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Structural discordance in HIV-1 Vpu from brain isolate alarms amyloid fibril forming behavior: A computational perspective

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**HIGHLIGHTS:**

- HIV-1 Vpu protein derived from brain isolate is predicted to encapsulate a stretch of amino acids possessing aggregating potential
- The residues in the predicted amyloid region of brain derived HIV-1 Vpu exhibits ambiguity in their secondary structure
- The molecular simulation of brain derived HIV-1 Vpu presents a conformational transition from  $\alpha$ -helix to  $\beta$ -sheet highlighting its prospective role in amyloidogenicity and underlying neurodegeneration in HIV associated dementia

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