Building 3D structure of protein from predicted distances

As the Minifold model predicts the distances and angles from primary sequences of proteins, the predicted distances can be utilised to create a 3D model of the protein once it is converted into the suitable format.

To model the 3D structure of a single protein(for example:- 1GOU)

1. create the PSSM(.pssm) file for the protein of interest such as 1GOU using POSSUM webserver:- possum.erc.monash.edu
2. create a notebook file and copy the required libraries and function utilities from pretrain_model_pssm_l_*_l.ipynb
3. load the protein sequence of interest
4. load its pssm file and copy the piece of code from modify_pssm.py with necessary editings
5. load the trained model
6. predict the distances of the protein using model.predict()
7. copy the piece of code from RR_format.py to the same notebook file
8. edit the code using the resultant predictions
9. save the RR formatted file as "protein_sequence_ofinterest.rr/.txt"
10. use the RR formatted file as input for 3D structure modelling software GDFuzz3D:- http://www.genesilico.pl/gdserver/GDFuzz3D/

Results obtained from GDFuzz3D for the protein sequence 1GOU