About

The extended version of LPTD software (LPTD_GUI_2) can be used for any protein in which the atomic model and the predicted secondary structure from the cryo-EM map are provided by the user. In the following the description of how one can utilize the LPTD for such proteins is elaborated.

Getting Started

1. Download or clone LPTD to your computer
2. Start MATLAB (R2020a)
3. Double-click on “LPTD_GUI_2.fig”
4. You can find a screen as below:

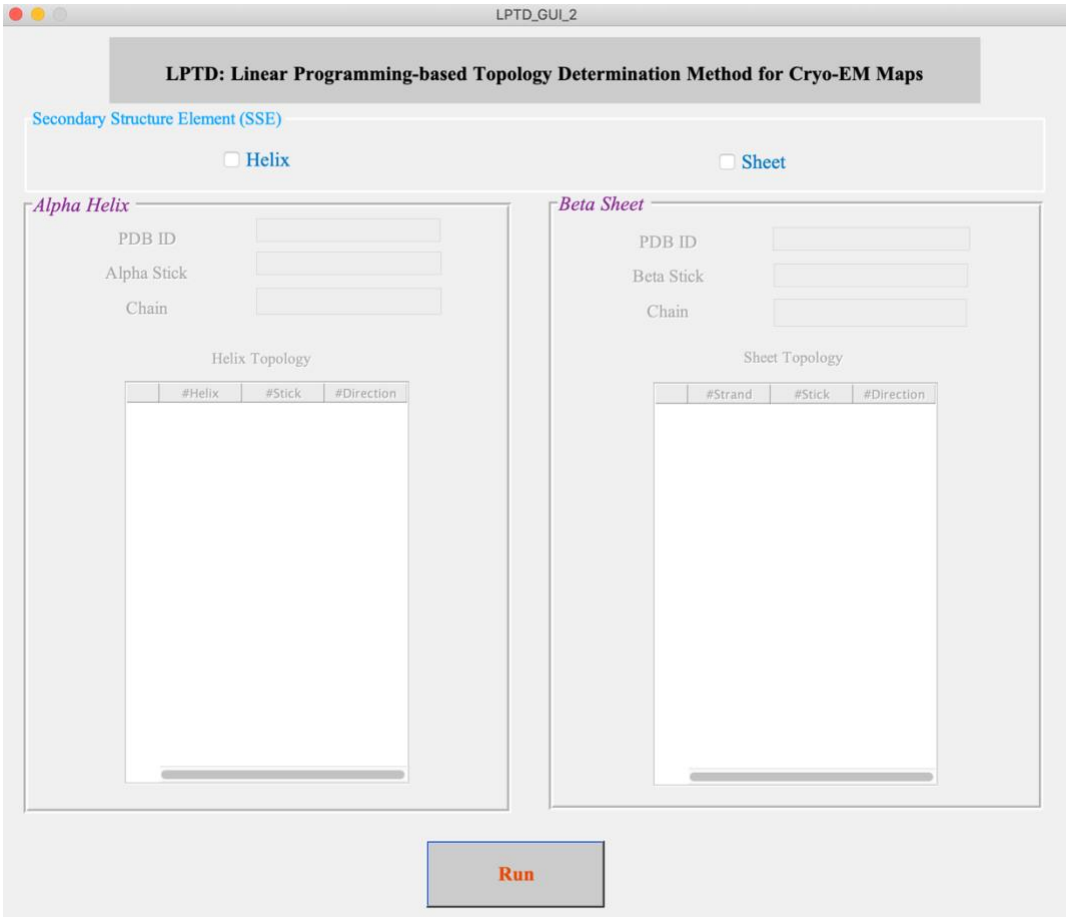

Fig. 1. LPTD graphical user interface (LPTD_GUI_2)

5. From the secondary structure element (SSE) menu, which is shown in blue, choose the ‘Helix’ or ‘Sheet’ button to find the ‘Helix Topology’ or ‘Sheet Topology’.

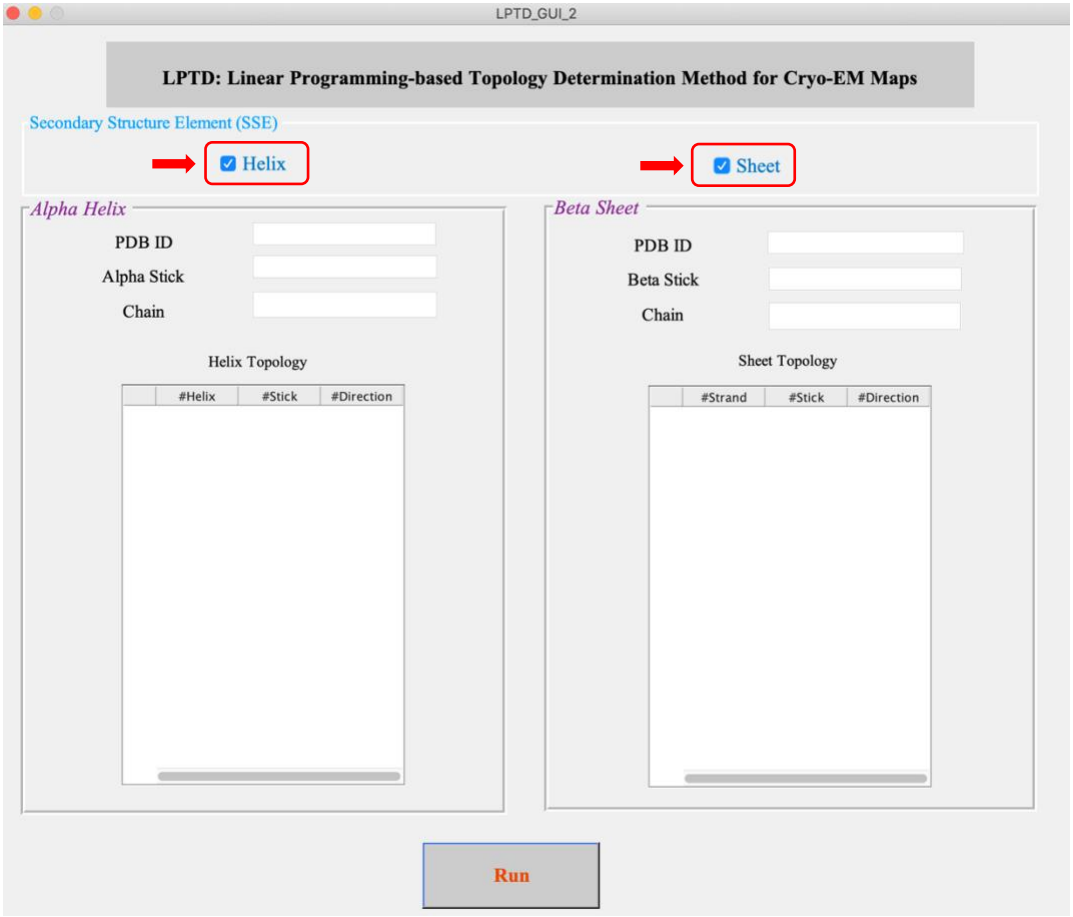

Fig. 2. Selection of helix, sheet, or both of them in the LPTD_GUI_2

After selecting helix/sheet, one can insert alpha-helix/beta-sheet information in the relevant panels. As shown in Fig. 2, each panel is divided into three sections including the 'PDB ID' for inserting the atomic model (prepared based on the Protein Data Bank format), the 'Alpha Stick' for inserting the predicted alpha sticks extracted from the cryo-EM map (prepared based on the format, which is described in Fig. 5), and 'chain' for inserting the chain of the protein.

6. In case the helix button is chosen as depicted in Fig. 3, one can enter the name of the atomic model in the 'PDB ID' section. As an example, we select one protein arbitrary with PDB ID 3u3h.

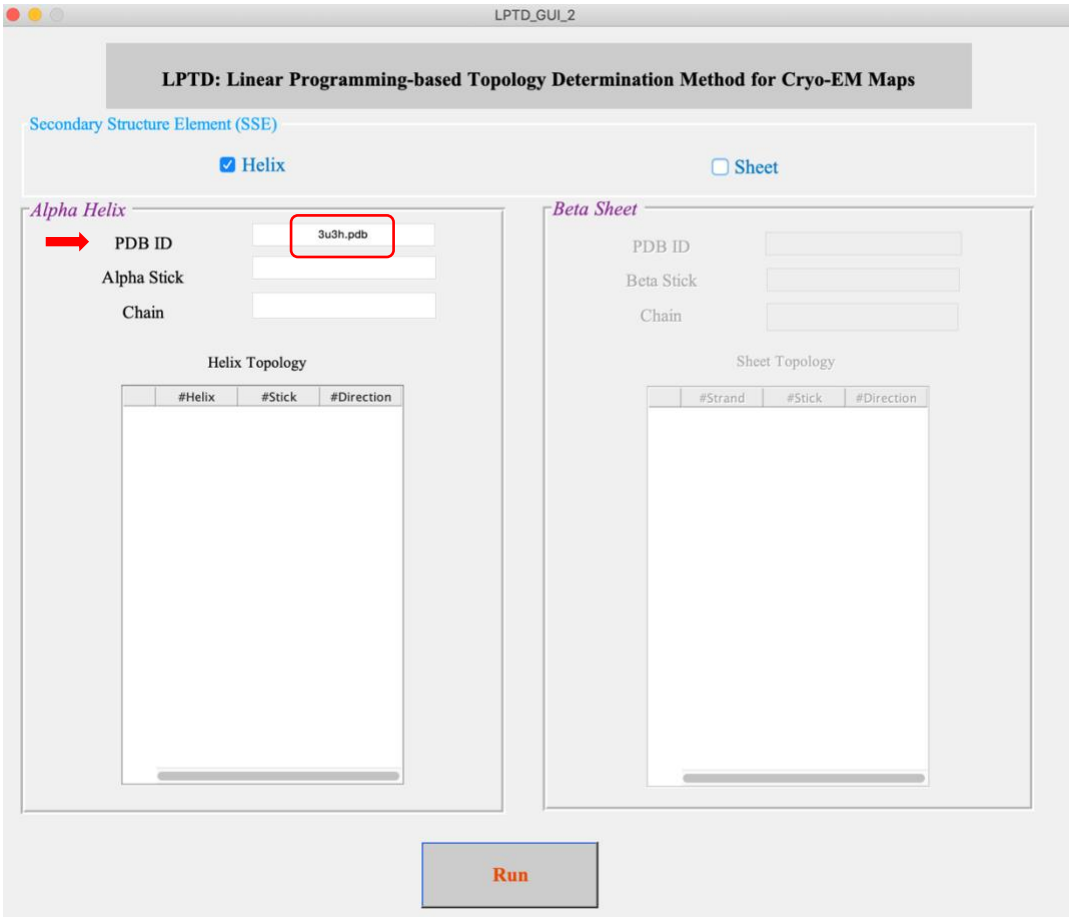

Fig. 3. Substituting the PDB ID of the protein in the LPTD graphical user interface (LPTD_GUI_2)

7. Enter the name of the extracted stick file (.csv file) in the ‘Alpha Stick’ section of Fig. 4 that is provided based on the format described in Fig. 5.

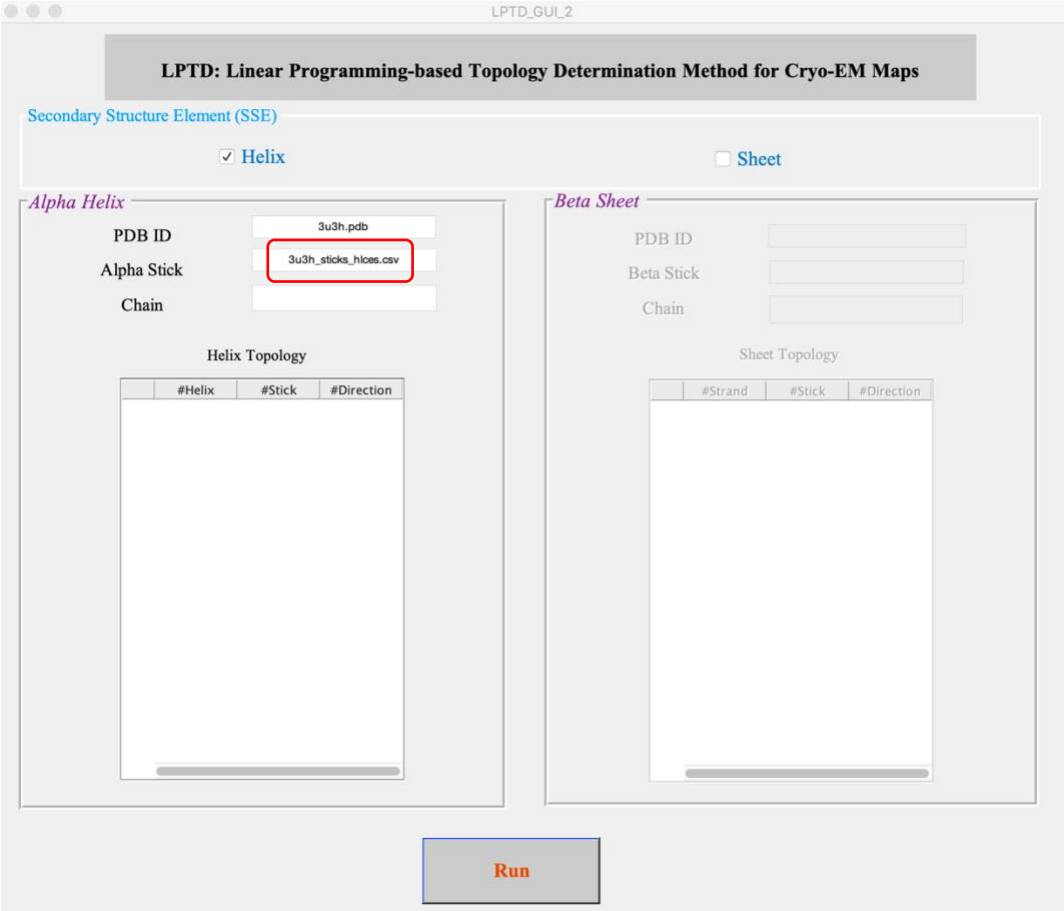

Fig. 4. Substituting the alpha stick in the LPTD graphical user interface (LPTD_GUI_2)

As shown in Fig. 5, the excel file containing the coordinate voxels of predicted secondary structures (SSEs) extracted from the cryo-EM map (.mrc file) as well as the index of the SSEs (SSE's number).

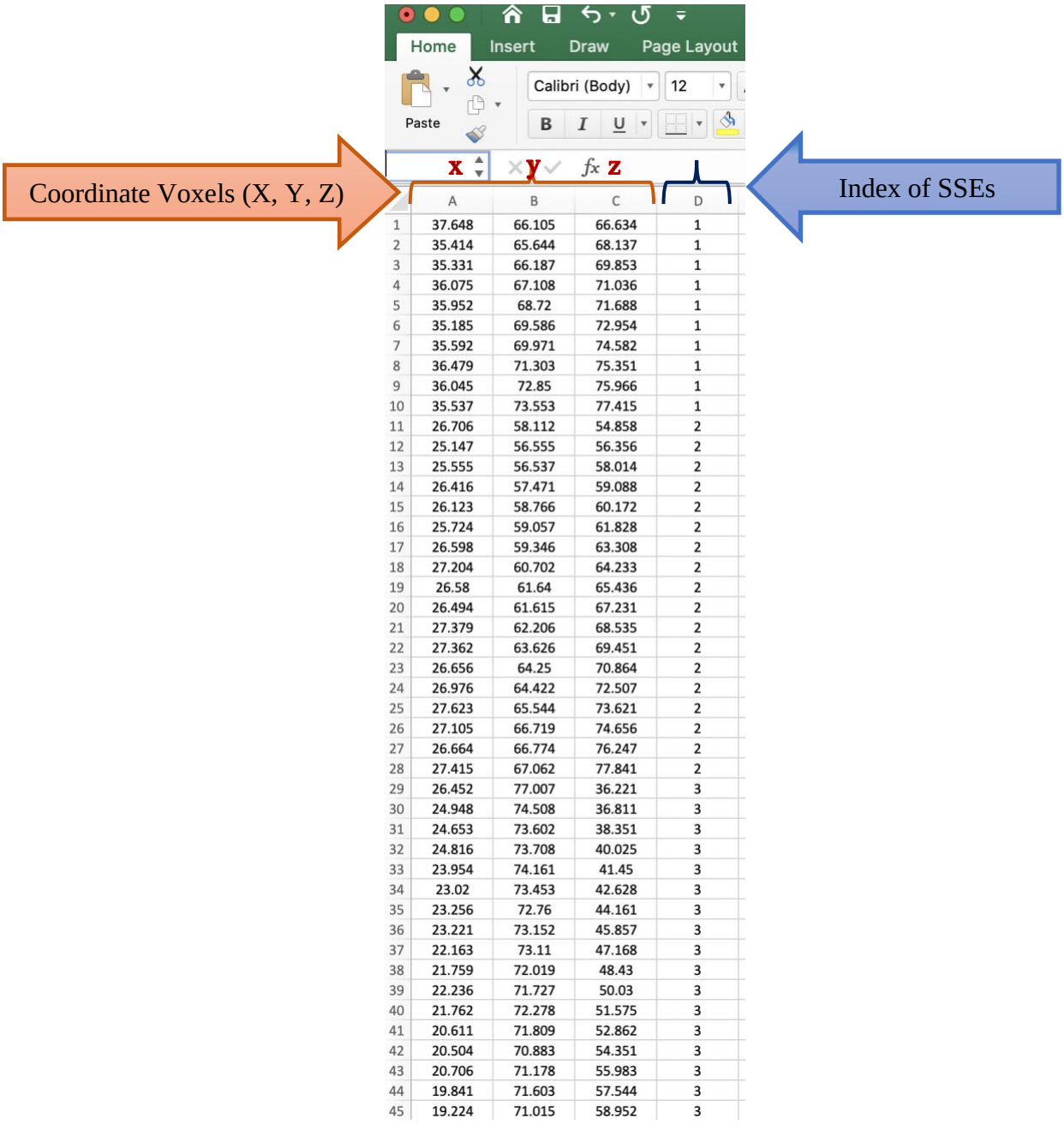

Fig. 5. The format of coordinate voxels in excel file (.csv)

8. Enter the chain of the protein in the 'Chain' section as depicted in Fig. 6.

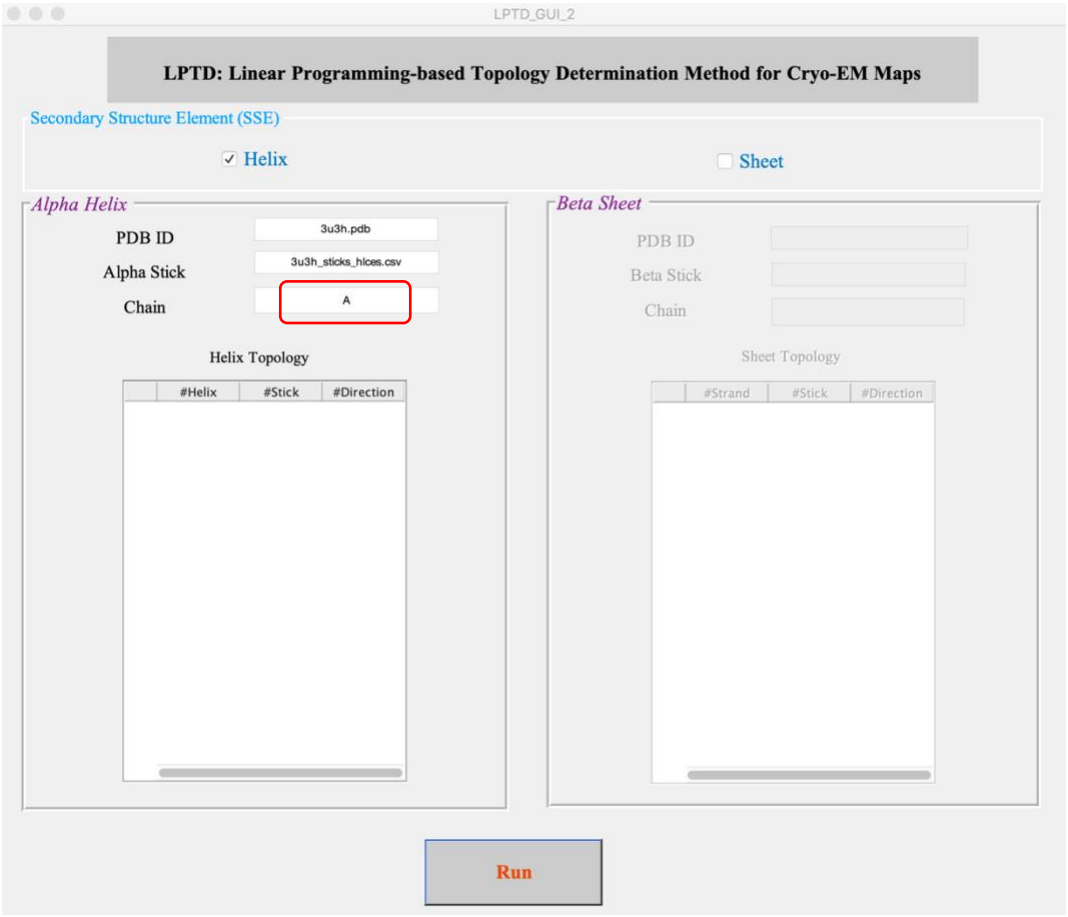

Fig. 6. Substituting the chain of the protein in the LPTD graphical user interface (LPTD_GUI_2)

9. If your protein doesn't have beta-sheet press the Run button, otherwise, select the sheet button to continue as depicted in Fig 7. Similar to the alpha helix panel, this panel is divided into three sections including the 'PDB ID' section for inserting the atomic model, the 'Beta Stick' section for inserting the beta strand extracted from the cryo-EM map, and 'chain' section for inserting the chain of the protein.

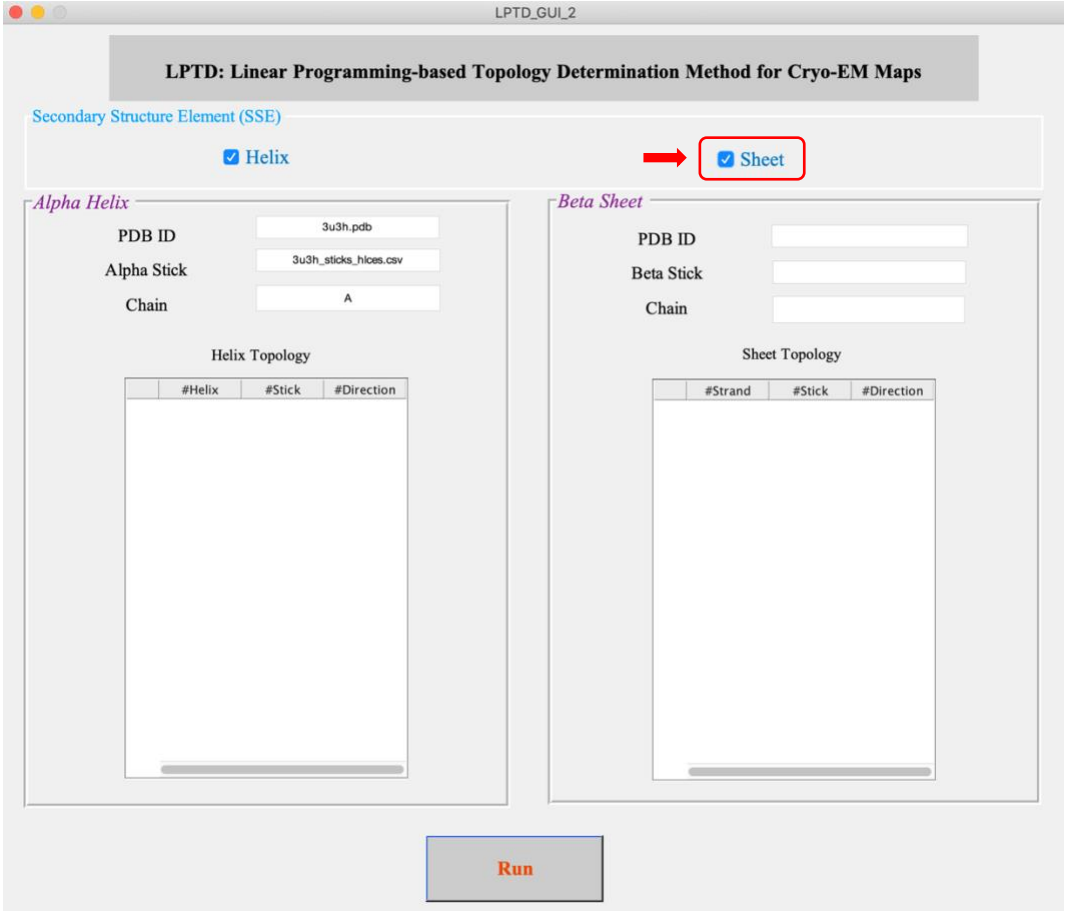

Fig. 7. Selection of the sheet button in the LPTD graphical user interface (LPTD_GUI_2)

10. Enter the name of the atomic model in 'PDB ID' section as depicted in Fig. 8:

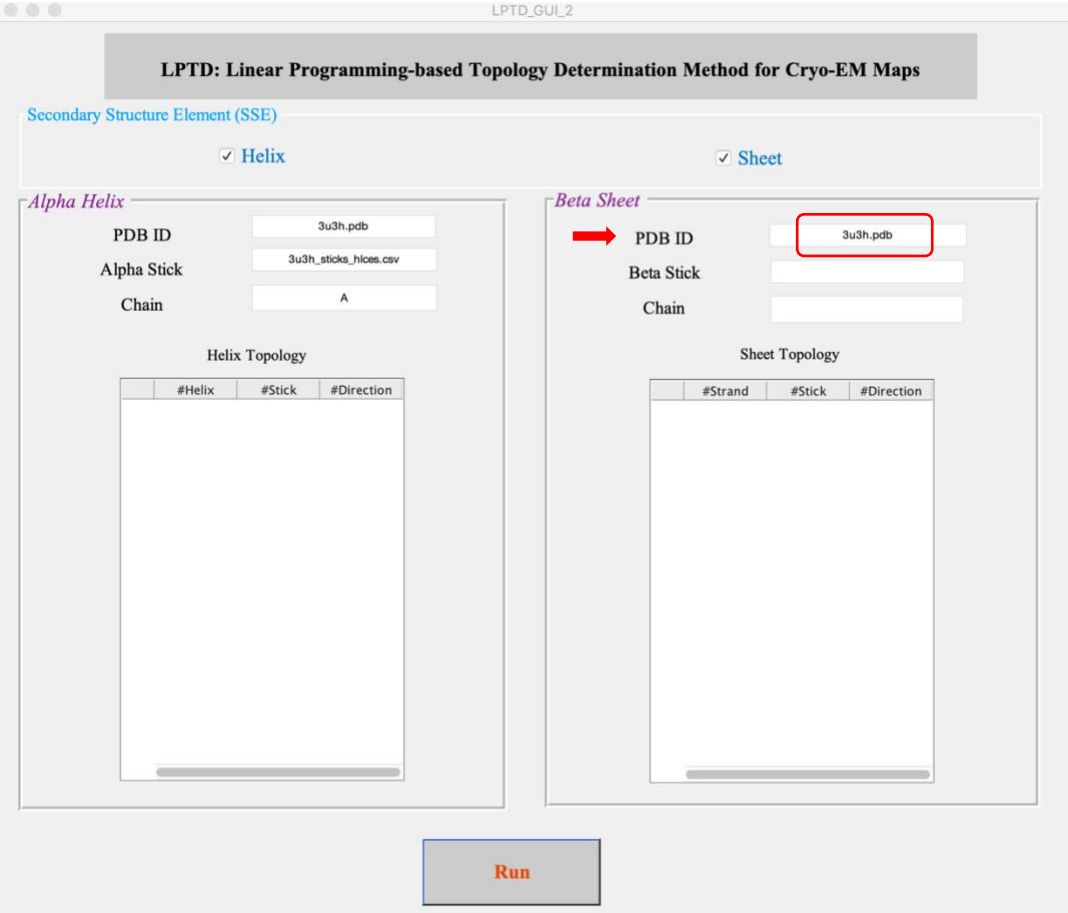

Fig. 8. Substituting the PDB ID of the protein in the LPTD graphical user interface (LPTD_GUI_2)

11. Enter the name of the beta-strand file in the 'Beta Stick' section as depicted in Fig. 9:

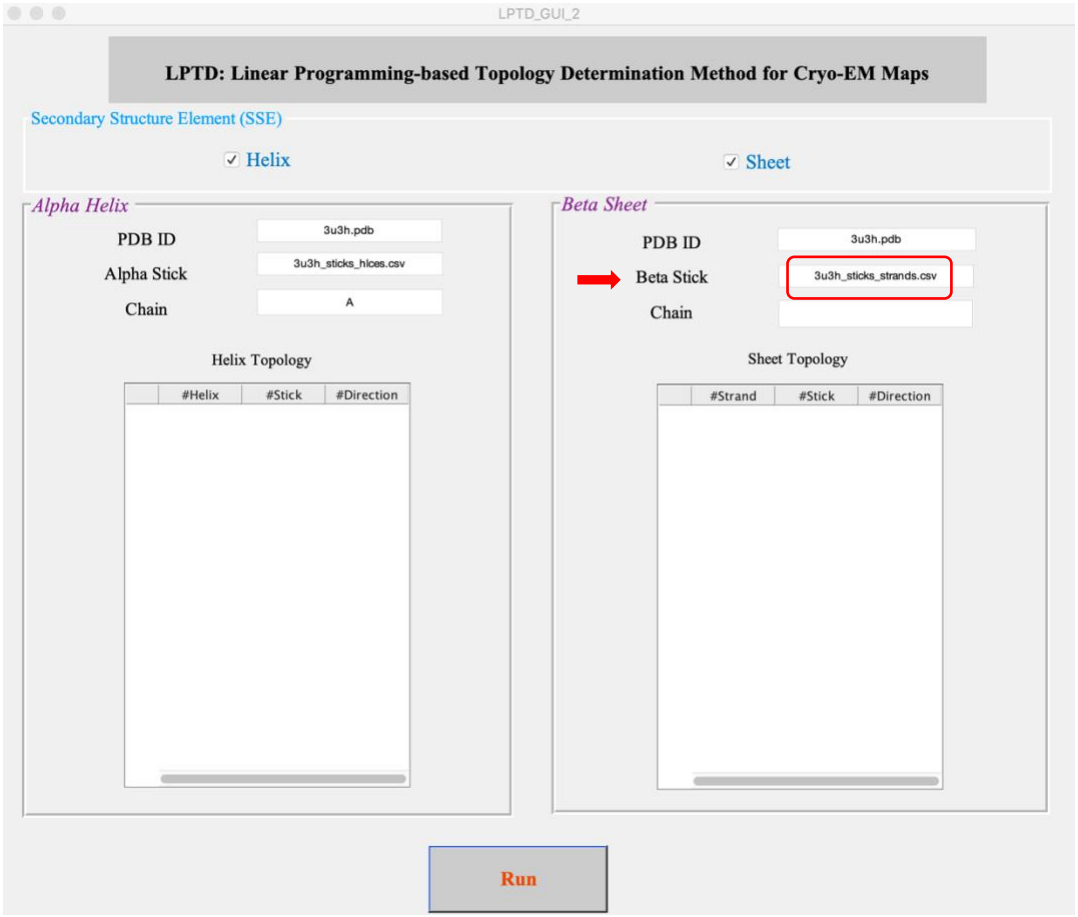

Fig. 9. Substituting the beta-stick in the LPTD graphical user interface (LPTD_GUI_2)

12. Enter the chain of the protein in the 'Chain' section as depicted in Fig. 10:

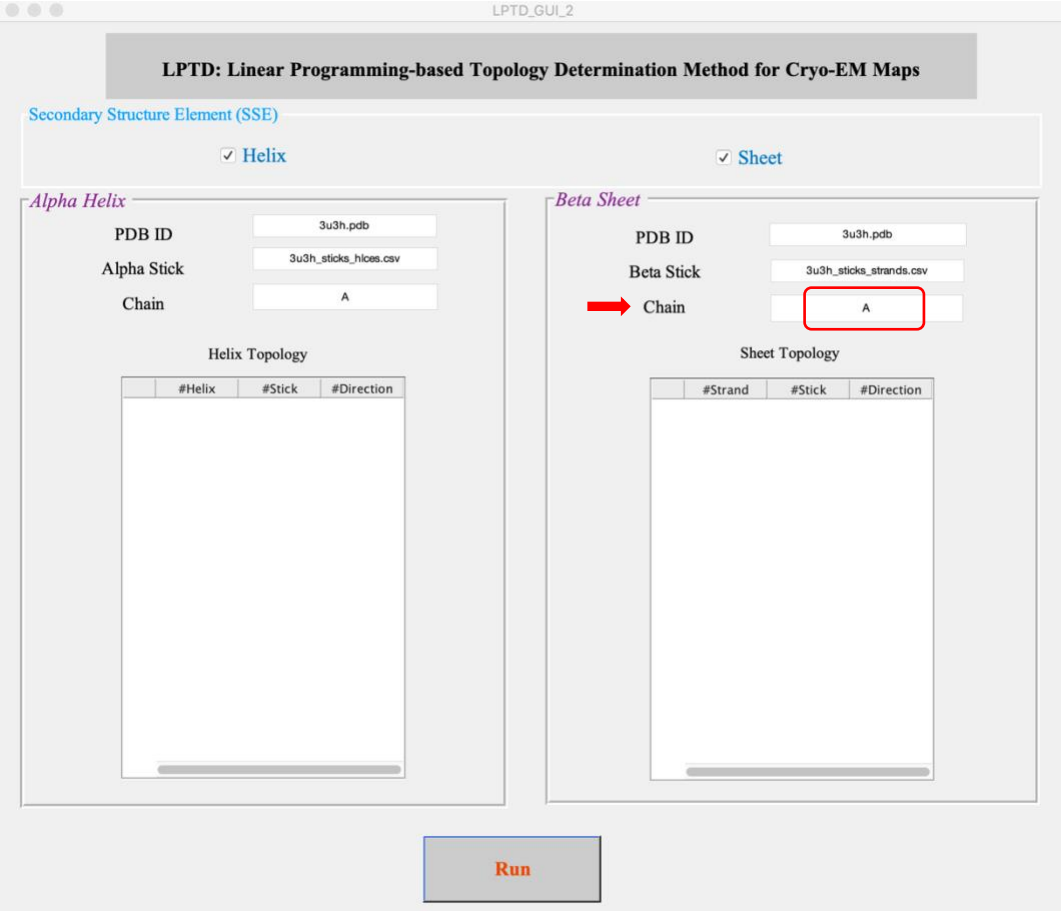

Fig. 10. Substituting the chain of the protein in LPTD graphical user interface (LPTD_GUI_2)

13. Pressing the Run button, as shown in Fig 11, will show the helix topology and sheet topology tables. In the helix topology table, the first column (#Helix) represents the order of the helices in the atomic model, the second column (#stick) indicates the matched alpha stick, which is extracted from the cryo-EM map, and the last column (#Direction) represents the direction of the alpha stick in a forward (1) or backward (-1) direction. One can scroll up and down in the helix topology table to see all matched pairs. Similarly, in the sheet topology table, the first column (#Strand) represents the order of the beta-strand in the atomic model, the second column (#Stick) indicates the matched strand stick, and the last column (#Direction) represents the direction of the strand stick in a forward (1) or backward (-1) direction. Moreover, the extracted helices and sticks will be plotted and shown as depicted in Figs. 12 and 13.

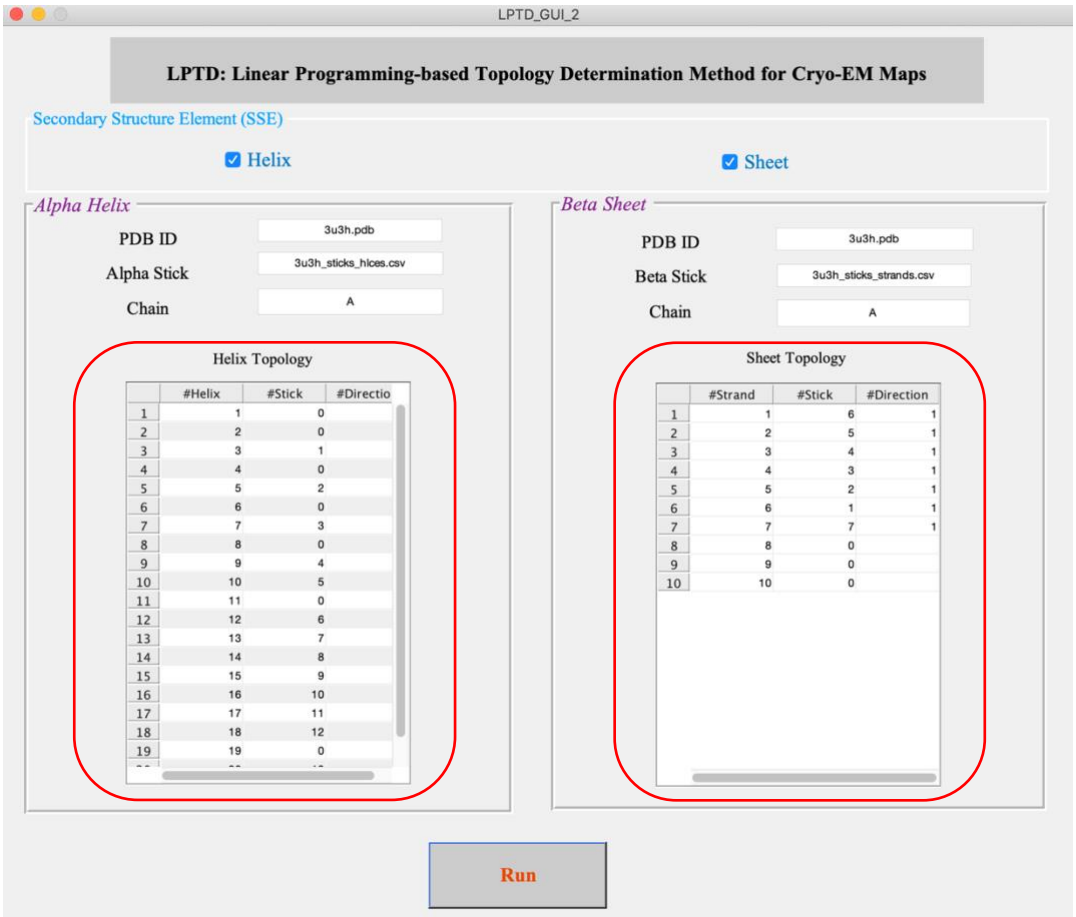

Fig. 11. Results of LPTD obtained by LPTD_GUI_2

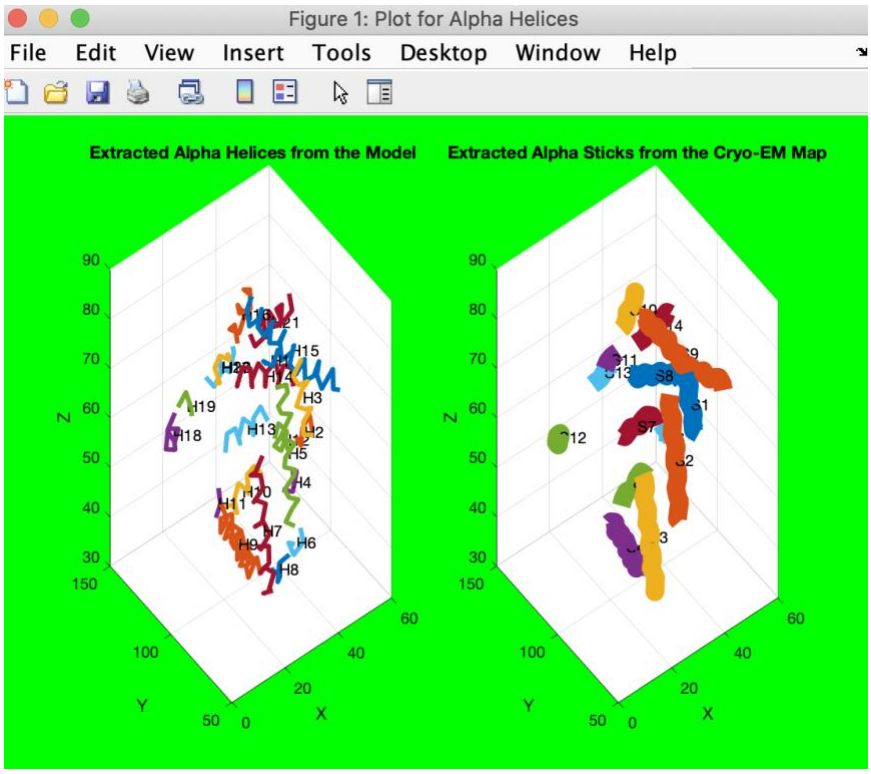

Fig. 12. Plots of alpha-helices obtained by LPTD_GUI_2

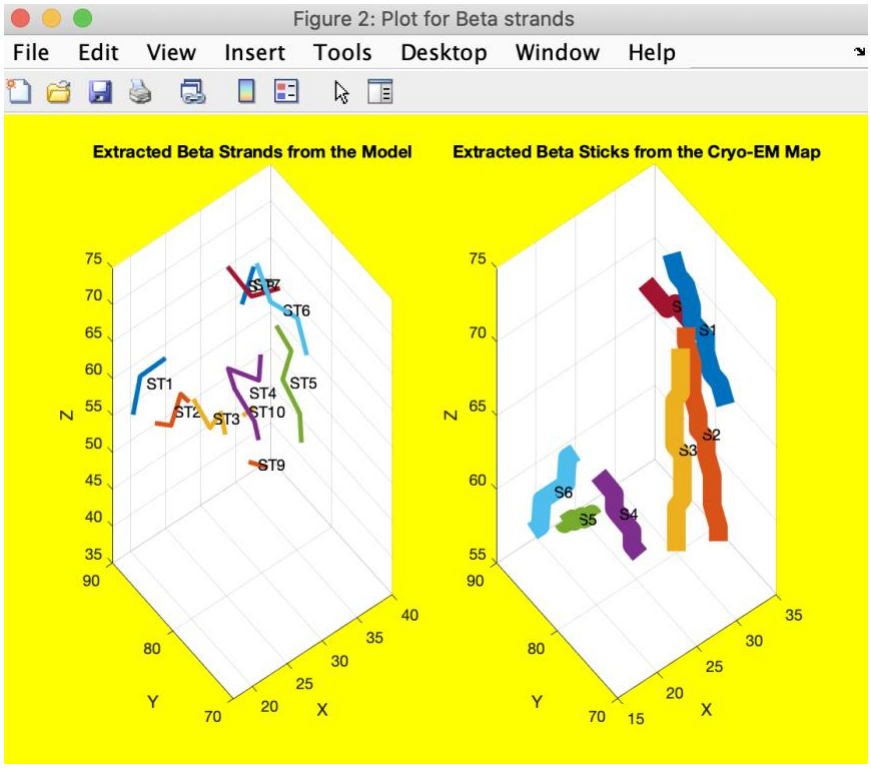

Fig. 13. Plots of beta strands obtained by LPTD_GUI_2