SUPPLEMENTARY MATERIAL for ^{1}H, ^{15}N, ^{13}C, and ^{13}CO Assignments and Secondary Structure Determination of ZipA by Franklin J. Moy, Elizabeth Glasfeld and Robert Powers

Table S1 ^{15}N, ^{13}C, ^{13}CO and ^{1}H resonance assignments for ZipA at pH 6.0 and 30°C.[a]

Residue	N	CO	Cα	Cβ	Others
M1	- (-)	172.1	55.0 (4.14)	32.9 (2.18)	Cγ 30.7 (2.62)
D2	124.9 (8.82)	175.4	54.4 (4.69)	41.3 (2.69,2.56)	
K3	123.0 (8.41)	-	54.3 (4.60)	32.6 (1.83,1.74)	Cγ 24.6 (1.49);Cδ 29.1 (1.73) ;Cε 39.4 (3.02)
P4	- (-)	176.7	62.9 (4.44)	32.2 (2.33, 1.88)	Cγ 27.4 (2.04);Cδ 50.6 (3.82,3.61)
K5	122.2 (8.44)	176.5	56.0 (4.29)	33.5 (1.80,1.73)	Cγ 25.2 (1.49);Cδ 29.0 (1.72);Cε 42.2 (3.02)
R6	124.2 (8.79)	174.7	56.2 (4.25)	31.1 (1.81,1.74)	Cγ 27.3 (1.73,1.66);Cδ 44.0 (3.20,3.12)
K7	120.1 (8.38)	175.7	56.3 (4.29)	33.5 (1.96,1.74)	Cγ 25.6 (1.52,1.38);Cδ 29.1 (1.68); Cε 42.0(2.99)
E8	116.4 (7.75)	174.3	54.7 (5.07)	32.9 (2.18,2.07)	Cγ 35.0 (2.17)
A9	120.8 (8.95)	174.7	51.9 (4.63)	22.9 (1.20)	
V10	118.9 (8.28)	175.0	61.4 (4.85)	33.9 (1.98)	Cγ 21.2 (0.98)
I11	129.5 (9.11)	175.0	58.4 (4.26)	37.0 (2.10)	Cγ 26.9 (1.51,1.16);Cγm 17.1 (0.51); Cδ 10.0 (0.67)
I12	127.3 (8.43)	175.4	61.0 (4.9	41.9 (1.68)	Cγ 28.6 (1.59,0.89);Cγm 18.3 (0.85); Cδ 13.7 (0.87)
M13	124.4 (9.33)	173.1	54.9 (4.75)	36.1 (1.96,1.80)	Cγ 32.6 (2.53,2.12);Cε 18.4 (1.64)
N14	118.4 (9.14)	173.9	52.6 (5.77)	43.6 (2.44,2.30)	Nd2 (7.12,6.64)
V15	121.6 (9.07)	173.6	62.0 (4.80)	32.6 (1.85)	Cγ 21.4 (0.86);20.0 (0.62)
A16	128.2 (8.82)	176.2	49.8 (5.36)	24.4 (1.35)	
A17	119.4 (7.97)	178.6	51.4 (4.32)	19.9 (1.29)	
H18	118.2 (8.86)	174.8	56.8 (4.38)	29.2 (3.28,3.04)	Cδ2 120.0 (7.41) Cε1 136.7 (8.43)
H19	119.6 (8.85)	176.2	57.9 (4.40)	28.5 (3.31,3.23)	Cδ2 119.9 (7.32)
G20	113.9 (8.81)	173.7	45.2 (4.23,3.62)		
S21	115.5 (8.09)	-	57.0 (4.85)	65.7 (3.88)	
E22	116.4 (8.30)	175.5	55.6 (4.37)	33.8 (1.91,1.65)	Cγ 36.7 (2.27)
L23	120.1 (9.06)	176.2	53.8 (4.51)	42.3 (1.99,1.10)	Cγ 26.7 (1.77) Cδ 26.6 (0.75);21.7 (0.71)
N24	121.0 (8.57)	175.2	54.4 (4.32)	40.0 (2.85,2.70)	Nδ2 113.5 (7.81,7.13)
G25	116.7 (8.20)	173.8	47.5 (2.78,2.27)		
E26	122.1 (8.17)	179.0	60.1 (3.95)	29.2 (2.13)	Cγ 36.7 (2.29)
L27	120.0 (7.98)	180.0	57.4 (4.13)	42.0 (1.69)	Cγ 27.3 (1.58);Cδ 24.6 (1.00);23.9 (0.99)
L28	120.6 (8.43)	178.2	58.2 (3.87)	42.2 (2.03)	Cγ 26.7 (1.37);Cδ 26.6 (0.85) ;22.8 (0.70)
L29	118.6 (8.87)	179.9	58.4 (3.70)	40.5 (1.94,1.35)	Cγ 26.8 (2.09);Cδ 26.1 (1.01) ;22.0 (0.68)
N30	117.6 (7.79)	177.5	56.7 (4.46)	38.3 (2.89,2.83)	
S31	116.9 (8.12)	177.3	62.3 (4.18)	63.2 (3.84,3.80)	
I32	122.1 (8.49)	178.2	65.8 (3.40)	38.3 (1.43)	Cγ 28.4 (1.44,0.48);Cγm 17.2 (-0.14);

					Cδ 14.3 (-0.06)
Q33	119.8 (7.76)	181.2	59.1 (4.44)	28.4 (2.33)	Cγ 34.8 (2.64,2.53)
Q34	120.8 (8.41)	177.2	58.5 (4.15)	28.4 (2.27)	Cγ 34.2 (2.61,2.51)
A35	119.3 (7.66)	176.9	52.0 (4.47)	18.3 (1.73)	
G36	105.3 (7.87)	173.7	45.8 (4.01,3.88)		
F37	117.0 (7.64)	175.8	58.9 (4.43)	40.5 (2.99,2.77)	Cδ 132.6 (7.16);Cε 130.9 (7.07);Cζ (7.20)
I38	120.0 (9.23)	176.8	59.3 (4.83)	41.3 (2.06)	Cγ 27.0 (1.59,1.47);Cγm 17.5 (1.11); Cδ 12.6 (0.84)
F39	133.4 (9.51)	176.0	59.4 (3.69)	39.1 (2.78,2.69)	Cδ 131.3 (6.33);Cε 131.0 (7.18); Cζ 130.0 (7.36)
G40	113.9 (7.70)	172.5	46.8 (4.08,3.89)		
D41	127.1 (8.71)	177.1	56.2 (4.34)	40.9 (2.46)	
M42	115.8 (8.90)	174.3	56.9 (4.02)	29.0 (2.52,2.33)	Cγ 32.7 (2.53,2.34)
N43	111.7 (8.25)	173.1	55.2 (3.91)	35.6 (3.60,3.22)	Cγ (7.33,7.17)
I44	108.4 (6.52)	173.4	60.0 (4.98)	40.0 (2.86)	Cγ 25.2 (1.15,0.81);Cγm 18.2 (1.21); Cδ 14.5 (1.02)
Y45	115.3 (8.04)	176.0	58.4 (4.90)	42.8 (2.78)	Cδ 132.5 (6.58);Cε 118.2 (6.20)
H46	115.4 (9.00)	173.9	55.4 (5.27)	33.9 (3.00,2.52)	Cδ2 120.1 (6.93);Cε1 137.9 (7.88)
R47	128.0 (8.82)	174.8	53.9 (4.43)	30.7 (0.25,-0.20)	Cγ 27.3 (0.88);Cδ 42.5 (2.73,2.69)
H48	126.5 (9.67)	173.5	54.5 (4.90)	29.6 (3.14,2.89)	Cδ2 120.9 (7.12)
L49	120.9 (8.11)	177.0	58.2 (3.97)	43.4 (1.89,1.41)	Cγ 27.0 (1.66);Cδ 25.5 (0.94);23.9 (1.02)
S50	110.1 (7.76)	-	54.8 (5.09)	63.9 (3.90,3.81)	
P51	- (-)	175.2	64.6 (4.34)	31.9 (2.32,2.08)	Cγ 27.3 (2.07,2.01);Cδ 51.5 (3.99,3.87)
D52	114.5 (7.67)	177.0	53.5 (4.46)	39.9 (2.99,2.59)	
G53	107.5 (7.88)	172.7	45.1 (4.05,3.24)		
S54	115.6 (7.82)	174.1	58.6 (4.29)	64.4 (3.88,3.81)	
G55	106.3 (8.30)	-	44.7 (4.31,3.88)		
P56	- (-)	175.9	62.7 (4.31)	32.3 (1.95,1.33)	Cγ 26.8 (1.35,1.14);Cδ 49.6 (3.40,3.20)
A57	122.5 (8.44)	176.4	52.0 (3.41)	18.3 (0.87)	
L58	122.1 (8.99)	177.3	55.9 (4.38)	44.0 (1.18)	Cγ 26.8 (1.37); Cδ 25.5 (0.69);Cγ 21.6 (0.81)
F59	110.0 (7.07)	174.4	55.6 (5.07)	40.1 (3.54,3.13)	Cδ 132.8 (6.92);Cε 131.0 (7.07); Cζ 128.7 (6.83)
S60	115.5 (8.64)	182.2	58.6 (5.37)	66.0 (3.62,2.32)	
L61	124.6 (8.77)	173.4	55.0 (5.53)	46.6 (1.13,0.83)	Cγ 27.3 (1.32);Cδ 27.9 (-0.08);26.0 (0.61)
A62	128.3 (9.57)	175.6	49.6 (5.26)	23.6 (1.68)	
N63	121.7 (8.83)	176.6	52.6 (4.65)	38.2 (2.39,1.26)	Nδ2 (7.28,6.87)
M64	123.7 (8.67)	176.9	59.0 (4.05)	34.0 (1.87,1.69)	Cγ 34.3 (2.39,2.17);Cε 16.8 (1.86)
V65	116.7 (7.02)	176.0	61.6 (3.98)	32.4 (1.88)	Cγ 21.0 (1.14);21.0 (1.03)
K66	129.5 (8.63)	-	55.8 (4.12)	31.5 (1.78)	Cγ 25.0 (1.58,1.42);Cδ 26.8(1.57,1.51); Cε 41.1 (2.75,2.63)
P67	- (-)	176.5	63.9 (4.61)	33.5 (2.47,2.23)	Cγ 24.5 (2.01,1.83);Cδ 49.7 (3.63,3.52)
G68	114.4 (9.16)	173.6	45.6 (4.33,4.17)		
T69	107.6 (6.88)	174.6	60.2 (4.58)	71.0 (4.63)	Cγ 22.6 (1.33)
F70	115.2 (8.60)	174.5	56.7 (4.77)	43.1 (3.03,2.75)	Cγ 132.9 (7.45);Cδ 130.4 (7.31);

					Cε 128.5 (6.90)
D71	118.9 (8.33)	-	50.5 (4.96)	42.1 (2.80,2.52)	
P72	- (-)	176.9	64.0 (4.02)	32.0 (1.88,1.71)	Cγ 26.6 (1.18,1.34);Cδ 50.8 (3.50,3.05)
E73	114.8 (7.97)	176.4	56.0 (4.23)	29.5 (2.16,1.89)	Cγ 36.2 (2.24)
M74	122.2 (7.82)	174.6	55.5 (4.44)	32.4 (2.13,1.89)	Cγ 32.3 (2.58,2.49);Cε 25.9 (1.01)
K75	121.8 (8.28)	175.9	56.2 (4.47)	33.7 (1.87,1.74)	Cγ 25.0 (1.42);Cδ 29.0 (1.67);Cε 42.2 (3.00)
D76	119.1 (8.31)	174.0	53.6 (4.77)	40.0 (2.86,2.64)	
F77	118.2 (7.85)	173.4	56.0 (5.10)	41.0 (3.30,3.17)	Cδ 132.9 (7.12);Cε 130.8 (7.24); Cζ 129.2 (7.17)
T78	111.0 (8.46)	173.6	59.9 (4.99)	71.9 (4.14)	Cγ 21.3 (1.11)
T79	113.4 (8.09)	-	56.4 (5.39)	69.0 (4.65)	Cγ 21.6 (1.11)
P80	- (-)	176.4	64.5 (4.57)	32.5 (2.49,2.04)	Cγ 27.2 (2.03,1.89);Cδ 52.2 (4.23,3.78)
G81	106.2 (8.53)	183.0	46.9 (5.02,4.03)		
V82	107.0 (9.04)	173.4	58.7 (5.24)	35.2 (2.40)	Cγ 24.8 (1.12);17.7 (0.72)
T83	119.9 (9.27)	172.5	61.5 (4.99)	71.9 (3.64)	Cγ 22.0 (1.16)
I84	128.3 (9.13)	173.9	59.8 (5.36)	40.0 (1.55)	Cγ 28.2 (1.61,0.76);Cγm 18.5 (1.04); Cδ 14.2 (0.71)
F85	121.6 (9.00)	173.3	54.7 (6.08)	42.8 (2.88,2.74)	Cδ 132.7 (6.97);Cε 131.0 (7.24); Cζ 132.9 (7.12)
M86	121.4 (9.03)	174.3	54.4 (4.99)	39.0 (2.35,2.24)	Cγ 31.4 (3.00,2.51)
Q87	127.5 (9.12)	174.8	55.8 (4.86)	29.9 (2.18)	Cγ 34.3 (2.45,2.41)
V88	119.6 (8.81)	-	58.1 (4.52)	34.0 (2.03)	Cγ 22.6 (0.99);20.9 (0.90)
P89	- (-)	175.9	63.0 (4.72)	35.6 (2.39,2.17)	Cγ 25.3 (1.94,1.81);Cδ 50.9 (3.77)
S90	118.2 (9.90)	173.7	56.9 (4.60)	64.9 (4.19,4.06)	
Y91	121.5 (8.37)	175.5	58.8 (4.42)	39.8 (2.96,2.77)	Cδ 133.3 (7.09);Cε 118.2 (6.87)
G92	112.2 (7.89)	172.7	45.1 (3.87,3.41)		
D93	121.5 (8.50)	176.3	53.1 (4.67)	41.3 (2.91,2.53)	
E94	125.5 (9.99)	178.8	61.6 (3.99)	30.0 (1.97)	Cγ 37.6 (2.60)
L95	118.3 (8.25)	180.1	58.0 (4.27)	40.9 (1.98,1.70)	Cγ 27.7 (1.71);Cδ 24.6 (1.03) ;23.8 (0.95)
Q96	121.6 (7.81)	179.5	58.4 (4.19)	27.9 (2.27,2.20)	Cγ 33.7 (2.49,2.46)
N97	120.8 (8.79)	177.1	55.9 (4.45)	37.7 (3.14,2.83)	
F98	120.7 (8.50)	175.7	61.2 (3.97)	39.0 (3.29,3.16)	Cδ 131.5 (7.04);Cε 129.2 (7.25); Cζ 130.7 (7.02)
K99	119.3 (7.58)	179.2	59.9 (3.67)	31.8 (2.02,1.96)	Cγ 25.4 (1.73,1.45);Cδ 29.5 (1.72); Cε 42.1 (3.02)
L100	119.8 (7.70)	179.5	57.4 (4.17)	41.8 (1.99,1.89)	Cγ 27.2 (1.76);Cδ 23.9 (0.91);23.6 (0.95)
M101	125.7 (8.41)	177.0	59.9 (2.78)	32.3 (1.67,0.87)	Cγ 32.3 (1.77,1.35);Cε 18.2 (1.83)
L102	120.0 (8.00)	178.3	57.7 (3.76)	41.6 (1.56,0.76)	Cγ 26.8 (1.38);Cδ 26.1 (0.83);23.0 (0.82)
Q103	117.0 (7.97)	-	58.9 (3.99)	28.7 (2.18,2.06)	Cγ 34.2 (2.48,2.27)
S104	116.4 (8.28)	174.8	63.0 (4.36)	63.0 (4.27,3.93)	
A105	124.2 (8.46)	178.4	55.4 (3.67)	18.2 (1.30)	
Q106	115.4 (8.41)	177.9	58.3 (3.75)	28.6 (2.18,2.04)	Cγ 33.9 (2.48,2.33)
H107	117.4 (8.34)	177.4	58.9 (4.42)	28.5 (3.41)	Cδ2 119.0 (7.22)
I108	118.4 (8.20)	177.4	65.4 (3.66)	38.4 (1.67)	Cγ 28.5 (1.90);Cγm16.3 (0.64);Cδ 14.6 (0.56)

A109	119.6 (8.40)	179.5	56.2 (3.45)	18.1 (1.27)	
D110	116.8 (8.43)	179.0	57.1 (4.39)	40.4 (2.85,2.70)	
E111	119.1 (7.89)	178.9	59.0 (4.07)	29.7 (2.14,2.03)	Cγ 36.1 (2.36,2.21)
V112	108.8 (8.16)	175.7	60.4 (4.47)	32.3 (2.42)	Cγ 19.6 (0.87);21.1 (0.90)
G113	110.5 (7.66)	175.2	46.6 (4.08,3.90)		
G114	107.3 (8.77)	176.0	42.9 (4.63,3.15)		
V115	115.3 (9.00)	175.4	59.6 (4.55)	35.6 (1.87)	Cγ 21.4 (0.70);19.3 (0.65)
V116	123.5 (8.42)	175.1	62.7 (4.60)	31.5 (2.04)	Cγ 21.9 (0.85);22.3 (0.76)
L117	126.4 (9.36)	176.4	51.7 (5.19)	46.7 (1.59,1.33)	Cγ 26.3 (1.55);Cδ 26.3 (0.66);22.1 (0.63)
D118	119.5 (9.27)	177.5	52.3 (4.93)	42.5 (3.39,2.98)	
D119	116.0 (8.57)	177.0	56.0 (4.02)	39.6 (3.27,2.83)	
Q120	121.1 (8.59)	174.7	54.5 (4.43)	28.8 (2.39,1.90)	Cγ 33.9 (2.29)
R121	111.9 (8.18)	174.1	58.2 (3.54)	25.7 (2.17,1.97)	Cγ 28.2 (1.58,1.26);Cδ 43.2 (3.10)
R122	119.1 (8.54)	176.8	54.2 (4.66)	31.2 (2.10,1.83)	Cγ 27.2 (1.64);Cδ 43.2 (3.22)
M123	121.4 (8.68)	177.7	57.0 (4.24)	32.1 (2.07,2.04)	Cγ 32.0 (2.71,2.61)
M124	125.0 (8.19)	175.3	55.9 (4.58)	31.4 (2.09,1.85)	Cγ 32.1 (2.54) ;Cε 16.9 (2.11)
T125	114.9 (7.01)	-	58.4 (5.04)	70.6 (4.69)	Cγ 21.6 (1.33)
P126	- (-)	179.6	65.1 (4.29)	31.9 (2.48,1.98)	Cγ 27.9 (2.24,2.08);Cδ 50.7 (3.92)
Q127	117.3 (8.38)	178.0	59.4 (4.02)	27.4 (2.18,1.98)	Cγ 33.8 (2.54,2.43)
K128	123.6 (7.90)	179.9	56.8 (4.09)	31.1 (2.15,1.84)	Cγ 22.0 (1.01,0.66);Cδ 26.1 (1.90,1.37); Cε 40.5 (3.68)
L129	117.7 (7.79)	180.0	58.7 (4.29)	41.6 (2.06,1.60)	Cγ 26.9 (1.97);Cδ 25.8 (0.99);24.9 (1.15)
R130	118.9 (7.70)	178.0	59.1 (4.09)	29.5 (2.04,1.97)	Cγ 27.5 (1.77,1.70);Cδ 43.2 (3.25)
E131	121.6 (7.97)	179.8	59.7 (4.10)	29.3 (2.20)	Cγ 36.3 (2.49)
Y132	117.4 (8.58)	178.2	59.4 (4.35)	38.6 (3.19,2.51)	Cδ 131.8 (7.25);Cε 120.5 (7.04)
Q133	116.3 (7.57)	177.8	59.7 (3.48)	28.9 (2.22,2.03)	Cγ 36.0 (2.28,1.77)
D134	121.5 (8.60)	179.3	57.5 (4.45)	39.8 (2.97,2.68)	
I135	123.2 (8.18)	177.6	65.5 (3.72)	37.8 (2.06)	Cγ 29.2 (1.90,1.00);Cγm 17.2 (0.70); Cδ 13.6 (0.93)
I136	118.8 (7.73)	177.5	66.5 (3.31)	37.8 (1.88)	Cγ 29.9 (1.90,0.70);Cγm 18.3 (0.77); Cδ 14.5 (0.56)
R137	118.3 (8.17)	178.0	60.0 (3.88)	30.3 (1.98)	Cγ 28.3 (1.84,1.69);Cδ 43.2 (3.27)
E138	120.2 (8.19)	179.0	59.6 (4.05)	29.5 (2.24)	Cγ 36.1 (2.45,2.25)
V139	119.5 (8.20)	179.1	65.4 (3.93)	31.3 (2.00)	Cγ 22.6 (0.76);22.2 (0.67)
K140	121.0 (8.35)	179.8	59.2 (4.04)	31.1 (1.99,1.89)	Cγ 24.0 (1.68,1.52);Cδ 28.4 (1.78,1.64); Cε 41.1 (3.12)
D141	120.1 (8.35)	178.3	56.5 (4.47)	40.4 (2.83,2.70)	
A142	121.7 (8.17)	178.2	53.8 (4.21)	19.6 (1.50)	
N143	115.8 (7.62)	173.4	53.5 (4.7	40.7 (2.96,2.65)	
A144	129.4 (7.41)	-	54.4 (4.1	19.8 (1.46)	

Footnotes to Table S1

[a]In each column, ^{15}N and ^{13}C shifts are listed first, and the corresponding ^{1}H shifts are given in parentheses. ^{1}H, ^{13}C and ^{15}N chemical shifts are referenced according to the method of Wishart et al. 1995.