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Supplementary Table 1. Alignment tensor of ubiquitin-SH₆ as a function of pH.^a

pH	conc. ^c	α	β	γ	$10^4 A_{zz}$	$10^4 A_{yy}$	$10^4 A_{xx}$
4.65	5%	37.5	21.2	34.4	-6.20	3.76	2.44
6.18	4.8%	33.0	23.2	29.6	-7.48	4.88	2.60
6.75	4.6%	32.0	27.5	25.5	-7.26	4.77	2.49
7.50	5.0%	31.3	31.1	27.8	-10.86	7.02	3.84

^a Using bicelles in 93% H₂O, 7% D₂O, with a 30:10:1 ratio of DMPC:DHPC:CTAB, at 310 K.

The Euler angles α , β , and γ define the alignment tensor relative to the coordinate frame of the 1.8-Å X-ray structure.¹⁶

^b Molar ratios of lipids. M = [DMPC]; H = [DHPC]; C = [CTAB]; MA = [myristic acid].

^c Weight by volume for M+H+C in water.

Supplementary Table 2. Alignment tensor of aprotinin in charged bicelles.^a

M:H:C ^b	conc. ^c	α	β	γ	$10^4 A_{zz}$	$10^4 A_{yy}$	$10^4 A_{xx}$
30:10:0	5%	153.3	92.7	58.7	5.47	-0.93	-4.54
30:10:1	3.5%	154.6	86.0	77.1	1.92	-0.58	-1.33
30:10:2	4.5%	154.8	77.8	93.6	2.53	-0.51	-2.02

^a Using bicelles in 93% H₂O, 7% D₂O, at pH 6.75, 310 K. The Euler angles α , β , and γ define the alignment tensor relative to the coordinate frame of the crystal X-ray/neutron structure (Wlodawer, A.; Walter, J.; Huber, R.; Sjolin, L. *J. Mol. Biol.* **1984**, *180*, 301-329).

^b Molar ratios of lipids. M = [DMPC]; H = [DHPC]; C = [CTAB].

^c Weight by volume for M+H+C+MA in water.

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Supplementary Table 3. Angles of intersection for the two cones of N-H vector orientations compatible with the D_{NH} dipolar couplings measured in ubiquitin in liquid crystalline phases consisting of 3:1:0 and 30:10:1 ratios of DMPC:DHPC:CTAB. Only the angle for the intersection closest to the true N-H orientation is given.

Q2	1		
I3	-25		
F4	32		
V5	19		
K6	-3		
T7	-14		
L8	2		
G10	73		
K11	11	D58	-26
T12	-19	Y59	-21
I13	6	N60	-23
T14	-25	I61	-2
L15	29	Q62	-15
E16	-14	K63	-24
V17	-6	E64	-53
E18	1	S65	-8
S20	12	T66	45
D21	-13	L67	42
T22	63	H68	-51
I23	-83	L69	-43
N25	-9	V70	-55
V26	-2	L71	44
K27	-59		
A28	31		
K29	0		
I30	-84		
D32	-28		
K33	24		
E34	-64		
G35	-17		
I36	-3		
D39	-43		
Q40	-29		
Q41	14		
R42	83		
L43	29		
I44	72		
F45	21		
G47	-77		
K48	-9		
Q49	-9		
L50	-73		
E51	-4		
D52	-50		
R54	9		
T55	1		
L56	50		
S57	-27		

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Supplementary Table 4. Angles of intersection for the two cones of N-H vector orientations compatible with the D_{NH} dipolar couplings measured in aprotinin in liquid crystalline phases consisting of 3:1:0 and 15:5:1 ratios of DMPC:DHPC:CTAB. Only the angle for the intersection closest to the true N-H orientation is given.

Residue	Angle (°)
F4	16
C5	-3
L6	51
E7	47
Y10	61
G12	-34
C14	50
A16	-31
R17	-33
I18	25
I19	-13
R20	-80
Y21	24
F22	2
Y23	72
N24	5
A25	22
K26	25
A27	20
G28	15
L29	-32
C30	17
Q31	-37
T32	-47
F33	79
V34	-52
Y35	56
G36	-6
C38	13
A40	-30
K41	57
R42	17
N43	28
N44	7
F45	11
S47	-25
A48	18
E49	-8
D50	9
C51	-17
M52	5
R53	-1
T54	15
C55	18
G56	47