

Supplementary Material

Sparse Isotopic Labeling for NMR Characterization of HtpG, the *E. coli* Hsp90

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Table S1. RDC data and assignments for full-length HtpG at 37° C, pH 9.0

peak	Assignment	¹³ C (ppm)	¹ H (ppm)	Peg RDC	error	Phage RDC	error
X1C-H	A537	23.6	1.22	3.7	2.2	-1.9	2.6
X2C-H	A165	23.4	1.39	2.9	4.6	2.6	1.6
X3C-H	A403	23.0	1.43	4.5	3.1	-2.3	4.8
X4C-H	A134	22.4	0.94	-8.3	4.1	-6.9	4.4
X5C-H	A143	20.2	1.19	0.2	2.3	-6.0	2.1
X6C-H	A144	19.8	1.35	2.1	1.5	7.6	1.6
X7C-H	A232	19.7	0.44	-25.1	1.8	-18.3	1.5
X8C-H	A387	19.5	0.64	18.1	3.9	16.7	2.2
X9C-H	A439*	19.3	1.54	-11.8	2.6	-4.6	1.5
X10C-H	A397	19.3	1.71	-24.6	2.0	-18.3	2.2
X11C-H	A157	19.2	1.64	-18.8	2.1	-11.0	2.1
X12C-H	A205	19.0	1.38				
X13C-H	A98	18.8	1.36				
X14C-H	A284*	18.8	1.49	40.7	2.8		
X15C-H	A557	18.7	1.45	-2.6	0.9		
X16C-H	A42	18.7	1.71	3.9	3.4	4.1	2.5
X17C-H	A368*	18.6	1.29	-15.8	1.2	-8.6	1.2
X18C-H		18.6	1.38	-0.0	0.8	3.3	0.9
X19C-H	A43	18.5	1.60				
X20C-H	A39*	18.4	1.46	1.4	1.1	-0.9	0.4
X21C-H	A556*	18.5	1.43	16.6	6.7		
X22C-H	A603	18.5	1.59			25.6	1.3
X23C-H		18.5	1.53			4.8	1.4
X24C-H	A114	18.5	1.45				
X25C-H	A435*	18.4	1.26	-16.4	1.1		
X26C-H	A50	18.4	0.86	-2.9	1.5	-2.3	1.5
X27C-H		18.3	1.34	0.6	2.0	-0.8	0.7
X28C-H	A543*	18.2	1.39	6.0	1.1	-0.1	1.4
X29C-H		18.1	1.46	-1.1	0.7	0.7	0.6
X30C-H		18.1	1.71	8.8	1.7	5.0	1.6
X31C-H	A254*	18.0	1.39	-22.3	2.3	-15.1	1.2
X32C-H		17.9	1.50	-3.9	1.4	-2.9	0.9
X33C-H		17.8	1.29	28.7	4.2	15.6	2.3
X34C-H	A517	17.8	1.53	2.9	1.5	6.2	1.8
X35C-H	A130	17.6	1.04	32.8	2.0	16.4	1.9
X36C-H	A580	17.3	1.37	-3.3	2.8	-2.2	2.5
X37C-H	A580	17.1	1.30	-6.7	2.9	-2.0	2.2
X38C-H	A581	16.9	0.52	0.3	2.9	-0.2	4.8
X39C-H	A581	16.8	0.59	4.2	3.1	3.8	2.4
X40C-H	A411*	16.9	1.14	30.1	12.7	28.6	5.8

Assignments of moderate confidence, all others are high confidence

Table S2. Alanine chemical shifts for single domains of HtpG at 35 °C, pH 7.5

N-terminal domain

Residue Number	Residue Name	H	N	CO	CA	CB	HB	HA
39	ALA	7.50	123.9	178.8	55.0	18.7	1.45	4.26
42	ALA	8.18	122.7	181.5	54.9	18.9	1.74	4.20
43	ALA	8.47	124.3	178.8	55.3	19.1	1.63	4.16
50	ALA	8.75	120.1	178.8	52.5	18.4	0.86	4.06
98	ALA	8.07	125.2	177.8	52.9	19.2	1.36	4.26
114	ALA	8.16	123.5	178.5	53.3	18.9	1.43	4.26
130	ALA	7.81	123.9	178.3	54.8	18.9	0.93	3.57
134	ALA	7.68	124.9	175.1	51.1	23.0	0.95	5.11
143	ALA	8.69	129.9	178.5	51.0	20.3	1.21	5.01
144	ALA	8.71	123.9	177.9	52.5	19.9	1.37	4.09
157	ALA	8.59	129.0	177.1	51.8	19.5	1.60	5.24
165	ALA	9.40	126.3	174.6	51.4	23.8	1.38	4.79
205	ALA	8.49	127.8	176.3	52.2	19.2	1.40	4.46

Middle domain

Residue Number	Residue Name	H	N	CO	CA	CB	HB	HA
403	ALA					23.1	1.44	

C-terminal domain

Residue Number	Residue Name	H	N	CO	CA	CB	HB	HA
517	ALA	8.05	120.6	179.4	54.5	18.0	1.52	4.14
537	ALA	6.95	116.9	175.3	51.0	23.6	1.26	5.12
543	ALA	8.28	124.9	177.8	53.3	19.1	1.39	4.24
551	ALA	8.08	122.2	179.5	54.6	18.4	1.48	4.18
555	ALA	8.02	123.0	179.3	53.7	18.7	1.46	4.30
556	ALA	8.00	122.1	178.0	53.3	18.7	1.47	4.26
557	ALA	7.84	120.8	178.2	52.5	18.9	1.46	4.37
580	ALA	7.27	122.1	178.8	55.7	17.3	1.31	3.64
581	ALA	8.20	117.8	179.2	54.8	17.3	0.68	3.93
587	ALA	8.26	123.1	180.7	55.2	17.9	1.55	4.28
600	ALA	7.73	122.3	181.0	54.7	18.0	1.55	4.26
603	ALA	8.04	119.4	179.1	55.0	18.5	1.55	3.83