Supporting Information

Phenyl-Ring Dynamics in Proteins and Amyloid Fibrils: the Consistent Microscopic-Order-Macroscopic-Disorder Perspective

Eva Meirovitch[1, *] Zhichun Liang[2] and Jack H. Freed[2]

[1]The Mina and Everard Goodman Faculty of Life Sciences, Bar-Ilan University, Ramat-Gan 5290002 Israel; [2]Baker Laboratory of Chemistry and Chemical Biology, Cornell University, Ithaca, NY 14853-1301, U.S.A

*Corresponding author: eva.meirovitch@biu.ac.il, phone: 972-3-531-8049

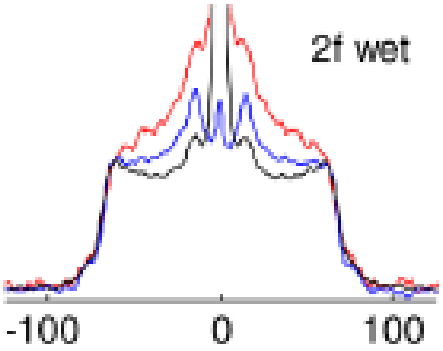

Figure S1. ^{2}H quadrupole-echo spectra of F19 in the hydrated 2-fold-symmetric striated-ribbon $A\beta_{40}$ amyloid fibril-variant (2fw) at 278 (black), 295 (blue) and 308 (red) K.[1]

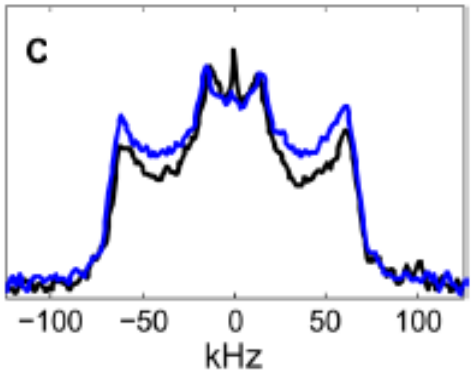

Figure S2. ^{2}H quadrupole-echo spectra of F58 at 295 K in hydrated (black) and dry (blue) HP36.[2]

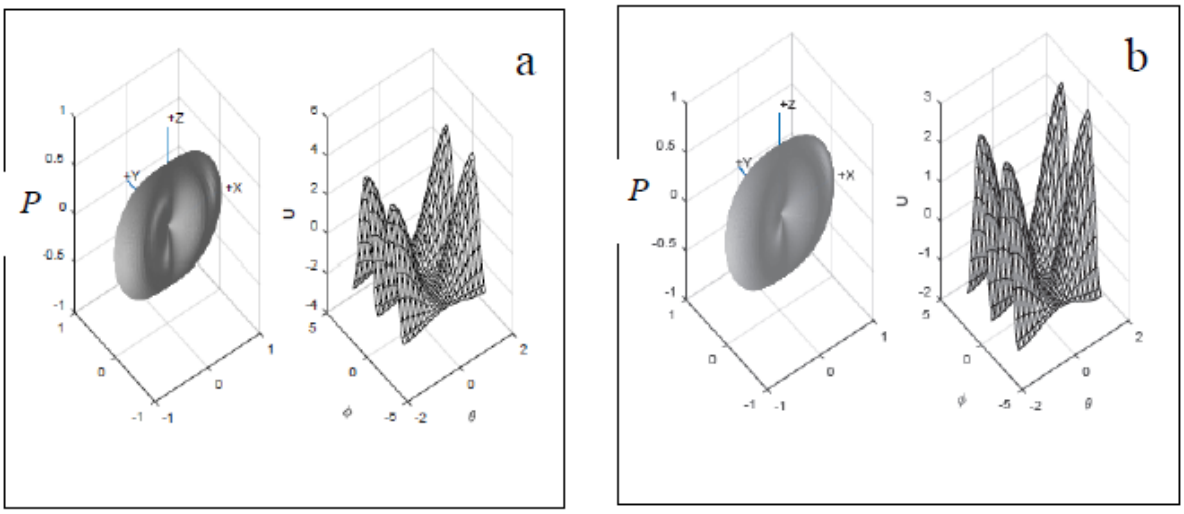

Figure S3. 3D plots of the potential $u = -1.8D_{00}^2 - 2.6(D_{02}^2 + D_{0-2}^2)$, and the corresponding probability density, $P = \exp(-u)$ (part a); 3D plots of the potential $u = -1.2D_{00}^2 - 1.8\,(D_{02}^2 + D_{0-2}^2)$, and the corresponding probability density, $P = \exp(-u)$ (part b).

References

1. Vugmeyster, L.; Clark, M. A.; Falconer, I. B.; Ostrovsky, D.; Gantz, D.; Qiang, W. Flexibility and Solvation of Amyloid-β Hydrophobic Cores. *J. Biol. Chem.* **2016**, *291*, 18484-18495.

2. Vugmeyster, L.; Ostrovsky, D.; Villafranca, T.; Sharp, J.; Xu, W.; Lipton, A. S.; Hoatson, G. L.; Vold, R. L. Dynamics of Hydrophobic Core Phenylalanine Residues Probed by Solid-State Deuteron NMR. *J. Phys. Chem. B* **2015**, *119*, 14892-14904.