ATOM	100 P DAA 6	15.060 13.659 14.706 1.00 10.00	<u>P</u>
ATOM	101 OP1 DA A 6	14.114 12.694 15.318 1.00 10.00	0
ATOM	102 OP2 DA A 6	16.053 13.109 13.762 1.00 10.00	0
ATOM	103 O5' DA A 6	14.197 14.848 14.023 1.00 10.00	0
ATOM	104 C5' DA A 6	13.168 15.423 14.895 1.00 10.00	C
ATOM	105 C4' DA A 6	12.160 16.099 14.010 1.00 10.00	C
ATOM	106 O4' DA A 6	12.788 17.233 13.398 1.00 10.00	0
ATOM	107 C3' DA A 6	11.539 15.272 12.883 1.00 10.00	C
ATOM	108 O3' DA A 6	10.115 15.440 12.877 1.00 10.00	0
ATOM	109 C2' DA A 6	12.266 15.763 11.646 1.00 10.00	C
ATOM	110 C1' DA A 6	12.558 17.191 11.965 1.00 10.00	C
ATOM	111 N9 DA A 6	13.775 17.791 11.392 1.00 10.00	N
ATOM	112 C8 DA A 6	15.001 17.245 11.178 1.00 10.00	C
ATOM	113 N7 DA A 6	15.882 18.098 10.683 1.00 10.00	N
ATOM	114 C5 DA A 6	15.184 19.294 10.598 1.00 10.00	C
ATOM	115 C6 DA A 6	15.554 20.575 10.156 1.00 10.00	C
ATOM	116 N6 DAA 6	16.769 20.924 9.713 1.00 10.00	N
ATOM	117 N1 DAA 6	14.605 21.532 10.221 1.00 10.00	N
ATOM	118 C2 DA A 6	13.382 21.243 10.650 1.00 10.00	C
ATOM	119 N3 DAA 6	12.922 20.063 11.106 1.00 10.00	N
ATOM	120 C4 DA A 6	13.887 19.126 11.047 1.00 10.00	C
ATOM	366 P DT B 19	15.275 30.434 4.030 1.00 10.00	<u>P</u>
ATOM	367 OP1 DT B 19	14.401 31.249 3.131 1.00 10.00	0
ATOM	368 OP2 DT B 19	16.559 31.031 4.453 1.00 10.00	0
ATOM	369 O5' DT B 19	14.398 30.065 5.351 1.00 10.00	0
ATOM	370 C5' DT B 19	13.150 29.372 5.104 1.00 10.00	C
ATOM	371 C4' DT B 19	12.966 28.356 6.184 1.00 10.00	<u>C</u>
ATOM	372 O4' DT B 19	13.470 27.050 6.276 1.00 10.00	0
ATOM	373 C3' DT B 19	12.498 28.839 7.545 1.00 10.00	C
ATOM	374 O3' DT B 19	11.095 29.170 7.506 1.00 10.00	0
ATOM	375 C2' DT B 19	12.884 27.730 8.476 1.00 10.00	C
ATOM	376 C1' DT B 19	13.222 26.542 7.610 1.00 10.00	C
ATOM	377 N1 DTB 19	14.411 25.807 8.085 1.00 10.00	N
<u>ATOM</u>	378 C2 DT B 19	14.233 24.573 8.678 1.00 10.00	C

ATOM	379 O2	DT B 19	13.155 24.022	8.847 1.00 10.00	0
ATOM	380 N3	DT B 19	15.401 23.980	9.068 1.00 10.00	N
ATOM	381 C4	DT B 19	16.689 24.455	8.964 1.00 10.00	C
ATOM	382 O4	DT B 19	17.622 23.771	9.381 1.00 10.00	0
ATOM	383 C5	DT B 19	16.777 25.752	8.346 1.00 10.00	С
ATOM	384 C7	DT B 19	18.116 26.399	8.177 1.00 10.00	С
ATOM	385 C6	DT B 19	15.665 26.361	7.942 1.00 10.00	С

- Given above are ATOMIC CO-ORDINATES of 1 base pair in B DNA DUPLEX.
 - a. Which nucleotide bases are involved in base pairing?
 - b. Calculate the distance between the two carbons attached to base in each individual chain A and B.
 - c. Calculate the distance between the HYDROGEN BOND DONOR ATOMS in the base pair for ALL HB pairs.
 - d. Calculate the TORSION ANGLES: α ; β ; γ ; δ ; χ ;
 - e. Calculate the helix DIAMETER.
 - f. Can you calculate the base pair inclination?
 - g. Can you determine the SUGAR PUCKER?

h.

2. The above DNA structure co-ordinates were obtained from 114d.pdb file. Download this file and VIEW the DNA structure in 3D using software like PYMOL.

