TABLES

Table S1: Acquisition and Processing Parameters for NMR Emperiments recorded on CBD_{N1}.

Experiment	nucleus	acq. pts (complex)	spectral width (Hz)	carrier freq. (ppm)	processing	matrix dim. (real points)	reference
^{1}H-^{15}N HSQC	t_1=^{15}N	128	1450	120.59	ss (70°)	1024	Bodenhausen & Ruben, 1980
	t_2=$^{1}H^{N}$	1024	6500	4.67	tdc, gm (10), poly	1024	Kay et al., 1992
^{1}H-^{15}N HMQC-J	t_1=^{15}N	341	1450	120.59	gm (2, 5, 10, 15)	4096	Kay & Bax, 1990
	t_2=$^{1}H^{N}$	1024	6500	4.67	tdc, gm (5), poly	1024	
^{1}H-^{13}C HSQC	t_1=^{13}C	512	8050	43.03	sb (72°), poly	1024	
(aliphatic)	t_2=^{1}H	1024	6500	4.67	tdc, sb (72°), pol	1024	
^{1}H-^{13}C HSQC	t_1=$^{13}C^{ct}$	236	8050	43.03	lp, ss (90°), poly	1024	Vuister & Bax, 1992
(aliphatic)	t_2=^{1}H	1024	6500	4.67	tdc, ss(90°), poly	1024	Santoro & King, 1992
^{1}H-^{13}C HSQC	t_1=$^{13}C^{ct}$	101	6200	125.47	lp, ss (80°)	1024	Vuister & Bax, 1992
(aromatic)	t_2=^{1}H	1024	6500	4.67	tdc, gm(10°)	1024	Santoro & King, 1992
^{15}N NOESY-HSQC	t_1=^{1}H	128	6500	4.67	lp, sb (72°)	512	Marion et al., 1989b

(125 msec mixing time)	t_2=^{15}N	54	1450	120.59	lp, sb (72°)	128	Zuiderweg & Fesik, 1989
	t_3=^{1}H^{N}	512	6500	4.67	tdc, sb (72°), poly	256	
^{15}N TOCSY-HSQC	t_1=^{1}H	108	6500	4.67	lp, sb (80°)	512	Marion et al., 1989c
(40, 72 msec mixing times)	t_2=^{15}N	54	1450	120.59	lp, sb (80°)	128	
	t_3=^{1}H^{N}	512	6500	4.67	tdc, sb (80°), poly	256	
HNHB	t_1=^{1}H	96	6500	4.67	lp, sb (80°)	256	Archer et al., 1991
	t_2=^{15}N	54^{ct}	1450	120.59	lp, sb (80°)	128	
	t_3=^{1}H^{N}	512	6500	4.67	tdc, sb(80°), poly	256	
HNCO	t_1=^{13}C'	64	1170	174.71	lp, ss (90°)	256	Ikura et al., 1990
	t_2=^{15}N	35^{ct}	1450	120.59	lp, sb (90°)	128	Muhandiram & Kay, 1994
	t_3=^{1}H^{N}	512	6500	4.67	tdc, sb (60°), poly	128	
HNCACB	t_1=^{13}C$^{\alpha\beta}$	45	8050	43.04	lp, ss (90°)	256	Wittekind & Müller, 1993
	t_2=^{15}N	35^{ct}	1450	120.59	lp, sb (80°)	128	
	t_3=^{1}H^{N}	512	6500	4.67	tdc, sb (90°), poly	256	
CBCA(CO)NH	t_1=^{13}C$^{\alpha\beta}$	53	8050	43.04	lp, ss (90°)	256	Grzesiek & Bax, 1992
	t_2=^{15}N	35^{ct}	1450	120.59	lp, ss (70°)	128	

	t_3=$^1H^N$	512	6500	4.67	tdc, sb (60°), poly	256	
CBCACO(CA)HA	t_1=$^{13}C'$	56	1050	176.95	lp, ss (90°)	256	Kay, 1993
	t_2=$^{13}C^{\alpha\beta}$	64^{ct}	8050	43.04	lp, ss (90°)	128	
	t_3=$^1H^{\alpha}$	512	6500	4.67	sb (60°), poly	256	
H(CCO)NH	t_1=^1H	64	6500	3.15	lp, sb (80°)[a], poly	256	Logan et al., 1992
10.0 msec DIPSI	t_2=^{15}N	35	1450	120.59	lp, ss (72°), poly	128	Montelione et al. 1992
	t_3=$^1H^N$	512	4050	4.67	sol, sb (80°), poly	256	Grzesiek et al., 1993a
C(CO)NH	t_1=^{13}C	64	8050	43.04	lp, sb (72°), poly	256	Logan et al., 1992
10.0 msec DIPSI	t_2=^{15}N	35	1450	120.59	lp, ss (72°), poly	128	Grzesiek et al., 1993a
	t_3=$^1H^N$	512	6500	4.67	sol, sb (72°), poly	256	
HCCH-TOCSY	t_1=^1H	96	4050	3.15	lp, sb (72°)[a], poly	256	Bax et al., 1990
12.2 msec DIPSI	t_2=^{13}C	40^{ct}	4025	43.04	lp, sb (72°), poly	256	Kay et al., 1993
	t_3=^1H	512	6500	4.67	sol, sb (72°), poly	256	
HCCH-COSY	t_1=^1H	128	4050	3.15	lp, sb (72°)[a], poly	256	Kay et al., 1990
	t_2=^{13}C	31	4025	43.04	lp, sb (72°), poly	256	Ikura et al., 1991
	t_3=^1H	512	6500	4.67	sol, sb (72°), poly	256	

CBCACO(CA)HA	t_1=^{13}C'	38	1864	43.04	lp, ss (72°), poly	256	Kay, 1993
-for sidechain NH_2	t_2=$^{13}C^{\alpha\beta\gamma}$	56^{ct}	8050	43.04	lp, ss (72°), poly	256	
	t_3=$^1H^{\beta\gamma}$	512	6500	4.67	sb (72°), poly	520	
HNCO	t_1=^{13}C'	44	1864	176.47	lp, ss (72), poly	128	Ikura et al., 1990
-for sidechain NH_2	t_2=^{15}N	28^{ct}	1450	120.59	lp, ss (72°), poly	128	Muhandiram & Kay, 1994
	t_3=$^1H^N$	512	6500	4.67	sol, sb (72°), poly	512	Schleucher et al., 1994
(Hβ)Cβ(CγCδ)Hδ	t_1=^{13}C	32^{ct}	4000	35.0	lp, ss (80°)	512	Yamakazi et al., 1993
	t_2=^{1}H	512	6500	4.67	tdc, gm (-10)	1024	
(Hβ)Cβ(CγCδCε)Hε	t_1=^{13}C	32^{ct}	4000	35.0	lp, ss (80°)	512	Yamakazi et al., 1993
	t_2=^{1}H	512	6500	4.67	tdc, gm (-10)	1024	
^{1}H-^{1}H-clean TOCSY	t_1=^{1}H	300-320	6500	4.67	ss (65°)	2048	Griesinger et al., 1988
(70 msec MLEV-17)	t_2=^{1}H	1024	6500	4.67	tdc, ss (75°), poly	2048	
^{1}H-^{1}H NOESY	t_1=^{1}H	231-474	6500	4.67	sb (90°)	2048	Macura et al., 1981
(85, 150 msec mixing time)	t_2=^{1}H	1024	6500	4.67	sb (90°), poly	2048	

$^{13}C/^{15}N$ NOESY-HSQC	$t_1={}^1H$	128	6500	4.67	lp, sb (72°), poly	256	Pascal et al., 1994
(50, 85 msec mixing time)	$t_2={}^{13}C$	30	3000	66.99	lp, sb (72°), poly	128	
	$t_3={}^1H$	512	6500	4.67	tdc, sb(72°), poly	256	
4D ^{13}C-^{13}C NOESY	$t_1={}^1H$	64	5000	3.20	lp, sb (80°), poly	128	Clore et al., 1991
(150 msec mixing time)	$t_2={}^{13}C$	16	3000	66.99	lp, sb (90°)	64	
	$t_3={}^{13}C$	16	3000	66.99	lp, sb (90°)	64	
	$t_4={}^1H$	256	6500	3.20	ss (80°), poly	256	
Long Range CC Correlation	$t_1={}^{13}C$	48	8050	43.04	lp, ss (110°)	128	Bax et al., 1992
	$t_2={}^{13}C$	51^{ct}	2512	43.04	lp, ss (110°)	128	
	$t_3={}^1H$	512	6500	4.67	sb (110°), poly	256	
^{13}C-{^{15}N} spin echo HSQC	$t_1={}^{13}C$	310	5530	34.99	gm (4)	1024	Grzesiek et al., 1993b
	$t_2={}^1H$	512	6500	4.67	gm (5), poly	1024	
^{13}C-{$^{13}C'$} spin echo HSQC	$t_1={}^{13}C$	310	5530	34.99	gm (4),poly	1024	Vuister et al., 1993
	$t_2={}^1H$	512	6500	4.67	gm (5), poly	1024	

ct=constant time; lp=linear prediction (or mirror image linear prediction with constant-time); ss=sinebell squared (degrees shifted); sb=sinebell (degrees shifted); gm=Lorenztian-to-Gaussian multiplication with a maximum at approximately 0.1 of the acquisition time (Hz line broadening); poly=polynomial baseline flattening; tdc=time domain convolution; sol=solvent filter.

[a]4342 degree first order phase shift applied to the FID prior to linear prediction to shift the carrier position.

Table S2. Assignment of the ^{1}H, ^{13}C, and ^{15}N NMR spectra of CBD_{N1} in the presence of cellotetraose (35 °C, pH* 5.90).

residue	^{15}N (H^N)	C'	$^{13}C^{\alpha}$ (H^{α})	$^{13}C^{\beta}$ (H^{β})^a	other
A1		172.89	52.13 (4.19)	19.56 (1.56)	
S2	118.27 (8.39)		57.78 (5.13)	64.48 (4.66)	
P3		177.36	65.38 (4.54)	32.51 (1.98, 2.60)	γ 28.12 (2.15, 2.35) δ 51.65 (4.05, 4.34)
I4	109.59 (7.26)	175.34	61.39 (4.50)	37.63 (2.26)	γ^2 18.78 (0.95) γ^1 26.49 (1.19, 1.34) δ^1 15.04 (0.91)
G5	112.30 (8.12)	174.84	43.80 (3.90, 4.62)		
E6	125.2 0(9.43)	178.72	59.29 (4.01)	29.48 (2.23)	γ 36.28 (2.46) δ 183.2
G7	112.45 (10.39)		45.68 (3.28, 4.40,)		
T8	105.13 (7.07)	176.55	60.75 (4.47)	70.17 (4.47)	γ^2 (1.18)
F9	119.10 (8.05)	174.83	60.52 (4.51)	34.92 (2.86, 2.97)*	δ 131.5 (7.38) ε 131.74 (6.86) ζ 128.44 (5.86)
D10	118.47 (7.83)	177.12	56.24 (4.43)	40.96 (2.70, 2.58)*	γ 179.94
D11	118.76 (8.81)	175.76	53.03 (4.81)	41.08 (2.72, 2.65)*	γ 180.84
G12	110.62 (7.70)		44.89 (3.86, 4.70)		
P13		175.59	64.41 (4.52)	32.35 (2.04, 2.48)	γ 26.83 (2.04, 2.12) δ 49.49 (3.61, 3.89)
E14	117.23 (8.75)	176.13	57.14 (3.90)	27.81 (2.61)	γ 36.25 (2.36,2.58) δ 183.8
G15	106.97 (8.19)	175.05	45.52 (3.79, 4.09)		
W16	125.76 (8.33)	176.03	59.53 (4.46)	29.12 (3.37, 2.96)*	δ^1 129.3 (8.02) ε^1 132.79 (11.04) ζ^2 113.52 (7.22) ζ^3 121.0 (6.95) ε^3 121.04 (7.39) η^2 122.5 (6.98)

V17	116.62 (9.23)	173.61	59.97 (4.69)	36.13 (2.26)	γ^1 21.71 (1.04) γ^2 19.89 (0.97)
A18	124.30 (8.56)	176.42	49.87 (5.65)	23.74 (1.43)	
Y19	119.18 (8.86)	174.36	56.07 (5.13)	41.38 (3.09, 2.95)*	δ 133.7 (6.81) ε 117.3 (6.70)
G20	111.62 (9.01)	173.77	45.83 (3.82, 4.72)		
T21	108.29 (7.07)	174.70	60.73 (4.09)	69.85 (4.51)	γ^2 22.85 (0.81)
D22	123.07 (8.65)	176.21	53.09 (4.74)	40.04 (2.08, 2.71)*	γ 179.4
G23	113.60 (7.70)		44.04 (3.89, 4.26)		
P24		177.71	62.37 (4.52)	32.85 (2.15, 2.33)	γ 26.78 (1.93, 2.06) δ 49.29 (3.59, 3.64)
L25	120.89 (8.22)	175.22	55.84 (4.16)	42.45 (1.47, 1.55)	γ 26.31 (1.81) δ^1 25.55 (0.86) δ^2 23.64 (1.57)
D26	124.10 (8.42)	176.58	53.19 (5.03)	44.49 (2.62)	γ 180.9
T27	117.65 (8.86)	177.65	61.34 (5.51)	68.21 (4.69)	γ^2 21.49 (0.82)
S28	123.57 (8.75)	176.54	62.84 (4.12)	(3.95)	
T29	113.12 (8.46)	176.10	62.27 (4.46)	70.44 (4.46)	γ^2 21.21 (1.18)
G30	112.01 (8.23)	171.27	45.30 (3.75, 4.28)		
A31	124.90 (7.37)	173.39	49.93 (4.39)	21.7 (1.04)	
L32	124.52 (8.25)	175.29	54.81 (3.86)	40.16 (-0.63, 0.68)*	γ 27.2 (0.73) δ^1 26.10 (0.27) δ^2 25.30 (0.14)
C33	126.39 (8.60)	174.26	55.00 (6.13)	47.35 (2.96, 2.75)*	
V34	116.72 (9.02)	172.14	58.88 (4.39)	35.87 (1.71)	γ^1 22.36 (0.57) γ^2 18.81 (0.41)
A35	127.51 (8.28)	175.47	50.60 (4.42)	19.23 (1.34)	

V36	129.50 (9.11)		59.54 (3.82)	32.00 (0.80)	γ^1 20.79 (0.80) γ^2 21.20 (-0.30)
P37		176.69	62.36 (4.43)	32.42 (1.91, 2.24)	γ 27.29 (1.91) δ 51.87 (3.55, 3.82)
A38	123.83 (8.55)	169.78	52.59 (3.91)	18.77 (1.51)	
G39	109.67 (8.40)	175.05	46.79 (3.83)		
S40	114.71 (7.43)	173.07	58.99 (4.06)	65.23 (4.12, 3.84)*	
A41	124.79 (8.65)	177.82	50.09 (4.44)	21.48 (1.34)	
Q42	124.10 (8.42)	176.51	57.31 (3.25)	27.87 (1.48, 1.35)*	γ 32.33 (0.59, 1.46) δ 179.5 ε^2 112.31 (6.41, 6.80)
Y43	122.08 (9.41)	177.82	59.97 (4.07)	36.38 (3.27)	δ 132.6 (6.97) ε 118.3 (6.74)
G44	110.34 (8.56)	172.94	49.47 (3.80, 4.30)		
V45	116.63 (7.11)	175.25	59.33 (4.54)	35.27 (1.58)	γ^1 21.84 (0.77) γ^2 21.77 (0.95)
G46	117.65 (7.83)	179.66	46.21 (3.68, 4.65)		
V47	120.81 (8.60)	175.26	61.48 (5.13)	35.09 (1.97)	γ^1 22.23 (1.00) γ^2 22.73 (0.86)
V48	122.63 (9.59)	173.26	59.28 (5.58)	36.96 (2.01)	γ^1 22.70 (0.95) γ^2 21.60 (1.01)
L49	128.41 (8.66)	175.02	52.95 (4.09)	41.12 (-1.51, 0.64)	γ 26.61 (0.70) δ^1 22.00 (0.22) δ^2 26.45 (0.51)
N50	124.84 (8.38)	175.88	52.92 (5.02)	40.27 (2.47, 2.75)*	γ 173.46 δ^2 113.79 (7.20, 6.68)
G51	111.04 (8.29)	173.44	46.65 (4.03, 4.17)		
V52	125.18 (7.54)	172.93	61.30 (3.76)	33.60 (1.45)	γ^1, γ^2 21.09 (0.62)
A53	128.04 (7.89)	177.22	51.32 (4.27)	19.57 (1.36)	
I54	125.22 (8.51)	174.90	56.71 (4.26)	39.83 (1.50)	γ^1 25.48 (0.95, 1.45) γ^2 18.55 (0.70) δ^1 8.60 (0.15)

E55	128.06 (8.84)	175.24	54.61 (4.60)	31.50 (1.96)	γ 35.74 (2.23) δ 183.6
E56	127.82 (8.18)	177.42	57.97 (3.40)	28.92 (1.64)	γ 34.95 (1.99) δ 182.2
G57	115.48 (9.09)	174.35	44.87 (3.49, 4.32)		
T58	122.00 (8.08)	172.39	63.38 (4.16)	69.41 (4.39)	γ^2 21.21 (0.56)
T59	126.56 (8.47)	172.31	62.70 (4.80)	69.28 (3.78)	γ^2 21.66 (0.94)
Y60	128.06 (8.84)	174.96	56.58 (4.98)	43.68 (1.41, 2.47)	δ 133.0 (6.61) ε 117.7 (6.83)
T61	116.08 (8.84)	174.11	61.86 (5.24)	71.55 (3.86)	γ^2 22.23 (1.08)
L62	132.71 (9.58)	174.09	53.79 (5.38)	44.76 (1.42, 2.11)*	γ 28.41 (1.80) δ^1 23.12 (1.20) δ^2 26.17 (0.80)
R63	127.76 (9.31)	175.05	53.94 (5.73)	34.56 (1.84)	γ 28.18 (1.70) δ 43.56 (1.70) ε 118.32 (8.82)
Y64	115.18 (8.18)	172.56	58.03 (4.90)	40.13 (3.65, 2.71)*	δ 132.8 (6.63) ε 117.32 (6.50)
T65	118.00 (8.86)	173.83	61.02 (5.37)	70.02 (3.86)	γ^2 21.86 (1.02)
A66	128.89 (8.54)	176.91	50.46 (5.63)	24.61 (1.47)	
T67	117.76 (8.73)	172.01	61.76 (4.52)	71.58 (3.78)	γ^2 21.61 (0.97)
A68	129.41 (8.44)	177.18	50.21 (5.75)	25.65 (1.46)	
S69	113.12 (8.46)	173.71	59.74 (4.27)	63.74 (3.95)	
T70	118.3 (7.35)	170.06	59.44 (4.36)	70.22 (3.94)	γ^2 18.17 (0.53)
D71	122.74 (7.40)	175.55	54.42 (4.97)	39.86 (2.55)	γ 180.3
V72	125.73 (7.82)	171.87	60.24 (4.16)	34.68 (1.17)	γ^1 17.80 (-0.45) γ^2 20.44 (0.15)
T73	125.36 (7.64)	173.50	61.46 (4.92)	70.12 (3.75)	γ^2 21.45 (0.91)

V74	115.64 (7.11)	173.17	57.82 (3.50)	31.48 (2.68)	γ^1 23.54 (0.93) γ^2 18.07(0.77)
R75	121.90 (7.58)	174.01	54.99 (5.47)	34.31 (2.06, 1.93)*	γ 27.17 (1.36) δ 44.63 (3.31) ε 116.12 (7.29)
A76	131.15 (8.22)	176.16	50.41 (5.15)	20.73 (0.78)	
L77	125.20 (9.34)	174.48	53.47 (4.96)	45.80 (1.60, 1.97)	γ 25.05 (1.82) δ^1 25.75 (0.77) δ^2 26.93 (0.69)
V78	120.86 (8.17)	176.66	61.53 (5.06)	32.97 (1.62)	γ^1 20.83 (0.84) γ^2 20.83 (0.89)
G79	116.70 (8.75)	171.66	47.40 (4.10, 4.97)		
Q80	117.22 (8.02)	177.93	55.61 (3.43)	31.78 (1.72, 1.32)*	γ 35.97 (1.32, 1.57) δ 179.76 ε^2 117.13 (6.81, 8.84)
N81	124.48 (9.18)	174.24	51.56 (4.76)	36.26 (2.07, 2.67)*	γ 177.84 δ^2 116.60 (8.08)
G82	110.35 (7.01)	170.64	43.91 (3.28, 3.79)		
A83	124.45 (7.91)		51.21 (3.34)	16.89 (1.11)	
P84		175.73	64.08 (4.39)	32.95 (2.05, 2.46)	γ 24.85 (1.63, 1.91) δ 49.57 (3.38)
Y85	124.62 (9.43)	176.09	60.36 (4.02)	34.94 (3.09, 3.38)*	δ 133.7 (7.10) ε 118.0 (6.6)
G86	109.38 (8.99)	172.30	45.55 (3.67, 4.09)		
T87	107.21 (7.70)	175.28	60.55 (5.28)	72.88 (4.24)	γ^2 22.80 (1.19)
V88	110.32 (8.35)	174.96	60.46 (4.54)	33.26 (2.42)	γ^1 21.83 (1.01) γ^2 19.97 (0.76)
L89	124.53 (7.36)	174.41	55.06 (4.10)	44.02 (0.03, 1.01)	γ 27.19 (1.30) δ^1 23.04 (0.74) δ^2 25.88 (0.62)
D90	129.12 (8.62)	175.30	54.61 (4.84)	41.60 (2.55, 2.85)*	γ 181.3
T91	116.69 (8.37)	173.91	59.87 (4.88)	73.89 (4.22)	γ^2 22.87 (1.09)
S92	117.91 (8.64)		54.14 (5.79)	64.68 (3.70)	

P93		175.25	62.82 (4.30)	32.63 (1.73, 2.25)	γ 26.43 (1.69, 1.98) δ 49.52 (3.38, 3.45)
A94	125.73 (7.82)	177.29	51.52 (4.64)	18.83 (1.29)	
L95	126.35 (9.14)	176.31	53.36 (4.75)	45.24 (1.78, 1.35)*	γ 27.00 (1.75) δ 27.69 (0.82) δ 22.80 (0.83)
T96	115.65 (8.91)	174.08	60.14 (4.82)	71.52 (4.38)	γ^2 20.47 (1.15)
S97	115.89 (8.23)	175.09	59.46 (4.79)	63.25 (3.76, 4.05)*	
E98	124.46 (7.78)		53.13 (4.75)	30.74 (1.81, 1.96)*	γ 35.80 (2.22) δ 183.9
P99		176.90	63.36 (4.33)	31.63 (1.72, 1.94)	γ 27.50 (1.97, 2.09) δ 50.47 (3.74, 3.84)
R100	125.51 (8.06)	174.23	55.05 (4.55)	33.31 (1.81, 1.99)*	γ 27.84 (1.51) δ 43.82 (3.14, 3.34) ε 115.90 (7.44)
Q101	127.12 (8.50)	175.34	55.51 (4.69)	29.00 (2.08, 1.89)*	γ 34.47 (2.27) δ 180.9 ε^2 113.71 (6.61, 7.31)
V102	132.90 (9.26)	175.28	62.41 (3.92)	32.91 (0.55)	γ^1 21.89 (0.84) γ^2 20.58 (0.63)
T103	122.41 (8.12)	174.19	60.87 (5.15)	71.24 (3.93)	γ^2 21.62 (1.10)
E104	127.02 (9.38)	175.34	54.53 (4.97)	33.29 (1.86, 2.19)*	γ (2.42)
T105	123.29 (8.86)	174.37	61.68 (5.75)	70.85 (3.87)	γ^2 21.78 (1.13)
F106	125.20 (9.34)	172.19	55.82 (5.11)	41.54 (3.03, 3.25)*	δ (6.96) ε 128.2 (6.72)
T107	121.41 (9.14)	175.58	61.89 (4.81)	69.38 (3.90)	γ^2 21.48 (1.00)
A108	132.06 (8.83)	178.47	54.38 (4.34)	20.07 (1.86)	
S109	119.19 (8.14)	171.92	57.66 (4.54)	63.90 (4.30, 3.99)*	
A110	124.36 (7.18)	172.96	51.05 (4.28)	23.00 (1.06)	
T111	115.08 (7.80)	175.00	60.26 (4.74)	71.32 (3.90)	γ^2 22.06 (1.30)

Y112	129.18 (9.44)		50.81 (5.66)	39.50 (2.60, 3.22)*	δ 131.54 (6.97) ε 116.8 (6.29)
P113		174.93	61.72 (4.73)	33.22 (2.25, 2.37)	γ 26.78 (2.39, 2.47) δ (4.10)
A114	119.13 (8.41)	176.95	53.20 (3.85)	19.68 (1.41)	
T115	111.01 (7.2)		57.68 (4.71)	70.57 (4.06)	γ^2 21.26 (1.20)
P116		176.63	63.27 (4.51)	32.49 (2.45)	γ 27.05 (2.01,) δ 50.61 (3.53, 3.82)
A117	124.93 (8.18)	177.76	50.14 (4.60)	22.23 (1.88, 1.52)	
A118	126.55 (8.56)	177.98	54.67 (3.93)	17.74 (1.34)	
D119	117.59 (8.41)	175.30	54.32 (4.01)	40.33 (2.77)	γ 181.3
D120	120.10 (7.59)		52.17 (5.07)	41.93 (2.81, 2.22)*	γ 180.0
P121		175.09	62.59 (4.18)	32.38 (1.22, 1.87)	γ 26.78 (1.45, 1.56) δ 49.29 (3.55, 3.66)
E122	121.34 (9.30)	175.46	54.35 (4.38)	29.81 (1.26, 1.93)	γ 35.82 (2.18, 2.37) δ 182.0
G123	107.86 (7.69)	174.50	45.06 (4.06, 4.25)		
Q124	120.68 (9.27)	174.24	53.57 (5.61)	32.52 (1.66)	γ 33.20 (1.67, 2.11) δ 179.4 ε^2 113.66 (8.42)
I125	121.96 (8.20)	174.45	60.73 (4.64)	40.03 (1.57)	γ^1 27.71 (1.57, 1.77) γ^2 17.76 (0.92) δ^1 15.36 (1.03)
A126	127.97 (8.93)	174.62	51.06 (5.34)	22.56 (1.12)	
F127	122.26 (9.13)	175.77	56.91 (5.02)	39.88 (3.12, 2.51)*	δ 131.08 (6.91) ε 131.09 (6.55) ζ 128.4 (5.89)
Q128	123.94 (9.39)	175.77	55.85 (4.82)	29.61 (2.42, 2.12)*	γ 33.62 (2.31, 2.55) δ 179.6 ε^2 113.44 (6.84, 7.68)
L129	119.56 (8.07)	177.14	54.57 (4.98)	43.70 (1.10, 1.99)	γ 27.19 (1.74) δ^1 25.76 (0.47) δ^2 23.10 (0.98)
G130	108.65 (8.00)	174.63	44.45 (3.72, 4.13)		

G131	111.26 (8.12)	173.89	45.88 (3.34, 3.52)		
F132	120.32 (6.98)	175.45	59.66 (4.51)	40.87 (2.34, 3.45)*	δ 131.8 (7.11) ε 131.3 (7.35) ζ 129.53 (7.25)
S133	113.37 (7.80)	175.65	56.38 (4.57)	64.72 (3.45, 3.52)*	
A134	134.02 (9.12)	178.72	54.59 (4.32)	18.83 (1.47)	
D135	120.51 (7.99)	175.06	53.71 (4.75)	42.71 (2.46, 2.87)*	γ 179.9
A136	122.68 (8.25)	178.05	52.07 (4.58)	19.81 (1.48)	
W137	120.37 (8.19)	172.86	56.34 (4.63)	29.55 (3.23)	δ^1 119.9 (7.49) ε^1 131.44 (10.19) ζ^2 113.13 (7.57) ζ^3 130.9 (6.55) η^2 123.07 (6.92) ε^3 128.39 (5.89)
T138	115.16 (9.07)	173.12	61.21 (4.93)	72.40 (3.88)	γ^2 21.69 (1.05)
L139	129.72 (8.37)	175.61	53.25 (5.19)	44.63 (1.34, 1.59)*	γ 27.50 (1.32) δ^1 24.08 (0.91) δ^2 26.30 (0.61)
C140	123.07 (8.72)	173.15	55.68 (5.63)	47.53 (2.72, 2.41)*	
L141	127.07 (9.06)	174.36	52.74 (5.05)	47.06 (0.90, 1.03)	γ 26.05 (0.96) δ^1 24.70 (-0.16) δ^2 23.89 (0.01)
D142	120.31 (9.01)	173.37	51.43 (5.18)	44.56 (2.39, 2.51)*	γ 183.9
D143	124.06 (9.03)	176.23	55.72 (4.28)	39.66 (2.60)	γ 181.4
V144	120.40 (8.53)	176.62	60.77 (5.28)	33.40 (2.06)	γ^1 21.46 (1.26) γ^2 21.54 (1.03)
A145	129.71 (9.51)	174.35	52.60 (4.38)	23.54 (1.44)	
L146	122.49 (7.61)	174.71	54.44 (5.41)	44.49 (1.25, 2.02)*	γ 27.99 (1.55) δ^1 24.46 (1.06) δ^2 26.80 (0.76)
D147	128.06 (8.84)	175.58	53.27 (5.19)	44.62 (2.54, 2.79)*	γ 179.3
S148	116.39 (8.66)	174.35	56.94 (4.65)	65.30 (3.57)	

E149	123.65 (8.20)	176.05	55.97 (4.28)	30.02 (1.78, 1.96)*	γ 35.53 (2.13) δ 183.2
V150	122.76 (8.03)	175.71	62.08 (4.08)	33.13 (2.01)	γ^1 21.26 (0.88) γ^2 21.26 (0.88)
E151	126.98 (8.32)	175.20	56.28 (4.29)	30.12 (1.90, 2.04)*	γ 35.99 (2.26) δ 180.8
L152	131.64 (7.83)		56.75 (4.17)	43.55 (1.53)	γ 27.33 (1.53) δ (0.92) δ (0.86)

[a] asterisk denotes stereospecifically assigned β protons, reported as $H^{\beta 2}$ and $H^{\beta 3}$, respectively. Otherwise all other methylene protons are listed by ascending chemical shift. Leucine and valine residues for which the methyls are not stereospecifically assigned are reported as δ and γ, respectively.

SUPPLEMENTARY FIGURE LEGEND

Figure S1. **(A)** Distribution of NOE restraints per residue. Filled bars represent the number of long range NOEs ($|i - j| > 4$), open bars represent the sum of non-trivial intraresidue, sequential and short range NOEs ($1 < |i - j| \leq 4$). For every restraint the originating and destination residues were each counted once. **(B, C, D)** Angular order parameters $S\phi$, $S\psi$, and $S\chi 1$ for the ϕ and ψ main chain, and side chain $\chi 1$ dihedral angles, respectively, observed in the final ensemble of 25 structures (Hyberts et al., 1992). **(E, F)** The rms deviation for all heavy atoms and main chain atoms, respectively, for the ensemble of 25 structures, aligned against the average structure obtained by superimposing residues 4-148. The locations of the ten β-strands are indicated on the top of the figure.

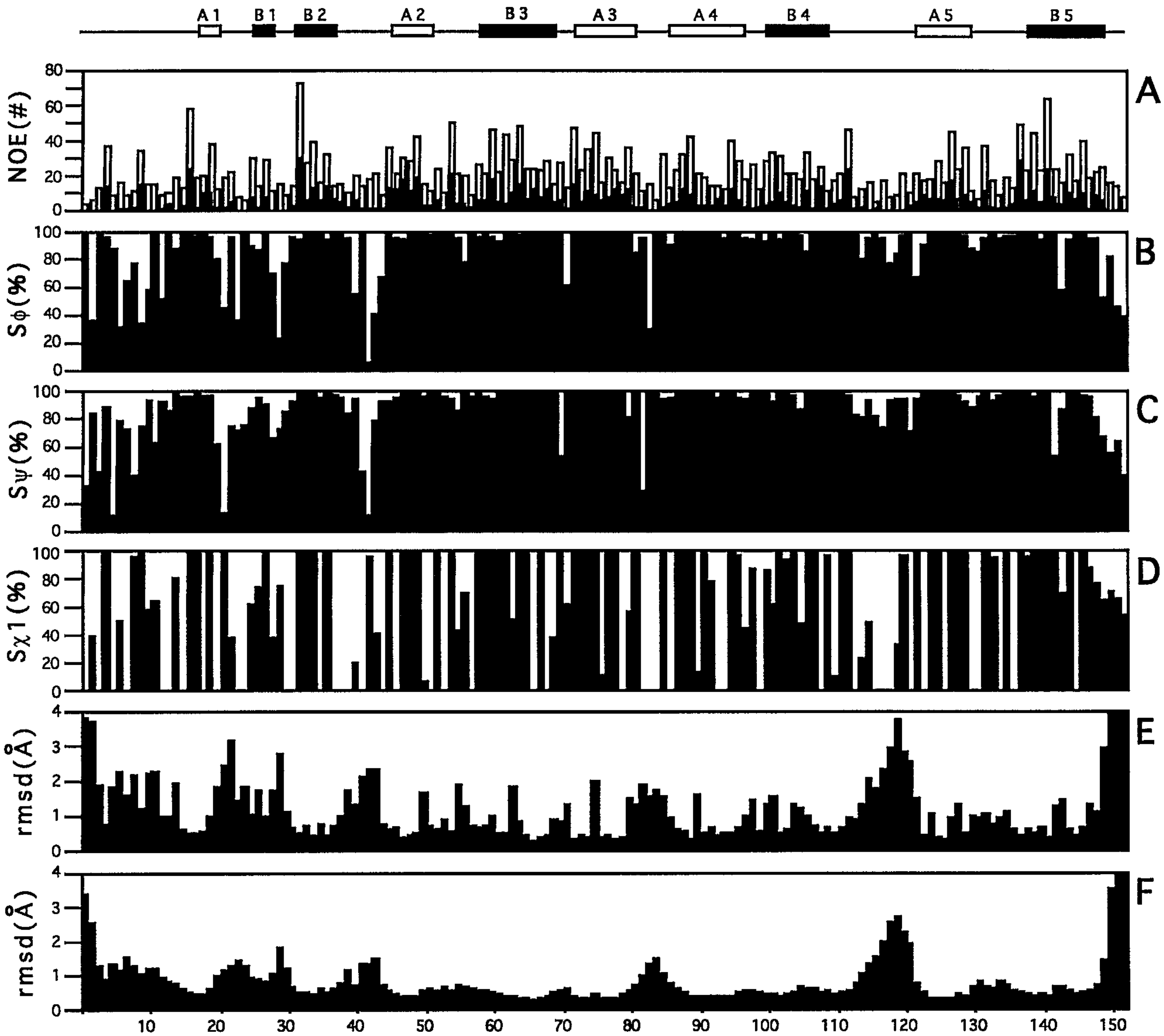

FIGURE S1
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Structure of the N-terminal