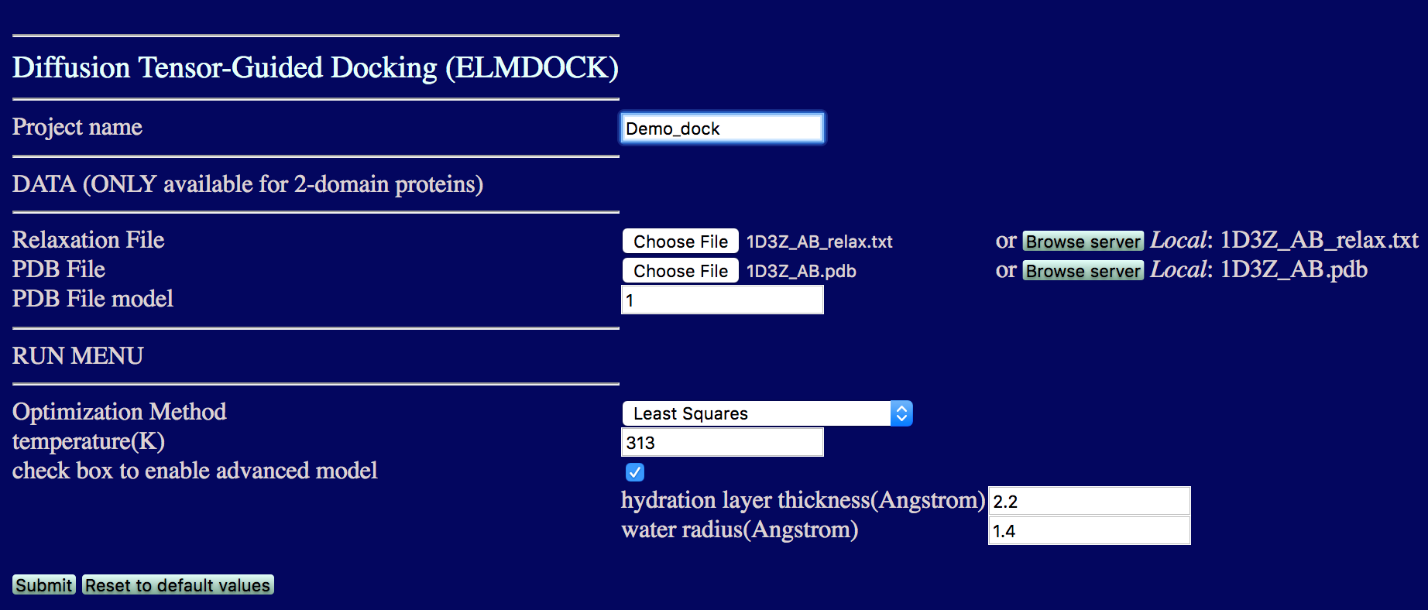
## Diffusion Tensor-Guided Docking (ELMDOCK)

This module performs a rigid-body docking of macromolecular complexes guided by experimental rotational diffusion tensors using the program ELMDOCK [7,8].

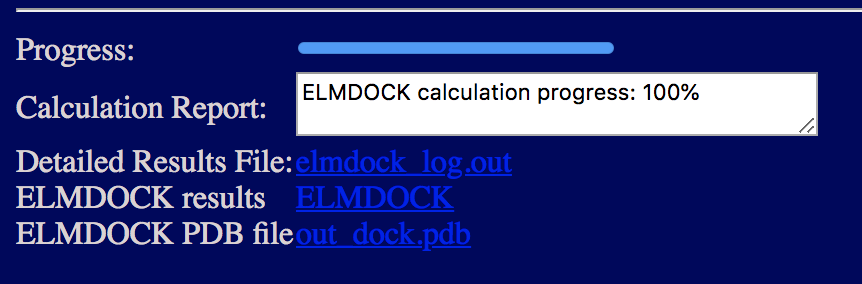
Caution: this part is currently designed only for 2-domain/component systems.

Please use the examples “diUb\_AB\_relax.txt” and “diUb\_AB.pdb” to go through the process.

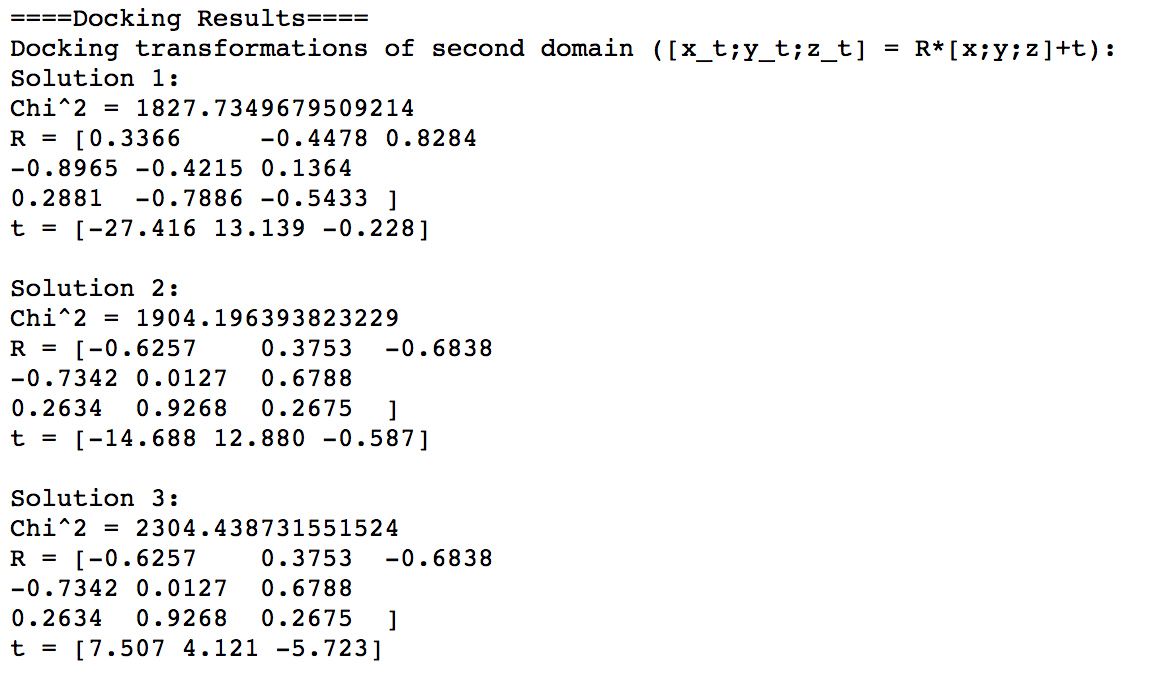


* **Project name:** The name of the folder to store all the results
* **Relaxation File:** Upload a text file containing spin relaxation data. The format of the data file is the same as spelled above in the ROTDIF & Dynamics Analysis, except that it has to contain data for two molecules (chainID), and the chainID letters must match those in the PDB file.
* **PDB File:** Upload the starting coordinate file to be used for the docking. The file must contain coordinates for both molecules (chainID) listed in the relaxation data file.
* **PDB File model:** If the coordinate file contains more than one structural model, please specify the model you want to analyze. The default model number is 1.
* **Temperature:** The desired temperature (in K) of the aqueous medium. The value of the temperature could vary from complex to complex and might need to be adjusted to avoid steric clashes. For the diUb\_AB example provided we suggest 301 K
* **Advanced model:** As in the ELM Predictor, these options are designed for advanced adjustment of the hydration layer thickness and the water radius. It is recommended that you use the default values.

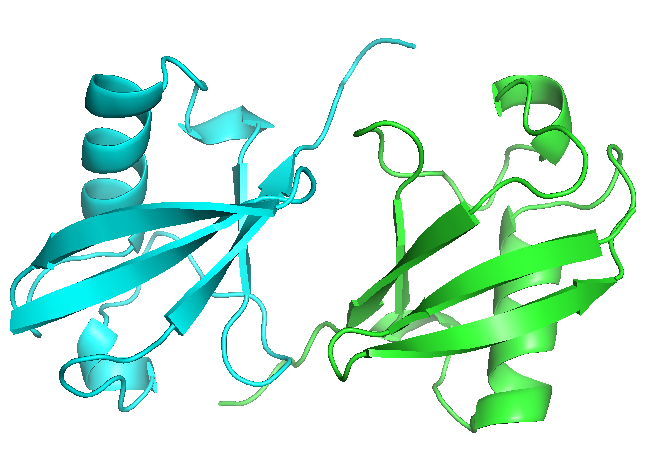
After you uploaded all the files, click the Submit button. You can download the following 3 files after the docking is finished.



* **Detailed Results File:** elmdock\_log.out. This file contains the records of all the details.
* **ELMDOCK results:** ELMDOCK. This file contains the following information on the found solutions:



* **ELMDOCK PDB file:** out\_dock.pdb. After the docking is completed ELMDOCK will start *Jmol* viewer that allows you to visualize the results. Alternatively, you can download this coordinate file and view it in a molecular viewing program. Here is the view from PyMol. The temperature is set to be 301K.



# Exercise

This exercise includes diffusion-guided rigid-body docking of two ubiquitin molecules using 15N relaxation data for K48-linked di-ubiquitin [7, 9]. Use files “diUb\_AB.pdb” (starting coordinates) and “diUb\_AB\_relax.txt” (relaxation data) to run ELMDOCK. (Note that diUb\_AB.pdb contains two arbitrarily positioned ubiquitin molecules. The atom coordinates for each ubiquitin molecule are from PDB ID 1D3Z)

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