

SUPPLEMENTARY MATERIAL for ^1H , ^{13}C and ^{15}N Assignments for *Archaeoglobus fulgidis* Protein AF2095. by

Robert Powers, Thomas B. Acton, Yiwen Chiang, Rajan Paranj, John R. Cort, Michael A. Kennedy, Jinfeng Liu,

LiChung Ma, Burkhard Rost and Gaetano T. Montelione

Table S1 ^{15}N , ^{13}C , ^{13}CO and ^1H resonance assignments for AF2095 at pH 6.5 and 40°C.^a

Residue	N	CO	C α	C β	Others
M1	-(-)	-	-(-)	-(-)	
T2	-(-)	179.7	61.7(4.15)	69.3(4.20)	C γ 21.5(1.33)
L3	126.5(9.39)	173.9	54.2(4.93)	44.7(1.04,1.94)	C γ 27.3(1.83);C δ 27.1(0.88);C δ 23.5(0.69)
K4	117.1(8.95)	178.7	55.5(4.91)	37.2(1.72,1.56)	C γ 24.1(1.17,1.06);C δ 30.0(1.57); C ϵ 41.1(2.63)
Q5	123.1(8.42)	176.4	54.4(4.68)	35.1(1.82,1.73)	C γ 35.5(1.58);N ϵ -(7.36,5.29)
V6	125.8(8.80)	176.9	60.6(4.92)	34.7(1.70)	C γ 21.5(0.73);C γ 22.2(0.82)
I7	128.0(8.94)	176.9	60.9(4.79)	40.7(1.67)	C γ 30.3(1.32,1.13);C γ_m 20.9(0.73); C δ 15.0(0.83)
V8	127.5(9.16)	175.4	60.1(4.68)	32.3(1.92)	C γ 20.9(0.68);C γ 23.8(0.76)
V9	119.7(8.79)	175.3	59.0(4.94)	34.4(2.10)	C γ 19.2(0.78);C γ 21.2(0.83)
R10	119.5(7.68)	174.7	55.5(4.36)	32.8(1.62)	C γ 26.4(1.74);C δ 44.4(3.26)
D11	122.1(9.04)	173.5	54.3(4.89)	43.4(2.55,2.48)	
D12	115.4(8.88)	174.2	54.7(4.40)	39.1(2.81)	
L13	118.0(6.80)	-	54.2(4.31)	43.0(1.31,1.67)	C γ 27.4(1.50);C δ 22.8(0.76)
K14	119.9(8.20)	-	55.6(4.07)	30.0(1.81)	C γ 24.8(-);C δ 29.4(-);C ϵ 42.4(-)
L15	120.0(7.69)	-	53.9(4.48)	43.8(1.29)	
S16	-(-)	175.8	57.8(4.44)	64.3(3.22,3.13)	
R17	120.5(8.83)	171.9	60.5(3.91)	30.7(1.84)	C γ 27.4(1.61);C δ 43.7(3.23)
G18	106.5(8.67)	175.1	47.0(3.58,4.03)		
K19	120.8(7.37)	170.7	58.6(4.10)	32.5(2.00,1.81)	C γ 25.8(1.54,1.48);C δ 28.4(1.71); C ϵ 42.4(3.00)
L20	121.5(8.81)	172.0	58.6(3.86)	41.4(1.84,1.54)	C γ 27.1(1.57);C δ 25.1(0.84);C δ 24.1(0.84)
A21	119.3(7.76)	171.9	55.5(3.76)	17.5(1.45)	
V22	115.3(7.41)	174.1	67.5(3.08)	31.2(2.16)	C γ 21.8(0.70);C γ 23.8(0.85)
Q23	116.0(7.62)	172.0	58.1(3.76)	27.6(2.08)	C γ 33.6(2.34);N ϵ -(6.43,5.51)
V24	117.6(7.80)	173.7	65.9(3.38)	31.0(2.16)	C γ 20.9(0.69);C γ 22.8(0.85)
A25	122.6(7.97)	171.4	55.4(3.96)	18.6(1.27)	
H26	116.3(8.68)	171.8	56.9(4.46)	31.5(3.24,3.11)	
A27	119.5(7.85)	172.5	54.7(3.46)	19.9(1.35)	
A28	119.4(8.31)	169.7	54.6(4.10)	19.4(1.53)	
I29	117.6(7.53)	173.0	63.8(3.55)	36.1(2.47)	C γ 28.4(1.70,1.39);C γ_m 16.6(0.52);

I30	119.4(7.94)	172.2	65.7(3.54)	37.8(1.76)	C δ 11.2(0.83) C γ 29.3(1.50,1.40);C γ_m 16.6(0.69); C δ 13.0(0.78)
G31	104.5(8.47)	174.7	47.3(3.48)		
Y32	122.6(7.98)	172.9	63.4(3.50)	38.7(3.37,3.03)	C δ 132.6(7.05);C ϵ 118.1(6.86)
L33	118.7(8.63)	171.4	57.5(3.76)	42.2(1.88,1.46)	C γ 26.9(1.89);C δ 26.4(0.80);C δ 22.5(0.90)
K34	115.1(7.39)	174.0	56.9(4.14)	33.8(1.88,1.49)	C γ 25.1(1.40);C δ 28.7(1.70);C ϵ 42.1(3.02)
S35	114.8(7.08)	178.1	59.9(4.35)	64.8(3.73,3.54)	
D36	122.9(9.01)	173.3	54.9(4.35)	43.4(2.80,2.58)	
S37	119.9(8.59)	173.8	61.8(3.85)	62.8(3.96)	
S38	118.6(8.32)	173.6	61.4(4.36)	62.4(4.01,3.93)	
L39	125.6(8.20)	170.9	58.6(4.09)	42.9(1.81,1.52)	C γ 27.9(1.65);C δ 25.4(0.82);C δ 25.7(0.98)
R40	116.2(8.56)	173.4	59.1(4.15)	28.5(2.00,1.37)	C γ 25.4(1.69);C δ 43.4(3.00)
R41	121.8(7.25)	172.4	59.1(4.34)	30.2(2.08)	C γ 26.7(1.84,1.79);C δ 43.0(3.32)
K42	121.1(7.64)	172.0	59.4(4.15)	32.0(1.96)	C γ 24.8(1.51);C δ 29.0(1.72);C ϵ 42.1(3.00)
W43	118.6(8.44)	171.0	60.8(4.19)	27.6(3.85,2.93)	C δ_1 126.7(6.99);N ϵ_1 132.6(10.80) C ζ_3 120.6(7.90);C ζ_2 114.9(7.08); C η_2 122.5(7.14)
L44	121.2(8.16)	170.0	58.9(3.44)	41.9(2.14,1.57)	C γ 27.0(2.06);C δ 23.5(0.58);C δ 26.4(0.98)
D45	121.8(8.41)	172.5	57.3(4.35)	40.2(2.97,2.77)	
E46	116.8(7.62)	174.1	56.1(4.32)	30.4(2.44,2.11)	C γ 35.5(2.74)
G47	106.7(7.59)	176.6	45.0(3.46,4.21)		
Q48	119.7(8.30)	176.1	52.4(-)	28.8(-)	C γ 31.0(1.03)
K49	118.0(8.38)	171.7	58.8(4.09)	33.0(2.00)	C γ 25.4(1.62);C δ 29.3(1.73);C ϵ 42.1(3.02)
K50	125.1(9.05)	175.6	54.7(6.01)	39.5(1.52,1.73)	C γ 23.8(1.24);C δ 30.6(1.57);C ϵ 41.4(2.63)
V51	119.0(8.25)	177.0	61.1(4.29)	36.1(1.92)	C γ 20.9(0.95)
V52	125.6(8.13)	175.6	60.8(5.33)	32.9(1.90)	C γ 22.5(0.85)
L53	128.6(8.99)	175.4	53.0(4.95)	45.7(1.59,1.37)	C γ 27.4(1.48);C δ 26.4(0.83);C δ 23.1(0.75)
K54	117.4(8.22)	174.9	54.5(5.51)	36.3(1.59)	C γ 23.8(1.24);C δ 29.7(1.57); C ϵ 41.7(2.85,2.96)
V55	111.7(8.12)	174.2	58.9(4.79)	34.9(2.43)	C γ 18.9(0.68);C γ 22.5(0.80)
K56	117.8(8.50)	174.9	57.8(4.35)	33.6(1.90)	C γ 24.4(1.50);C δ 29.0(1.70);C ϵ 41.7(3.00)
S57	107.6(7.14)	176.3	56.7(4.84)	67.0(4.25,3.92)	
L58	122.3(8.98)	172.6	57.7(3.96)	41.3(1.87,1.43)	C γ 26.7(1.54);C δ 25.4(0.99);C δ 23.1(0.84)
E59	118.3(8.77)	170.3	60.5(3.87)	28.7(2.08,1.92)	C γ 36.2(2.37,2.27)
E60	119.5(7.91)	171.4	59.4(4.06)	30.6(2.00)	C γ 36.8(2.34,2.27)
L61	121.4(7.62)	172.0	59.0(3.74)	42.4(2.09,1.54)	C γ 26.5(1.44);C δ 25.8(0.66);C δ 26.4(0.59)
L62	117.1(8.63)	170.4	57.1(3.91)	40.6(1.82,1.29)	C γ 26.4(1.76);C δ 25.1(0.85);C δ 21.2(0.71)
G63	109.2(8.14)	173.5	47.4(3.95)		
I64	123.6(7.77)	173.2	63.5(3.76)	36.6(2.09)	C γ 28.7(1.51,1.39);C γ_m 17.6(0.73); C δ 13.1(0.78)
K65	120.7(7.75)	172.7	60.5(3.69)	33.4(2.00,1.71)	C γ 24.8(1.22);C δ 30.0(1.57);C ϵ 41.7(2.90)
H66	115.3(8.33)	172.7	58.3(4.54)	28.3(3.36)	
K67	121.6(8.26)	171.1	59.4(4.03)	32.4(1.99,1.92)	C γ 25.1(1.46);C δ 29.0(1.74);C ϵ 42.1(2.95)

A68	120.8(8.43)	170.9	55.5(3.96)	18.3(1.37)	
E69	118.6(8.32)	169.3	59.4(4.15)	28.9(2.25,2.05)	C γ 36.5(2.55,2.44)
S70	117.6(8.09)	175.4	61.5(4.28)	62.8(4.01,3.92)	
L71	120.9(7.18)	173.4	54.6(4.43)	42.9(1.66)	C γ 27.1(1.70);C δ 23.1(0.83);C δ 25.8(0.79)
G72	107.4(7.86)	175.8	45.8(4.08,3.76)		
L73	119.9(7.43)	174.0	53.8(4.25)	42.8(1.43,1.13)	C γ 27.3(1.48);C δ 26.4(0.76);C δ 24.1(0.84)
V74	123.8(9.06)	174.8	64.1(3.75)	32.0(1.67)	C γ 21.5(1.00);C γ 22.8(0.72)
T75	116.6(7.78)	176.4	58.8(5.70)	73.4(3.96)	C γ 22.2(1.20)
G76	105.2(8.02)	179.3	44.6(4.41,3.30)		
L77	121.7(8.47)	173.5	54.0(4.98)	45.1(1.95,1.40)	C γ 27.4(1.71);C δ 24.8(0.80);C δ 26.4(0.80)
V78	121.2(8.15)	176.3	62.5(3.96)	33.0(2.05)	C γ 21.2(0.71);C γ 22.5(0.90)
Q79	124.8(7.83)	176.1	54.5(4.68)	32.5(1.82,1.73)	C γ 34.2(2.09,1.91);N ϵ -(6.73,7.31)
D80	123.5(9.19)	174.2	53.4(4.74)	43.3(2.88,2.74)	
A81	128.6(8.69)	171.8	53.7(4.25)	18.6(1.43)	
G82	105.4(8.79)	176.7	45.7(4.14,3.71)		
L83	-(-)	-	-(-)	-(-)	
T84	-(-)	-	-(-)	-(-)	
E85	-(-)	-	-(-)	-(-)	
V86	-(-)	-	-(-)	-(-)	
P87	-(-)	-	-(-)	-(-)	
P88	-(-)	172.9	64.0(4.28)	31.7(2.33,1.88)	C γ 27.4(2.10);C δ 50.9(3.62,3.96)
G89	112.1(8.89)	175.7	45.0(3.50,4.10)		
T90	118.0(7.40)	176.9	64.9(3.98)	69.6(3.82)	C γ 21.8(1.02)
I91	129.5(8.59)	174.2	60.6(4.57)	38.6(1.68)	C γ 27.4(-);C γ_m 18.9(0.83);C δ 13.4(0.91)
T92	116.4(8.56)	175.9	62.2(4.20)	69.5(3.99)	C γ 21.8(1.34)
A93	118.6(7.12)	175.3	51.4(5.28)	21.3(1.08)	
V94	117.3(8.81)	177.9	59.2(5.13)	36.6(1.76)	C γ 20.5(0.83);C γ 21.8(0.82)
V95	124.3(8.58)	178.4	58.0(5.18)	35.2(1.65)	C γ 16.0(0.80);C γ 22.2(0.80)
I96	125.5(9.02)	174.7	59.7(4.84)	41.2(1.54)	C γ 27.1(1.39);C γ_m 19.9(0.72);C δ 14.3(0.56)
G97	111.7(8.31)	-	43.4(4.15,3.35)		
P98	-(-)	175.7	60.2(4.26)	35.0(0.09,-0.04)	C γ 24.1(1.07,0.42);C δ 49.2(3.11,1.81)
D99	118.2(8.44)	175.9	52.7(4.40)	44.7(2.55,2.45)	
E100	123.0(11.15)	171.7	57.4(4.29)	30.2(2.17,1.84)	C γ 35.9(2.45,2.38)
E101	125.8(8.64)	-	60.9(3.71)	29.8(2.09,2.03)	C γ 36.2(2.21)
R102	116.2(8.85)	172.0	59.0(4.10)	29.9(1.86,1.93)	C γ 27.1(1.69);C δ 43.4(3.21)
K103	117.5(7.12)	172.6	59.1(4.06)	33.8(1.81)	C γ 25.4(1.47);C δ 29.7(1.65);C ϵ 42.1(3.00)
I104	117.7(7.64)	171.7	64.7(3.47)	37.9(1.62)	C γ 29.3(1.59);C γ_m 18.2(0.77);C δ 13.7(0.65)
D105	119.7(8.71)	172.0	56.6(4.34)	39.4(2.61)	
K106	118.6(7.16)	172.7	58.8(4.04)	32.5(1.96)	C γ 25.1(1.50);C δ 29.0(1.71);C ϵ 42.1(2.99)
V107	115.2(7.89)	173.4	64.0(3.90)	32.5(2.25)	C γ 22.5(0.89)
T108	106.4(7.77)	174.2	62.5(4.14)	68.4(4.39)	C γ 22.2(0.89)
G109	109.6(7.93)	176.4	46.8(3.88)		
N110	116.9(8.16)	175.1	52.8(4.84)	38.8(2.82,2.69)	N δ 112.2(7.41,6.74)
L111	122.1(7.72)	-	53.8(4.59)	41.6(1.84,1.49)	C γ -(1.71);C δ -(0.88)
P112	-(-)	174.6	62.4(4.87)	34.8(1.71)	C γ 24.4(1.96,1.78);C δ 50.2(3.58,3.47)

L113	122.7(8.64)	173.2	55.9(4.26)	42.0(1.61)	C γ 27.1(1.59);C δ 23.8(0.84);C δ 25.1(0.84)
L114	122.7(8.15)	173.7	54.9(4.30)	42.7(1.52)	C γ 26.7(1.59);C δ 23.5(0.85);C δ 24.8(0.90)
K115	122.3(8.12)	174.6	56.1(4.27)	32.9(1.76)	C γ 24.1(1.38);C δ 29.0(1.69);C ϵ 42.1(2.98)
L116	123.7(8.11)	173.5	55.3(4.29)	42.5(1.56,26.70)	C γ -(1.56);C δ 23.5(0.99);C δ 24.8(0.81)
E117	121.5(8.20)	174.4	56.2(4.26)	30.7(1.86)	C γ 35.9(2.20)
H118	119.6(8.40)	176.9	55.3(4.67)	29.5(3.19,3.07)	
H119	125.4(8.24)	171.7	57.2(4.45)	29.7(3.22,3.13)	
H120	-(-)	-	-(-)	-(-)	
H121	-(-)	-	-(-)	-(-)	
H122	-(-)	-	-(-)	-(-)	
H123	-(-)	-	-(-)	-(-)	

Footnotes to Table S1

^aIn each column, ¹⁵N and ¹³C shifts are listed first, and the corresponding ¹H shifts are given in parentheses. ¹H, ¹³C and ¹⁵N chemical shifts are referenced according to the method of Wishart et al.

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