Degradation of fungal prion HET-s(218-289) induces formation of a generic amyloid fold

William Wan, Holger Wille, Jan Stöhr, Ulrich Baxa, Stanley B. Prusiner, and Gerald Stubbs

SUPPORTING MATERIAL

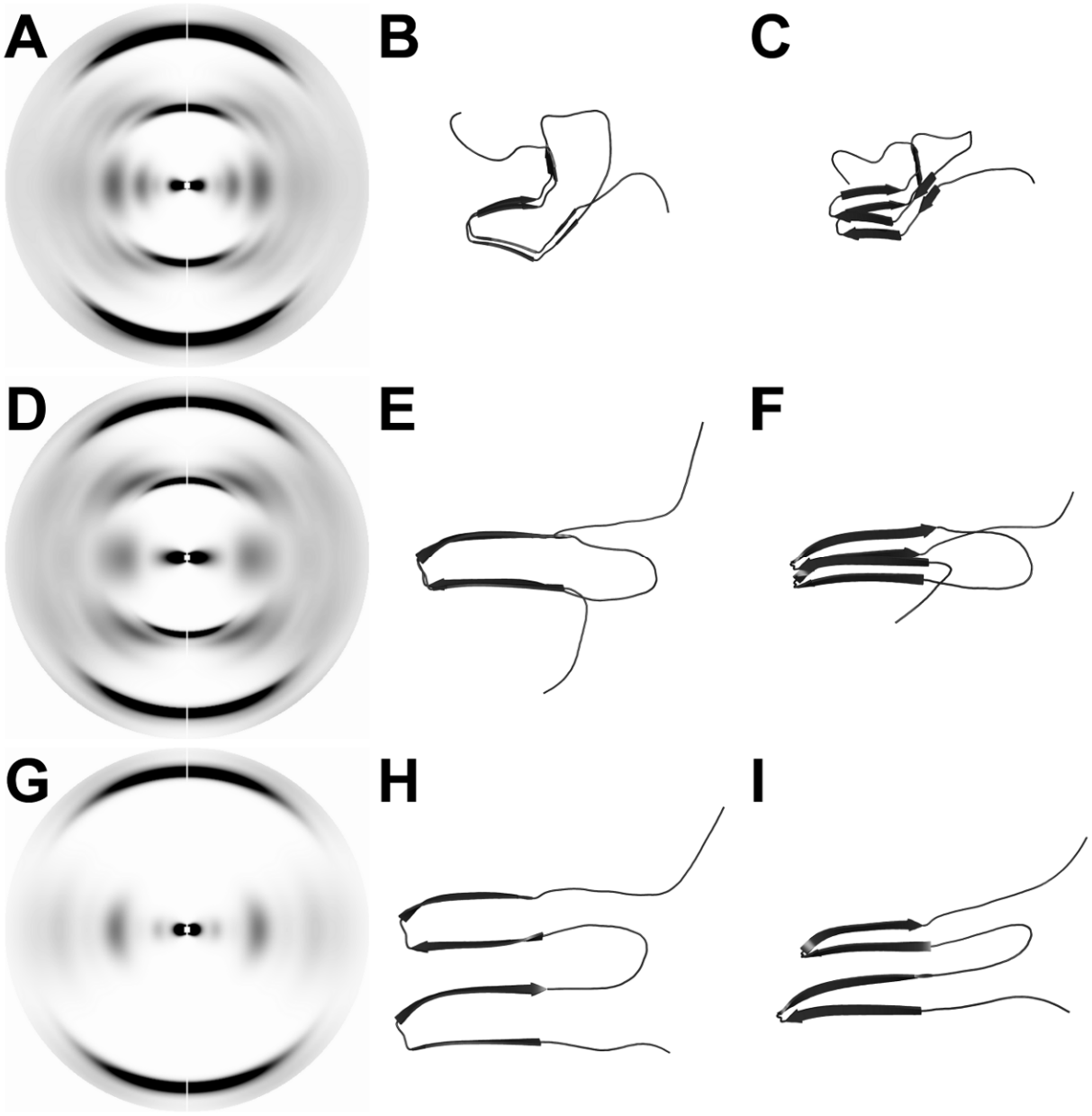

Figure S1. Examples of diffraction patterns calculated from solenoidal and stacked-sheet structures. (*A*) Diffraction pattern calculated from the two-layer solenoidal HET-s structure (1). (*B*) Axial view of the subunit used to calculate (*A*). (*C*) Transverse view of the subunit in (*B*). (*D*) Diffraction pattern calculated from a fibril constructed from a stacked β-sheet subunit in which the axial repeat consisted of two layers of β-strands. (*E*) Axial view of the subunit used to calculate (*D*). (*F*) Transverse view of the subunit in (*E*). (*G*) Diffraction pattern calculated from a fibril constructed from a stacked β-sheet subunit in which the axial repeat consisted of a single layer of β-strands. (*H*) Axial view of the subunit used to calculate (G). (I) Transverse view of the subunit in (H). Meridional diffracted intensity at 9.5 Å is prominent in (*A*) and (*D*). Equatorial intensity is dominated by diffraction at about 10 Å in (*D*) and (*G*), in distinct contrast to (*A*). Diffraction patterns were calculated using the program DISORDER from the FiberNet website (www.fiberdiffraction.org). Models in (E), (F), (H), and (I) were constructed from the HET-s(218-289) amino acid sequence using SwissPDBViewer (2) and visualized using PyMOL (3). These models are hypothetical, and are presented only for the purpose of illustrating the effect of the different types of β-sheet structure on the diffraction patterns. They have not been optimized, other than to avoid unacceptable bond lengths, angles, and close interatomic contacts.

SUPPORTING REFERENCES

1. Van Melckebeke, H., C. Wasmer, A. Lange, E. Ab, A. Loquet, A. Böckmann, and B. H. Meier. 2010. Atomic-resolution three-dimensional structure of HET-s(218−289) amyloid fibrils by solid-state NMR spectroscopy. *J. Am. Chem. Soc.* 132:13765–13775.
2. Guex, N., and M. C. Peitsch. 1997. SWISSMODEL and SWISSPDB VIEWER: an environment for protein modeling. *Electrophoresis* 18:2714–2723.
3. The PyMOL Molecular Graphics System, Version 1.2r1 (Schrödinger, LLC., Portland, OR).