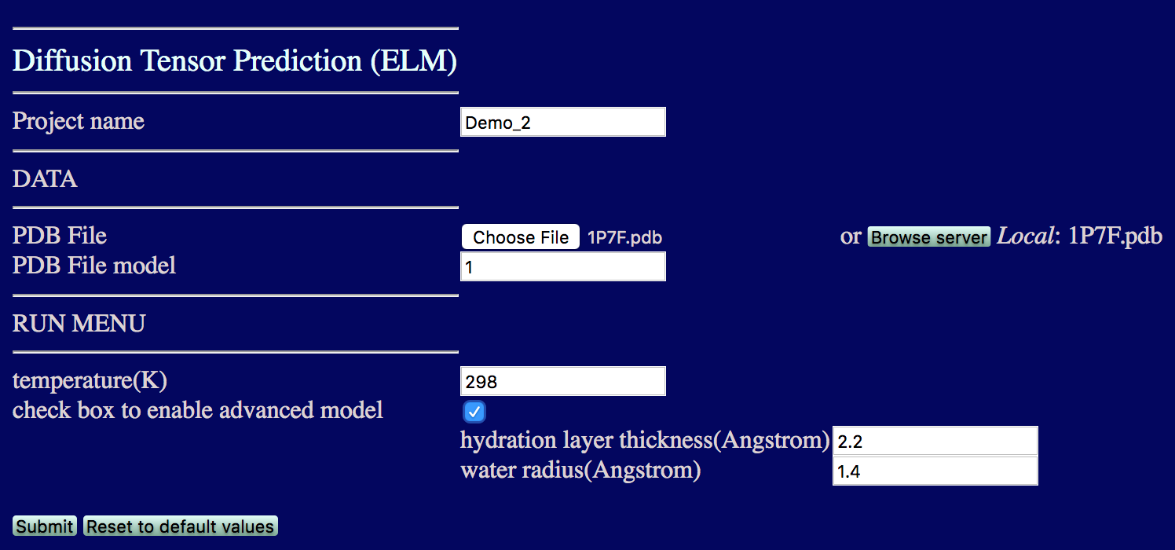
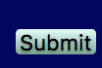
## Diffusion Tensor Prediction Module (ELM)

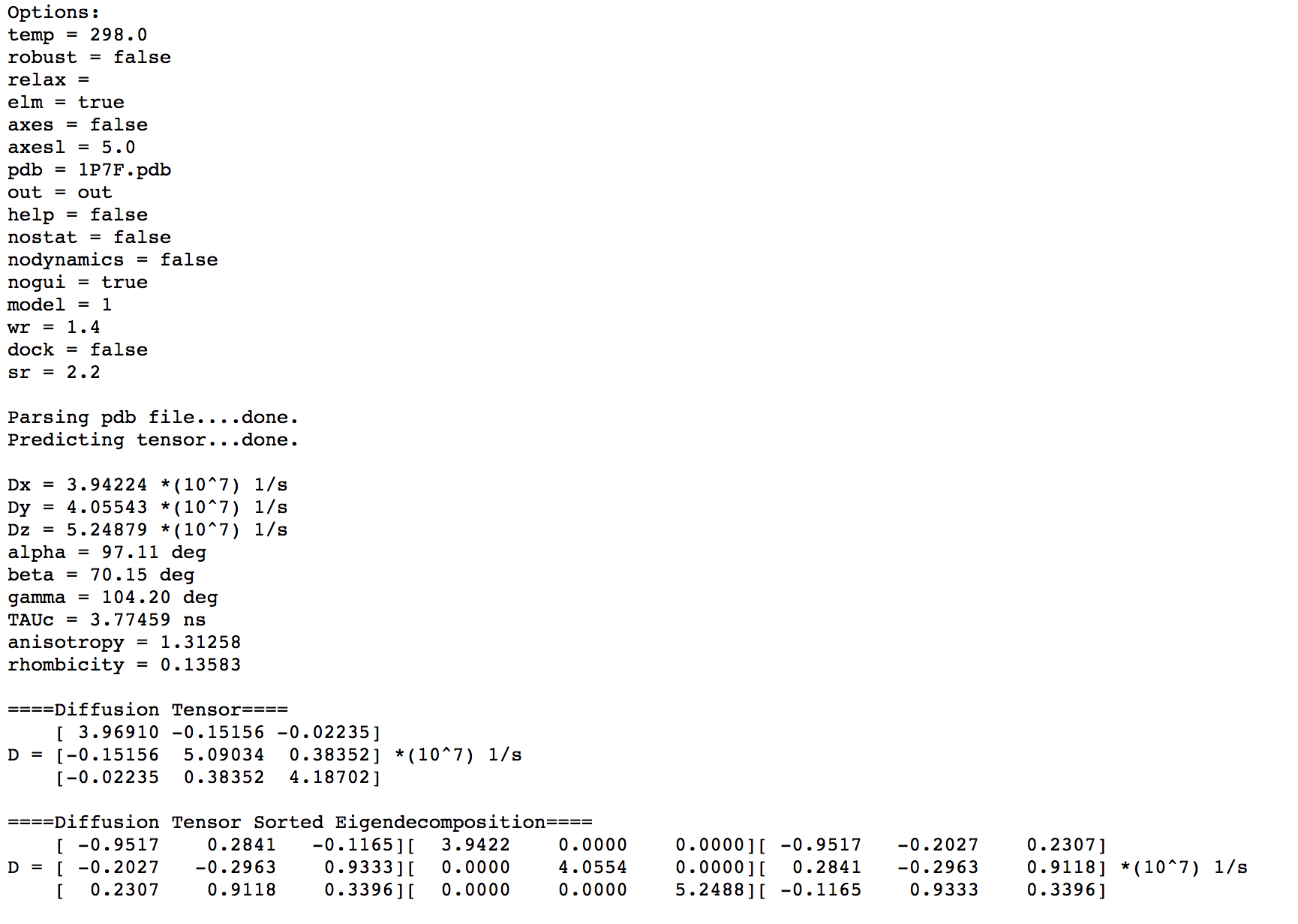
This module performs *ab initio* prediction of the rotational diffusion tensor of a macromolecule directly from the atom coordinates using an ellipsoid model (ELM) representation [6].



* **Project name:** The name of the folder to store all the results
* **PDB File:** Upload the coordinate file to be used for diffusion tensor prediction
* **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. Please note that the program assumes that molecule of interest is tumbling in water, and the empirical formula for the water viscosity used here [6, 12] is valid in the range from 273K to 373 K.
* **check box to enable advanced model:** 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.

Click . After the progress has completed, you should be able to see and download a file “ELM prediction” containing the output of the diffusion tensor prediction.

It looks like:



# Exercise

This exercise includes prediction of the rotational diffusion tensor for the B3 domain of protein G (GB3). Use coordinate file “1P7F.pdb” to run the ELM module.

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