

Folding of Small Proteins Using Constrained Molecular Dynamics

Gouthaman S. Balaraman,[†] In-Hee Park,[†] Abhinandan Jain,[‡] and Nagarajan Vaidehi[†]

[†] Division of Immunology, Beckman Research Institute of the City of Hope, Duarte, CA 91010, USA.

[‡] Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, USA

Supporting Material

1. We calculated the helicity of the WALP16 peptide using the helical backbone torsions from experiments. These values are $\phi = -62^\circ$ and $\psi = -41^\circ$. The helicity calculated using these angles are shown in red and the helicity calculated using $\phi = -57^\circ$ and $\psi = -47^\circ$ is shown in blue. It is seen that the trend in helicity is the same in both the cases.

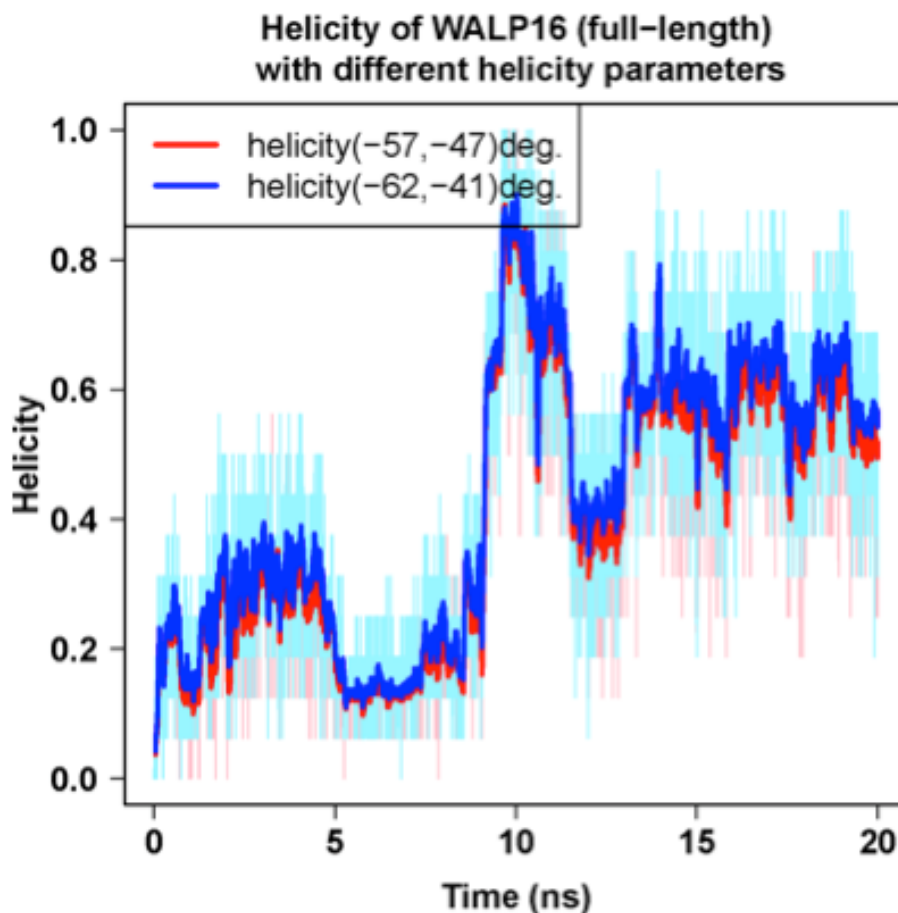


Figure S1. Calculated helicity comparison for the full-length WALP16 (Δ 1-18) using two different helicity parameter set; Red and blue lines are moving averages (50 points average) from the raw helicity data (pink and cyan, respectively).