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Table SM1: Chemical Shifts (ppm from TSP) of peptide 4 in aqueous solution at 5°C and pH 4.3.

	NH	$C_\alpha H$	$C_\beta H$	other
Ile 1		3.85	1.94	$C_\gamma H$ 1.45, 1.16; $C_\gamma H_3$ 0.97; $C_\delta H_3$ 0.89
Tyr 2	8.80	4.67	2.97, 2.90	$C_\delta H$ 7.06, 7.06; $C_\varepsilon H$ 6.81, 6.81
Ser 3	8.36	4.44	3.68, 3.68	
Asn 4	8.54	4.67	2.84, 2.74	$N_\delta H_2$ 7.64, 7.02
Ser 5	8.48	4.41	3.92, 3.84	
Asp 6	8.29	4.65	2.78, 2.72	
Gly 7	8.25	3.91, 3.79		
Val 8	7.76	4.10	1.97	$C_\gamma H_3$ 0.82, 0.82
Trp 9	8.60	4.86	3.34, 3.15	$N_{\varepsilon 1}H$ 10.12; $C_{\delta 1}H$ 7.22; $C_{\varepsilon 3}H$ 7.54; $C_{\zeta 3}H$ 7.11; $C_{\eta 2}H$ 7.22; $C_{\zeta 2}H$ 7.47
Thr 10	7.95	4.19	4.16	$C_\gamma H_3$ 1.14

Table SM2: Chemical Shifts (ppm from TSP) of peptide 5 in aqueous solution at 5°C and pH 4.3.

	NH	$C_\alpha H$	$C_\beta H$	other
Ile 1		3.88	1.96	$C_\gamma H$ 1.47, 1.19; $C_\gamma H_3$ 0.98; $C_\delta H_3$ 0.90
Tyr 2	8.83	4.61	3.01, 2.90	$C_\delta H$ 7.06, 7.06; $C_\varepsilon H$ 6.79, 6.79
Ser 3	8.10	4.33	3.66, 3.60	
Ala 4	8.39	4.43	1.37	
Pro 5		4.36	2.29, 1.91	$C_\gamma H$ 2.03, 2.03; $C_\delta H$ 3.82, 3.67
Asp 6	8.41	4.61	2.80, 2.75	
Gly 7	8.36	3.96, 3.88		
Thr 8	7.97	4.30	4.12	$C_\gamma H_3$ 1.10
Trp 9	8.37	4.86	3.38, 3.25	$N_{\varepsilon 1}H$ 10.14; $C_{\delta 1}H$ 7.25; $C_{\varepsilon 3}H$ 7.63; $C_{\zeta 3}H$ 7.14; $C_{\eta 2}H$ 7.23; $C_{\zeta 2}H$ 7.48
Thr 10	7.92	4.20	4.20	$C_\gamma H_3$ 1.13

Table SM3: Chemical Shifts (ppm from TSP) of peptide 6 in aqueous solution at 5°C and pH 4.3.

	NH	$C_\alpha H$	$C_\beta H$	other
Ile 1		3.87	1.97	$C_\gamma H$ 1.47, 1.21; $C_\gamma H_3$ 0.99; $C_\delta H_3$ 0.93
Tyr 2	8.82	4.56	2.92, 2.86	$C_\delta H$ 6.99, 6.99; $C_\varepsilon H$ 6.77, 6.77
Ser 3	8.13	4.35	3.71, 3.71	
Ala 4	8.45	4.17	1.40	
Lys 5	8.29	4.23	1.78, 1.72	$C_\gamma H$ 1.41, 1.41; $C_\delta H$ 1.63, 1.63; $C_\varepsilon H$ 2.94, 2.94; $N_\zeta H$ 7.55
Ala 6	8.32	4.31	1.40	
Gly 7	8.42	3.93, 3.87		
Thr 8	7.84	4.36	4.14	$C_\gamma H_3$ 1.10
Trp 9	8.38	4.85	3.41, 3.25	$N_{\varepsilon 1}H$ 10.16; $C_{\delta 1}H$ 7.26; $C_{\varepsilon 3}H$ 7.66; $C_{\zeta 3}H$ 7.16; $C_{\eta 2}H$ 7.24; $C_{\zeta 2}H$ 7.48
Thr 10	7.87	4.23	4.18	$C_\gamma H_3$ 1.14

Table SM4: Chemical Shifts (ppm from TSP) of peptide 7 in aqueous solution at 5°C and pH 4.3.

	NH	$C_\alpha H$	$C_\beta H$	other
Ile 1		3.89	1.95	$C_\gamma H$ 1.48, 1.20; $C_\gamma H_3$ 0.98; $C_\delta H_3$ 0.91
Tyr 2	8.80	4.75	2.91, 2.85	$C_\delta H$ 7.04, 7.04; $C_\varepsilon H$ 6.76, 6.76
Ser 3	8.44	4.68	3.70, 3.70	
Tyr 4	8.56	4.48	2.84, 2.74	$C_\delta H$ 6.95, 6.95; $C_\varepsilon H$ 6.76, 6.76
Asn 5	8.49	4.56	2.81, 2.68	$N_\delta H$ 7.62, 6.92
Gly 6	7.50	4.00, 3.66		
Lys 7	8.00	4.38	1.68, 1.68	$C_\gamma H$ 1.23, 1.23; $C_\delta H$ 1.58, 1.58; $C_\varepsilon H$ 2.81, 2.81; $N_\zeta H$ 7.50
Thr 8	8.26	4.57	4.16	$C_\gamma H_3$ 1.15
Trp 9	8.49	4.88	3.30, 3.10	$N_{\varepsilon 1}H$ 10.13; $C_{\delta 1}H$ 7.23; $C_{\varepsilon 3}H$ 7.52; $C_{\zeta 3}H$ 7.12; $C_{\eta 2}H$ 7.20; $C_{\zeta 2}H$ 7.40
Thr 10	8.08	4.22	4.22	$C_\gamma H_3$ 1.16

Table SM5. Medium and long-range NOE connectivities observed for peptide 4 in aqueous solution (pH 4.3, 5 °C).

^{1}H resonance in		[a]NOE intensity
Residue i	Residue j	
C_γ'H Ile1	NH Ser3	vw
$C_\gamma H_3$ Ile1	NH Ser3	vw
$C_\delta H_3$ Ile1	NH Ser3	vw
C_γH3 Ile1	$C_{\beta\beta}$'H Ser3	vw
C_δH3 Ile1	$C_{\beta\beta}$'H Ser3	vw
C_βH Ile1	$C_{\varepsilon 3}$H Trp9	vw
C_γ'H Ile1	$C_{\varepsilon 3}$H Trp9	vw
C_γH Ile1	$C_{\varepsilon 3}$H Trp9	vw
$C_\gamma H_3$ Ile1	$C_{\varepsilon 3}$H Trp9	vw
$C_\delta H_3$ Ile1	$C_{\varepsilon 3}$H Trp9	vw
C_εH Tyr2	$N_{\delta 1}$H Asn4	vw
C_αH Tyr2[b]	$C_{\varepsilon 3}$H Trp9	w
C_αH Tyr2[b]	$C_{\zeta 3}$H Trp9	w
C_αH Tyr2[b]	C_αH Trp9	m
C_εH Tyr2	$C_{\varepsilon 3}$H Trp9	vw
C_εH Tyr2	C_βH Trp9	w
$C_{\beta\beta}$'H Ser3	NH Ser5	w
$C_{\beta\beta}$'H Ser3	C_βH Asp6	w
$C_{\beta\beta}$'H Ser3	NH Gly7	vw
$C_{\beta\beta}$'H Ser3	NH Val8	vw
C_αH Ser3	C_αH Val8	vw
$C_{\beta\beta}$'H Ser3	C_γH Val8	vw
C_αH Ser3	C_αH Trp9	w-m
$N_{\delta 1}$H Asn4	C_βH Val8	w
C_αH Ser5	NH Gly7	w
NH Asp6	NH Val8	vw
C_βH Asp6	C_γH Val8	w
C_βH Val8	NH Thr10	vw
C_γH Val8	NH Thr10	w
C_γH Val8	C_αH/C_βH Thr10	w

[a]NOE intensities are classified as strong, s; medium, m; intermediate between weak and medium, w-m; weak, w; and very weak, vw.

[b]NOEs involving C_αH Tyr2 are not unambiguous due to the coincidence of its chemical shift with that of C_αH Asn4. The assignment to C_αH Tyr2 is based on the presence of equivalent NOEs which could be unambiguously assigned to C_αH Tyr2 in peptide 3.[8]

Table SM6. Medium and long-range NOE connectivities observed for peptide 5 in aqueous solution (pH 4.3, 5 °C).

^{1}H resonance in		[a]NOE Intensity
Residue i	Residue j	
C_βH Ile1	NH Ser3	vw
C_γ'H Ile1	NH Ser3	w
C_γH3 Ile1	NH Ser3	vw
C_δH3 Ile1	NH Ser3	w
C_γH3 Ile1	C_αH Ser3	w
C_βH Ile1	$C_{\varepsilon 3}$H Trp9	vw
C_γ'H Ile1	$C_{\varepsilon 3}$H Trp9	vw
C_γH3 Ile1	$C_{\varepsilon 3}$H Trp9	w
C_δH3 Ile1	$C_{\varepsilon 3}$H Trp9	w
C_βH Tyr2	NH Ala4	w
C_δH Tyr2	C_αH Ala4	w
C_δH Tyr2	C_βH Ala4	w
C_δH Tyr2	NH Ala4	w
C_εH Tyr2	C_αH Ala4	s
C_εH Tyr2	C_βH Ala4	s
C_εH Tyr2	NH Ala4	w
C_εH Tyr2	C_δ'H Pro5	m
C_δH Tyr2	C_αH Trp9	vw
C_εH Tyr2	$C_{\varepsilon 3}$H Trp9	w
C_αH Tyr2	C_αH Trp9	w-m
C_δH Tyr2	C_γH Thr10	vw
C_εH Tyr2	C_γH Thr10	w
NH Tyr2	NH Thr10	w
$C_{\beta\beta'}$H Ser3	$C_{\beta\beta'}$H Asp6	w
C_αH Ser3	C_αH Trp9	w-m
C_αH Ser3	C_β'H Trp9	w
C_βH Ala4	NH Gly7	w
C_βH Ala4	C_βH Thr8	m
C_βH Ala4	NH Thr8	w
C_βH Ala4	$C_{\zeta 2}$H Trp9	w
C_βH Pro5	NH Gly7	w
C_δH Pro5	C_γH Thr8	w
C_αH Asp6	NH Thr8	w
$C_{\beta\beta'}$H Asp6	NH Thr8	w
$C_{\beta\beta'}$H Asp6	C_γH Thr8	w

Table SM6. cont.

$C_{\alpha\alpha'}H$ Gly7	$C_{\zeta 2}H$ Trp9	w

[a]NOE intensities are classified as strong, s; medium, m; intermediate between weak and medium, w-m; weak, w; and very weak, vw.

Table SM7. Medium and long-range NOE connectivities observed for peptide 6 in aqueous solution (pH 4.3, 5 °C).

^{1}H resonance in		[a]NOE Intensity
Residue i	Residue j	
C_αH Ile1	NH Ser3	vw
C_γH3 Ile1	NH Ser3	vw
C_γH3 Ile1	$C_{\beta\beta'}$H Ser3	w
C_δH3 Ile1	$C_{\beta\beta'}$H Ser3	vw
C_γH3 Ile1	NH Ala4	vw
C_αH Ile1	$C_{\varepsilon 3}$H Trp9	vw
C_δH Tyr2	C_αH Ala4	w
C_δH Tyr2	NH Ala4	w
C_εH Tyr2	C_αH Ala4	m
C_εH Tyr2	NH Ala4	w
C_εH Tyr2	$C_{\alpha\alpha'}$H Gly7	w
C_δH Tyr2	C_αH Trp9	vw
C_δH Tyr2	$C_{\varepsilon 3}$H Trp9	w
C_δH Tyr2	$C_{\varepsilon 1}$H Trp9	vw
C_δH Tyr2	$C_{\zeta 2}$H Trp9	w
C_εH Tyr2	$C_{\zeta 2}$H Trp9	w
C_εH Tyr2	$C_{\varepsilon 3}$H Trp9	w
C_αH Tyr2	C_αH Trp9	m
C_αH Tyr2	$C_{\varepsilon 3}$H Trp9	vw
$C_{\beta\beta'}$H Ser3	NH Lys5	w
$C_{\beta\beta'}$H Ser3	NH Ala6	w
$C_{\beta\beta'}$H Ser3	NH Gly7	vw
$C_{\beta\beta'}$H Ser3	NH Thr8	w
NH Ser3	NH Thr8	w-m
C_αH Lys5	NH Gly7	vw
$C_{\delta\delta'}$H Lys5	$C_{\varepsilon 3}$H Trp9	vw
$C_{\varepsilon\varepsilon'}$H Lys5	$C_{\zeta 2}$H Trp9	vw
$C_{\alpha\alpha'}$H Gly7	$C_{\zeta 3}$H Trp9	w

[a]NOE intensities are classified as strong, s; medium, m; intermediate between weak and medium, w-m; weak, w; and very weak, vw.

Table SM8. Medium and long-range NOE connectivities observed for peptide 7 in aqueous solution indicating in which of the two β-hairpin 2:2 structures they are satisfied.

^{1}H resonance in		β-hairpin 2:2	
Residue i	Residue j	type I' turn	type II' turn
C_βH Ile1	NH Ser 3	yes	yes
C_βH Ile1	$C_{\beta\beta'}$H Ser 3	yes	yes
C_γH Ile1	NH Ser 3	yes	yes
C_γH Ile1	$C_{\beta\beta'}$H Ser 3	yes	yes
$C_\gamma H_3$ Ile1	NH Ser 3	yes	yes
$C_\gamma H_3$ Ile1	C_αH Ser 3	yes	yes
$C_\gamma H_3$ Ile1	$C_{\beta\beta'}$H Ser 3	yes	yes
$C_\delta H_3$ Ile1	NH Ser 3	yes	yes
$C_\delta H_3$ Ile1	C_αH Ser 3	yes	yes
$C_\delta H_3$ Ile1	$C_{\beta\beta'}$H Ser 3	yes	yes
$C_\gamma H_3$ Ile1	NH Tyr4	yes	yes
$C_\delta H_3$ Ile1	NH Tyr4	yes	yes
C_βH Ile1	C_βH Thr8	yes	no
C_γH Ile1	C_βH Thr8	yes	no
$C_\gamma H_3$ Ile1	C_αH Thr8	yes	no
$C_\gamma H_3$ Ile1	C_βH Thr8	yes	no
$C_\delta H_3$ Ile1	C_αH Thr8	yes	no
$C_\delta H_3$ Ile1	C_βH Thr8	yes	no
C_αH Ile1	$C_{\varepsilon 3}$H Trp9	no	yes
C_αH Ile1	$C_{\zeta 3}$H Trp9	no	yes
C_αH Ile1	$C_{\eta 2}$H Trp9	no	yes
C_βH Ile1	NH Trp9	no	yes
C_βH Ile1	$C_{\varepsilon 3}$H Trp9	no	yes
$C_\gamma H_3$ Ile1	NH Trp9	no	yes
$C_\gamma H_3$ Ile1	$C_{\delta 1}$H Trp9	no	yes
$C_\gamma H_3$ Ile1	$C_{\varepsilon 3}$H Trp9	no	yes
$C_\gamma H_3$ Ile1	$C_{\zeta 2}$H Trp9	no	yes
$C_\gamma H_3$ Ile1	$C_{\zeta 3}$H Trp9	no	yes
$C_\gamma H_3$ Ile1	$C_{\eta 2}$H Trp9	no	yes
$C_\delta H_3$ Ile1	NH Trp9	no	yes
$C_\gamma H_3$ Ile1	$C_{\delta 1}$H Trp9	no	yes
$C_\delta H_3$ Ile1	$C_{\varepsilon 3}$H Trp9	no	yes
$C_\delta H_3$ Ile1	$C_{\zeta 2}$H Trp9	no	yes
$C_\delta H_3$ Ile1	$C_{\zeta 3}$H Trp9	no	yes

Table SM8. cont.

$C_{\delta}H_3$ Ile1	$C_{\eta 2}H$ Trp9	no	yes
$C_{\alpha}H$ Ile1	$C_{\alpha}H$ Thr10	yes	no
$C_{\beta}H$ Ile1	$C_{\alpha}H$ Thr10	yes	no
$C_{\gamma}H$ Ile1	$C_{\alpha}H$ Thr10	yes	no
$C_{\gamma}H_3$ Ile1	NH Thr10	yes	no
$C_{\gamma}H_3$ Ile1	$C_{\alpha}H$ Thr10	yes	no
$C_{\delta}H_3$ Ile1	$C_{\alpha}H$ Thr10	yes	no
$C_{\delta}H$ Tyr2	NH Tyr4	yes	yes
$C_{\delta}H$ Tyr2	$C_{\alpha}H$ Tyr4	yes	yes
$C_{\delta}H$ Tyr2	$C_{\beta}H$ Tyr4	yes	yes
$C_{\delta}H$ Tyr2	$C_{\beta\beta'}H$ Lys7	yes	no
$C_{\delta}H$ Tyr2	$C_{\gamma\gamma'}H$ Lys7	yes	no
$C_{\delta}H$ Tyr2	$C_{\delta\delta'}H$ Lys7	yes	no
NH Tyr2	NH Trp9	yes	no
NH Tyr2	$C_{\beta 3}H$ Trp9	yes	no
$C_{\alpha}H$ Tyr2	$C_{\varepsilon 3}H$ Trp9	yes	no
$C_{\beta 2}H$ Tyr2	$C_{\beta 2}H$ Trp9	yes	no
$C_{\beta 2}H$ Tyr2	$C_{\varepsilon 3}H$ Trp9	yes	no
$C_{\beta 2}H$ Tyr2	$C_{\zeta 2}H$ Trp9	yes	no
$C_{\beta 3}H$ Tyr2	$C_{\varepsilon 3}H$ Trp9	yes	no
$C_{\delta}H$ Tyr2	$C_{\alpha}H$ Trp9	yes	no
$C_{\delta}H$ Tyr2	$C_{\beta 2}H$ Trp9	yes	no
$C_{\delta}H$ Tyr2	$C_{\beta 3}H$ Trp9	yes	no
$C_{\delta}H$ Tyr2	$C_{\varepsilon 1}H$ Trp9	yes	no
$C_{\beta 2}H$ Tyr2	NH Thr10	yes	yes
$C_{\delta}H$ Tyr2	$C_{\alpha}H$ Thr10	yes	yes
$C_{\alpha}H$ Ser3	$C_{\alpha}H$ Thr8	yes	no
$C_{\beta\beta'}H$ Ser3	NH Thr8	yes	no
$C_{\beta\beta'}H$ Ser3	$C_{\alpha}H$ Thr8	yes	no
$C_{\beta\beta'}H$ Ser3	$C_{\gamma}H_3$ Thr8	yes	no
$C_{\alpha}H$ Ser3	NH Trp9	yes	no
$C_{\alpha}H$ Ser3	$C_{\delta 1}H$ Trp9	yes	no
$C_{\alpha}H$ Ser3	$C_{\varepsilon 3}H$ Trp9	yes	no
$C_{\alpha}H$ Ser3	$C_{\zeta 3}H$ Trp9	yes	no
$C_{\alpha}H$ Ser3	$C_{\eta 2}H$ Trp9	yes	no
$C_{\beta\beta'}H$ Ser3	$C_{\zeta 3}H$ Trp9	yes	no
$C_{\beta\beta'}H$ Ser3	$C_{\eta 2}H$ Trp9	yes	no

Table SM8. cont.

NH Ser3	NH Thr10	no	yes
NH Tyr4	NH Lys7	yes	no
NH Tyr4	$C_{\beta\beta'}$H Lys7	yes	no
C_{α}H Tyr4	NH Lys7	yes	no
NH Tyr4	$C_{\delta 1}$H Trp9	no	yes
NH Tyr4	$C_{\varepsilon 1}$H Trp9	no	yes
NH Tyr4	$C_{\zeta 3}$H Trp9	no	yes
C_{α}H Tyr4	C_{α}H Trp9	no	yes
C_{α}H Tyr4	$C_{\varepsilon 3}$H Trp9	no	yes
$C_{\beta 2}$H Tyr4	$C_{\delta 1}$H Trp9	no	yes
$C_{\beta 2}$H Tyr4	$C_{\zeta 3}$H Trp9	no	yes
$C_{\beta 2}$H Tyr4	$C_{\eta 2}$H Trp9	no	yes
$C_{\beta 3}$H Tyr4	$C_{\eta 2}$H Trp9	no	yes
C_{δ}H Tyr4	$C_{\varepsilon 1}$H Trp9	no	yes
NH Asn5	NH Lys7	yes	no
C_{α}H Asn5	NH Lys7	yes	no
$C_{\beta 2}$H Asn5	NH Lys7	yes	yes
$C_{\beta 3}$H Asn5	NH Lys7	yes	yes
$N_{\delta 1}$H Asn5	$C_{\gamma\gamma'}$H Lys7	yes	yes
$N_{\delta 1}$H Asn5	$C_{\delta\delta'}$H Lys7	yes	yes
NH Asn5	NH Thr8	no	yes
$N_{\delta 2}$H Asn5	NH Thr8	no	yes
NH Lys7	$C_{\varepsilon 1}$H Trp9	yes	no
C_{α}H Lys7	$C_{\delta 1}$H Trp9	yes	yes
C_{α}H Lys7	$C_{\varepsilon 3}$H Trp9	yes	yes
C_{α}H Lys7	$C_{\zeta 2}$H Trp9	yes	yes
C_{α}H Lys7	$C_{\zeta 3}$H Trp9	yes	yes
C_{α}H Lys7	$C_{\eta 2}$H Trp9	yes	yes
$C_{\beta\beta'}$H Lys7	NH Trp9	yes	yes
$C_{\beta\beta'}$H Lys7	$C_{\delta 1}$H Trp9	yes	no
$C_{\beta\beta'}$H Lys7	$C_{\zeta 2}$H Trp9	yes	yes
$C_{\beta\beta'}$H Lys7	$C_{\zeta 3}$H Trp9	yes	yes
$C_{\beta\beta'}$H Lys7	$C_{\eta 2}$H Trp9	yes	yes
$C_{\gamma\gamma'}$H Lys7	NH Trp9	yes	yes
$C_{\gamma\gamma'}$H Lys7	$C_{\delta 1}$H Trp9	yes	yes
$C_{\gamma\gamma'}$H Lys7	$C_{\zeta 2}$H Trp9	yes	yes
$C_{\gamma\gamma'}$H Lys7	$C_{\zeta 3}$H Trp9	yes	yes

Table SM8 .cont.

$C_{\gamma\gamma'}H$ Lys7	$C_{\eta 2}H$ Trp9	yes	yes
$C_{\delta\delta'}H$ Lys7	$C_{\delta 1}H$ Trp9	yes	yes
$C_{\delta\delta'}H$ Lys7	$C_{\zeta 2}H$ Trp9	yes	yes
$C_{\delta\delta'}H$ Lys7	$C_{\zeta 3}H$ Trp9	yes	yes
$C_{\delta\delta'}H$ Lys7	$C_{\eta 2}H$ Trp9	yes	yes