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Table S1. The ^1H , ^{15}N and ^{13}C assignments of apo-CRABP II at pH 7.3 and 25°C.

Residue	^{15}N	CO	C^α	C^β	Others
P1			63.0 (4.32)	33.2 (2.37, 1.91)	H^γ 2.10, 2.08; H^δ 3.32, 3.25
N2		171.9	52.7 (5.03)	39.3 (2.95, 2.89)	
F3	121.9 (9.82)	173.5	60.4 (4.32)	32.3 (3.28, 2.70)	2, 6H 7.42; 3, 5H 7.16; 4H 7.34
S4	112.5 (8.49)	171.8	60.7 (4.70)	64.5 (4.30, 3.99)	
G5	110.6 (9.22)	167.9	44.9 (3.96, 3.76)		
N6	118.6 (8.15)	171.5	53.0 (5.52)	40.2 (2.69, 2.52)	
W7	123.3 (9.35)	172.5	56.7 (5.14)	32.2 (3.06, 2.66)	2H 6.78; 4H 7.07; 5H 6.82; 6H 7.23; 7H 7.12 H^ϵ 9.20; N^ϵ 124.6
K8	123.2 (10.17)	172.4	54.1 (5.28)	36.1 (1.90, 1.85)	H^γ 1.63, 1.52; H^δ 1.37, 1.33; H^ϵ 2.85
I9	125.6 (9.05)	173.3	55.5 (3.92)	33.6 (1.76)	H^γ 1.65, 1.56; H^δ 0.48; H^m 1.39
I10	118.8 (9.24)	173.3	61.3 (4.61)	41.8 (1.83)	H^m 0.87
R11	120.8 (7.57)				
S12	115.8 (8.33)	171.0	62.8 (5.12)	(3.61, 3.43)	
E13	124.0 (8.71)		61.7 (4.80)	40.1 (2.19, 2.08)	H^γ 1.93
N14	117.8 (9.25)		55.7 (4.95)	41.4 (3.31, 3.22)	H^δ 7.35, 7.00; N^δ 109.8
F15	119.3 (8.72)		55.3 (4.59)	33.7 (2.98, 2.85)	2, 6H 7.14; 3, 5H 6.84; 4H 6.93
E16	117.4 (8.36)	172.1	63.2 (3.30)	32.6 (1.96)	H^γ 2.16
E17	118.5 (8.36)	175.9	59.6 (3.68)	28.1 (1.84, 1.73)	H^γ 2.38, 2.19
L18	121.4 (7.59)	174.9	58.5 (3.73)	42.4 (2.17, 1.34)	H^γ 0.81; H^δ 0.74, 0.70
L19	114.5 (7.36)	176.0	57.6 (3.62)	41.1 (1.62, 1.56)	H^γ 1.12; H^δ 0.36, 0.32
K20	118.9 (8.18)	178.3	60.5 (3.83)	32.6 (1.93, 1.61)	H^γ 1.35, 1.14; H^ϵ 2.91
V21	121.3 (7.83)	174.9	66.0 (3.78)	31.7 (2.15)	H^γ 1.10, 0.95
L22	117.5 (7.24)	173.6	55.4 (3.91)	41.5 (1.39)	H^δ 0.49
G23	106.5 (7.69)	172.0	45.9 (3.96, 3.58)		
V24	121.4 (7.62)	173.6	63.3 (3.72)	31.7 (1.45)	H^γ 0.83
N25	127.9 (8.68)	172.8	54.2 (4.38)	39.3 (3.09, 2.74)	H^δ 7.73, 6.91; N^δ 112.3
V26	120.3 (8.47)	173.4	66.7 (3.46)	32.1 (2.03)	H^γ 0.96, 0.91
M27	119.7 (7.95)		58.5 (4.14)	32.0 (2.07, 2.01)	H^γ 2.59, 2.46
L28	118.6 (7.82)		(4.08)	(1.63, 1.32)	H^γ 1.09; H^δ 0.82, 0.76
R29			(4.32)	(2.20, 1.97)	H^γ 1.74; H^δ 2.70
K30	116.5 (7.66)	177.7	59.6 (3.87)	32.2 (1.89, 1.81)	H^γ 1.68, 1.59
I31	119.2 (7.16)		64.3 (3.72)	39.2 (1.80)	H^m 0.88; H^δ 0.80
A32	122.6 (8.54)				
V33	116.7 (8.66)		66.6 (3.62)	(2.07)	H^γ 0.94
A34	121.0 (7.31)		(4.08)	(1.38)	
A35	121.6 (8.44)		(4.21)	(1.38)	
A36		174.8	52.2	19.1	
S37	113.9 (7.43)		60.4 (4.70)	(4.23, 4.02)	
K38					
P39					
A40	123.9 (8.71)	174.4	51.9 (4.96)	20.9 (1.45)	
V41	125.2 (7.93)	171.5	61.2 (5.13)	35.3 (1.73)	H^γ 0.63, 0.46
E42	130.0 (9.30)	172.1	54.6 (5.36)	33.4 (2.06, 1.99)	H^γ 2.25
I43	123.1 (9.30)	173.9	60.0 (5.34)	40.8 (2.27)	H^γ 1.66; H^m 0.85; H^δ 0.51
K44	128.9 (9.56)	170.8	56.4 (4.60)	35.3 (1.87, 1.76)	H^γ 1.54, 1.41; H^δ 1.33, 1.24
Q45	128.0 (8.58)	172.2	53.9 (4.45)	30.6 (1.82, 1.71)	H^γ 2.03; H^ϵ 7.83, 7.11; N^ϵ 106.8
E46	128.9 (8.53)	173.5	55.1 (4.37)	31.0 (1.62, 1.26)	H^γ 2.02
G47	117.9 (9.10)	170.6	48.0 (3.94, 3.58)		
D48	126.6 (8.54)	172.5	54.5 (5.18)	42.1 (3.15, 2.68)	
T49	116.7 (8.08)	170.1	63.0 (4.70)	69.6 (4.14)	H^γ 0.99
F50	124.2 (9.08)	173.1	57.6 (4.56)	44.6 (1.65)	2, 6H 6.48; 3, 5H 7.08; 4H 6.81
Y51	122.5 (8.35)	172.8	56.3 (5.24)	41.0 (3.01, 2.70)	2, 6H 6.94; 3, 5H 6.61
I52	123.3 (8.41)	171.6	61.0 (4.60)	40.4 (1.84)	H^γ 1.26; H^m 0.80; H^δ 0.31
K53	133.1 (9.30)	172.0	54.5 (5.08)	34.9 (1.76, 1.58)	H^γ 1.17; H^δ 0.44, 0.29; H^ϵ 2.84
T54	124.4 (8.85)		62.1 (4.88)	70.0 (3.86)	H^γ 0.94
S55	122.7 (9.43)		58.0 (5.30)	65.0 (3.83, 3.74)	
T56	124.0 (8.71)		(4.85)	(4.61)	H^γ 1.07
T57		173.5	64.9 (4.00)	66.7 (4.23)	H^γ 1.27
V58			62.2 (4.16)	(1.96)	H^γ 0.79, 0.74

Residue	¹⁵ N	CO	C ^α	C ^β	Others
R59					
T60	123.5 (8.58)		60.3 (5.20)	71.7 (3.90)	H ^γ 1.06
T61			60.1 (4.61)	71.7 (3.97)	H ^γ 1.06
E62	122.9 (8.73)		(4.98)	(2.02, 1.91)	
I63		170.5	59.5 (4.88)	42.2 (1.85)	H ^γ 1.16, 1.01; H ^{γm} 1.09; H ^δ 0.80
N64	120.4 (8.10)	169.7	52.3 (5.56)	42.8 (2.54, 2.50)	H ^δ 7.62, 6.92; N ^δ 113.1
F65	117.2 (8.34)	169.1	55.9 (4.65)	39.8 (2.15)	2, 6H 6.24; 3, 5H 6.52; 4H 6.32
K66	120.8 (9.32)	175.2	53.9 (4.65)	35.4 (1.63, 1.49)	H ^γ 1.45, 1.28; H ^ε 2.92
V67	127.5 (9.01)	174.1	67.1 (3.23)	31.9 (1.85)	H ^γ 0.64, 0.43
G68	114.9 (8.91)	170.7	45.7 (4.38, 3.61)		
E69	120.2 (7.94)	171.5	54.9 (4.77)	35.3 (2.16, 1.96)	H ^γ 2.19
E70	130.3 (9.21)	172.6	57.6 (4.88)	31.4 (1.99, 1.91)	H ^γ 2.20, 2.13
F71	121.4 (9.06)	169.5	55.8 (5.11)	41.4 (3.53, 3.20)	2, 6H 7.32; 3, 5H 6.82; 4H 6.52
E72	119.6 (8.67)	173.1	55.3 (5.05)	31.9 (2.02, 1.91)	H ^γ 2.30, 2.13
E73	122.4 (8.44)	171.6	55.3 (4.73)	29.7 (2.02, 1.90)	H ^γ 2.14, 2.14
Q74	117.9 (7.59)	174.3	54.2 (5.30)	33.1 (1.73, 1.70)	H ^γ 2.17, 1.99; H ^ε 7.49, 6.70; N ^ε 110.3
T75	111.8 (9.18)	175.4	62.4 (4.55)	71.2 (4.16)	H ^γ 1.03
V76	122.4 (9.18)		65.6 (3.82)	32.1 (2.00)	H ^γ 1.01, 0.81
D77	112.0 (8.54)				
G78	107.2 (7.93)		45.9 (4.10, 3.55)		
R79	121.0 (7.86)	171.4	54.0	29.8	
P80		173.6	63.8 (4.66)	33.0 (2.38, 1.86)	H ^γ 2.15, 1.99
C81	118.8 (8.87)	168.5	55.9 (5.05)	31.6 (2.58)	
K82	120.0 (8.87)	173.0	54.5 (4.73)	34.3 (1.54, 1.47)	H ^γ 1.26, 1.22; H ^δ 1.03
S83	124.9 (9.06)	168.7	58.7 (4.86)	68.0 (2.78, 1.54)	
L84	120.7 (7.36)	173.7	54.9 (4.23)	45.2 (2.00, 1.58)	H ^γ 1.17; H ^δ 0.68, 0.51
V85	130.1 (9.20)	171.5	60.6 (4.35)	32.6 (1.35)	H ^γ 0.23, 0.02
K86	123.8 (8.47)	173.3	54.2 (4.48)	36.9 (1.61, 1.43)	H ^γ 1.26, 1.12
W87	120.2 (8.65)	174.9	57.0 (5.11)	29.5 (3.22, 2.99)	2H 7.30; 4H 7.98; 5H 6.95; 6H 7.21; 7H 7.62 H ^ε 10.66; N ^ε 129.6
E88	127.7 (9.21)	173.3	58.0 (4.35)	32.3 (1.80, 1.66)	H ^γ 1.99
S89	112.5 (8.59)	171.2	57.0 (4.55)	65.0 (4.11, 3.98)	
E90	116.7 (8.71)	173.1	59.1 (3.66)	29.5 (1.84, 1.78)	H ^γ 2.08
N91	111.2 (8.05)	171.3	52.9 (4.96)	40.4 (3.15, 2.85)	H ^δ 7.50, 6.83; N ^δ 112.6
K92	120.1 (7.84)	171.0	56.7 (5.46)	37.2 (1.98, 1.47)	H ^γ 1.22; H ^δ 1.10; H ^ε 2.68
M93	127.0 (9.35)	171.0	53.4 (5.18)	35.1 (1.99)	H ^γ 2.19, 2.08; H ^ε 0.41
V94	119.3 (8.86)	170.0	60.3 (4.30)	34.9 (1.77)	H ^γ 0.73, 0.70
C95	127.3 (8.85)	171.4	55.6 (4.48)	27.9 (0.36, -0.28)	
E96	127.7 (7.70)	172.6	55.2 (4.31)	31.6 (1.81, 1.73)	H ^γ 2.14, 1.95
Q97	121.0 (7.43)	173.1	54.7 (4.91)	30.8 (1.75)	H ^γ 2.43, 2.02; H ^ε 7.38, 6.71; N ^ε 114.4
K98	123.1 (8.94)	172.9	54.7 (4.60)	35.0 (2.10)	H ^γ 1.96, 1.78; H ^δ 1.24; H ^ε 3.16, 2.84
L99	126.1 (8.78)	175.4	56.0 (4.00)	42.0 (1.98, 1.63)	H ^γ 1.36; H ^δ 0.86, 0.65
L100	121.9 (7.77)	174.8	57.0 (4.07)	42.5 (1.64, 1.47)	H ^γ 1.35; H ^δ 0.80, 0.76
K101	117.4 (8.05)	172.7	55.4 (4.37)	34.9 (1.72, 1.61)	H ^γ 1.37, 1.27
G102	108.6 (8.18)	169.7	45.1 (4.02, 3.71)		
E103	117.2 (8.10)	173.1	54.9 (4.60)	32.9 (1.96, 1.78)	H ^γ 2.10
G104	109.1 (8.14)		45.5 (4.10, 3.90)		
P105		172.8	62.7 (4.48)	32.7 (2.03, 1.33)	H ^γ 1.84, 1.76; H ^δ 3.60, 3.29
K106	123.5 (8.58)	175.1	56.6 (4.38)	32.6 (1.81, 1.51)	H ^γ 1.35, 1.30;
T107	118.7 (8.79)	170.8	60.1 (5.36)	72.5 (4.46)	H ^γ 1.13
S108	112.3 (7.80)	171.2	57.3 (4.63)	66.8 (3.86, 3.78)	
W109	116.3 (8.21)	171.8	56.1 (5.76)	33.1 (3.48, 3.29)	2H 6.89; 4H 6.90; 5H 6.35; 6H 6.43; 7H 6.59 H ^ε 11.37; N ^ε 137.8
T110	111.2 (9.56)	171.7	61.0 (5.24)	72.2 (4.16)	H ^γ 1.09
R111	120.1 (8.79)	170.9	56.1 (5.57)	35.6 (1.85, 1.50)	H ^γ 1.35, 1.23; H ^δ 3.00
E112	123.3 (8.87)	170.5	53.9 (5.78)	34.9 (1.94)	H ^γ 2.03
L113	126.4 (8.25)	175.1	52.8 (5.28)	43.9 (1.25)	H ^γ 0.94; H ^δ 0.51, 0.44
T114	116.9 (9.35)		(4.76)	(4.70)	H _γ 1.25
N115		173.1	55.5 (4.44)	38.1 (2.79, 2.76)	H ^δ 7.67, 6.95; N ^δ 112.6
D116	115.7 (7.75)	173.5	54.3 (4.74)	41.2 (2.79, 2.39)	
G117	107.6 (7.96)	171.7	46.1 (4.17, 3.69)		
E118	117.5 (7.43)	172.0	(4.98)	(2.02, 1.98)	

Residue	^{15}N	CO	C^α	C^β	Others
L119	124.6 (8.73)	172.6	53.4 (5.08)	43.3 (0.89)	H^γ 0.44; H^δ 0.18, -0.36
I120	125.2 (9.47)		60.8 (4.83)	39.4 (1.77)	H^γ 1.35; H^γ 0.75; H^δ 0.99
L121	135.5 (9.88)	172.8	53.3 (5.56)	45.3 (2.15)	H^γ 1.22; H^δ 0.85, 0.74
T122	120.1 (9.13)	171.4	60.4 (5.76)	71.0 (4.03)	H^γ 1.06
M123	121.7 (9.29)	171.5	55.1 (5.14)	38.3 (1.84, 1.81)	H^γ 2.55, 2.28
T124	115.2 (8.26)	172.1	60.7 (5.46)	71.2 (3.93)	H^γ 0.96
A125	125.3 (8.39)	172.7	51.6 (4.84)	21.3 (1.03)	
D126	122.4 (9.28)	172.7	57.3 (4.14)	39.6 (2.72)	
D127	121.1 (8.48)	172.8	54.7 (4.50)	41.4 (2.66)	
V128	123.4 (8.41)	171.2	63.6 (3.95)	32.9 (2.14)	H^γ 0.92, 0.69
V129	125.7 (8.38)	172.9	61.4 (4.50)	34.4 (1.83)	H^γ 0.77, 0.69
C130	129.4 (9.56)		56.4 (5.16)	35.4 (3.00, 2.66)	
T131	124.6 (8.11)		(5.13)	(3.74)	H^γ 0.98
R132	128.3 (9.77)		(5.01)	(1.78, 1.67)	H^γ 1.50
V133	122.2 (8.50)	171.2	62.2 (4.90)	(1.66)	H^γ 0.85, 0.80
Y134	127.2 (9.79)	172.5	56.5 (5.59)	43.6 (3.23, 3.01)	2, 6H 6.82; 3, 5H 6.37
V135	112.1 (9.55)	172.8	59.7 (5.33)	36.2 (2.36)	H^γ 1.04, 0.85
R136	123.2 (8.55)	174.5	57.3 (3.89)	30.3 (1.29, 1.11)	H^γ 0.59, 0.06; H^δ 2.70, 2.79
E137	125.6 (8.08)	178.7	58.9 (3.86)	31.6 (1.80, 1.68)	H^γ 2.05, 1.90