

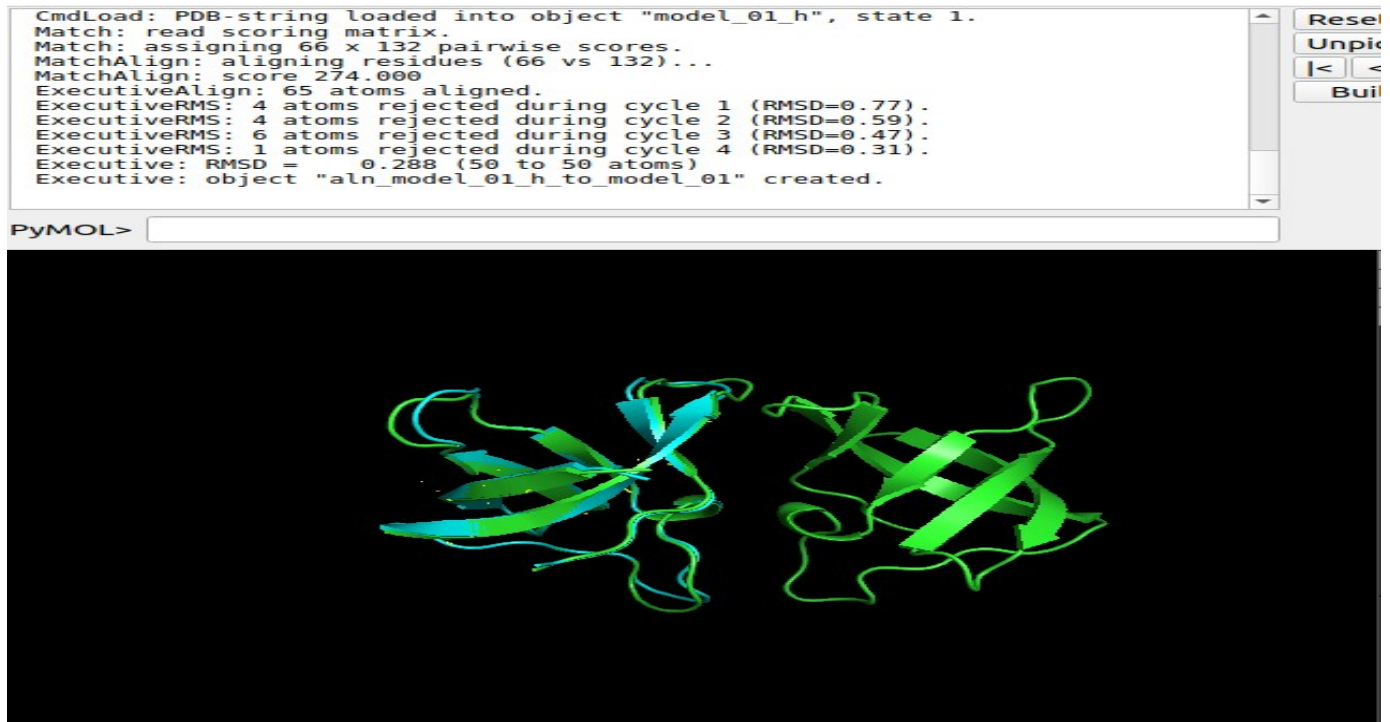
BT305 Lab Assignment 6

Name: Vansh

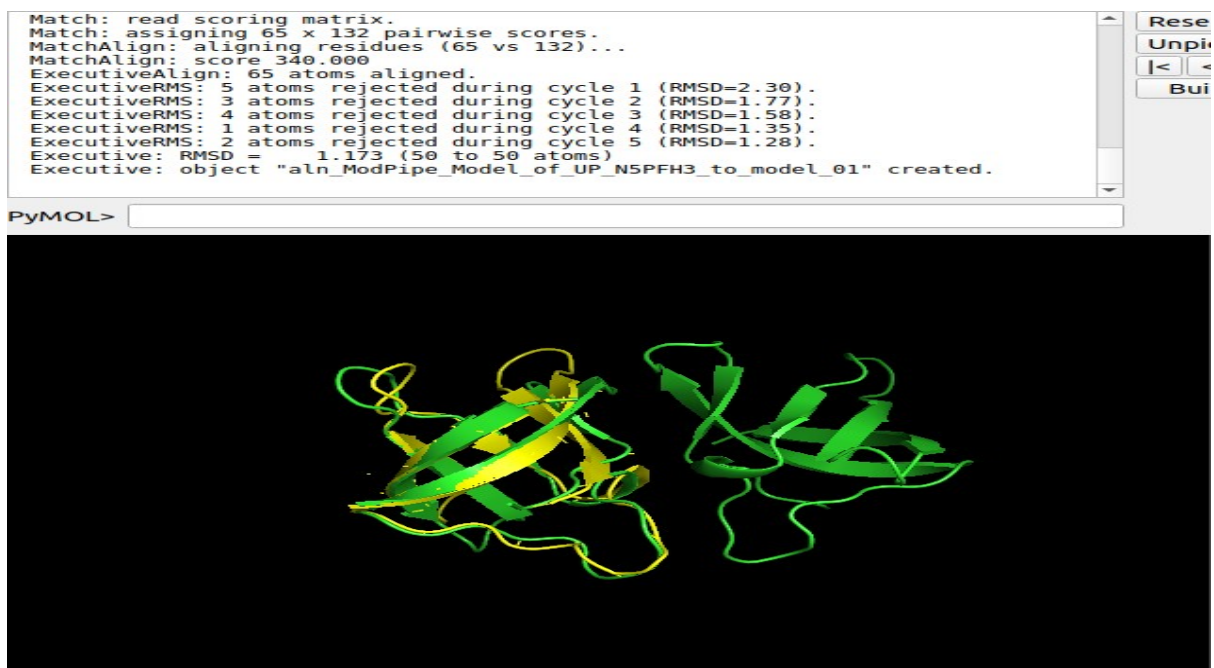
Roll no. 210106082

Model 1: Major Cold shock protein from Staphylococcus aureus

Comparison between original sequence and
homologue(RMSD:0.288)



Comparison between original sequence and ModWeb(RMSD:1.173)

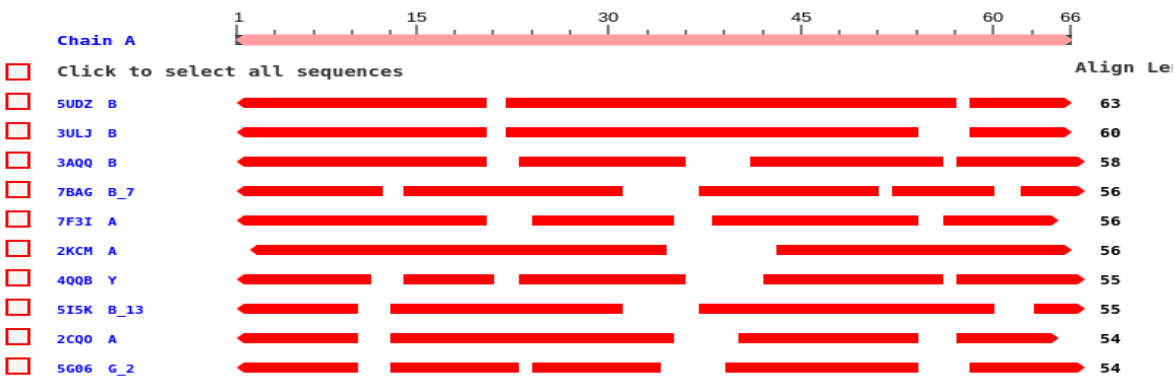


Comparison between homologue and ModWeb(RMSD:0.848)

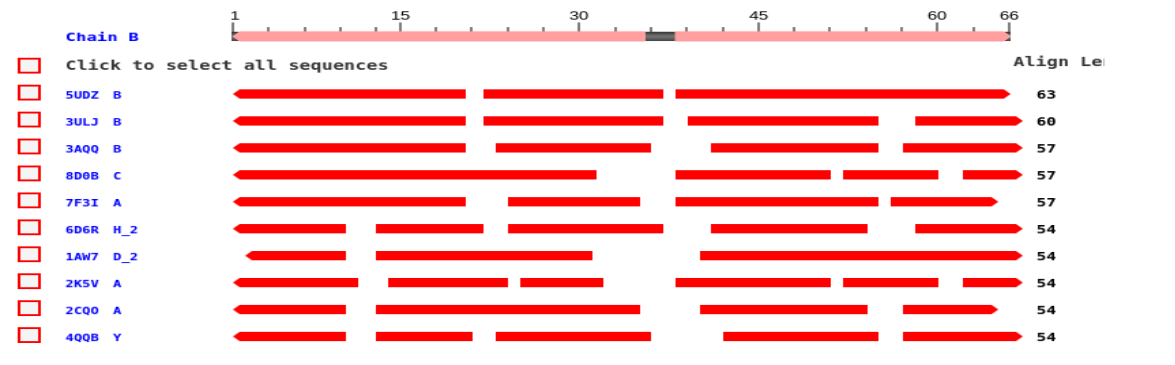


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In the graphics below the red regions are aligned segments.



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<input type="checkbox"/>	PDB C D	Alignment Length	SCORE	RMSD	Identity	Description
<input type="checkbox"/>	5UDZ B	63	10.41	1.34	39.7	Human LIN28A in complex with let-7f-1 microRNA pre-element
<input type="checkbox"/>	3ULJ B	60	10.84	1.19	41.7	Crystal Structure Of Apo Lin28b Cold Shock Domain
<input type="checkbox"/>	3A00 B	58	11.28	0.88	32.8	Crystal Structure Of Human Crhsp-24
<input type="checkbox"/>	7BAG B	56	8.30	2.45	10.7	C3b in complex with CP40
<input type="checkbox"/>	7F3I A	56	10.09	0.71	53.6	Crystal structure of human YBX2 CSD in complex with m5C RNA in space group P212121
<input type="checkbox"/>	2KCM A	56	9.60	1.58	28.6	Solution NMR structure of the N-terminal OB-domain of SO_1732 from Shewanella oneidensis. Northeast Structural Genomics Consortium Target SoR210A
<input type="checkbox"/>	400B Y	55	9.48	1.02	30.9	Structural basis for the assembly of the SXL-UNR translation regulatory complex
<input type="checkbox"/>	5I5K B	55	8.88	2.55	5.5	Structure of complement C5 in complex with eculizumab
<input type="checkbox"/>	2C00 A	54	9.28	1.86	20.4	Solution structure of the S1 RNA binding domain of human hypothetical protein FLJ11067
<input type="checkbox"/>	5G06 G	54	7.29	1.66	14.8	Cryo-em Structure Of Yeast Cytoplasmic Exosome

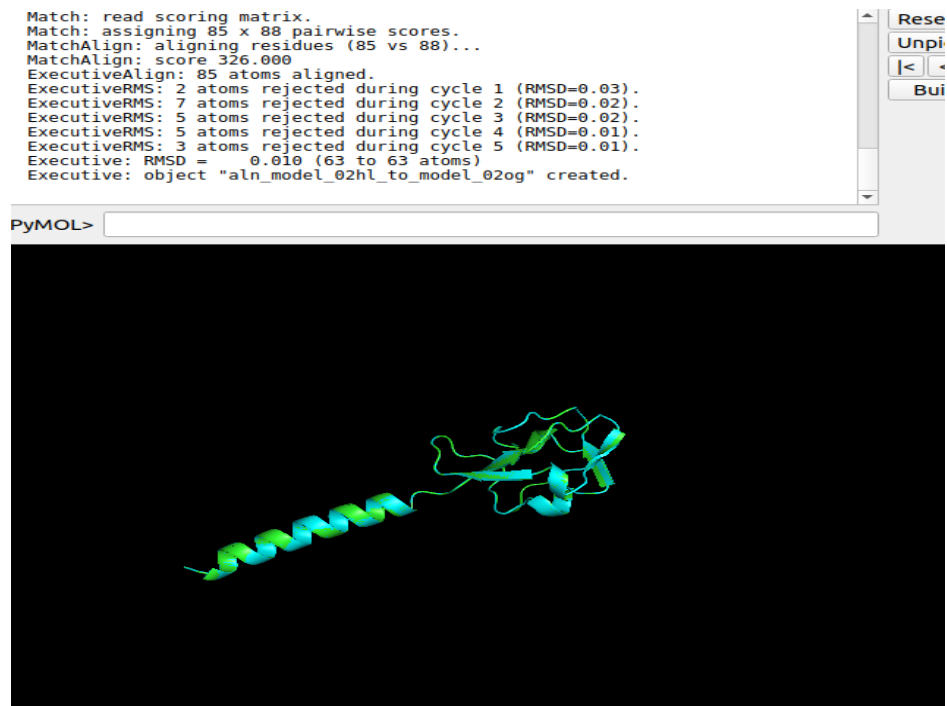
<input type="checkbox"/>	PDB C D	Alignment Length	SCORE	RMSD	Identity	Description
<input type="checkbox"/>	5UDZ B	63	10.58	1.36	39.7	Human LIN28A in complex with let-7f-1 microRNA pre-element
<input type="checkbox"/>	3ULJ B	60	10.75	1.31	40.0	Crystal Structure Of Apo Lin28b Cold Shock Domain
<input type="checkbox"/>	3A00 B	57	11.37	0.71	33.3	Crystal Structure Of Human Crhsp-24
<input type="checkbox"/>	8D0B C	57	7.81	2.31	7.0	Human CST-DNA polymerase alpha/primase preinitiation complex bound to 4xTEL-foldback template
<input type="checkbox"/>	7F3I A	57	10.11	0.70	54.4	Crystal structure of human YBX2 CSD in complex with m5C RNA in space group P212121
<input type="checkbox"/>	6D6R H	54	8.77	1.66	22.2	Human nuclear exosome-MTR4 RNA complex - composite map after focused reconstruction
<input type="checkbox"/>	1AWZ D	54	7.26	2.14	14.8	Q136A MUTANT OF TOXIC SHOCK SYNDROME TOXIN-1 FROM S. AUREUS
<input type="checkbox"/>	2K5V A	54	10.03	1.93	11.1	SOLUTION NMR STRUCTURE OF the second OB-fold domain of replication protein A from Methanococcus maripaludis. NORTHEAST STRUCTURAL GENOMICS TARGET MRF110B
<input type="checkbox"/>	2C00 A	54	8.87	1.84	20.4	Solution structure of the S1 RNA binding domain of human hypothetical protein FLJ11067
<input type="checkbox"/>	400B Y	54	9.18	0.90	31.5	Structural basis for the assembly of the SXL-UNR translation regulatory complex

Model 2: Antifreeze protein from *Pachycara brachycephalum*

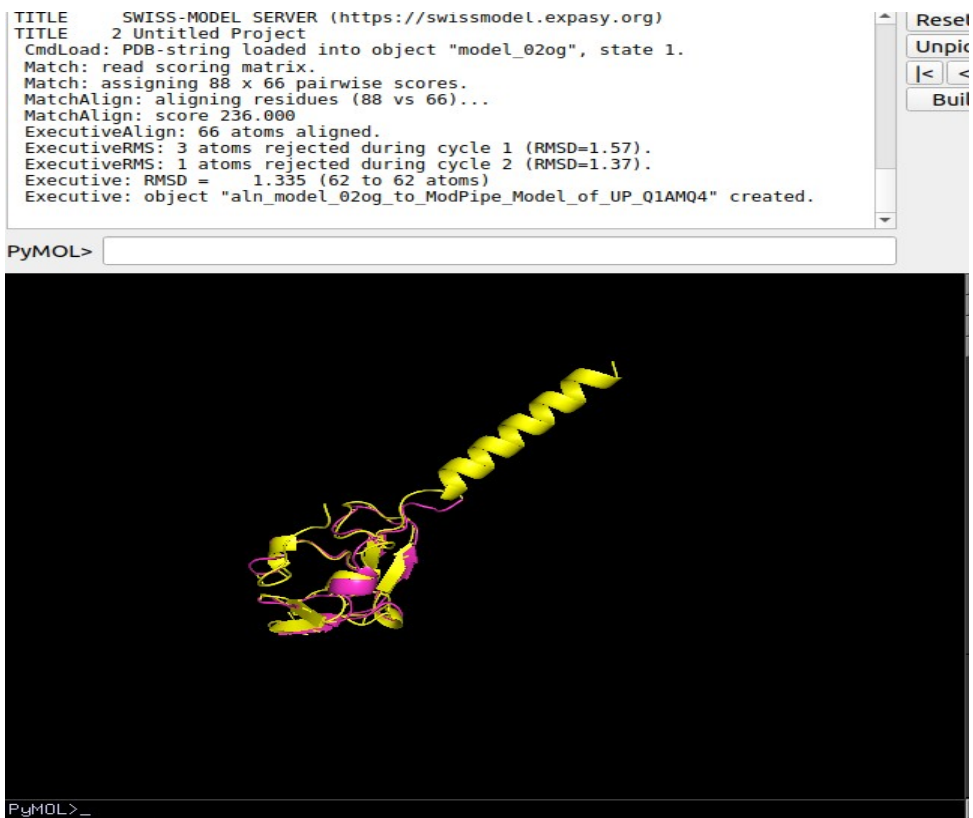
Comparison between original sequence and homologue(RMSD:0.840)



Comparison between original sequence and ModWeb(RMSD:0.010)

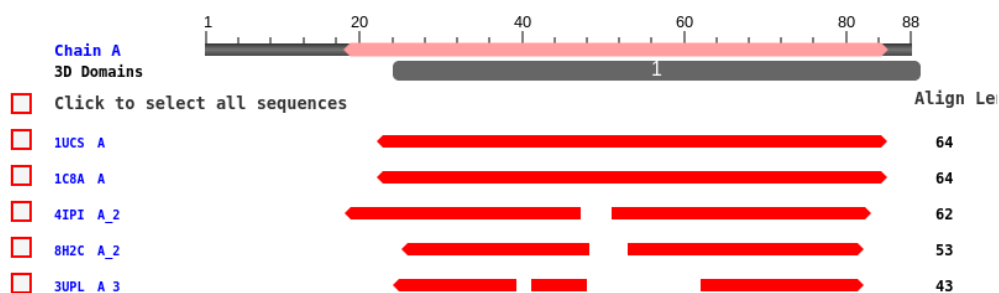


Comparison between homologue and ModWeb(RMSD:1.335)



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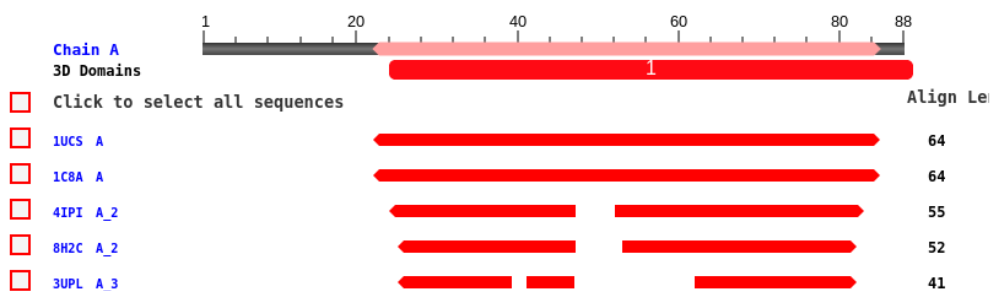


Citing VAST: Gibrat JF, Madej T, Bryant SH, "Surprising similarities in structure comparison", *Curr Opin Struct Biol.* 1996 Jun; 6(3):377-85.

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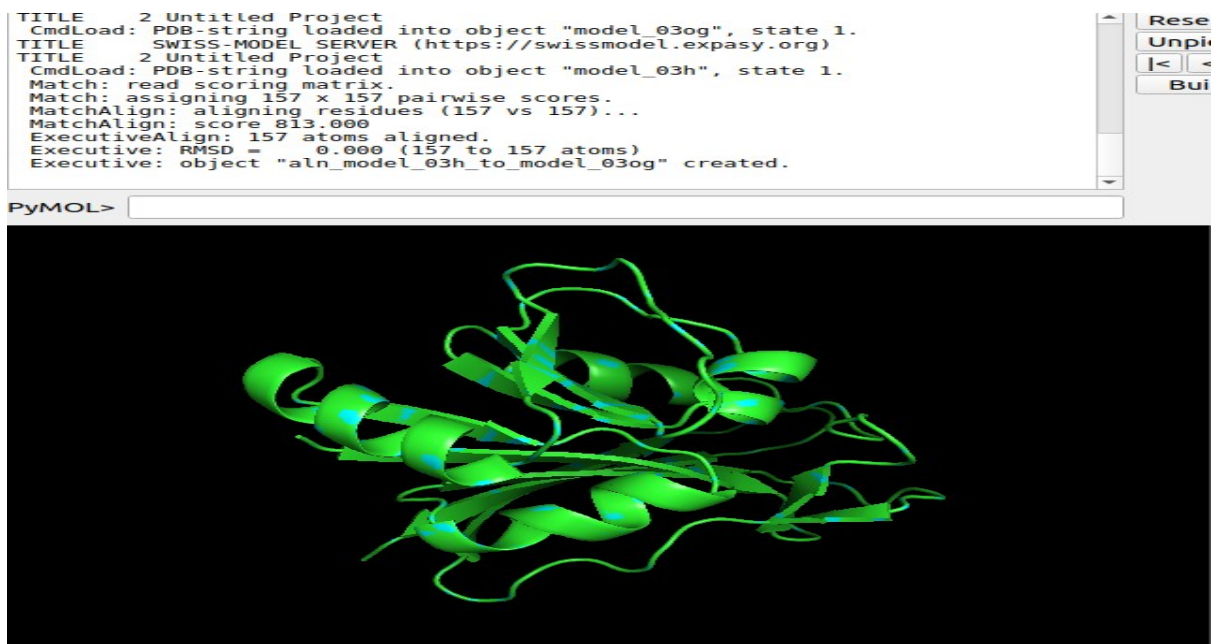
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<input type="checkbox"/>	<u>PDB C D</u>	<u>Alignment Length</u>	<u>SCORE</u>	<u>RMSD</u>	<u>Identity</u>	<u>Description</u>
<input type="checkbox"/>	<u>1UCS</u> A	64	7.33	0.60	64.1	Type III Antifreeze Protein RD1 from an Antarctic Eel Pout
<input type="checkbox"/>	<u>1C8A</u> A	64	8.09	1.35	64.1	NMR STRUCTURE OF INTRAMOLECULAR DIMER ANTIFREEZE PROTEIN RD3, 40 SA STRUCTURES
<input type="checkbox"/>	<u>4IPI</u> A	62	6.92	1.75	17.7	Crystal Structure of R314A N-acetyl Neuraminic Acid Synthase from Neisseria meningitidis with Malate bound
<input type="checkbox"/>	<u>8H2C</u> A	53	5.52	1.09	13.2	Crystal structure of the pseudaminic acid synthase PseI from Campylobacter jejuni
<input type="checkbox"/>	<u>3UPL</u> A	43	7.71	1.26	14.0	Crystal Structure Of The Brucella Abortus Enzyme Catalyzing The First Committed Step Of The Methylerythritol 4-Phosphate Pathway

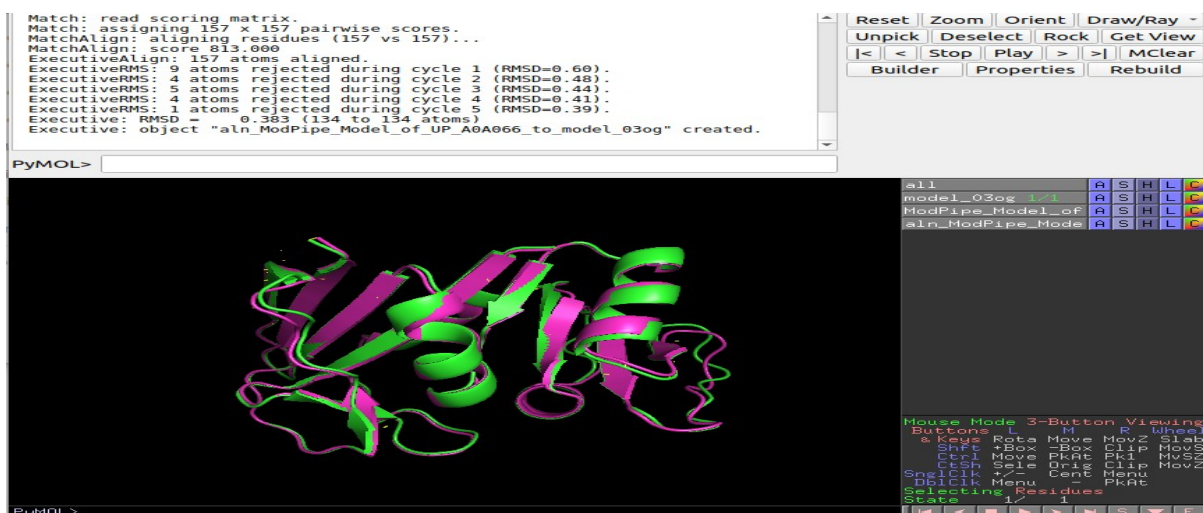
<input type="checkbox"/>	<u>PDB C D</u>	<u>Alignment Length</u>	<u>SCORE</u>	<u>RMSD</u>	<u>Identity</u>	<u>Description</u>
<input type="checkbox"/>	<u>1UCS</u> A	64	7.33	0.60	64.1	Type III Antifreeze Protein RD1 from an Antarctic Eel Pout
<input type="checkbox"/>	<u>1C8A</u> A	64	8.09	1.35	64.1	NMR STRUCTURE OF INTRAMOLECULAR DIMER ANTIFREEZE PROTEIN RD3, 40 SA STRUCTURES
<input type="checkbox"/>	<u>4IPI</u> A	55	6.55	0.90	18.2	Crystal Structure of R314A N-acetyl Neuraminic Acid Synthase from Neisseria meningitidis with Malate bound
<input type="checkbox"/>	<u>8H2C</u> A	52	5.52	1.04	13.5	Crystal structure of the pseudaminic acid synthase PseI from Campylobacter jejuni
<input type="checkbox"/>	<u>3UPL</u> A	41	7.71	1.09	14.6	Crystal Structure Of The Brucella Abortus Enzyme Catalyzing The First Committed Step Of The Methylerythritol 4-Phosphate Pathway

Model 3: Dihydrofolate reductase from Vibrio cholerae

Comparison between original sequence and homologue(RMSD:0.0)



Comparison between original sequence and ModWeb(RMSD:0.383)

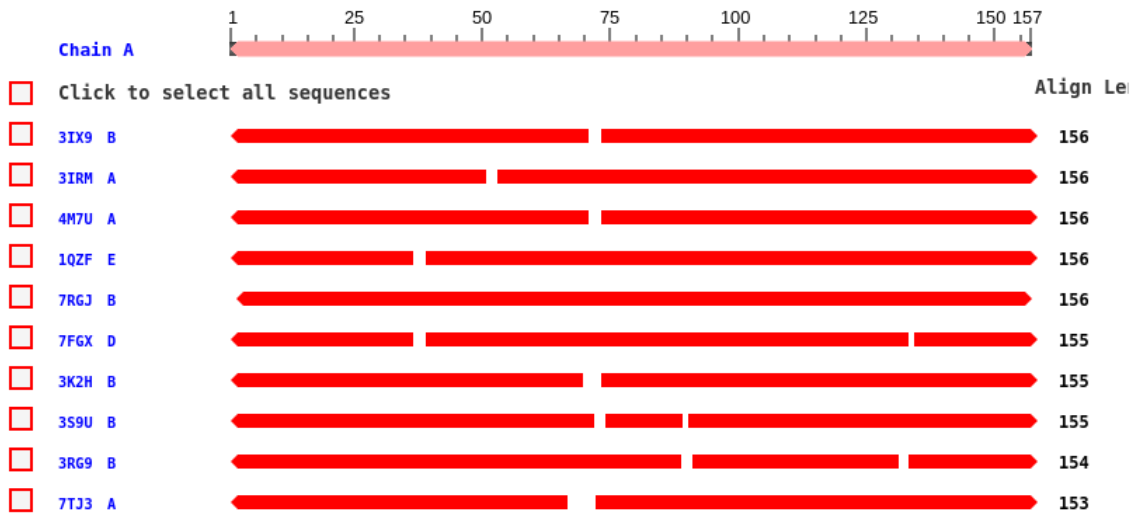


Comparison between homologue and ModWeB(RMSD:0.383)



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<input type="checkbox"/>	PDB C D	Alignment Length	SCORE	RMSD	Identity	Description
<input type="checkbox"/>	3IX9 B	156	20.34	1.51	28.2	Crystal structure of Streptococcus pneumoniae dihydrofolate reductase - Sp9 mutant
<input type="checkbox"/>	3IRM A	156	15.47	2.01	23.1	Trypanosoma cruzi Dihydrofolate Reductase-Thymidylate Synthase COMPLEXED WITH Cycloguanil
<input type="checkbox"/>	4M7U A	156	18.12	1.67	31.4	Dihydrofolate reductase from Enterococcus faecalis complexed with NADP(H)
<input type="checkbox"/>	1QZF E	156	20.90	1.61	33.3	Crystal structure of DHFR-TS from Cryptosporidium hominis
<input type="checkbox"/>	7RGJ B	156	21.27	0.30	91.7	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"/>	7FGX D	155	21.80	1.69	29.0	Toxoplasma gondii dihydrofolate reductase thymidylate synthase (TgDHFR-TS) complexed with P39, NADPH and dUMP
<input type="checkbox"/>	3K2H B	155	21.12	1.59	26.5	Co-crystal structure of dihydrofolate reductase/thymidylate synthase from Babesia bovis with dUMP, Pemetrexed and NADP
<input type="checkbox"/>	3S9U B	155	20.92	1.50	31.6	Bacillus anthracis Dihydrofolate Reductase bound to propargyl-linked TMP analog, UCP120J
<input type="checkbox"/>	3RG9 B	154	22.60	1.67	25.3	Trypanosoma Brucei Dihydrofolate Reductase (tbdhfr) In Complex With Wr99210
<input type="checkbox"/>	7TJ3 A	153	23.43	1.71	34.0	Crystal structure of a dihydrofolate reductase folA from Stenotrophomonas maltophilia bound to NADP and p218