SUPPLEMENTARY MATERIAL

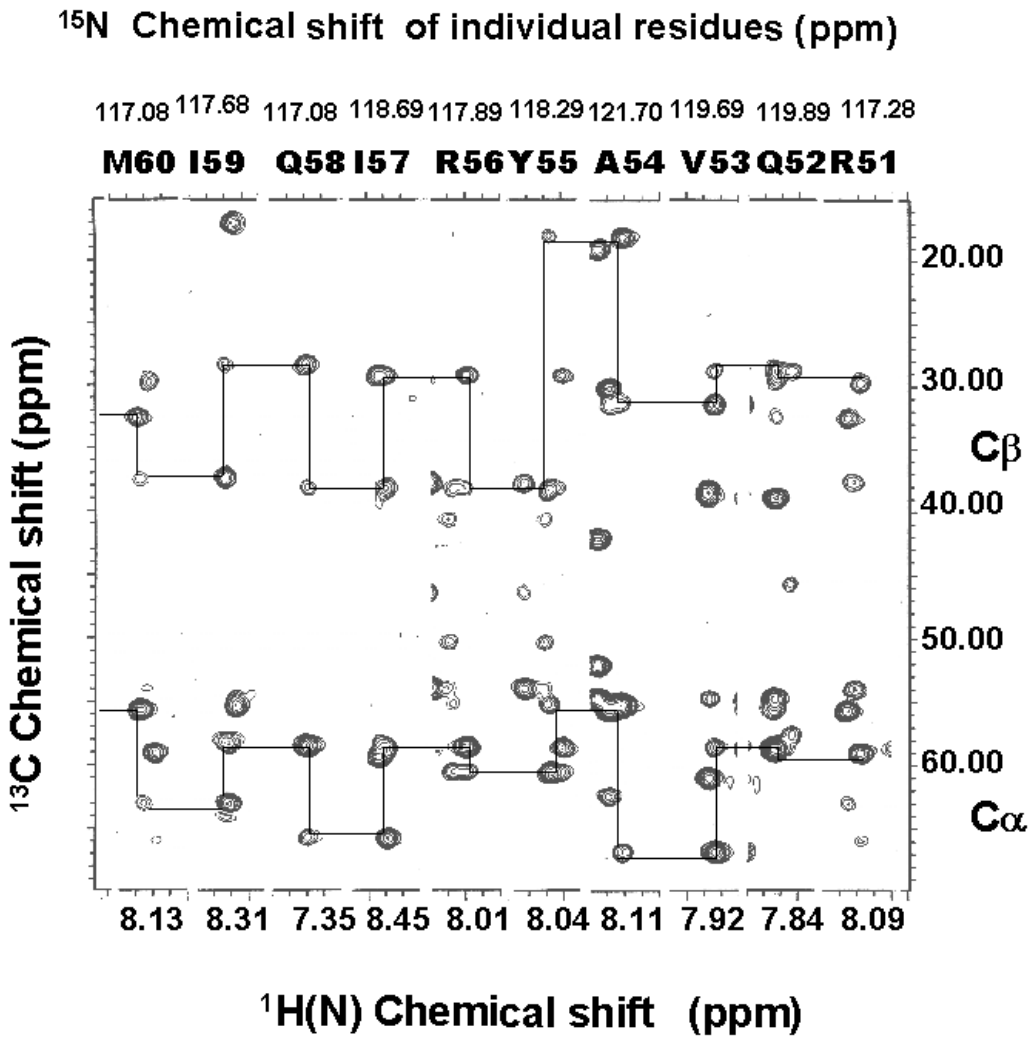

Figure S1. Series of strips from ^{15}N slices from the HNCACB spectrum of the CTD of NifA showing the crosspeaks due to NH coupling to the Cα and Cβ atoms in the backbone of the protein from the C-terminal (recognition) helix. The vertical lines within each strip connect the crosspeaks between the NH resonance (residue numbered on the top of the strip) to the Cα and Cβ resonances from the same residue (i) and the previous residue (i-1). The horizontal lines between the strips connect the crosspeaks arising from the same resonances, leading to the sequential assignments. i-1 crosspeaks are not observed in the strip from R51 because residue 50 is proline.

Table S1. Assignment of the backbone resonances of the C-terminal domain of NifA from *K. pneumoniae* in 10 mM sodium phosphate buffer, pH 6.6, containing 500 mM LiBr and 0.1 mM EDTA at 27 °C

Residue	^{15}N	NH	Hα	Hα2	Hβ1	Hβ2	Hβ3	Cα	Cβ	CO
Ala-8			4.36		1.4	1.4		52.4	19.07	176.75
Arg-7	125.22	7.9	4.47		1.82	1.82		56.31	30.62	176.036
Ile-6	123.32	8.31	3.99					61.11	38.44	176.037
Arg-5	125.91	8.41	4.36		1.81	1.81		55.99	30.63	175.22
Ala-4	126.11	8.35	4.34		1.4	1.4	1.4	52.63	19.085	177.611
Arg-3	120.89	8.39	4.36		1.91	1.82		56.48	30.61	176.979
Gly-2	110.33	8.48	4.03	4.03				45.25		177.69
Ser-1	115.3	8.23	4.47		3.89	3.89		58.32	63.62	174.16
Asp 1	122.08	8.36	4.64		2.69	2.69		54.08	40.99	175.49
Asn 2	119.09	8.29	4.99					51.18	38.7	
Pro 3										
Pro 4			4.43		1.92	1.92		62.77	31.8	177.133
Lys 5	121.48	8.29	4.27		1.79	1.63		56.06	32.85	176.35
Lys 5	122.3	8.51	4.27		1.79	1.63		56.06	32.85	176.35
Ala 6	124.91	8.28	4.31		1.37	1.37	1.37	52.69	18.91	177.53
Leu 7	121.5	8.18	4.47		1.63	1.79		54.85	42.12	177.29
Ala 8	124.91	8.28	4.36		1.42	1.42	1.42	52.75	18.9	177.69
Ser 9	114.69	8.23	4.55		3.91	3.91		58.32	63.63	174.39
Ser 10	117.5	8.32	4.55		3.91	3.91		58.38	63.86	174.39
Gly 11	110.64	8.23	4.13	4.13				44.1		
Pro 12			4.38		2.24	1.91		63.18	31.83	176.91
Ala 13	124.12	8.38	4.29		1.37	1.37	1.37	52.7	18.9	178
Glu 14	119.9	8.34	4.24		2.03	1.89		56.71	29.16	176.28
Asp 15	120.5	8.23	4.47		2.5	2.41		54.64	40.64	177.13
Gly 16	109.06	8.35	3.91	3.91				46.5		174.23
Trp 17	119.29	7.78	4.6		3.3	3.3		57.99	28.69	175.81
Leu 18	122.71	7.6	4.14		1.39	1.25		54.92	42.1	176.5
Asp 19	120.91	7.84	4.42		2.76	2.55		54.43	40.89	176.2
Asn 20	120.89	8.36	4.66		2.83	2.83		53.87	38.21	175.571
Ser 21	115.68	8.47	4.39		3.98	3.91		59.38	63.61	174.937
Leu 22	123.29	7.88	4.34		1.73	1.56		55.83	42.11	177.61
Asp 23	120.28	8.29	4.57		2.9	2.73		54.64	40.89	176.9
Glu 24	119.69	8.34	3.91		2.03	2.03		59.88	29.91	178.39
Arg 25	121.1	8.28	3.98		1.98	1.98		60.28	30.14	177.77
Gln 26	116.69	8.32	3.99		2.25	2.08		58.881	28.448	179.413
Arg 27	120.08	8.36	3.98		1.84	1.84		59.835	30.323	178.24
Leu 28	121.08	7.87	4.03		1.75	1.75		58.43	40.89	178.32
Ile 29	118.7	8.28	3.4		1.81			65.9	37.73	177.134
Ala 30	120.28	8.19	4.15		1.51	1.51	1.51	54.8	17.67	178.95
Ala 31	120.28	7.86	3.93		1.42	1.42	1.42	54.92	18.16	178.95
Leu 32	118.89	8.22	3.21		1.14	1.14		58.55	39.43	178.55
Glu 33	119.07	8.47	3.49		2.08	1.96		59.72	29.16	181.06
Lys 34	121.69	7.82	4		1.77	1.77		58.77	31.62	177.77
Ala 35	118.49	7.84	4.29		1.37	1.37	1.37	51.57	19.41	177.92
Gly 36	110.67	7.86	4.03	3.91				48.06		175.02
Trp 37	110.86	9.18	3.61		3.37	3.21		59.83	24.06	173.451
Val 38	118.88	6.93	4.26		2.24			62.18	31.36	177.76
Gln 39	130.54	9.29	3.56		2.07	2.07		61.39	28.19	178
Ala 40	119.3	9.23	3.94		1.49	1.49	1.49	55.32	17.95	179.8
Lys 41	116.28	6.82	4.19		1.98	1.98		58.66	32.59	178.47

Residue	^{15}N	NH	Hα	Hα2	Hβ1	Hβ2	Hβ3	Cα	Cβ	CO
Ala 42	122.9	7.91	3.73		1.11	1.11	1.11	55.09	16.97	178.285
Ala 43	117.29	8.29	3.58		1.3	1.3	1.3	55.82	16.95	178.78
Arg 44	116.09	7.05	4.19		1.98	1.98		59.06	29.42	179.81
Leu 45	118.89	7.58	4.1		1.93	1.35		57.65	41.4	178.86
Leu 46	115.67	7.55	4.29		1.58	1.58		54.81	43.82	177.29
Gly 47	109.27	7.88	3.98	3.98				47.11		174.47
Met 48	117.88	8.11	4.88		2.27	1.54		54.37	37.72	174.94
Thr 49	110.44	8.54	4.82					59.76	68.5	
Pro 50				3.98	2.29	2.29		66.22	31.59	178.78
Arg 51	117.28	8.09	4.15		2.01	1.79		59.38	29.66	178.79
Gln 52	119.9	7.82	4.19		2.1	2.44		58.99	29.87	179.33
Val 53	119.7	7.92	3.54		2.1			66.97	31.37	176.51
Ala 54	121.7	8.11	4.01		1.58	1.58	1.58	55.64	17.09	180.51
Tyr 55	118.47	8.04	4.38		3.28	3.07		60.89	38.22	177.29
Arg 56	117.89	8.01	3.79		1.84	1.84		58.99	29.16	178.08
Ile 57	118.7	8.45	3.51		1.96			65.96	38.2	177.45
Gln 58	117.077	7.35	4.2		2.24	2.24		58.83	28.2	179.96
Ile 59	117.69	8.31	3.99		1.75			63.4	37.25	178.08
Met 60	117.08	8.13	4.48		2.01	1.79		56.09	32.57	174.94
Asp 61	119.89	7.82	4.36		3.07	2.43		55.14	38.95	175.1
Ile 62	119.68	7.94	4.1		1.82			61.34	38.46	175.86
Thr 63	123.11	8.34	4.2		1.86			61.67	69.6	173.45
Met 64	126.12	8.39	4.24		?			52.85	31.75	172.08
Pro 65			4.2		1.96	1.58		62.68	31.6	175.96
Arg 66	121.48	8.15	4.27		1.82	1.7		55.98	30.15	175.18
Leu 67	130.15	7.86						56.653	43.097	

Lys5 shows two sets of resonances, presumably from *cis* and *trans* conformations of Pro4, and both sets of shifts are given. The estimated errors are: for ^{15}N – 0.13 ppm, $^{1}H_N$ – 0.015 ppm, Hα/Hβ- 0.14 ppm, Cα-0.11 ppm, Cβ - 0.65 ppm, C' –0.15 ppm.