8K00: Interface Residue-Level Analysis (IDP Chain, Reference Coordinates)
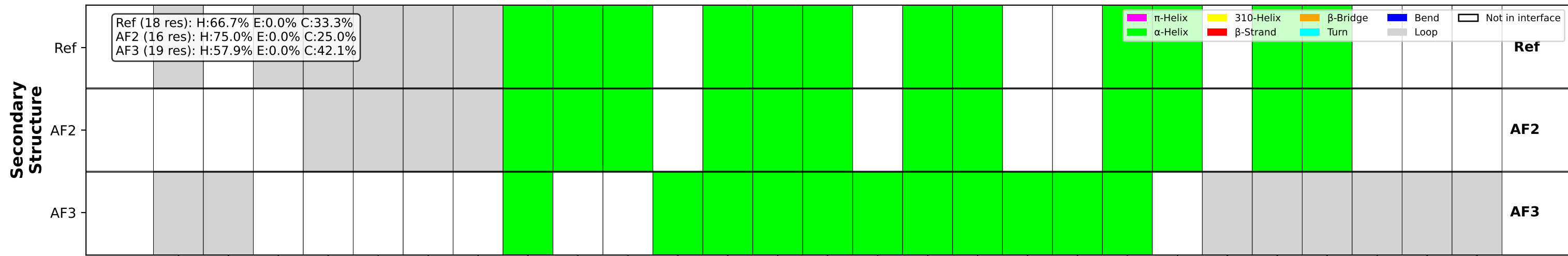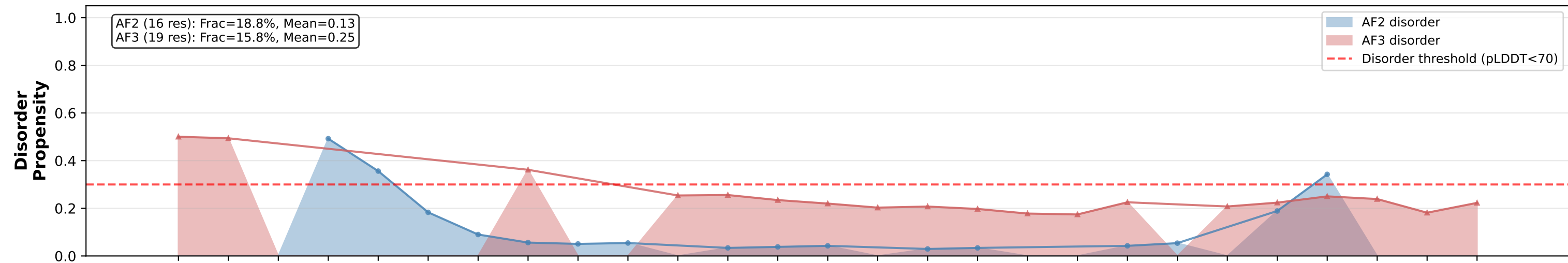
A Secondary Structure

Ref (18 res): H:66.7% E:0.0% C:33.3%
AF2 (16 res): H:75.0% E:0.0% C:25.0%
AF3 (19 res): H:57.9% E:0.0% C:42.1%

Legend: π-Helix, 310-Helix, β-Bridge, Bend, Not in interface, α-Helix, β-Strand, Turn, Loop

B Disorder Propensity

AF2 (16 res): Frac=18.8%, Mean=0.13
AF3 (19 res): Frac=15.8%, Mean=0.25

AF2 disorder
AF3 disorder
Disorder threshold (pLDDT<70)

C Hydropathy (Kyte-Doolittle)

Ref: Mean=-0.47 | Hydrophobic=33.3%
AF3: Mean=-0.27 | Hydrophobic=36.8%

Hydrophobic (+) [AF3], Hydrophobic (+) [AF2], Hydrophobic (+) [Ref]
Hydrophilic (−) [AF3], Hydrophilic (−) [AF2], Hydrophilic (−) [Ref]

Residue Position (Reference Numbering)

G533³, T534³, S536ʳ, G537ʳ², S538ʳ², A539ʳ², F540ʳ², D543, D544ʳ², L545ʳ², M546³, S547, I548, D549, L550³, A551, E552, Q553³, M554³, A555, N556ʳ², D557³, S558, D559, S561³, I562³, S563³

Markers: ʳ=Ref only, ²=AF2 only, ³=AF3 only, ʳ²=Ref+AF2, ʳ³=Ref+AF3, ²³=AF2+AF3, (none)=All three