Manual for StrandTwister_v2

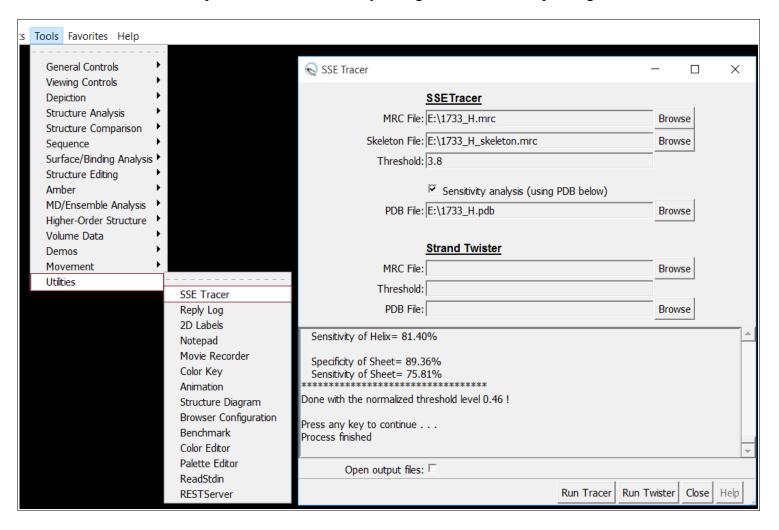
Usage within USCF Chimera

Setup:

To use StrandTwister in Chimera, copy the folder "SSETracer" from "SSETracer_Chimera" into Chimera's "share" folder.

StrandTwister will be available for use under Tools \rightarrow Utilities \rightarrow SSE Tracer.

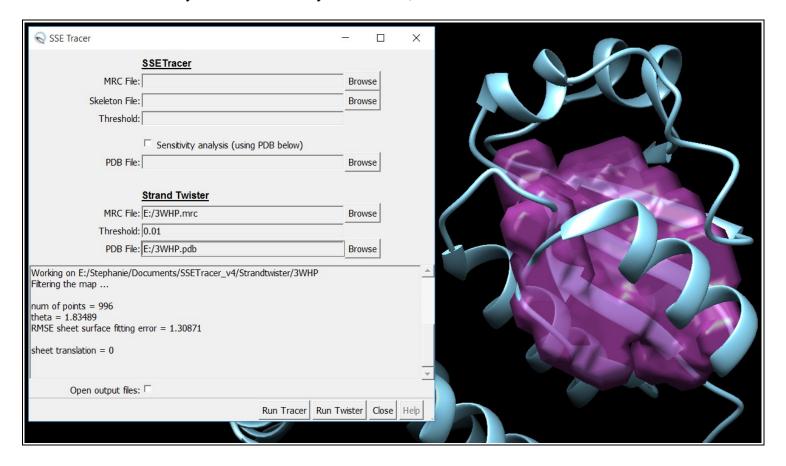
StrandTwister input files can be selected by hitting each field's corresponding "Browse" button.



Required input:

Density mrc file for a single beta sheet Threshold PDB model file

The threshold parameter corresponds with the threshold of the sheet density map. If the input MRC density voxels have already been filtered, the threshold can be set to 0.



To run:

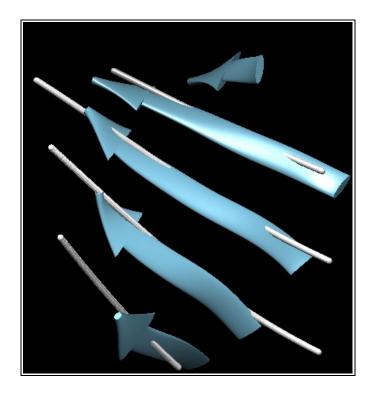
After providing the necessary files and threshold value, hit the button "Run Twister".

Output:

Output will be located in the same directory as the density mrc file, in a subdirectory named after the mrc file.

Example: Input file 3WHPsht35.mrc will result in an output directory 3WHPsht35twist.

StrandTwister will output the Top ten detected beta-traces as PDB files. Detected beta-traces will be labeled as "pdbID trans # orient *.pdb"



Example of outputted beta-trace 3WHP_trans_1_orient_30, displayed as white lines.

Usage with Command Line

To use StrandTwister in command line, run with "strandtwister_v2_command <pdb> <mrc> <threshold>". Note that the input files must include the path but not the file extension. Required inputs and provided output files are the same as in the GUI version.