

Table 1S. Summary of parameters describing the status of individual chains – as standalone units and as part of larger structures (where the 3D Gaussian is constructed for a protofibril and for a superfibril respectively). * – only the 30–100 fragment, which exhibits amyloid-like properties, is subjected to analysis. Underscores indicate that the given amyloid does not form a superfibril; D_{KL} values for T, R and H distribution treated as target distribution for O distribution allowing the RD calculation.

RD					D_{KL}	AMYLOID
T-O-R	T-O-H	O T	O R	O H		
CHAIN AS PART OF SUPERFIBRIL						
CHAIN AS PART OF PROTOFIBRIL						
0.554	0.475	0.163	0.131	0.180	$A\beta(15-40)$ D23N (2MPZ)	
0.607	0.620	0.242	0.156	0.148	$A\beta(1-40)$ E22 Δ (2MVX)	
0.565	0.594	0.218	0.168	0.149	$A\beta(11-42)$ (5KK3)	
0.747	0.697	0.701	0.236	0.304	TAU (5O3L)	
0.761	0.722	0.738	0.231	0.284	TAU (5O3O)	
0.728	0.666	0.576	0.214	0.288	TAU (5O3T)	
CHAIN AS INDIVIDUAL UNIT						
0.491	0.487	0.135	0.140	0.142	$A\beta(15-40)$ D23N (2MPZ)	
0.649	0.686	0.315	0.170	0.144	$A\beta(1-40)$ E22 Δ (2MVX)	
0.513	0.620	0.175	0.166	0.107	<u>$A\beta(11-42)$ (2MXU)</u>	
0.569	0.600	0.230	0.174	0.153	$A\beta(11-42)$ (5KK3)	
0.664	0.595	0.422	0.213	0.287	TAU (5O3L)	
0.661	0.607	0.424	0.217	0.274	TAU (5O3O)	
0.688	0.618	0.471	0.213	0.291	TAU (5O3T)	
0.506	0.588	0.254	0.247	0.178	<u>ASYN (2N0A*)</u>	

Table 2S. Summary of FOD parameters for amyloid protofibrils. Underscores indicate that the given amyloid does not form a superfibril; * – only the 30-100 fragment, which exhibits amyloid-like properties, is subjected to analysis. D_{KL} values for T, R and H distribution treated as target distribution for O distribution allowing the RD calculation.

RD		D_{KL}			AMYLOID
T-O-R	T-O-H	O T	O R	O H	PDB ID
0.614	0.600	0.241	0.151	0.160	A β (15-40) D23N (2MPZ)
0.639	0.659	0.335	0.188	0.173	A β (1-40) E22 Δ (2MVX)
0.680	0.756	0.369	0.173	0.118	<u>Aβ (11-42) (2MXU)</u>
0.608	0.623	0.277	0.178	0.168	A β (11-42) (5KK3)
0.652	0.564	0.425	0.227	0.329	TAU (5O3L)
0.652	0.577	0.430	0.229	0.315	TAU (5O3O)
0.674	0.584	0.469	0.226	0.333	TAU (5O3T)
0.531	0.598	0.286	0.252	0.192	<u>ASYN (2N0A*)</u>

Table 3S. Summary of FOD parameters for superfibrils. D_{KL} values for T, R and H distribution treated as target distribution for O distribution allowing the RD calculation.

RD		D_{KL}			AMYLOID
T-O-R	T-O-H	O T	O R	O H	
0.578	0.494	0.194	0.141	0.199	A β (15-40) D23N (2MPZ)
0.590	0.592	0.252	0.174	0.173	A β (1-40) E22 Δ (2MVX)
0.620	0.652	0.280	0.171	0.149	A β (11-42) (5KK3)
0.730	0.662	0.677	0.250	0.345	TAU (5O3L)
0.745	0.687	0.712	0.243	0.323	TAU (5O3O)
0.724	0.641	0.599	0.228	0.335	TAU (5O3T)

Table 4S. FOD parameters for amyloids consisting of two or three protofibrils. In the case of 5O3T, due to its asymmetric conformation, residues no. 321 and 323 are contributed by one protofibril, while the remaining residues belong to its partner. Underscores indicate that the interface residues form a beta fold. D_{KL} values for T, R and H distribution treated as target distribution for O distribution allowing the RD calculation.

RD					D_{KL}	AMYLOID	
T-O-R	T-O-H	O T	O R	O H	AMYLOID	Residues in interface	
0.424	0.155	0.073	0.100	0.400	A β (15-40) D23N	17,28,29,31,38,40	
0.454	0.313	0.117	0.141	0.257	A β (1-40) E22 Δ	3,4,13,28-30,37-40	
0.595	0.707	0.243	0.165	0.100	A β (11-42))	11, 13, 15, 17, 34-38	
0.388	0.532	0.188	0.297	0.165	TAU (5O3L)	331-336, <u>338</u>	
0.401	0.550	0.345	0.514	0.282	TAU (5O3O)	331-336	
0.538	0.314	0.357	0.307	0.779	TAU (5O3T)	<u>321, 323</u> / 313, 15,317	