Steps for typical MD using the AMBER16 GUI

1. Open Linux terminal and type ‘perl GUI_DROIDS_START.pl’ to open GUI
2. specify query and reference PDB files in your DROIDS folder
3. Specify number of production run samples to take (note: should be >30)
4. Check box for solvation method (note: explicit takes longer and uses considerably more memory)
5. Specify the length of heating, equilibration, and each production run (note: energy minimization step is hard coded)
6. Create MD control files
7. Click on the alignment button and USCF Chimera will open and you will be prompted at terminal to use MatchMaker and Match->Align to create a Clustal (.aln) file as well as to choose the residue from which you want to reference your atom correlations. Simply close Chimera to continue on. NOTE: make sure the sequence files and structure files reference the same amino acid at the start of the chain. Occasionally, PDB files don’t exactly match the reposited sequences. Edit your alignment file accordingly.
8. Create/check your topology and coordinate files using teLeap button. Read the terminal output carefully here.
9. Launch MD runs (note: MD runs can be monitored at the main Linux and GPU surveillance terminals. The cpptraj GUI will open upon completion)

Cpptraj GUI

1. Re-enter PDB and MD control parameters as specified
2. Using GUI, make ccptraj control files, atom info files, atom fluctuation files.
3. Click ‘prepare/parse files for DROIDS’ and follow directions on main Linux terminal.
4. DROIDS GUI will open when step 3 and 4 is done.

DROIDS analysis GUI

1. Enter PDB ID’s, length of protein, and number of frames for movies.
2. Choose visualization options for Chimera protein representation, types of motion to analyze, type of K-S test result to view, corresponding color scheme, and method of multiple test correction.
3. Run statistical tests (note: R graphics plots and data files will appear in resulting folder for each analysis)
4. Create chimera attribute file and display these results on static PDB structure in the Chimera viewer
5. Render movies on XYZ axes of the reference PDB and display in DROIDS movie viewer