Table 2. C–N distances in TTR(105–115) fibrils

Atoms		Measured NMR distance used in structure calculation, Å	Range of distances in ensemble of NMR structures, Å*
Y105 C^{β}	T106 N	3.3 ± 0.33	3.06–3.13
Y105 C^{γ}	Y105 N	3.18 ± 0.20†	3.01–3.33
	T106 N	>3.5†	4.12–4.44
T106 C^{β}	I107 N	3.5 ± 0.35	3.29–3.45
T106 C^{γ}	T106 N	3.6 ± 0.36	3.77–3.82
	I107 N	3.2 ± 0.32	3.31–3.52
I107 C^{β}	A108 N	3.4 ± 0.34	3.27–3.30
I107 $C^{\gamma 1}$	I107 N	3.1 ± 0.31	3.06–3.13
	A108 N	4.0 ± 0.40	4.43–4.45
I107 $C^{\gamma 2}$	I107 N	3.8 ± 0.38	3.80–3.82
	A108 N	3.1 ± 0.31	3.06–3.13
I107 C^{δ}	I107 N	4.6 ± 0.46	4.17–4.42
	A108 N	5.7 ± 0.57	5.65–5.75
A108 C'	L110N	$4.25^{+0.45}_{-0.15}$‡	4.16–4.46
A108 C^{β}	A109 N	3.5 ± 0.35	3.29–3.45
A109 C^{β}	L110 N	3.3 ± 0.33	3.31–3.53
L110 C^{β}	L111 N	3.6 ± 0.36	3.33–3.58
L110 $C^{\delta 1}$	L110 N	4.2 ± 0.42	4.30–4.45
	L111 N	3.4 ± 0.34	3.50–3.72
L111 C^{α}	L110N	$4.56^{+0.62}_{-0.12}$‡	4.60–4.79
L111 C^{β}	S112 N	3.8 ± 0.20†	3.53–3.54
L111 C^{γ}	L111 N	3.0 ± 0.30	2.95–3.02
	S112 N	4.6 ± 0.46	4.83–4.85
L111 $C^{\delta 1}$	L111 N	> 3.5	4.33–4.44
	S112 N	> 3.5	5.93–6.00
L111 $C^{\delta 2}$	L111 N	3.2 ± 0.32	3.45–3.54
	S112 N	5.5 ± 0.55	4.95–5.02
S112 C'	Y114N	$4.06^{+0.36}_{-0.06}$‡	4.00–4.17
P113 C^{β}	P113 N	2.4 ± 0.24	—

Atoms		Measured NMR distance used in structure calculation, Å	Range of distances in ensemble of NMR structures, Å*
	Y114 N	3.7 ± 0.37	3.33–3.46
P113 C^{γ}	P113 N	2.3 ± 0.23	—
	Y114 N	> 3.5	4.31–4.66
P113 C^{δ}	S112 N	3.2 ± 0.32	3.61–3.62
Y114 C^{γ}	Y114 N	> 2.8†	3.13–3.80
S115 C^{α}	Y114N	$5.0^{+1.8}_{-0.5}$ ‡	4.73–4.85

Experimental NMR distances are compared with corresponding distances in the ensemble of 20 low-energy structures calculated using simulated annealing molecular dynamics in CNS (1). A total of 35 distances used in the structure calculation are in the 3-6 Å regime and depend on at least one dihedral angle. Unless otherwise indicated distances were determined using the 3D *z*-filtered transferred-echo double-resonance technique (2) in uniformly ^{13}C,^{15}N-labeled fibrils.

*As evaluated by MOLMOL (3).

†Distance determined by using frequency selective REDOR (4) in uniformly ^{13}C,^{15}N-labeled fibrils.

‡Distance determined by using REDOR (5) in selectively ^{13}C,^{15}N-labeled fibrils (6). Uncertainties include the potential contribution from intermolecular dipolar couplings as discussed in ref. 6.

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