In [15]:
```
##Citation
#Jumper, J., Evans, R., Pritzel, A. et al. Highly accurate protein structure predict
#Mihaly Varadi, Stephen Anyango, Mandar Deshpande, Sreenath Nair, Cindy Natassia, Ga
#https://alphafold.ebi.ac.uk/entry/A0A6J3EQU8
#https://biopython.org/docs/1.75/api/Bio.PDB.Residue.html
#https://biopython.org/docs/1.75/api/Bio.PDB.Atom.html
```

In [16]:
```
import os #Bring the os to check working directory
os.getcwd()
```

Out[16]:
```
'C:₩₩Users₩₩panky₩₩Desktop₩₩pLDDT'
```

In [17]:
```
from Bio.PDB import * #Bring the Bio.PDB for ananlysis, Bio.PDB is included in Biop
```

In [18]:
```
##Set up the PDB file
par = PDBParser() #Set PDBParser() to par for convenient
protein = par.get_structure("MRGPRX2", "AF-A0A6J3EQU8-F1-model_v3.pdb") #Load the PD
```

In [19]:
```
protein #Check the file
```

Out[19]:
```
<Structure id=MRGPRX2>
```

In [20]:
```
print(dir(protein)) #Check the module
```

```
['__class__', '__contains__', '__delattr__', '__delitem__', '__dict__', '__dir__',
'__doc__', '__eq__', '__format__', '__ge__', '__getattribute__', '__getitem__', '__g
t__', '__hash__', '__init__', '__init_subclass__', '__iter__', '__le__', '__len__',
'__lt__', '__module__', '__ne__', '__new__', '__reduce__', '__reduce_ex__', '__repr_
_', '__setattr__', '__sizeof__', '__str__', '__subclasshook__', '__weakref__', '_gen
erate_full_id', '_id', '_reset_full_id', 'add', 'atom_to_internal_coordinates', 'cen
ter_of_mass', 'child_dict', 'child_list', 'copy', 'detach_child', 'detach_parent',
'full_id', 'get_atoms', 'get_chains', 'get_full_id', 'get_id', 'get_iterator', 'get_
level', 'get_list', 'get_models', 'get_parent', 'get_residues', 'has_id', 'header',
'id', 'insert', 'internal_to_atom_coordinates', 'level', 'parent', 'set_parent', 'tr
ansform', 'xtra']
```

In [21]:
```
print(protein.header["name"]) #Check the header name
print(protein.header["release_date"]) #Check the release date
```

```
alphafold monomer v2.0 prediction for mas-related g-protein coupled receptor member
x2 (a0a6j3equ8)
1909-01-08
```

In [22]:
```
model = protein.get_models() #Get model to use PDB file easily
model
```

Out[22]:
```
<generator object Structure.get_models at 0x000002847D5E67A0>
```

In [23]:
```
models = list(model) #Make model as list
```

In [24]:
```
models
```

Out[24]:
```
[<Model id=0>]
```

In [25]:
```
chains = list(models[0].get_chains()) #Check the numer of chain
chains #In this case, the protein has one chain
```

Out[25]:
```
[<Chain id=A>]
```

In [26]:
```
residue = list(chains[0].get_residues()) #Set the chain number and get residue data
len(residue) #Check the number of residues
```

Out[26]:
```
330
```

In [27]:
```
a=residue[1].get_resname() #Use .get_resname() to extract residue name
print(a)
```

```
ASP
```

In [28]:
```
##Generate the sequence of protein
#Create the dictionary to make shorter amioacids sequence
d= {'CYS': 'C', 'ASP': 'D', 'SER': 'S', 'GLN': 'Q', 'LYS': 'K',
     'ILE': 'I', 'PRO': 'P', 'THR': 'T', 'PHE': 'F', 'ASN': 'N',
     'GLY': 'G', 'HIS': 'H', 'LEU': 'L', 'ARG': 'R', 'TRP': 'W',
     'ALA': 'A', 'VAL':'V', 'GLU': 'E', 'TYR': 'Y', 'MET': 'M'}

#len(residue)
nr_0=range(0,len(residue)) #Select the residue range, be aware of that python starts
R=[] #Create the empty list
for i in nr_0: #Repeat the for loop
    rr=residue[i].get_resname() #Get the name of each residue
    rrs=str(rr) #Convert residue name object to string
    nrr=d[rrs] #Bring the simple code from dictionary above
    R.append(nrr) #Add the code to list
```

In [29]:
```
seq="".join(R) #Use "".join() to make continuous sequence with no space
print(seq) #View the result sequence
len(seq) #Check the length of sequence
```

```
MDPTIPAWGTKSTTMNGDDQALPLLCGKETLIPVLLILFIGLVGLVGNAVVLWFLGFHMRRNAFSVYVLSLAGADFLCLCFQII
DCLAYLSDFYHSLYTYFPSFLTAMITCAYLAGLNILSAISAERCLSVLCPIWYRCRRPRHLSTVMCALLWAVSLLLSILEGKFC
GFLFTDGDSGWCQTFDFITAAWLIFLFVVLCGSSLALLVRILCGSRKMPLTRLYVTILLTVLVFLLCGLPFGIQWFLILWIWKN
FDDFLCHIHPVSLVLSSLNSSANPIIYFFVGSFRQQWRLRQPTLKLALQRALQDTAEVDHSEGSFRQDTLEMSGSSLV
```

Out[29]:
```
330
```

In [30]:
```
##Draw the pLDDT plot
atoms = list(residue[1].get_atoms()) #Check atoms in each residue
atoms
```

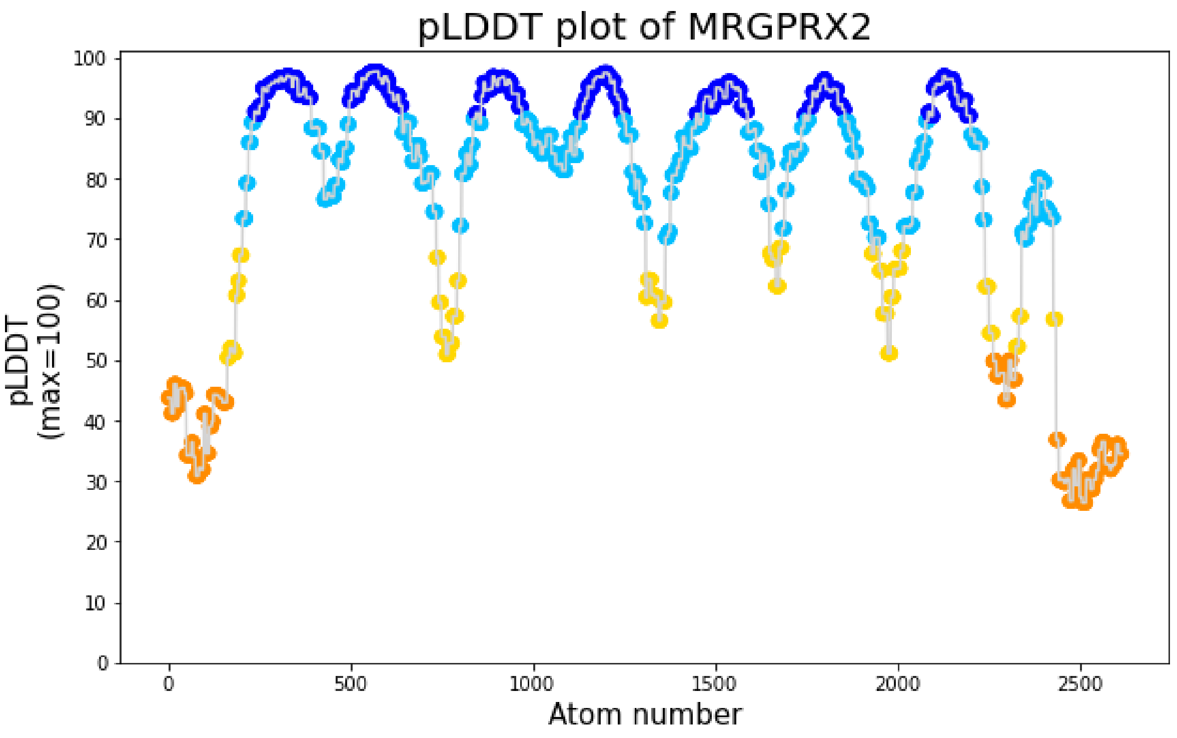
Out[30]:
```
[<Atom N>,
 <Atom CA>,
 <Atom C>,
 <Atom CB>,
 <Atom O>,
 <Atom CG>,
 <Atom OD1>,
 <Atom OD2>]
```

In [31]:
```
atoms[1].get_bfactor() #Get the data in b factor column, in alphfold PDB files, pLDD
```

Out[31]:
```
41.16
```

In [32]:
```
#Prepare the x-value and y-value for plot
X=[] #Create the empty list
Y=[] #Create the empty list
nr=range(0,len(residue)) #Select the residue range, remember the len(residue)
N=nr[0] #Set the base value for for loop
for i in nr: #Repeat the for loop
    atoms_1=list(residue[i].get_atoms()) #Extract the atom list of each residue
    for k in atoms_1: #Additional for loop for atoms list
        bb=k.get_bfactor() #Get pLDDT value for each atom
        Y.append(bb) #Add pLDDT to y-value list
        N=N+1 #Create x-value which means atom number
        X.append(N) #Add atom numer to x-value list
```

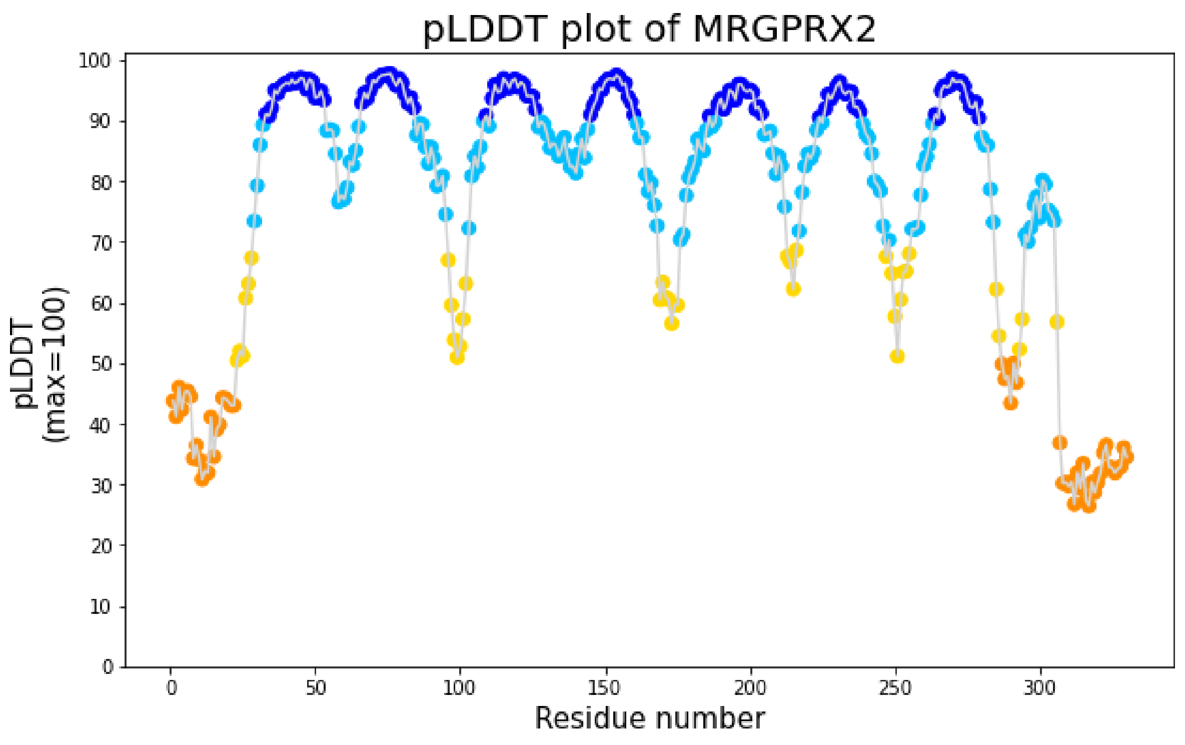
In [33]:
```
#Draw the plot
import matplotlib.pyplot as plt #Bring the matplotlib to draw the plot
import matplotlib as mpl
ids=str(protein) #Make the string of protein name
pn=ids[14:-1] #Extract the name

#plot
fig, ax = plt.subplots(figsize=(10, 6)) #Set the size of figure
cmaps = mpl.colors.ListedColormap(['darkorange','gold','deepskyblue','b']) #Set the
bounds = [0,50,70,90,100] #Set the bound for colormap
norms = mpl.colors.BoundaryNorm(bounds,cmaps.N) #Set the norm for colormap
ax.plot(X,Y,color='lightgrey') #Set the color of line plot
ax.scatter(X,Y,s=50,c=Y,cmap=cmaps,norm=norms) #Draw the scatter plot and set the co
ax.set_title("pLDDT plot of "+pn, fontsize=20) #Set the title and fontsize
ax.set_xlabel("Atom number",fontsize=15) #Set the x label and fontsize
ax.set_ylabel("pLDDT₩n(max=100)",fontsize=15) #Set the y label and fontsize, remeber
plt.yticks(range(0, 109,10)) #Custom the y sticks
plt.show() #Show the plot
```



In [34]:
```
#Use the residue number to view the pLDDT value
X1=[] #Create the empty list
Y1=[] #Create the empty list
nr_1=range(0,len(residue)) #Select the residue range, remember the len(residue)
N1=nr_1[0] #Set the base value for for loop
for i in nr_1: #Repeat the for loop
    atoms1=list(residue[i].get_atoms()) #Extract the atom list of each residue
    bb=atoms1[0].get_bfactor() #All pLDDT value is same in on residue, just use the
    Y1.append(bb) #Add pLDDT to y-value list
    N1=N1+1 #Create x-value which means residue number
    X1.append(N1) #Add residue numer to x-value list
```

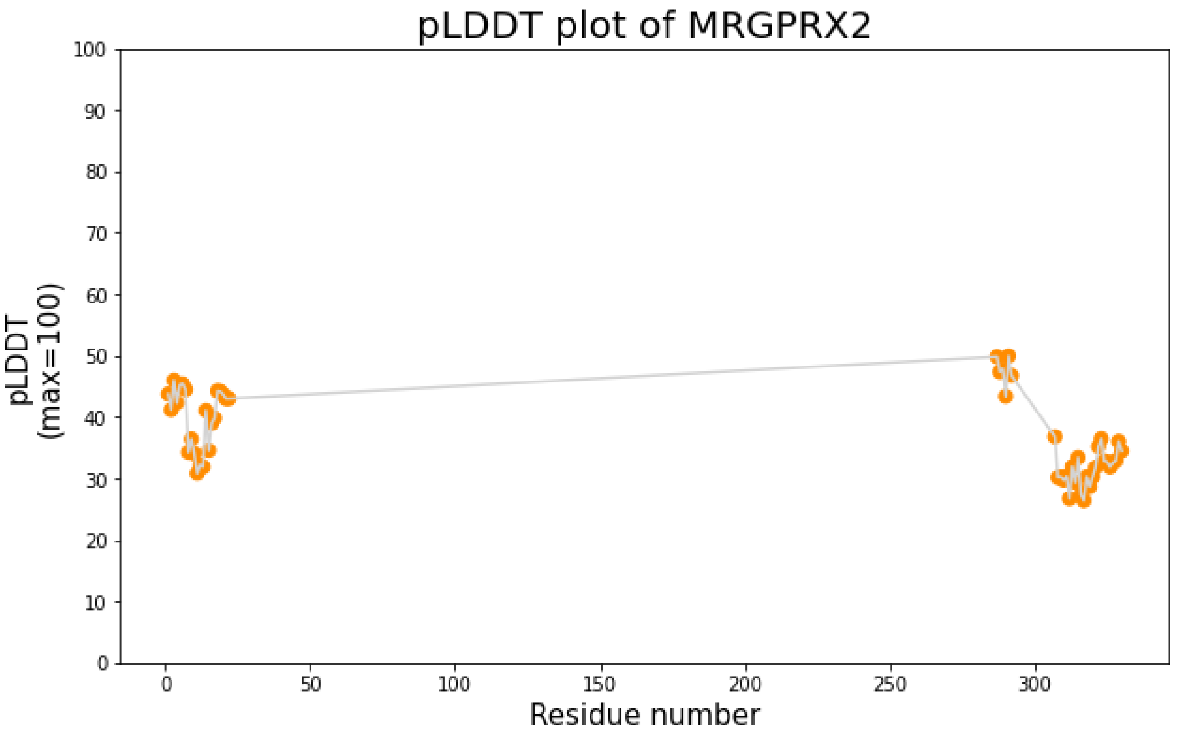
In [35]:
```
#Draw the plot
import matplotlib.pyplot as plt #Bring the matplotlib to draw the plot
import matplotlib as mpl
ids=str(protein) #Make the string of protein name
pn=ids[14:-1] #Extract the name
```

```
#plot
fig, ax = plt.subplots(figsize=(10, 6)) #Set the size of figure
cmaps = mpl.colors.ListedColormap(['darkorange','gold','deepskyblue','b']) #Set the
bounds = [0,50,70,90,100] #Set the bound for colormap
norms = mpl.colors.BoundaryNorm(bounds,cmaps.N) #Set the norm for colormap
ax.plot(X1,Y1,color='lightgrey') #Set the color of line plot
ax.scatter(X1,Y1,s=50,c=Y1,cmap=cmaps,norm=norms) #Draw the scatter plot and set the
ax.set_title("pLDDT plot of "+pn, fontsize=20) #Set the title and fontsize
ax.set_xlabel("Residue number",fontsize=15) #Set the x label and fontsize
ax.set_ylabel("pLDDT₩n(max=100)",fontsize=15) #Set the y label and fontsize, remeber
plt.yticks(range(0, 109,10)) #Custom the y sticks
plt.show() #Show the plot
```



In [36]:
```
##Extract the residue number, pLDDT<50
X2=[] #Create the empty list
Y2=[] #Create the empty list
nr_2=range(0,len(residue)) #Select the residue range, remember the len(residue)
cr_s2=0 ##Set the criteria of pLDDT
cr_e2=50 ##Set the criteria of pLDDT
for i in nr_2: #Repeat the for loop
    atoms1=list(residue[i].get_atoms()) #Extract the atom list of each residue
    bb=atoms1[0].get_bfactor() #All pLDDT value is same in on residue, just use the
    if bb >= cr_s2 and bb < cr_e2:
        Y2.append(bb) #Add pLDDT to y-value list
        N2=i+1 #Create x-value which means residue number
        X2.append(N2) #Add residue numer to x-value list
```

In [37]:
```
#Draw the plot
import matplotlib.pyplot as plt #Bring the matplotlib to draw the plot
import matplotlib as mpl
ids=str(protein) #Make the string of protein name
pn=ids[14:-1] #Extract the name

#plot
fig, ax = plt.subplots(figsize=(10, 6)) #Set the size of figure
cmaps = mpl.colors.ListedColormap(['darkorange','gold','deepskyblue','b']) #Set the
bounds = [0,50,70,90,100] #Set the bound for colormap
norms = mpl.colors.BoundaryNorm(bounds,cmaps.N) #Set the norm for colormap
ax.plot(X2,Y2,color='lightgrey') #Set the color of line plot
ax.scatter(X2,Y2,s=50,c=Y2,cmap=cmaps,norm=norms) #Draw the scatter plot and set the
ax.set_title("pLDDT plot of "+pn, fontsize=20) #Set the title and fontsize
ax.set_xlabel("Residue number",fontsize=15) #Set the x label and fontsize
ax.set_ylabel("pLDDT₩n(max=100)",fontsize=15) #Set the y label and fontsize, remeber
plt.yticks(range(0, 109,10)) #Custom the y sticks
plt.show() #Show the plot

#View the residue number
print('0<pLDDT<50')
print('Total:',len(X2))
print(X2)
```



```
0<pLDDT<50
Total: 52
[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 287,
288, 289, 290, 291, 292, 307, 308, 309, 310, 311, 312, 313, 314, 315, 316, 317, 318,
319, 320, 321, 322, 323, 324, 325, 326, 327, 328, 329, 330]
```

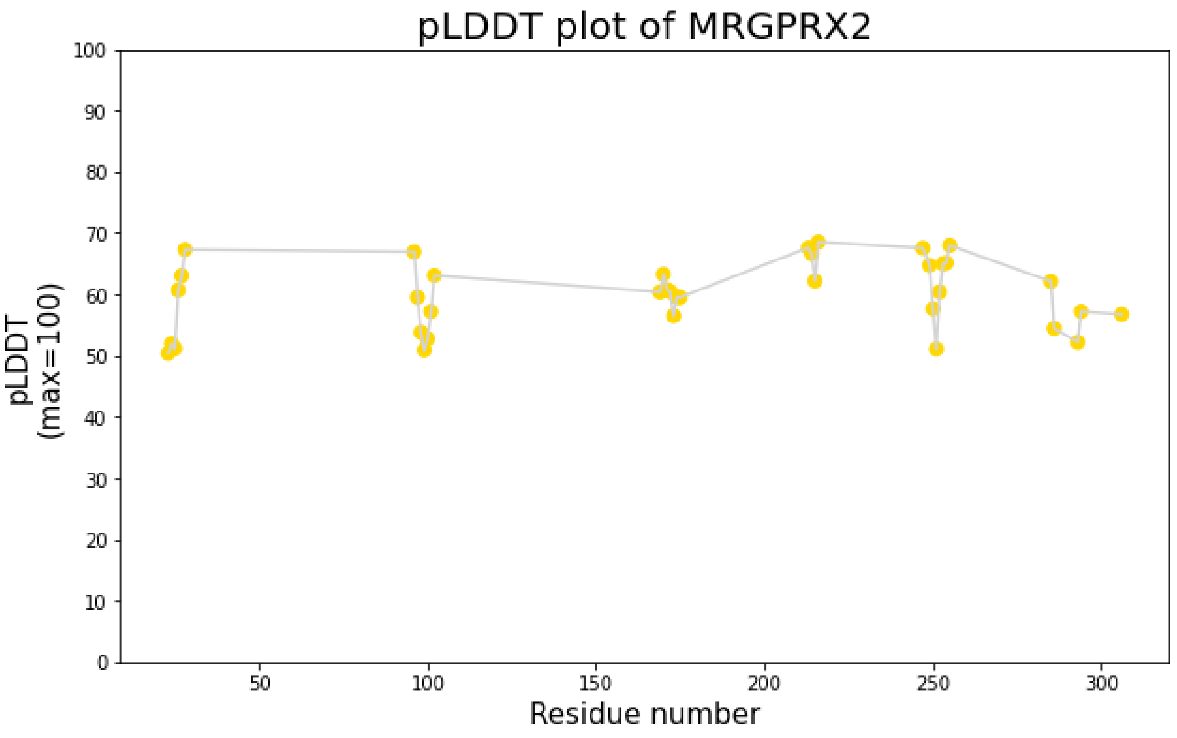
In [38]:

```
##Extract the residue number, 50<pLDDT<70
X3=[] #Create the empty list
Y3=[] #Create the empty list
nr_3=range(0,len(residue)) #Select the residue range, remember the len(residue)
cr_s3=50 ##Set the criteria of pLDDT
cr_e3=70 ##Set the criteria of pLDDT
for i in nr_3: #Repeat the for loop
    atoms1=list(residue[i].get_atoms()) #Extract the atom list of each residue
    bb=atoms1[0].get_bfactor() #All pLDDT value is same in on residue, just use the
    if bb >= cr_s3 and bb < cr_e3:
        Y3.append(bb) #Add pLDDT to y-value list
        N2=i+1 #Create x-value which means residue number
        X3.append(N2) #Add residue numer to x-value list
```

In [39]:

```
#Draw the plot
import matplotlib.pyplot as plt #Bring the matplotlib to draw the plot
import matplotlib as mpl
ids=str(protein) #Make the string of protein name
pn=ids[14:-1] #Extract the name

#plot
fig, ax = plt.subplots(figsize=(10, 6)) #Set the size of figure
cmaps = mpl.colors.ListedColormap(['darkorange','gold','deepskyblue','b']) #Set the
```

```
bounds = [0,50,70,90,100] #Set the bound for colormap
norms = mpl.colors.BoundaryNorm(bounds,cmaps.N) #Set the norm for colormap
ax.plot(X3,Y3,color='lightgrey') #Set the color of line plot
ax.scatter(X3,Y3,s=50,c=Y3,cmap=cmaps,norm=norms) #Draw the scatter plot and set the
ax.set_title("pLDDT plot of "+pn, fontsize=20) #Set the title and fontsize
ax.set_xlabel("Residue number",fontsize=15) #Set the x label and fontsize
ax.set_ylabel("pLDDT₩n(max=100)",fontsize=15) #Set the y label and fontsize, remeber
plt.yticks(range(0, 109,10)) #Custom the y sticks
plt.show() #Show the plot

#View the residue number
print('50<pLDDT<70')
print('Total:',len(X3))
print(X3)
```



```
50<pLDDT<70
Total: 37
[23, 24, 25, 26, 27, 28, 96, 97, 98, 99, 100, 101, 102, 169, 170, 171, 172, 173, 17
4, 175, 213, 214, 215, 216, 247, 249, 250, 251, 252, 253, 254, 255, 285, 286, 293, 2
94, 306]
```

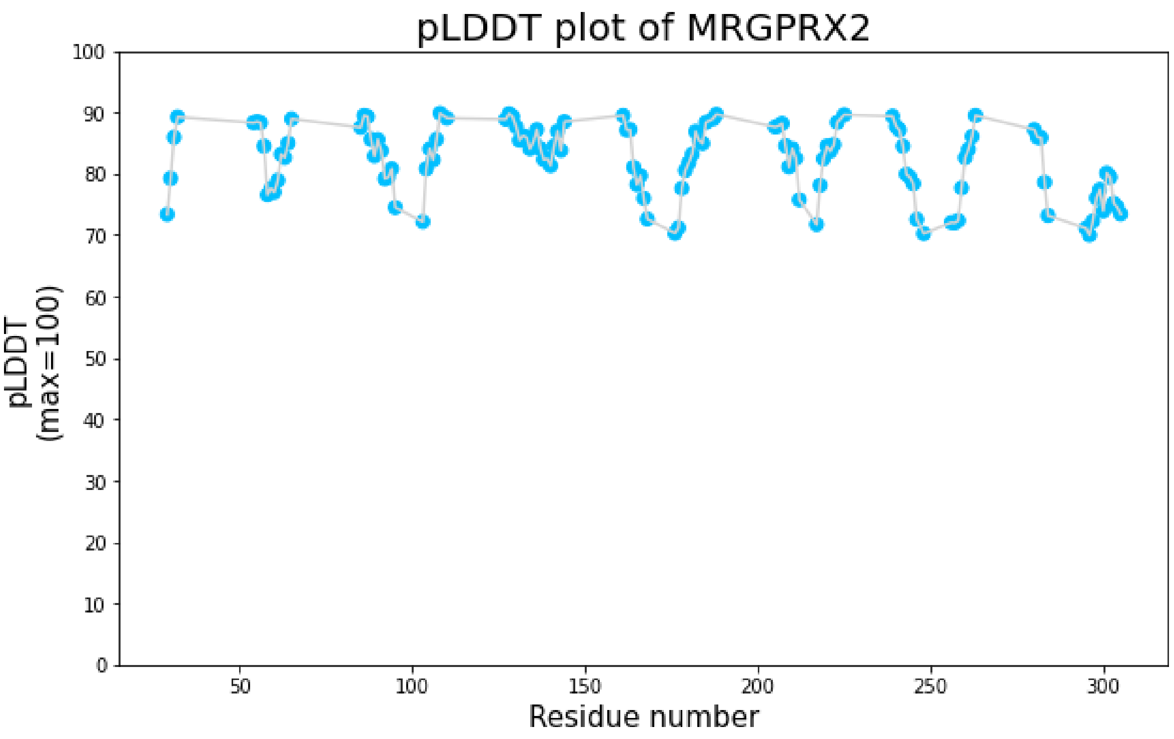
In [40]:

```
##Extract the residue number, 70<pLDDT<90
X4=[] #Create the empty list
Y4=[] #Create the empty list
nr_4=range(0,len(residue)) #Select the residue range, remember the len(residue)
cr_s4=70 ##Set the criteria of pLDDT
cr_e4=90 ##Set the criteria of pLDDT
for i in nr_4: #Repeat the for loop
    atoms1=list(residue[i].get_atoms()) #Extract the atom list of each residue
    bb=atoms1[0].get_bfactor() #All pLDDT value is same in on residue, just use the
    if bb >= cr_s4 and bb < cr_e4:
        Y4.append(bb) #Add pLDDT to y-value list
        N2=i+1 #Create x-value which means residue number
        X4.append(N2) #Add residue numer to x-value list
```

In [41]:

```
#Draw the plot
import matplotlib.pyplot as plt #Bring the matplotlib to draw the plot
import matplotlib as mpl
ids=str(protein) #Make the string of protein name
pn=ids[14:-1] #Extract the name
```

```
#plot
fig, ax = plt.subplots(figsize=(10, 6)) #Set the size of figure
cmaps = mpl.colors.ListedColormap(['darkorange','gold','deepskyblue','b']) #Set the
bounds = [0,50,70,90,100] #Set the bound for colormap
norms = mpl.colors.BoundaryNorm(bounds,cmaps.N) #Set the norm for colormap
ax.plot(X4,Y4,color='lightgrey') #Set the color of line plot
ax.scatter(X4,Y4,s=50,c=Y4,cmap=cmaps,norm=norms) #Draw the scatter plot and set the
ax.set_title("pLDDT plot of "+pn, fontsize=20) #Set the title and fontsize
ax.set_xlabel("Residue number",fontsize=15) #Set the x label and fontsize
ax.set_ylabel("pLDDT₩n(max=100)",fontsize=15) #Set the y label and fontsize, remeber
plt.yticks(range(0, 109,10)) #Custom the y sticks
plt.show() #Show the plot

#View the residue number
print('70<pLDDT<90')
print('Total:',len(X4))
print(X4)
```

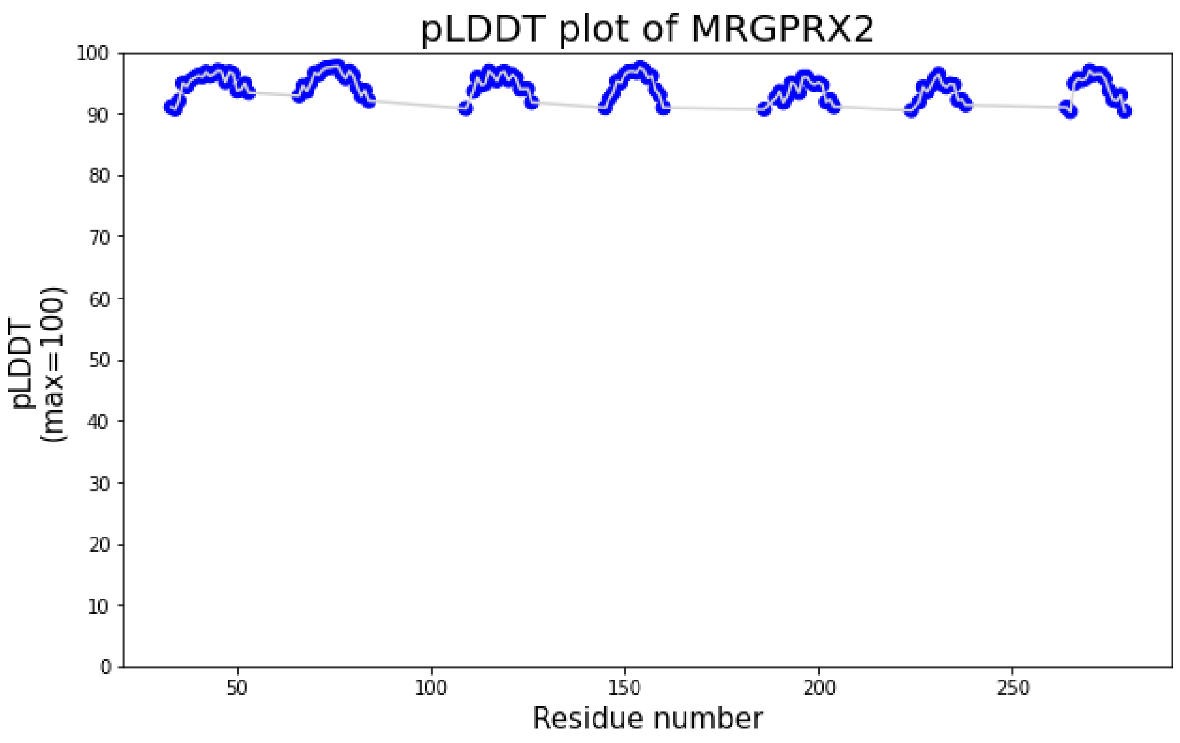


```
70<pLDDT<90
Total: 121
[29, 30, 31, 32, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 85, 86, 87, 88, 89,
90, 91, 92, 93, 94, 95, 103, 104, 105, 106, 107, 108, 110, 127, 128, 129, 130, 131,
132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 161, 162, 163, 164,
165, 166, 167, 168, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 187, 188, 205,
206, 207, 208, 209, 210, 211, 212, 217, 218, 219, 220, 221, 222, 223, 225, 239, 240,
241, 242, 243, 244, 245, 246, 248, 256, 257, 258, 259, 260, 261, 262, 263, 280, 281,
282, 283, 284, 295, 296, 297, 298, 299, 300, 301, 302, 303, 304, 305]
```

In [42]:

```
##Extract the residue number, 90<pLDDT<100
X5=[] #Create the empty list
Y5=[] #Create the empty list
nr_5=range(0,len(residue)) #Select the residue range, remember the len(residue)
cr_s5=90 ##Set the criteria of pLDDT
cr_e5=100 ##Set the criteria of pLDDT
for i in nr_5: #Repeat the for loop
    atoms1=list(residue[i].get_atoms()) #Extract the atom list of each residue
    bb=atoms1[0].get_bfactor() #All pLDDT value is same in on residue, just use the
    if bb >= cr_s5 and bb < cr_e5:
        Y5.append(bb) #Add pLDDT to y-value list
        N2=i+1 #Create x-value which means residue number
        X5.append(N2) #Add residue numer to x-value list
```

In [43]:
```
#Draw the plot
import matplotlib.pyplot as plt #Bring the matplotlib to draw the plot
import matplotlib as mpl
ids=str(protein) #Make the string of protein name
pn=ids[14:-1] #Extract the name

#plot
fig, ax = plt.subplots(figsize=(10, 6)) #Set the size of figure
cmaps = mpl.colors.ListedColormap(['darkorange','gold','deepskyblue','b']) #Set the
bounds = [0,50,70,90,100] #Set the bound for colormap
norms = mpl.colors.BoundaryNorm(bounds,cmaps.N) #Set the norm for colormap
ax.plot(X5,Y5,color='lightgrey') #Set the color of line plot
ax.scatter(X5,Y5,s=50,c=Y5,cmap=cmaps,norm=norms) #Draw the scatter plot and set the
ax.set_title("pLDDT plot of "+pn, fontsize=20) #Set the title and fontsize
ax.set_xlabel("Residue number",fontsize=15) #Set the x label and fontsize
ax.set_ylabel("pLDDT₩n(max=100)",fontsize=15) #Set the y label and fontsize, remeber
plt.yticks(range(0, 109,10)) #Custom the y sticks
plt.show() #Show the plot

#View the residue number
print('90<pLDDT<100')
print('Total:',len(X5))
print(X5)
```



```
90<pLDDT<100
Total: 120
[33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53,
66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 109, 11
1, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 145, 1
46, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 186, 189,
190, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204, 224, 226,
227, 228, 229, 230, 231, 232, 233, 234, 235, 236, 237, 238, 264, 265, 266, 267, 268,
269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279]
```