**README**

**Louis R. Hollingsworth IV1-3, Anne M. Brown2,4, Richard D. Gandour3,5,\* and David R. Bevan2,5,\*.**

This file is intended to provide a brief overview of the contents of this archive. For additional information, please contact the authors.

**File Tree Structure and Description**

**Clusters**

* Cluster size document: # frames binned into each cluster (0.2 nm RMSD cutoff)
* Amber and Charmm folders: Contain dominant clusters for each replicate of Amber and Charmm gp120 simulations, respectively

**Docking**

* Docking Box: Docking box vectors for each protein
* Docking Results: Docking scores for ligands docked into structures prior to MD simulations
* Docking\_preMD: Docking to Homology models
  + Largebox: Largebox.txt -- Vina configuration file for the larger box for each protein
  + Ligands: Contains pdbqt files for every ligand (enantiomer, protonation state = 112 total)
  + Receptors: PDBQT files of the receptors used to dock
  + Results
    - Grouped by ligand then by box (large box = docked to entire protein, V3 = V3 loop only). Output log file (with scores) and output poses (pdbqt files) separated into different folders
  + V3: Vina configuration file vina docking boxes around each V3 loop
* Docking\_postMD: Docking to cluster structures following MD simulations

Largebox: Largebox.txt -- Vina configuration file for the larger box for each protein

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  + Receptors: PDBQT files of the receptors used to dock
  + Results
    - Grouped by ligand then by box (large box = docked to entire protein, V3 = V3 loop only). Output log file (with scores) and output poses (pdbqt files) separated into different folders
  + V3: Vina configuration file vina docking boxes around each V3 loop

**Eigenvector**

* Eigenvectors extremes (with interpolation between states) for each structure (pdb files)

**Figures**

* Many of the figures in the paper and supplemental information

**GP120\_FST**

* Sequences of each gp120 in the paper (other than the published sequence for the 2B4C crystal structure)

**Homology Model**

* Homology models, starting coordinates for MD simulations

**RMSD**

* Amber and Charmm folders: Contain root-mean-squared-deviation (RMSD) graphs for each replicate of Amber and Charmm gp120 simulations, respectively. Also, each contains RMSD block averages.

**RMSF**

* Amber and Charmm folders: Contain root-mean-squared-fluctuation (RMSF) graphs for each replicate of Amber and Charmm gp120 simulations, respectively.

**V1/V2-V3 Loop Distance**

* Amber and Charmm folders: Contain measured distance (backbone) between the V1/V2 and V3 loops (center of mass) for Amber and Charmm simulations