NAME: Aditya Jindal
ROLL NUMBER: 210106004
BT305 Lab Assignments

INDEX

BT305 Assignment 2

Name: Aditya Jindal
Roll No.: 210106004
Date: 17 January 2024

1)

2)

3)

4)

5)
A) Amino acids having large side chains, sidechains with CG, CD etc atoms = 76
(lucine(LEU), isoleucine(ILE), tryptophan(TRP), tyrosine(TYR), phenylalanine(PHE))
B) Acidic side chains(negative charge) = 49
C) Basic side chains(positive charge) = 41
D) Net charge = -8

6)
A) Total number of amino acids = 322
B) Total number of alanines = 26
C) Total number of tryptophans = 10
D) Total number of amino acids with polar side chains = 78
(glycine (GLY), threonine (THR), glutamine (GLN), tyrosine (TYR), cysteine (CYS), serine (SER), asparagine (ASN))

7)
X coordinates sum = 50656.1
Y coordinates sum = 157120
Z coordinates sum = 89316.1

BT307 LAB 3

Name: Aditya Jindal
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%)	-

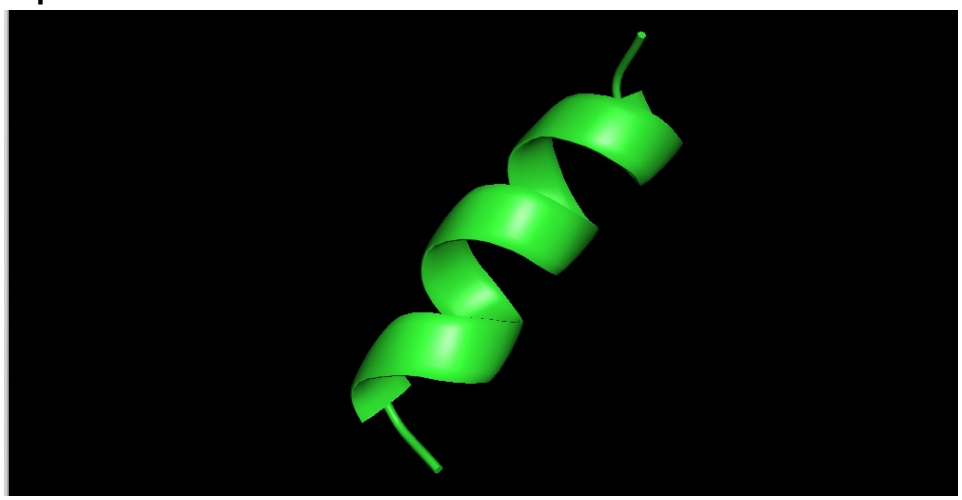
Expected values obtained from Morris AL, MacArthur MW, Hutchinson EG and Thornton JM. Proteins. 1992 Apr;12(4):345-364.

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

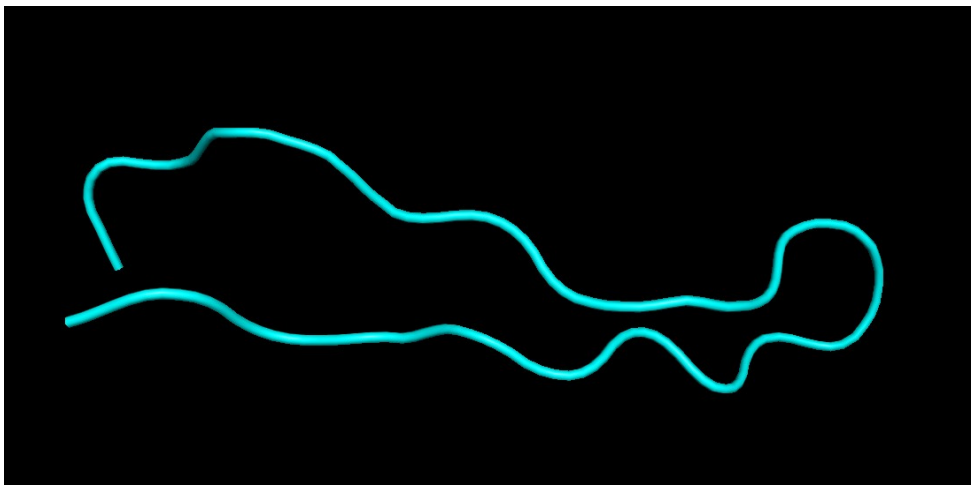
Screenshot

2)

Alpha helix



Beta sheet



BT307 LAB 4

Name: Aditya Jindal
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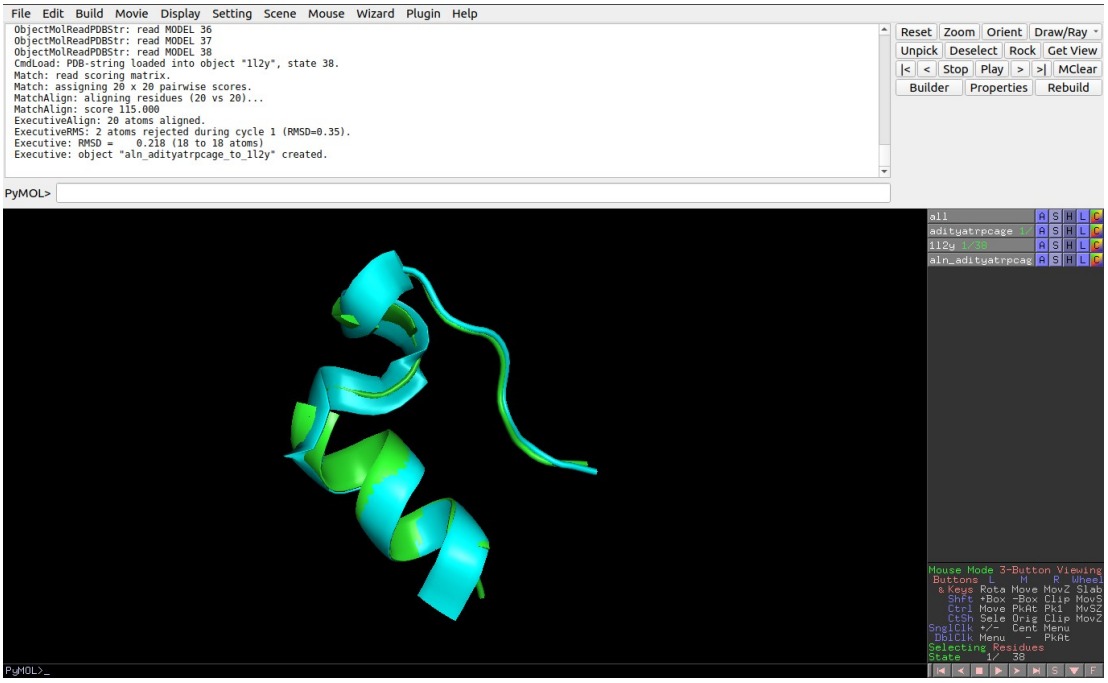
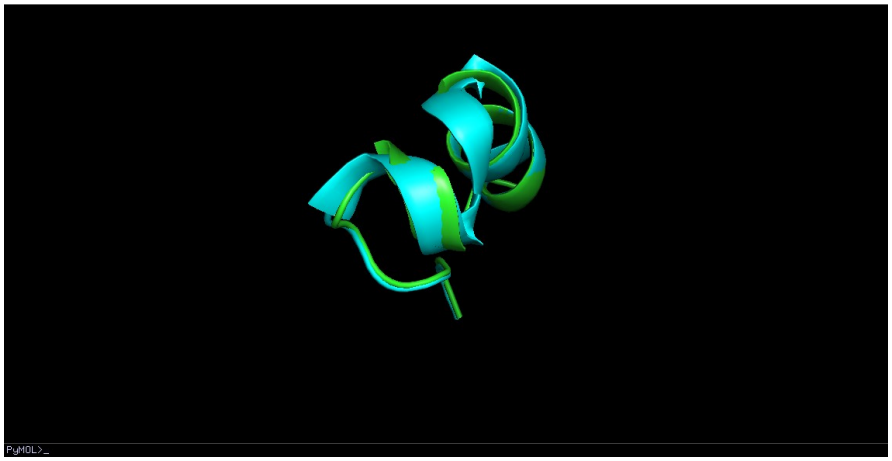
Root Mean Square Deviation(RMSD) = 0.218





BT305 LAB 5

Name: Aditya Jindal
Roll No.: 210106004

1)
Total relative Solvent Accessible Surface Area(SASA):
Alpha helix = 1712.39
Beta sheet = 2669.05
Protein G = 3712.8
Trpcage = 1859.4

2)
Average per residue solvent accessible surface area:
Alpha helix = 122.31
Beta sheet = 121.32
Protein G = 66.3
Trpcage = 93.0

3)
Per-residue solvent accessible surface area gives a measure of how much each residue in the protein is exposed to the solvent on average.
Protein G < Trpcage < Beta sheet < Alpha helix

4) If we change the probe radius from 1.4 to 1.0:
Absolute SASA values:
Alpha helix = 1627.27
Beta sheet = 2529.59
Protein G = 3735.83
Trpcage = 1759.20

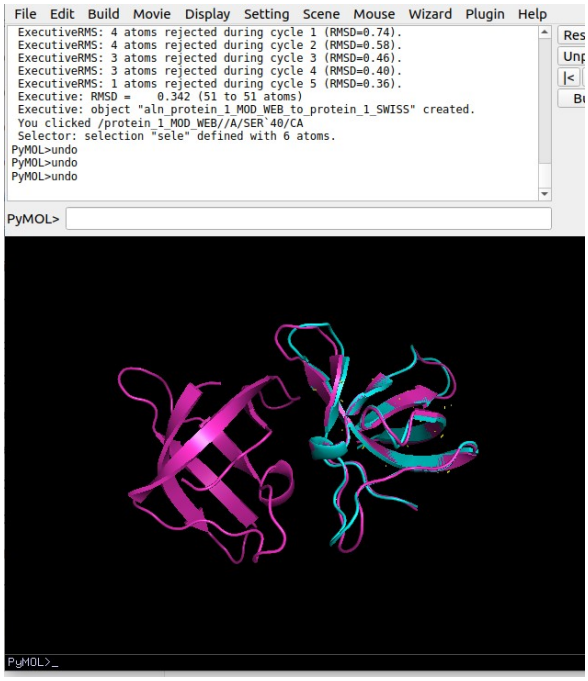
Relative SASA values:
Alpha helix = 0.95
Beta sheet = 0.94
Protein G = 1
Trpcage = 0.94

5.) In both cases trp is buried as it is a hydrophobic residue, so it is less exposed to the solvent.

BT305 LAB 6

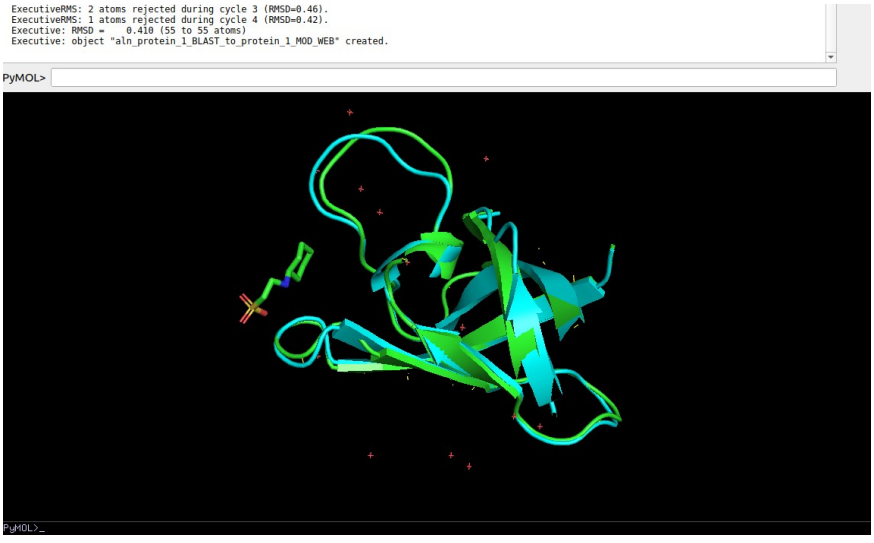
Name: Aditya Jindal
Roll No.: 210106004

MODEL 1 : Major Cold shock protein from Staphylococcus aureus
Aligning SWISS model and ModWeb model



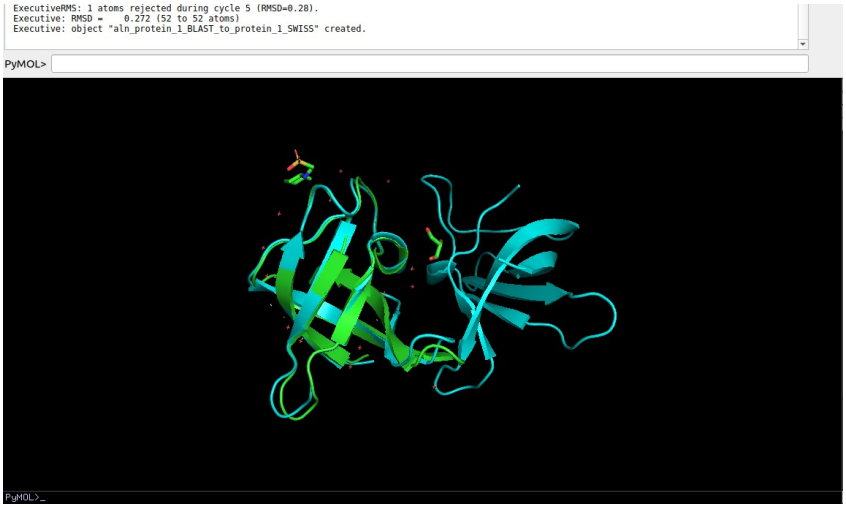
RMSD = 0.342

Aligning BLAST homologous model and ModWeb model



RMSD = 0.410

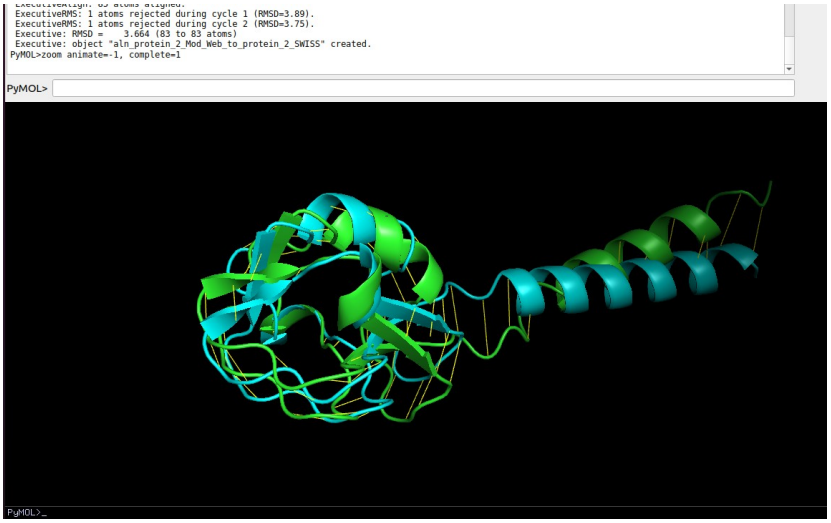
Aligning BLAST homologous model and SWISS model



RMSD = 0.272

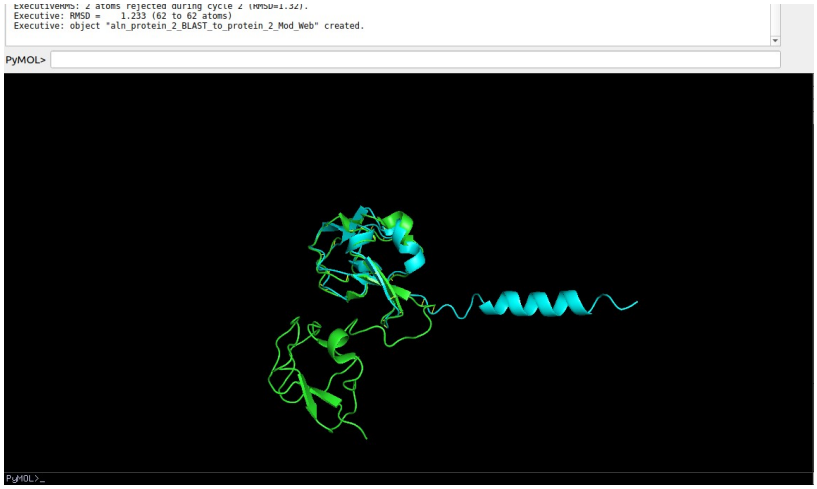
MODEL 2 : Antifreeze protein from Pachycara brachycephalum

Aligning SWISS model and ModWeb model



RMSD = 3.664

Aligning BLAST homologous model and ModWeb model



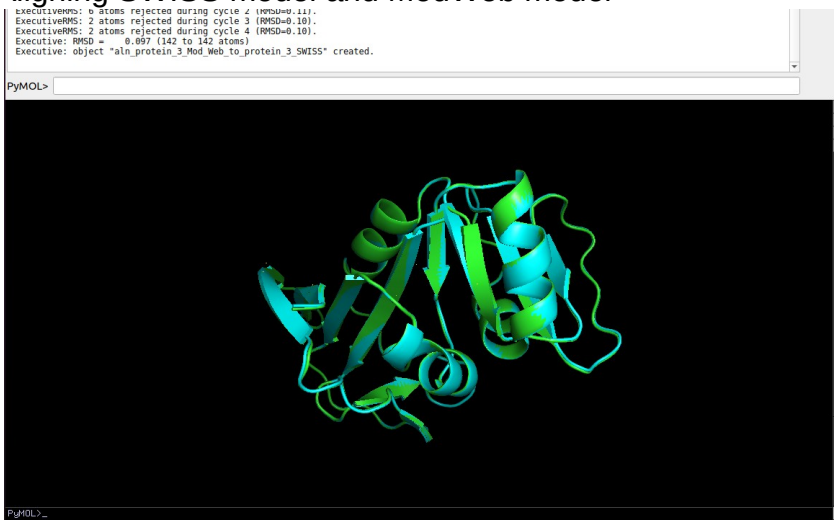
RMSD = 1.233

Aligning BLAST homologous model and SWISS model

RMSD = 1.202

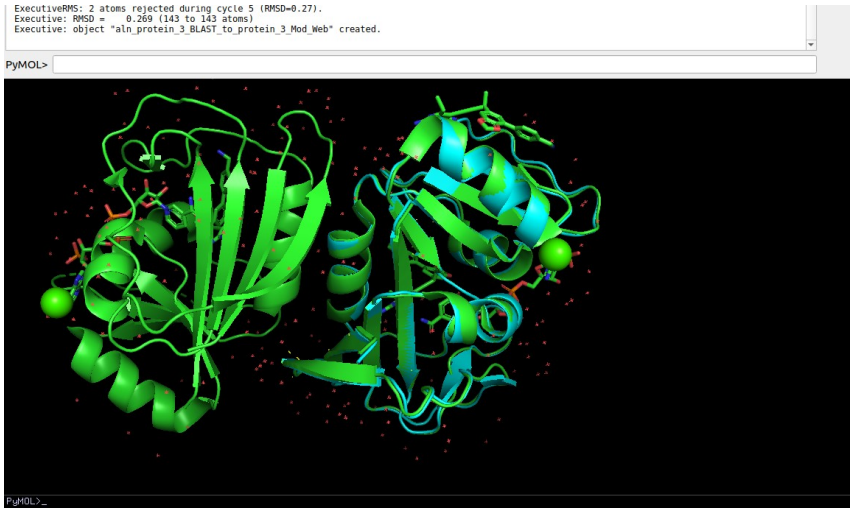
MODEL 3 - Dihydrofolate reductase from Vibrio cholerae

Aligning SWISS model and ModWeb model



RMSD = 0.097

Aligning BLAST homologous model and ModWeb model



RMSD = 0.269

Aligning BLAST homologous model and SWISS model

RMSD = 0.289

VAST Scores:

Model 1:

☐	PDB C D	Alignment Length	SCORE	RMSD	Identity	Description
☐	7F3I A	54	10.12	0.66	40.7	Crystal structure of human YBX2 CSD in complex with m5C RNA in space group P212121
☐	1SRO A	59	9.94	2.14	23.7	S1 RNA BINDING DOMAIN, NMR, 20 STRUCTURES
☐	3AQQ B	57	9.94	0.97	28.1	Crystal Structure Of Human Crhsp-24
☐	5UDZ B	55	9.66	0.96	36.4	Human LIN28A in complex with let-7f-1 microRNA pre-element
☐	3ULJ B	53	9.64	0.84	37.7	Crystal Structure Of Apo Lin28b Cold Shock Domain
☐	1X65 A	52	9.62	1.30	21.2	Solution structure of the third cold-shock domain of the human KIAA0885 protein (UNR PROTEIN)
☐	6Y96 A	49	9.59	1.26	26.5	solution structure of cold-shock domain 9 of drosophila Upstream of N-Ras (Unr)
☐	2VNU D	40	9.51	1.40	10.0	Crystal Structure Of Sc Rrp44
☐	3G05 A	50	9.35	1.41	10.0	Crystal structure of a multidomain protein with nucleic acid binding domains (sp_0946) from streptococcus pneumoniae tigr4 at 1.40 A resolution
☐	7YM0 A	46	9.34	1.46	10.9	Crystal structure of the recombination mediator protein RecO from Campylobacter jejuni

Model 2:

	PDB C D	Alignment Length	SCORE	RMSD	Identity	Description
☐	1C8A A	134	20.97	0.00	100.0	NMR STRUCTURE OF INTRAMOLECULAR DIMER ANTIFREEZE PROTEIN RD3, 40 SA STRUCTURES
☐	1A0J B	27	7.61	1.95	7.4	THE SH3 DOMAIN OF EPS8 EXISTS AS A NOVEL INTERTWINED DIMER

Model 3:

	PDB C D	Alignment Length	SCORE	RMSD	Identity	Description
☐	7RGJ B	153	24.25	0.56	98.0	DfrA1 complexed with NADPH and 5-(3-(7-(4-(aminomethyl)phenyl)benzo[d][1,3]dioxol-5-yl)but-1-yn-1-yl)-6-ethylpyrimidine-2,4-diamine (UCP1223)
☐	1DIU A	149	24.15	1.44	25.5	DIHYDROFOLATE REDUCTASE (E.C.1.5.1.3) COMPLEX WITH BRODIMOPRIM-4,6-DICARBOXYLATE
☐	3ROA B	152	23.80	1.63	27.0	Candida glabrata dihydrofolate reductase complexed with NADPH and 6-ethyl-5-[(3R)-3-[3-methoxy-5-(morpholin-4-yl)phenyl]but-1-yn-1-yl]pyrimidine-2,4-diamine (UCP1004)
☐	7TJ3 A	154	23.34	1.85	33.8	Crystal structure of a dihydrofolate reductase folA from Stenotrophomonas maltophilia bound to NADP and p218
☐	3IX9 B	153	23.33	1.53	27.5	Crystal structure of Streptococcus pneumoniae dihydrofolate reductase - Sp9 mutant
☐	3TQ8 A	152	23.28	1.47	31.6	Structure Of The Dihydrofolate Reductase (fola) From Coxiella Burnetii In Complex With Trimethoprim
☐	1CZ3 B	144	22.55	1.82	22.2	DIHYDROFOLATE REDUCTASE FROM THERMOTOGA MARITIMA
☐	3F0U X	145	22.26	1.40	31.7	Staphylococcus aureus F98Y mutant dihydrofolate reductase complexed with NADPH and 2,4-Diamino-5-[3-(3-methoxy-5-phenylphenyl)but-1-ynyl]-6-methylpyrimidine
☐	3RG9 B	152	21.83	1.60	27.0	Trypanosoma Brucei Dihydrofolate Reductase (tbdhfr) In Complex With Wr99210
☐	6CXK A	149	21.58	1.70	28.9	E. coli DHFR substrate complex with Dihydrofolate

BT305 LAB 7

Name: Aditya Jindal
Roll No.: 210106004

1)
1PGB
Initial:
phi & psi angles of 4th residue : -129.838 126.485
phi & psi angles of 8th residue : -86.0263 179.722
Deviation After EM:
phi & psi angles of 4th residue : 7.438 6.42
phi & psi angles of 8th residue : -41.5487 -11.122
Deviation After MD:
phi & psi angles of 4th residue : 19.884 11.112
phi & psi angles of 8th residue : -56.2887 21.131

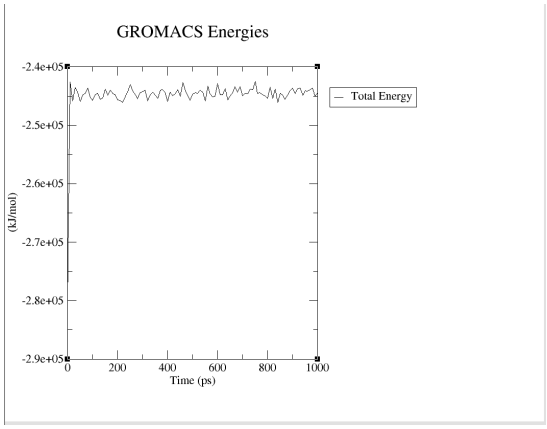
TRP Cage
Initial:
phi & psi angles of 4th residue : -61.5746 -42.7245
phi & psi angles of 8th residue : -73.2076 -18.7175
Deviation After EM:
phi & psi angles of 4th residue : 7.3421 8.5531
phi & psi angles of 8th residue : 3.9723 -9.5835
Deviation After MD:
phi & psi angles of 4th residue : -4.7935 11.4069
phi & psi angles of 8th residue : -96.2384 128.3735

Alpha-Helix
Initial:
phi & psi angles of 4th residue : -64.6311 -34.1108
phi & psi angles of 8th residue : -61.6178 -42.1426
Deviation After EM:
phi & psi angles of 4th residue : 11.6488 -7.0309
phi & psi angles of 8th residue : 3.2649 -13.0852
Deviation After MD:
phi & psi angles of 4th residue : 18.9604 -41.948
phi & psi angles of 8th residue :8.5922 -2.2798

Beta-Sheet

Initial:
phi & psi angles of 4th residue : -103.326 122.067
phi & psi angles of 8th residue : -72.7477 -36.7
Deviation After EM:
phi & psi angles of 4th residue : 17.3887 5.357
phi & psi angles of 8th residue : 5.4159 3.3185
Deviation After MD:
phi & psi angles of 4th residue : 1.763 -78.5052
phi & psi angles of 8th residue : 132.75 -38.07

2)
A) Total Energy:
Beta sheet:



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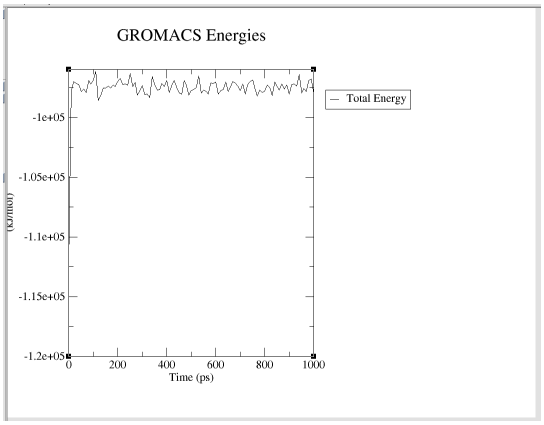

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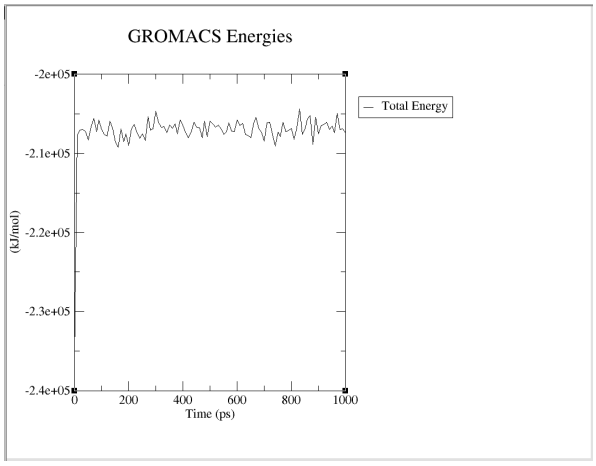

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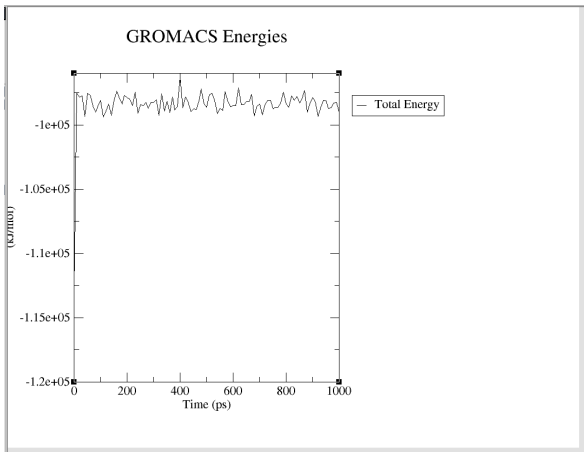
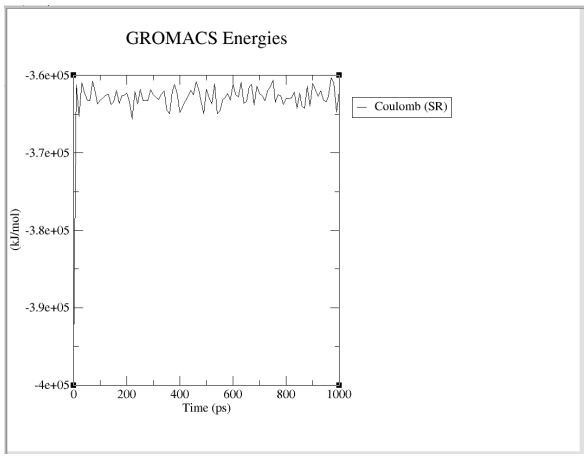
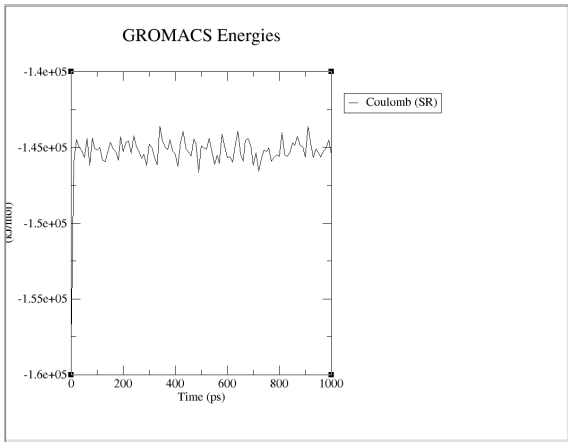


B) Coul-SR:

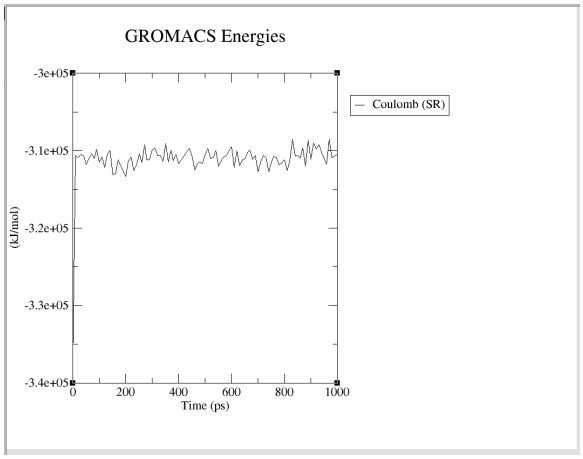
Beta sheet:



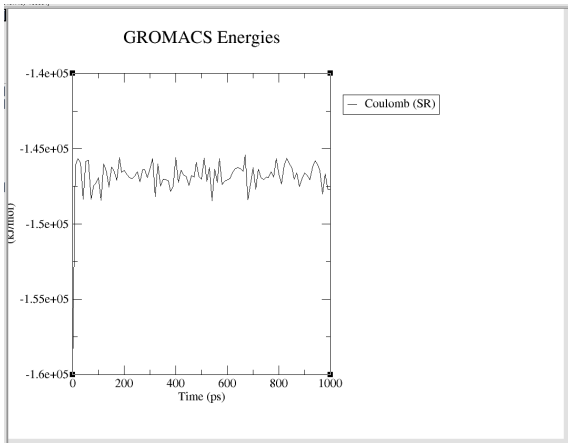
Helix:



PGB:

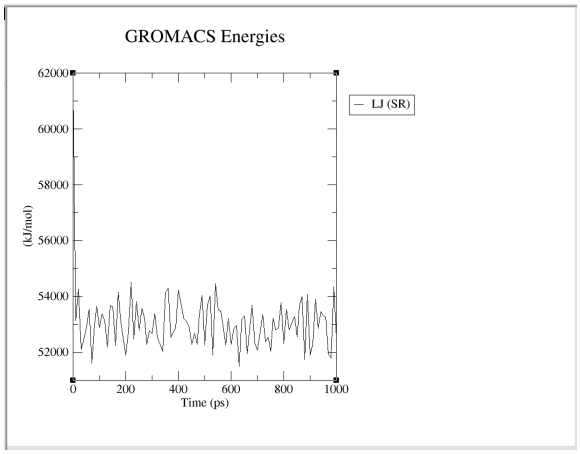


TRP:

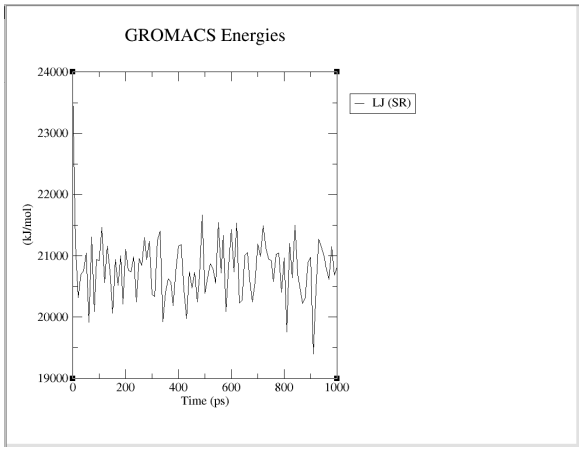


C) LJ-SR:

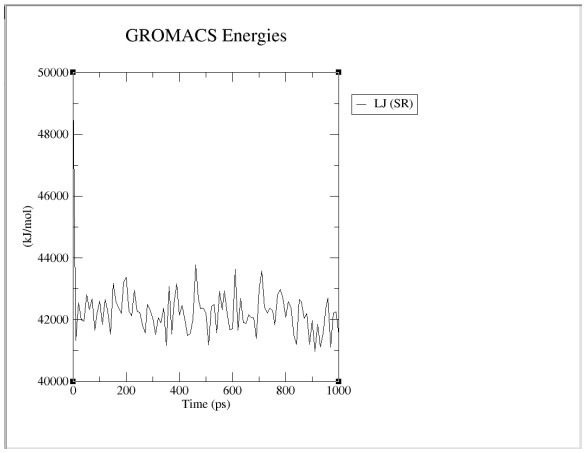
Beta sheet:



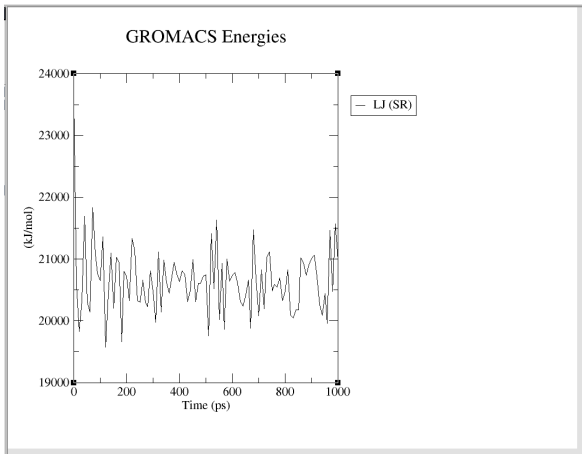
Helix:



PGB:



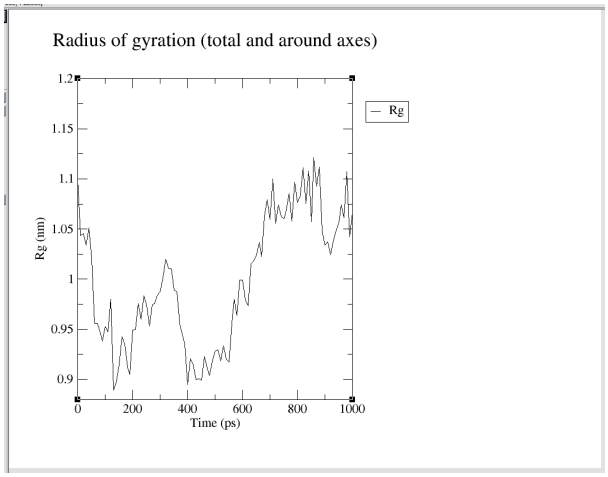
TRP:



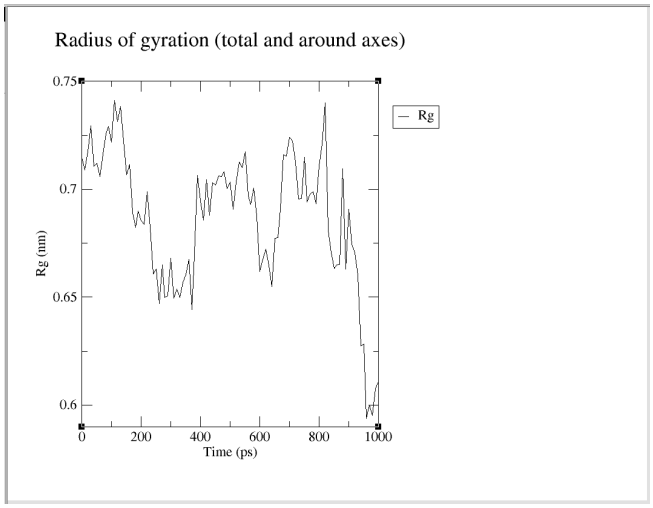
4) Radius of Gyration

The radius of Gyration of TRP: 0.538806
The radius of Gyration of PGB: 0.70167
The radius of Gyration of Helix: 0.382169
The radius of Gyration of BetaSheet: 0.938183

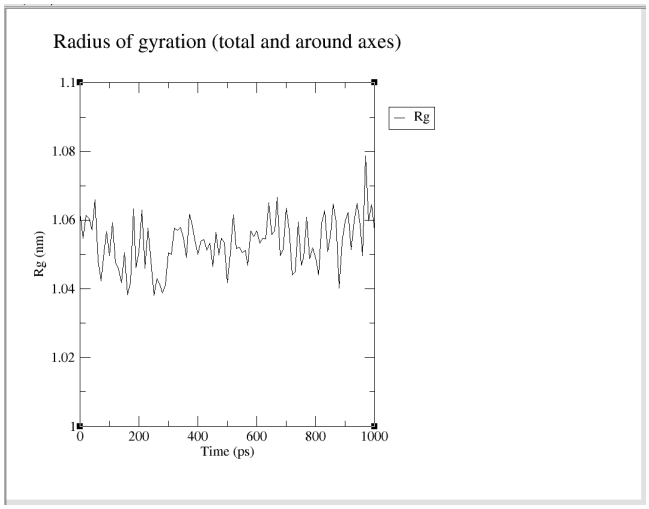
Beta sheet:



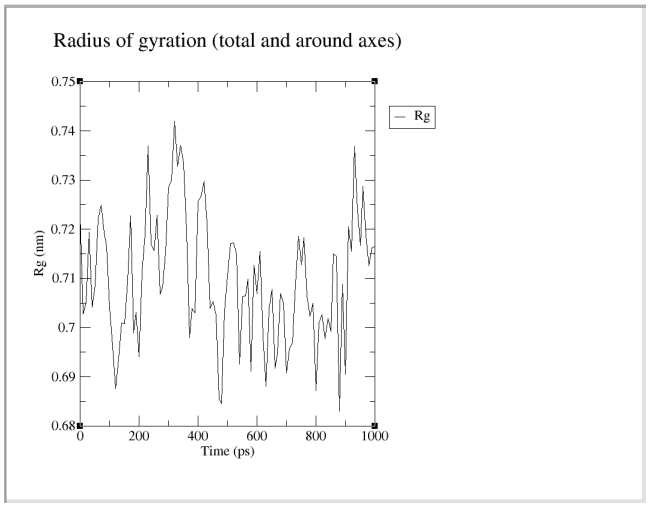
Helix:


Radius of gyration (total and around axes)
Rg
Rg (nm)
Time (ps)
0.75
0.7
0.65
0.6
0
200
400
600
800
1000

PGB:


Radius of gyration (total and around axes)
Rg
Rg (nm)
Time (ps)
1.1
1.08
1.06
1.04
1.02
1
0
200
400
600
800
1000

TRP:


Radius of gyration (total and around axes)
Rg
Rg (nm)
Time (ps)
0.75
0.74
0.73
0.72
0.71
0.7
0.69
0.68
0
200
400
600
800
1000

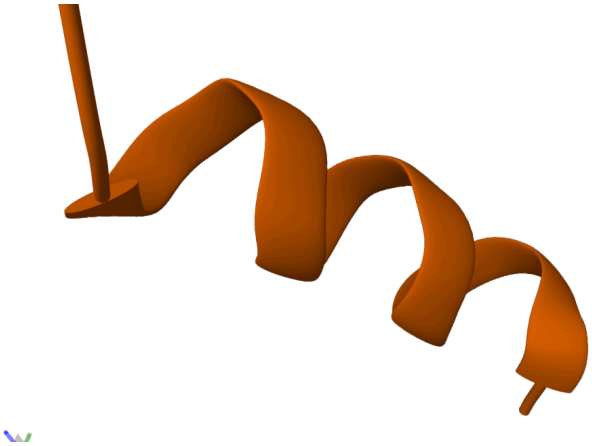
5)

Beta Sheet:
Number of clusters for cutoff 0.15=17

Number of clusters for cutoff 0.1=57

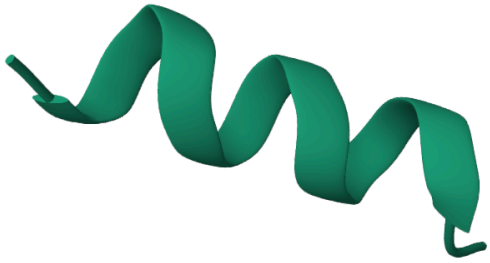
Number of clusters for cutoff 0.30=3

Helix:
Number of clusters for cutoff 0.15=6



Number of clusters for cutoff 0.1=15

Number of clusters for cutoff 0.30=1

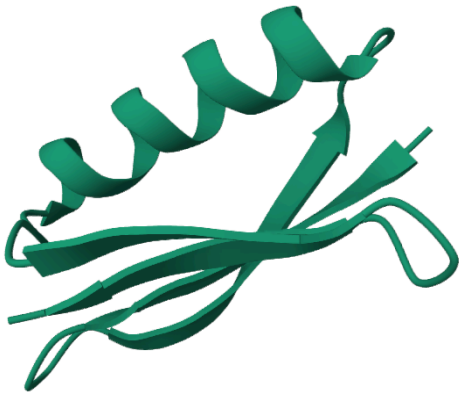


PDB:

Number of clusters for cutoff 0.15=3

Number of clusters for cutoff 0.1=19

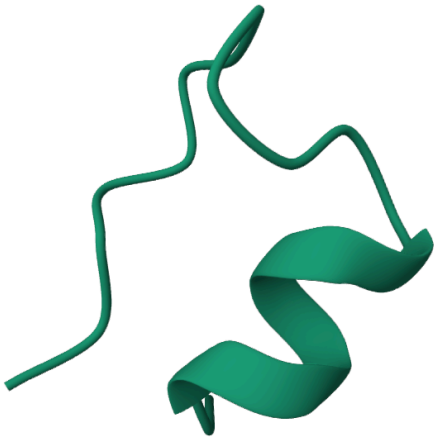
Number of clusters for cutoff 0.30=1



TRP:
Number of clusters for cutoff 0.15=10

Number of clusters for cutoff 0.1=40

Number of clusters for cutoff 0.30=1



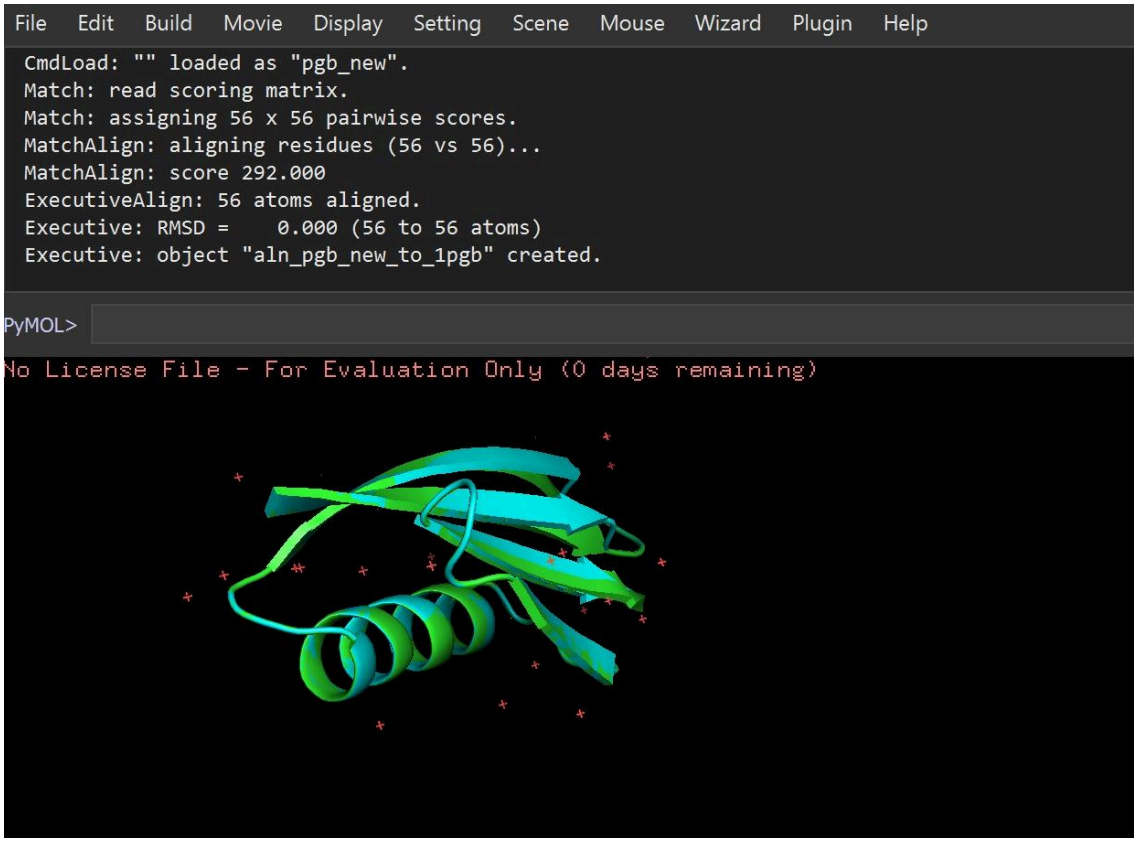
BT305 LAB 8

Name: Aditya Jindal
Roll No.: 210106004

Section 1
From the video, we can observe that the Trpcage protein at 363 K is more actively moving around the space and water molecules than the protein at 300 K.

Section 2
Exercise 1:
1)
Trpcage:

1PGB:



2)

ALA: N[C@H](C(=O)N[C@H](C=O)C)C
PHE: N[C@H](C=O)Cc1ccccc1
GLU: N[C@H](C=O)CCC(=O)O
LYS: N[C@H](C=O)CCCCN

Exercise 2:

Q) Convert trp.pdb to smiles format:

Ans

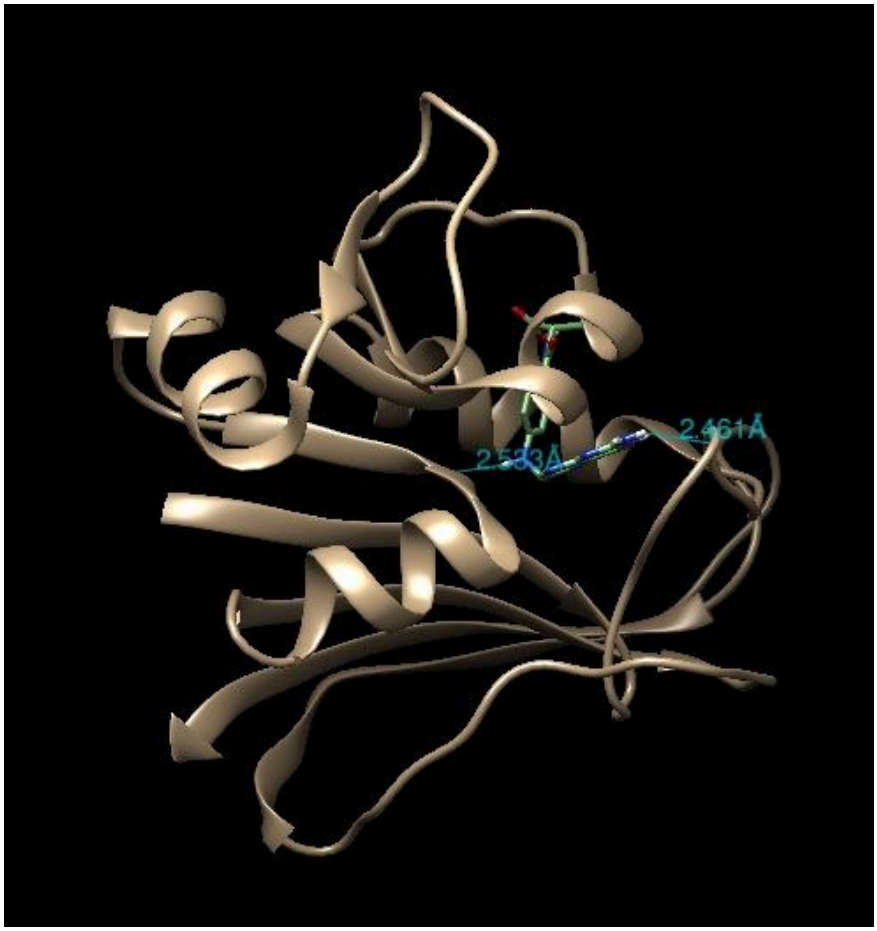
N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)NCC(=O)NCC(=O)N1[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)NCC(=O)N[C@H](C(=O)N2[C@H](C(=O)N3[C@H](C(=O)N4[C@H](C(=O)N[C@H](C=O)CO)CCC4)CCC3)CCC2)CCCNC(=[NH2])N)C)CO)CCC1)CC(=O)OO)CCCC[NH3])CC(C)C)Cc1c[nH]c2c1cccc2)CCC(=O)N)[C@H](CC)C)Cc1ccc(cc1)O)CC(C)C)CC(=O)N

BT305 LAB 9

Name: Aditya Jindal
Roll No.: 210106004

1)
A) Binding Energy of most probable conformation: -8.8

B) Residue present in ligand binding sites: Iso-Leucine, Histidine, Alanine



C) Nature of Amino Acids present in ligand binding sites:
Iso-Leucine: Non-polar aromatic amino acids
Histidine: Basic Amino Acid
Alanine: Non-polar amino acid

E)
Target-Based Docking
Binding Energy: 201.2

Number Of Residues: 1
Residues: ASP

Blind Docking
Binding Energy: -8.8
Number Of Residues: 3
Residues: MET, HIS, ILE

Target-Based Docking: