

BIOCHEMISTRY

including biophysical chemistry & molecular biology

Biochemistry, 1996, 35(16), 5145-5157, DOI:[10.1021/bi952897w](https://doi.org/10.1021/bi952897w)

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1996 American Chemical Society

SUPPLEMENTARY MATERIAL

Figure S1. ^1H - ^{15}N HSQC of 0.8 mM ^{15}N -labeled wild type IKE coat protein in 400 mM ^2H -SDS, 95% H_2O , 5% D_2O , pH 4.5, 45°C.

Figure S2. Decay (+, •) and buildup curves (x, o) arising from the slow exchange at Trp 29. Solid and dashed lines indicate magnetization originating on the major (+, o) and minor (•, x) species respectively.

Table S1. ^{15}N T_1 , T_2 and NOE values at 500 MHz, and T_2 values at 600 MHz.

Table S2. S^2 , τ_e and R_{ex} values determined from ^{15}N T_1 , T_2 and NOE values at 500 MHz, and T_2 values at 600 MHz. The values of R_{ex} represent exchange contributions to the ^{15}N linewidths as measured at 500 MHz (^1H frequency).

Table S3. Amide exchange rates and protection factors for the IKE coat protein in 400 mM MPG micelles, pH 4.5, 45°C.

Table S4. Chemical shift assignments of the IKE coat protein in 400 mM MPG micelles, pH 4.5, 45°C.

R-5157-m2

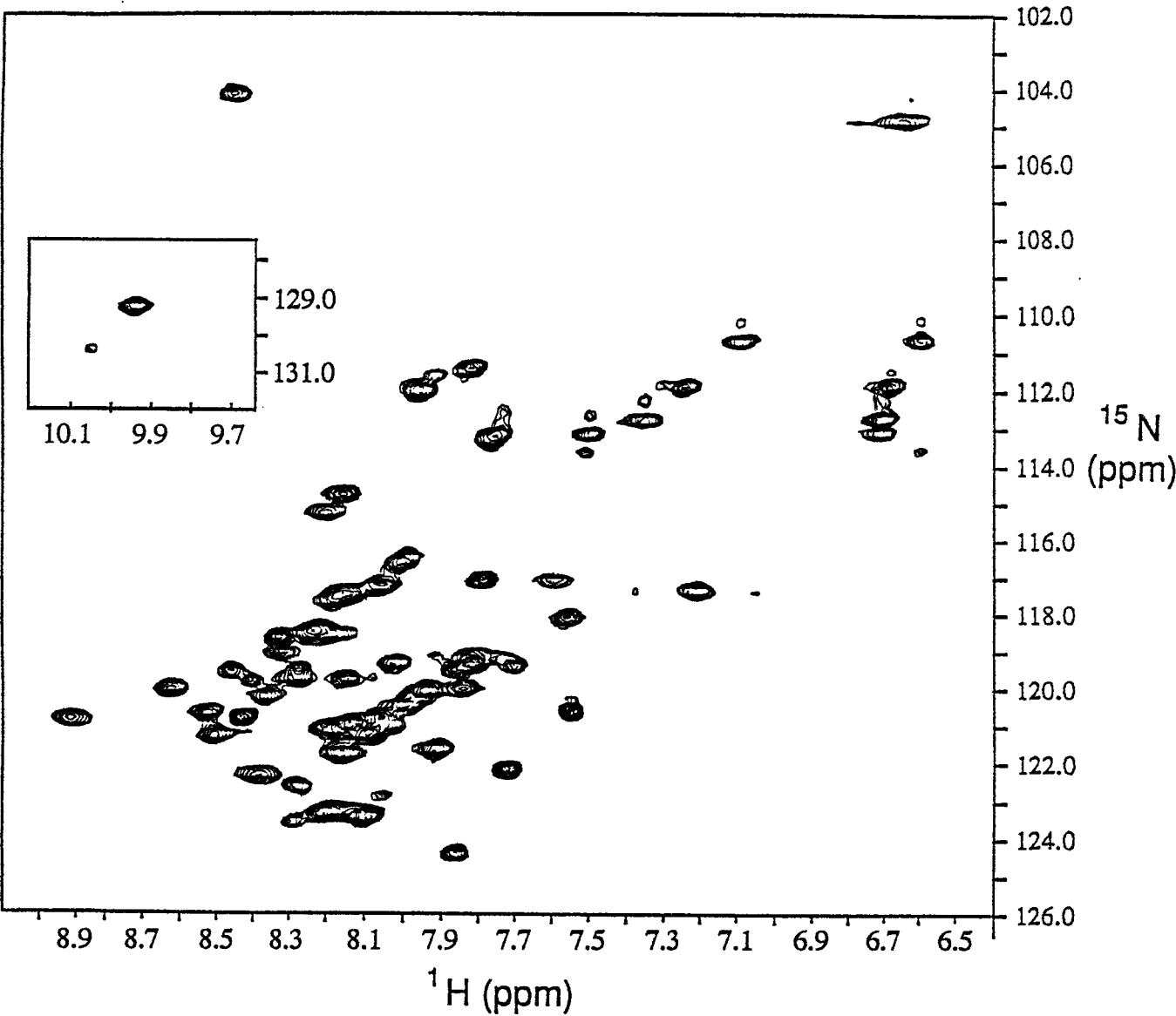
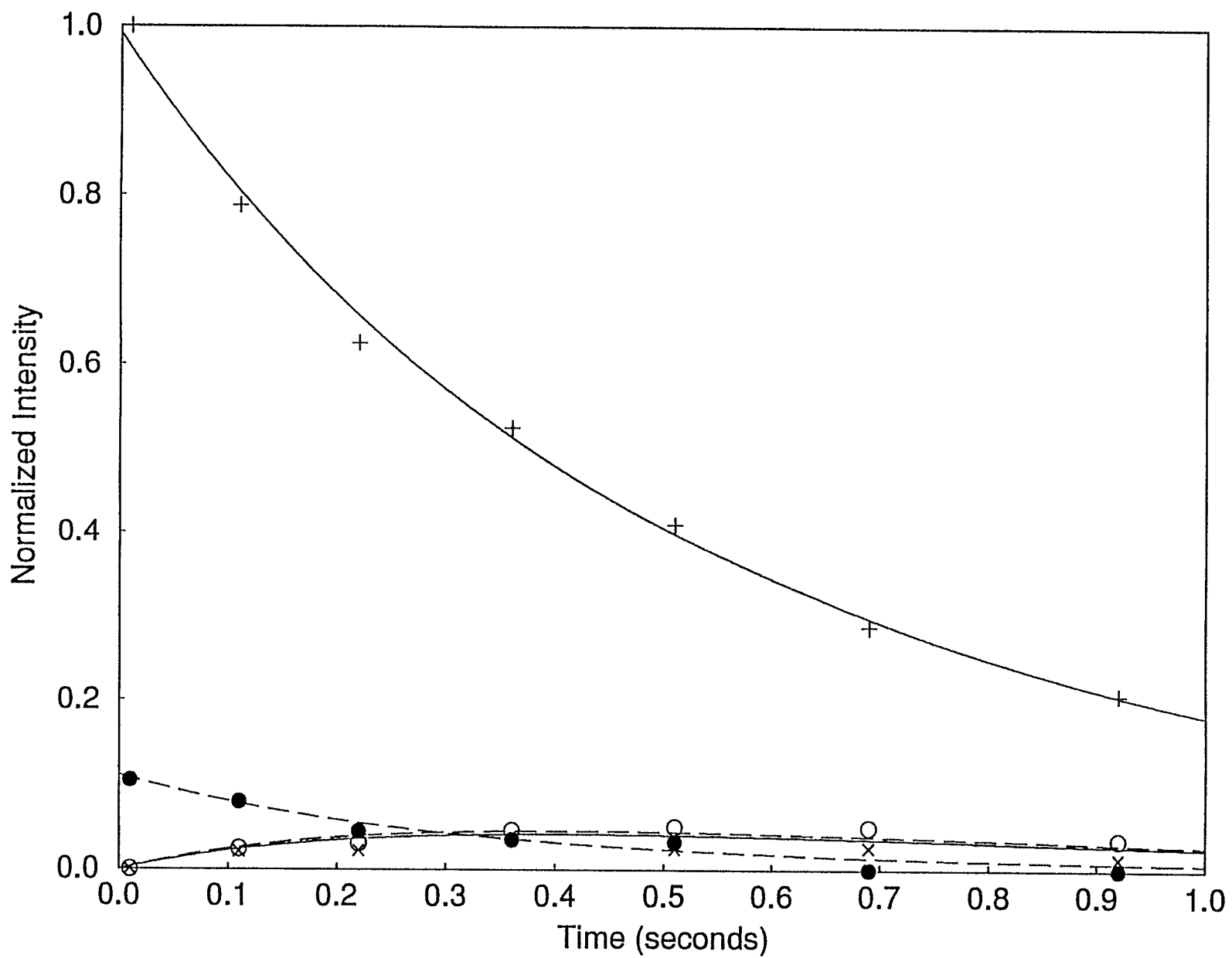


Figure S1

K-5157-M2

Figure S2



K- 5157-M4

Table S1. ^{15}N T_1 , T_2 and NOE values at 500, and T_2 values at 600 MHz (^1H frequency). T_1 and T_2 values are in seconds.

Residue	500 MHz			600 MHz
	$T_1(\text{sd})$	NOE(sd)	$T_2(\text{sd})$	$T_2(\text{sd})$
1				
2	0.692 (0.043)	-0.748 (0.007)	0.273 (0.001)	0.361 (0.006)
3				
4	0.679 (0.017)	-0.237 (0.005)	0.185 (0.003)	0.191 (0.005)
5	0.702 (0.021)	-0.095 (0.012)	0.122 (0.002)	0.113 (0.002)
6				
7	0.690 (0.019)	0.167 (0.019)	0.091 (0.001)	0.087 (0.001)
8	0.642 (0.021)	0.256 (0.020)	0.074 (0.001)	0.068 (0.001)
9				
10				
11	0.699 (0.051)	0.465 (0.051)	0.054 (0.001)	0.050 (0.001)
12	0.748 (0.034)	0.502 (0.041)	0.049 (0.001)	0.045 (0.001)
13	0.746 (0.033)	0.526 (0.042)	0.049 (0.001)	0.046 (0.000)
14	0.835 (0.031)	0.530 (0.050)	0.048 (0.001)	0.044 (0.001)
15				
16	0.785 (0.034)	0.571 (0.062)	0.046 (0.001)	0.046 (0.002)
17	0.819 (0.013)	0.396 (0.062)	0.048 (0.002)	0.043 (0.001)
18	0.844 (0.061)	0.637 (0.084)	0.045 (0.001)	0.040 (0.001)
19	0.794 (0.042)	0.386 (0.022)	0.042 (0.001)	0.042 (0.002)
20				
21	0.824 (0.038)	0.597 (0.062)	0.041 (0.001)	0.038 (0.002)
22	0.892 (0.043)	0.614 (0.091)	0.040 (0.001)	0.037 (0.001)
23				
24	0.854 (0.025)	0.479 (0.071)	0.045(0.001)	0.040 (0.002)
25	0.892 (0.040)	*	0.043(0.002)	0.039 (0.002)
26	0.802 (0.041)	0.509 (0.095)	0.042(0.001)	0.036 (0.001)
27	0.749 (0.050)	0.456 (0.091)	0.042(0.002)	*
28	0.622 (0.082)	0.440 (0.139)	0.036(0.004)	0.027 (0.004)
29	0.729 (0.042)	0.493 (0.099)	0.043(0.002)	0.041 (0.003)
30				
31	*	0.615 (0.361)	0.027 (0.002)	0.025 (0.005)
32	0.764 (0.043)	0.485 (0.116)	0.037 (0.002)	0.034 (0.003)
33				
34				
35				
36	0.769 (0.071)	0.565 (0.270)	0.049(0.003)	0.042(0.007)
37				
38	0.872 (0.056)	0.522 (0.118)	0.040 (0.001)	0.040 (0.002)
39	0.832 (0.067)	0.611 (0.085)	0.045 (0.003)	0.042 (0.001)
40	0.876 (0.047)	0.530 (0.110)	0.039 (0.001)	0.039 (0.001)
41	0.935 (0.047)	0.577 (0.116)	0.043 (0.002)	0.038 (0.003)
42	0.834 (0.041)	0.471 (0.090)	0.044 (0.001)	0.039 0.002)
43	0.844 (0.032)	0.598 (0.065)	0.047 (0.001)	0.040 (0.001)
44				
45	0.992 (0.036)	0.557 (0.057)	0.043 (0.002)	0.040 (0.002)
46	0.789 (0.040)	0.659 (0.065)	0.046 (0.001)	0.044 (0.001)
47	0.878 (0.033)	0.446 (0.051)	0.047 (0.001)	0.044 (0.001)

48	0.803 (0.034)	0.459 (0.043)	0.050 (0.001)	0.049 (0.001)
49	0.685 (0.026)	0.554 (0.070)	0.066 (0.001)	0.062 (0.001)
50	0.601 (0.017)	0.213(0.010)	0.108(0.001)	0.104 (0.001)
51	0.623 (0.012)	-0.002(0.007)	0.158(0.001)	0.153 (0.001)
52	0.689 (0.015)	-0.326(0.005)	0.238(0.002)	0.246 (0.003)
53	0.956 (0.028)	-0.613(0.009)	0.304(0.004)	0.317 (0.006)

* values not determined

Table S2. S^2 , τ_e , R_{ex} , τ_s and S_f^2 values determined from ^{15}N T_1 , T_2 and NOE values at 500 MHz, and T_2 values at 600 MHz (^1H frequency). Values of the correlation times τ_e and τ_s are given in ns, values of R_{ex} are given in s^{-1} .

Residue	$S^2(\text{sd})$	$\tau_e(\text{sd})$	$R_{ex}(\text{sd})$	$S^2(\text{sd})$	$\tau_s(\text{sd})$	$S_f^2(\text{sd})$
1						
2*				0.09 (0.01)	0.85 (0.01)	0.88 (0.06)
3						
4*				0.18 (0.00)	1.08 (0.01)	0.78 (0.02)
5				0.34 (0.01)	1.07 (0.01)	0.83 (0.02)
6						
7				0.47 (0.01)	1.21 (0.03)	0.87 (0.01)
8				0.60 (0.01)	1.23 (0.04)	0.98 (0.02)
9						
10						
11	0.87 (0.01)	0.87 (0.34)				
12	0.84 (0.03)	1.10 (0.23)	2.31 (0.50)			
13	0.85 (0.03)	1.16 (0.21)	1.72 (0.44)			
14	0.92 (0.02)	0.59 (0.26)	1.57 (0.38)			
15						
16	0.89 (0.03)	1.04 (0.32)	2.21 (0.63)			
17	0.87 (0.02)	0.61 (0.09)	2.48 (0.52)			
18	0.94 (0.04)	0.73 (0.62)	2.67 (0.75)			
19*	0.87 (0.03)	0.61 (0.21)	4.77 (0.63)			
20						
21	0.93 (0.03)	0.74 (0.56)	4.76 (0.69)			
22	0.94 (0.04)	0.19 (0.31)	4.61 (0.72)			
23						
24	0.91 (0.02)	0.36 (0.18)	3.23 (0.54)			
25						
26	0.88 (0.04)	0.86 (0.35)	5.35 (0.75)			
27						
28	0.67 (0.17)	1.54 (2.10)	13.22 (3.27)			
29	0.82 (0.06)	1.23 (0.35)	5.15 (1.19)			
30						
31						
32	0.84 (0.06)	1.04 (0.40)	8.40 (1.26)			
33						
34						
35						
36	0.94 (0.05)	2.33 (1.97)				
37						
38	0.93 (0.04)	0.31 (0.46)	4.90 (0.91)			
39	0.94 (0.04)	0.68 (0.54)	2.20 (0.71)			
40*	0.94 (0.03)	0.30 (0.27)	4.07 (0.70)			
41	0.87 (0.04)	0.09 (0.09)	4.76 (0.99)			
42	0.90 (0.03)	0.56 (0.29)	3.64 (0.63)			
43	0.93 (0.02)	0.67 (0.39)	2.26 (0.48)			
44						
45	0.83 (0.03)	0.06 (0.03)	4.87 (0.88)			
46	0.92 (0.03)	1.26 (1.64)	1.61 (0.52)			

K-5157-M7

47	0.90 (0.02)	0.27 (0.10)	1.82 (0.34)			
48	0.89 (0.03)	0.63 (0.21)	0.73 (0.47)			
49				0.68 (0.01)	1.79 (0.36)	0.93 (0.02)
50				0.37 (0.01)	1.44 (0.02)	0.87 (0.02)
51*				0.22 (0.00)	1.27 (0.01)	0.81 (0.01)
52*				0.12 (0.00)	1.06 (0.01)	0.75 (0.01)
53*				0.10 (0.00)	0.88 (0.01)	0.58 (0.01)

* The reported model did not fit one or more of the measured relaxation parameters to within 1.96 times their experimental error.

Table S3. Amide exchange rates (k_{prot} [min^{-1}]) for IKe coat protein in 400 mM MPG at 45°C. Protection factors ($P=k_{\text{rc}}/k_{\text{prot}}$) were determined based on calculated exchange values for a random coil, k_{rc} , using the method of Bai et al. (1993)^a.

residue	k_{prot}	protection factor
1		
2		
3		
4		
5		
6		
7		
8		
9		
10		
11	0.404	108.94
12	0.287	88.22
13	0.066	558.08
14	0.168	300.77
15		
16		
17	0.066	413.09
18	0.022	1346.30
19	0.246	236.21
20		
21	0.050	1636.20
22	0.011	903.38
23		
24	0.035	258.79
25	0.005	1164.70
26	0.121	589.75
27	0.384	308.04
28	0.138	506.39
29	0.318	100.25
30		
31	0.090	65.60
32	0.135	55.42
33		
34		
35		
36	0.241	31.05
37	0.030	245.24
38	0.049	766.32
39	0.149	646.17
40	0.047	429.70
41	0.003	1963.00
42	0.002	3008.60
43	0.007	4945.90
44		
45	0.002	8696.70
46	0.044	1233.50
47	0.014	4449.50
48	0.060	656.95

K-5157-mg

49

50

51

52

53

^aThe exchange rates for residues 2, 4, 5, 7, 8, 16, and 49-53 could not be measured due to rapid exchange. Exchange rates at residues 6, 9, 10, 15, 20, 23, 33, 34, 35 and 44 were not measured due to resonance overlap.

Table S4. Backbone and side chain assignments for IKe coat protein in 400 mM MPG, pH4.5, 45°C^a

Residue	N	NH	CO	C α	H α	C β	H β	other
Ala-1			173.19	51.60	4.09	19.29	1.46	
Glu-2	121.28	8.56	175.40	54.08	4.66	28.74	2.13/1.93	C γ 33.70, H γ 2.41
Pro-3			176.29	63.47	4.41	31.84	1.91/2.26	C γ 27.11, H γ 2.01, C δ 50.33, H δ 3.77/3.70
Asn-4	118.54	8.34	174.93	53.37	4.62	38.82	2.85	N δ 113.3, H δ 7.56/6.75
Ala-5	123.97	8.15	178.08	53.51	4.23	19.08	1.44	
Ala-6	121.49	8.20	178.17	53.82	4.24	18.84	1.43	
Thr-7	112.00	7.89	175.55	63.92	4.03	68.75	4.15	C γ 22.38, H γ 1.16
Asn-8	121.56	8.12	176.11	54.58	4.60	38.56	2.79	N δ 112.8, H δ 7.43/6.71
Tyr-9	120.39	8.08	177.14	60.36	4.35	38.30	3.06	C δ 130.56, H δ 7.04, C ϵ 116.61, H ϵ , 6.76
Ala-10	121.38	8.18	178.53	54.96	4.05	18.43	1.48	
Thr-11	112.45	7.98	176.24	65.72	3.92	68.60	4.25	C γ 21.98, H γ 1.24
Glu-12	121.75	7.97	178.54	58.60	4.13	28.21	2.13	C γ 33.47, H γ 2.52/2.46
Ala-13	122.98	8.25	179.15	54.78	4.12	18.32	1.42	
Met-14	117.15	8.18	177.58	58.57	4.12	32.59	2.15	C γ 32.53, H γ 2.65/2.55

Table S4 (Cont'd) Backbone and side chain assignments for IKe coat protein in 400 mM MPG, pH4.5, 45°C

Residue	N	NH	CO	C α	H α	C β	H β	other
Asp-15	118.55	8.29	178.03	56.08	4.43	38.96	2.86/2.94	
Ser-16	116.28	8.02	176.16	61.51	4.34	63.24	3.98/4.06	
Leu-17	122.36	8.12	177.86	57.70	4.12	42.12	1.62/1.84	C γ *, H γ (2.11) , C δ 24.37, H δ 0.88
Lys-18	118.70	8.20	177.33	60.29	3.84	32.23	1.98	C γ 25.52, H γ 1.44, C δ *, H δ 1.59/1.74, C ϵ 41.74, H ϵ 2.94
Thr-19	113.75	7.84	177.45	66.09	3.89	68.91	4.28	C γ 21.75, H γ 1.24
Gln-20	120.33	8.06	177.95	58.47	4.11	28.78	2.12	C γ *, H γ 2.44, N δ 112.60, H δ 7.09/6.61
Ala-21	121.64	8.46	178.55	55.25	4.05	18.46	1.47	
Ile-22	117.25	8.11	*	64.54	3.67	37.34	1.98	C γ *, H γ (1.76) , C γ m 17.38, H γ m 0.96, C δ *, H δ *
Asp-23	*	*	(179.31)	(53.89)	4.42	(40.59)	2.96	
Leu-24	120.97	8.02	179.34	57.95	*	42.28	1.65	C γ *, H γ *, C δ *, H δ 0.91
Ile-25	119.41	8.33	177.29	64.47	3.85	38.06	2.03	C γ *, H γ 1.76, C γ m 17.90, H γ m 1.00, C δ *, H δ *
Ser 26	115.09	8.22	175.19	61.13	4.29	63.30	(4.05)	
Gln-27	118.04	7.63	176.62	56.73	4.32	29.60	2.10/2.19	C γ 33.92, H γ 2.46, N δ 110.2 , H δ 7.25/ 6.70

Table S4 (Cont'd) Backbone and side chain assignments for IKE coat protein in 400 mM MPG, pH4.5, 45°C

Residue	N	NH	CO	Cα	Hα	Cβ	Hβ	other
Thr-28	112.81	7.76	175.18	63.69	4.27	69.63	4.02	Cγ 21.89, Hγ 1.07
Trp-29	124.01	8.32	174.20	58.45	4.74	28.58	3.35	Hring 7.00/7.44/6.89 Nin 130.20, Hin 10.01
Pro-30			*	62.70	*	31.50	(1.92)	Cγ *, Hγ (2.07) , Cδ *, Hδ (3.25)
Val-31	116.78	7.60	176.63	63.85	3.96	32.00	2.24	Cγ 21.22, Hγ 0.98
Val-32	120.30	7.84	*	64.28	3.77	31.67	2.05	Cγ * , Hγ *
Thr-33	*	(8.06)	*	(65.69)	(3.95)	(73.21)	(5.24)	Cγ * , Hγ (1.27)
Thr-34	*	*	*	(65.52)	*	(68.70)	*	Cγ * , Hγ (1.22)
Val-35	119.62	7.71	178.62	65.28	3.80	31.95	2.35	Cγ * , Hγ 1.01
Val-36	121.32	7.69	177.78	65.62	3.85	31.75	2.18	Cγ 22.11, Hγ 1.05
Val-37	119.37	7.86	176.76	66.20	3.79	31.46	2.16	Cγ * , Hγ 0.94
Ala-38	121.59	8.32	178.86	55.45	3.94	18.27	1.45	
Gly-39	103.32	7.94	175.81	47.09	3.81			
Leu-40	122.62	7.73	178.05	57.88	4.14	42.07	1.92/1.71	Cγ 27.20, Hγ 1.75, Cδ * , Hδ 0.91

K-5157-M1c

Table S4 (Cont'd) Backbone and side chain assignments for IKe coat protein in 400 mM MPG, pH4.5, 45°C

Residue	N	NH	CO	C α	H α	C β	H β	other
Val-41	118.47	8.06	177.33	67.02	3.56	31.25	2.27	C γ 23.13, H γ 1.07/0.93
Ile-42	119.29	8.16	177.61	65.09	3.75	37.53	1.98	C γ *, H γ 1.74, C γ m 17.47, H γ m 0.98, C δ *, H δ 0.85
Arg-43	119.31	7.79	179.07	59.68	3.98	30.03	2.00/1.89	C γ 27.75, H γ 1.87/1.63, C δ 43.42, H δ 3.19, N1 *, HN1 7.35, N2 *, HN2 7.36, N3 *, HN3 6.75
Leu-44	120.31	8.14	178.00	57.80	4.08	41.76	1.93/1.64	C γ 26.75, H γ 1.81, C δ 24.18, H δ 0.90
Phe-45	119.38	8.55	178.19	61.46	4.24	39.00	3.32/3.22	Cring 128.99, Hring 7.18
Lys-46	119.47	8.45	178.35	59.15	3.95	32.11	1.91/1.96	C γ 26.50, H γ 1.54/1.78, C δ 29.3, H δ 1.72, C ϵ 42.00, H ϵ 2.98
Lys-47	119.70	7.77	177.95	58.48	4.02	32.10	1.72/1.82	C γ 24.73, H γ 1.08/1.26, C δ 28.92, H δ 1.57/1.48, C ϵ 41.77, H ϵ 2.85
Phe-48	116.53	7.84	176.12	59.34	4.50	39.67	3.20/2.90	Cring 129.50, Hring 7.25
Ser-49	113.88	7.90	174.64	59.46	4.25	63.56	3.59/3.78	
Ser-50	117.02	7.76	174.31	58.99	4.41	63.55	3.93	
Lys-51	122.13	7.89	175.74	56.03	4.33	32.75	1.88/1.78	C γ 24.65, H γ 1.46, C δ 28.90, H δ 1.68, C ϵ 42.15, H ϵ 2.99

K-5157-M12

Table S4 (Cont'd) Backbone and side chain assignments for IKe coat protein in 400 mM MPG, pH4.5, 45°C

Residue	N	NH	CO	C α	H α	C β	H β	other
Ala-52	124.63	7.96	176.37	52.38	4.36	19.35	1.36	
Val-53	120.77	7.50	179.34	62.46	4.10	33.06	2.11	C γ 1 20.02, H γ 1 0.89, C γ 2 21.51, H γ 2 0.91

^aTentative chemical shifts are indicated in parenthesis. ¹H and ¹³C chemical shifts are referenced relative to external TSP at 0 ppm, while ¹⁵N shifts are referenced relative to liquid ammonia at 0 ppm.

K-5157-M14