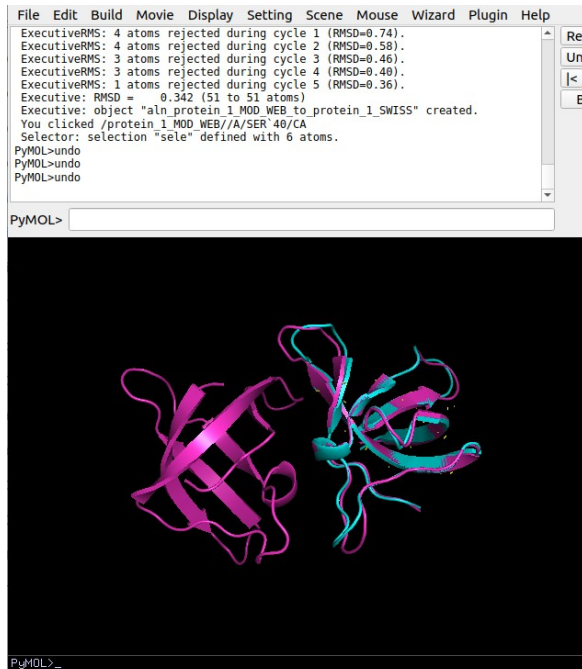


BT305 LAB 6

Name: Aditya Jindal

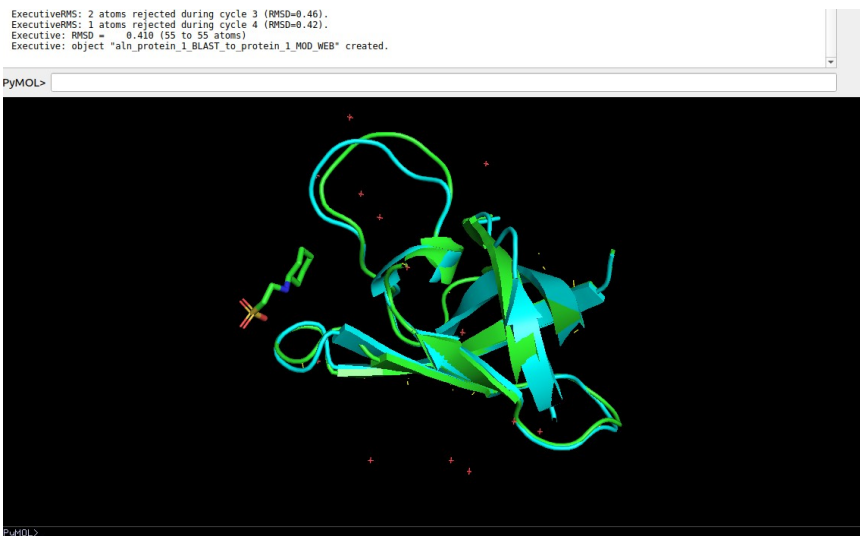
Roll No.: 210106004

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



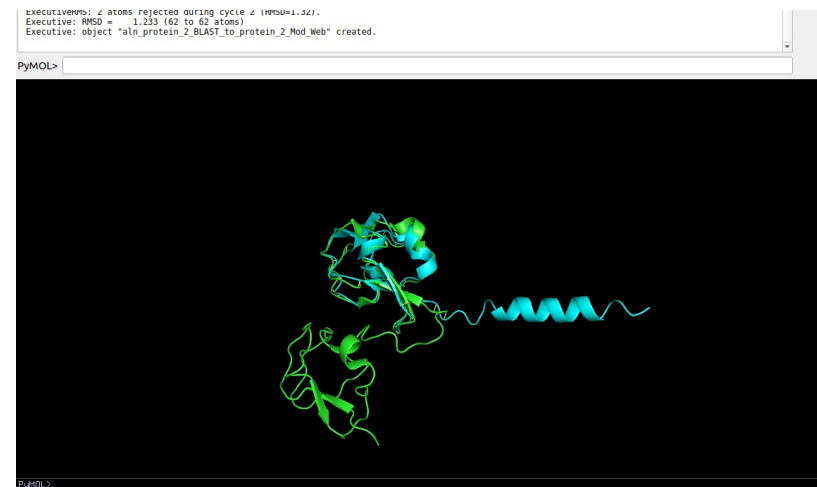
RMSD = 0.272

MODEL 2 : Antifreeze protein from *Pachycara brachycephalum* Aligning SWISS model and ModWeb model



RMSD = 3.664

Aligning BLAST homologous model and ModWeb model

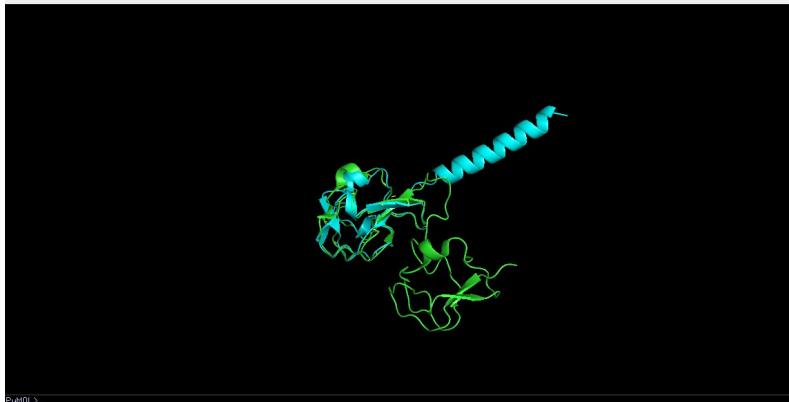


RMSD = 1.233

Aligning BLAST homologous model and SWISS model

```
ExecutiveRMS: 1 atoms rejected during cycle 3 (RMSD=1.24).  
Executive: RMSD = 1.202 (61 to 61 atoms)  
Executive: object "aln_protein_2_BLAST_to_protein_2_SWISS" created.
```

PyMOL>



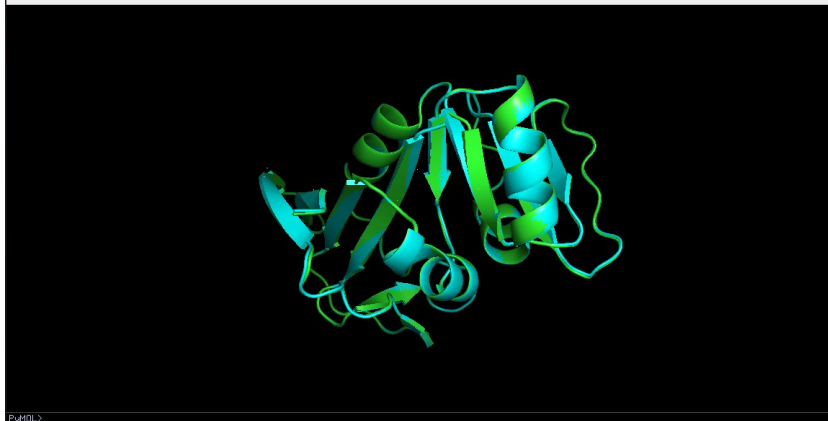
RMSD = 1.202

MODEL 3 - Dihydrofolate reductase from Vibrio cholerae

Aligning SWISS model and ModWeb model

```
ExecutiveRMS: 0 atoms rejected during cycle 2 (RMSD=0.11).  
ExecutiveRMS: 2 atoms rejected during cycle 3 (RMSD=0.10).  
ExecutiveRMS: 2 atoms rejected during cycle 4 (RMSD=0.10).  
Executive: RMSD = 0.097 (142 to 142 atoms)  
Executive: object "aln_protein_3_Mod_Web_to_protein_3_SWISS" created.
```

PyMOL>

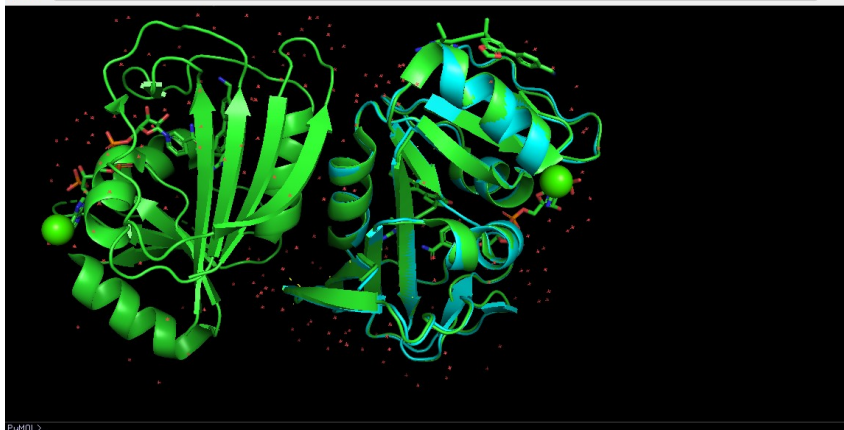


RMSD = 0.097

Aligning BLAST homologous model and ModWeb model

```
ExecutiveRMS: 2 atoms rejected during cycle 5 (RMSD=0.27).  
Executive: RMSD = 0.269 (143 to 143 atoms)  
Executive: object "aln_protein_3_BLAST_to_protein_3_Mod_Web" created.
```

PyMOL>



RMSD = 0.269

Aligning BLAST homologous model and SWISS model



RMSD = 0.289

VAST Scores:

Model 1:

<input type="checkbox"/>	<u>PDB C D</u>	<u>Alignment Length</u>	<u>SCORE</u>	<u>RMSD</u>	<u>Identity</u>	<u>Description</u>
<input type="checkbox"/>	7F3I A	54	10.12	0.66	40.7	Crystal structure of human YBX2 CSD in complex with m5C RNA in space group P212121
<input type="checkbox"/>	1SR0 A	59	9.94	2.14	23.7	S1 RNA BINDING DOMAIN, NMR, 20 STRUCTURES
<input type="checkbox"/>	3A0Q B	57	9.94	0.97	28.1	Crystal Structure Of Human Crhsp-24
<input type="checkbox"/>	5UDZ B	55	9.66	0.96	36.4	Human LIN28A in complex with let-7f-1 microRNA pre-element
<input type="checkbox"/>	3ULJ B	53	9.64	0.84	37.7	Crystal Structure Of Apo Lin28b Cold Shock Domain
<input type="checkbox"/>	1X65 A	52	9.62	1.30	21.2	Solution structure of the third cold-shock domain of the human KIAA0885 protein (UNR PROTEIN)
<input type="checkbox"/>	6Y96 A	49	9.59	1.26	26.5	solution structure of cold-shock domain 9 of drosophila Upstream of N-Ras (Unr)
<input type="checkbox"/>	2VNU D	40	9.51	1.40	10.0	Crystal Structure Of Sc Rrp44
<input type="checkbox"/>	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
<input type="checkbox"/>	7YMO A	46	9.34	1.46	10.9	Crystal structure of the recombination mediator protein RecO from Campylobacter jejuni

Model 2:

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

Model 3:

<input type="checkbox"/>	<u>PDB C D</u>	<u>Alignment Length</u>	<u>SCORE</u>	<u>RMSD</u>	<u>Identity</u>	<u>Description</u>
<input type="checkbox"/>	<u>7RGJ</u> 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)
<input type="checkbox"/>	<u>1DIU</u> A	149	24.15	1.44	25.5	DIHYDROFOLATE REDUCTASE (E.C.1.5.1.3) COMPLEX WITH BRODIMOPRIM-4,6-DICARBOXYLATE
<input type="checkbox"/>	<u>3R0A</u> 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)
<input type="checkbox"/>	<u>7TJ3</u> A	154	23.34	1.85	33.8	Crystal structure of a dihydrofolate reductase folA from Stenotrophomonas maltophilia bound to NADP and p218
<input type="checkbox"/>	<u>3IX9</u> B	153	23.33	1.53	27.5	Crystal structure of Streptococcus pneumoniae dihydrofolate reductase - Sp9 mutant
<input type="checkbox"/>	<u>3TQ8</u> A	152	23.28	1.47	31.6	Structure Of The Dihydrofolate Reductase (folA) From Coxiella Burnetii In Complex With Trimethoprim
<input type="checkbox"/>	<u>1CZ3</u> B	144	22.55	1.82	22.2	DIHYDROFOLATE REDUCTASE FROM THERMOTOGA MARITIMA
<input type="checkbox"/>	<u>3F0U</u> 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
<input type="checkbox"/>	<u>3RG9</u> B	152	21.83	1.60	27.0	Trypanosoma Brucei Dihydrofolate Reductase (tbdhfr) In Complex With Wr99210
<input type="checkbox"/>	<u>6CXK</u> A	149	21.58	1.70	28.9	E. coli DHFR substrate complex with Dihydrofolate