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

Subject name: Computational Structural Biology (BT60007)
Time: 3 hrs. Max. Marks: 50 No. of Students: 30

Answer all the questions. No query will be entertained regarding the questions during exam

1. What is the ratio of energies of electrostatic interaction between histidine and glutamate residue separated by 5 Angstroms within the interior of a protein (dielectric constant = 8) to that on the surface of a protein (dielectric constant = 80)? [3]

2. If the rise of the alpha helix is 0.15 nm/residue. Calculate the pitch for alpha helix. Assuming alpha helix is having 18 residues per 5 turns. [2]

3. Describe in details three components of a docking software. Explain three types of scoring functions that are used in molecular docking. [3+3]

4. Name different search algorithms used in molecular docking programs. Describe any one of these approaches in details. [1+3]

5. Explain with diagram different torsion angles used to describe DNA conformation. Write down the equation to calculate Tilt, Twist and Roll for changing DNA conformation. [3+2]

Q6. A) What is icosahedron? Explain the symmetry elements in an icosahedron? What is lattice triangulation number? Discuss how the size of the virus capsids depends on the lattice triangulation number.

[1+2+1+1=5]

B) In the following part of the virus capsid generate the symmetry related ASN 18 using the symmetry elements three and five given in the matrix below. The coordinates of the residues and the transformation matrices are given below.

[5+5=10]

ATOM	47	N	SER A	17	-5.946	51.495	25.629	1.00	61.12	N
ATOM	48	CA	SER A	17	-6.566	52.078	26.823	1.00	46.62	C
ATOM	49	C	SER A	17	-6.323	53.584	26.755	1.00	37.94	C
ATOM	50	O	SER A	17	-5.202	54.012	26.495	1.00	36.14	O
ATOM	51	CB	SER A	17	-5.915	51.529	28.104	1.00	44.98	C
ATOM	52	OG	SER A	17	-6.613	51.936	29.259	1.00	39.85	O
ATOM	58	N	ASN A	18	-7.344	54.391	26.985	1.00	28.24	N
ATOM	59	CA	ASN A	18	-7.164	55.835	26.908	1.00	21.25	C
ATOM	60	C	ASN A	18	-7.323	56.521	28.254	1.00	16.15	C
ATOM	61	O	ASN A	18	-7.280	57.751	28.319	1.00	14.83	O

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ATOM     62  CB  ASN A  18      -8.183  56.448  25.935  1.00 24.28           C
ATOM     63  CG  ASN A  18      -7.837  56.231  24.458  1.00 25.65           C
ATOM     64  OD1 ASN A  18      -8.738  56.174  23.643  1.00 28.85           O
ATOM     65  ND2 ASN A  18      -6.553  56.134  24.107  1.00 28.45           N
ATOM     72  N   VAL A  19      -7.551  55.748  29.313  1.00 12.90           N
ATOM     73  CA  VAL A  19      -7.709  56.346  30.632  1.00 11.37           C
ATOM     74  C   VAL A  19      -6.840  55.634  31.657  1.00  9.64           C
ATOM     75  O   VAL A  19      -6.315  54.555  31.403  1.00 10.10           O
ATOM     76  CB  VAL A  19      -9.184  56.270  31.161  1.00 12.10           C
ATOM     77  CG1 VAL A  19     -10.127  57.200  30.374  1.00 13.49           C
ATOM     78  CG2 VAL A  19      -9.717  54.843  31.173  1.00  9.84           C
ATOM     88  N   VAL A  20      -6.682  56.286  32.806  1.00 10.73           N
ATOM     89  CA  VAL A  20      -5.927  55.712  33.906  1.00 10.52           C
ATOM     90  C   VAL A  20      -6.686  54.465  34.386  1.00 10.87           C
ATOM     91  O   VAL A  20      -7.927  54.430  34.387  1.00 11.63           O
ATOM     92  CB  VAL A  20      -5.813  56.690  35.113  1.00  9.34           C
ATOM     93  CG1 VAL A  20      -4.867  57.824  34.795  1.00  8.61           C
ATOM     94  CG2 VAL A  20      -7.171  57.289  35.496  1.00 10.24           C
ATOM    104  N   THR A  21      -5.957  53.410  34.734  1.00 10.35           N
ATOM    105  CA  THR A  21      -6.578  52.186  35.233  1.00 11.35           C
ATOM    106  C   THR A  21      -5.857  51.761  36.511  1.00 11.35           C
ATOM    107  O   THR A  21      -4.685  52.088  36.710  1.00 10.58           O
ATOM    108  CB  THR A  21      -6.527  51.047  34.211  1.00 10.27           C
ATOM    109  OG1 THR A  21      -5.176  50.892  33.780  1.00 12.84           O
ATOM    110  CG2 THR A  21      -7.415  51.370  33.005  1.00 11.04           C

BIOMT1   2  0.500000  0.309017  0.809017        0.00000
BIOMT2   2  0.309017  0.809017 -0.500000        0.00000
BIOMT3   2 -0.809017  0.500000  0.309017        0.00000
BIOMT1   3 -0.309017  0.809017  0.500000        0.00000
BIOMT2   3  0.809017  0.500000 -0.309017        0.00000
BIOMT3   3 -0.500000  0.309017 -0.809017        0.00000
BIOMT1   4 -0.309017  0.809017 -0.500000        0.00000
BIOMT2   4  0.809017  0.500000  0.309017        0.00000
BIOMT3   4  0.500000 -0.309017 -0.809017        0.00000
BIOMT1   5  0.500000  0.309017 -0.809017       -2.00000
BIOMT2   5  0.309017  0.809017  0.500000        0.00000
BIOMT3   5  0.809017 -0.500000  0.309017        0.36000
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Q7. In the following structure based sequence alignment, calculate the average entropy of the target sequence. Also find out which residues are evolving faster and which are evolving slower. Write a python code for the same. [5+2+5+2+5+5=15]

39