BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI (RAJ.) FIRST SEMESTER 2023-2024 BIO F417, BIOMOLECULAR MODELING MID-SEMESTER EXAMINATION

TOTAL WEITAGE 25% Date: 14.10.2023 DURATION: 90Mins. (Part A & Part B) Total Marks (35+15) =50

- Answer <u>Part A</u> and <u>Part B</u> in separate answer sheets.
- Irrelevant answers may attract a penalty.

PART – A (CLOSED BOOK) (Max. duration: 60 mins., Max. Marks 35)

1. Write notes on i) Levinthal Paradox ii) Ramachandran plot iii) DNA structural descriptor iv) Turns and loops v) Amphipathic helix. [2X5=10]

2. a) Why do we call β -strand as extended conformation? Explain why we do not see single β -strand in protein structure. [3]

b) List down all possible stability and instability factors of collagen structure. [2]

c) Explain why α -helix have particular significance in DNA binding motifs, including helix-turn-helix motifs, leucine zipper motifs and zinc finger motifs. [2]

d) Which way polyproline helices are different from conventional secondary structures? [2]

3. a) The following average structural parameters are obtained from the crystal structure of a DNA with sequence "CGCGCGCGCGCG". Identify the structure and justify your answer. [3]

X-displacement: -5.28 Å; Propeller Twist: 13.7°; Rise (Step): 3.4 Å; Inclination: 20.7°; Pseudorotation torsion angle: 18.3°.

b) Identify the sugar pucker and glycosidic torsion angle of the following nucleotide. Do you think this nucleotide will be part of above DNA structure (Q.3a)? Justify your answer. [2+2]



c) Explain how the Twist and Rise of a DNA structure are interlinked. [3]
d) Diagrammatically show transition of ³T₂ sugar pucker to ²T₃ sugar pucker via ^oE sugar pucker. [6]

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PART – B (OPEN BOOK) (Max. duration: 30 mins., Max. Marks 15)

1. a) Explain (with proper diagram) the conformational restriction of di-proline with
respect to di-glycine. (Only consider ϕ and ψ).[6]b) In order to choose a preferred rotameric form of amino acid side chain what factors
one should consider?[2]c) In nature γ -turns are frequently observed however the longer helix with i to i+2
hydrogen bond is never observed. Explain.[2]

2.The following schematic figure of DNA double strand was first proposed by Watson-Crick in their famous paper on 1953.

a) What structural operation will lead conversion of this DNA form into A-form? [3]

[2]

b) Explain possible reasons for rigid Pu/Pu or Py/Py step?


