Title:	Conformational and Solvation Dynamics of an Amyloidogenic Intrinsically Disordered Domain of a Melanosomal Protein.
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Abstract:	The conformational plasticity of intrinsically disordered proteins (IDPs) allows them to adopt a range of conformational states that can be important for their biological functions. The driving force for the conformational preference of an IDP emanates from an intricate interplay between chain–chain and chain–solvent interactions. Using ultrafast femtosecond and picosecond time-resolved fluorescence measurements, we characterized the conformational and solvation dynamics around the N- and C-terminal segments of a disordered repeat domain of a melanosomal protein Pmel17 that forms functional amyloid responsible for melanin biosynthesis. Our time-resolved fluorescence anisotropy results revealed slight compaction and slower rotational dynamics around the amyloidogenic C-terminal segment when compared to the proline-rich N-terminal segment of the repeat domain. The compaction of the C-terminal region was also associated with the restrained mobility of hydration water as indicated by our solvation dynamics measurements. Our findings indicate that sequence-dependent chain–solvent interactions govern both the conformational and solvation dynamics that are crucial in directing the conversion of a highly dynamic IDP into an ordered amyloid assembly. Such an interplay of amino acid composition-dependent conformational and solvation dynamics might have important physicochemical consequences in specific water–protein, ion–protein, and protein–protein interactions involved in amyloid formation and phase transitions.
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