BT307 LAB 3

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Roll No.: 210106004

1)

DIHEDRAL ANGLES

Statistic	Observed	Expected
Mean Helix Phi	-69.3 sd=9.2	-65.3 sd=11.9
Mean Helix Psi	-34.2 sd=16.9	-39.4 sd=25.5
# res with Gauche+ Chi	23 (50%)	25 (55%)
# res with Gauche- Chi	7 (15%)	9 (20%)
# res with Trans Chi	16 (34%)	11 (25%)
Mean Chi Gauche+	-65.4 sd=12.0	-66.7 sd=15.0
Mean Chi Gauche-	60.6 sd=15.9	64.1 sd=15.7
Mean Chi Trans	167.0 sd=11.7	168.6 sd=16.8
Std. dev of chi pooled	12.50	15.70
Mean Omega (|omega|>90)	179.0 sd=2.4	180.0 sd=5.8
# res with |omega|<90	1 (1%)	-

Expected values obtained from Morris AL, MacArthur MW, Hutchinson EG and Thornton JM. Proteins. 1992 Apr;12(4):345-364.

RES. NUM.	RES. NAME	SCND STRUC	HBOND	BTURN	RES. ASA	FRAC. ASA	RES. VOL.	FRAC. VOL.	PHI	PSI	OMEGA	PRBLM
Chain A												
1	MET	BCC C	20A		132.6	0.61	161.6	0.98	0.0	145.0	-179.5	
2	THR	BBB B			73.4	0.47	110.9	0.92	-94.1	130.2	178.8	
3	TYR	BBB B	18A,18A		7.9	0.03	196.1	1.00	-118.9	150.3	179.2	
4	LYS	BBB B	52A,50A		64.3	0.28	174.1	1.03	-119.1	154.1	174.8	
5	LEU	BBB B	16A,16A		0.0	0.00	161.1	0.98	-130.2	126.6	175.6	
6	ILE	BBB B	54A,52A		68.1	0.34	153.4	0.95	-102.9	122.2	-178.0	
7	LEU	BBB B	14A,14A		5.6	0.03	180.4	1.10	-103.0	122.4	178.2	
			B	56A,54A	56.5	0.32	110.6	0.90	-130.5	61.3	179.3	
			C	12A	1.8	0.02	66.2	1.03	-85.4	179.9	-178.8	
10	LYS	CCC C			172.4	0.75	173.9	1.03	-73.0	-36.6	-178.2	
11	THR	CBC C			124.7	0.80	108.3	0.90	-108.3	-37.9	-180.0	
12	LEU	CBC C	9A		48.4	0.23	166.0	1.01	-109.5	127.6	178.9	
13	LYS	CBC C			139.2	0.60	162.6	0.96	-132.4	146.4	178.5	
14	GLY	CCC C	7A,7A		37.1	0.43	58.6	0.91	143.3	-158.0	-177.9	
15	GLU	BBB B			99.6	0.52	128.2	0.93	-143.3	143.3	174.9	
16	THR	BBB B	5A,5A		53.5	0.34	126.1	1.05	-140.4	163.5	179.6	
17	THR	BBB B			73.8	0.47	115.7	0.96	-132.0	172.1	176.5	
18	THR	BBB B	3A,3A		33.8	0.22	123.2	1.02	-158.6	156.1	176.1	
19	GLU	BBB B			127.2	0.66	123.0	0.89	-100.1	135.9	178.0	
20	ALA	BBB B	1A		12.2	0.10	82.0	0.93	-152.5	155.5	-179.8	
21	VAL	CCC C			131.3	0.76	120.8	0.88	-69.4	-39.4	179.7	
22	ASP	CCH C	25A,26A		65.2	0.40	102.2	0.86	-146.8	-179.3	-178.2	
23	ALA	HHH H	26A,27A		29.9	0.24	83.3	0.94	-69.2	-32.2	179.8	
24	ALA	HHH H	27A,28A		61.7	0.50	76.4	0.86	-73.5	-27.7	180.0	
25	THR	HHH H	22A,29A		38.5	0.25	109.5	0.91	-75.9	-40.4	179.9	
26	ALA	HHH H	22A,30A		0.1	0.00	87.1	0.99	-65.9	-35.9	178.1	
27	GLU	HHH H	23A,31A		58.9	0.31	130.7	0.95	-64.4	-34.0	178.7	
28	LYS	HHH H	24A,32A		128.6	0.56	169.5	1.00	-64.6	-56.7	-179.5	
29	VAL	HHH H	25A,33A		75.7	0.44	133.6	0.98	-65.1	-35.6	179.9	
30	PHE	HHH H	26A,34A		4.4	0.02	195.3	1.00	-66.6	-41.0	176.5	
31	LYS	HHH H	27A,35A		95.0	0.41	166.4	0.98	-61.6	-44.9	178.2	
32	GLN	HHH H	28A,36A		125.2	0.63	193.1	1.33	-62.2	-42.0	179.9	V
33	TYR	HHH H	29A,37A		74.3	0.30	193.7	0.99	-63.8	-40.0	-179.4	
34	ALA	HHH H	30A,39A		1.9	0.02	98.7	1.12	-68.0	-44.6	178.4	
35	ASN	HHH H	31A,38A	I	113.7	0.65	115.4	0.93	-66.6	-31.3	-179.5	
36	ASP	HHH H	32A,33A	I	116.7	0.72	106.1	0.89	-73.0	-27.3	-179.1	
37	ASN	HCH H	33A,34A	I	70.6	0.40	121.3	0.98	-98.9	20.4	178.2	
38	GLY	CCC C	35A	I	62.8	0.72	59.0	0.92	61.9	15.5	-179.9	
39	VAL	CCC C	34A,37A		9.2	0.05	163.5	1.20	-84.0	133.6	-177.7	
40	ASP	BCC C			124.0	0.77	123.5	1.04	-142.1	94.0	-179.6	
41	GLY	BCC C			22.7	0.26	61.1	0.95	-140.7	-157.5	177.9	
42	GLU	BBB B	55A,55A		138.5	0.72	130.4	0.95	-92.4	146.1	-176.1	
43	TRP	BBB B			67.0	0.25	212.6	0.91	-119.1	142.9	173.5	
44	THR	BBB B	53A,53A		86.6	0.56	112.3	0.93	-134.2	154.9	178.4	
45	TYR	BBB B			78.0	0.32	181.4	0.93	-138.7	127.9	179.8	
46	ASP	BBB B	50A,51A		70.2	0.43	112.3	0.94	-118.3	110.0	-178.2	
47	ASP	CCC C			82.4	0.51	102.8	0.86	-75.1	-11.3	177.2	
48	ALA	CCC C	46A		89.7	0.73	75.2	0.85	-81.7	-17.0	179.5	
49	THR	CCC C	46A		88.8	0.57	106.4	0.88	-132.3	-1.0	176.8	
50	LYS	CCC C	46A,4A		69.5	0.30	171.9	1.02	57.8	42.6	-177.5	
51	THR	BBB B	46A		17.8	0.11	122.4	1.01	-120.9	130.8	175.9	
52	PHE	BBB B	4A,6A		4.2	0.02	190.3	0.97	-101.1	151.4	171.8	
53	THR	BBB B	44A,44A		35.5	0.23	129.0	1.07	-138.4	143.4	176.5	
54	VAL	BBB B	6A,8A		0.1	0.00	142.6	1.04	-125.7	126.6	-178.1	
55	THR	BBB B	42A,42A		58.6	0.38	120.3	1.00	-123.3	125.6	177.9	
56	GLU	BBB B	8A		83.3	0.43	137.8	1.00	-95.0	148.7	0.0	C

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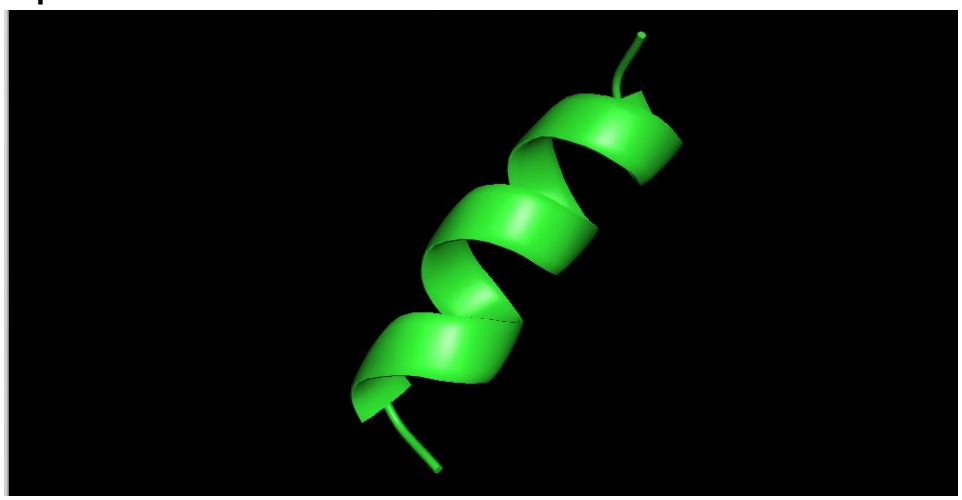
Alpha helix



Beta sheet