

Supplementary Information

Cryo-EM structure of disease-related prion fibrils provides insights into seeding barriers

Qiuye Li, Christopher P. Jaronec, and Witold K. Surewicz

Supplementary Table 1: Cryo-EM data collection, refinement and validation statistics

	huPrP23-144 fibrils (EMDB-24514) (PDB 7RL4)	moPrP23-144 fibrils (polymorph 1) (EMDB-27458) (PDB 8DJA)
Data collection and processing		
Magnification	105,000	105,000
Voltage (kV)	300	300
Electron exposure (e-/Å ²)	53	52
Defocus range (µm)	-0.8 to -1.5	-0.8 to -1.5
Pixel size (Å)	0.828	0.828
Symmetry imposed	C2	C2
Initial particle images (no.)	349,164	76,825
Final particle images (no.)	46,803	10,628
Map resolution (Å)	2.86	3.92
FSC threshold	0.143	0.143
Map resolution range (Å)	2.80 to 4.49	3.90 to 10.63
Refinement		
Initial model used (PDB code)	De novo	De novo
Model resolution (Å)	3.02	4.49
FSC threshold	0.5	0.5
Map sharpening <i>B</i> factor (Å ²)	-82.42	-58.39
Model composition		
Non-hydrogen atoms	4,620	4,600
Protein residues	680	680
Ligands	0	0
<i>B</i> factors (Å ²)		
Protein	88.57	164.65
R.m.s. deviations		
Bond lengths (Å)	0.015	0.006
Bond angles (°)	1.390	1.080
Validation		
MolProbity score	2.20	2.41
Clashscore	11.94	24.46
Poor rotamers (%)	0	0
Ramachandran plot		
Favored (%)	87.50	90.62
Allowed (%)	12.50	9.38
Disallowed (%)	0	0