BT305 LAB 8

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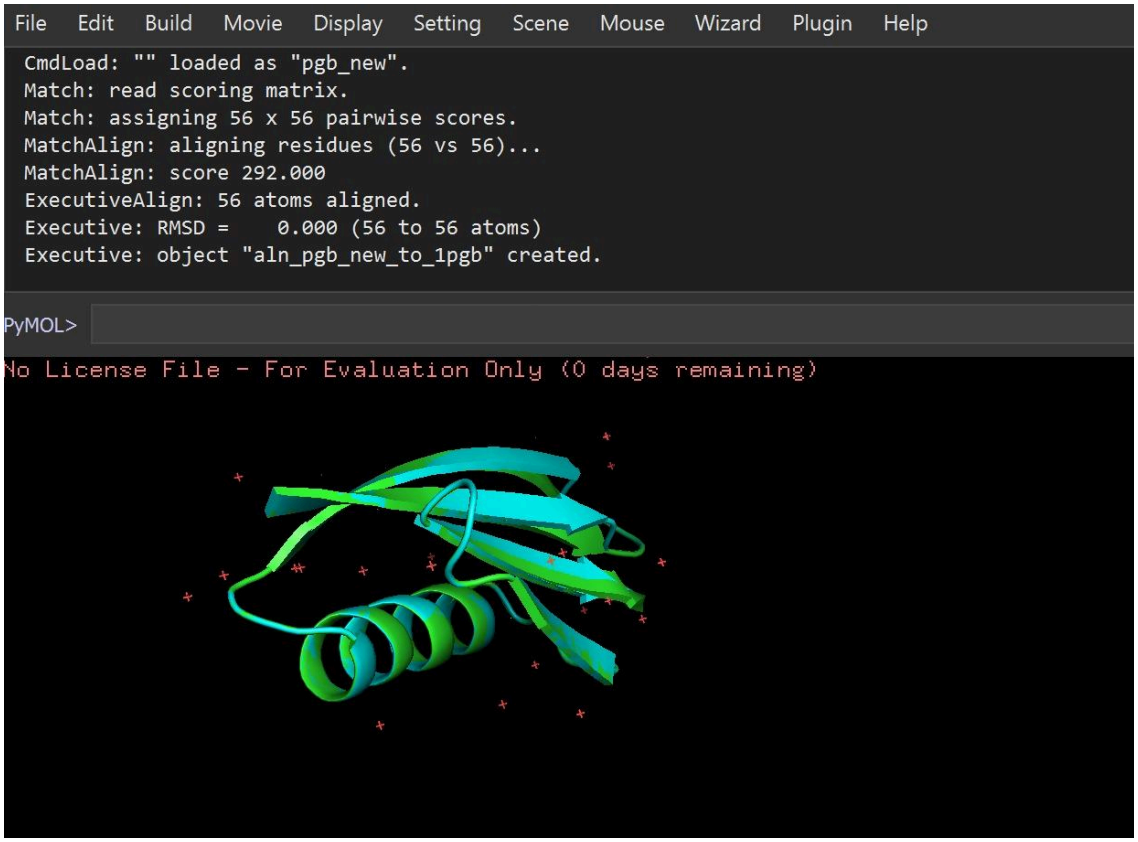
Section 1
From the video, we can observe that the Trpcage protein at 363 K is more actively moving around the space and water molecules than the protein at 300 K.

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