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Refining protein structure with DeepRefiner

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ABSTRACT

Post model refinement and structural analysis is a useful later step in homology modeling. DeepRefiner uses deep learning models to optimize a given structure to try to improve the realism.

This protocol was developed for JMU students taking course in Biochemistry.

The DeepRefiner method:
Shuvo, M.H., Gulfam, M., and Bhattacharya, D. DeepRefiner: high-accuracy protein structure refinement by deep network calibration. In preparation.

PROTOCOL CITATION

Chris Berndsen 2021. Refining protein structure with DeepRefiner. **protocols.io** https://protocols.io/view/refining-protein-structure-with-deeprefiner-brnwm5fe

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MATERIALS TEXT

A protein structure file in PDB format
Internet access
An email address

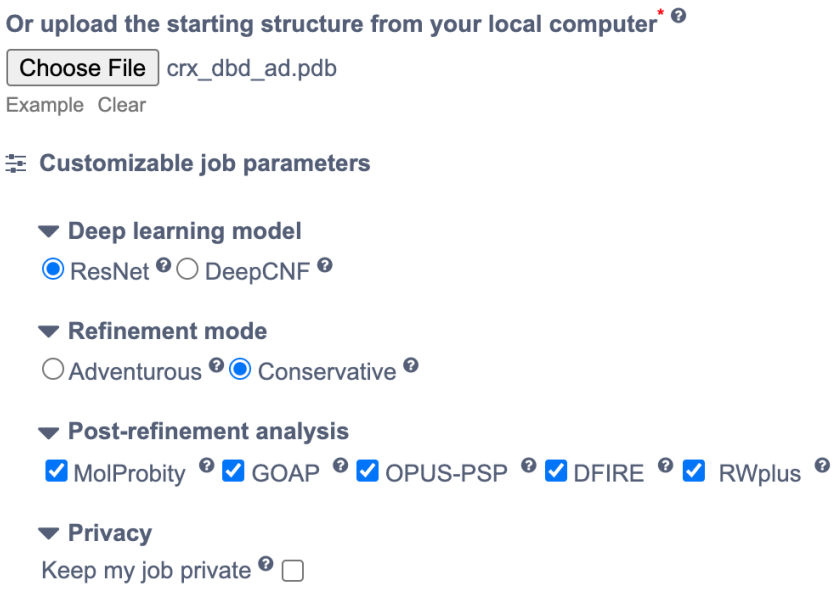
BEFORE STARTING

Make sure you have a biomolecule structure in PDB format

1 Navigate to the DeepRefiner server: http://watson.cse.eng.auburn.edu/DeepRefiner/

2 Provide your email and a job name where required. Record the job name as a note on this step.

3 Upload your .pdb file where designated and set job parameters. Suggested initial settings are shown below and they can be altered as needed.



3.1 Make note of any parameter changes in a note on this step.

4 Press the Run DeepRefiner button to begin refinement and minimization.

4.1 An email will be sent to the address provided initially. The job will complete in 12 to 96 hours depending on the number of jobs in the queue and protein site..

5 When the server returns with the result. Navigate to the URL provided in the email to view and download the results.

6 Select the Download button first to retrieve a .zip file containing all of the models and analysis.

Upload this file to OSF named as:

```
DeepRefiner_[Group_name]_[sequence_name].txt
```

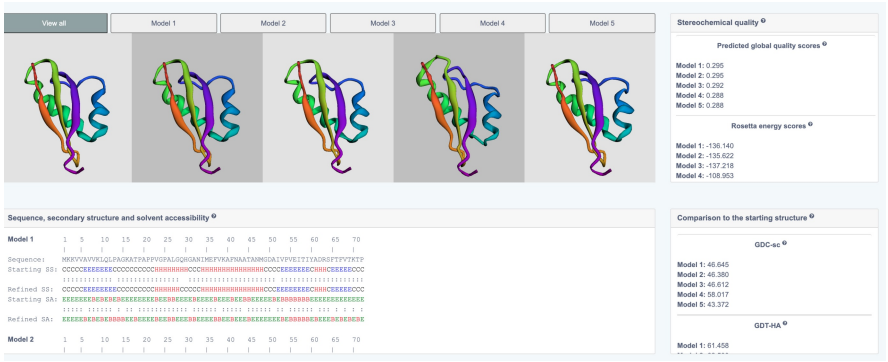
Replace [Group_name] with your name/group name without the brackets. Replace [sequence_name] with the name of the sequence.

6.1 Indicate your OSF file location as a link within a note on this step.

THIS IS YOUR DATA FILE FOR THE SEARCH!

7 Press the Show the Prediction button to see the analysis of your refined models.

8 The resulting page shows renderings of 1 to 5 models generated by the server along with an analysis of model quality.



8.1 More details on the analysis can be found on the FAQ site for DeepRefiner under the Automated results analysis tab: http://watson.cse.eng.auburn.edu/DeepRefiner/help.php

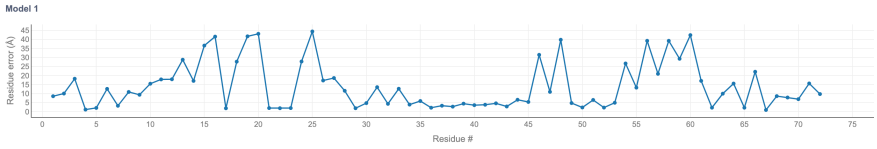
Also, hovering the cursor over the ? mark next to each analysis method shows a summary of what the numbers should trend towards for a better model.

8.2 The results from each method are contained in the .zip folder downloaded in step 6 as .txt files.

9 Visually compare the structures. It is likely that they look similar, however not any models that show distinct differences.

Note any differences as a note in this step.

10 Look at the Predicted Local Quality plots and note any regions of 5 or more amino acids that show poor quality. If those areas show up in all of the models, this may be an area that is not as trustworthy.



Predicted local quality plot. The region spanning amino acids 10 to 20 and 54 to 61 are potential areas of poor model quality or refinement.

Note any problem areas as a table or note in this step.

11 In the stereochemical quality box, compare the scores across the models. Note any models which show scores >10% off from the other models as a note in this step.

11.1 Ideally, a good model has a predicted global quality score > 0.5.

12 Record any results or conclusions in your notebook and include your notes from this procedure and remember to save this protocol as a PDF on OSF.