3D Data Processing in Structural Biology

תרגיל 4

מגישים:

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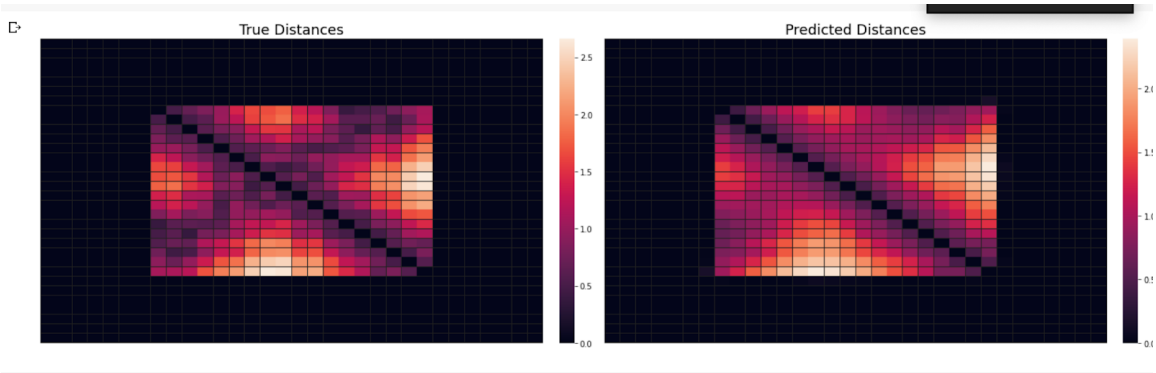
שאלה 1

```
Parameters:
CONV_1D_SIZE = 11

# number of ResNet blocks for the first ResNet and the kernel size.
RESNET_1_BLOCKS = 3
RESNET_1_SIZE = (11, 11)
# learning rate and batch size.
LR = 0.001
BATCH = 32
# number of ResNet blocks for the second ResNet, dilation list to
repeat and the kernel size.
RESNET_2_BLOCKS = 3  # good start may be 3/5/7
DILATION = [1,2,4]
RESNET_2_SIZE = (3,3)  # good start may be (3,3)/(5,5)/(7,7)

# percentage of dropout for the dropout layer
DROPOUT = 0.2 # good start may be 0.1-0.5

# number of epochs
EPOCHS = 20
```

שאלה 2

Total params: 1,467,155
Trainable params: 1,465,811
Non-trainable params: 1,344

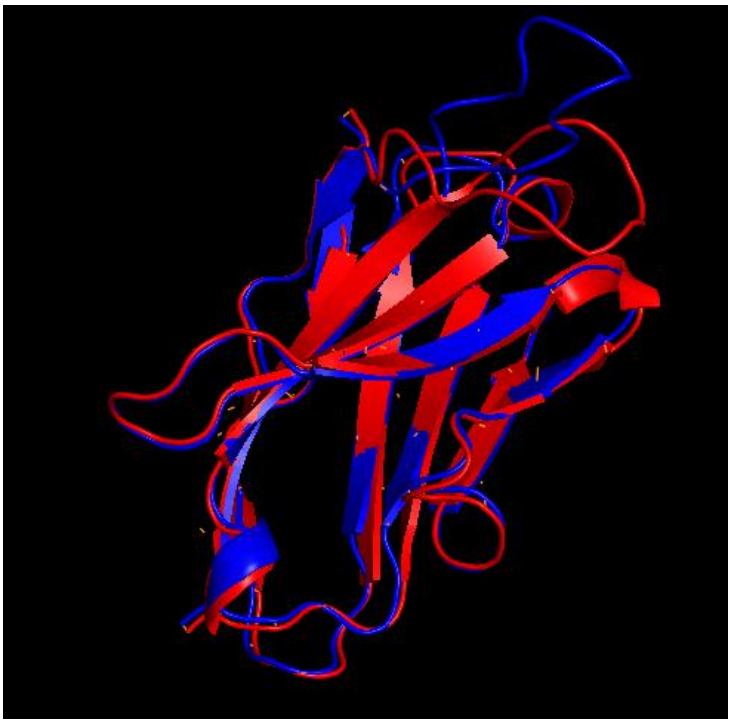


שאלה 3

total score of your model: 1639.418
phi: 0.007
omega, theta: 90.969

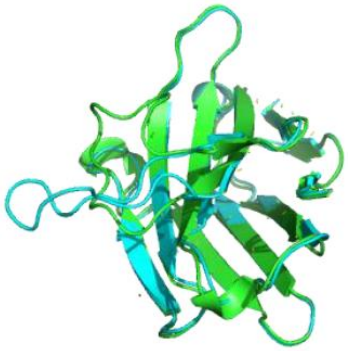
שאלה 4

המודל באדום, ה-REF בכחול :



מבחנת הRMSD נראה שיש שיפור מתרגיל 3 אך לא שיפור ניכר לצערנו, מבחנת ההתאמה המבנית דווקא כן נראה שיש שיפור – לא מספיק בלולאה (CDR3)

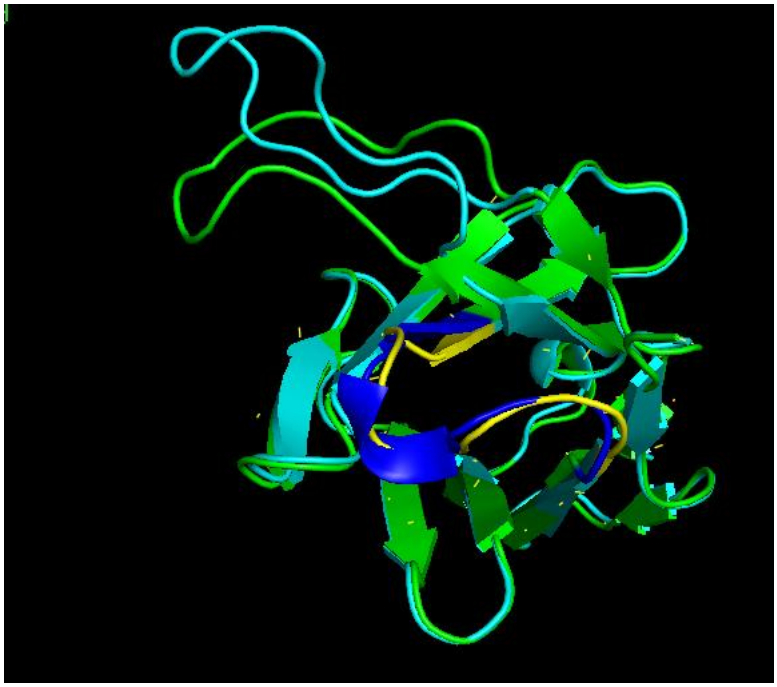
תזכורת זה מה שיצא לנו בתרגיל 3:



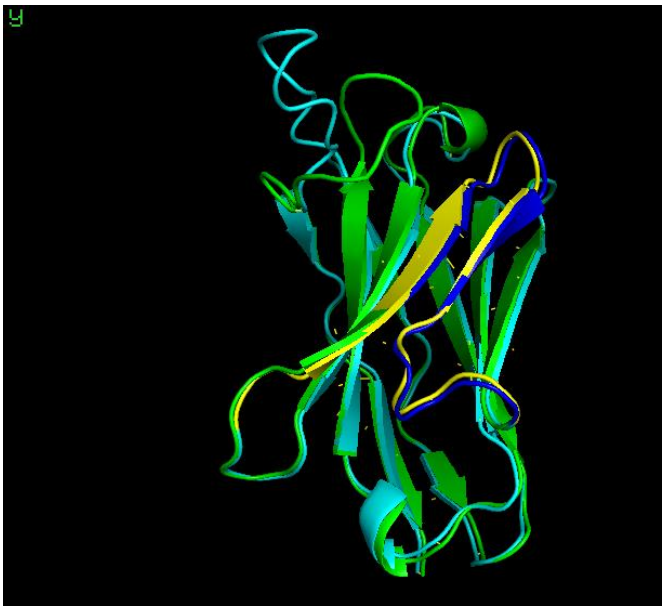
ה-RMSD שהתקבל ב-PyMOL הוא: 0.515

בתמונות הבאות נתמקד ב3 החלקים בנפרד, בכל תמונה החלק הרלוונטי צבוע בכחול במודל וצהוב בref

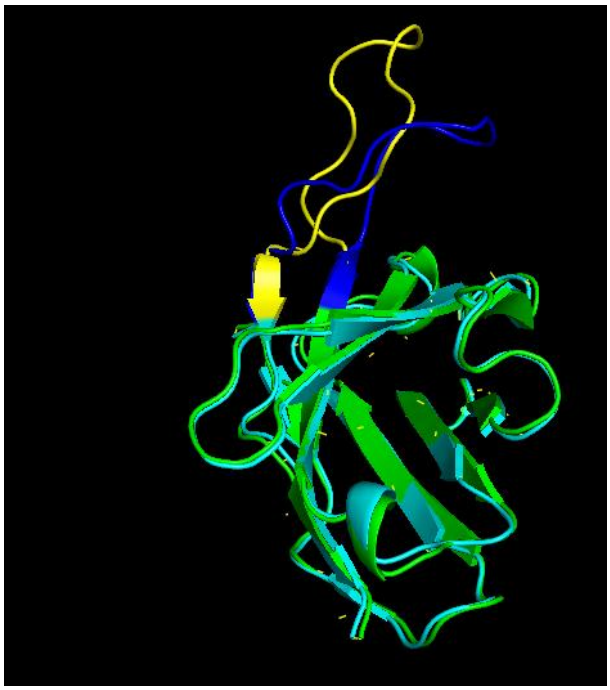
H1



H2



H3



<u>שאלה 5</u>
הRMSD שהתקבל: 0.507

```
MatchAlign: score 688.000
ExecutiveAlign: 125 atoms aligned.
ExecutiveRMS: 9 atoms rejected during cycle 1 (RMSD=2.21).
ExecutiveRMS: 4 atoms rejected during cycle 2 (RMSD=0.95).
ExecutiveRMS: 3 atoms rejected during cycle 3 (RMSD=0.58).
ExecutiveRMS: 2 atoms rejected during cycle 4 (RMSD=0.53).
ExecutiveRMS: 1 atoms rejected during cycle 5 (RMSD=0.52).
Executive: RMSD =    0.507 (106 to 106 atoms)
```