PROTAC mutation section

This section of the tool helps the user to mutate the amino acid sequence of the target protein binding site of the PROTAC molecule.

1) Structure Input:

It takes the input of the PDB ID or structure from the local system, the output file saving location, and the desired output file format (PDB/mmCIF/mol2)

2) Minimization (optional):

Takes the number of steps of Steepest Descent and Conjugate Gradient to run minimization of the mutated structure. This step is optional.

(Note: An Increased number of steps and structure complexity may increase the time of minimization.)

3) Mutation mode:

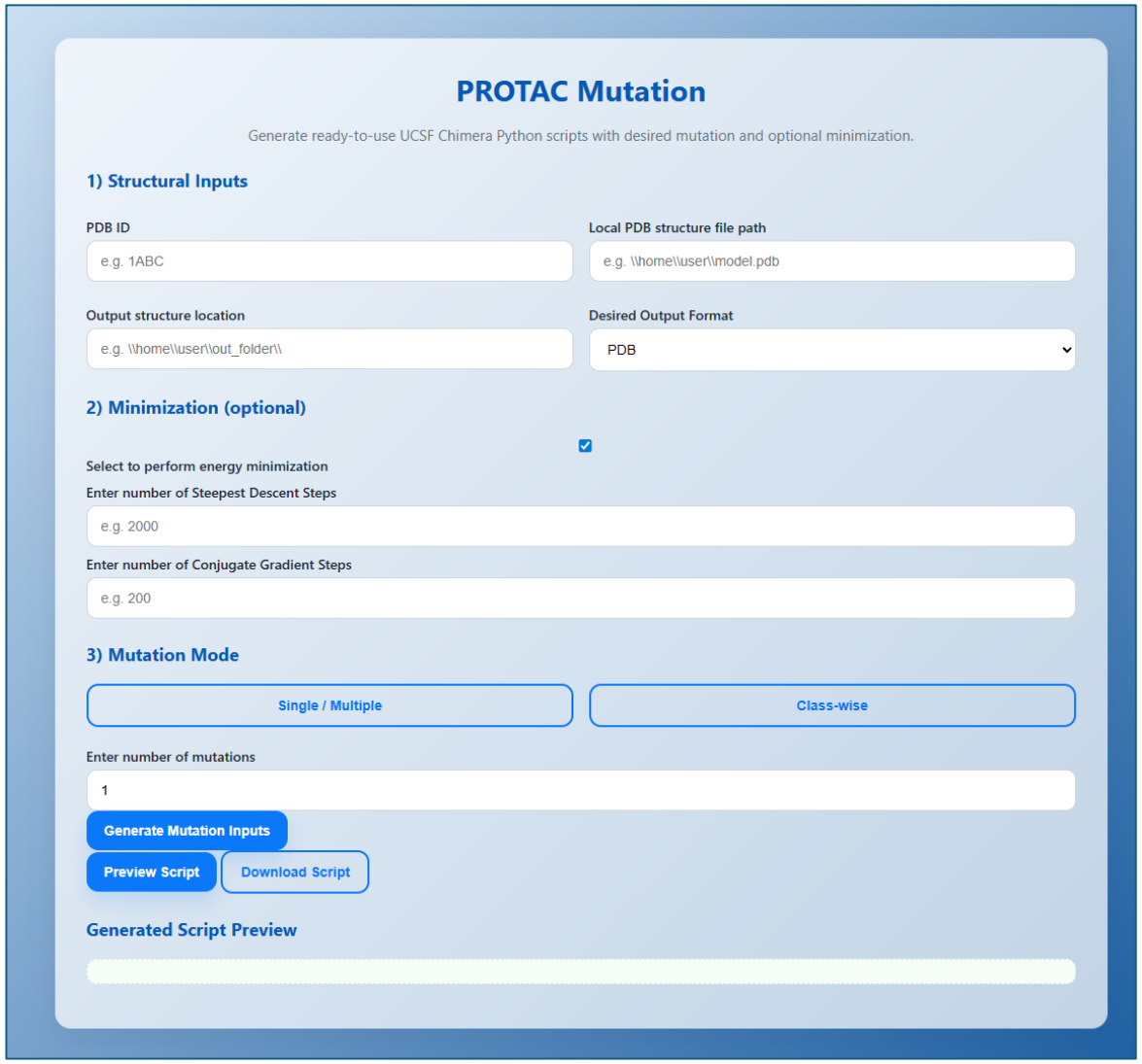
Allows users to select the type of mutation they want to perform on the structure. It includes,

Single or multiple mutation: Mutate one or more amino acids with any other amino acid. (Discussed in detail in the next section)

Class-wise mutation: Mutate one or more amino acids to all amino acids of any class. (Discussed in detail in the next section)

Enter the number of amino acids that you want to mutate and generate fields for input entry.

The user may also visualize the generated Python script and download it to directly run in Chimera 1.19+ for mutation and minimization, and save the final structures in the desired folder in the desired format.



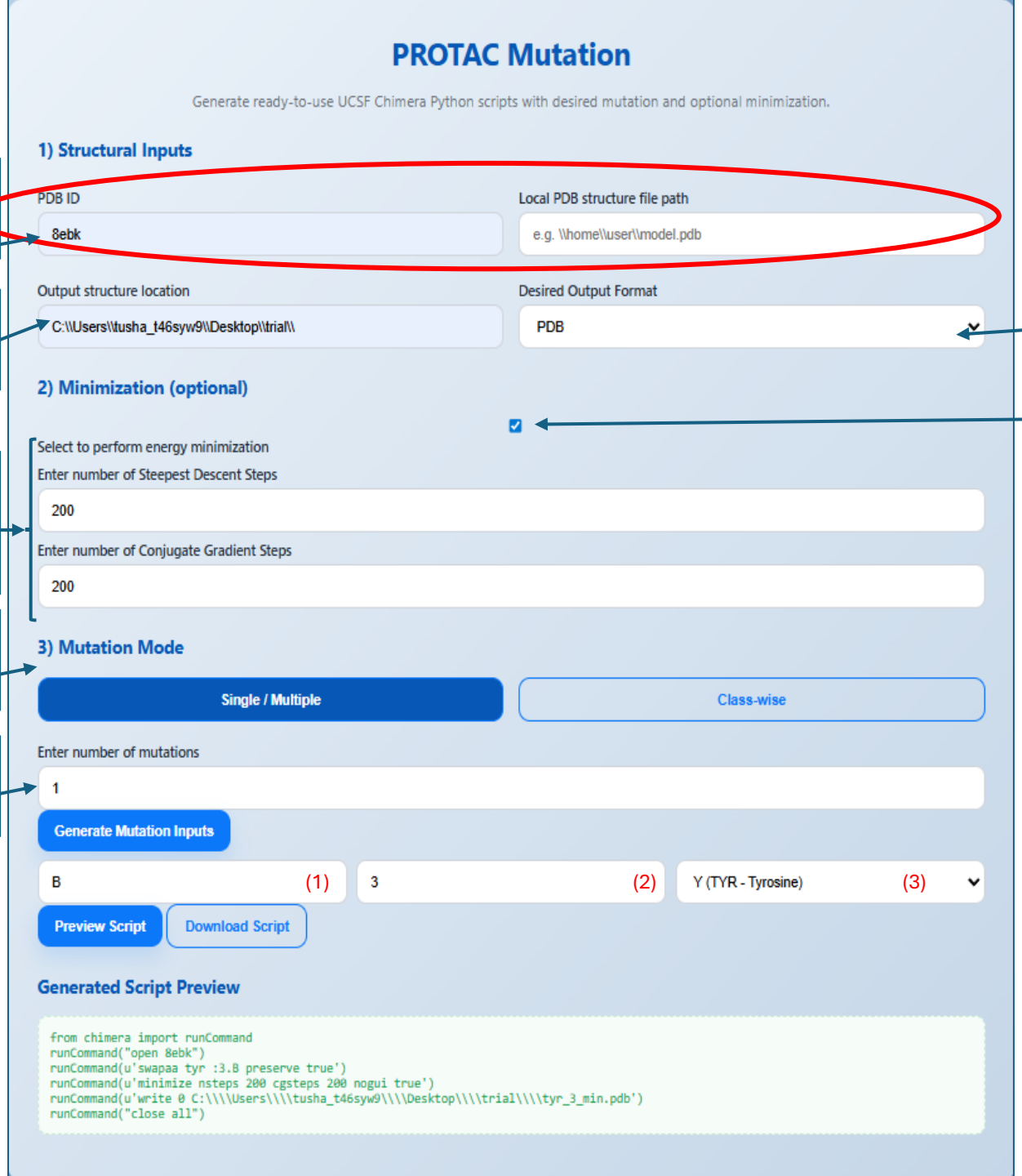
PDB ID or enter pdb structure location from local system

Enter preferred output file saving location

Enter the steps of steepest descent and conjugate gradient for minimization

Select the type of mutation to conduct on desired amino acids

Enter the number of amino acids to mutate



Choose desired output format

Check the box if you want to run minimization on output structures

For the case of single/multiple mutation mode :

1. Enter the Chain ID of the desired amino acid to mutate
2. Enter the residue ID or residue number of the amino acid
3. Choose the amino acid you wish to mutate to

Repeat the same for all the entries

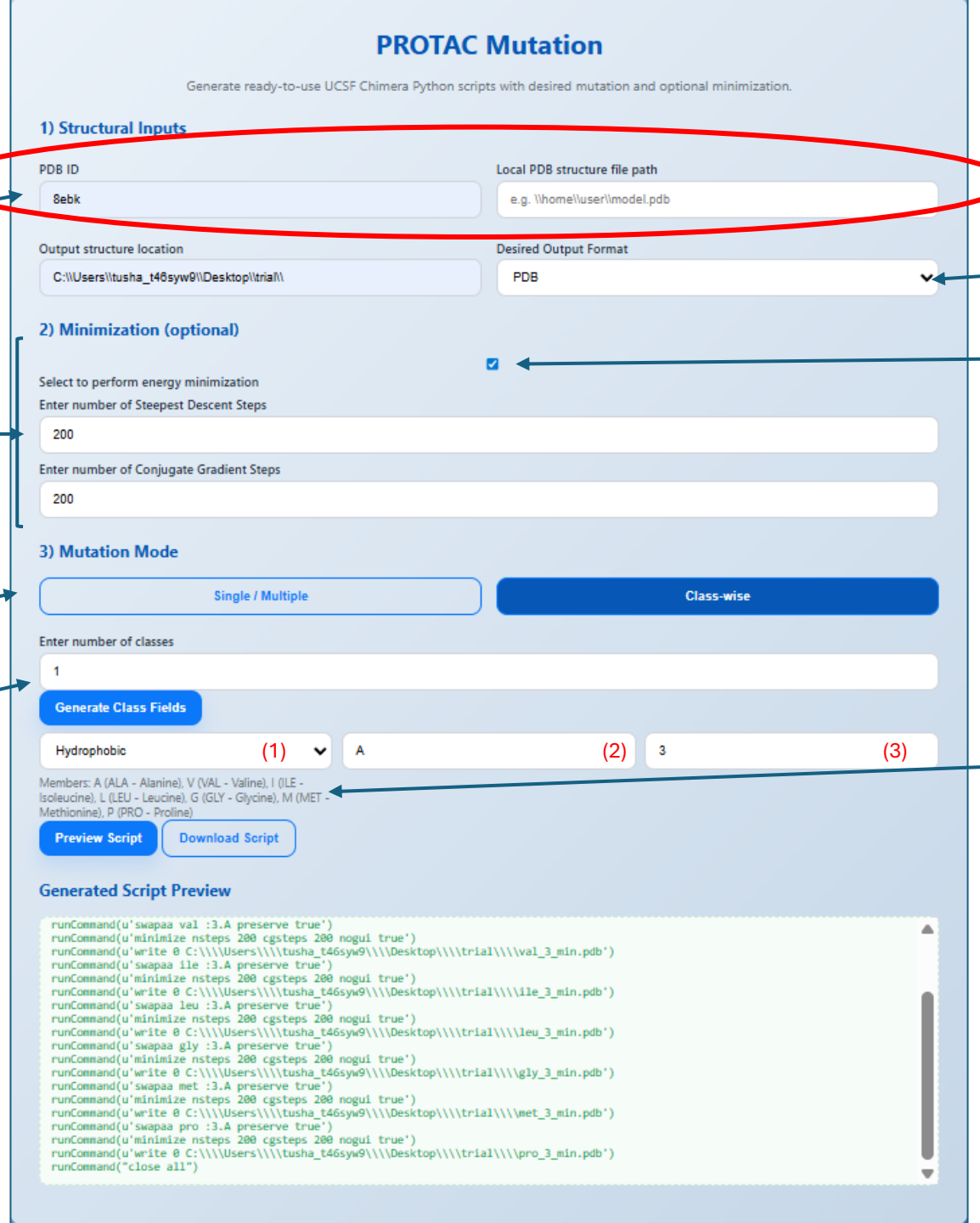
PDB ID or enter pdb structure location from local system

Enter preferred output file saving location

Enter the steps of steepest descent and conjugate gradient for minimization

Select the type of mutation to conduct on desired amino acids

Enter the number of amino acids to mutate



Choose desired output format

Check the box if you want to run minimization on output structures

For the case of class-wise mutation mode :

1. Enter the preferred class of amino acid (all amino acids of each class are listed for reference)
2. Enter the chain ID for the amino acid
3. Enter the residue ID or residue number of the amino acid

Repeat the same for all the entries