Supporting Material for:

Segmental polymorphism in a functional amyloid

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Contains Figs. S1-S4 and Tables S1-S6

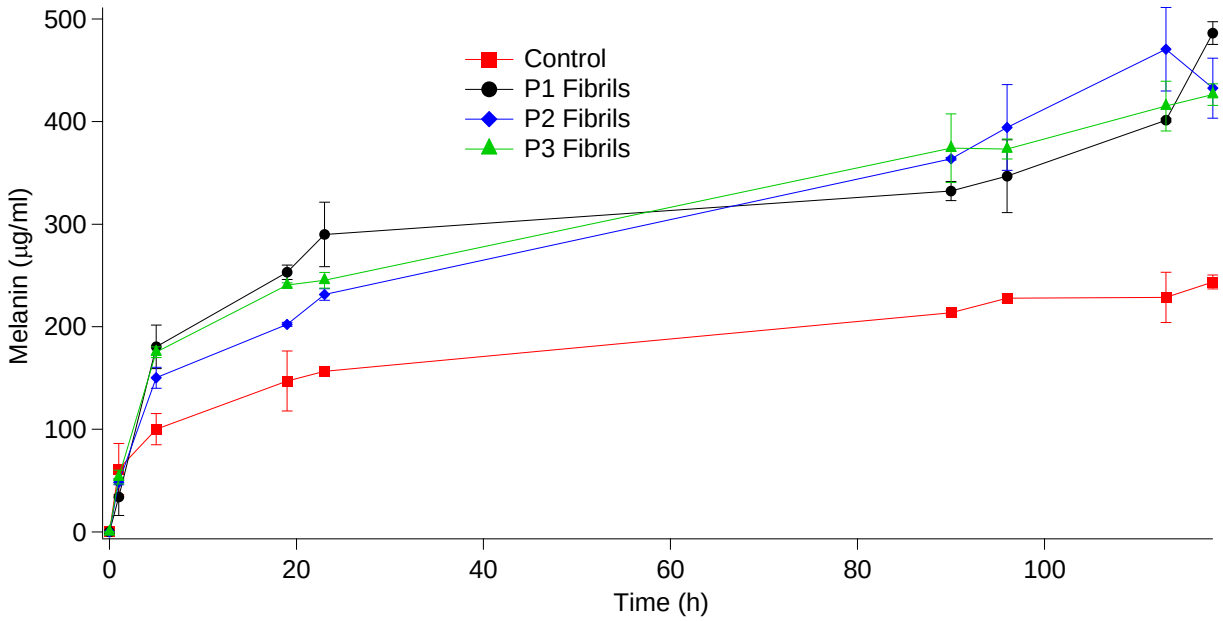

Figure S1: Acceleration of melanin synthesis by Pmel17:RPT fibrils. A time course of melanin synthesis *in vitro* shows that P1, P2 and P3 fibrils enhance the rate of melanin formation when compared with no fibrils (control). Assays followed the protocol described by McGlinchey *et al*. (Proc. Natl. Acad. Sci. U. S. A., vol.106, pp. 13731-13736, year 2009). Briefly, P1, P2 or P3 fibrils (9.0 µM) were added to 5 mM DL-DOPA in 0.20 mL of 20 mM K acetate buffer, 100 mM NaCl, pH 5.0. Tyrosinase (2 µg) was added to initiate the reactions, followed by incubation at 37^{o} C with agitation (600 rpm). Reactions were stopped by centrifugation, and pellets containing the melanin product were resuspended in 1 M NaOH and heated at 60° C for 5 min. Absorbance at 400 nm was used to measure melanin concentration. Synthetic melanin was used to calibrate the absorbance. P1, P2, and P3 fibrils in these assays were aliquots of the samples used for solid state NMR measurements.

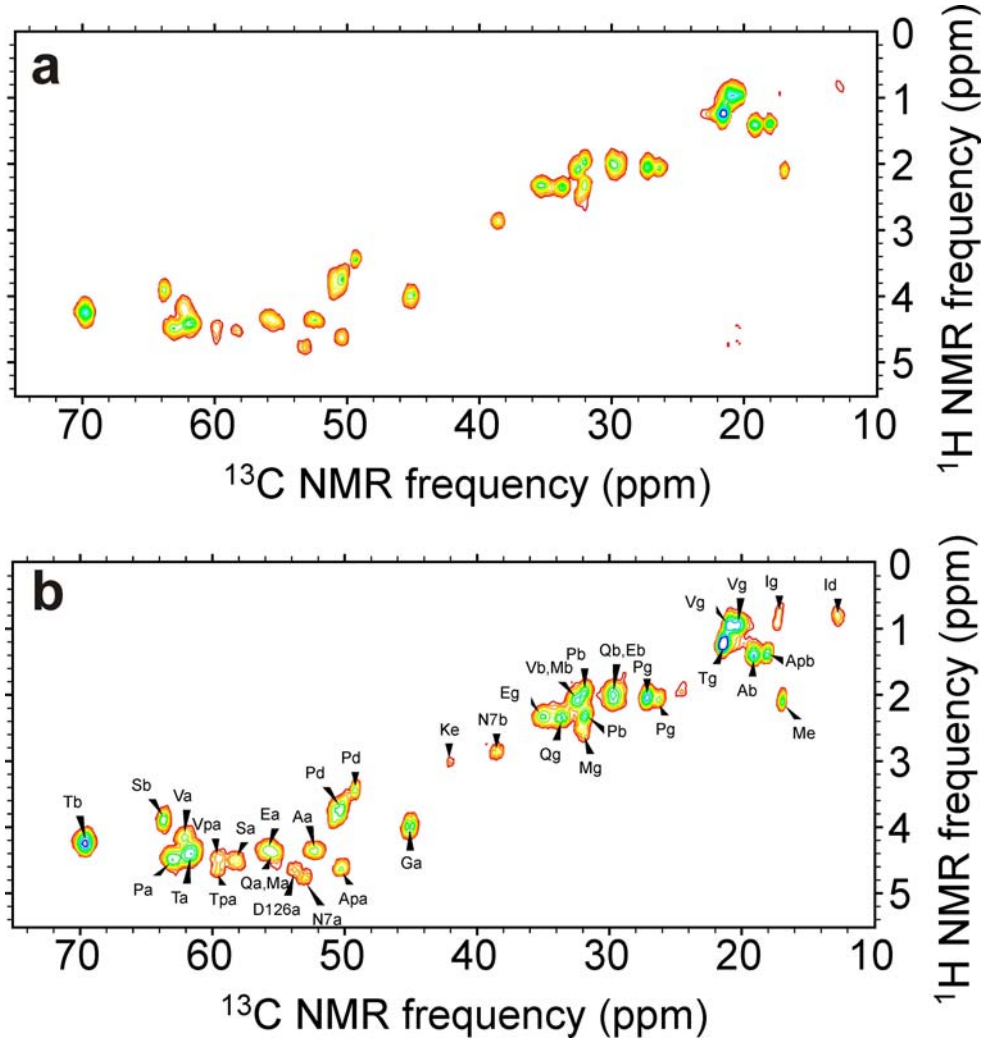

Figure S2: 2D ^{1}H-^{13}C INEPT spectra of Pmel17:RPT fibrils. Spectra for P1 (a) and P2 (b) fibrils are shown, in which signals arise from a subset of residues outside the fibril core that are highly mobile. Residue-type assignments are based on random coil chemical shifts for various residues types, and are therefore the same in both spectra. Unique assignments for N7 and D126 are possible because the Pmel17:RPT sequence contains single Asn and Asp residues. Residues that precede a Pro are indicated by "p"; "a", "b", "g", "d", and "e" indicate signals from α-, β-, γ-, δ-, and ε-carbons.

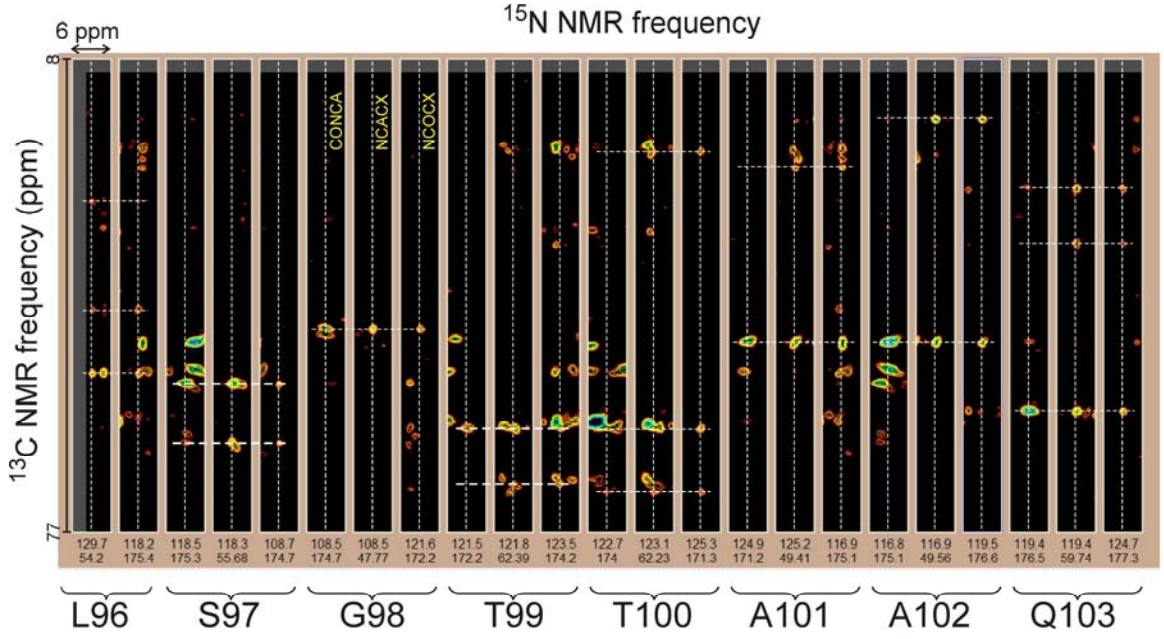

Figure S3: Representative regions of 2D ^{15}N-^{13}C planes from 3D CONCA, NCACX, and NCOCX spectra of P2 fibrils. These regions display the sequential connections among chemical shifts for residues 96-103. For each residue k, regions that contain signals at the $^{13}C_\alpha$ chemical shift of residue k are shown. The CONCA region contains signals at the ^{13}CO chemical shift of residue k-1 (t_1 dimension, not shown), the ^{15}N chemical shift of residue k (t_2 dimension), and the $^{13}C_\alpha$ chemical shift of residue k (t_3 dimension); the NCACX region contains signals at the backbone ^{15}N chemical shift of residue k (t_1 dimension), the $^{13}C_\alpha$ chemical shift of residue k (t_2 dimension, not shown), and the backbone ^{13}CO, $^{13}C_\alpha$. and sidechain ^{13}C chemical shifts of residue k (t_3 dimension); the NCOCX region contains signals at the backbone ^{15}N chemical shift of residue k+1 (t_1 dimension), the backbone ^{13}CO chemical shift of residue k (t_2 dimension, not shown), and the backbone ^{13}CO, $^{13}C_\alpha$. and sidechain ^{13}C chemical shifts of residue k (t_3 dimension). Assignments for residues 86-111 were determined unambiguously by the Monte Carlo/simulated annealing algorithm in the program MCASSIGN2.

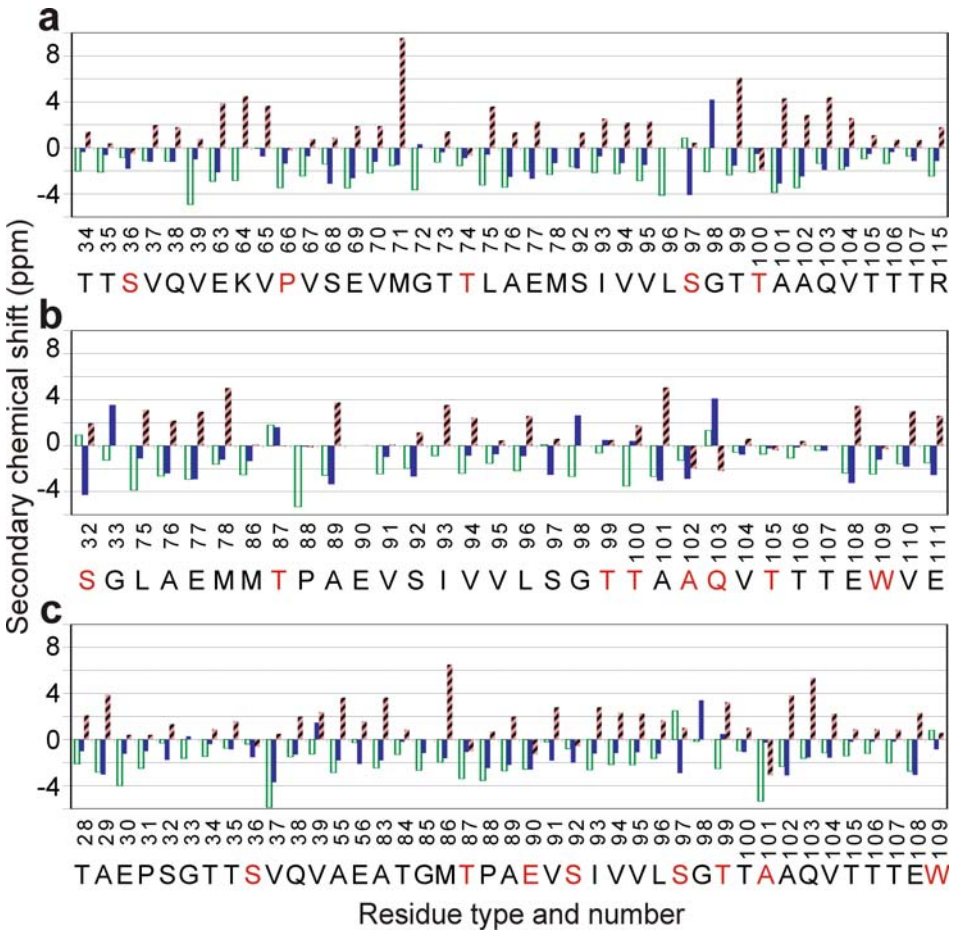

Figure S4: Secondary chemical shifts in Pmel17:RPT fibrils. Secondary shifts (*i.e.*, differences between experimentally determined ^{13}C shifts and random coil values) are shown for the unambiguously assigned residues of P1 (a), P2 (b) and P3 (c) fibrils. Results are shown for backbone ^{13}CO (open bars), $^{13}C_{\alpha}$ (solid bars), and $^{13}C_{\beta}$ (striped bars) sites. Red lettering indicates residues with secondary shifts that indicate non-β-strand conformations. Note that secondary chemical shifts for Gly residues do not correlate with secondary structure, so conclusions can not be drawn for Gly residues.

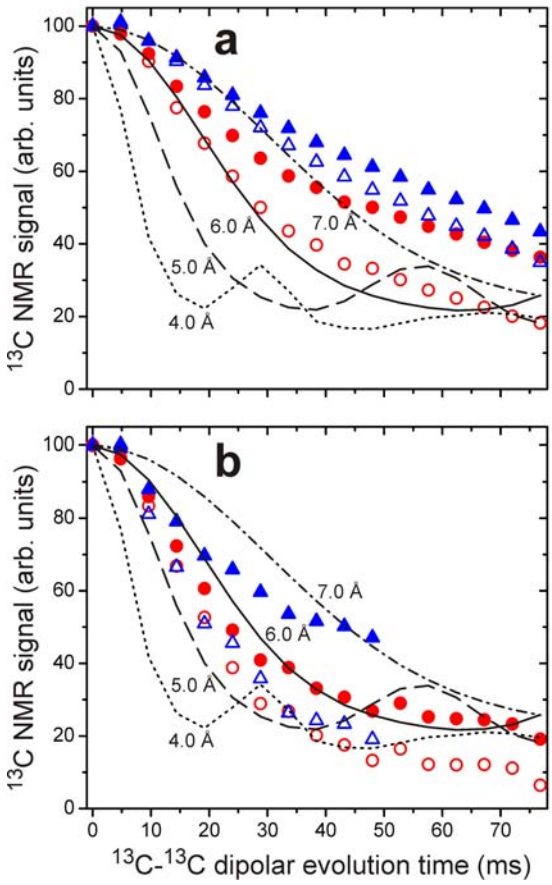

Figure S5: Measurements of ^{13}C-^{13}C dipole-dipole couplings in Pmel17:RPT fibrils. The fibrils were ^{13}C-labeled only at backbone carbonyl sites of all Met (triangles) or all Leu (circles) residues. Measurements were performed on lyophilized fibrils (a) and on fibrils that were rehydrated by addition of H_2O to the lyophilized samples within the MAS rotors (b). Solid symbols are the raw experimental data, with signal amplitudes at zero dipolar evolution time normalized to 100. Curves are ideal numerical simulations for linear chains of dipole-coupled ^{13}C nuclei with the indicated spacings. Hollow symbols are the experimental data after subtraction of signal contributions from natural-abundance ^{13}C nuclei at carbonyl and carboxyl sites. Natural-abundance contributions are assumed to decay linearly to 70% of their initial values over the full 76.8 ms evolution time, as indicated by measurements on unlabeled samples. In the lyophilized samples, natural-abundance signals for Met-labeled and Leu-labeled samples are taken to be 24% and 35% of the total ^{13}C NMR signals, respectively, calculated from the 1.1% natural-abundance level and the numbers of labeled and unlabeled carbonyl and carboxyl sites in Pmel17:RPT. In the rehydrated samples, natural-abundance signals for Met-labeled and Leu-labeled samples are taken to be 45% and 20%, respectively, adjusted to cancel experimental signal components that apparently decay slowly in the PITHIRDS-CT data. In the lyophilized state, it is reasonable to assume that all carbonyl and carboxyl sites contribute to the data, regardless of whether these sites are in the cross-β structure of the fibrils. In the rehydrated state, it is reasonable to assume that only sites in the cross-β structure contribute to the data. The observation that the major fraction of the signal from rehydrated fibrils decays on the 30 ms time scale characteristic of 5 Å ^{13}C-^{13}C distances is consistent with a parallel β-sheet structure in Pmel17:RPT fibrils.

Table S1: Signals from 3D solid state NMR spectra of P1 fibrils, used as input for MCASSIGN2. Each row is one multidimensional signal. Columns are chemical shifts (in ppm) of backbone amide nitrogens, α-carbons, carbonyl carbons, β-carbons, and γ-carbons, uncertainties in the chemical shifts, signal degeneracies, and possible residue-type assignments. Absent values are indicated by #.

NCACX spectrum

ν(N)	ν(Ca)	ν(C)	ν(Cb)	ν(Cg)	δ(N)	δ(Ca)	δ(C)	δ(Cb)	δ(Cg)	deg.	type
113.4	56.4	173.7	#	#	0.4	0.2	0.3	#	#	1	K
114.0	59.0	174.7	#	#	0.3	0.2	0.3	#	#	1	V
118.5	54.0	174.6	42.7	#	0.3	0.2	0.3	0.3	#	1	M
104.0	45.4	171.3	#	#	0.4	0.2	0.3	#	#	1	G
113.8	61.5	173.4	71.3	21.0	0.3	0.2	0.3	0.3	0.3	1	T
117.3	61.1	173.1	69.2	#	0.3	0.2	0.3	0.2	#	1	T
122.2	54.5	174.4	46.0	#	0.3	0.2	0.3	0.2	#	1	L
121.3	49.9	174.3	20.4	#	0.3	0.2	0.3	0.2	#	1	A
118.0	54.1	174.6	32.2	#	0.3	0.2	0.3	0.2	#	1	E
118.1	61.4	172.8	67.8	#	0.3	0.2	0.3	0.3	#	1	T
124.7	49.5	173.9	23.3	#	0.3	0.2	0.3	0.2	#	1	A
120.3	50.1	174.3	22.0	#	0.3	0.2	0.3	0.2	#	1	A
122.1	54.9	174.0	#	#	0.3	0.2	0.3	#	#	1	R
121.5	60.3	174.2	41.5	#	0.3	0.2	0.3	0.3	#	1	I
124.3	56.5	174.0	63.3	#	0.4	0.3	0.4	0.2	#	1	S
121.5	54.2	173.6	32.6	#	0.3	0.2	0.3	0.4	#	1	QE
118.1	61.4	172.6	71.2	#	0.3	0.2	0.3	0.6	#	1	T
123.0	53.9	174.0	#	#	0.3	0.4	0.3	#	#	1	M
122.0	61.6	173.7	#	#	0.3	0.2	0.3	#	#	1	V
120.0	56.6	173.0	65.1	#	0.3	0.2	0.3	0.2	#	1	S
114.4	54.3	175.6	64.2	#	0.3	0.2	0.3	0.2	#	1	S
111.5	60.3	174.3	36.3	21.9	0.4	0.3	0.4	0.6	0.4	1	V
117.0	55.2	173.3	64.9	#	0.3	0.2	0.3	0.4	#	1	S
122.3	60.7	173.5	35.2	22.1	0.4	0.3	0.4	0.4	0.4	1	V
120.4	53.8	174.7	33.8	#	0.3	0.2	0.3	0.3	#	1	QEMKR
121.8	61.4	173.8	70.8	#	0.3	0.2	0.3	0.3	#	1	T
121.8	61.4	173.5	70.5	#	0.4	0.3	0.4	0.2	#	1	T
118.8	54.5	174.7	#	#	0.4	0.3	0.4	#	#	1	QE
122.0	53.8	174.5	32.1	#	0.3	0.2	0.3	0.3	#	1	QEKRMW
121.5	54.6	173.6	33.9	#	0.4	0.3	0.4	0.4	#	1	QEKRMW
118.0	49.3	172.8	#	#	0.3	0.2	0.3	#	#	1	AG
107.6	60.2	172.3	76.0	#	0.3	0.2	0.3	0.3	#	1	T
121.4	60.5	174.4	35.5	20.5	0.4	0.3	0.4	0.2	0.4	1	V
125.2	60.9	174.1	35.0	20.8	0.3	0.2	0.3	0.2	0.4	1	V
124.4	61.2	174.0	35.0	22.0	0.4	0.2	0.3	0.2	0.4	1	V
123.5	54.0	173.0	31.8	#	0.6	0.2	0.3	0.3	#	1	E
118.6	58.8	170.0	33.4	#	0.3	0.2	0.3	0.5	#	1	V
122.9	53.9	175.1	#	#	0.3	0.2	0.3	#	#	1	M
121.4	59.5	174.6	36.5	20.8	0.4	0.5	0.4	0.3	0.3	1	V

NCOCX spectrum

ν(N)	ν(Ca)	ν(C)	ν(Cb)	ν(Cg)	δ(N)	δ(Ca)	δ(C)	δ(Cb)	δ(Cg)	deg.	type
113.7	56.2	173.9	#	#	0.3	0.2	0.3	#	#	1	K
103.6	54.0	174.8	42.2	#	0.5	0.2	0.3	0.4	#	1	M
114.0	45.5	171.2	#	#	0.3	0.2	0.3	#	#	1	G
117.1	61.4	173.5	71.2	21.1	0.3	0.2	0.3	0.4	0.4	1	T
122.1	60.9	173.0	69.1	#	0.3	0.2	0.3	0.2	#	1	T
121.0	54.5	174.4	#	#	0.3	0.2	0.3	#	#	1	L
118.0	50.1	174.5	20.5	#	0.3	0.2	0.3	0.3	#	1	A
124.5	61.3	172.6	67.9	#	0.3	0.2	0.3	0.2	#	1	T
120.5	49.4	174.0	23.5	#	0.3	0.2	0.3	0.3	#	1	A
120.6	50.0	174.4	#	#	0.3	0.2	0.3	#	#	1	A
113.3	54.9	173.7	32.7	#	0.3	0.2	0.3	0.4	#	1	R
125.3	60.4	174.3	41.2	#	0.3	0.2	0.3	0.4	#	1	I
125.0	56.5	173.5	63.3	#	0.4	0.3	0.4	0.4	#	1	S
121.8	60.8	174.6	#	#	0.3	0.2	0.3	#	#	1	V
118.1	61.6	172.6	#	#	0.4	0.3	0.4	#	#	1	T
121.5	56.5	172.8	65.2	#	0.5	0.2	0.3	0.3	#	1	S
117.6	54.2	175.3	64.3	#	0.3	0.2	0.3	0.3	#	1	S
116.3	59.2	175.0	#	#	0.4	0.2	0.3	#	#	1	V
122.1	62.1	173.9	#	#	0.3	0.2	0.3	#	#	1	P
122.9	55.2	173.0	64.5	#	0.3	0.2	0.3	0.4	#	1	S
122.1	60.6	173.4	#	#	0.4	0.3	0.4	#	#	1	V
123.2	53.9	174.5	#	#	0.3	0.2	0.3	#	#	1	E
119.0	53.7	174.9	33.8	#	0.4	0.2	0.4	0.4	#	1	QEMKRW
122.3	54.0	173.9	#	#	0.3	0.2	0.3	#	#	1	QE
121.3	61.2	174.0	71.0	#	0.3	0.2	0.3	0.3	#	1	T
121.2	61.6	173.2	70.5	#	0.4	0.3	0.4	0.2	#	1	T
124.1	61.3	172.6	70.2	#	0.3	0.2	0.3	0.2	#	1	T
118.8	61.1	175.2	#	#	0.4	0.3	0.4	#	#	1	V
119.7	53.6	174.6	32.0	#	0.3	0.2	0.3	0.4	#	1	QEMKRW
107.8	49.3	172.9	#	#	0.3	0.2	0.3	#	#	1	AG
118.0	60.4	172.3	#	#	0.3	0.2	0.3	#	#	1	VPT
122.6	60.8	174.2	35.2	#	0.3	0.2	0.3	0.4	#	1	V
118.6	60.9	174.1	34.6	#	0.3	0.2	0.3	0.4	#	1	V
124.1	53.9	173.0	#	#	0.4	0.2	0.3	#	#	1	E
121.0	59.9	174.6	35.9	#	0.4	0.3	0.4	0.4	#	1	V
116.9	61.4	174.0	#	#	0.3	0.2	0.3	#	#	1	V
109.6	53.9	174.8	#	#	0.5	0.4	0.4	#	#	1	M

CONCA spectrum

ν(N)	ν(Ca)	ν(C)	ν(Cb)	ν(Cg)	δ(N)	δ(Ca)	δ(C)	δ(Cb)	δ(Cg)	deg.	type
113.9	56.2	173.8	#	#	0.4	0.2	0.3	#	#	1	K
113.9	59.0	173.7	#	#	0.3	0.2	0.3	#	#	1	V
118.6	53.8	174.3	#	#	0.3	0.2	0.3	#	#	1	M
104.1	45.4	174.9	#	#	0.4	0.2	0.3	#	#	1	G
114.1	61.4	171.3	#	#	0.3	0.2	0.3	#	#	1	T
117.1	60.8	173.5	#	#	0.3	0.2	0.3	#	#	1	T
122.1	54.6	173.4	#	#	0.3	0.2	0.3	#	#	1	L
121.0	50.1	174.3	#	#	0.3	0.2	0.3	#	#	1	A
118.1	53.9	174.4	#	#	0.3	0.2	0.3	#	#	1	E
118.4	61.2	172.5	#	#	0.3	0.2	0.3	#	#	1	T
124.6	49.4	172.4	#	#	0.3	0.2	0.3	#	#	1	A
120.6	50.1	173.9	21.9	#	0.3	0.2	0.3	0.4	#	1	A
117.8	61.1	172.9	#	#	0.3	0.2	0.3	#	#	1	VT
121.9	60.4	173.1	#	#	0.3	0.2	0.3	#	#	1	I
124.4	60.9	173.8	#	#	0.4	0.3	0.4	#	#	1	V
121.8	54.8	174.4	#	#	0.3	0.2	0.3	#	#	1	QEKRMW
122.3	61.6	173.8	#	#	0.3	0.2	0.3	#	#	1	V
122.1	53.6	173.8	#	#	0.3	0.2	0.3	#	#	1	QEMKRW
120.0	56.5	173.6	#	#	0.3	0.2	0.3	#	#	1	S
114.5	54.2	173.5	#	#	0.3	0.2	0.3	#	#	1	S
116.8	61.9	174.9	#	#	0.4	0.2	0.3	#	#	1	P
116.8	55.1	173.9	#	#	0.3	0.2	0.3	#	#	1	S
122.4	60.9	173.9	#	#	0.4	0.3	0.4	#	#	1	V
123.1	54.3	174.8	#	#	0.3	0.4	0.3	#	#	1	M
121.6	61.3	174.3	#	#	0.4	0.4	0.4	#	#	1	VT
121.8	61.4	173.4	#	#	0.6	0.6	0.6	#	#	1	T
121.0	60.8	174.6	#	#	0.3	0.2	0.3	#	#	1	V
123.2	54.0	173.3	#	#	0.3	0.2	0.3	#	#	1	E
118.0	49.3	175.5	#	#	0.3	0.2	0.3	#	#	1	AG
107.9	60.2	172.8	#	#	0.3	0.2	0.3	#	#	1	TP
124.4	60.9	173.4	#	#	0.3	0.2	0.3	#	#	1	V
125.4	61.0	174.3	#	#	0.3	0.2	0.3	#	#	1	V
121.2	59.1	174.5	#	#	0.4	0.3	0.4	#	#	1	V
118.5	58.8	175.0	#	#	0.4	0.3	0.4	#	#	1	V
109.4	54.0	174.8	#	#	0.5	0.4	0.5	#	#	1	S
120.3	53.8	174.4	#	#	0.5	0.4	0.5	#	#	1	Q

Table S2: Signals from 3D solid state NMR spectra of P2 fibrils, used as input for MCASSIGN2. Each row is one multidimensional signal. Columns are chemical shifts (in ppm) of backbone amide nitrogens, α-carbons, carbonyl carbons, β-carbons, and γ-carbons, uncertainties in the chemical shifts, signal degeneracies, and possible residue-type assignments. Absent values are indicated by #.

NCACX spectrum

ν(N)	ν(Ca)	ν(C)	ν(Cb)	ν(Cg)	δ(N)	δ(Ca)	δ(C)	δ(Cb)	δ(Cg)	deg.	type
129.7	54.2	175.6	44.9	29.1	0.3	0.2	0.3	0.3	0.3	1	L
118.3	55.7	174.7	64.4	#	0.3	0.2	0.3	0.2	#	1	S
108.4	47.8	172.3	#	#	0.3	0.2	0.3	#	#	1	G
116.9	49.6	176.5	17.1	#	0.3	0.2	0.3	0.2	#	1	A
119.4	59.8	177.3	27.2	35.1	0.3	0.2	0.3	0.3	0.3	1	Q
124.7	61.4	175.8	33.5	21.9	0.3	0.2	0.3	0.3	0.3	1	V
114.0	56.3	173.7	29.3	#	0.3	0.2	0.3	0.6	#	1	WQEKR
119.2	53.4	174.3	33.3	#	0.3	0.2	0.3	0.6	#	1	QEMKR
125.4	54.1	173.8	#	#	0.3	0.2	0.3	#	#	1	QEMKR
125.6	61.2	174.1	35.4	21.5	0.4	0.2	0.3	0.3	0.3	1	V
125.6	61.1	175.5	42.4	28.6	0.3	0.2	0.3	0.3	0.3	1	I
114.7	48.7	173.7	#	#	0.3	0.2	0.3	#	#	1	G
121.8	62.2	174.0	70.4	#	0.3	0.2	0.3	0.4	#	1	T
125.1	49.5	175.2	24.2	#	0.3	0.2	0.3	0.2	#	1	A
125.8	50.1	175.2	21.4	#	0.3	0.2	0.3	0.2	#	1	A
117.2	61.6	173.9	70.6	21.3	0.3	0.2	0.3	0.5	0.4	1	T
123.2	62.2	171.1	71.6	21.8	0.3	0.2	0.3	0.4	0.4	1	T
125.7	61.7	173.9	69.5	20.9	0.3	0.2	0.3	0.4	0.3	1	T
112.4	60.5	174.7	36.0	21.4	0.3	0.2	0.3	0.3	0.3	1	V
115.1	53.9	175.5	65.7	#	0.3	0.2	0.3	0.5	#	1	S
117.0	55.7	172.7	65.1	#	0.3	0.2	0.3	0.3	#	1	S
124.8	61.8	173.7	70.2	21.5	0.4	0.2	0.3	0.3	0.8	1	T
125.3	61.6	174.9	33.4	20.7	0.3	0.2	0.3	0.3	0.3	1	V
116.8	53.7	173.7	32.9	#	0.3	0.2	0.3	0.5	#	1	QEMKR
123.8	49.1	175.2	22.9	#	0.3	0.2	0.3	0.2	#	1	A
118.0	63.2	#	#	#	0.5	0.2	#	#	#	1	P
121.3	54.0	175.1	32.5	#	0.3	0.2	0.3	0.6	#	1	QEMKRW
124.2	61.5	174.4	69.8	22.6	0.3	0.2	0.3	0.3	0.3	1	T
125.6	54.1	173.8	45.1	28.5	0.3	0.2	0.3	0.6	0.4	1	L
114.2	61.3	#	#	#	0.3	0.2	#	#	#	1	VIT
108.4	48.7	174.3	#	#	0.3	0.2	0.3	#	#	1	G
119.1	54.2	174.7	37.9	#	0.3	0.2	0.3	0.5	#	1	MQE

NCOCX spectrum

ν(N)	ν(Ca)	ν(C)	ν(Cb)	ν(Cg)	δ(N)	δ(Ca)	δ(C)	δ(Cb)	δ(Cg)	deg.	type
118.2	54.2	175.4	44.9	28.9	0.3	0.2	0.3	0.4	0.5	1	L
108.6	55.8	174.7	64.4	#	0.3	0.2	0.3	0.3	#	1	S
121.6	47.7	172.2	#	#	0.3	0.2	0.3	#	#	1	G
119.5	49.7	176.6	17.1	#	0.3	0.2	0.3	0.2	#	1	A
124.7	59.8	177.3	27.2	35.1	0.3	0.2	0.3	0.3	0.5	1	Q
125.9	61.4	175.8	33.5	21.7	0.3	0.2	0.3	0.4	0.4	1	V
112.2	56.3	173.6	#	#	0.3	0.2	0.3	#	#	1	WQEKR
114.4	53.3	174.2	33.4	#	0.3	0.2	0.3	0.5	#	1	QEMKR
125.4	61.4	173.8	35.3	#	0.3	0.2	0.3	0.4	#	1	V
125.9	54.1	173.8	33.0	#	0.3	0.2	0.3	0.5	#	1	QEMKRW
125.7	61.1	175.5	42.3	28.6	0.3	0.2	0.3	0.4	0.5	1	I
101.9	48.6	173.6	#	#	0.3	0.2	0.3	#	#	1	G
116.9	49.6	175.1	24.1	#	0.3	0.2	0.3	0.4	#	1	A
116.9	50.1	175.0	21.3	#	0.3	0.2	0.3	0.4	#	1	A
121.8	61.8	173.7	71.3	21.5	0.3	0.2	0.3	0.5	0.4	1	T
125.3	62.3	171.3	71.6	21.8	0.3	0.2	0.3	0.3	0.3	1	T
125.2	61.5	174.1	69.4	20.9	0.3	0.2	0.3	0.4	0.5	1	T
121.3	60.4	174.8	35.7	21.3	0.3	0.2	0.3	0.4	0.5	1	V
114.7	54.0	175.3	65.8	#	0.3	0.2	0.4	0.3	#	1	S
125.5	55.6	172.8	64.8	#	0.3	0.2	0.3	0.3	#	1	S
123.5	62.3	174.2	70.2	20.6	0.3	0.2	0.3	0.4	0.4	1	T
117.2	61.2	173.9	33.0	21.6	0.4	0.2	0.3	0.5	0.4	1	V
124.3	61.6	173.7	70.2	21.5	0.4	0.2	0.3	0.5	0.6	1	T
129.6	61.4	174.7	33.4	20.6	0.3	0.2	0.3	0.3	0.3	1	V
119.0	53.7	173.7	32.8	#	0.3	0.2	0.3	0.5	#	1	QEMKR
125.7	54.1	173.8	45.7	#	0.3	0.2	0.3	0.4	#	1	L
116.9	49.2	175.1	22.8	#	0.3	0.2	0.3	0.4	#	1	A
118.5	61.3	174.8	69.8	22.6	0.3	0.2	0.3	0.4	0.4	1	T
123.5	63.4	172.2	#	#	0.3	0.2	0.3	#	#	1	P
119.1	61.4	174.3	69.8	22.5	0.3	0.2	0.3	0.3	0.3	1	T
124.8	61.8	172.4	71.2	#	0.4	0.3	0.4	0.4	#	1	T

CONCA spectrum

ν(N)	ν(Ca)	ν(C)	ν(Cb)	ν(Cg)	δ(N)	δ(Ca)	δ(C)	δ(Cb)	δ(Cg)	deg.	type
129.6	54.2	174.7	45.2	#	0.3	0.2	0.3	0.4	#	1	L
118.5	55.8	175.3	64.4	#	0.3	0.2	0.3	0.5	#	1	S
108.5	47.7	174.7	#	#	0.3	0.2	0.3	#	#	1	G
116.8	49.6	175.1	#	#	0.3	0.2	0.3	#	#	1	A
119.5	59.8	176.5	#	#	0.3	0.2	0.3	#	#	1	Q
124.5	61.5	177.4	33.5	#	0.3	0.2	0.3	0.4	#	1	V
112.2	60.4	173.6	36.0	#	0.3	0.2	0.3	0.4	#	1	V
119.0	53.4	174.2	#	#	0.3	0.2	0.3	#	#	1	QEMKR
126.1	61.4	175.7	35.3	#	0.4	0.2	0.3	0.4	#	1	V
125.5	61.0	172.4	42.3	28.5	0.3	0.2	0.3	0.5	0.4	1	I
121.5	62.1	173.9	#	#	0.3	0.2	0.3	#	#	1	VT
114.6	48.6	175.8	#	#	0.3	0.2	0.4	#	#	1	G
124.9	49.4	171.2	#	#	0.3	0.2	0.3	#	#	1	A
125.8	50.1	173.6	21.1	#	0.3	0.2	0.3	0.4	#	1	A
114.0	56.3	174.2	#	#	0.3	0.2	0.3	#	#	1	SMEQWKR
123.1	62.1	174.0	71.5	#	0.3	0.2	0.3	0.4	#	1	T
126.0	61.5	175.7	69.3	#	0.3	0.2	0.3	0.4	#	1	T
125.6	61.5	173.8	33.3	#	0.3	0.2	0.3	0.4	#	1	V
121.5	62.4	172.2	#	#	0.3	0.2	0.3	#	#	1	TV
125.9	53.9	173.4	45.7	#	0.3	0.2	0.3	0.7	#	1	L
125.4	61.6	173.9	#	#	0.8	0.8	0.8	#	#	1	VT
123.9	49.2	171.8	#	#	0.3	0.2	0.3	#	#	1	A
116.6	53.7	175.3	#	#	0.3	0.2	0.3	#	#	1	LQEMWKR
117.1	56.6	175.4	#	#	0.3	0.2	0.3	#	#	1	SQEMWKR
117.0	61.8	174.2	#	#	0.3	0.2	0.3	#	#	1	VT
118.3	63.1	175.2	#	#	0.3	0.2	0.3	#	#	1	PT
121.7	54.1	174.7	#	#	0.3	0.2	0.3	#	#	1	QEMKRW
125.2	54.0	171.8	#	#	0.3	0.2	0.3	#	#	1	MQEWKR
119.3	54.2	173.6	#	#	0.3	0.2	0.3	#	#	1	MQE
124.3	61.2	173.5	69.8	#	0.3	0.2	0.3	0.5	#	1	T
116.9	55.6	173.8	#	#	0.3	0.2	0.3	#	#	1	SQEMWKR
114.0	61.2	176.6	#	#	0.3	0.2	0.3	#	#	1	VIT
115.3	54.2	175.0	#	#	0.3	0.2	0.3	#	#	1	S
125.5	61.5	173.7	69.7	#	0.3	0.2	0.3	0.4	#	1	T
108.8	48.5	174.7	#	#	0.4	0.4	0.4	#	#	1	G

Table S3: Signals from 3D solid state NMR spectra of P3 fibrils, used as input for MCASSIGN2. Each row is one multidimensional signal. Columns are chemical shifts (in ppm) of backbone amide nitrogens, α-carbons, carbonyl carbons, β-carbons, and γ-carbons, uncertainties in the chemical shifts, signal degeneracies, and possible residue-type assignments. Absent values are indicated by #.

NCACX spectrum

ν(N)	ν(Ca)	ν(C)	ν(Cb)	ν(Cg)	δ(N)	δ(Ca)	δ(C)	δ(Cb)	δ(Cg)	deg.	type
117.1	61.6	173.3	70.7	20.8	0.3	0.3	0.2	0.4	0.4	1	T
108.6	44.0	172.2	#	#	0.3	0.1	0.1	#	#	1	G
114.4	53.7	174.3	39.5	#	0.3	0.1	0.1	0.3	#	1	MQE
115.5	58.7	169.8	68.7	22.4	0.3	0.3	0.3	0.3	0.3	1	T
131.8	60.9	#	#	#	0.3	0.3	#	#	#	1	P
120.6	50.4	175.1	21.1	#	0.3	0.2	0.2	0.2	#	1	A
117.6	60.4	176.1	35.8	22.4	0.3	0.3	0.3	0.3	0.3	1	V
123.9	56.2	173.7	63.2	#	0.3	0.1	0.3	0.3	#	1	S
124.6	59.9	173.7	41.6	#	0.3	0.5	0.3	0.3	#	1	I
122.7	53.8	174.9	43.9	#	0.3	0.4	1.2	0.4	#	1	L
112.8	55.4	177.2	64.8	#	0.3	0.4	0.4	0.4	#	1	S
116.0	48.6	174.6	#	#	0.3	0.3	0.2	#	#	1	G
119.5	60.8	173.6	70.9	21.1	0.3	0.2	0.2	0.3	0.3	1	T
121.9	52.0	172.3	16.0	#	0.3	0.2	0.2	0.4	#	1	A
116.4	49.3	175.5	23.0	#	0.3	0.1	0.3	0.4	#	1	A
120.4	60.8	172.5	71.9	21.8	0.5	0.2	0.2	0.3	0.3	1	T
122.7	49.5	174.9	23.0	#	0.3	0.1	0.3	0.4	#	1	A
118.6	52.9	170.8	29.6	#	0.3	0.4	0.4	0.4	#	1	QE
112.5	56.5	174.2	65.0	#	0.3	0.1	0.3	0.3	#	1	S
110.8	45.3	173.2	#	#	0.3	0.2	0.4	#	#	1	G
117.0	61.4	173.2	70.7	20.8	0.4	0.2	0.2	0.3	0.3	1	T
119.3	58.5	170.4	33.4	22.6	0.3	0.3	0.3	0.3	0.3	1	V
123.0	61.7	173.4	70.6	21.6	0.2	0.3	0.3	0.3	0.4	1	T
119.5	56.8	174.0	63.1	#	0.6	0.2	0.2	0.3	#	1	S
121.8	60.7	174.9	35.0	21.8	0.3	0.2	0.4	0.2	0.5	1	V
120.5	50.7	175.2	22.8	#	0.3	0.1	0.3	0.4	#	1	A
112.4	62.3	172.1	73.1	21.9	0.3	0.4	0.3	0.3	0.3	1	T
123.1	61.3	173.5	34.9	21.6	0.3	0.3	0.4	0.2	0.4	1	V
124.5	54.4	173.8	30.5	#	0.3	0.6	0.4	0.4	#	1	QEMKRW
117.5	54.5	176.4	#	#	0.3	0.3	0.4	#	#	1	QE
123.0	53.8	173.7	32.2	#	0.3	0.4	0.4	0.4	#	1	QEMKRW
125.9	61.2	174.0	35.2	21.3	0.3	0.2	0.2	0.3	0.3	1	V
122.5	53.9	173.9	34.2	#	0.3	0.2	0.4	0.4	#	1	QEMKRW
118.7	54.1	174.4	34.5	#	0.3	0.4	0.4	0.6	#	1	QEMKRW
125.5	61.1	174.2	35.3	21.4	0.3	0.2	0.2	0.3	0.4	1	V
121.1	54.0	174.1	28.6	#	0.3	0.4	0.4	0.3	#	1	QEKRW
111.9	45.0	173.1	#	#	0.3	0.3	0.3	#	#	1	G
113.0	56.7	176.9	#	#	0.3	0.2	0.2	#	#	1	QEKRWS
123.3	61.5	173.0	70.6	20.5	0.3	0.2	0.2	0.4	0.4	1	T
123.3	61.6	172.8	70.6	23.0	0.3	0.2	0.2	0.4	0.4	1	T
123.0	61.7	173.4	70.6	20.6	0.3	0.3	0.3	0.3	0.4	1	T

NCOCX spectrum

ν(N)	ν(Ca)	ν(C)	ν(Cb)	ν(Cg)	δ(N)	δ(Ca)	δ(C)	δ(Cb)	δ(Cg)	deg.	type
108.6	61.7	173.5	70.6	20.7	0.2	0.2	0.2	0.4	0.3	1	T
114.4	43.9	172.2	#	#	0.1	0.2	0.1	#	#	1	G
115.4	53.8	174.4	39.3	#	0.2	0.2	0.2	0.4	#	1	MQE
131.8	58.7	169.8	68.9	#	0.2	0.2	0.2	0.3	#	1	T
120.5	60.9	173.6	32.8	27.4	0.2	0.3	0.2	0.3	0.3	1	P
121.0	50.3	175.1	21.1	#	0.2	0.2	0.2	0.3	#	1	A
123.7	60.4	176.1	35.6	22.2	0.2	0.2	0.2	0.3	0.3	1	V
124.9	56.3	173.8	63.2	#	0.3	0.2	0.2	0.3	#	1	S
125.5	59.8	173.8	41.6	27.1	0.2	0.2	0.2	0.2	0.3	1	I
112.7	53.8	176.4	44.2	#	0.2	0.2	1.1	0.4	#	1	L
116.2	55.3	177.1	64.8	#	0.6	0.2	0.4	0.3	#	1	S
112.6	48.4	174.7	#	#	0.6	0.2	0.2	#	#	1	G
119.8	62.2	172.2	73.0	21.7	0.5	0.2	0.2	0.2	0.3	1	T
122.0	60.8	173.8	70.7	21.0	0.5	0.2	0.2	0.4	0.4	1	T
116.5	52.5	172.3	#	#	0.2	0.5	0.2	#	#	1	A
118.5	49.5	175.4	22.9	#	0.4	0.4	0.4	0.3	#	1	A
123.0	61.5	173.4	70.7	21.7	0.4	0.4	0.4	0.5	0.8	1	T
122.4	60.8	172.7	71.9	21.5	0.3	0.3	0.2	0.3	0.5	1	T
118.6	49.5	175.0	23.0	#	0.2	0.2	0.2	0.3	#	1	A
129.4	53.0	171.1	#	#	0.3	0.2	0.2	#	#	1	E
112.6	62.3	174.9	32.5	#	0.2	0.2	0.2	0.4	#	1	P
110.4	56.6	174.3	65.3	#	0.4	0.2	0.2	0.2	#	1	S
116.6	45.3	173.1	#	#	0.5	0.2	0.5	#	#	1	G
118.7	61.3	173.1	#	21.2	0.2	0.5	0.2	#	0.5	1	T
119.2	61.0	174.0	71.5	21.6	0.2	0.5	0.2	0.5	0.5	1	T
119.2	56.7	174.3	63.2	#	0.4	0.2	0.3	0.3	#	1	S
122.5	61.1	174.1	35.1	#	0.4	0.4	0.4	0.4	#	1	V
117.4	50.6	175.2	22.7	#	0.4	0.2	0.4	0.3	#	1	A
122.6	61.3	173.8	35.1	21.7	0.2	0.4	0.3	0.4	0.4	1	V
117.9	54.6	173.8	30.6	#	0.2	0.2	0.2	0.4	#	1	QEMKRW
119.8	54.6	176.3	#	#	0.5	0.3	0.5	#	#	1	QE
112.9	53.4	174.0	32.2	#	0.2	0.2	0.2	0.4	#	1	QEMKRW
123.6	54.1	173.9	34.5	#	0.2	0.2	0.2	0.4	#	1	QEMKRW
125.9	61.0	174.0	35.2	21.3	0.2	0.2	0.2	0.3	0.3	1	V
117.4	54.0	174.1	28.6	#	0.3	0.4	0.2	0.3	#	1	QEKRW
122.3	44.8	173.1	#	#	0.2	0.2	0.2	#	#	1	G
123.3	60.6	175.4	35.3	22.2	0.4	0.2	0.4	0.4	0.4	1	V
119.6	56.6	176.9	#	#	0.2	0.2	0.2	#	#	1	QEKRWS
122.0	54.2	174.4	35.0	#	0.4	0.2	0.4	0.6	#	1	QEMKRW
123.0	61.6	173.4	70.9	20.6	0.4	0.4	0.4	0.4	0.3	1	T
123.2	61.5	172.6	70.7	#	0.2	0.2	0.4	0.4	#	1	T
123.2	61.5	172.8	#	22.9	0.2	0.2	0.2	#	0.4	1	T

CONCA spectrum

ν(N)	ν(Ca)	ν(C)	ν(Cb)	ν(Cg)	δ(N)	δ(Ca)	δ(C)	δ(Cb)	δ(Cg)	deg.	type
117.1	61.5	175.4	#	#	0.3	0.3	0.3	#	#	1	T
108.5	43.9	173.4	#	#	0.1	0.1	0.1	#	#	1	G
114.4	53.8	172.3	#	#	0.1	0.1	0.1	#	#	1	MQE
115.3	58.8	174.3	#	#	0.3	0.3	0.3	#	#	1	T
131.6	60.7	169.8	#	#	0.3	0.3	0.3	#	#	1	P
120.6	50.2	173.9	#	#	0.3	0.2	0.2	#	#	1	A
121.1	54.0	175.0	#	#	0.3	0.3	0.3	#	#	1	E
123.7	56.3	176.1	#	#	0.3	0.3	0.3	#	#	1	S
124.7	60.0	173.9	#	#	0.3	0.3	0.3	#	#	1	I
122.4	54.0	174.2	#	#	0.3	0.3	0.3	#	#	1	L
112.8	55.5	176.5	#	#	0.3	0.3	1.2	#	#	1	S
116.0	48.5	177.0	#	#	0.3	0.3	0.3	#	#	1	G
112.3	62.3	174.8	#	#	0.3	0.3	0.3	#	#	1	T
119.7	60.6	172.2	#	#	0.3	0.3	0.3	#	#	1	T
121.7	52.2	173.8	#	#	0.3	0.3	0.3	#	#	1	A
116.5	49.4	172.7	#	#	0.3	0.3	0.4	#	#	1	A
122.6	49.4	172.5	#	#	0.3	0.3	0.3	#	#	1	A
118.8	53.0	175.0	#	#	0.3	0.3	0.3	#	#	1	QE
129.3	62.3	170.7	#	#	0.3	0.3	0.3	#	#	1	P
112.7	56.6	174.7	#	#	0.3	0.3	0.3	#	#	1	S
110.5	45.5	174.4	#	#	0.3	0.3	0.3	#	#	1	G
117.0	61.5	173.5	#	#	0.3	0.3	0.3	#	#	1	T
118.5	60.9	173.4	#	#	0.3	0.3	0.3	#	#	1	T
119.3	56.8	173.9	#	#	0.3	0.3	0.3	#	#	1	S
119.4	58.5	174.3	#	#	0.3	0.3	0.3	#	#	1	V
123.0	61.8	173.7	#	#	0.3	0.3	0.3	#	#	1	T
119.8	56.9	176.3	#	#	0.3	0.3	0.3	#	#	1	S
120.4	50.9	175.7	#	#	0.3	0.3	0.3	#	#	1	A
122.8	61.2	174.5	#	#	0.3	0.3	0.3	#	#	1	V
119.4	61.0	176.9	#	#	0.3	0.3	0.3	#	#	1	VT
122.1	60.6	174.3	#	#	0.3	0.3	0.3	#	#	1	V
117.7	60.3	173.9	#	#	0.3	0.3	0.3	#	#	1	V
122.5	53.8	173.3	#	#	0.3	0.3	0.3	#	#	1	QEMKRWL
124.4	54.8	172.5	#	#	0.3	0.3	0.3	#	#	1	QEMKRW
122.8	61.6	173.1	#	#	0.3	0.3	0.3	#	#	1	VT
117.7	54.4	174.8	#	#	0.3	0.3	0.3	#	#	1	QEMKRW
125.8	61.0	174.2	#	#	0.3	0.3	0.3	#	#	1	V
125.2	61.0	173.8	#	#	0.3	0.3	0.3	#	#	1	V
123.1	53.4	172.6	#	#	0.3	0.3	0.3	#	#	1	QEMKRW
111.6	45.2	174.7	#	#	0.3	0.3	0.3	#	#	1	G
117.6	60.4	173.7	#	#	0.3	0.3	0.3	#	#	1	VT

Table S4: Chemical shift assignments for backbone amide nitrogens, carbonyl carbons, α-carbons, and β-carbons in P1 fibrils. Only assignments that were identical in all high-scoring MCASSIGN2 runs are listed. ^{15}N shifts are relative to liquid NH_3. ^{13}C shifts are relative to DSS. The last three columns are secondary shifts (relative to random coil values given by Wishart *et al*., J. Biomolec. NMR **5**, 67-81, 1995).

Residue	ν(N)	ν(C)	ν(Ca)	ν(Cb)	δδ(C)	δδ(Ca)	δδ(Cb)
T34	118.1	172.7	61.5	71.2	-2.0	-0.4	1.4
T35	118.0	172.6	61.2	70.2	-2.1	-0.6	0.4
S36	124.2	173.8	56.5	63.3	-0.8	-1.8	-0.5
V37	124.7	175.2	61.0	34.9	-1.1	-1.2	2.0
Q38	118.8	174.8	54.5	31.2	-1.2	-1.2	1.8
V39	118.6	170.0	58.8	33.4	-4.9	-1.0	0.8
E63	121.5	173.7	54.5	33.8	-2.9	-2.1	3.9
K64	113.7	173.8	56.2	37.6	-2.8	0.0	4.5
V65	113.9	174.9	59.1	36.6	0.0	-0.7	3.7
P66	116.6	173.9	62.0	31.9	-3.5	-1.4	-0.2
V67	122.1	173.9	61.5	33.7	-2.4	-0.7	0.8
S68	116.9	173.2	55.2	64.7	-1.4	-3.1	0.9
E69	123.2	173.1	54.0	31.8	-3.5	-2.6	1.9
V70	124.3	174.1	61.0	34.8	-2.2	-1.2	1.9
M71	118.6	174.8	53.9	42.5	-1.5	-1.5	9.6
G72	103.9	171.3	45.4	0.0	-3.6	0.3	0.0
T74	114.0	173.5	61.4	71.3	-1.2	-0.4	1.5
T74	117.2	173.2	60.9	69.2	-1.5	-0.9	-0.7
L75	122.1	174.4	54.5	46.0	-3.2	-0.6	3.6
A76	121.1	174.4	50.0	20.5	-3.4	-2.5	1.4
E77	118.0	174.6	53.9	32.2	-2.0	-2.7	2.3
M78	123.1	174.0	54.1	0.0	-2.3	-1.3	0.0
S92	120.0	173.0	56.5	65.2	-1.6	-1.8	1.4
I93	121.6	174.3	60.4	41.4	-2.1	-0.7	2.6
V94	125.3	174.1	60.9	35.1	-2.2	-1.3	2.2
V95	122.4	173.5	60.7	35.2	-2.9	-1.5	2.3
L96	122.1	173.5	0.0	0.0	-4.1	0.0	0.0
S97	114.5	175.5	54.2	64.3	0.9	-4.1	0.5
G98	117.9	172.8	49.3	0.0	-2.1	4.2	0.0
T99	107.8	172.4	60.3	75.9	-2.3	-1.5	6.1
T100	118.2	172.6	61.3	67.9	-2.1	-0.5	-2.0
A101	124.6	173.9	49.4	23.4	-3.9	-3.1	4.3
A102	120.5	174.4	50.0	22.0	-3.5	-2.5	2.9
Q103	120.5	174.7	53.8	33.8	-1.3	-1.9	4.4
V104	121.1	174.4	60.6	35.5	-1.9	-1.6	2.6
T105	121.7	173.8	61.3	70.9	-0.9	-0.5	1.1
T106	121.6	173.4	61.5	70.5	-1.3	-0.3	0.7
T107	121.2	174.0	60.7	70.5	-0.7	-1.1	0.7

Table S5: Chemical shift assignments for backbone amide nitrogens, carbonyl carbons, α-carbons, and β-carbons in P2 fibrils. Only assignments that were identical in all high-scoring MCASSIGN2 runs are listed. ^{15}N shifts are relative to liquid NH_3. ^{13}C shifts are relative to DSS. The last three columns are secondary shifts (relative to random coil values given by Wishart *et al*., J. Biomolec. NMR **5**, 67-81, 1995).

Residue	ν(N)	ν(C)	ν(Ca)	ν(Cb)	δδ(C)	δδ(Ca)	δδ(Cb)
S32	115.2	175.5	54.0	65.8	0.9	-4.3	2.0
G33	114.7	173.7	48.6	0.0	-1.3	3.5	0.0
L75	125.8	173.7	54.0	45.5	-3.9	-1.1	3.1
A76	125.8	175.2	50.1	21.3	-2.6	-2.4	2.2
E77	116.8	173.7	53.7	32.9	-2.9	-2.9	3.0
M78	119.1	174.7	54.2	37.9	-1.6	-1.2	5.0
M86	125.3	173.8	54.1	33.0	-2.5	-1.3	0.1
T87	125.7	175.0	61.4	69.8	1.8	1.6	-0.1
P88	118.3	172.0	63.2	32.0	-5.3	-0.1	-0.1
A89	123.7	175.2	49.2	22.9	-2.6	-3.3	3.8
E90	117.0	176.6	56.6	29.9	0.0	0.0	0.0
V91	114.1	173.9	61.2	33.0	-2.5	-1.0	0.1
S92	117.0	172.6	55.6	65.0	-2.0	-2.7	1.2
I93	125.5	175.5	61.1	42.3	-0.9	0.0	3.5
V94	125.8	173.9	61.3	35.3	-2.4	-0.9	2.4
V95	125.4	174.8	61.5	33.4	-1.5	-0.7	0.5
L96	129.6	175.4	54.2	45.0	-2.2	-0.9	2.6
S97	118.3	174.7	55.8	64.4	0.1	-2.5	0.6
G98	108.5	172.2	47.7	0.0	-2.7	2.6	0.0
T99	121.6	174.1	62.3	70.3	-0.6	0.5	0.5
T100	123.3	171.2	62.2	71.6	-3.5	0.4	1.8
A101	125.1	175.1	49.5	24.2	-2.7	-3.0	5.1
A102	116.8	176.5	49.6	17.1	-1.3	-2.9	-2.0
Q103	119.4	177.3	59.8	27.2	1.3	4.1	-2.2
V104	124.6	175.7	61.4	33.5	-0.6	-0.8	0.6
T105	125.8	174.0	61.6	69.4	-0.7	-0.2	-0.4
T106	125.1	173.6	61.7	70.2	-1.1	-0.1	0.4
T107	124.3	174.3	61.4	69.8	-0.4	-0.4	0.0
E108	119.1	174.2	53.4	33.4	-2.4	-3.2	3.5
W109	114.1	173.6	56.3	29.3	-2.5	-1.2	-0.3
V110	112.2	174.7	60.4	35.9	-1.6	-1.8	3.0
E111	121.4	175.1	54.1	32.5	-1.5	-2.6	2.6

Table S6: Chemical shift assignments for backbone amide nitrogens, carbonyl carbons, α-carbons, and β-carbons in P3 fibrils. Only assignments that were identical in all high-scoring MCASSIGN2 runs are listed. ^{15}N shifts are relative to liquid NH_3. ^{13}C shifts are relative to DSS. The last three columns are secondary shifts (relative to random coil values given by Wishart *et al*., J. Biomolec. NMR **5**, 67-81, 1995).

Residue	ν(N)	ν(C)	ν(Ca)	ν(Cb)	δδ(C)	δδ(Ca)	δδ(Cb)
T28	120.4	172.6	60.8	71.9	-2.1	-1.0	2.1
A29	122.6	175.0	49.5	23.0	-2.8	-3.0	3.9
E30	118.7	170.9	53.0	29.6	-4.0	-1.2	0.4
P31	129.4	174.8	62.3	32.5	-2.5	-1.0	0.4
S32	112.6	174.3	56.5	65.2	-0.3	-1.8	1.4
G33	110.6	173.3	45.4	0.0	-1.6	0.3	0.0
T34	116.9	173.2	61.4	70.7	-1.5	-0.4	0.9
T35	118.6	174.0	61.0	71.4	-0.8	-0.9	1.6
S36	119.3	174.2	56.8	63.2	-0.4	-1.5	-0.7
V37	119.3	170.4	58.5	33.4	-5.9	-3.7	0.5
Q38	117.7	174.5	54.4	31.4	-1.5	-1.3	2.0
V39	123.0	173.7	61.3	35.0	-1.3	1.5	2.4
A55	120.5	174.9	50.7	22.8	-2.9	-1.8	3.7
E56	117.6	176.3	54.5	31.5	-0.3	-2.1	1.6
A83	120.5	175.3	50.7	22.8	-2.5	-1.8	3.7
T84	117.2	173.4	61.6	70.7	-1.3	-0.2	0.9
G85	108.6	172.2	43.9	0.0	-2.7	-1.2	0.0
M86	114.4	174.3	53.8	39.4	-2.0	-1.6	6.5
T87	115.4	169.8	58.7	68.8	-3.4	-1.1	-1.0
P88	131.7	173.8	60.8	32.8	-3.6	-2.5	0.7
A89	120.6	175.1	50.3	21.1	-2.7	-2.2	2.0
E90	121.1	174.0	54.0	28.6	-2.6	-2.6	-1.3
V91	117.6	176.1	60.4	35.7	-0.2	-1.8	2.8
S92	123.8	173.8	56.3	63.2	-0.8	-2.0	-0.6
I93	124.7	173.8	59.9	41.6	-2.6	-1.2	2.8
V94	125.4	174.1	61.0	35.3	-2.2	-1.2	2.4
V95	125.9	174.1	61.1	35.2	-2.2	-1.1	2.3
L96	122.5	176.0	53.9	44.1	-1.6	-1.2	1.7
S97	112.8	177.1	55.4	64.8	2.5	-2.9	1.0
G98	116.1	174.7	48.5	0.0	-0.2	3.4	0.0
T99	112.4	172.2	62.3	73.1	-2.5	0.5	3.3
T100	119.7	173.7	60.7	70.8	-1.0	-1.1	1.0
A101	121.9	172.4	52.2	16.0	-5.4	-0.3	-3.1
A102	116.5	175.5	49.4	23.0	-2.4	-3.1	3.9
Q103	118.6	174.4	54.2	34.8	-1.6	-1.6	5.4
V104	122.0	175.2	60.6	35.2	-1.2	-1.6	2.3
T105	123.2	173.3	61.6	70.7	-1.4	-0.2	0.9
T106	122.9	173.5	61.6	70.7	-1.2	-0.2	0.9
T107	123.1	172.7	61.6	70.7	-2.0	-0.2	0.9
E108	123.1	173.9	53.5	32.2	-2.8	-3.1	2.3
W109	113.0	176.9	56.7	30.2	0.8	-0.9	0.6