Argument	Function
python3 **$dir_py**/run_pipeline.py	The initial command that executes the Python script found at $dir_py - thus running the pipeline.
-s $dir_run/[PDBNAME]_af2.pdb	Sets the initial PDB that the pipeline will run on to the designated file. In practice, [PDBNAME] will be replaced with the PDB ID of the target PPI (e.g. 1DAN).
-o $dir_run/output_[PDBNAME]	Sets the output directory of the pipeline. If this directory does not exist, it will be created.
-i fullrun	Informs the program what steps of the pipeline should be run. In this case, the fullrun command causes the setup, the initial relaxation step and the mutagenesis step to occur.
-mm mut_file -m $dir_run/[PDBNAME]_mutfile.txt	Informs the program that it should be reading mutations in from a mutfile as opposed to saturation mutagenesis, and designates a .txt file to be read in for that purpose. See Section 4.4 for more details on mutfiles.
--chainid ABCD --run_struc ABCD	Designates which chain or chains of the target complex should be subject to analysis. In this study, all chains will be included here, so the parameter ABCD will be changed to accommodate the IDs of every chain.
--overwrite_path True	Tells the program to overwrite existing data in the output directory if there is any. Used in case a run causes errors and needs to be repeated.
--slurm_partition sbinlab_ib	Tells the program which partition in the computing cluster to use. Must be the same as in the batch file parameters.
--dump_pdb True	Tells the program to export and save all mutant PDBs.