02)	0.0 (0.0)
Lys49	0.73 (0.05)	0.0 (0.2)	0.72 (0.07)	0.8 (0.3)
Asp50	0.78 (0.06)	0.4 (0.2)		
Ala51	0.76 (0.04)	0.0 (0.1)	0.91 (0.01)	0.0 (0.1)
Asp52	0.73 (0.11)	1.2 (0.4)	0.98 (0.02)	0.2 (0.2)
Ala53	0.81 (0.07)	1.1 (0.2)	0.98 (0.01)	0.1 (0.2)
Val54	0.91 (0.02)	0.0 (0.1)	0.91 (0.07) [c]	0.5 (0.3) [c]
Asp55	0.93 (0.04)	0.5 (0.2)	0.97 (0.03)	0.7 (0.2)
Lys56	0.95 (0.02)	0.7 (0.2)		
Val57	0.94 (0.03)	0.3 (0.3)	0.96 (0.03)	0.1 (0.2)
Met58	0.98 (0.02)	0.6 (0.2)	0.95 (0.04)	0.5 (0.2)

Lys59	0.97 (0.03)	0.6 (0.2)	0.97 (0.02)	0.5 (0.1)
Glu60	0.93 (0.03)	0.6 (0.2)	0.96 (0.02)	0.5 (0.1)
Leu61	0.95 (0.03)	0.4 (0.3)	0.94 (0.05)	0.5 (0.2)
Asp62	0.93 (0.03)	0.2 (0.2)	0.91 (0.02)	0.4 (0.2)
Glu63	0.89 (0.02)	0.1 (0.2)	0.90 (0.01)	0.5 (0.1)
Asp64	0.87 (0.05)	0.2 (0.2)	0.91 (0.02)	0.0 (0.0)
Gly65	0.64 (0.08)	0.4 (0.4)	0.87 (0.03)	0.0 (0.0)
Asp66	0.70 (0.07)	0.3 (0.2)	0.85 (0.08)	0.3 (0.3)
Gly67	0.66 (0.08)	0.6 (0.4)	0.92 (0.05)	0.1 (0.2)
Glu68	0.87 (0.04)	0.3 (0.1)	0.88 (0.03)	0.0 (0.0)
Val69	0.93 (0.06)	0.3 (0.3)	0.91 (0.05)	0.4 (0.3)
Asp70	0.96 (0.03)	0.4 (0.2)	0.92 (0.05)	0.5 (0.3)
Phe71	0.92 (0.05)	0.7 (0.3)	0.94 (0.05)	0.6 (0.2)
Gln72	0.94 (0.03)	0.5 (0.2)	0.93 (0.04)	0.2 (0.3)
Glu73	0.98 (0.02) [c]	0.4 (0.1) [c]	0.94 (0.01)	0.5 (0.1)
Tyr74	0.91 (0.06)	0.7 (0.3)	0.87 (0.07)	0.9 (0.3)
Val75	0.92 (0.04)	1.0 (0.1)	0.89 (0.06)	0.9 (0.3)
Val76	0.98 (0.01)	0.7 (0.2)	0.93 (0.05)	0.6 (0.2)
Leu77	0.93 (0.03)	1.5 (0.1)	0.79 (0.04) [c]	0.0 (0.0) [c]
Val78	0.95 (0.03) [c]	0.1 (0.1) [c]	0.93 (0.06) [c]	0.6 (0.3) [c]
Ala79	0.79 (0.05)	1.0 (0.2)	0.87 (0.04)	0.7 (0.2)
Ala80	0.91 (0.04)	0.1 (0.2)		
Leu81	0.92 (0.03)	1.0 (0.1)	0.97 (0.03)	0.6 (0.2)
Thr82	0.90 (0.04)	1.0 (0.1)	0.95 (0.05)	0.7 (0.3)
Val83	0.89 (0.04)	1.0 (0.1)	0.79 (0.08)	1.2 (0.3)
Ala84	0.94 (0.03)	0.9 (0.2)	0.93 (0.05)	0.9 (0.3)
Cys85	0.93 (0.04)	1.1 (0.2)		
Asn86	0.90 (0.04)	1.0 (0.1)	0.90 (0.03)	0.4 (0.2)
Asn87	0.94 (0.03)	1.4 (0.2)		
Phe88	0.96 (0.03)	0.6 (0.2)		
Phe89	0.96 (0.04)	0.7 (0.3)	0.94 (0.05)	1.3 (0.3)
Trp90	0.93 (0.05)	0.5 (0.2)		
Glu91	0.79 (0.05) [a]	0.0 (0.0) [a]	0.71 (0.02) [d]	0.0 (0.0) [d]

Asn92	0.60 (0.03) [a]	0.0 (0.0) [a]		
Ser93	0.32 (0.01) [a]	0.1 (0.1) [a]	0.22 (0.01) [d]	0.0 (0.0) [d]

[a] The model-free approach parameters were determined together with the residue dependent correlation times $\tau_{R,i}$. For Ser2, Glu91, Asn92, and Ser93 they were equal to 7.9 ns, 7.7 ns, 6.8 ns, and 4.5 ns, respectively.

[b] The model-free approach parameters were calculated from the data measured at 9.4 T solely assuming that the anisotropic overall tumbling was determined independently.

[c] The model-free approach parameters were calculated from the data measured at 11.7 T solely assuming that the anisotropic overall tumbling was determined independently.

[d] The model-free approach parameters were determined together with the residue dependent correlation times $\tau_{R,i}$. For Glu91 and Ser93 they were equal to 5.2 ns and 4.7 ns, respectively.