A Native Disulfide Stabilizes Non-Native Helical Structures in Partially Folded States of Equine β-Lactoglobulin

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Supporting Information

Table S1. Chemical Shifts for NMR Resonances of CHIBLΔF in 0.1 M Phosphoric Acid, pH 1.8, 90% H_2O/10% D_2O at 12 ºC

Residue		chimical shifts (ppm)					
		CO	CA	HA	CB	HN	N
97	T	173.73	62.05	4.32	69.91	8.67	118.67
98	D	175.29	52.74	4.72	38.36	8.67	122.17
99	Y	176.48	60.29	4.32	38.48	8.41	121.67
100	K	177.89	58.45	3.88	32.45	8.17	119.92
101	N	176.97	54.97	4.57	38.46	8.04	118.03
102	Y	178.17	61.26	4.17	38.72	8.06	120.31
103	L	178.08	58.13	3.90	42.25	8.34	120.92
104	F	177.95	60.83	4.20	39.29	7.95	118.64
105	L	178.87	58.07	3.88	42.25	7.93	119.30
106	C	177.35	58.85	4.27	38.18	8.09	118.17
107	M	178.21	56.77	4.23	31.88	8.29	118.67
108	K	177.39	58.04	3.98	32.40	7.79	120.17
109	N	174.90	53.25	4.68	39.10	7.67	115.42
110	A	177.45	53.09	4.25	19.21	7.65	123.92
111	A	177.88	52.85	4.39	19.98	8.53	123.92
112	T	173.75	58.36	4.83	70.23	7.50	109.42
113	P	179.49	64.84		32.14		
114	G	176.46	46.53	3.88		8.70	107.31
115	Q	178.16	57.65	4.18	28.94	7.94	120.67
116	S	176.55	61.11	4.16	62.97	8.23	116.17
117	L	179.95	57.88	4.11	41.97	7.92	121.92
118	V	178.32	65.95	3.82	31.90	7.60	119.38
119	C	176.92	57.31	4.57	37.50	8.06	117.48
120	Q	178.34	59.01	4.07	28.34	8.21	119.17
121	Y	178.98	60.38	4.31	38.07	7.98	120.67
122	L	179.47	57.76	3.98	42.29	8.67	122.17
123	A	179.49	54.86	4.24	19.21	8.34	121.36
124	R	178.43	58.69	4.16	30.30	7.89	117.72
125	T	175.89	65.00	3.99	69.42	7.91	113.92

	126	Q	177.72	57.80	4.16	28.15	8.07	120.67
	127	M	178.37	58.48	4.05	32.61	7.93	119.91
	128	V	177.85	65.31	3.82	32.57	8.06	120.53
	129	D	177.24	55.16	4.48	37.54	8.33	119.42
	130	E	177.94	58.48	4.16	27.85	8.28	120.42
	131	E	178.69	58.37	4.12	28.09	8.11	119.67
	132	I	178.23	64.20	3.82	38.88	8.07	120.41
	133	M	178.37	57.70	4.34	32.38	7.99	119.92
	134	E	178.41	58.23	4.12	28.59	8.20	119.17
	135	K	177.85	58.23		32.13	8.06	120.42
	136	F	176.69	59.07	4.49	39.56	8.08	119.42
	137	R	177.17	57.33	4.17	30.59	8.07	120.92
	138	R	176.71	57.04	4.20	30.75	8.17	121.17
	139	A	177.98	52.53	4.24	19.21	8.07	123.92
	140	L	177.56	55.18	4.25	42.30	8.05	120.92
	141	Q	174.24	53.90	4.56	28.87	8.24	122.17
	142	P	177.05	63.26		32.25		
143(tag)		L	177.62	55.29	4.25	42.29	8.34	122.06
144(tag)		E	175.94	55.42	4.24	29.41	8.27	120.92
145(tag)		H	174.21	55.65	4.61	29.19	8.77	122.92
146(tag)		H	174.24	55.77	4.64	29.57	8.81	121.42
147(tag)		H	174.35	55.22	4.61	29.46	8.69	119.67
148(tag)		H	174.40	55.66	4.65	29.57	8.86	120.92
149(tag)		H	174.44	55.44	4.62	29.66	8.82	120.17
150(tag)		H	174.34	55.33	4.54	29.46	8.58	119.42

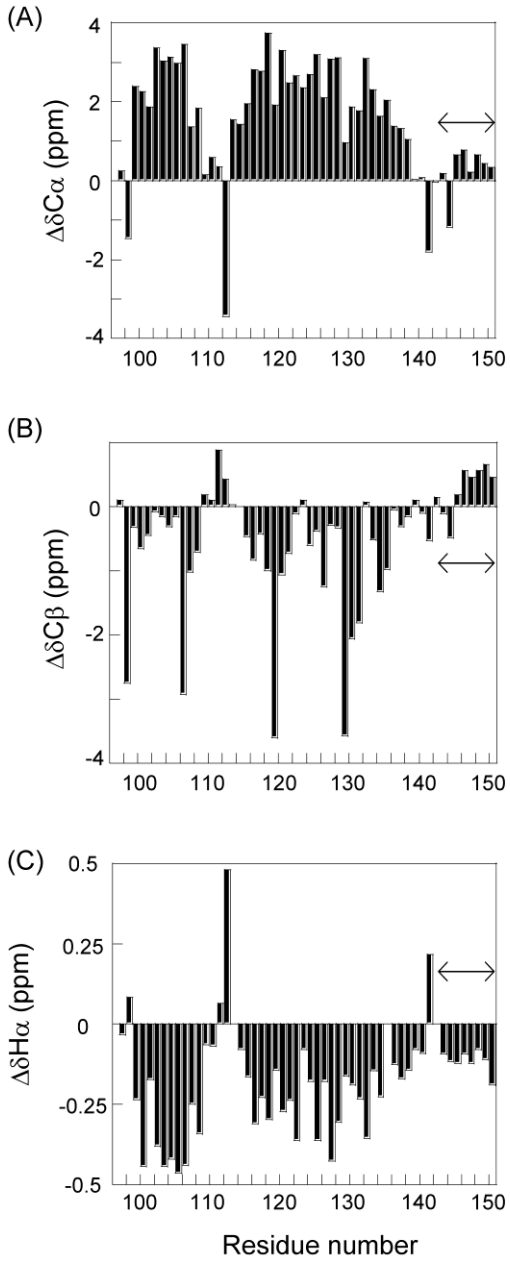

Figure S1: Chemical shift deviations from random coil values for (A) $^{13}C\alpha$ (B) $^{13}C\beta$ and (C) $^{1}H\alpha$ CHIBLΔF resonances. Double arrows indicate the hexahistidine sequences.