Database Pipeline

Input:
Uniprot ID + mutation(s)

1.
Do we have a Provean MSA for this protein?

DB

no → Run Provean to construct a multiple sequence alignment for the specified protein.

yes

2.
Do we have homology models for all domains in this protein?

DB

no → Run Modeller to create homology models for all domains in this protein.

yes

3.
Do we have homology models for all interactions involving this protein?

DB

no → Run Modeller to create homology models of all pairs of domains mediating interactions involving this protein.

yes

4.
Does the specified mutation fall inside a domains for which we have a structural template?

no → **Return None.** ELASPIC only works for mutations that fall inside domains.

yes

5.
Have the features and ΔΔG values been calculated for the specified mutation(s)?

DB

no → Run FoldX and other programs and internal scripts to calculate all the features required by the machine learning classifier. Run the classifier to predict a value of ΔΔG for every mutation and every domain / domain pair.

yes

Success!
Return the predicted ΔΔG caused by the mutation for all domains and domain-domain interactions