

About

LPTD software has been built using MATLAB R2020a. The LPTD is an automatic topology determination method for intermediate resolution cryo-EM maps.

Getting Started

1. Download or clone LPTD to your computer
2. Start MATLAB (R2020a)
3. Double-click on “LPTD_GUI_1.fig”
4. You can find a screen as below:

LPTD: Linear Programming-based Topology Determination Method for Cryo-EM Maps

Secondary Structure Element (SSE)

☐ Helix ☐ Sheet

Alpha Helix

PDB ID:
Alpha Stick:
Chain:
Native Helix Topology:

Helix Topology

#Helix	#Stick	#Direction

Beta Sheet

PDB ID:
Strand Stick:
Chain:
Native Sheet Topology:

Sheet Topology

#Strand	#Stick	#Direction

Run

Results

Precision	Recall	F-measure	Accuracy	Rank
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

Fig. 1. LPTD graphical user interface (LPTD_GUI_1)

- From the secondary structure element (SSE) menu, which is shown in blue, choose the 'Helix' or 'Sheet' button as depicted below in red to find the 'Helix Topology' or 'Sheet Topology'.

The screenshot shows the LPTD_GUI_1 window. At the top, the title bar reads 'LPTD_GUI_1'. Below it, a header bar contains the text 'LPTD: Linear Programming-based Topology Determination Method for Cryo-EM Maps'. The main area is titled 'Secondary Structure Element (SSE)' in blue. Below this title, there are two buttons: 'Helix' and 'Sheet', both highlighted with red boxes and red arrows pointing to them. Below the 'Helix' button is the 'Alpha Helix' section, which includes input fields for 'PDB ID', 'Alpha Stick', 'Chain', and 'Native Helix Topology'. Below these fields is a 'Helix Topology' table with columns '#Helix', '#Stick', and '#Direction'. Below the 'Sheet' button is the 'Beta Sheet' section, which includes input fields for 'PDB ID', 'Strand Stick', 'Chain', and 'Native Sheet Topology'. Below these fields is a 'Sheet Topology' table with columns '#Strand', '#Stick', and '#Direction'. At the bottom center of the interface is a 'Run' button. Below the 'Run' button is a 'Results' section with five columns: 'Precision', 'Recall', 'F-measure', 'Accuracy', and 'Rank', each with an empty input field.

Fig. 2. Selection of helix, sheet, or both of them in LPTD_GUI_1

As reported in Table 1, for some proteins such as proteins with PDB IDs 1ICX, 1OZ9, 4OXW, 1YD0, 2Y4Z, 3FIN, 4CHV, 6EM3, 5UZH, 3C91, 5O8O, 5M50, 5KBU, 6UXW, both helices and sheets are contained. Hence, one can choose both the 'Helix' and 'Sheet' buttons.

No	PDB ID	Helix	Sheet	No	PDB ID	Helix	Sheet
1	1FLP	✓		15	4R9A		✓
2	1NG6	✓		16	3FIN	✓	✓
3	2XB5	✓		17	4CHV	✓	✓
4	1BZ4	✓		18	5I1M	✓	

5	3ACW	✓		19	6F36	✓	
6	1A7D	✓		20	6EM3	✓	✓
7	3ODS	✓		21	4UE4	✓	
8	3HJL	✓		22	5UZH	✓	✓
9	1ICX	✓	✓	23	3C91	✓	✓
10	1OZ9	✓	✓	24	5O8O	✓	✓
11	4OXW	✓	✓	25	5M50	✓	✓
12	1YD0	✓	✓	26	5KBU	✓	✓
13	2Y4Z	✓	✓	27	6UXW	✓	✓
14	4YOK		✓				

Table 1: The data set, in which proteins contain helix, sheet or both of them

After selecting helix/sheet, one can insert alpha-helix/beta-sheet information in the relevant panels. As shown in Fig. 3, this part is divided into four sections including the 'PDB ID' for inserting the generated model of the sequence, 'Alpha Stick' for inserting the alpha sticks extracted from the cryo-EM map, 'chain' for inserting the chain of the protein, 'Native Helix Topology' for inserting the true topology for evaluating the method and computing the performance measurements and rank of the topology.

6. In case the helix button is chosen, one can therefore select one of the following generated atomic models and insert it in the 'PDB ID' section as depicted in Fig. 3. As an example, we have selected the protein with PDB ID 5m50.

{model_1flp.pdb, model_1ng6.pdb, model_2xb5.pdb, model_1bz4.pdb,
model_3acw.pdb, model_1a7d.pdb, model_3ods.pdb, model_3hjl.pdb,
model_1icx.pdb, model_1oz9.pdb, model_4oxw.pdb, model_1yd0.pdb,
model_2y4z.pdb, model_3fin.pdb, model_4chv.pdb, model_5iln.pdb,
model_6f36.pdb, model_6em3.pdb, model_4ue4.pdb, model_5uzb.pdb,
model_3c91.pdb, model_5o8o.pdb, **model_5m50.pdb**, model_5kbu.pdb,
model_6uxw.pdb}

LPTD: Linear Programming-based Topology Determination Method for Cryo-EM Maps

Secondary Structure Element (SSE)

☒ Helix ☐ Sheet

Alpha Helix

PDB ID:

Alpha Stick:

Chain:

Native Helix Topology:

Helix Topology

#Helix	#Stick	#Direction

Beta Sheet

PDB ID:

Strand Stick:

Chain:

Native Sheet Topology:

Sheet Topology

#Strand	#Stick	#Direction

Run

Results

Precision	Recall	F-measure	Accuracy	Rank
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

Fig. 3. Substituting the PDB ID of protein in the LPTD graphical user interface (LPTD_GUI_1)

- Choose the relevant alpha stick with the above-selected PDB ID from the following list and insert it in the 'Alpha Stick' section as depicted in Fig. 4.

{ 1flp_sticks_hlces.csv,
1bz4_sticks_hlces.csv,
3ods_stick_hlces.csv,
1oz9_sticks_hlces.csv,
2y4z_sticks_hlces.csv,
5i1m_sticks_hlces.csv,
4ue4_sticks_hlces.csv,
5o8o_sticks_hlces.csv,
6uxw_sticks_hlces.csv }

1ng6_sticks_hlces.csv,
3acw_stick_hlces.csv,
3hjl_stick_hlces.csv,
4oxw_sticks_hlces.csv,
3fin_sticks_hlces.csv,
6f36_sticks_hlces.csv,
5uzb_sticks_hlces.csv,
5m50_sticks_hlces.csv,

2xb5_stick_hlces.csv,
1a7d_sticks_hlces.csv,
1icx_sticks_hlces.csv,
1yd0_sticks_hlces.csv,
4chv_sticks_hlces.csv,
6em3_sticks_hlces.csv,
3c91_sticks_hlces.csv,
5kbu_sticks_hlces.csv,

LPTD_GUI_1

LPTD: Linear Programming-based Topology Determination Method for Cryo-EM Maps

Secondary Structure Element (SSE)

☒ Helix ☐ Sheet

Alpha Helix

PDB ID

→ Alpha Stick

Chain

Native Helix Topology

Helix Topology

#Helix	#Stick	#Direction

Beta Sheet

PDB ID

Strand Stick

Chain

Native Sheet Topology

Sheet Topology

#Strand	#Stick	#Direction

Run

Results

Precision	Recall	F-measure	Accuracy	Rank
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

Fig. 4. Substituting the alpha stick in the LPTD graphical user interface (LPTD_GUI_1)

8. Enter the chain of the protein from the following list and insert it in the 'Chain' section as depicted in Fig. 5.

```
{ 1flp_chain:A,  1ng6_chain:A,  2xb5_chain:A,  1bz4_chain:A,  3acw_chain:A,
  1a7d_chain:A,  3ods_chain:A,  3hjl_chain:A,  1icx_chain:A,  1oz9_chain:A,
  4oxw_chain:A,  1yd0_chain:A,  2y4z_chain:A,  3fin_chain:R,  4chv_chain:A,
  5i1m_chain:V,  6f36_chain:M,  6em3_chain:A,  4ue4_chain:C,  5uzb_chain:A,
  3c91_chain:A,  5o8o_chain:A,  5m50_chain:A,  5kbu_chain:A,  6uxw_chain:A }
```

LPTD_GUI_1

LPTD: Linear Programming-based Topology Determination Method for Cryo-EM Maps

Secondary Structure Element (SSE)

☒ Helix ☐ Sheet

Alpha Helix

PDB ID:

Alpha Stick:

Chain:

Native Helix Topology:

Helix Topology

#Helix	#Stick	#Direction

Beta Sheet

PDB ID:

Strand Stick:

Chain:

Native Sheet Topology:

Sheet Topology

#Strand	#Stick	#Direction

Run

Results

Precision	Recall	F-measure	Accuracy	Rank
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

Fig. 5. Substituting the chain of protein in the LPTD graphical user interface (LPTD_GUI_1)

9. Enter the native topology from the following list and insert it in the 'Native Helix Topology' section as depicted in Fig. 6.

{Topology_1FLP_helices.csv, Topology_1NG6_helices.csv, Topology_2XB5_helices.csv, Topology_1BZ4_helices.csv, Topology_3ACW_helices.csv, Topology_1AD7_helices.csv, Topology_3ODS_helices.csv, Topology_3HJL_helices.csv, Topology_1ICX_helices.csv, Topology_1OZ9_helices.csv, Topology_4OXW_helices.csv, Topology_1YD0_helices.csv, Topology_2Y4Z_helices.csv, Topology_3FIN_helices.csv, Topology_4CHV_helices.csv, Topology_5I1M_helices.csv, Topology_4UE4_helices.csv, Topology_5UZB_helices.csv, Topology_6F36_helices.csv, Topology_6EM3_helices.csv, Topology_3C91_helices.csv, Topology_5O8O_helices.csv, **Topology_5M50_helices.csv**, Topology_5KBU_helices.csv, Topology_6UXW_helices.csv}

LPTD_GUI_1

LPTD: Linear Programming-based Topology Determination Method for Cryo-EM Maps

Secondary Structure Element (SSE)

☒ Helix ☐ Sheet

Alpha Helix

PDB ID:

Alpha Stick:

Chain:

Native Helix Topology:

Helix Topology

#Helix	#Stick	#Direction

Beta Sheet

PDB ID:

Strand Stick:

Chain:

Native Sheet Topology:

Sheet Topology

#Strand	#Stick	#Direction

Run

Results

Precision	Recall	F-measure	Accuracy	Rank
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

Fig. 6. Substituting the topology of protein in the LPTD graphical user interface (LPTD_GUI_1)

10. If the protein has both helices and sheets according to Table 1, select the sheet button as depicted in Fig 7. Similar to the alpha helix panel, this part is divided into four sections including the 'PDB ID' for inserting the generated model of the sequence, 'Strand Stick' for inserting the beta-strand extracted from the cryo-EM map, 'chain' for inserting the chain of the protein, and 'Native Sheet Topology' for inserting the true (native) topology.

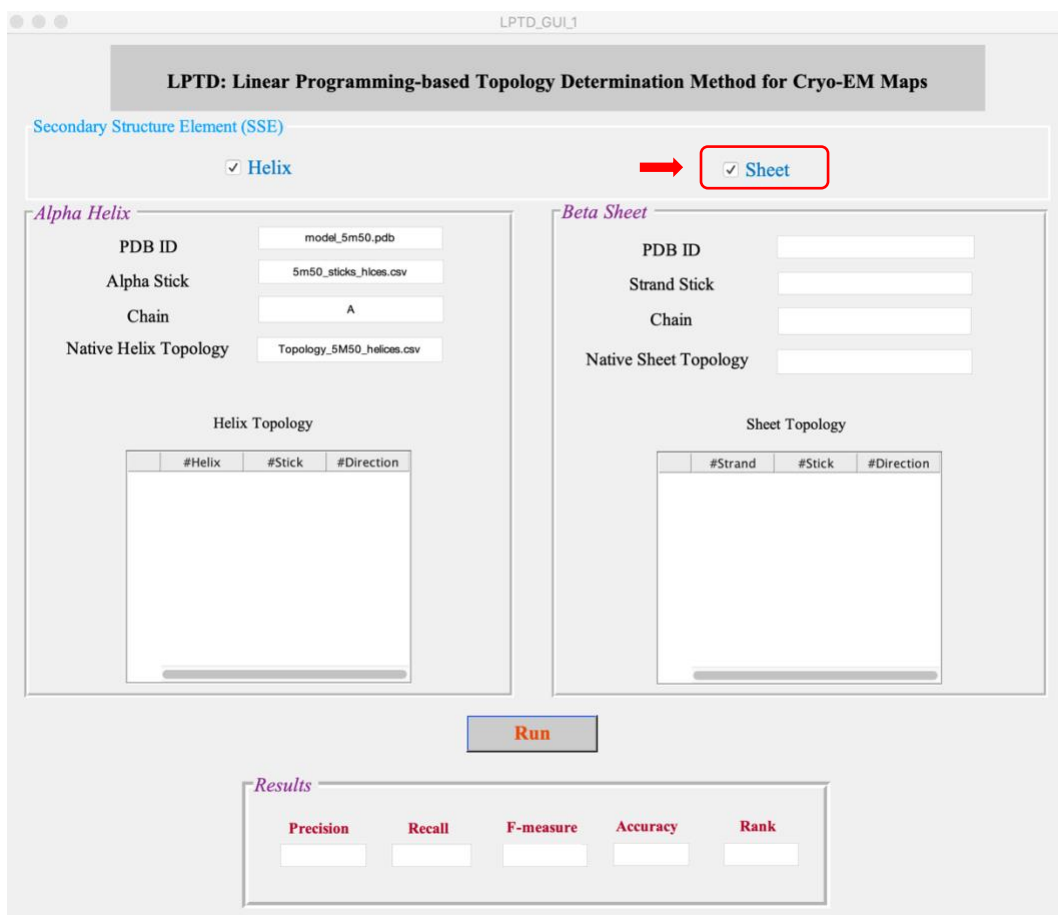


Fig. 7. Selection of beta sheet button in the LPTD graphical user interface (LPTD_GUI_1)

11. Choose the PDB ID of the protein from the following list and insert it in the 'PDB ID' section of the sheet panel as illustrated in Fig. 8:

{model_1icx.pdb, model_1oz9.pdb, model_4oxw.pdb, model_1yd0.pdb, model_2y4z.pdb, model_4yok.pdb, model_4r9a.pdb, model_3fin.pdb, model_4chv.pdb, model_6em3.pdb, model_5uzb.pdb, model_3c91.pdb, model_5o8o.pdb, **model_5m50.pdb**, model_5kbu.pdb, model_6uxw.pdb}

LPTD_GUI_1

LPTD: Linear Programming-based Topology Determination Method for Cryo-EM Maps

Secondary Structure Element (SSE)

☒ Helix ☒ Sheet

Alpha Helix

PDB ID:

Alpha Stick:

Chain:

Native Helix Topology:

Helix Topology

#Helix	#Stick	#Direction

Beta Sheet

→ PDB ID:

Strand Stick:

Chain:

Native Sheet Topology:

Sheet Topology

#Strand	#Stick	#Direction

Run

Results

Precision	Recall	F-measure	Accuracy	Rank
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

Fig. 8. Substituting the PDB ID of protein in the LPTD graphical user interface (LPTD_GUI_1)

12. Choose the beta-strand stick from the following list and insert it in the 'Strand Stick' section as depicted in Fig. 9:

{ 1icx_sticks_strands.csv,	1oz9_sticks_strands.csv,	4oxw_sticks_strands.csv,
1yd0_sticks_strands.csv,	2y4z_sticks_strands.csv,	4yok_sticks_strands.csv,
4r9a_sticks_strands.csv,	3fin_sticks_strands.csv,	4chv_sticks_strands.csv,
6em3_sticks_strands.csv,	5uzb_sticks_strands.csv,	3c91_sticks_strands.csv,
5o8o_sticks_strands.csv,	5m50_sticks_strands.csv,	5kbu_sticks_strands.csv,
6uxw_sticks_strands.csv}		

LPTD_GUI_1

LPTD: Linear Programming-based Topology Determination Method for Cryo-EM Maps

Secondary Structure Element (SSE)

☒ Helix ☒ Sheet

Alpha Helix

PDB ID:

Alpha Stick:

Chain:

Native Helix Topology:

Helix Topology

#Helix	#Stick	#Direction

Beta Sheet

PDB ID:

→ Strand Stick:

Chain:

Native Sheet Topology:

Sheet Topology

#Strand	#Stick	#Direction

Run

Results

Precision	Recall	F-measure	Accuracy	Rank
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

Fig. 9. Substituting the beta-strand stick in the LPTD graphical user interface (LPTD_GUI_1)

13. Select the chain of the protein from the following list and insert it in the 'Chain' section as depicted in Fig. 10:

{ 1icx_chain:A, 1oz9_chain:A, 4oxw_chain:A, 1yd0_chain:A, 2y4z_chain:A, 4yok_chain:A, 4r9a_chain:A, 3fin_chain:R, 4chv_chain:A, 6em3_chain:A, 5uzb_chain:A, 3c91_chain:A, 5o8o_chain:A, **5m50_chain:A**, 5kbu_chain:A, 6uxw_chain:A }

LPTD_GUI_1

LPTD: Linear Programming-based Topology Determination Method for Cryo-EM Maps

Secondary Structure Element (SSE)

☒ Helix
 ☒ Sheet

Alpha Helix

PDB ID:

Alpha Stick:

Chain:

Native Helix Topology:

Helix Topology

#Helix	#Stick	#Direction

Beta Sheet

PDB ID:

Strand Stick:

→ Chain:

A

Native Sheet Topology:

Sheet Topology

#Strand	#Stick	#Direction

Run

Results

Precision	Recall	F-measure	Accuracy	Rank
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

Fig. 10. Substituting the chain of protein in the LPTD graphical user interface (LPTD_GUI_1)

14. Enter the relevant native topology from the following list and insert it in the 'Native Topology' section as depicted in Fig. 11.

{Topology_1ICX_strands.csv, Topology_1OZ9_strands.csv, Topology_4OXW_strands.csv, Topology_1YD0_strands.csv, Topology_2Y4Z_strands.csv, Topology_4YOK_strands.csv, Topology_4R9A_strands.csv, Topology_3FIN_strands.csv, Topology_4CHV_strands.csv, Topology_6EM3_strands.csv, Topology_5UZZ_strands.csv, Topology_3C91_strands.csv, Topology_5O8O_strands.csv, **Topology_5M50_strands.csv**, Topology_5KBU_strands.csv, Topology_6UXW_strands.csv}

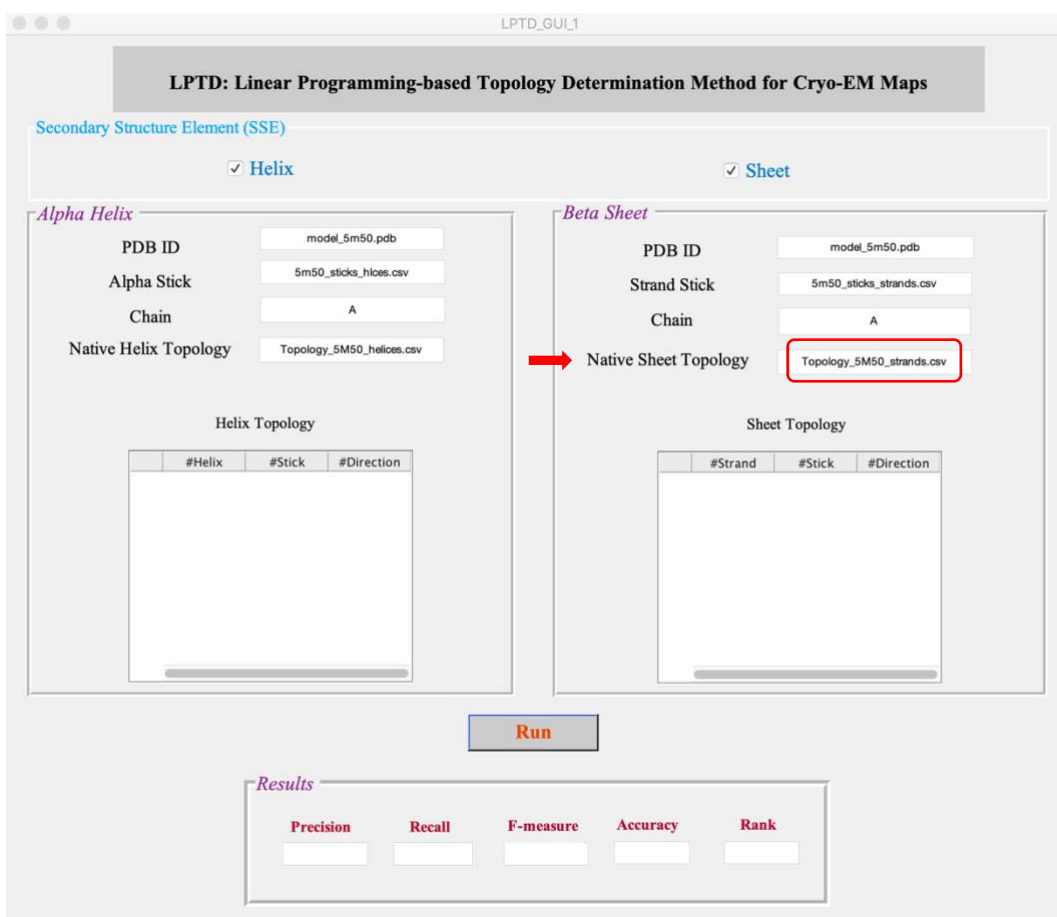


Fig. 11. Substituting the native topology of the sheet in the LPTD graphical user interface (LPTD_GUI_1)

15. Clicking on the Run button will show the helix topology and sheet topology tables as well as the performance measurements and rank of the correct topology obtained by LPTD as shown in Fig 12. In the helix topology table, the first column (#Helix) represents the order of the alpha helices in the sequence, 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 sequence, 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. 13 and 14.

LPTD_GUI_1

LPTD: Linear Programming-based Topology Determination Method for Cryo-EM Maps

Secondary Structure Element (SSE)

☒ Helix
☒ Sheet

Alpha Helix

PDB ID:

Alpha Stick:

Chain:

Native Helix Topology:

Helix Topology

	#Helix	#Stick	#Directio
1	1	1	
2	2	2	
3	3	3	
4	4	4	
5	5	5	
6	6	6	
7	7	7	
8	8	8	
9	9	9	
10	10	10	

Beta Sheet

PDB ID:

Strand Stick:

Chain:

Native Sheet Topology:

Sheet Topology

	#Strand	#Stick	#Directio
1	1	1	
2	2	2	
3	3	3	
4	4	4	
5	5	5	
6	6	6	
7	7	7	
8	8	8	
9	9	9	
10	10	10	

Results

Precision	Recall	F-measure	Accuracy	Rank
100	100	100	100	1

Fig. 12. Results of LPTD obtained by LPTD_GUI_1

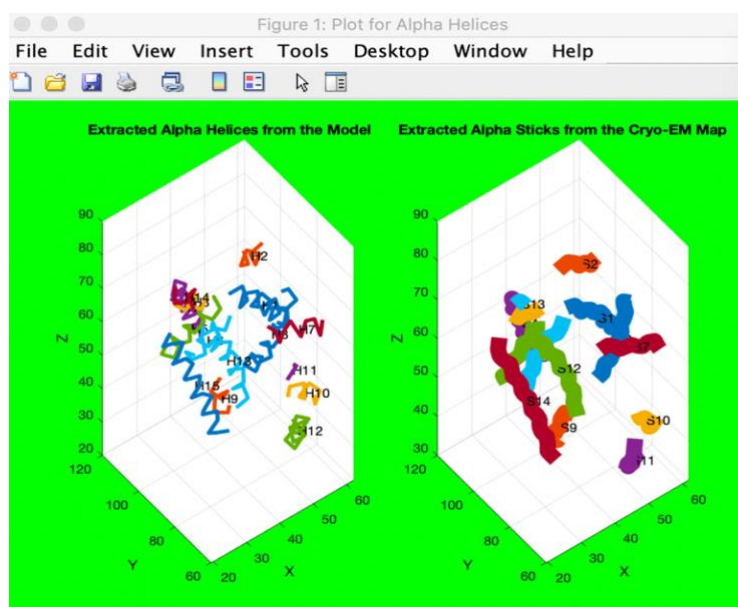


Fig. 13. Plots of alpha-helices obtained by LPTD_GUI_1

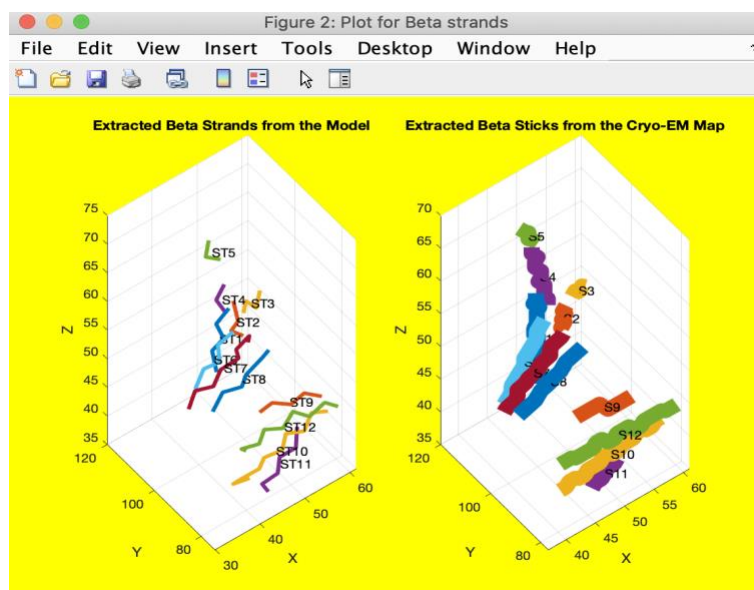


Fig. 14. Plots of beta-strands obtained by LPTD_GUI_1