



All-atom models of HIV-1 Env spike

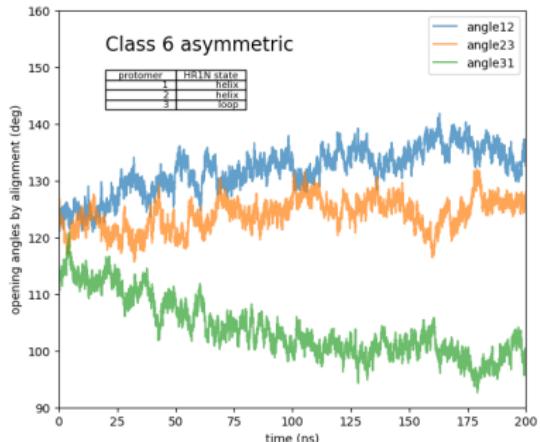
Cameron F. Abrams and Salsabil Abou-Hatab

March 21, 2024

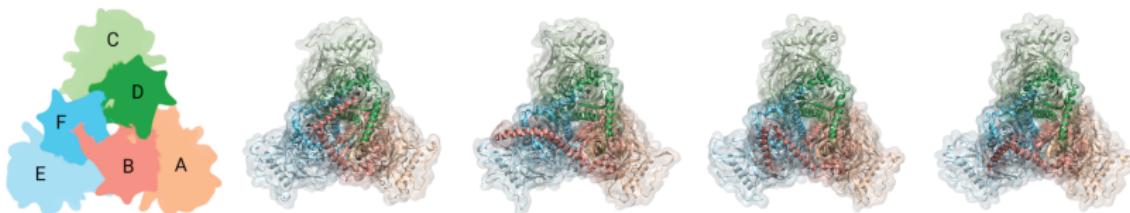
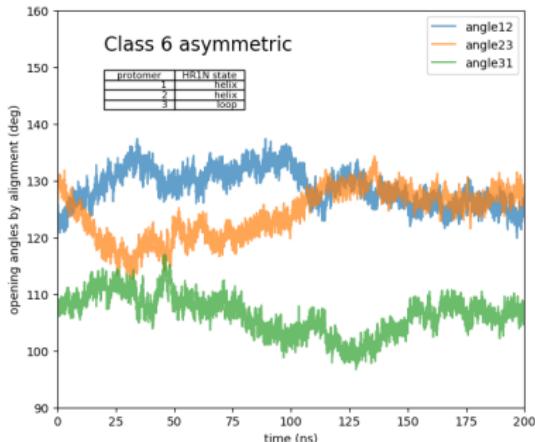
Drexel University, Department of Chemical and Biological Engineering

C6-FT-HHL (as-received Tri-FPPR class 6 cryo-EM model)

gp120 alignment



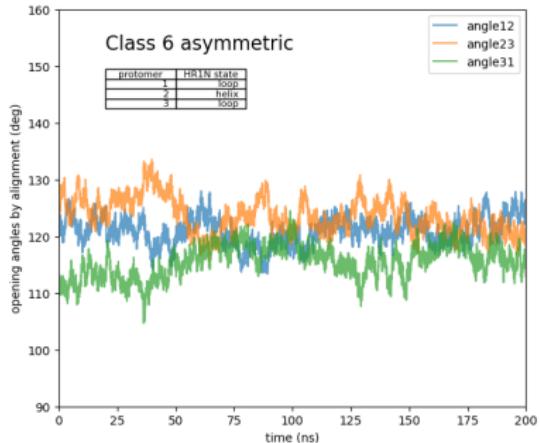
gp41 alignment



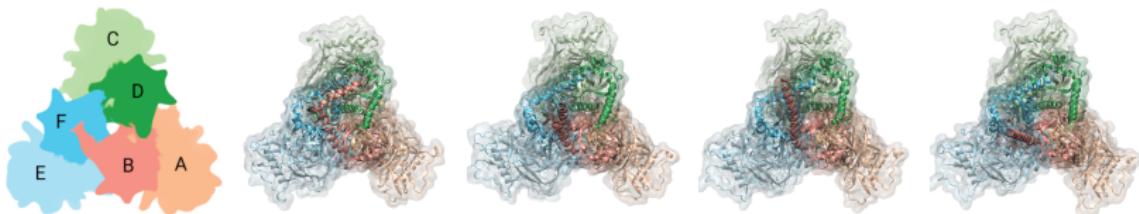
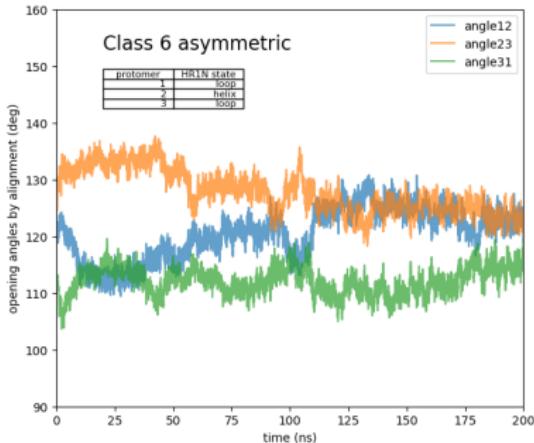
Protomer 1 MPER “flops out” and binds to protomer 3 gp41

C6-FT-LHL (HR1N unfolded in protomer 1 and 3)

gp120 alignment



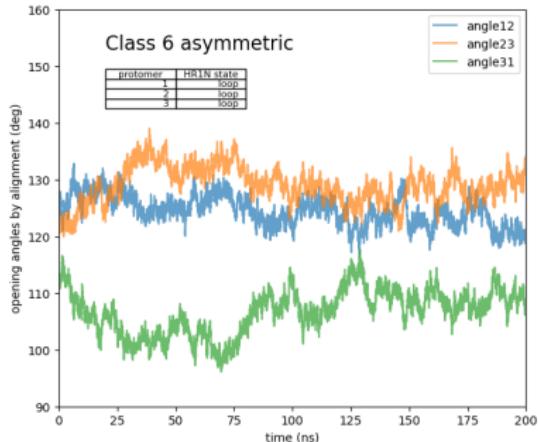
gp41 alignment



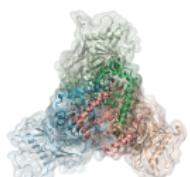
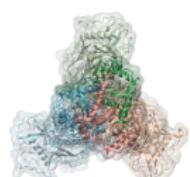
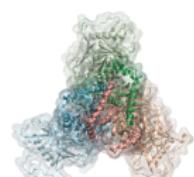
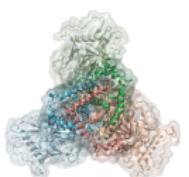
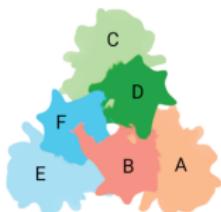
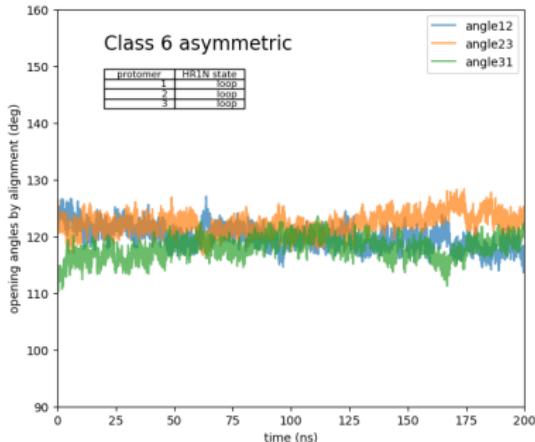
Protomer 1 α 9 and MPER become one helix

C6-FT-LLL (HR1N unfolded in all protomers)

gp120 alignment



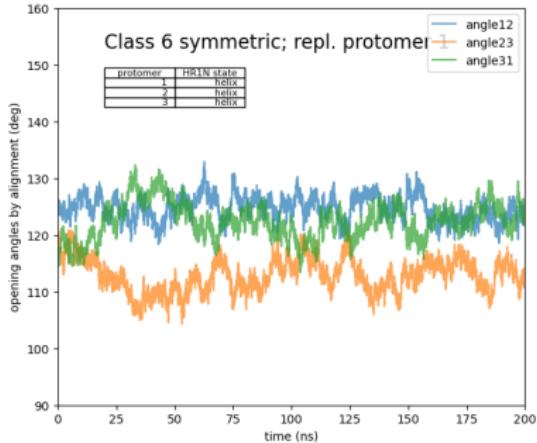
gp41 alignment



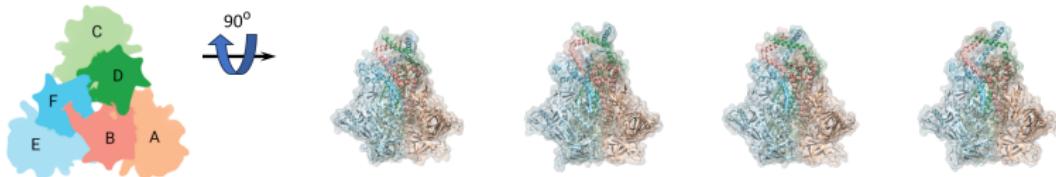
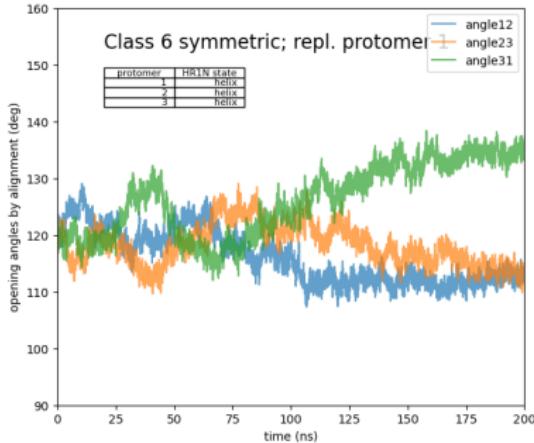
Protomer 1 MPER remains relatively stable

C6-S1-HHH (Protomer 1 replicated onto 2, 3)

gp120 alignment



gp41 alignment



Protomer 1 MPER remains relatively stable