DEPARTMENT OF BIOTECHNOLOGY
INDIAN INSTITUTE OF TECHNOLOGY KHARAGPUR
MID-SEMESTER EXAMINATION, Autumn 2017-18

Subject Name: Computational Structural Biology — Subject no. BT60007
Time: 2 hrs. — Max marks: 30 — No. of Students: 31

This question paper has two parts, Part A and Part B. No query on questions will be entertained during examination.

----------PART A----------

Answer all the questions.

1. Find the error, if any, from the following: [3]

a)
```
for i in line:
   for j in i:
       print i,j
```
b)
```
if item=0:
      print 'no item'
```
c)
```
source=open(1a06.pdb)
   for line in source
         print line
```

2. Append all the atom names of D68 in a list called 'atom_names'. [2]

```
ATOM   3207  N   GLU A  68     109.133  28.570  12.404  1.00 82.83           N
ATOM   3208  CA  GLU A  68     110.235  28.504  13.360  1.00 82.82           C
ATOM   3209  C   GLU A  68     110.613  29.875  13.928  1.00 83.06           C
ATOM   3210  O   GLU A  68     110.953  30.795  13.173  1.00 82.18           O
ATOM   3211  CB  GLU A  68     111.474  27.834  12.730  1.00 82.60           C
ATOM   3212  CG  GLU A  68     111.535  27.802  11.191  1.00 82.62           C
ATOM   3213  CD  GLU A  68     111.478  29.178  10.545  1.00 82.99           C
ATOM   3214  OE1 GLU A  68     112.497  29.904  10.564  1.00 81.61           O
ATOM   3215  OE2 GLU A  68     110.405  29.529  10.006  1.00 85.26           O
ATOM   3216  N   ASP A  69     110.519  30.010  15.253  1.00 83.22           N
ATOM   3217  CA  ASP A  69     110.864  31.250  15.956  1.00 82.74           C
ATOM   3218  C   ASP A  69     110.506  31.162  17.441  1.00 81.77           C
ATOM   3219  O   ASP A  69     109.960  30.158  17.896  1.00 81.01           O
ATOM   3220  CB  ASP A  69     110.144  32.457  15.332  1.00 83.13           C
ATOM   3221  CG  ASP A  69     110.730  33.783  15.779  1.00 82.77           C
ATOM   3222  OD1 ASP A  69     111.971  33.914  15.760  1.00 82.98           O
ATOM   3223  OD2 ASP A  69     109.958  34.684  16.166  1.00 82.13           O
```

Q3. Calculate the dihedral angles Phi and psi for GLN-12. Write a python code for the same.

[5+5+5=15]

	ATOM	1	N	TRP	A	10	109.622	32.123	34.299	1.00 55.67	N
	ATOM	2	CA	TRP	A	10	110.230	30.823	34.018	1.00 59.89	C
	ATOM	3	C	TRP	A	10	111.129	30.378	35.173	1.00 59.38	C
	ATOM	4	O	TRP	A	10	112.244	30.889	35.326	1.00 59.75	O
	ATOM	5	CB	TRP	A	10	111.103	30.865	32.755	1.00 58.85	C
	ATOM	6	CG	TRP	A	10	110.451	31.059	31.397	1.00 58.85	C
	ATOM	7	CD1	TRP	A	10	111.117	31.103	30.214	1.00 61.84	C
	ATOM	8	CD2	TRP	A	10	109.063	31.299	31.080	1.00 54.92	C
	ATOM	9	NE1	TRP	A	10	110.250	31.367	29.185	1.00 63.73	N
	ATOM	10	CE2	TRP	A	10	108.983	31.491	29.684	1.00 57.68	C
	ATOM	11	CE3	TRP	A	10	107.890	31.376	31.833	1.00 54.21	C
	ATOM	12	CZ2	TRP	A	10	107.781	31.756	29.021	1.00 56.60	C
	ATOM	13	CZ3	TRP	A	10	106.687	31.641	31.174	1.00 55.26	C
	ATOM	14	CH2	TRP	A	10	106.648	31.828	29.780	1.00 57.05	C
	ATOM	15	N	LYS	A	11	110.671	29.401	35.950	1.00 56.11	N
	ATOM	16	CA	LYS	A	11	111.460	28.912	37.067	1.00 53.54	C
(1)	ATOM	17	C	LYS	A	11	112.727	28.332	36.488	1.00 53.12	C
	ATOM	18	O	LYS	A	11	112.681	27.508	35.596	1.00 52.12	O
	ATOM	19	CB	LYS	A	11	110.726	27.806	37.812	1.00 54.96	C
	ATOM	20	CG	LYS	A	11	109.326	28.137	38.252	1.00 54.99	C
	ATOM	21	CD	LYS	A	11	108.675	26.892	38.855	1.00 58.65	C
	ATOM	22	CE	LYS	A	11	107.190	27.117	39.142	1.00 61.81	C
	ATOM	23	NZ	LYS	A	11	106.571	26.093	40.048	1.00 60.76	N
2	ATOM	24	N	GLN	A	12	113.866	28.821	36.933	1.00 57.60	N
3	ATOM	25	CA	GLN	A	12	115.118	28.292	36.434	1.00 58.40	C
4	ATOM	26	C	GLN	A	12	115.316	26.914	37.060	1.00 55.53	C
	ATOM	27	O	GLN	A	12	114.714	26.596	38.089	1.00 51.55	O
	ATOM	28	CB	GLN	A	12	116.276	29.230	36.779	1.00 61.32	C
	ATOM	29	CG	GLN	A	12	116.069	30.675	36.298	1.00 65.11	C
	ATOM	30	CD	GLN	A	12	115.828	30.783	34.797	1.00 65.33	C
	ATOM	31	OE1	GLN	A	12	116.651	30.352	33.986	1.00 65.19	O
	ATOM	32	NE2	GLN	A	12	114.696	31.362	34.424	1.00 65.21	N
5	ATOM	33	N	ALA	A	13	116.114	26.089	36.396	1.00 52.21	N
	ATOM	34	CA	ALA	A	13	116.404	24.748	36.850	1.00 48.40	C
	ATOM	35	C	ALA	A	13	117.772	24.390	36.306	1.00 49.57	C
	ATOM	36	O	ALA	A	13	118.077	24.685	35.151	1.00 53.26	O
	ATOM	37	CB	ALA	A	13	115.362	23.800	36.305	1.00 47.50	C
	ATOM	38	N	GLU	A	14	118.627	23.811	37.136	1.00 50.45	N
	ATOM	39	CA	GLU	A	14	119.959	23.419	36.668	1.00 53.77	C
	ATOM	40	C	GLU	A	14	119.855	22.260	35.666	1.00 51.28	C
	ATOM	41	O	GLU	A	14	120.592	22.204	34.677	1.00 50.62	O
	ATOM	42	CB	GLU	A	14	120.867	23.024	37.847	1.00 54.87	C
	ATOM	43	CG	GLU	A	14	122.327	22.816	37.453	1.00 59.76	C
	ATOM	44	CD	GLU	A	14	122.867	23.978	36.606	1.00 65.11	C
	ATOM	45	OE1	GLU	A	14	122.553	25.153	36.911	1.00 66.24	O
	ATOM	46	OE2	GLU	A	14	123.592	23.719	35.621	1.00 66.99	O
	ATOM	47	N	ASP	A	15	118.890	21.380	35.920	1.00 49.22	N
	ATOM	48	CA	ASP	A	15	118.630	20.210	35.106	1.00 45.70	C
	ATOM	49	C	ASP	A	15	117.177	19.879	35.390	1.00 42.44	C
	ATOM	50	O	ASP	A	15	116.786	19.809	36.543	1.00 44.26	O
	ATOM	51	CB	ASP	A	15	119.527	19.065	35.579	1.00 49.66	C
	ATOM	52	CG	ASP	A	15	119.609	17.916	34.576	1.00 56.59	C
	ATOM	53	OD1	ASP	A	15	118.828	17.884	33.597	1.00 58.84	O
	ATOM	54	OD2	ASP	A	15	120.482	17.039	34.771	1.00 60.93	O

----------PART B----------

Answer any two of the following questions

1. Describe the terms of a typical molecular mechanics force field. You should write down the equation, explain the variables, and explain with words what they represent. How temperature is controlled in molecular dynamics simulations? [5]

2. Describe all steps involved in setting up a molecular dynamics simulation of a protein with a ligand. You can assume that there is a crystal structure of the protein with the ligand. The purpose of the simulation is to analyze the dynamics of the protein. Try to be as detailed as possible. [5]

3. Sketch and describe the rugged energy landscape paradigm for protein folding. Write down the classical thermodynamics description of protein folding. [5]

----------END----------