1. Given below are ATOMIC CO-ORDINATES of atoms in protein (1L2Y.pdb)

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ATOM     76  N   GLN A   5      -4.907  -0.601  -1.645  0.00  0.00           N
ATOM     77  CA  GLN A   5      -4.122  -1.167  -2.743  0.00  0.00           C
ATOM     78  C   GLN A   5      -2.629  -1.321  -2.390  0.00  0.00           C
ATOM     79  O   GLN A   5      -1.986  -2.240  -2.884  0.00  0.00           O
ATOM     80  CB  GLN A   5      -4.292  -0.313  -4.013  0.00  0.00           C
ATOM     81  CG  GLN A   5      -4.244  -1.171  -5.290  0.00  0.00           C
ATOM     82  CD  GLN A   5      -5.576  -1.860  -5.585  0.00  0.00           C
ATOM     83  OE1 GLN A   5      -5.769  -3.044  -5.335  0.00  0.00           O
ATOM     84  NE2 GLN A   5      -6.532  -1.146  -6.152  0.00  0.00           N
ATOM     85  H   GLN A   5      -5.327   0.318  -1.763  0.00  0.00           H
ATOM     86  HA  GLN A   5      -4.517  -2.162  -2.940  0.00  0.00           H
ATOM     87 1HB  GLN A   5      -5.238   0.191  -3.969  0.00  0.00           H
ATOM     88 2HB  GLN A   5      -3.492   0.429  -4.053  0.00  0.00           H
ATOM     89 1HG  GLN A   5      -3.993  -0.539  -6.120  0.00  0.00           H
ATOM     90 2HG  GLN A   5      -3.458  -1.923  -5.205  0.00  0.00           H
ATOM     91 1HE2 GLN A   5      -6.389  -0.184  -6.408  0.00  0.00           H
ATOM     92 2HE2 GLN A   5      -7.392  -1.635  -6.335  0.00  0.00           H
ATOM     93  N   TRP A   6      -2.074  -0.459  -1.528  0.00  0.00           N
ATOM     94  CA  TRP A   6      -0.716  -0.631  -0.993  0.00  0.00           C
ATOM     95  C   TRP A   6      -0.631  -1.766   0.044  0.00  0.00           C
ATOM     96  O   TRP A   6       0.295  -2.579  -0.004  0.00  0.00           O
ATOM     97  CB  TRP A   6      -0.221   0.703  -0.417  0.00  0.00           C
ATOM     98  CG  TRP A   6       1.148   0.652   0.194  0.00  0.00           C
ATOM     99  CD1 TRP A   6       2.319   0.664  -0.482  0.00  0.00           C
ATOM    100  CD2 TRP A   6       1.508   0.564   1.606  0.00  0.00           C
ATOM    101  NE1 TRP A   6       3.371   0.560   0.411  0.00  0.00           N
ATOM    102  CE2 TRP A   6       2.928   0.515   1.710  0.00  0.00           C
ATOM    103  CE3 TRP A   6       0.779   0.524   2.812  0.00  0.00           C
ATOM    104  CZ2 TRP A   6       3.599   0.445   2.938  0.00  0.00           C
ATOM    105  CZ3 TRP A   6       1.439   0.433   4.053  0.00  0.00           C
ATOM    106  CH2 TRP A   6       2.842   0.407   4.120  0.00  0.00           C
ATOM    107  H   TRP A   6      -2.624   0.343  -1.242  0.00  0.00           H
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ATOM    108  HA  TRP A   6      -0.052  -0.908  -1.813  0.00  0.00          H
ATOM    109 1HB  TRP A   6      -0.206   1.425  -1.211  0.00  0.00          H
ATOM    110 2HB  TRP A   6      -0.921   1.044   0.344  0.00  0.00          H
ATOM    111  HD1 TRP A   6       2.412   0.733  -1.558  0.00  0.00          H
ATOM    112  HE1 TRP A   6       4.360   0.536   0.156  0.00  0.00          H
ATOM    113  HE3 TRP A   6      -0.299   0.571   2.773  0.00  0.00          H
ATOM    114  HZ2 TRP A   6       4.679   0.418   2.961  0.00  0.00          H
ATOM    115  HZ3 TRP A   6       0.862   0.400   4.966  0.00  0.00          H
ATOM    116  HH2 TRP A   6       3.334   0.360   5.081  0.00  0.00          H
ATOM    117  N   LEU A   7      -1.600  -1.860   0.967  0.00  0.00          N
ATOM    118  CA  LEU A   7      -1.641  -2.932   1.963  0.00  0.00          C
ATOM    119  C   LEU A   7      -1.847  -4.319   1.342  0.00  0.00          C
ATOM    120  O   LEU A   7      -1.144  -5.248   1.742  0.00  0.00          O
ATOM    121  CB  LEU A   7      -2.710  -2.645   3.033  0.00  0.00          C
ATOM    122  CG  LEU A   7      -2.301  -1.579   4.069  0.00  0.00          C
ATOM    123  CD1 LEU A   7      -3.475  -1.323   5.018  0.00  0.00          C
ATOM    124  CD2 LEU A   7      -1.093  -2.007   4.914  0.00  0.00          C
ATOM    125  H   LEU A   7      -2.316  -1.137   0.994  0.00  0.00          H
ATOM    126  HA  LEU A   7      -0.666  -2.978   2.445  0.00  0.00          H
ATOM    127 1HB  LEU A   7      -3.600  -2.308   2.537  0.00  0.00          H
ATOM    128 2HB  LEU A   7      -2.921  -3.571   3.572  0.00  0.00          H
ATOM    129  HG  LEU A   7      -2.061  -0.649   3.560  0.00  0.00          H
ATOM    130 1HD1 LEU A   7      -4.343  -0.992   4.449  0.00  0.00          H
ATOM    131 2HD1 LEU A   7      -3.725  -2.237   5.560  0.00  0.00          H
ATOM    132 3HD1 LEU A   7      -3.211  -0.549   5.739  0.00  0.00          H
ATOM    133 1HD2 LEU A   7      -1.270  -2.989   5.354  0.00  0.00          H
ATOM    134 2HD2 LEU A   7      -0.195  -2.045   4.300  0.00  0.00          H
ATOM    135 3HD2 LEU A   7      -0.922  -1.286   5.712  0.00  0.00          H
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a. Calculate the TORSION ANGLES: ϕ; ψ; for all
b. Calculate the distance between Cα atoms of Gln5; Trp6 and Leu7;
c. Indicate the secondary structure in which Gln-Trp-Leu are present

2. The below data from a simulated T-melt are presented for a protein folding transition. The Y_{obs} values are equal to the fraction of native protein (f_N), but they contain 2% Gaussian error. Plot the data and

describe the transition you observe. Calculate equilibrium constants and folding free energies at each temperature value from the Y_{obs} values, assuming that they are a direct measure of f_N. Plot the free energy values as a function of temperature.

T (K)	Y_{obs}	*T* (K)	Y_{obs}	*T* (K)	Y_{obs}
310	1.0091	324	0.8818	338	0.0834
312	1.0227	326	0.8028	340	0.0559
314	0.9903	328	0.6733	342	0.0294
316	0.9969	330	0.4964	344	0.0145
318	0.9793	332	0.3436	346	0.0229
320	0.9639	334	0.1972	348	0.0236
322	0.9369	336	0.1075	350	0.0221

3. Consider a simple two state model for a conformational transition from NATIVE (N) to DENATURED (D) protein.

a. Write the equilibrium constant for folding

b. Write expression for fluorescence intensity F_{obs} that is sensitive to state of the protein in the terms of fractional population of N (f_N) and D (f_D) states.

c. If fluorescence signal F is 0 for N state (F_N) and 100 for D state(F_D), show that: $f_N = \frac{F_{obs} - F_D}{F_N - F_D}$

d. Similarly derive expression for f_D.

e. Calculate f_N; f_D; and K_{fold} when F_{obs} = 60; 40; 80; 50;

4. Sketch a GREEK KEY MOTIF.

5. Draw a β–turn.

6. Draw and enumerate the different microstates for 0 and 1 H-H contacts in the sequence: H-P-P-P-P-H