

ASSIGNMENT-4

1. Download PDB file with ID '2wsc' from RCSB protein data bank(www.rcsb.org) and write a script that takes pdbfile name as input to retrieve the following information and write to 2wsc_output.txt.

- a. Title/Name of the protein.
- b. Total length of the protein/ number of residues in the given pdb
- c. No of chains present in protein and their names(Ascending order if chains are named numerically followed by alphabetical order)
- d. All aminoacid ratios present in the protein in alphabetical order.
ex: Ratio(Leu) = no of leucine present/total length of protein.
- e. Are there any unknown aminoacids present ? If so, mention total count.
- f. Are there any ligand molecules other than water ? If so, mention their names.
- g. Calculate all possible phi, psi, omega angles for the given pdb.

NOTE: Sample output file is provided, follow the same to generate your output file. The file 'Readme.txt' contains the description of the output file. Test files are also provided to check your scripts. Strictly follow the output format as mentioned.