

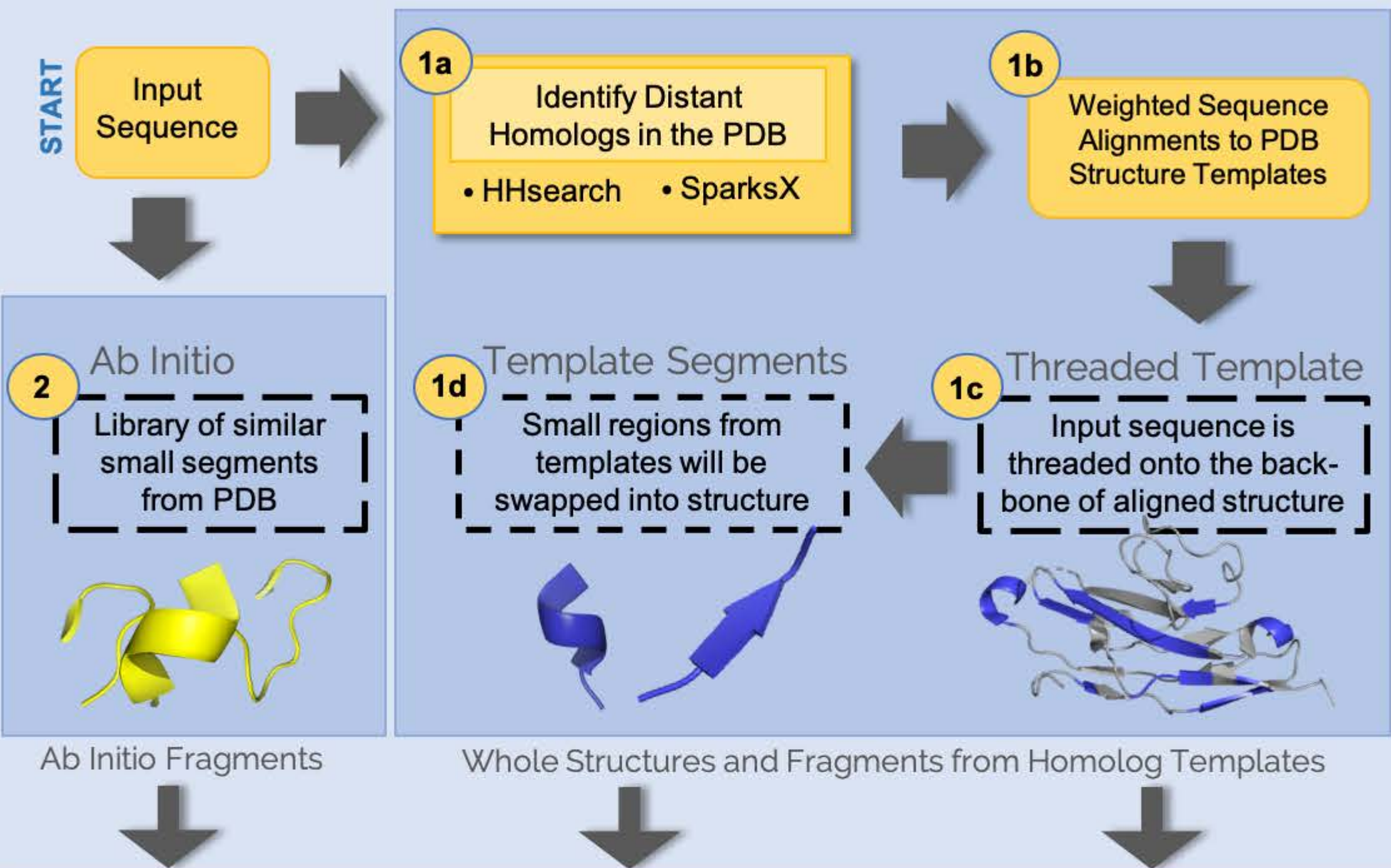


HOMOLOGY MODELING

From Sequence to Predicted Structure

TEMPLATE SEARCH

Input sequence is used to find similar structures to use as conformational sampling guides



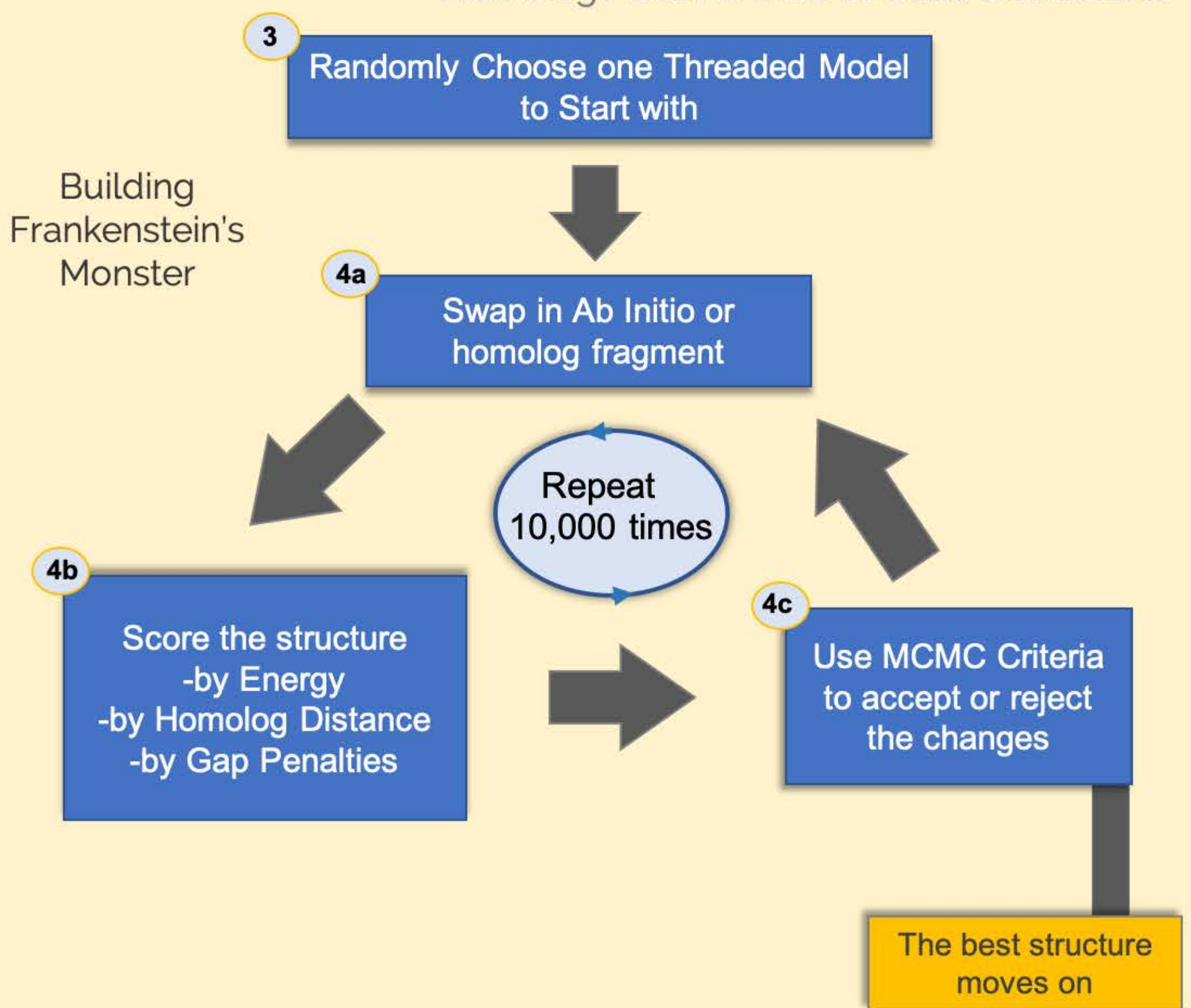
MODELING

Run 200 times

Produces a model for the entire input sequence, by testing out combinations of different whole templates, template segments, and Ab Initio fragments. Followed by structure optimization.

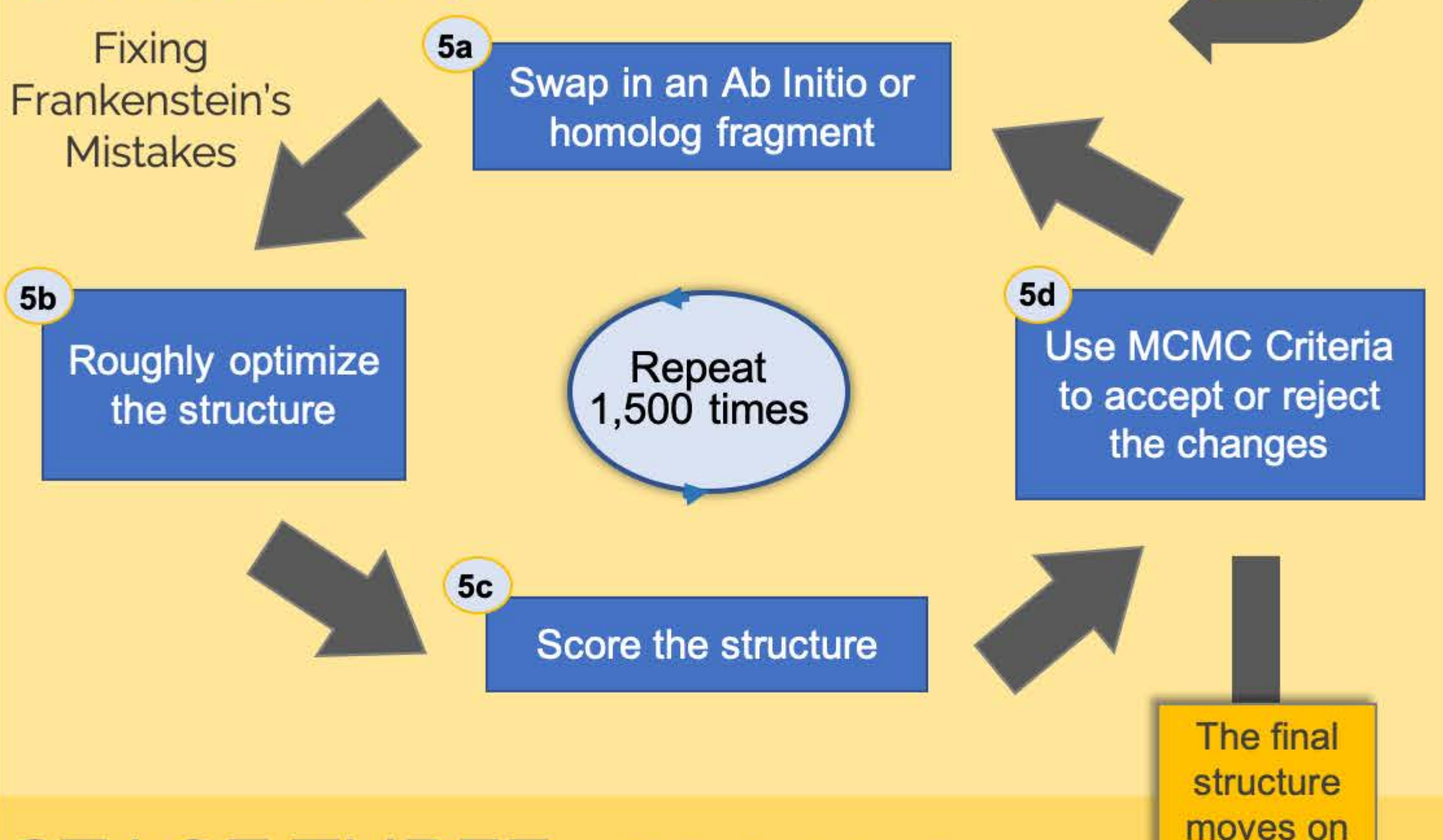
STAGE ONE

Find best combination of fragments from Homologs and Ab Initio to build a structure.



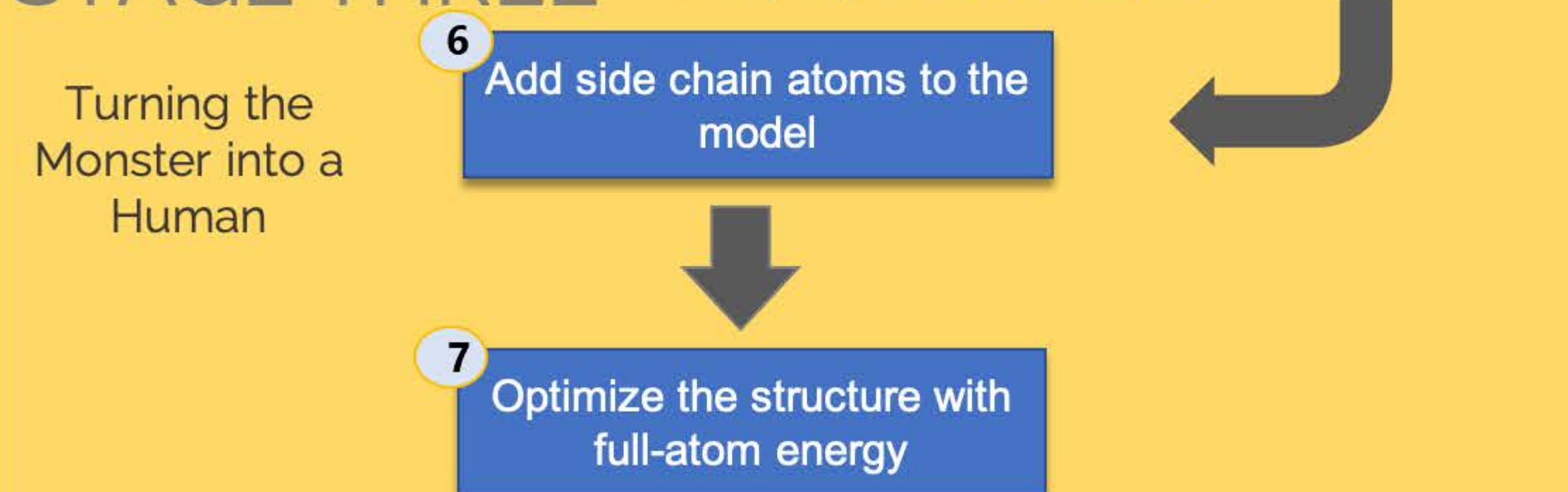
STAGE TWO

Optimize Structure in Centroid Mode



STAGE THREE

Fully Optimize Structure



Modeling Phase is Repeated 200X, Generating 200 Predicted Structures

CLUSTERING RESULTS

To better compare and understand the 200 predicted structures they are first clustered into groups based on shape

