

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.