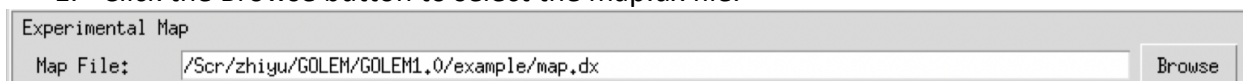
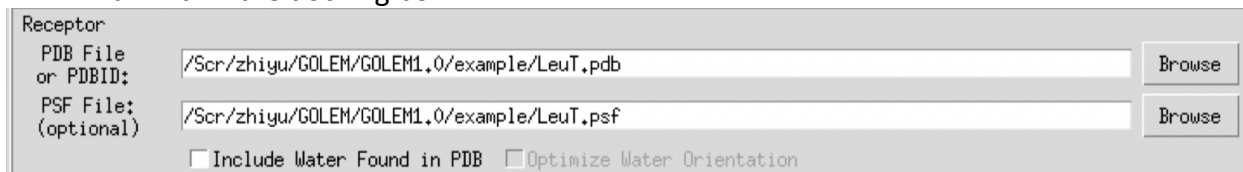


In this example case, you will use GOLEM to dock a leucine molecule into the bacterial leucine transporter LeuT. As an example, we are not using a real cryo-EM map, but a simulated map generated from an atomic X-ray crystal structure of leucine-bound LeuT (PDB ID: 2A65) so that you can compare the docking result to the leucine molecule modeled in the crystal structure.

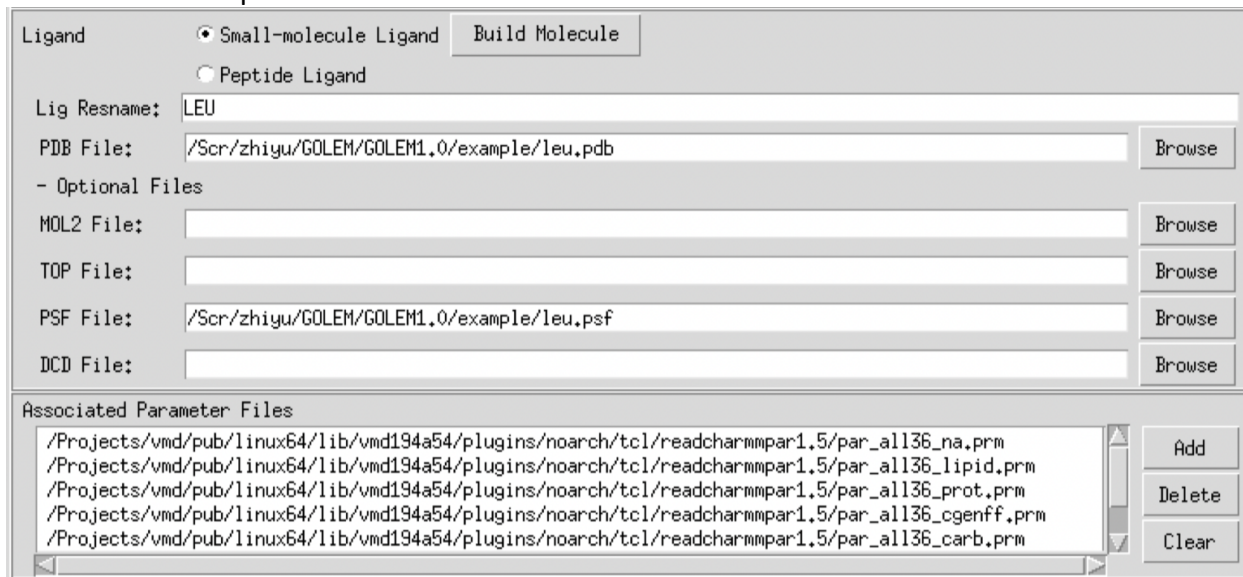
1. Click the Browse button to select the map.dx file.



2. Click the Browse buttons to select the PDB and PSF files of the receptor (protein).  
Uncheck “Include Water Found in PDB” to ignore water molecules in the receptor that fall within the docking box.



3. Select “Small-molecule Ligand”. Type Lig Resname “LEU”. It is the residue name of leucine in the CHARMM force field. Click the Browse buttons to select the PDB and PSF files of leucine. If you don’t see the entry of PSF File, click “Optional Files”. Because leucine is already included in the default CHARMM force field, there is no need to add additional parameter files.



4. Type “protein and resid 22 26 108 253 256” and click the Measure button. It will automatically calculate the min/max X/Y/Z values of the binding site residues to define the docking box. Click the Show button to visualize the docking box in VMD.

Docking box

Define From Atomselection:

Min X:  Min Y:  Min Z:  Max X:  Max Y:  Max Z:

5. Leave docking settings as default.

Docking Settings

☐ Fixed Side Chains      Ligand-map Coupling Factor:       Maximum number of water molecules:

☒ Flexible Side Chains      Water-map Coupling Factor:

6. Use the Browse buttons to specify the folder you want all output files to be placed in, and the path to NAMD executable in your computer. Modify NAMD options to maximize NAMD speed and compatibility.

NAMD Settings

Output Path:

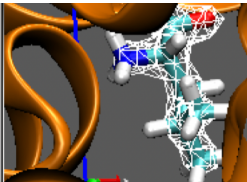
NAMD Path:

NAMD Options:

7. Click the Prepare button.

8. Click the Run! Button to perform docking. The docking procedure will continue until convergence or be terminated by clicking the Abort button. Top ten poses are listed and can be visualized by clicking.

Itera...	1st	2nd	3rd	4th	5th	6th	7th	8th	9th	10th
47	-11,1	-13,3	-68,6	-71,3	-81,2	-98,3	-142,3	-177,4	-180,5	-243,5
48	-11,1	-13,3	-60,3	-71,3	-81,2	-98,3	-138,9	-177,4	-180,5	-198,7
49	-11,1	-13,3	-60,3	-71,3	-81,2	-81,4	-136,5	-174,7	-177,4	-180,5
50	-11,1	-13,3	-60,3	-71,3	-75,5	-81,2	-134,9	-174,7	-177,4	-180,5
51	-11,1	-13,3	-60,3	-71,3	-75,5	-81,2	-133,3	-174,7	-177,4	-180,5



9. Load the original crystal structure PDB 2A65 to compare the docking result.