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

Subject Name: Computational Structural Biology
Time: 2 hrs.

Max marks: 30

Subject no. BT60007 No. of Students: 31

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

Answer all the questions.

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'

Append all the atom names of D68 in a list called 'atom names'.	[2]
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2207	1.7	CT 13		60		202					
	IN	GTO	A	68	109.133	28.570	12.404	1.00	82.83	N.	J
3208	CA	GLU	A	68	110.235	28.504	13.360	1.00	82 82		
3209	C	GLU	A	68	110.613	29.875					
3210	0	GLU	A	68						10.00	
3211	CB	GLU	A	68		(C)(C)(C) (C) (C)(C)(C)					
3212	CG	GLU	A	68							
3213	CD	GLU	A	68							
3214	OE1				STATE OF THE PARTY OF THE PARTY.						
3215	OE2	GLU	А	0.000						C)
3216	N	ASP	A							0)
3217	CA						100-100 N DHIDAGO.			N	1
3218										C	•
										C	:
						30.158	17.896	1.00	81.01	C)
	CB	ASP	A	69	110.144	32.457	15.332	1.00	83 13		
3221	CG	ASP	A	69	110.730	33 783					
3222	OD1	ASP	Α			CONTRACTOR DESCRIPTION OF THE PERSON OF THE	0000173 R M 100078			C	;
				10000			15.760	1.00	82.98	C)
3223	002	ASP	A	69	109.958	34.684	16.166	1.00	82.13		
	3210 3211 3212 3213 3214 3215 3216 3217 3218 3219 3220 3221	3208 CA 3209 C 3210 O 3211 CB 3212 CG 3213 CD 3214 OE1 3215 OE2 3216 N 3217 CA 3218 C 3219 O 3220 CB 3221 CG 3222 OD1	3208 CA GLU 3209 C GLU 3210 O GLU 3211 CB GLU 3212 CG GLU 3213 CD GLU 3214 OE1 GLU 3215 OE2 GLU 3216 N ASP 3217 CA ASP 3218 C ASP 3219 O ASP 3220 CB ASP 3221 CG ASP 3222 OD1 ASP	3208 CA GLU A 3209 C GLU A 3210 O GLU A 3211 CB GLU A 3212 CG GLU A 3213 CD GLU A 3214 OE1 GLU A 3215 OE2 GLU A 3216 N ASP A 3217 CA ASP A 3217 CA ASP A 3219 O ASP A 3220 CB ASP A 3221 CG ASP A 3221 CG ASP A	3208 CA GLU A 68 3209 C GLU A 68 3210 O GLU A 68 3211 CB GLU A 68 3212 CG GLU A 68 3213 CD GLU A 68 3214 OE1 GLU A 68 3215 OE2 GLU A 68 3216 N ASP A 69 3217 CA ASP A 69 3219 O ASP A 69 3220 CB ASP A 69 3221 CG ASP A 69 3221 CG ASP A 69 3222 OD1 ASP A 69	3208 CA GLU A 68 110.235 3209 C GLU A 68 110.613 3210 O GLU A 68 110.953 3211 CB GLU A 68 111.474 3212 CG GLU A 68 111.535 3213 CD GLU A 68 111.478 3214 OE1 GLU A 68 112.497 3215 OE2 GLU A 68 110.405 3216 N ASP A 69 110.519 3217 CA ASP A 69 110.506 3219 O ASP A 69 109.960 3220 CB ASP A 69 110.730 3222 OD1 ASP A 69 110.730 3222 OD1 ASP A 69 111.971	3208 CA GLU A 68 110.235 28.504 3209 C GLU A 68 110.613 29.875 3210 O GLU A 68 110.953 30.795 3211 CB GLU A 68 111.474 27.834 3212 CG GLU A 68 111.535 27.802 3213 CD GLU A 68 111.478 29.178 3214 OE1 GLU A 68 112.497 29.904 3215 OE2 GLU A 68 110.405 29.529 3216 N ASP A 69 110.519 30.010 3217 CA ASP A 69 110.519 30.010 3217 CA ASP A 69 110.864 31.250 3218 C ASP A 69 110.966 31.162 3219 O ASP A 69 109.960 30.158 3220 CB ASP A 69 110.730 33.783 3222 OD1 ASP A 69 111.971 33.914	3208 CA GLU A 68 110.235 28.504 13.360 3209 C GLU A 68 110.613 29.875 13.928 3210 O GLU A 68 110.953 30.795 13.173 3211 CB GLU A 68 111.474 27.834 12.730 3212 CG GLU A 68 111.535 27.802 11.191 3213 CD GLU A 68 111.478 29.178 10.545 3214 OE1 GLU A 68 112.497 29.904 10.564 3215 OE2 GLU A 68 110.405 29.529 10.006 3216 N ASP A 69 110.519 30.010 15.253 3217 CA ASP A 69 110.519 30.010 15.253 3218 C ASP A 69 110.864 31.250 15.956 3218 C ASP A 69 110.506 31.162 17.441 3219 O ASP A 69 109.960 30.158 17.896 3220 CB ASP A 69 110.144 32.457 15.332 3221 CG ASP A 69 110.730 33.783 15.779 3222 OD1 ASP A 69 111.971 33.914 15.760	3208 CA GLU A 68 110.235 28.576 12.404 1.00 3209 C GLU A 68 110.613 29.875 13.928 1.00 3210 O GLU A 68 110.953 30.795 13.173 1.00 3211 CB GLU A 68 111.474 27.834 12.730 1.00 3212 CG GLU A 68 111.535 27.802 11.191 1.00 3213 CD GLU A 68 111.478 29.178 10.545 1.00 3214 OE1 GLU A 68 112.497 29.904 10.564 1.00 3215 OE2 GLU A 68 110.405 29.529 10.006 1.00 3216 N ASP A 69 110.519 30.010 15.253 1.00 3217 CA ASP A 69 110.506 31.162 17.441 1.00 3218 C ASP A 69 110.506 31.162 17.441 1.00 3219 O ASP A 69 109.960 30.158 17.896 1.00 3220 CB ASP A 69 110.144 32.457 15.332 1.00 3221 CG ASP A 69 110.730 33.783 15.779 1.00 3222 OD1 ASP A 69 111.971 33.914 15.760 1.00	3208 CA GLU A 68	3208 CA GLU A 68

	MOTA	1	N	TRP		10	109.622	32.123	34.299	1.00 55.67	
	ATOM	2	CA	TRP		10	110.230	30.823	34.018	1.00 59.89	N
	MOTA	3	C	TRP		10	111.129	30.378	35.173	1.00 59.38	c
	MOTA	4	0	TRP		10	112.244	30.889	35.326	1.00 59.75	C
	ATOM	5	CB	TRP		10	111.103	30.865	32.755	1.00 58.85	0
	MOTA	6	CG	TRP		10	110.451	31.059	31.397	1.00 58.85	c
	MOTA	7		TRP		10	111.117	31.103	30.214	1.00 61.84	c
	MOTA	8		TRP		10	109.063	31.299	31.080	1.00 54.92	c
	ATOM	9		TRP		10	110.250	31.367	29.185	1.00 63.73	N
	MOTA	10		TRP		10	108.983	31.491	29.684	1.00 57.68	c
	MOTA	11		TRP		10	107.890	31.376	31.833	1.00 54.21	c
	ATOM	12		TRP		10	107.781	31.756	29.021	1.00 56.60	c
	MOTA	13	CZ3	TRP	A	10	106.687	31.641	31.174	1.00 55.26	c
	MOTA	14	CH2	TRP	A	10	106.648	31.828	29.780	1.00 57.05	c
	MOTA	15	N	LYS	A	11	110.671	29.401	35.950	1.00 56.11	N
	MOTA	16	CA	LYS		11	111.460	28.912	37.067	1.00 53.54	C
(1)	ATOM	17	<u>c</u>	LYS	A	11	112.727	28.332	36.488	1.00 53.12	C
	MOTA	18	0	LYS	A	11	112.681	27.508	35.596	1.00 52.12	0
	ATOM	19	CB	LYS		11	110.726	27.806	37.812	1.00 54.96	c
	ATOM	20	CG	LYS		11	109.326	28.137	38.252	1.00 54.99	c
	MOTA	21	CD	LYS		11	108.675	26.892	38.855	1.00 58.65	c
	ATOM	22	CE	LYS		11	107.190	27.117	39.142	1.00 61.81	c
	MOTA	23	NZ	LYS		11	106.571	26.093	40.048	1.00 60.76	N
2	ATOM	24	N	GLN		12	113.866	28.821	36.933	1.00 57.60	N
3	MOTA	25	CA	GLN		12	115.118	28.292	36.434	1.00 58.40	c
u	MOTA	26	c_	GLN		12	115.316	26.914	37.060	1.00 55.53	č
•	MOTA	27	0	GLN		12	114.714	26.596	38.089	1.00 51.55	ō
	MOTA	28	CB	GLN		12	116.276	29.230	36.779	1.00 61.32	c
	MOTA	29	CG	GLN		12	116.069	30.675	36.298	1.00 65.11	c
	MOTA	30	CD	GLN		12	115.828	30.783	34.797	1.00 65.33	С
	MOTA	31		GLN		12	116.651	30.352	33.986	1.00 65.19	0
	ATOM	32		GLN		12	114.696	31.362	34.424	1.00 65.21	N
5	ATOM	33	N	ALA		13	116.114	26.089	36.396	1.00 52.21	N
-	MOTA	34	CA	ALA		13	116.404	24.748	36.850	1.00 48.40	С
	ATOM	35	¢	ALA		13	117.772	24.390	36.306	1.00 49.57	С
	ATOM	36	0	ALA		13	118.077	24.685	35.151	1.00 53.26	0
	ATOM	37	СВ	ALA		13	115.362	23.800	36.305	1.00 47.50	С
	MOTA	38	N	GLU		14	118.627	23.811	37.136	1.00 50.45	N
	ATOM	39	CA	GLU		14	119.959	23.419	36,668	1.00 53.77	С
	MOTA	40	C	GLU	A	14	119.855	22.260	35.666	1.00 51.28	С
	ATOM	41	0	GLU		14	120.592	22.204	34.677	1.00 50.62	0
	MOTA	42	CB	GLU		14	120.867	23.024	37.847	1.00 54.87	С
	ATOM	43	CG	GLU	A	14	122.327	22.816	37.453	1.00 59.76	С
	MOTA	44	CD	GLU	A	14	122.867	23.978	36.606	1.00 65.11	С
	ATOM	45	OE1	GLU	A	14	122.553	25.153	36.911	1.00 66.24	0
	MOTA	46	OE2	GLU	A	14	123.592	23.719	35.621	1.00 66.99	0
	MOTA	47	N	ASP	A	15	118.890	21.380	35.920	1.00 49.22	N
	MOTA	48	CA	ASP	A	15	118.630	20.210	35.106	1.00 45.70	С
	MOTA	49	C	ASP		15	117.177	19.879	35.390	1.00 42.44	c
	MOTA	50	0	ASP		15	116.786	19.809	36.543	1.00 44.26	0
	MOTA	51	CB	ASP		15	119.527	19.065	35.579	1.00 49.66	c
	MOTA	52	CG	ASP		15	119.609	17.916	34.576	1.00 56.59	C
	MOTA	53		ASP		15	118.828	17.884	33.597	1.00 58.84	0
	MOTA	54	OD2	ASP	A	15	120.482	17.039	34.771	1.00 60.93	0

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]

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