Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: Folding and modulation of helical conformation of Glycophorin A by point mutations

Pei-Yin Lee,[†,§] Abhilash Sahoo,[‡,§] and Silvina Matysiak[*,¶]

†*Chemical Physics Program, University of Maryland, College Park, Maryland, USA*

‡*Biophysics Program, University of Maryland, College Park, Maryland, USA*

¶*Fischell Department of Bioengineering, University of Maryland, College Park, Maryland, USA*

§*P.l. and A.S. contributed equally to this work.*

E-mail: matysiak@umd.edu

Phone: +1 301-405-0313

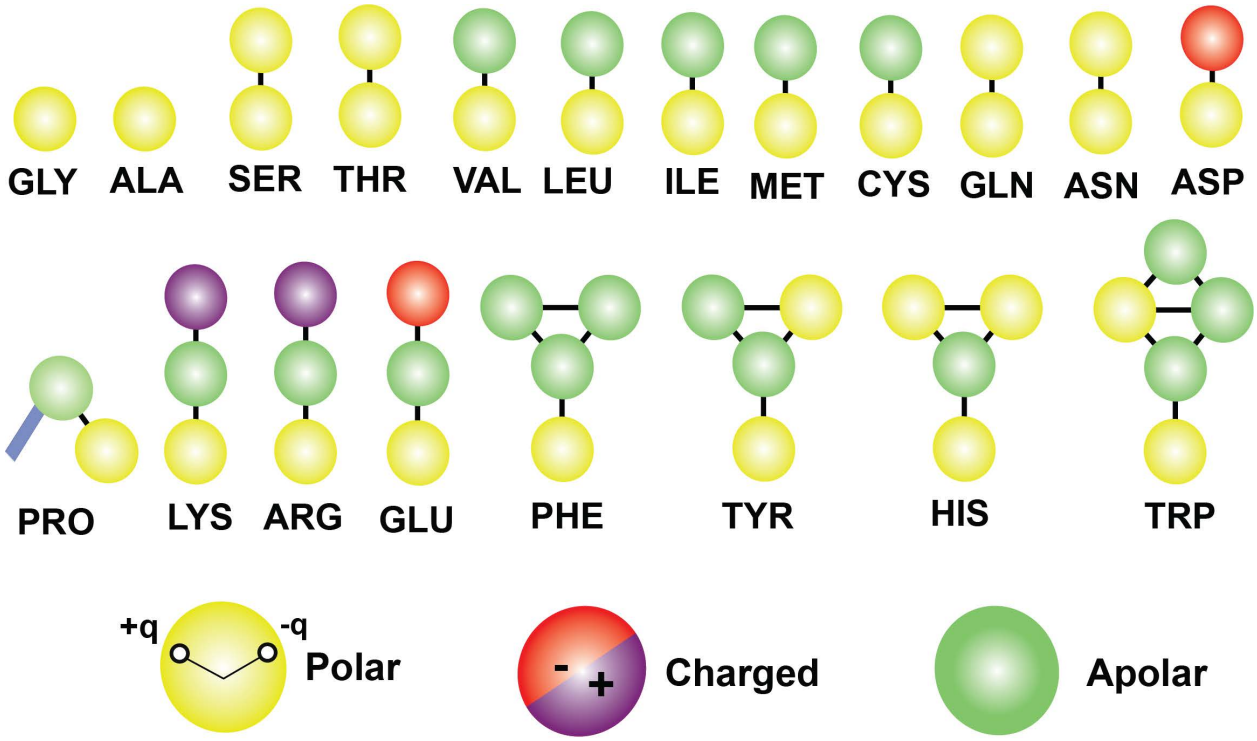

Figure S1: Schematic geometries of coarse-grained amino-acids and water. Polar beads are in yellow and carry two dummies.

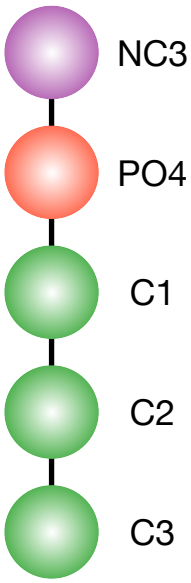

Figure S2: Coarse grained geometry of the DPC micelle. Apolar beads are in green, negatively charged bead is in red, and positively charged bead is in purple. The bead names are shown on the right.

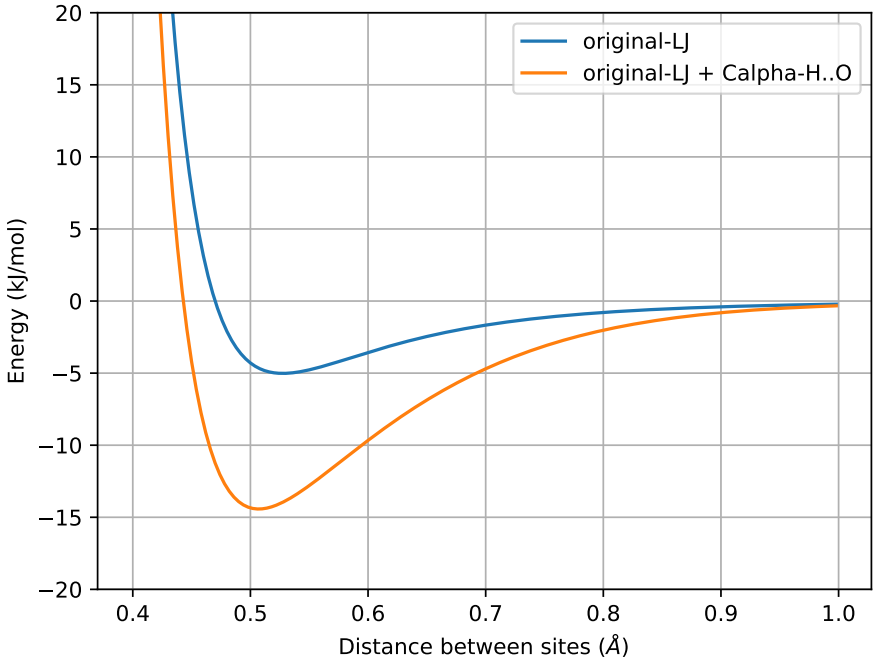

Figure S3: Interaction between Gly backbone of one monomer with Val/Leu backbone of the other monomer before (blue) and after (orange) addition of CαH..O interaction.

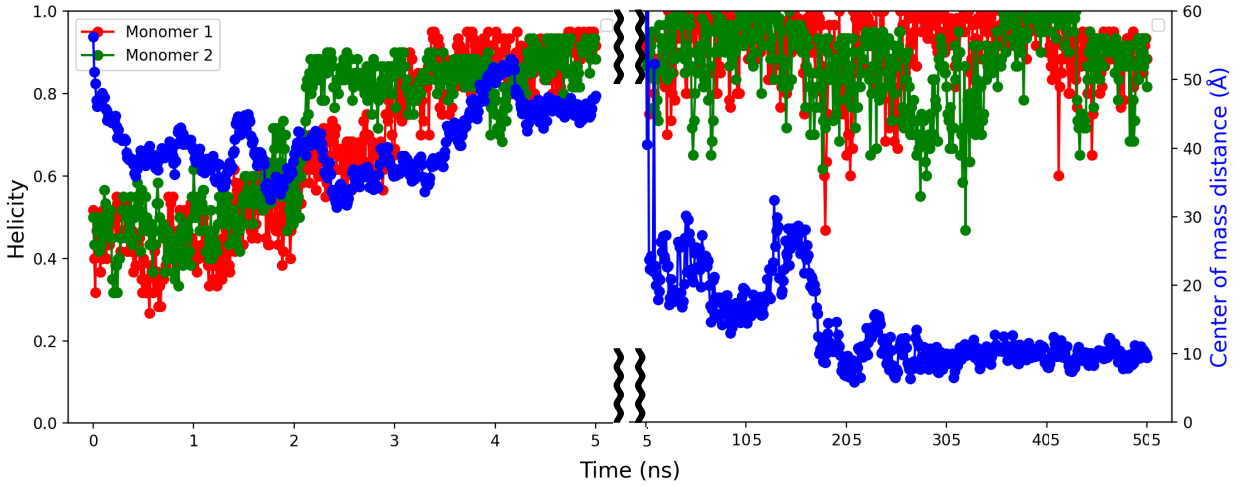

Figure S4: Time series of helicity for two WT GpA peptides and the center of mass distance between these two peptides for trial 2.

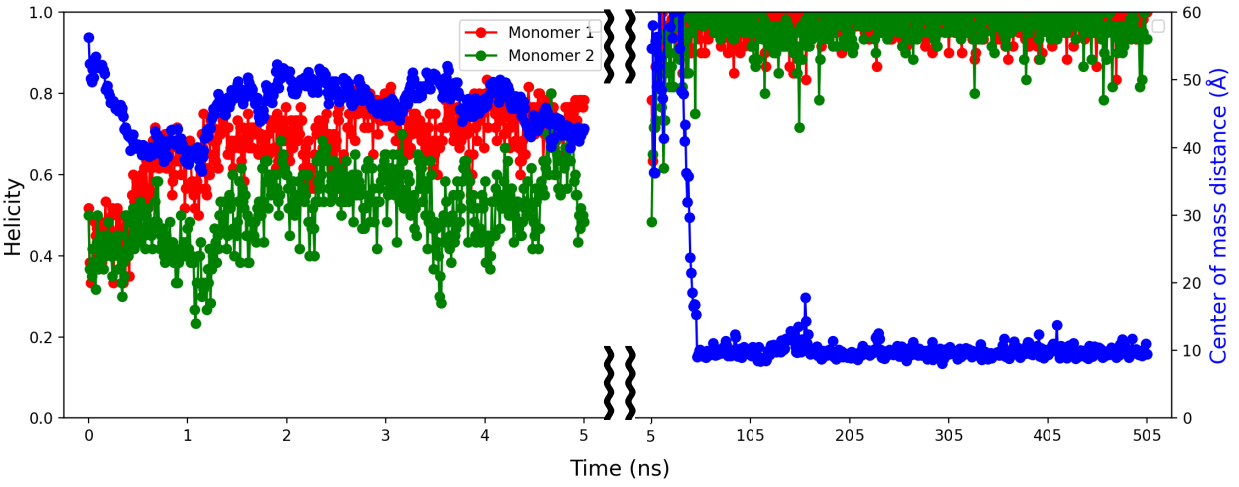

Figure S5: Time series of helicity for two WT GpA peptides and the center of mass distance between these two peptides for trial 3.

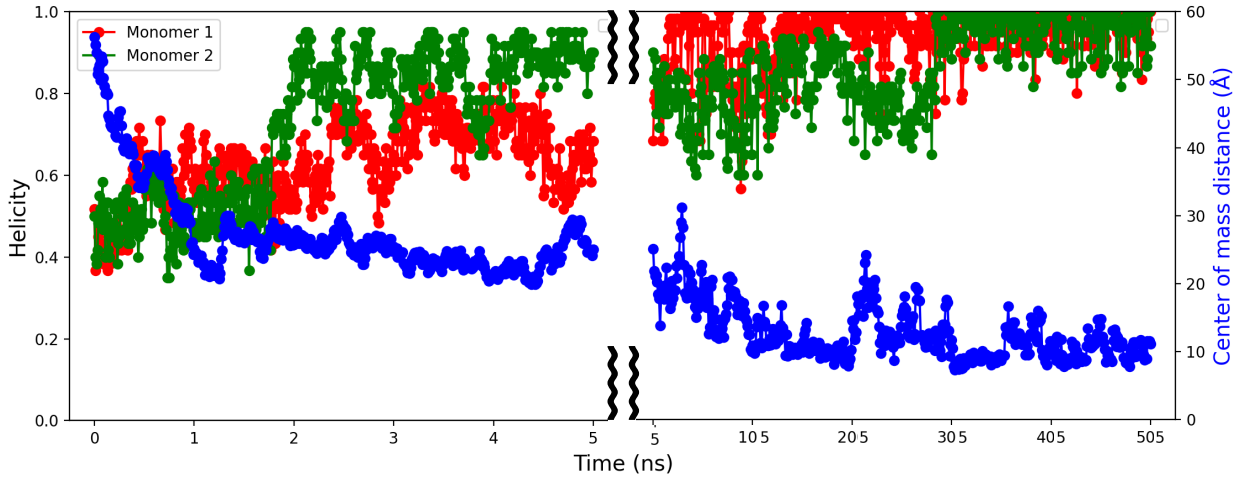

Figure S6: Time series of helicity for two WT GpA peptides and the center of mass distance between these two peptides for trial 4.

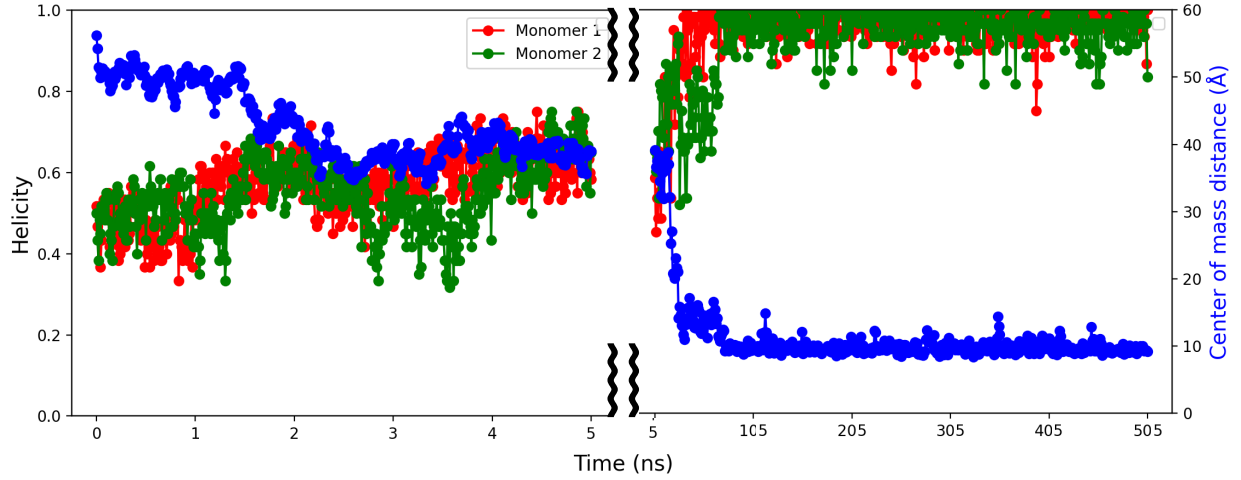

Figure S7: Time series of helicity for two WT GpA peptides and the center of mass distance between these two peptides for trial 5.

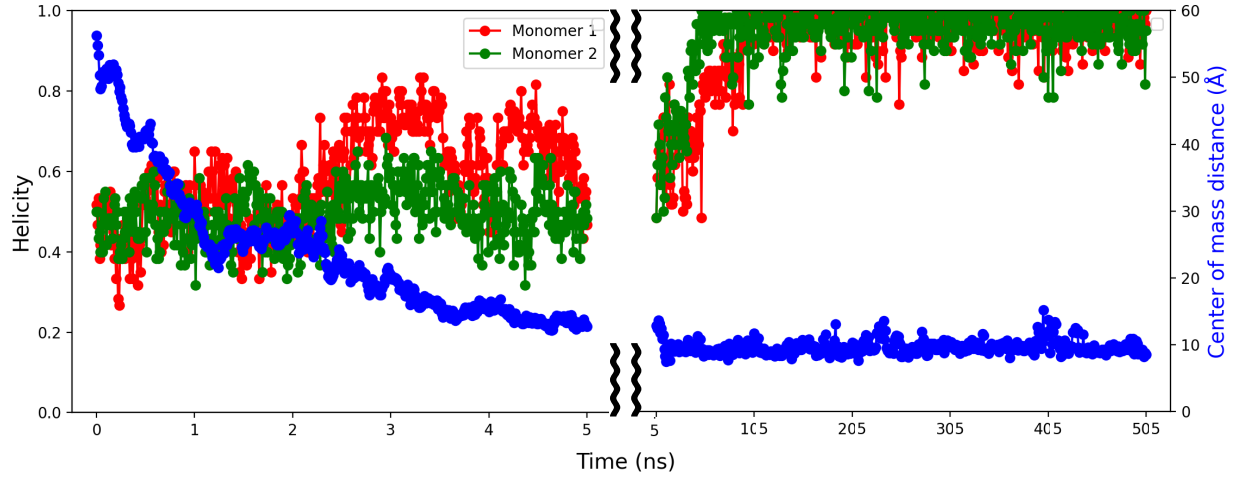

Figure S8: Time series of helicity for two WT GpA peptides and the center of mass distance between these two peptides for trial 6.

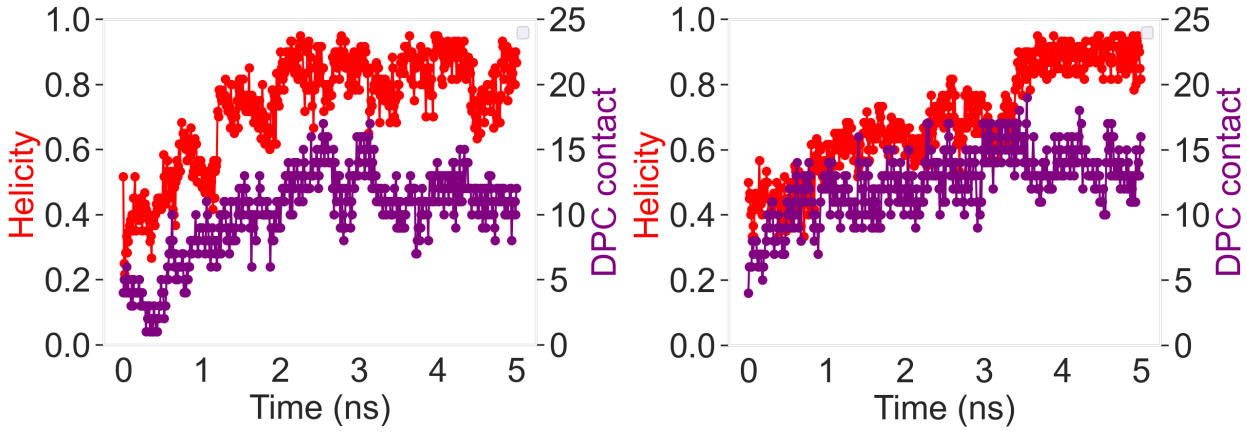

Figure S9: Helicity and number of DPC contacts time series for each of the GpA peptide in trial 1.

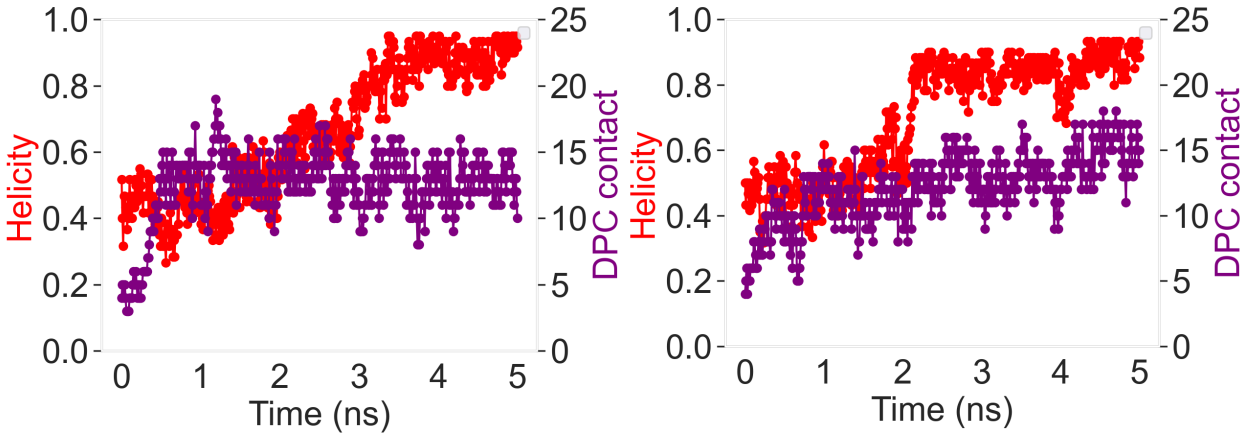

Figure S10: Helicity and number of DPC contacts time series for each of the GpA peptide in trial 2.

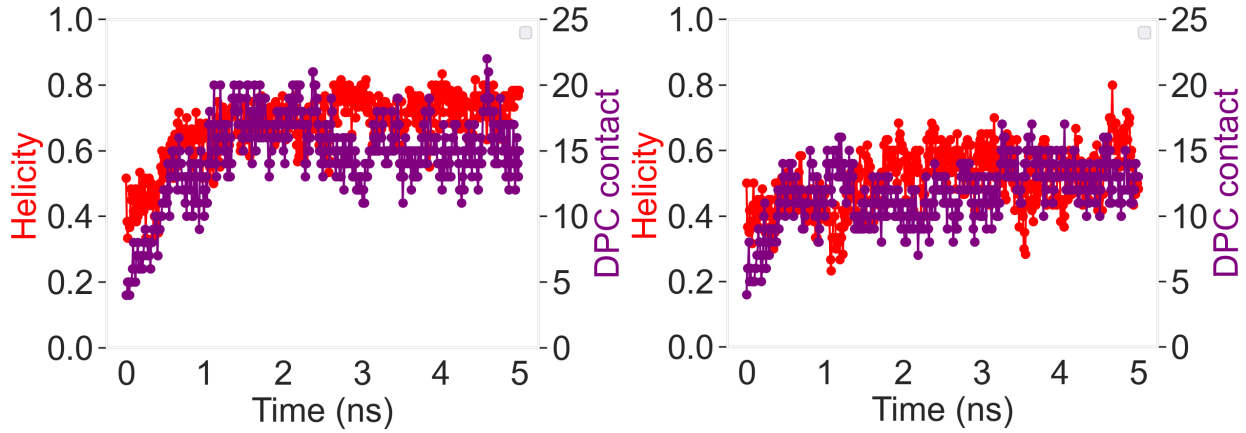

Figure S11: Helicity and number of DPC contacts time series for each of the GpA peptide in trial 3.

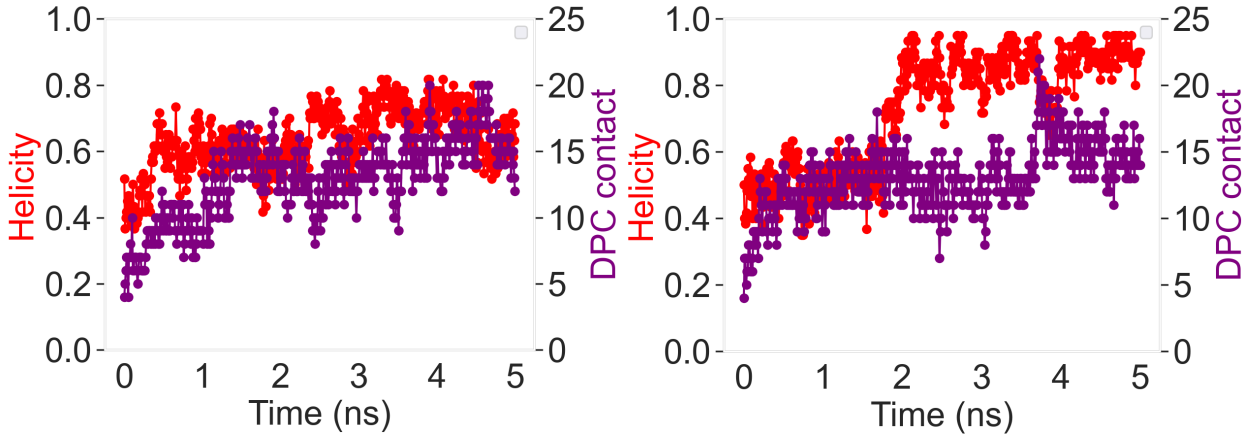

Figure S12: Helicity and number of DPC contacts time series for each of the GpA peptide in trial 4.

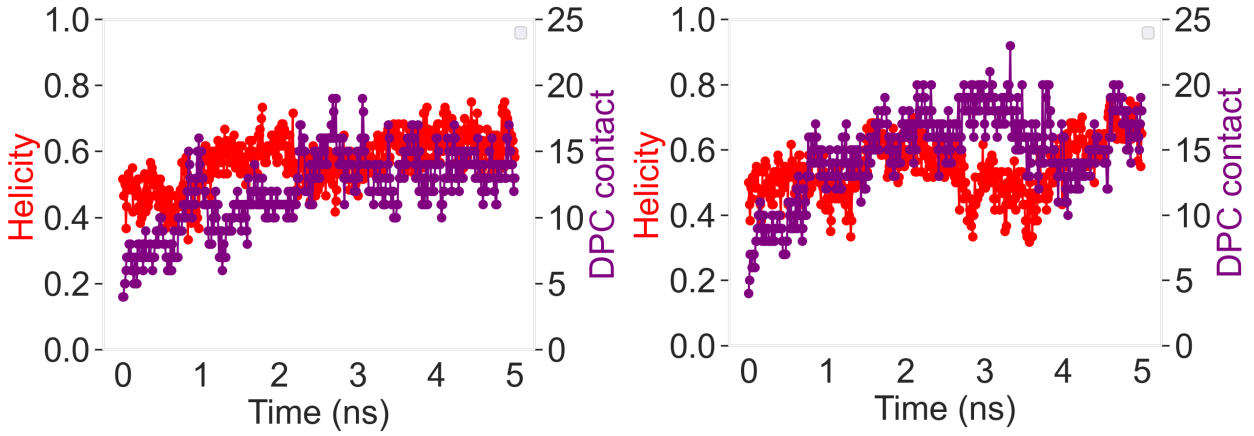

Figure S13: Helicity and number of DPC contacts time series for each of the GpA peptide in trial 5.

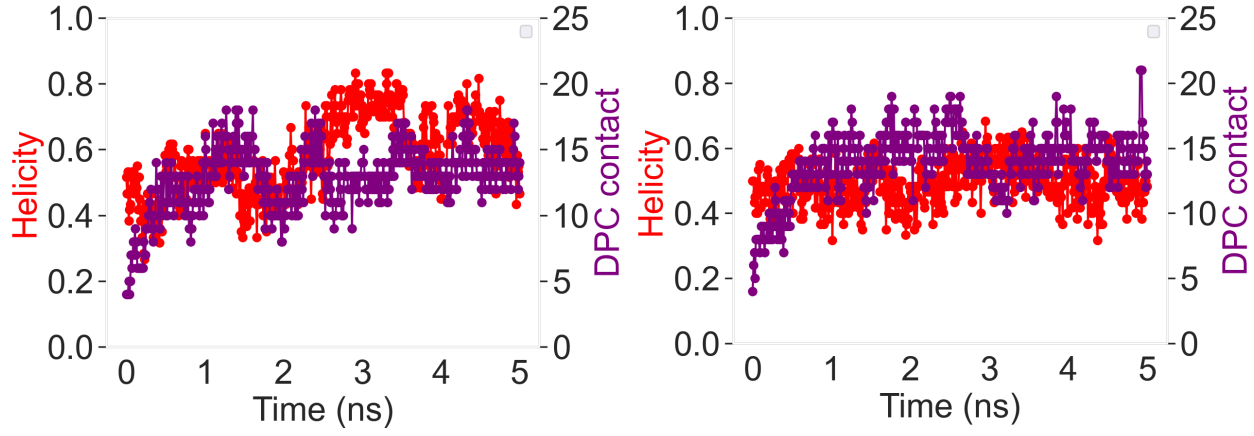

Figure S14: Helicity and number of DPC contacts time series for each of the GpA peptide in trial 6.