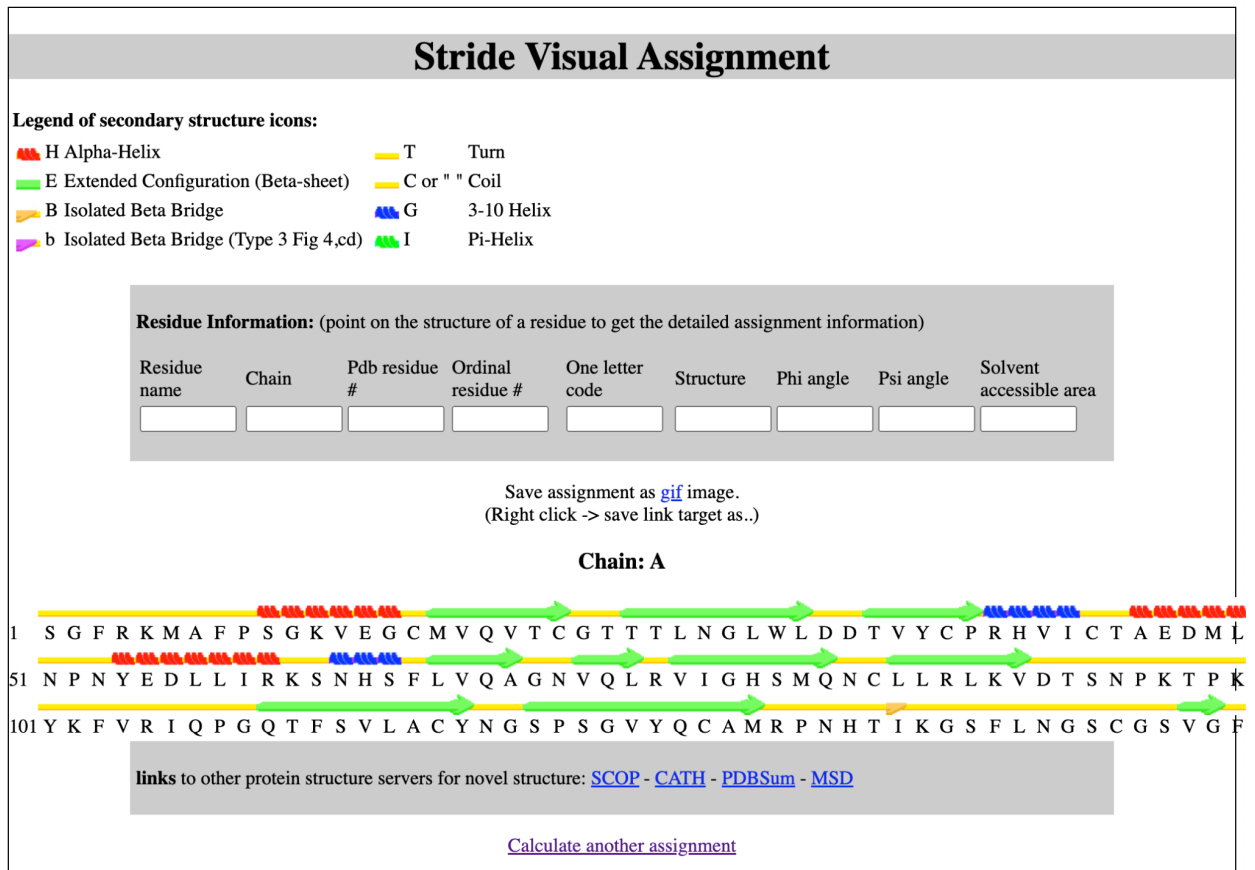## Question 1.

a) The python file for this problem has been attached in the folder with the name "iqb.py".

b)

```
1       SGFRKMAFPSGKVEGCMVQVTCGTTTLNGLWLDDTVYCPRHVICTAEDML        50
         HHHHHHHHHHHSSSSSSSSSSSSSSSSSHSSHHHSSSSSSSSHHSHHHHHHHH

51      NPNYEDLLIRKSNHSFLVQAGNVQLRVIGHSMQNCLLRLKVDTSNPKTPK       100
        H   HHHSSSHHHHSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS      HS

101     YKFVRIQPGQTFSVLACYNGSPSGVYQCAMRPNHTIKGSFLNGSCGSVGF       150
        SSSSSSSSSSSSSSSSSSSSS   SSSSSSHSSH    HHHHHH
```

Question 2.

a) The outputs received from the website given in the assignment have been attached below. The code for showing the regions differing has been attached in the folder with the name "iqb.py" and the result has been printed.

Stride Visual Assignment

Legend of secondary structure icons:

H Alpha-Helix		T	Turn	
E Extended Configuration (Beta-sheet)		C or " "	Coil	
B Isolated Beta Bridge		G	3-10 Helix	
b Isolated Beta Bridge (Type 3 Fig 4,cd)		I	Pi-Helix	

Residue Information: (point on the structure of a residue to get the detailed assignment information)

Residue name	Chain	Pdb residue #	Ordinal residue #	One letter code	Structure	Phi angle	Psi angle	Solvent accessible area

Save assignment as gif image.
(Right click -> save link target as..)

Chain: A

```
1   S G F R K M A F P S G K V E G C M V Q V T C G T T T L N G L W L D D T V Y C P R H V I C T A E D M L

51  N P N Y E D L L I R K S N H S F L V Q A G N V Q L R V I G H S M Q N C L L R L K V D T S N P K T P K

101 Y K F V R I Q P G Q T F S V L A C Y N G S P S G V Y Q C A M R P N H T I K G S F L N G S C G S V G F
```

links to other protein structure servers for novel structure: SCOP - CATH - PDBSum - MSD

Calculate another assignment

```
REM  -------------------- Secondary structure summary -------------------  ~~~~
REM                                                                         ~~~~
CHN  /home/proj/stride/tmp/tmpDOZs0apdb A                                   ~~~~
REM                                                                         ~~~~
REM           .         .         .         .         .                     ~~~~
SEQ  1    SGFRKMAFPSGKVEGCMVQVTCGTTTLNGLWLDDTVYCPRHVICTAEDML    50          ~~~~
STR       TTTT     HHHHHH EEEEEETTEEEEEEEEETTEEEEEGGGG   HHHHH              ~~~~
REM                                                                         ~~~~
REM           .         .         .         .         .                     ~~~~
SEQ  51   NPNYEDLLIRKSNHSFLVQAGNVQLRVIGHSMQNCLLRLKVDTSNPKTPK    100         ~~~~
STR         HHHHHHH  GGG EEEETTEEE EEEEEEETTEEEEEE    TTTT                  ~~~~
REM                                                                         ~~~~
REM           .         .         .         .         .                     ~~~~
SEQ  101  YKFVRIQPGQTFSVLACYNGSPSGVYQCAMRPNHTIKGSFLNGSCGSVGF    150         ~~~~
STR          TTTEEEEEEEEEETTEEEEEEEEEEETTTT B     TTTTTTTEE                 ~~~~
REM                                                                         ~~~~
REM                                                                         ~~~~
REM                                                                         ~~~~
LOC  AlphaHelix   SER    10 A      GLY    15 A                              ~~~~
LOC  AlphaHelix   ALA    46 A      LEU    50 A                              ~~~~
LOC  AlphaHelix   TYR    54 A      ARG    60 A                              ~~~~
LOC  310Helix     ARG    40 A      ILE    43 A                              ~~~~
LOC  310Helix     ASN    63 A      SER    65 A                              ~~~~
LOC  Strand       MET    17 A      CYS    22 A                              ~~~~
LOC  Strand       THR    25 A      LEU    32 A                              ~~~~
LOC  Strand       THR    35 A      PRO    39 A                              ~~~~
LOC  Strand       LEU    67 A      ALA    70 A                              ~~~~
LOC  Strand       VAL    73 A      LEU    75 A                              ~~~~
LOC  Strand       VAL    77 A      GLN    83 A                              ~~~~
LOC  Strand       LEU    86 A      VAL    91 A                              ~~~~
LOC  Strand       GLN   110 A      TYR   118 A                              ~~~~
LOC  Strand       SER   121 A      MET   130 A                              ~~~~
LOC  Strand       VAL   148 A      GLY   149 A                              ~~~~
LOC  TurnVIII     SER     1 A      ARG     4 A                              ~~~~
LOC  TurnII'      CYS    22 A      THR    25 A                              ~~~~
LOC  TurnII'      LEU    32 A      THR    35 A                              ~~~~
LOC  TurnIV       GLN    69 A      ASN    72 A                              ~~~~
LOC  TurnII'      ALA    70 A      VAL    73 A                              ~~~~
LOC  TurnII'      GLN    83 A      LEU    86 A                              ~~~~
LOC  TurnI        ASN    95 A      THR    98 A                              ~~~~
LOC  TurnII       GLN   107 A      GLN   110 A                              ~~~~
LOC  TurnIV       CYS   117 A      GLY   120 A                              ~~~~
LOC  TurnI'       TYR   118 A      SER   121 A                              ~~~~
LOC  TurnI        ARG   131 A      HIS   134 A                              ~~~~
LOC  TurnII       LEU   141 A      SER   144 A                              ~~~~
LOC  TurnII       SER   144 A      SER   147 A                              ~~~~
REM                                                                         ~~~~
REM  --------------- Detailed secondary structure assignment------------   ~~~~
REM                                                                         ~~~~
REM  |---Residue---|     |--Structure--|    |-Phi-|   |-Psi-|   |-Area-|    ~~~~
ASG  SER A    1    1    T          Turn     360.00    114.46     109.8      ~~~~
ASG  GLY A    2    2    T          Turn     -66.60    -24.47      91.7      ~~~~
ASG  PHE A    3    3    T          Turn    -142.74    102.86     188.2      ~~~~
ASG  ARG A    4    4    T          Turn     -81.84    140.92     191.0      ~~~~
ASG  LYS A    5    5    C          Coil     -71.44    131.66     170.8      ~~~~
ASG  MET A    6    6    C          Coil    -119.68    132.19     153.1      ~~~~
ASG  ALA A    7    7    C          Coil     -96.07    157.94      30.3      ~~~~
ASG  PHE A    8    8    C          Coil     -76.86    154.78     125.1      ~~~~
ASG  PRO A    9    9    C          Coil     -63.35    136.28     118.6      ~~~~
ASG  SER A   10   10    H     AlphaHelix    -94.72     -3.80      19.8      ~~~~
ASG  GLY A   11   11    H     AlphaHelix    -43.48    -49.99      47.8      ~~~~
ASG  LYS A   12   12    H     AlphaHelix    -62.41    -30.20     159.4      ~~~~
ASG  VAL A   13   13    H     AlphaHelix    -85.74    -32.57      20.3      ~~~~
ASG  GLU A   14   14    H     AlphaHelix    -54.10    -44.48      86.0      ~~~~
```

```
ASG   GLY A   15   15   H   AlphaHelix   -69.19      2.02    22.7   ~~~~
ASG   CYS A   16   16   C      Coil     -109.81     -5.96     3.0   ~~~~
ASG   MET A   17   17   E     Strand     -84.95    128.58    12.3   ~~~~
ASG   VAL A   18   18   E     Strand    -134.93    172.17     0.8   ~~~~
ASG   GLN A   19   19   E     Strand    -110.69    136.01    34.1   ~~~~
ASG   VAL A   20   20   E     Strand    -125.60    127.49     0.0   ~~~~
ASG   THR A   21   21   E     Strand    -123.98    145.70    25.1   ~~~~
ASG   CYS A   22   22   E     Strand    -149.99     97.50     7.2   ~~~~
ASG   GLY A   23   23   T      Turn      75.22    -133.71    70.0   ~~~~
ASG   THR A   24   24   T      Turn     -80.97     -8.44    150.1   ~~~~
ASG   THR A   25   25   E     Strand     -92.80    125.22    37.4   ~~~~
ASG   THR A   26   26   E     Strand    -132.11    130.84    38.5   ~~~~
ASG   LEU A   27   27   E     Strand    -149.46   -178.11     2.6   ~~~~
ASG   ASN A   28   28   E     Strand     -87.11    148.00     0.0   ~~~~
ASG   GLY A   29   29   E     Strand    -132.42    158.90     0.0   ~~~~
ASG   LEU A   30   30   E     Strand    -114.57    116.16    27.4   ~~~~
ASG   TRP A   31   31   E     Strand    -101.53    109.24    20.8   ~~~~
ASG   LEU A   32   32   E     Strand    -124.86    123.68     7.1   ~~~~
ASG   ASP A   33   33   T      Turn      57.67    -128.67    67.9   ~~~~
ASG   ASP A   34   34   T      Turn     -106.96     32.98    65.5   ~~~~
ASG   THR A   35   35   E     Strand    -132.36    136.75     5.6   ~~~~
ASG   VAL A   36   36   E     Strand    -116.13    122.15     0.0   ~~~~
ASG   TYR A   37   37   E     Strand    -103.50    138.77    23.5   ~~~~
ASG   CYS A   38   38   E     Strand    -158.15    162.74     3.1   ~~~~
ASG   PRO A   39   39   E     Strand     -59.39    136.76    24.1   ~~~~
ASG   ARG A   40   40   G    310Helix    -68.53    -17.27    47.7   ~~~~
ASG   HIS A   41   41   G    310Helix    -69.70     -0.49    61.7   ~~~~
ASG   VAL A   42   42   G    310Helix    -65.49    -22.40     0.0   ~~~~
ASG   ILE A   43   43   G    310Helix    -85.59     -2.95     5.5   ~~~~
ASG   CYS A   44   44   C      Coil      -97.82    146.40     4.9   ~~~~
ASG   THR A   45   45   C      Coil      -94.56    165.80    71.3   ~~~~
ASG   ALA A   46   46   H   AlphaHelix   -52.03    -34.54    95.4   ~~~~
ASG   GLU A   47   47   H   AlphaHelix   -76.97    -40.93   172.7   ~~~~
ASG   ASP A   48   48   H   AlphaHelix   -56.19    -34.39    48.2   ~~~~
ASG   MET A   49   49   H   AlphaHelix   -60.25    -29.59    69.8   ~~~~
ASG   LEU A   50   50   H   AlphaHelix   -57.38    -42.81   150.1   ~~~~
ASG   ASN A   51   51   C      Coil     -158.91     82.16   143.8   ~~~~
ASG   PRO A   52   52   C      Coil      -83.92    145.30    38.8   ~~~~
ASG   ASN A   53   53   C      Coil     -118.03     82.97    88.3   ~~~~
ASG   TYR A   54   54   H   AlphaHelix   -51.78    -47.45    30.0   ~~~~
ASG   GLU A   55   55   H   AlphaHelix   -55.27    -41.07   106.1   ~~~~
ASG   ASP A   56   56   H   AlphaHelix   -74.64    -39.13   100.2   ~~~~
ASG   LEU A   57   57   H   AlphaHelix   -67.69    -35.40    30.4   ~~~~
ASG   LEU A   58   58   H   AlphaHelix   -69.82    -38.22    17.3   ~~~~
ASG   ILE A   59   59   H   AlphaHelix   -53.22    -37.93   136.6   ~~~~
ASG   ARG A   60   60   H   AlphaHelix   -73.47     -4.57    81.0   ~~~~
ASG   LYS A   61   61   C      Coil     -100.59    162.43    58.6   ~~~~
ASG   SER A   62   62   C      Coil     -140.04    166.91    49.8   ~~~~
ASG   ASN A   63   63   G    310Helix    -52.49    -43.61    54.1   ~~~~
ASG   HIS A   64   64   G    310Helix    -68.45     -3.09   164.3   ~~~~
ASG   SER A   65   65   G    310Helix    -83.64    -12.88    35.2   ~~~~
ASG   PHE A   66   66   C      Coil     -109.76    125.90     8.3   ~~~~
ASG   LEU A   67   67   E     Strand    -108.63    103.79    72.9   ~~~~
ASG   VAL A   68   68   E     Strand    -102.20    124.42     0.2   ~~~~
ASG   GLN A   69   69   E     Strand    -127.78    121.72    52.4   ~~~~
ASG   ALA A   70   70   E     Strand    -105.45     98.67    19.3   ~~~~
ASG   GLY A   71   71   T      Turn      76.37    -110.38    61.9   ~~~~
ASG   ASN A   72   72   T      Turn     -111.47     -7.39   156.4   ~~~~
ASG   VAL A   73   73   E     Strand     -95.54    127.00    91.4   ~~~~
ASG   GLN A   74   74   E     Strand     -82.66    135.96   130.8   ~~~~
ASG   LEU A   75   75   E     Strand    -103.23    150.98    15.4   ~~~~
ASG   ARG A   76   76   C      Coil      -97.85    116.27    45.1   ~~~~
ASG   VAL A   77   77   E     Strand     -82.10    121.12    17.5   ~~~~
ASG   ILE A   78   78   E     Strand    -110.07     17.80    98.1   ~~~~
ASG   GLY A   79   79   E     Strand     172.56    149.48    17.5   ~~~~
```

```
ASG   HIS A    80   80     E      Strand   -145.03    136.63     57.4    ~~~~
ASG   SER A    81   81     E      Strand   -149.47    161.93     56.3    ~~~~
ASG   MET A    82   82     E      Strand   -106.62    134.81     55.4    ~~~~
ASG   GLN A    83   83     E      Strand   -127.80     94.16     67.6    ~~~~
ASG   ASN A    84   84     T      Turn       56.33   -125.01    143.6    ~~~~
ASG   CYS A    85   85     T      Turn      -90.68     11.45     83.0    ~~~~
ASG   LEU A    86   86     E      Strand   -109.49    151.90     65.5    ~~~~
ASG   LEU A    87   87     E      Strand   -102.71    126.56      1.0    ~~~~
ASG   ARG A    88   88     E      Strand   -105.21    110.04     60.0    ~~~~
ASG   LEU A    89   89     E      Strand   -103.64    117.22      0.0    ~~~~
ASG   LYS A    90   90     E      Strand    -82.61    128.77     73.2    ~~~~
ASG   VAL A    91   91     E      Strand   -115.86    159.65      1.2    ~~~~
ASG   ASP A    92   92     C      Coil      -80.48     -4.92     92.1    ~~~~
ASG   THR A    93   93     C      Coil     -125.19    133.62     60.7    ~~~~
ASG   SER A    94   94     C      Coil      -86.88    135.00     67.7    ~~~~
ASG   ASN A    95   95     T      Turn      -66.16    113.31      8.3    ~~~~
ASG   PRO A    96   96     T      Turn      -67.53    -13.15    114.9    ~~~~
ASG   LYS A    97   97     T      Turn     -104.37     13.14    149.9    ~~~~
ASG   THR A    98   98     T      Turn      -58.69    121.82     34.3    ~~~~
ASG   PRO A    99   99     C      Coil      -87.71    177.68     30.5    ~~~~
ASG   LYS A   100  100     C      Coil      -73.59    135.57    194.6    ~~~~
ASG   TYR A   101  101     C      Coil     -154.71    167.37     90.1    ~~~~
ASG   LYS A   102  102     C      Coil     -144.06    157.18    176.2    ~~~~
ASG   PHE A   103  103     C      Coil     -107.57    124.53    122.2    ~~~~
ASG   VAL A   104  104     C      Coil     -131.02    143.85    123.3    ~~~~
ASG   ARG A   105  105     C      Coil     -103.66    117.09    234.2    ~~~~
ASG   ILE A   106  106     C      Coil      -84.67    166.23     55.7    ~~~~
ASG   GLN A   107  107     T      Turn     -100.92    159.50    134.2    ~~~~
ASG   PRO A   108  108     T      Turn      -56.74    140.84     67.4    ~~~~
ASG   GLY A   109  109     T      Turn       93.56    -19.53     48.3    ~~~~
ASG   GLN A   110  110     E      Strand    -76.11    154.70     81.2    ~~~~
ASG   THR A   111  111     E      Strand   -108.98    164.60     87.8    ~~~~
ASG   PHE A   112  112     E      Strand   -167.18    163.20     30.1    ~~~~
ASG   SER A   113  113     E      Strand    -97.97    146.50      0.0    ~~~~
ASG   VAL A   114  114     E      Strand   -120.67    127.71      9.4    ~~~~
ASG   LEU A   115  115     E      Strand    -95.39     95.44      2.8    ~~~~
ASG   ALA A   116  116     E      Strand    -72.02    125.83      1.6    ~~~~
ASG   CYS A   117  117     E      Strand   -127.77    155.39      0.0    ~~~~
ASG   TYR A   118  118     E      Strand   -135.70    124.91     47.9    ~~~~
ASG   ASN A   119  119     T      Turn       56.35     32.54     92.8    ~~~~
ASG   GLY A   120  120     T      Turn       92.49     -2.33     12.4    ~~~~
ASG   SER A   121  121     E      Strand   -122.63    136.18     71.5    ~~~~
ASG   PRO A   122  122     E      Strand    -57.25    133.58     54.5    ~~~~
ASG   SER A   123  123     E      Strand   -108.11    -48.70     84.5    ~~~~
ASG   GLY A   124  124     E      Strand   -165.80    172.38     25.9    ~~~~
ASG   VAL A   125  125     E      Strand   -121.41    131.37     60.9    ~~~~
ASG   TYR A   126  126     E      Strand   -123.98    148.08    130.7    ~~~~
ASG   GLN A   127  127     E      Strand   -104.92    132.16     40.9    ~~~~
ASG   CYS A   128  128     E      Strand   -149.43   -177.06     23.9    ~~~~
ASG   ALA A   129  129     E      Strand   -133.56    153.35     27.4    ~~~~
ASG   MET A   130  130     E      Strand    -81.39    115.36     28.6    ~~~~
ASG   ARG A   131  131     T      Turn      -64.58    158.19     97.6    ~~~~
ASG   PRO A   132  132     T      Turn      -59.97    -28.93     88.5    ~~~~
ASG   ASN A   133  133     T      Turn      -88.15     19.32    104.9    ~~~~
ASG   HIS A   134  134     T      Turn       67.39     20.78    133.7    ~~~~
ASG   THR A   135  135     C      Coil     -112.69    174.51     68.2    ~~~~
ASG   ILE A   136  136     B      Bridge   -125.25    136.87     67.6    ~~~~
ASG   LYS A   137  137     C      Coil      -94.70    141.63    153.1    ~~~~
ASG   GLY A   138  138     C      Coil      155.94   -149.95     61.9    ~~~~
ASG   SER A   139  139     C      Coil     -150.13    109.45    108.1    ~~~~
ASG   PHE A   140  140     C      Coil     -110.48    136.19    107.1    ~~~~
ASG   LEU A   141  141     T      Turn      -94.95    168.97    118.0    ~~~~
ASG   ASN A   142  142     T      Turn      -59.75    117.64    162.4    ~~~~
ASG   GLY A   143  143     T      Turn      106.67     -2.04     14.5    ~~~~
ASG   SER A   144  144     T      Turn      -82.06    -15.64      7.2    ~~~~
```
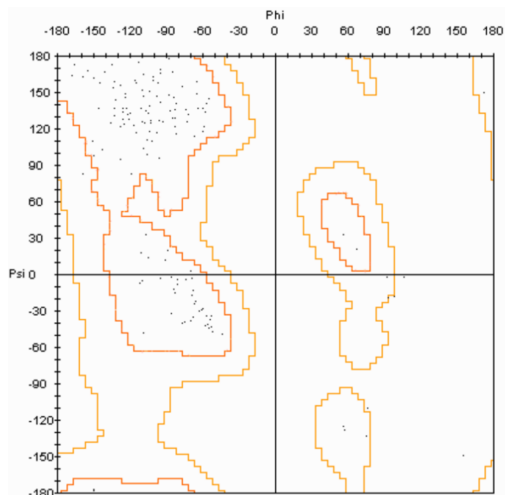
```
ASG   CYS A  145  145    T      Turn    -54.64   144.97   53.3    ~~~~
ASG   GLY A  146  146    T      Turn     98.38   -18.52   16.9    ~~~~
ASG   SER A  147  147    T      Turn    -64.46   148.70   23.9    ~~~~
ASG   VAL A  148  148    E      Strand  -114.56  157.71   36.2    ~~~~
ASG   GLY A  149  149    E      Strand  -108.29  146.66   40.3    ~~~~
ASG   PHE A  150  150    C      Coil    -158.18  360.00   72.3    ~~~~
```

Ramachandran Plot

b) Reasoning for the differences observed:

   i) We can clearly identify that the sequences are different at a lot of positions, this can be because of the fact that the website is predicting for single nucleotides as well, whereas we on the other hand are using a string with minimum length of 5, hence ignoring small sequences and giving us a different output.

   ii) The website is giving the final outputs based on a lot of criterias unlike our code which gives an output only with 'H', 'S' and ' '(blank) hence only checking these cases whereas the website's output has many letters indicating that they have inculcated more criterias to create the final sequence and thus have a higher accuracy than ours.

   iii) It can be seen at various indices where our code is outputting blank spaces, there are some letters in the website's output.

   iv) Our output is returning Hs and Ss at places where the website's output returns letters meaning that the few conditions that we checked have been overlapped by conditions of greater importance which we've not checked.