Assignment 3 - Clustering

November 29, 2024

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[1]:
```
# Import required Python libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt

from sklearn.cluster import KMeans
from sklearn.cluster import DBSCAN
```

[2]:
```
# Read the given CSV file
df = pd.read_csv('./data/data_assignment3.csv', delimiter=',')
```

[3]:
```
df.head()
```

[3]:

	residue name	position	chain	phi	psi
0	LYS	10	A	-149.312855	142.657714
1	PRO	11	A	-44.283210	136.002076
2	LYS	12	A	-119.972621	-168.705263
3	LEU	13	A	-135.317212	137.143523
4	LEU	14	A	-104.851467	95.928520

[4]:
```
print("The number of rows in the data frame is:", len(df))
```

```
The number of rows in the data frame is: 29369
```

[5]:
```
df = df.dropna()
```

[6]:
```
print("The number of rows in the data frame is:", len(df))
```

```
The number of rows in the data frame is: 29369
```

[7]:
```
df.describe()
```

[7]:

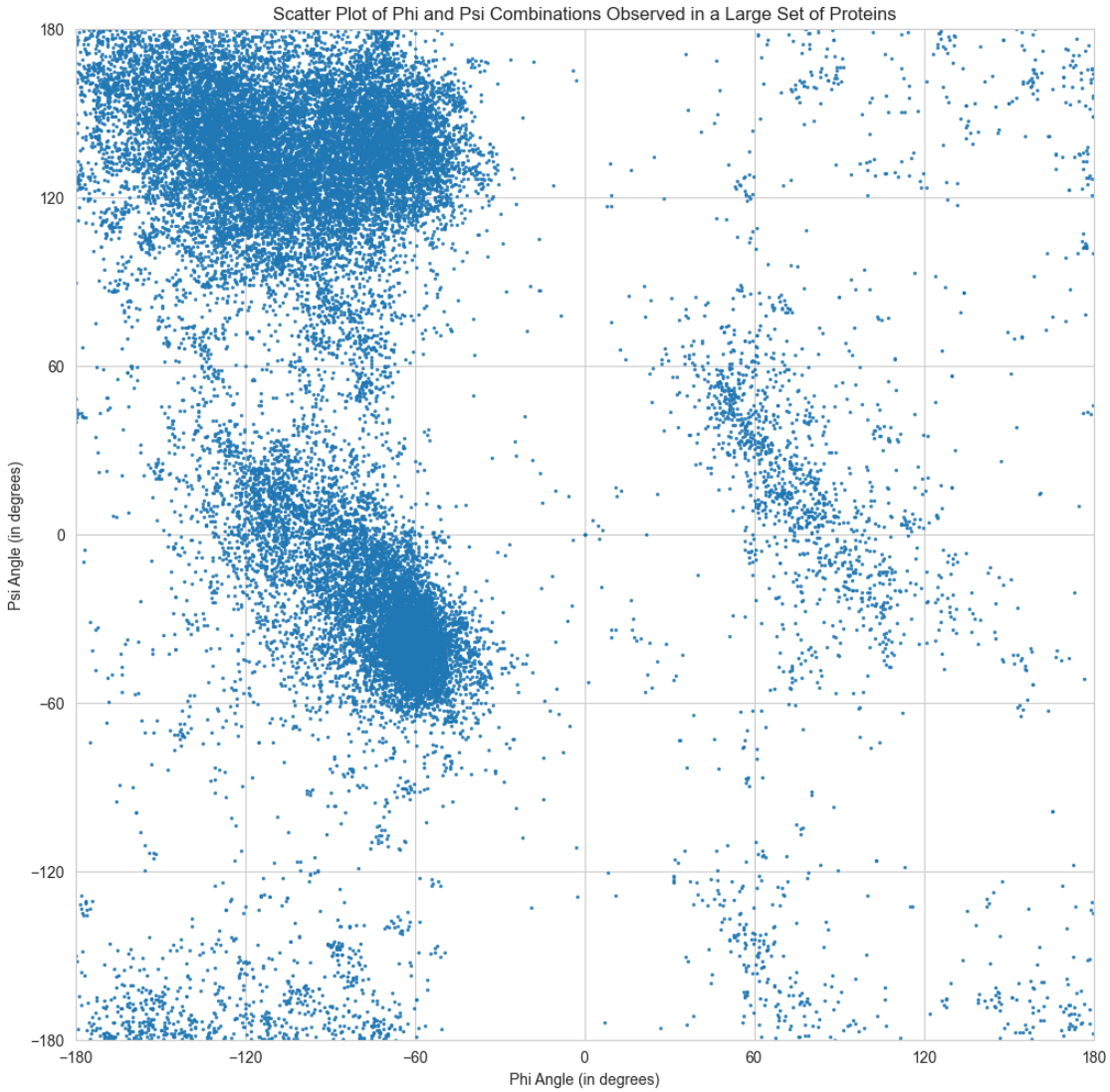
	position	phi	psi
count	29369.000000	29369.000000	29369.000000
mean	182.917634	-82.362440	64.251961
std	130.180669	56.848421	91.119597

```
min        1.000000   -179.991175   -179.995255
25%       84.000000   -118.089883    -24.299401
50%      151.000000    -85.198070    110.903019
75%      257.000000    -63.287290    141.154709
max      772.000000    179.973856    179.986259
```

1 Task 1: Show the distribution of phi and psi combinations using:

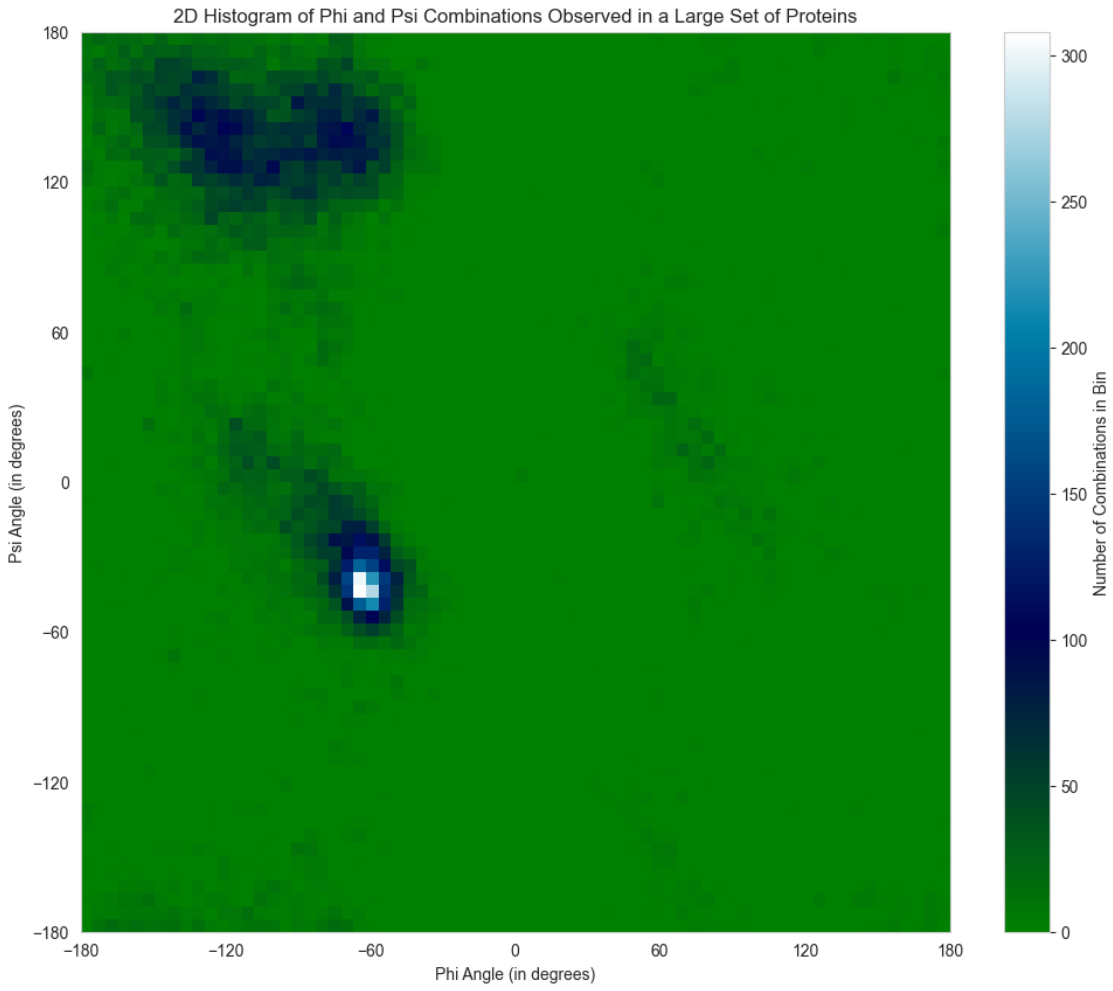
a. A scatter plot

[8]:
```
# Draw scatter plot of the data
plt.figure(figsize=(12, 12))
plt.scatter(df['phi'], df['psi'], s=2, alpha=0.8)
plt.xlim(-180, 180)
plt.ylim(-180, 180)
plt.xticks(range(-180, 181, 60))
plt.yticks(range(-180, 181, 60))
plt.xlabel('Phi Angle (in degrees)')
plt.ylabel('Psi Angle (in degrees)')

plt.title('Scatter Plot of Phi and Psi Combinations Observed in a Large Set of␣
 ↪Proteins')
plt.show()
```



b. A 2D histogram

[9]:
```
# Draw 2D histogram of the data
plt.figure(figsize=(12, 10))
plt.hist2d(df['phi'], df['psi'], bins=70, cmap='ocean')
plt.xticks(range(-180, 181, 60))
plt.yticks(range(-180, 181, 60))
plt.colorbar(label = "Number of Combinations in Bin")
plt.xlabel('Phi Angle (in degrees)')
plt.ylabel('Psi Angle (in degrees)')
plt.title('2D Histogram of Phi and Psi Combinations Observed in a Large Set of␣
 ↪Proteins')
plt.show()
```



2 Task 2: Use the K-means clustering method to cluster the phi and psi angle combinations in the data file.

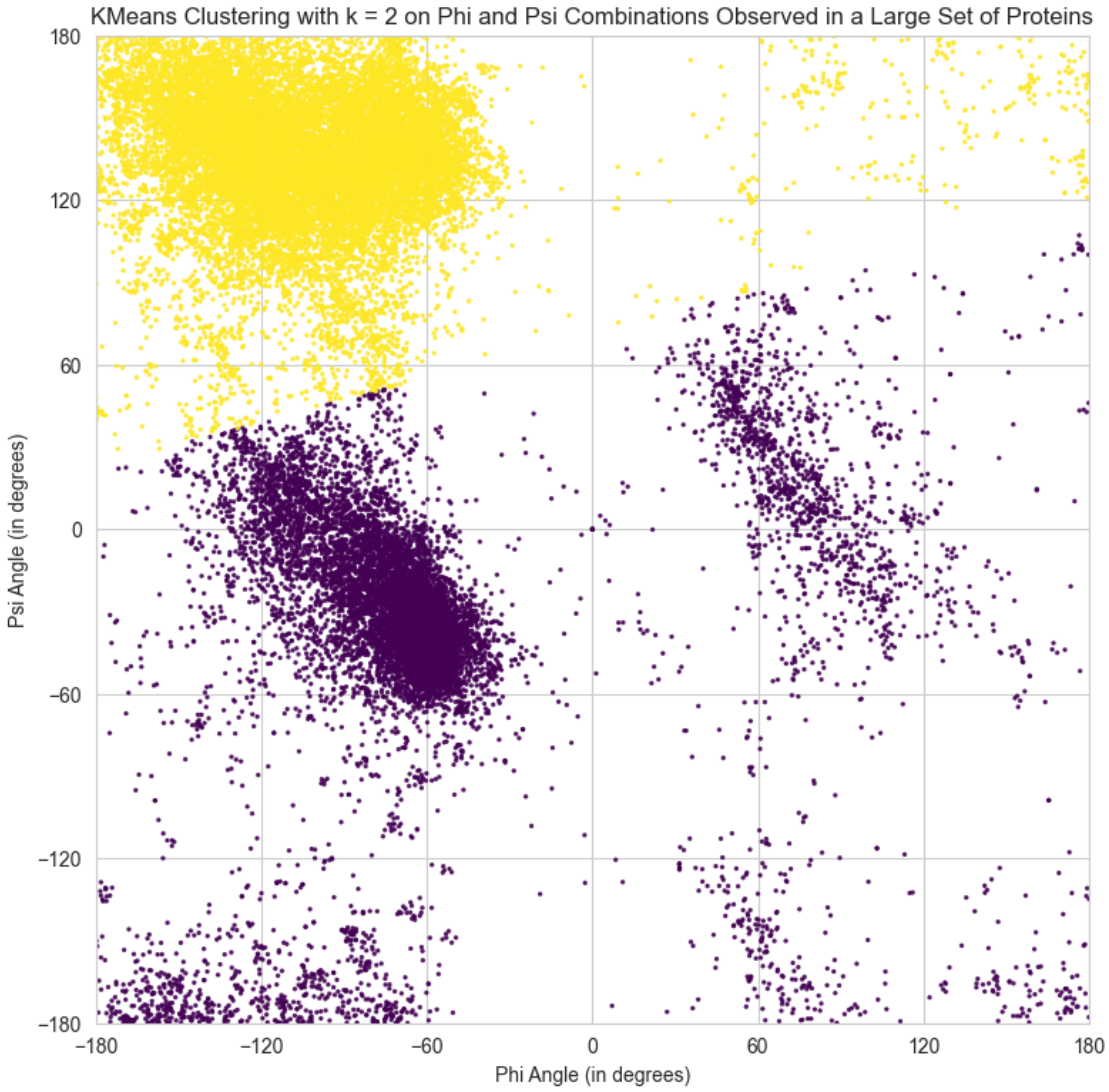
[10]:
```
X = df[['phi', 'psi']].copy()
```

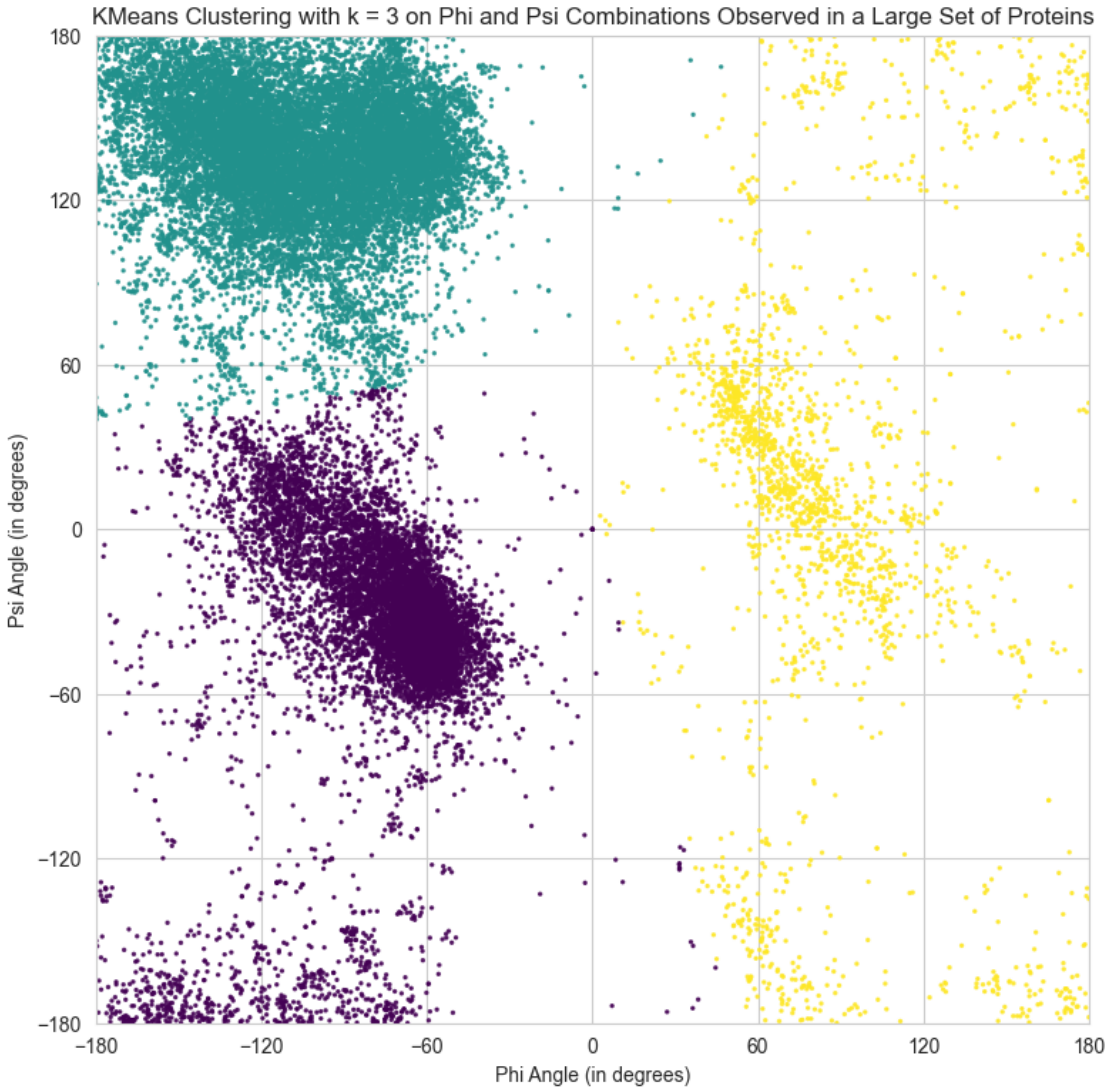
[11]:
```
# List that stores the sum of squared distances of samples to their closest␣
 ↪cluster center, weighted by the sample weights if given
inertia = []
```

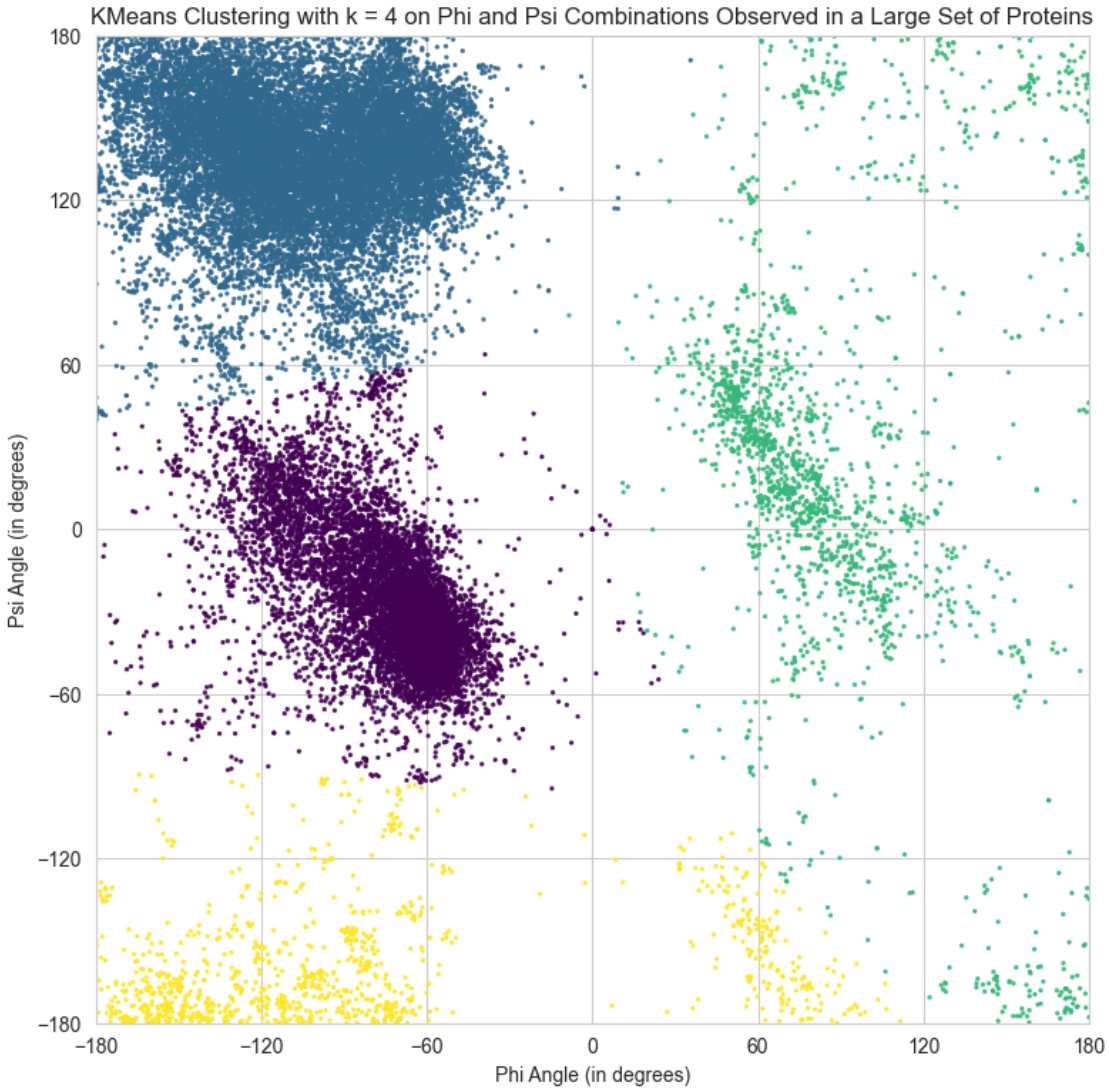
[12]:
```
def visualise_kmeans(k):
    kmeans = KMeans(n_clusters=k, n_init=10)
    kmeans.fit(X)
    y_kmeans = kmeans.predict(X)
    inertia.append(kmeans.inertia_)
```

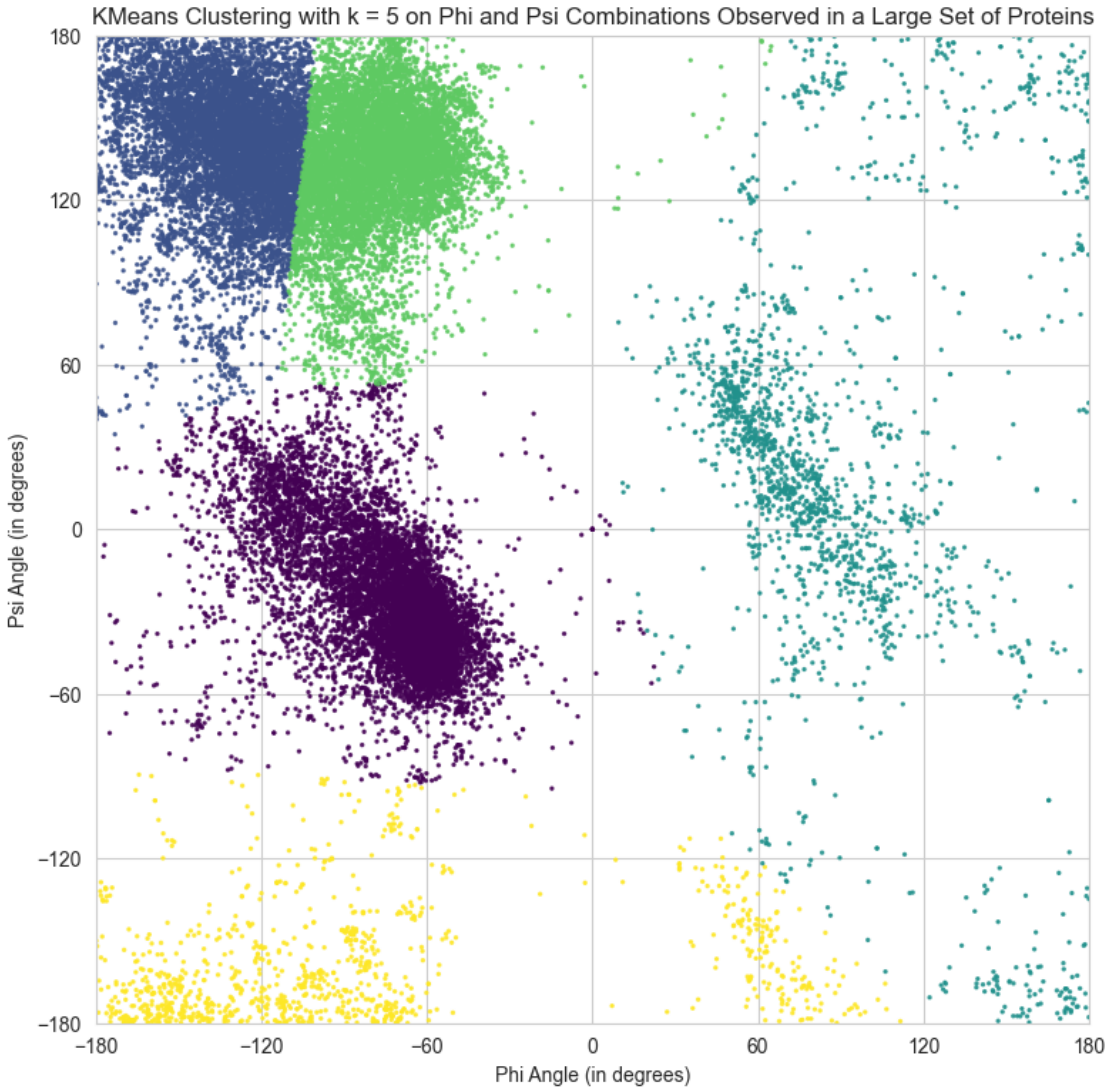
```
    plt.figure(figsize=(9, 9))
    plt.scatter(X['phi'], X['psi'], c=y_kmeans, s=2, alpha=0.8, cmap='viridis')
    plt.xlim(-180, 180)
    plt.ylim(-180, 180)
    plt.xticks(range(-180, 181, 60))
    plt.yticks(range(-180, 181, 60))
    plt.xlabel('Phi Angle (in degrees)')
    plt.ylabel('Psi Angle (in degrees)')

    plt.title(f'KMeans Clustering with k = {k} on Phi and Psi Combinations␣
 ↪Observed in a Large Set of Proteins')
    plt.show()
```

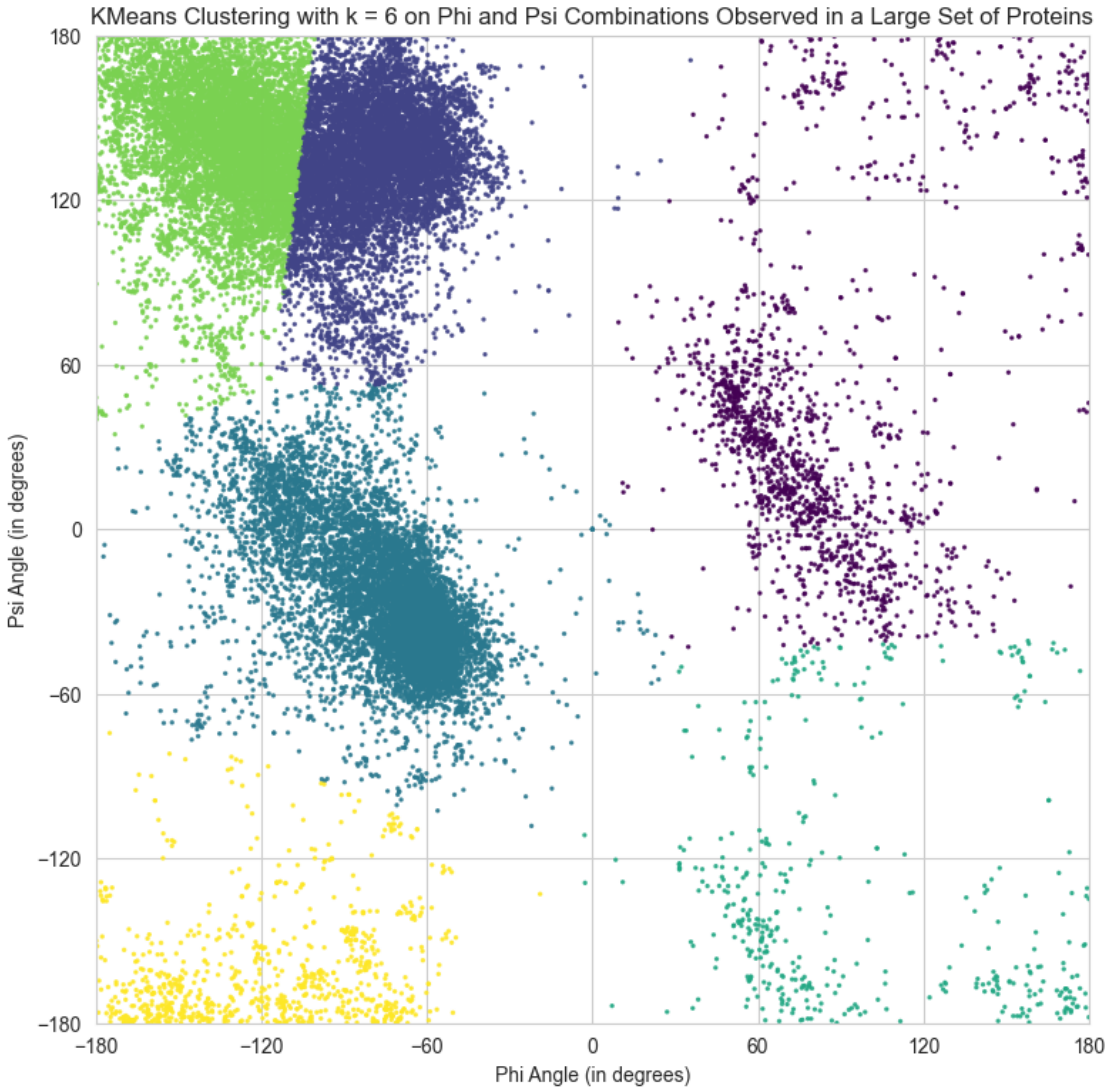
[13]:
```
for k in range(2, 11):
    visualise_kmeans(k)

plt.figure(figsize=(8, 8))
plt.plot(range(2, 11), inertia, marker='o')
plt.title('Elbow Method for KMeans Clustering on Phi and Psi Combinations␣
 ↪Observed in a Large Set of Proteins')
plt.xlabel('Number of Clusters (k)')
plt.ylabel('Inertia (WCSS)')
plt.show()
```

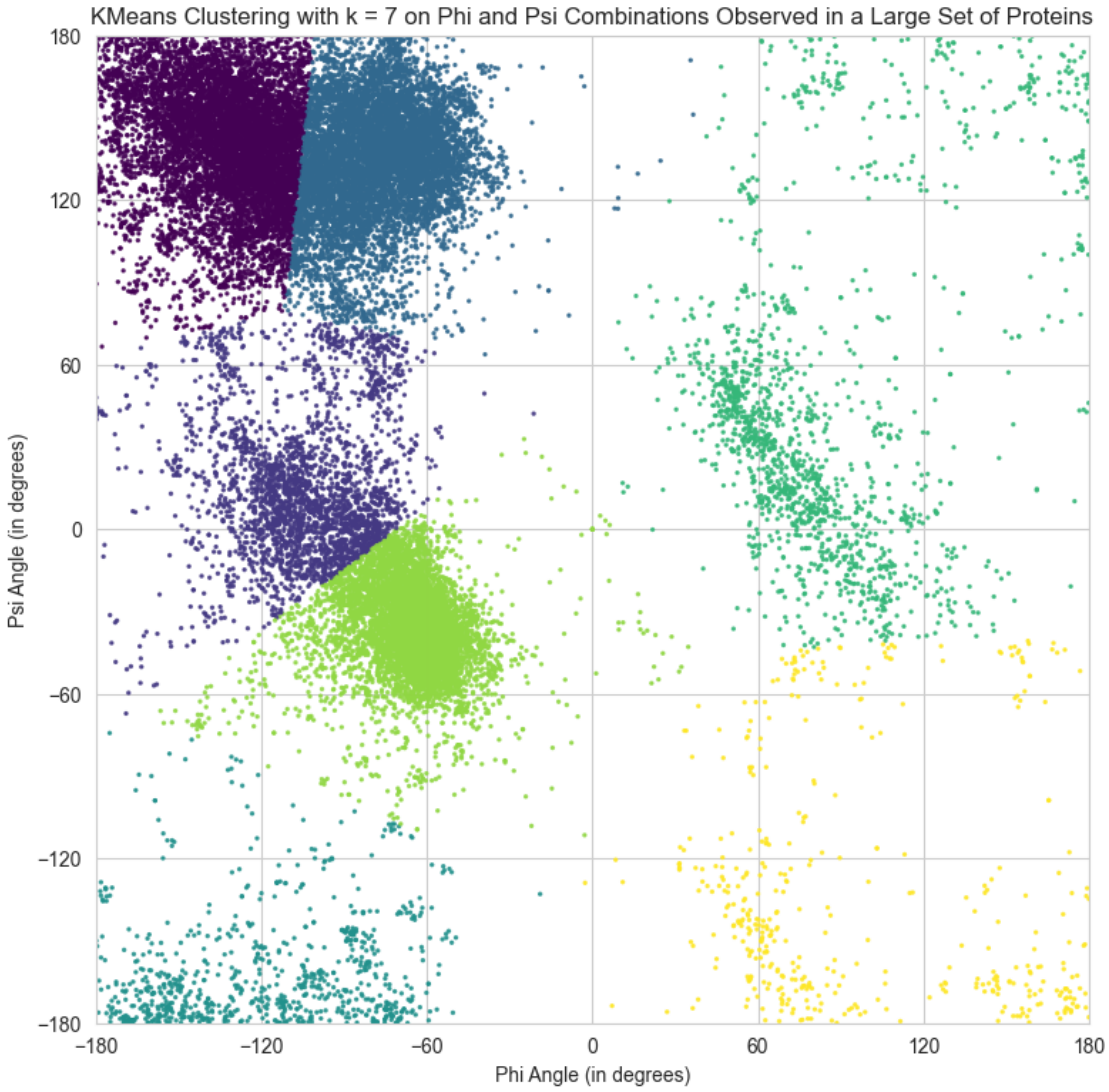

KMeans Clustering with k = 2 on Phi and Psi Combinations Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180

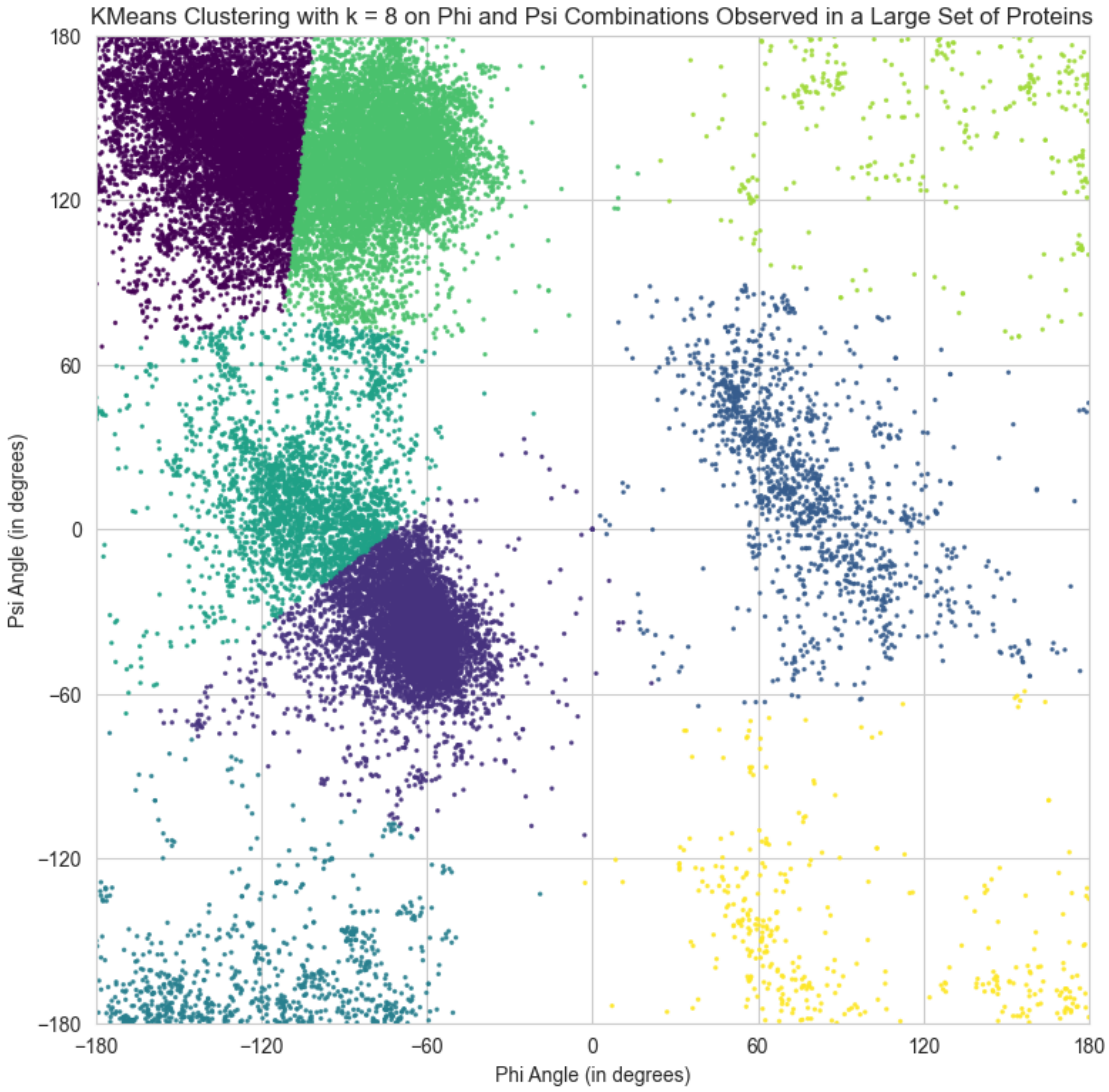

KMeans Clustering with k = 3 on Phi and Psi Combinations Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180

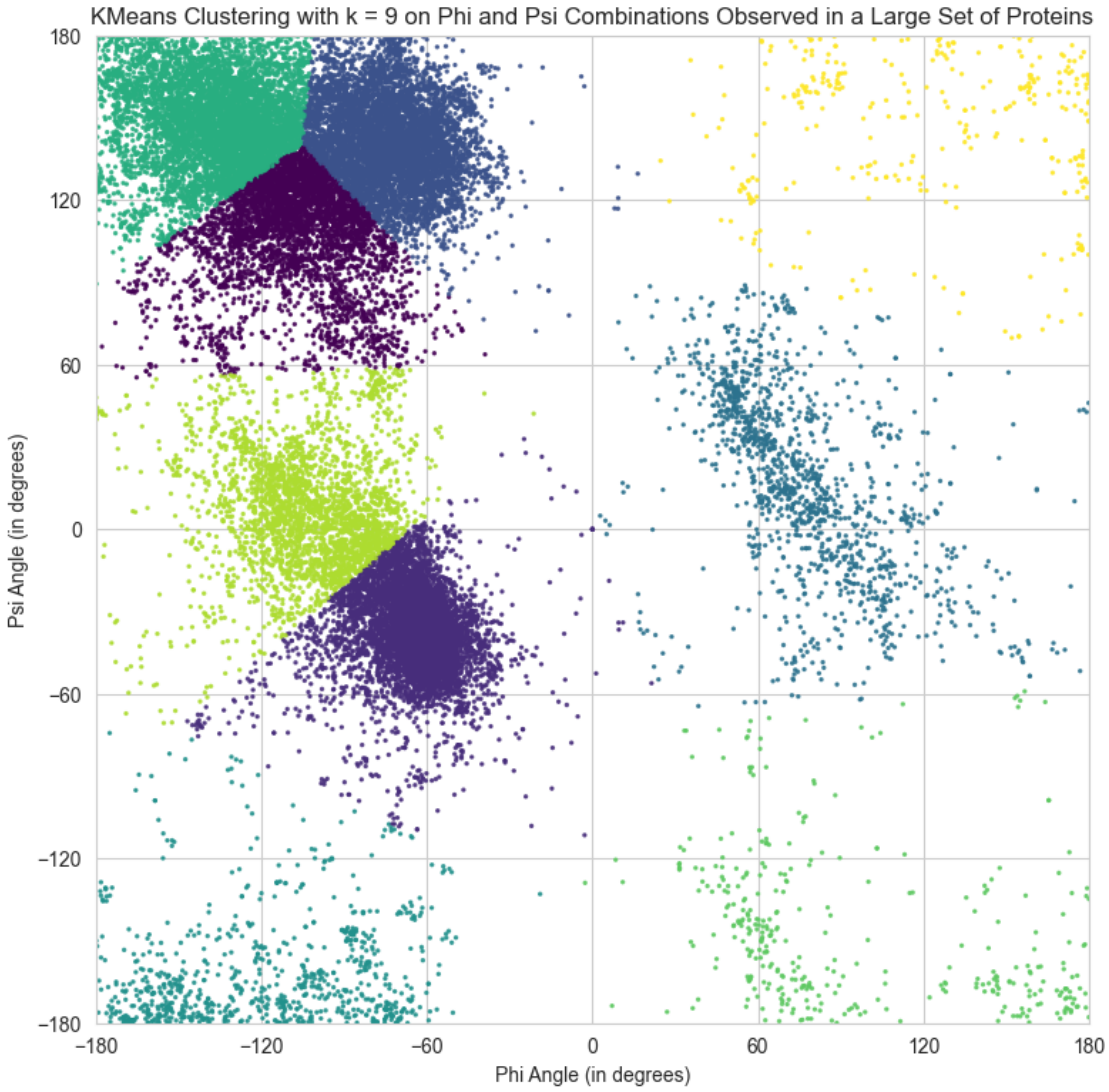

KMeans Clustering with k = 4 on Phi and Psi Combinations Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180

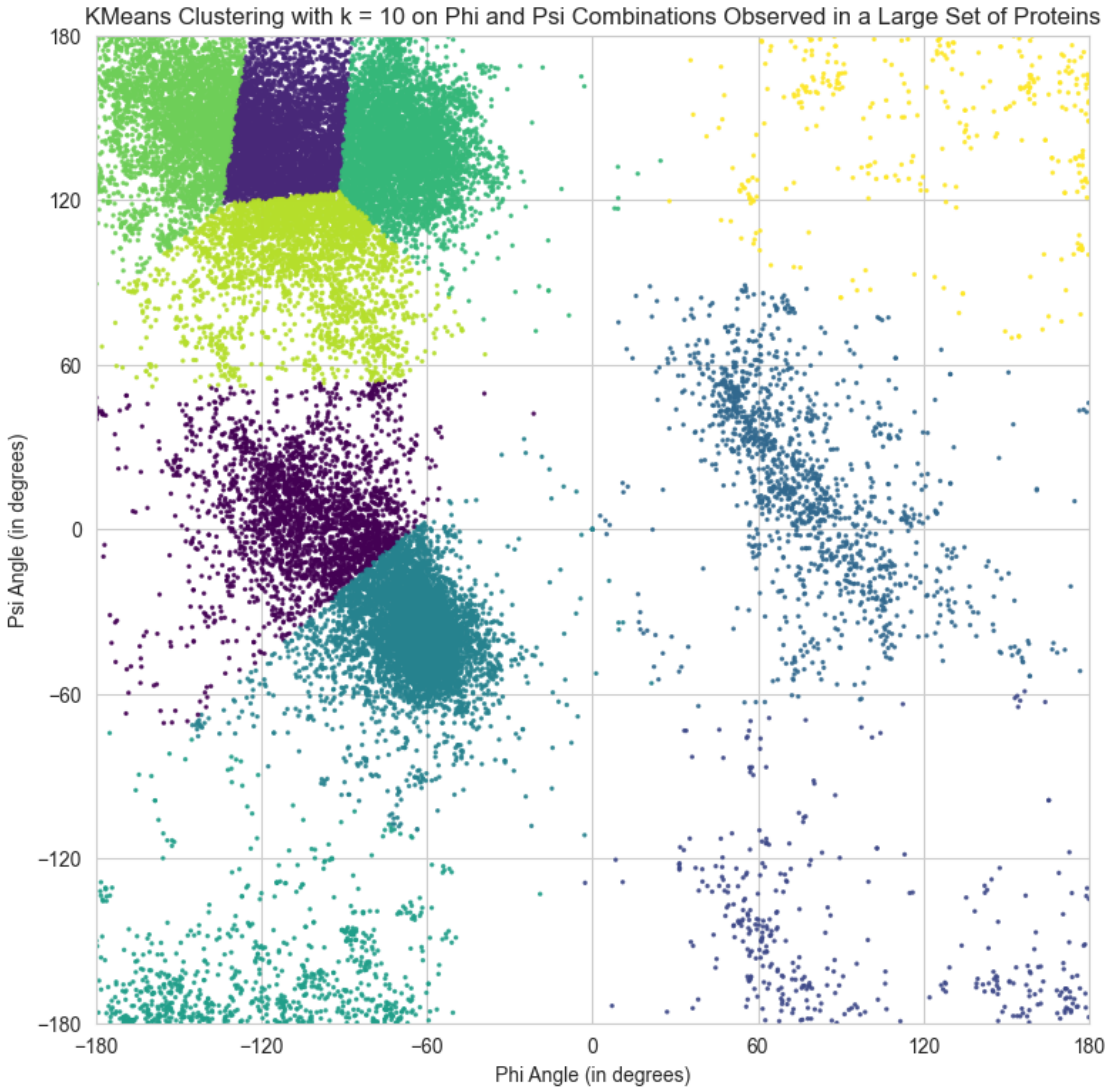

KMeans Clustering with k = 5 on Phi and Psi Combinations Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180

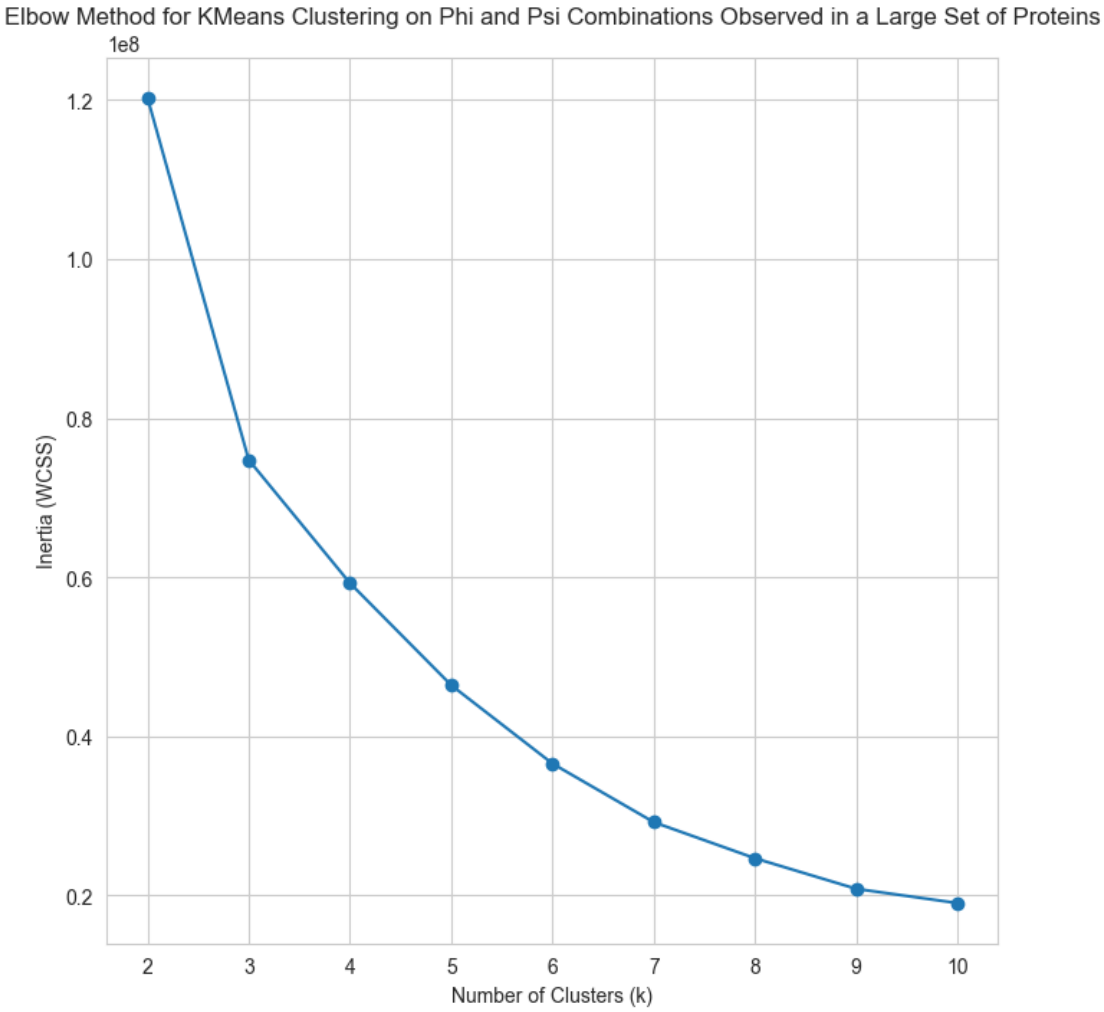

KMeans Clustering with k = 6 on Phi and Psi Combinations Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180


KMeans Clustering with k = 7 on Phi and Psi Combinations Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180


KMeans Clustering with k = 8 on Phi and Psi Combinations Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180


KMeans Clustering with k = 9 on Phi and Psi Combinations Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180


KMeans Clustering with k = 10 on Phi and Psi Combinations Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180

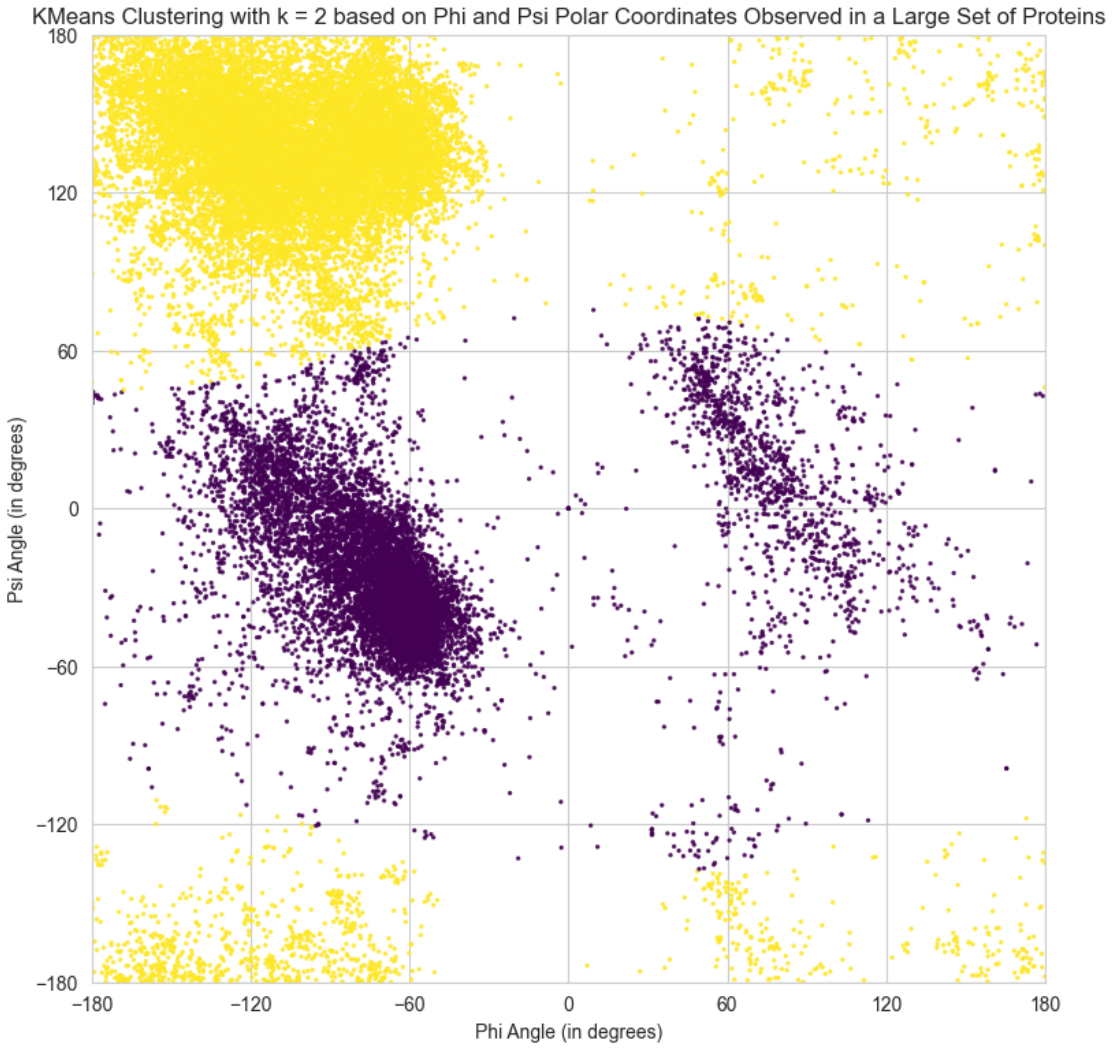


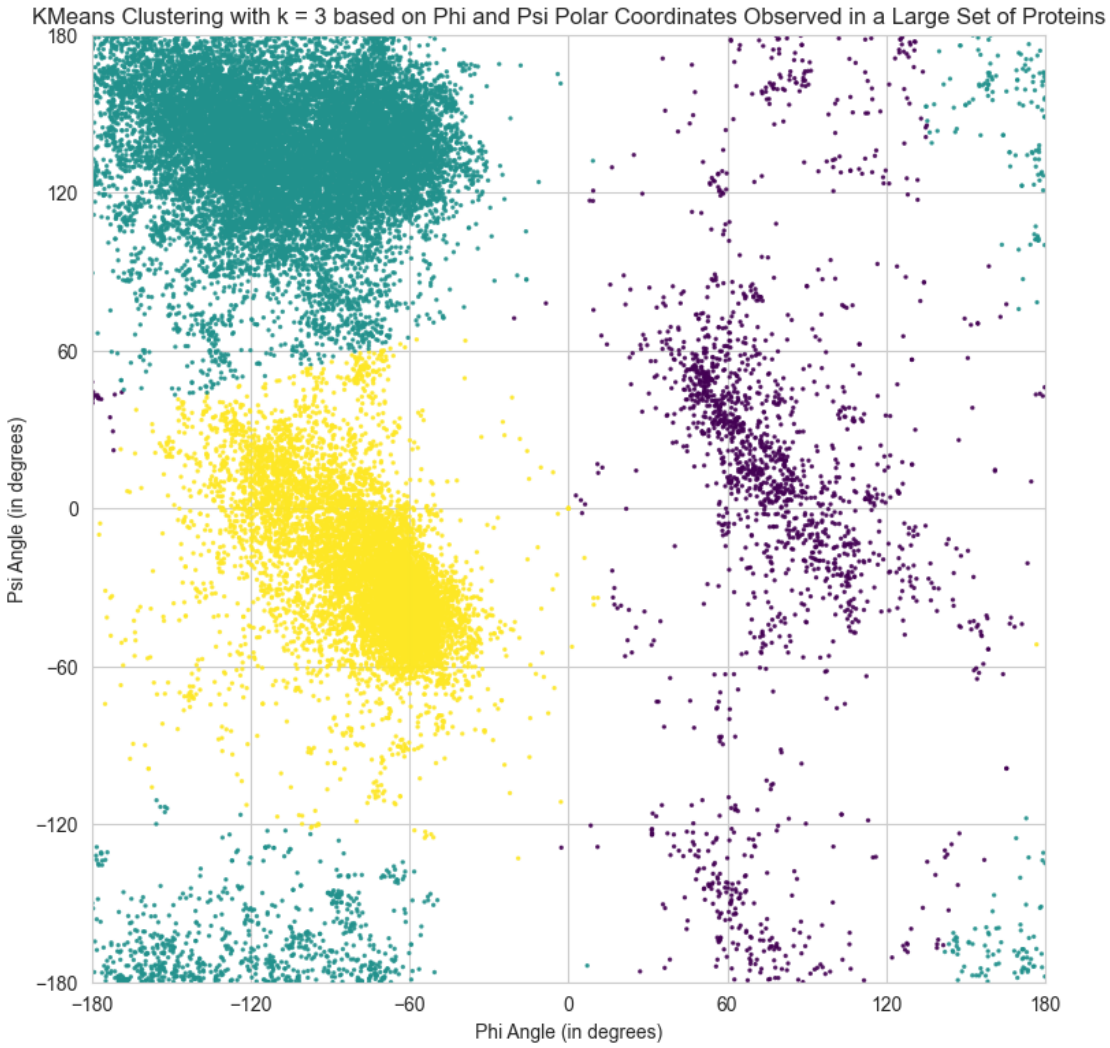
[14]:
```
# Transform to polar coordinates to tackle problem with periodicity
phi = df['phi'].values
psi = df['psi'].values

phi_cos = np.cos(np.radians(phi))
phi_sin = np.sin(np.radians(phi))
psi_cos = np.cos(np.radians(psi))
psi_sin = np.sin(np.radians(psi))

X_polar = np.column_stack((phi_cos, phi_sin, psi_cos, psi_sin))
inertia = []
```

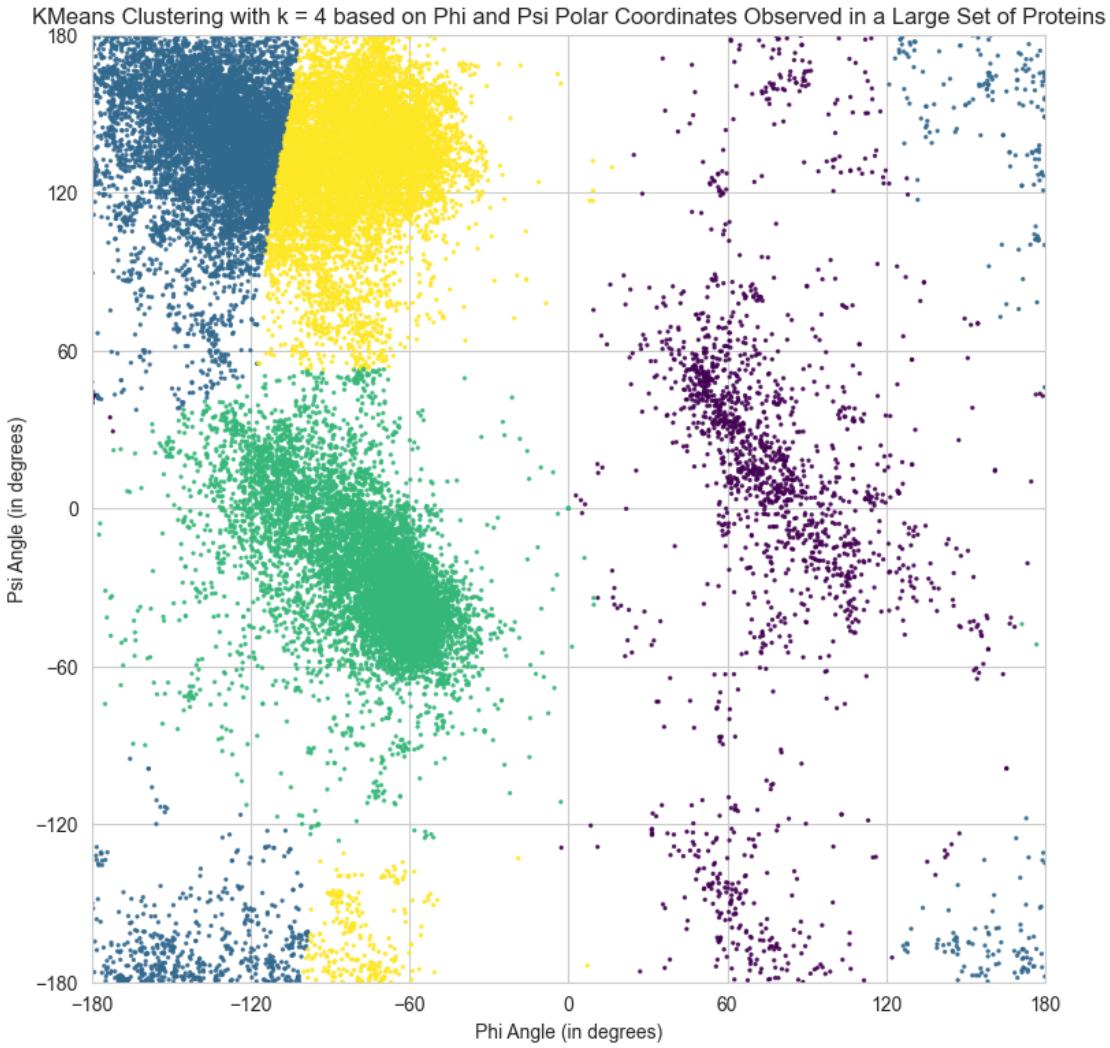
[15]:
```
def visualise_kmeans_polar(k):
    kmeans = KMeans(n_clusters=k, n_init=10, random_state=98)
    kmeans.fit(X_polar)
```

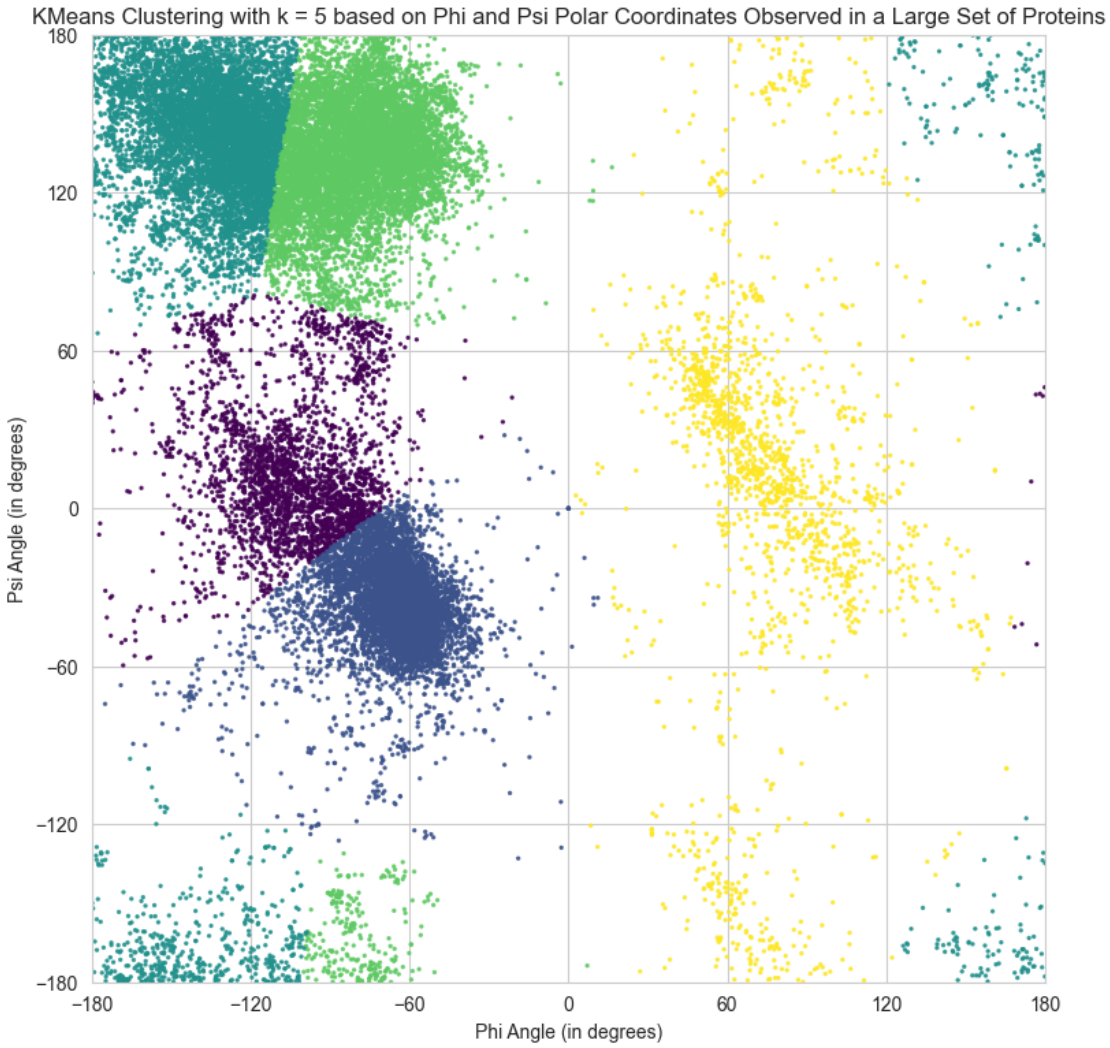
```
    y_kmeans = kmeans.predict(X_polar)
    inertia.append(kmeans.inertia_)

    plt.figure(figsize=(9, 9))
    plt.scatter(X['phi'], X['psi'], c=y_kmeans, s=2, alpha=0.8, cmap='viridis')
    plt.xlim(-180, 180)
    plt.ylim(-180, 180)
    plt.xticks(range(-180, 181, 60))
    plt.yticks(range(-180, 181, 60))
    plt.xlabel('Phi Angle (in degrees)')
    plt.ylabel('Psi Angle (in degrees)')

    plt.title(f'KMeans Clustering with k = {k} based on Phi and Psi Polar␣
 ↪Coordinates Observed in a Large Set of Proteins')
    plt.show()
```

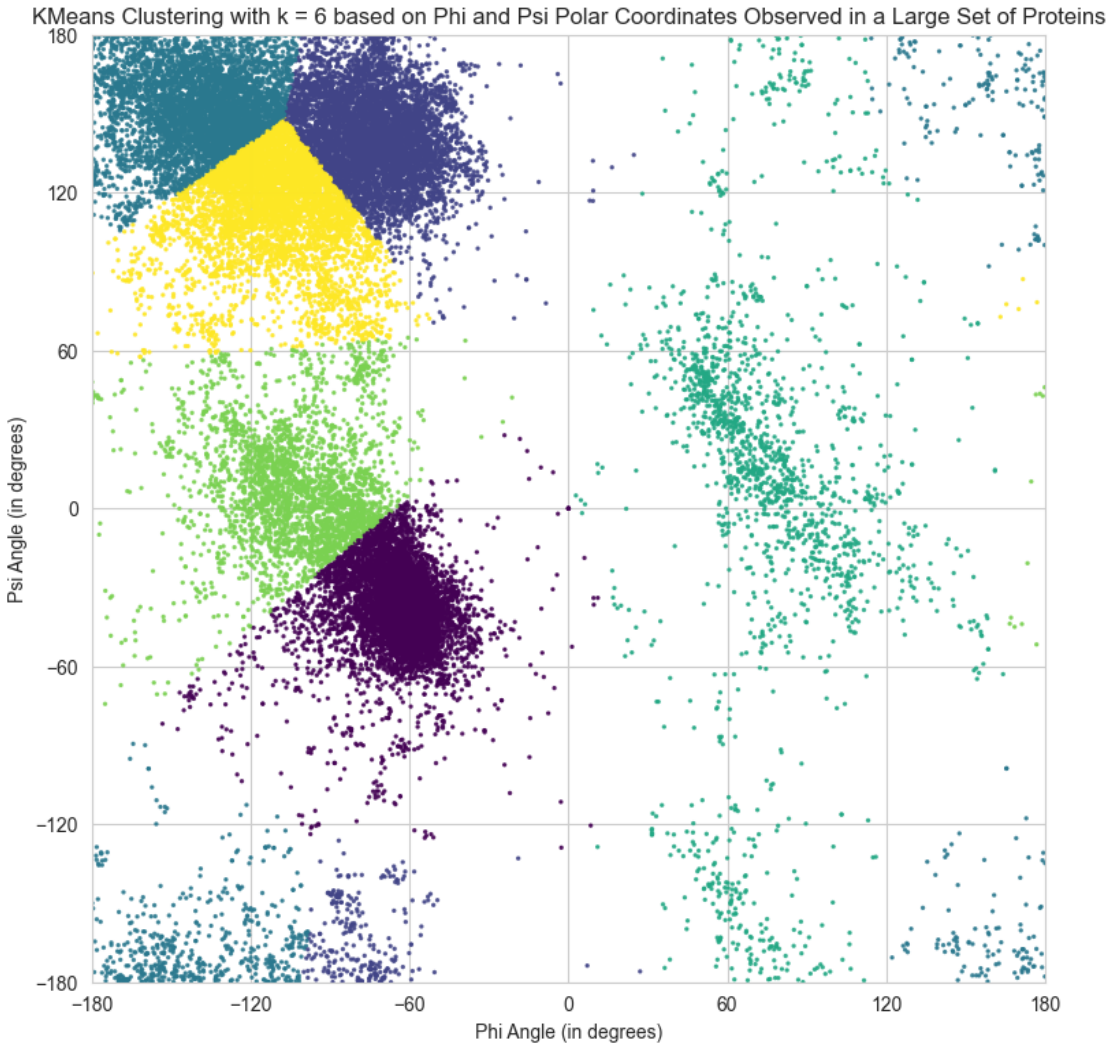
[16]:
```
for k in range(2, 11):
    visualise_kmeans_polar(k)

plt.figure(figsize=(8, 8))
plt.plot(range(2, 11), inertia, marker='o')
plt.title('Elbow Method for KMeans Clustering based on Phi and Psi Polar␣
 ↪Coordinates Observed in a Large Set of Proteins')
plt.xlabel('Number of Clusters (k)')
plt.ylabel('Inertia (WCSS)')
plt.show()
```

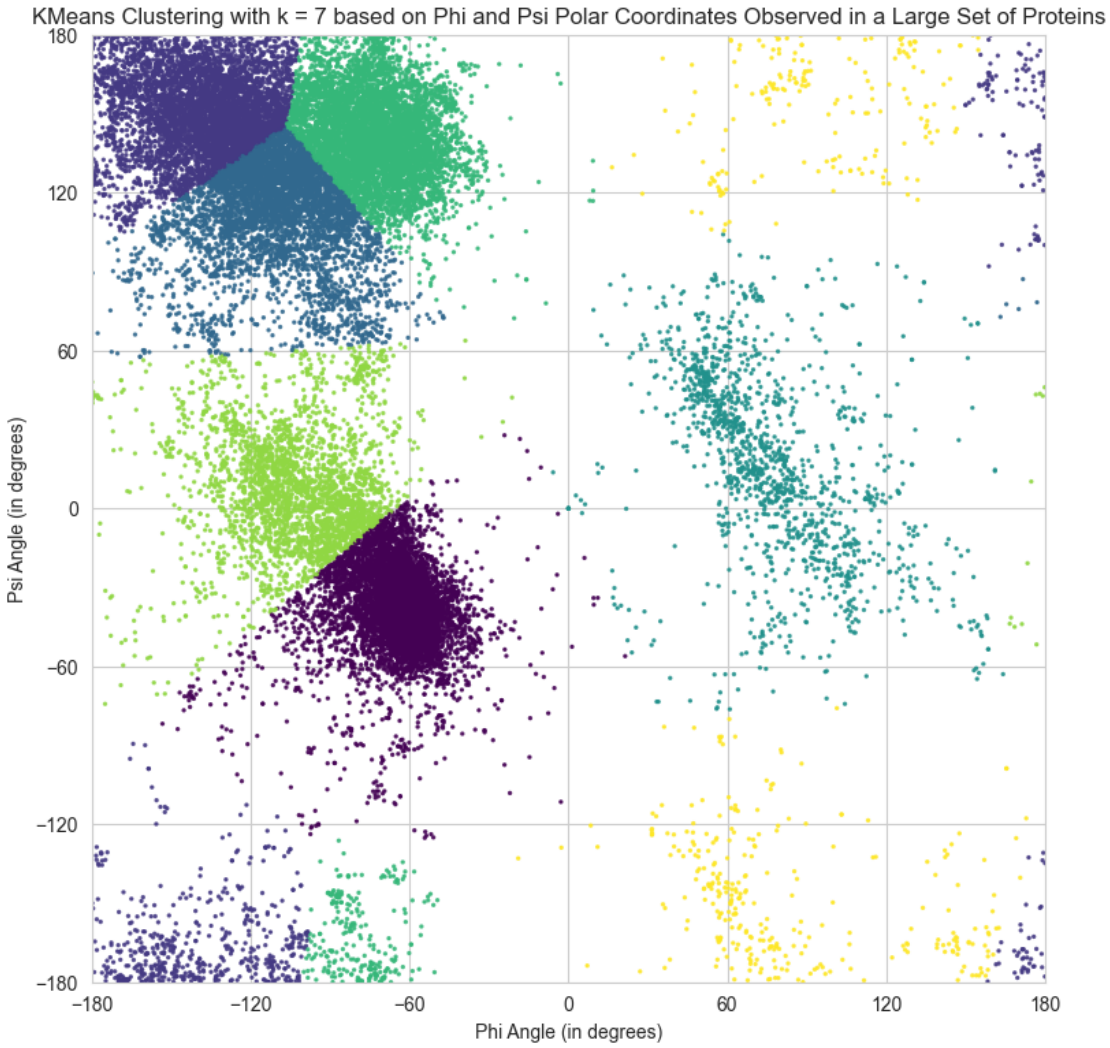

KMeans Clustering with k = 2 based on Phi and Psi Polar Coordinates Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180

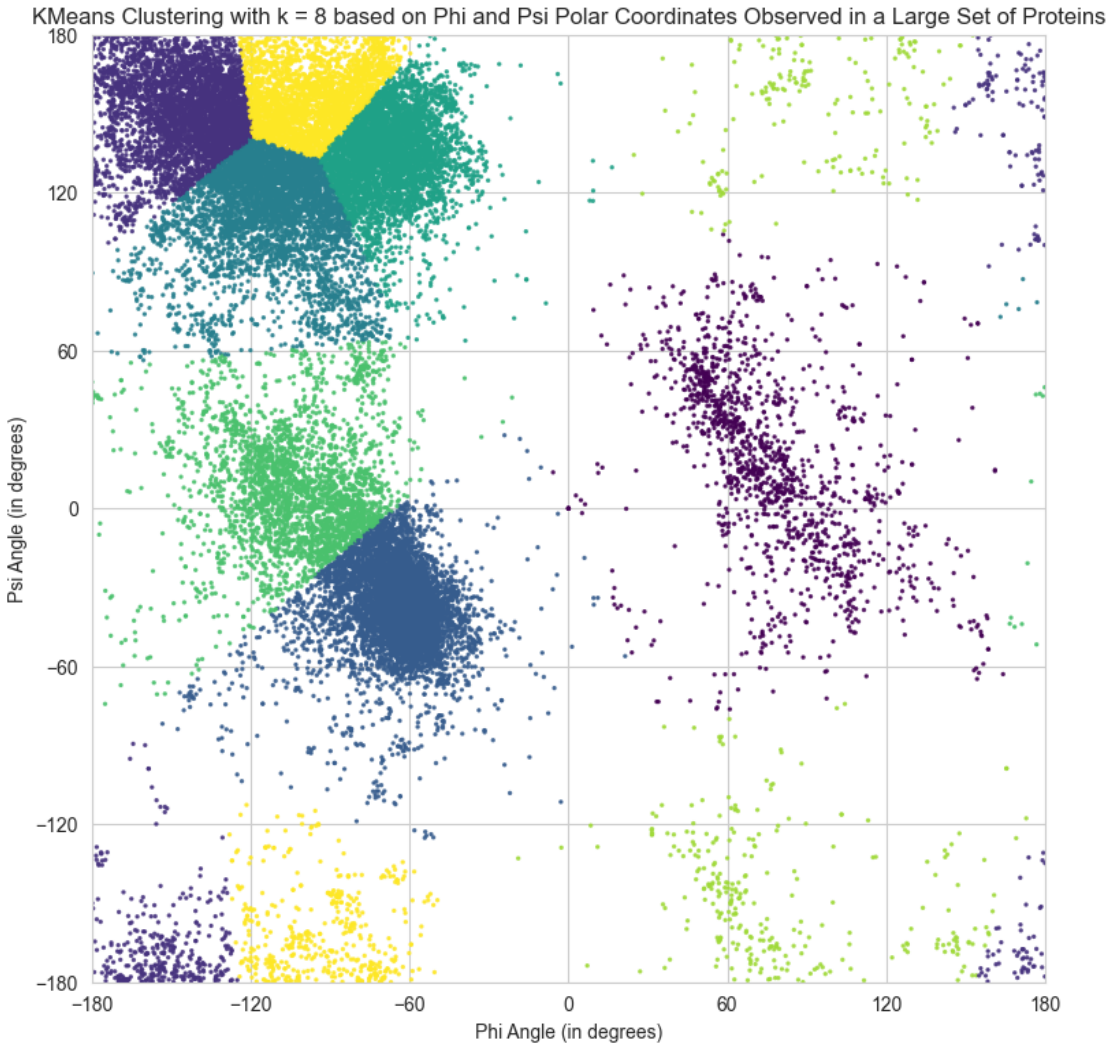

KMeans Clustering with k = 3 based on Phi and Psi Polar Coordinates Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180

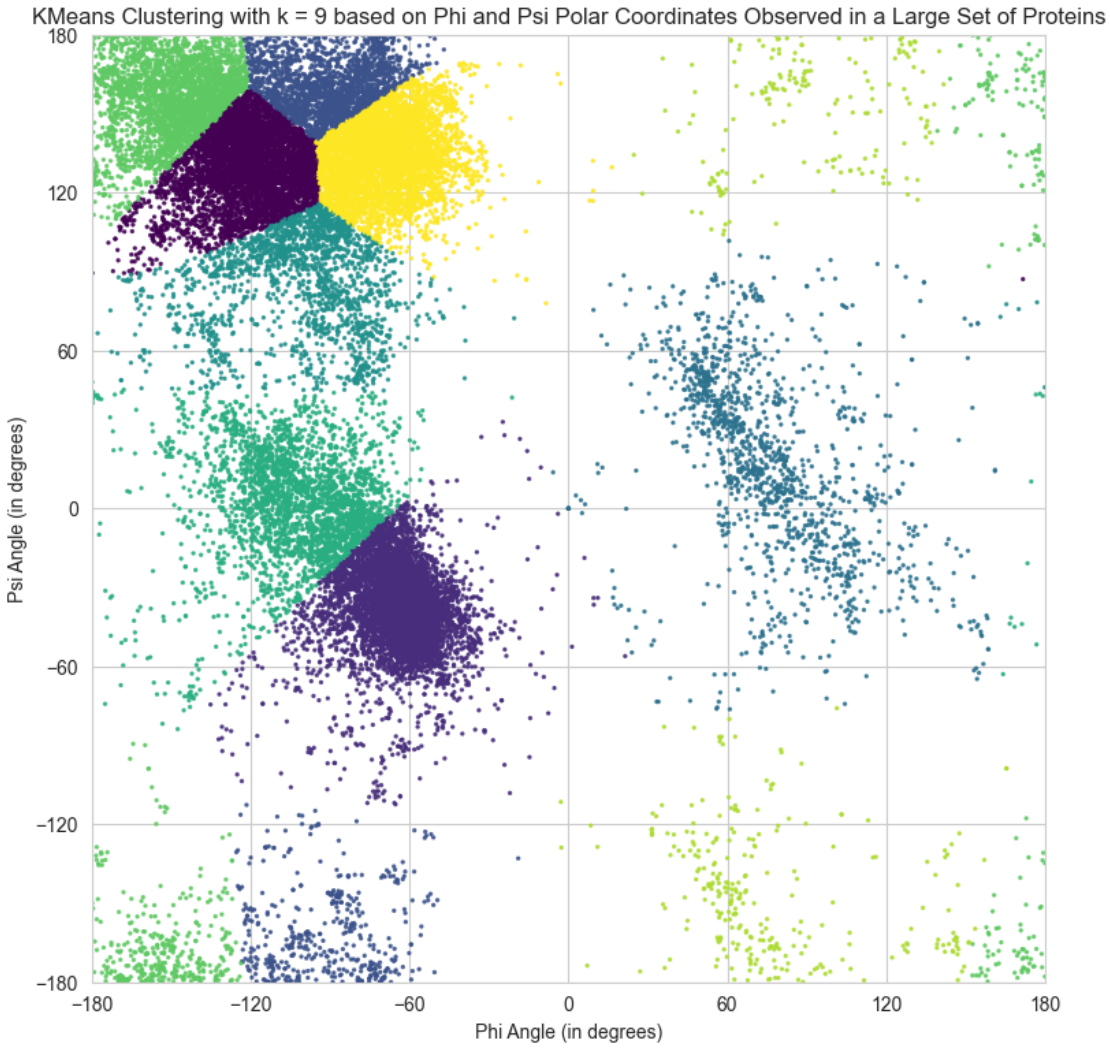

KMeans Clustering with k = 4 based on Phi and Psi Polar Coordinates Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180

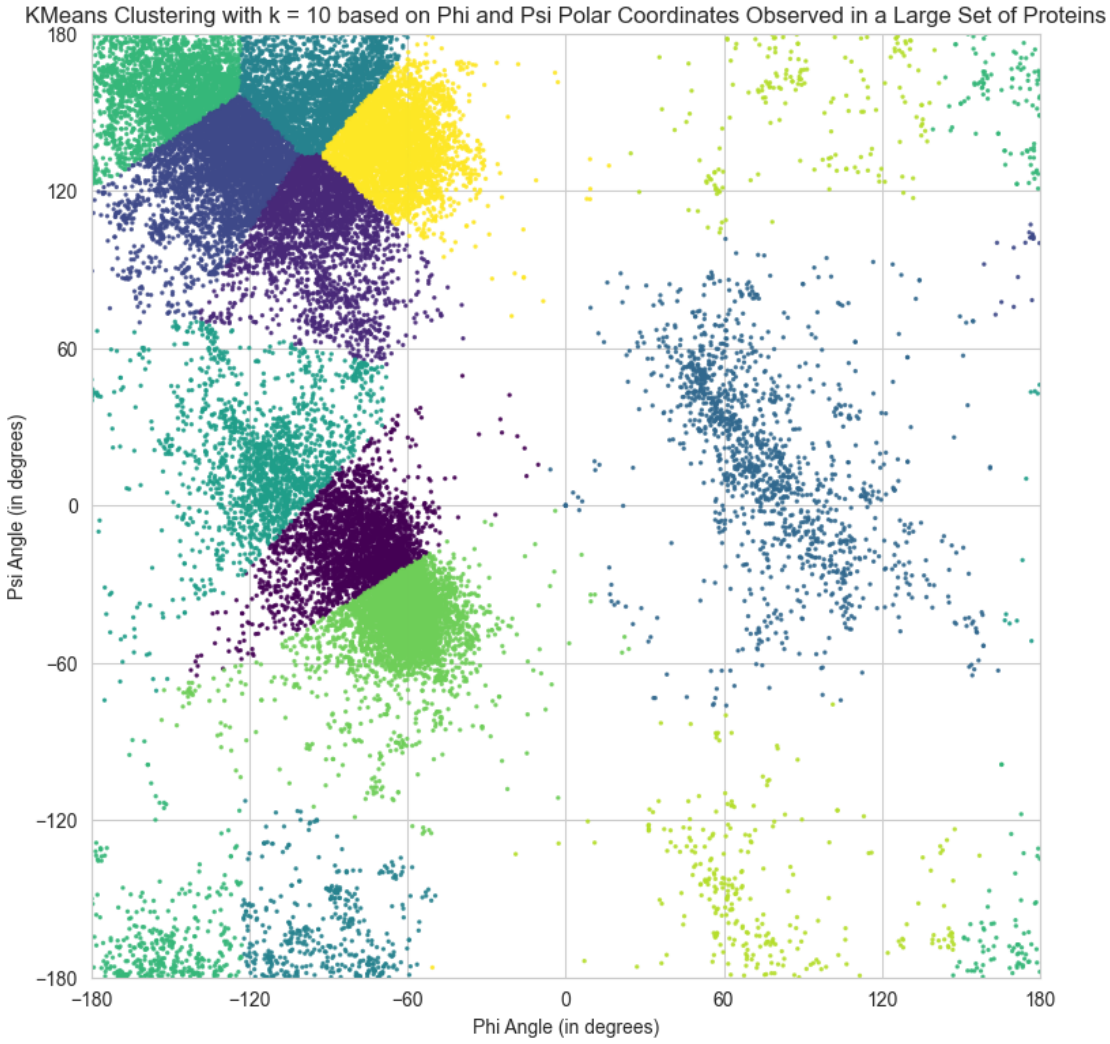

KMeans Clustering with k = 5 based on Phi and Psi Polar Coordinates Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180

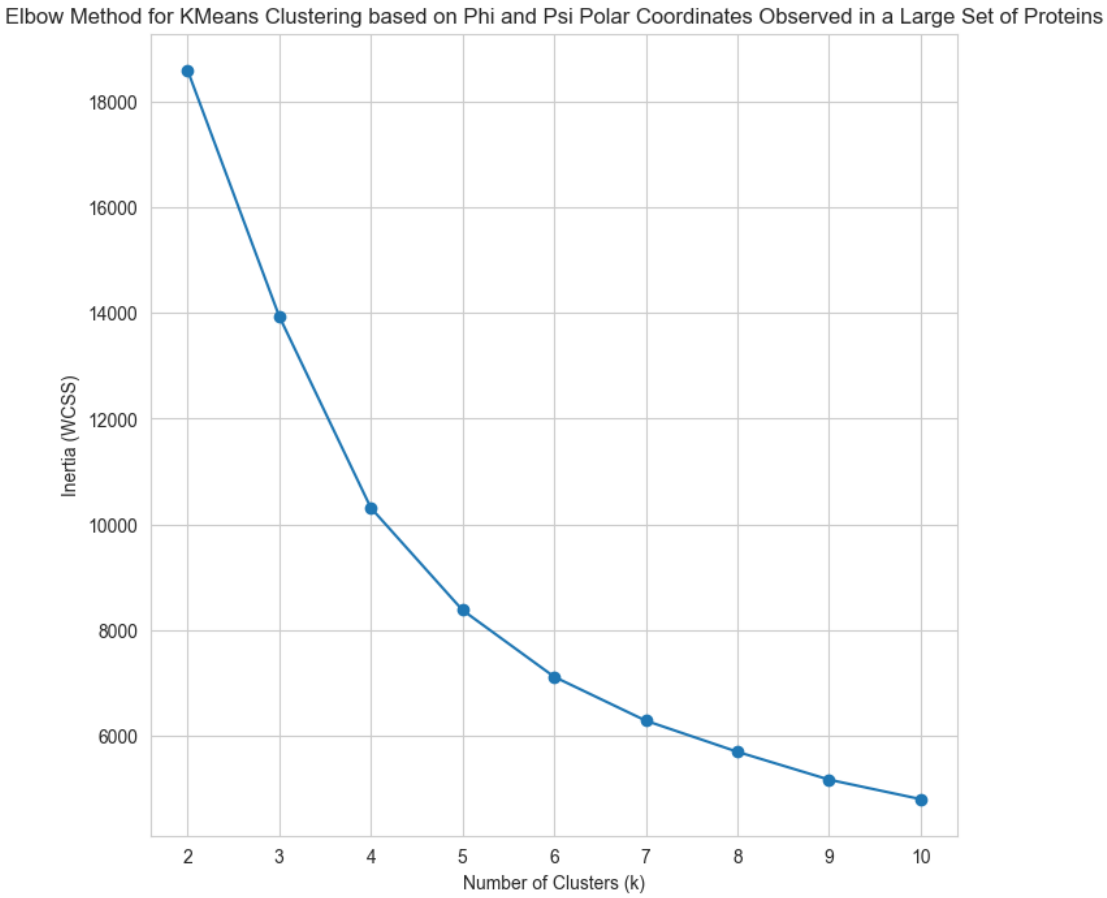

KMeans Clustering with k = 6 based on Phi and Psi Polar Coordinates Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180


KMeans Clustering with k = 7 based on Phi and Psi Polar Coordinates Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180


KMeans Clustering with k = 8 based on Phi and Psi Polar Coordinates Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180


KMeans Clustering with k = 9 based on Phi and Psi Polar Coordinates Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180

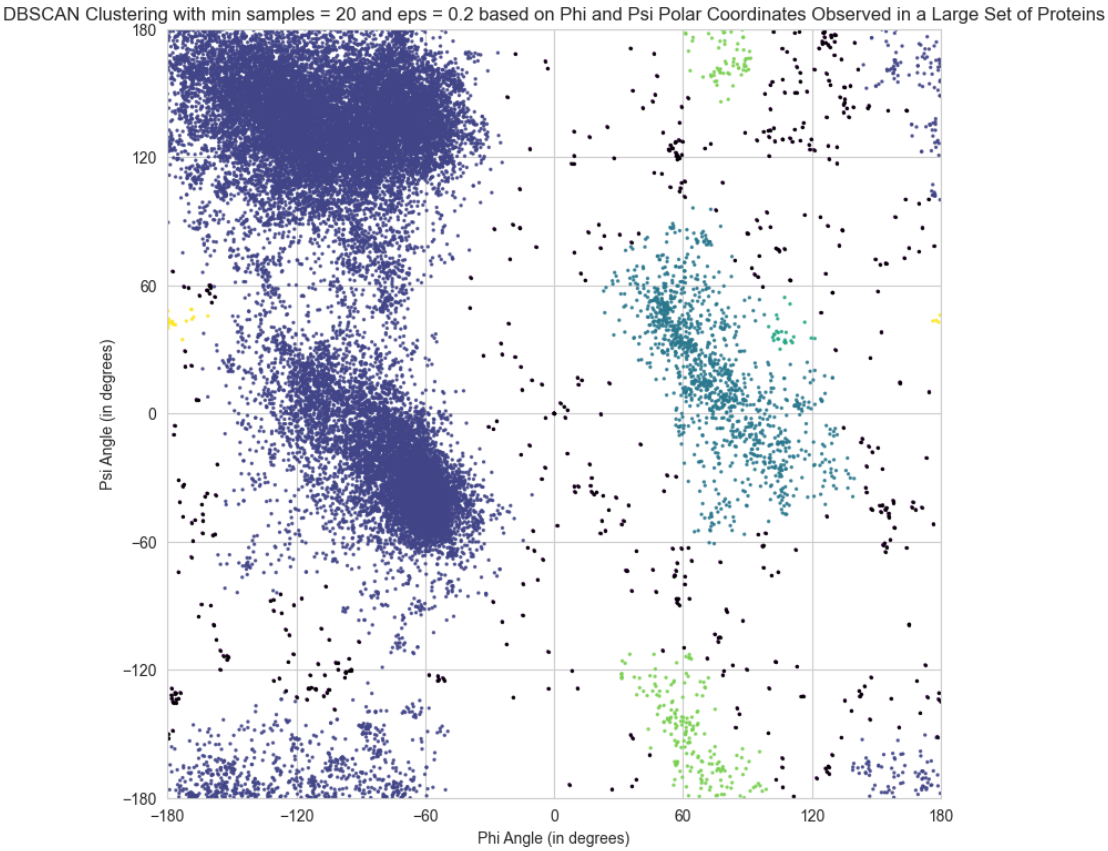

KMeans Clustering with k = 10 based on Phi and Psi Polar Coordinates Observed in a Large Set of Proteins
Psi Angle (in degrees)
Phi Angle (in degrees)
180
120
60
0
−60
−120
−180
−180
−120
−60
0
60
120
180



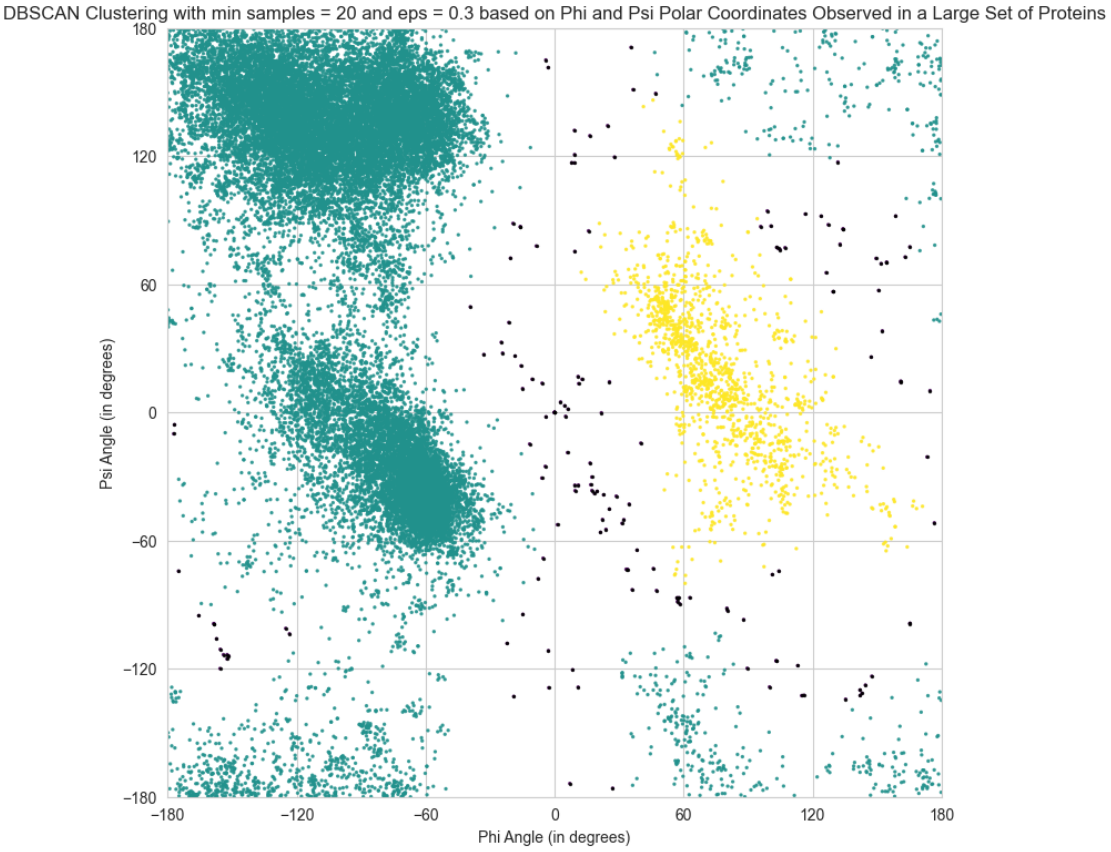
3 Task 3: Use the DBSCAN method to cluster the phi and psi angle combinations in the data file.

[17]:
```
# Performing DBSCAN for different values of min_samples and eps on phi and psi␣
 ↪polar coordinates data
for min_samples in [20, 30, 40, 50]:
    for eps in [0.2, 0.3, 0.4]:
        db = DBSCAN(eps=eps, min_samples=min_samples)
        y_db = db.fit_predict(X_polar)

        core_samples_mask = np.zeros_like(db.labels_, dtype=bool)
        core_samples_mask[db.core_sample_indices_] = True
        labels = db.labels_

        num_clusters = len(set(labels)) - (1 if -1 in labels else 0)
        num_outliers = list(labels).count(-1)
```

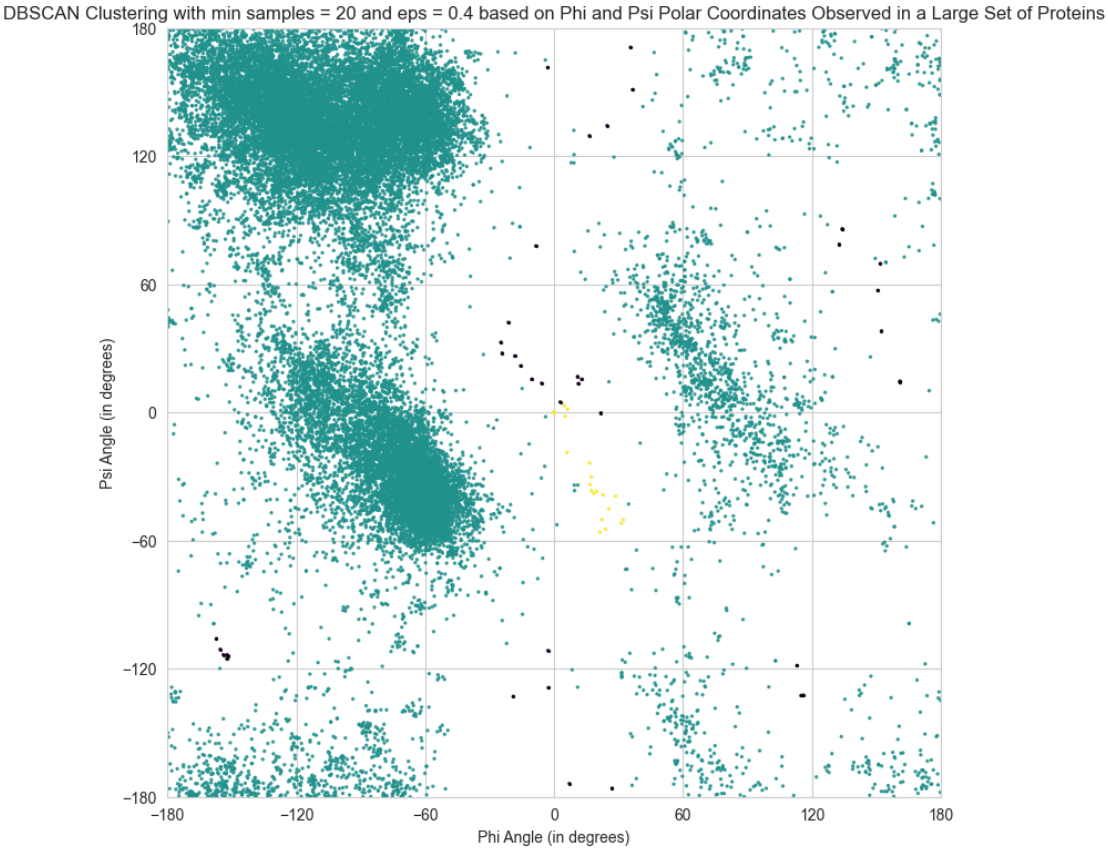
```
        plt.figure(figsize=(9, 9))
        plt.scatter(X['phi'], X['psi'], c=y_db, cmap='viridis', s=2, alpha=0.8)

        outliers_mask = labels == -1
        plt.scatter(X['phi'][outliers_mask], X['psi'][outliers_mask],␣
↪c='black', s=2, alpha=0.8)

        plt.xlim(-180, 180)
        plt.ylim(-180, 180)
        plt.xticks(range(-180, 181, 60))
        plt.yticks(range(-180, 181, 60))
        plt.xlabel('Phi Angle (in degrees)')
        plt.ylabel('Psi Angle (in degrees)')

        plt.title(f'DBSCAN Clustering with min samples = {min_samples} and eps␣
↪= {eps} based on Phi and Psi Polar Coordinates Observed in a Large Set of␣
↪Proteins')
        plt.show()

        print(f'Number of clusters: {num_clusters}')
        print(f'Number of outliers: {num_outliers}')
```



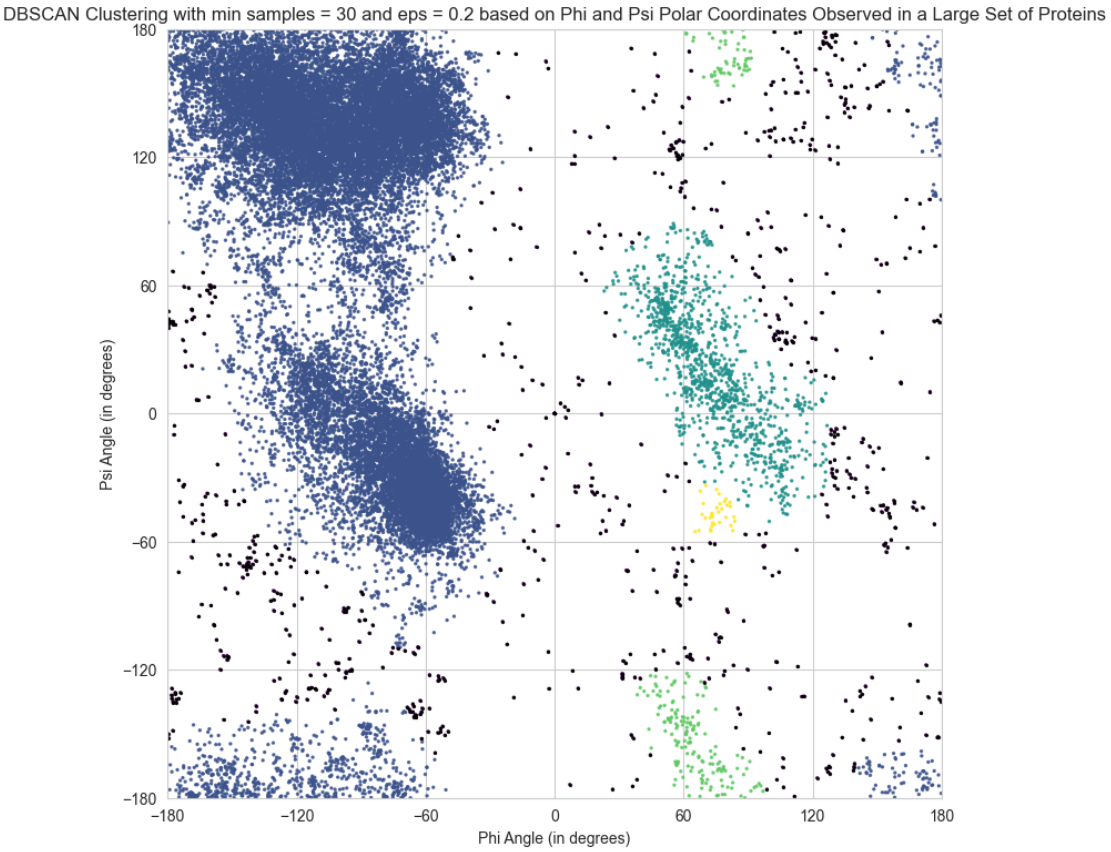
```
Number of clusters: 5
Number of outliers: 519
```



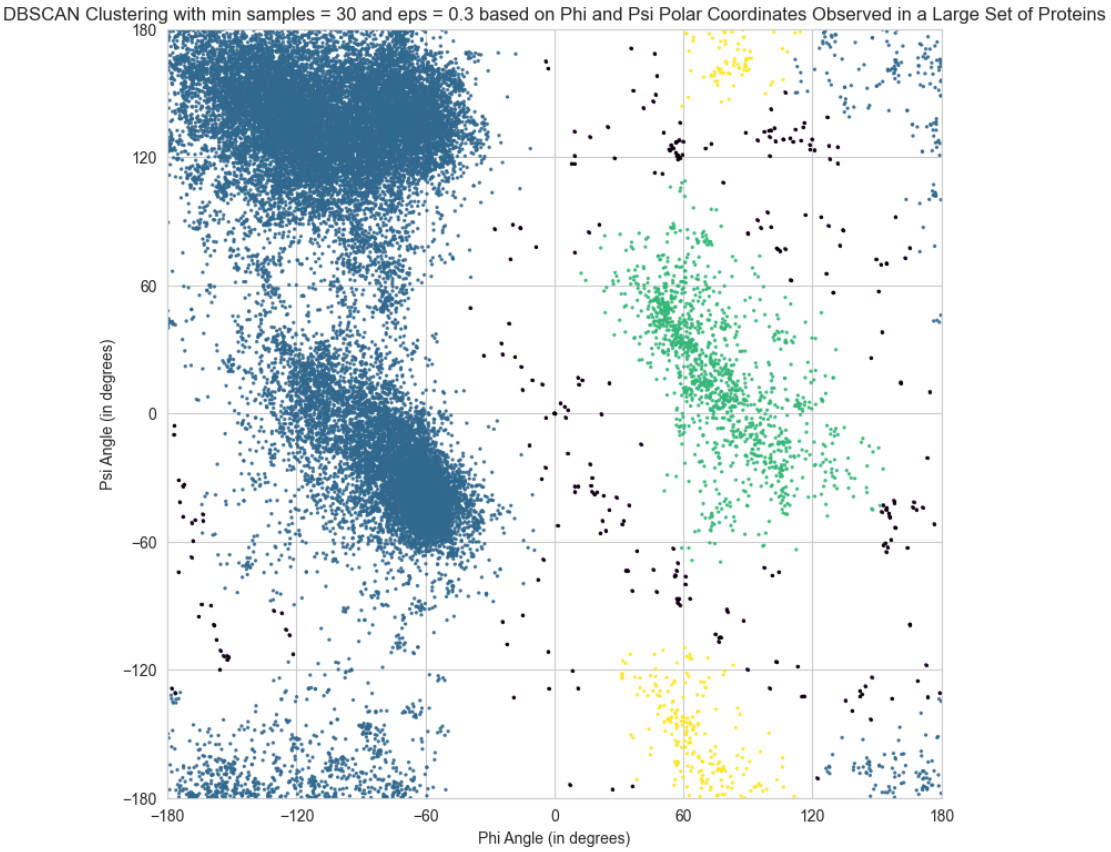

```
Number of clusters: 2
Number of outliers: 158
```



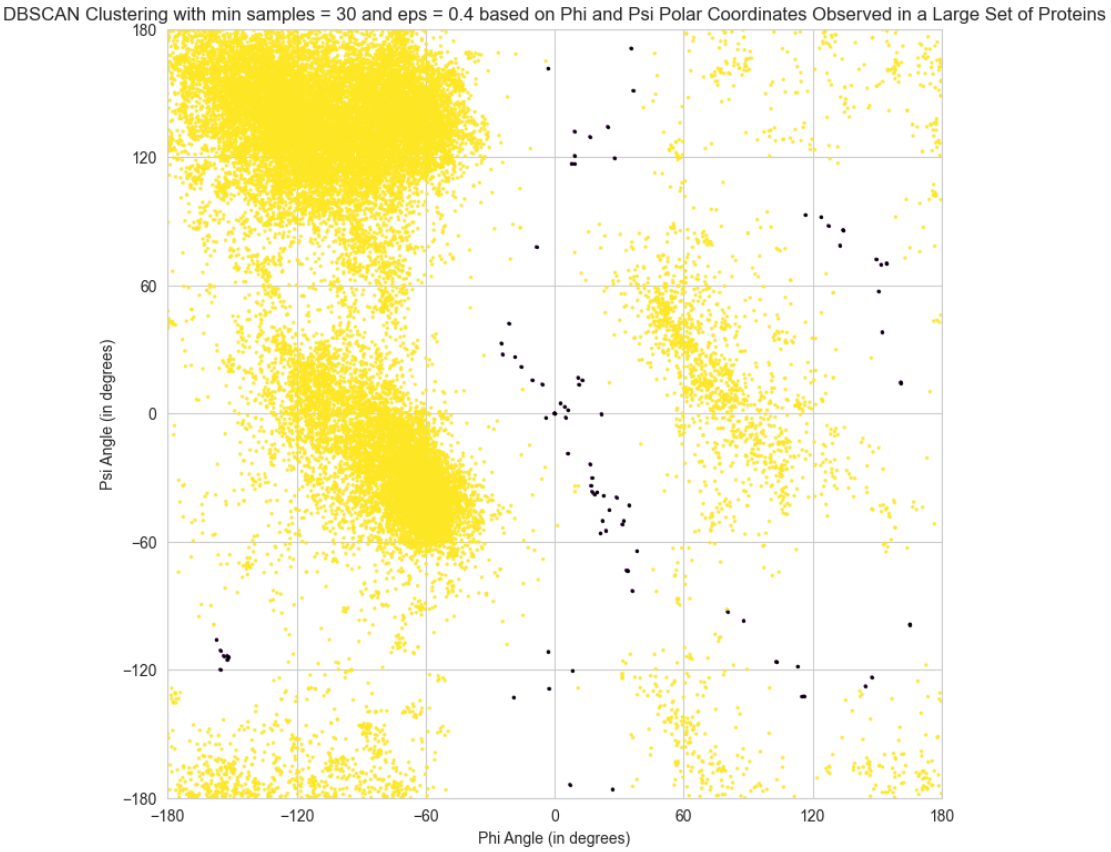

```
Number of clusters: 2
Number of outliers: 40
```



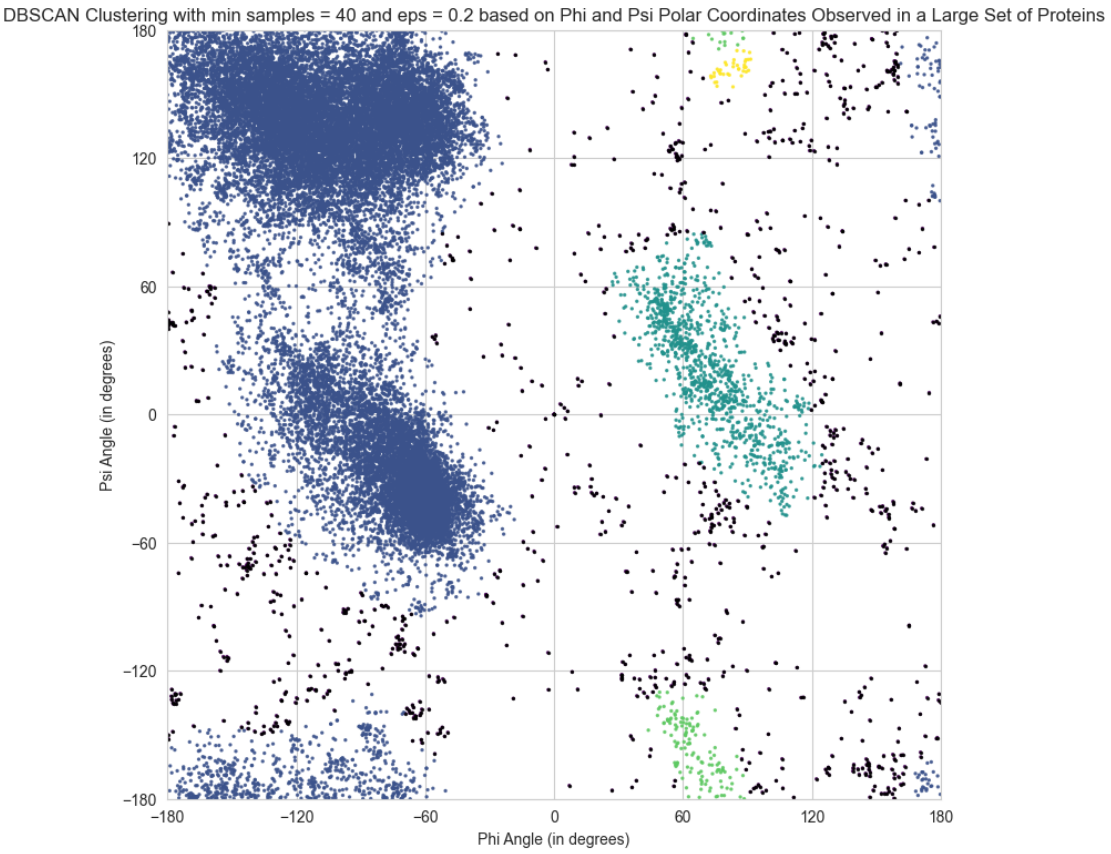

```
Number of clusters: 4
Number of outliers: 779
```



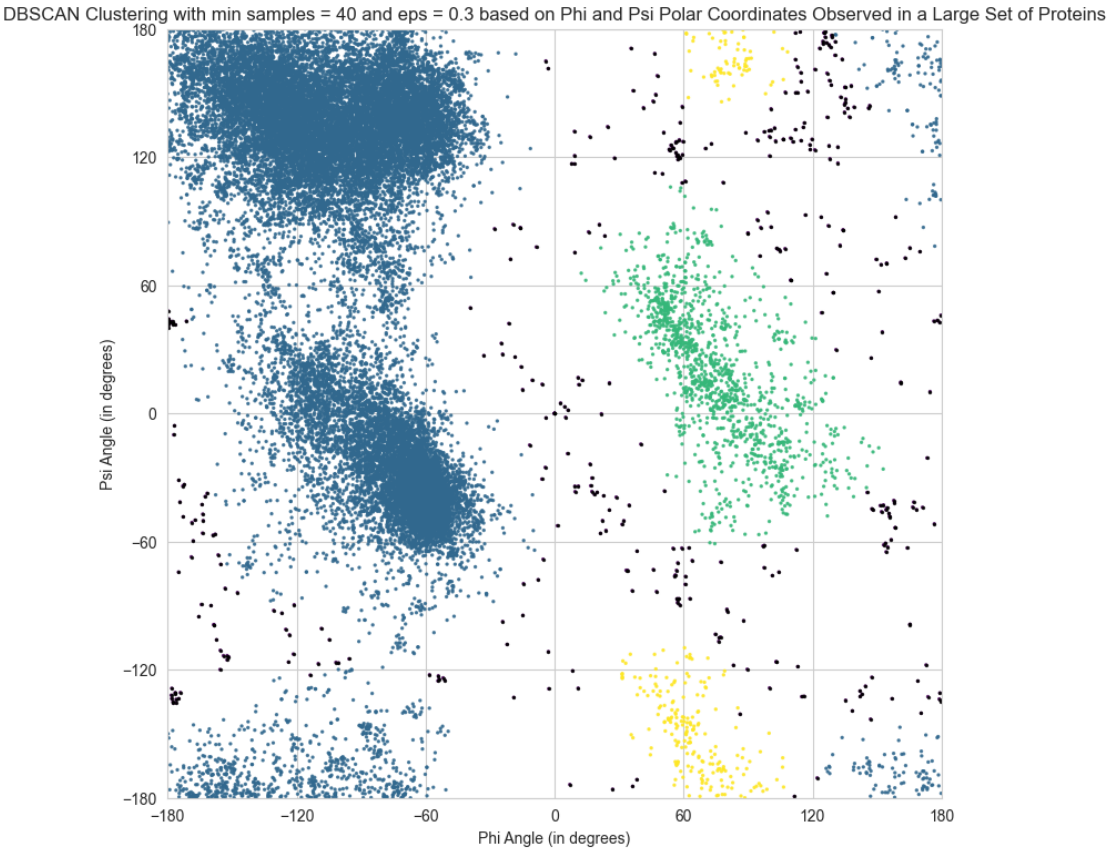

```
Number of clusters: 3
Number of outliers: 280
```



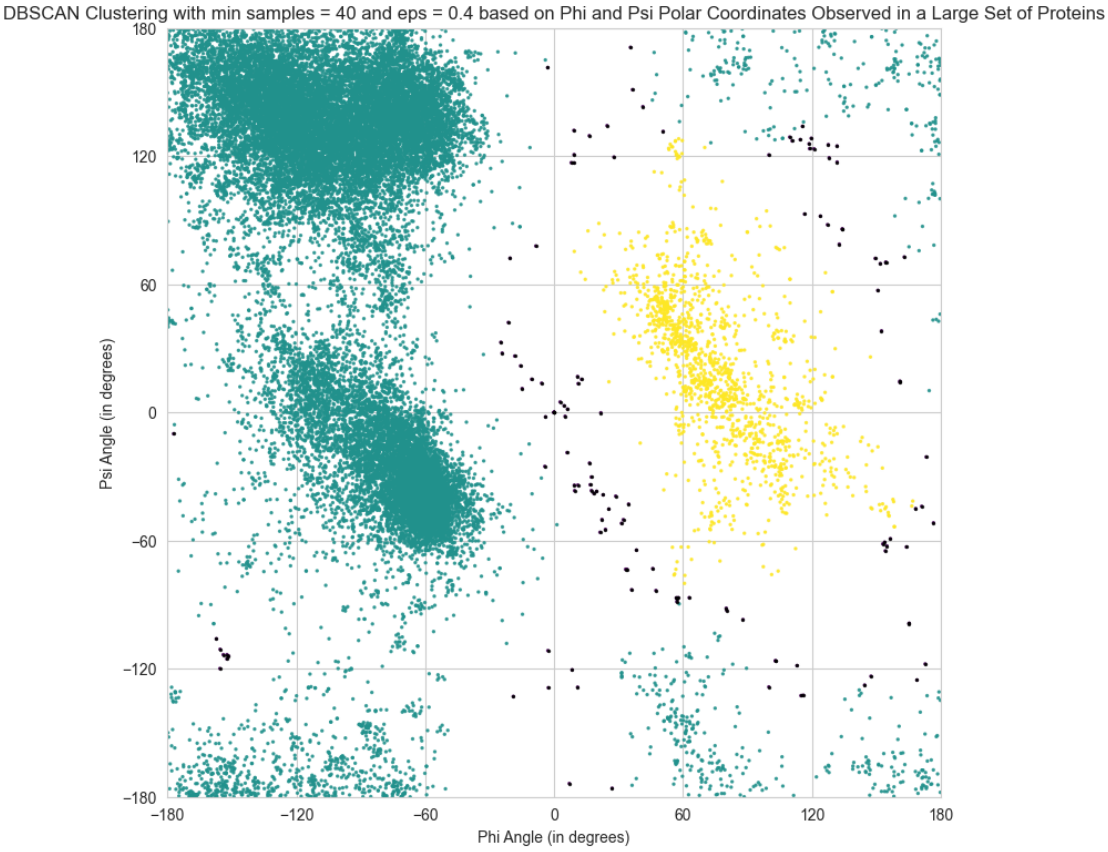

```
Number of clusters: 1
Number of outliers: 90
```



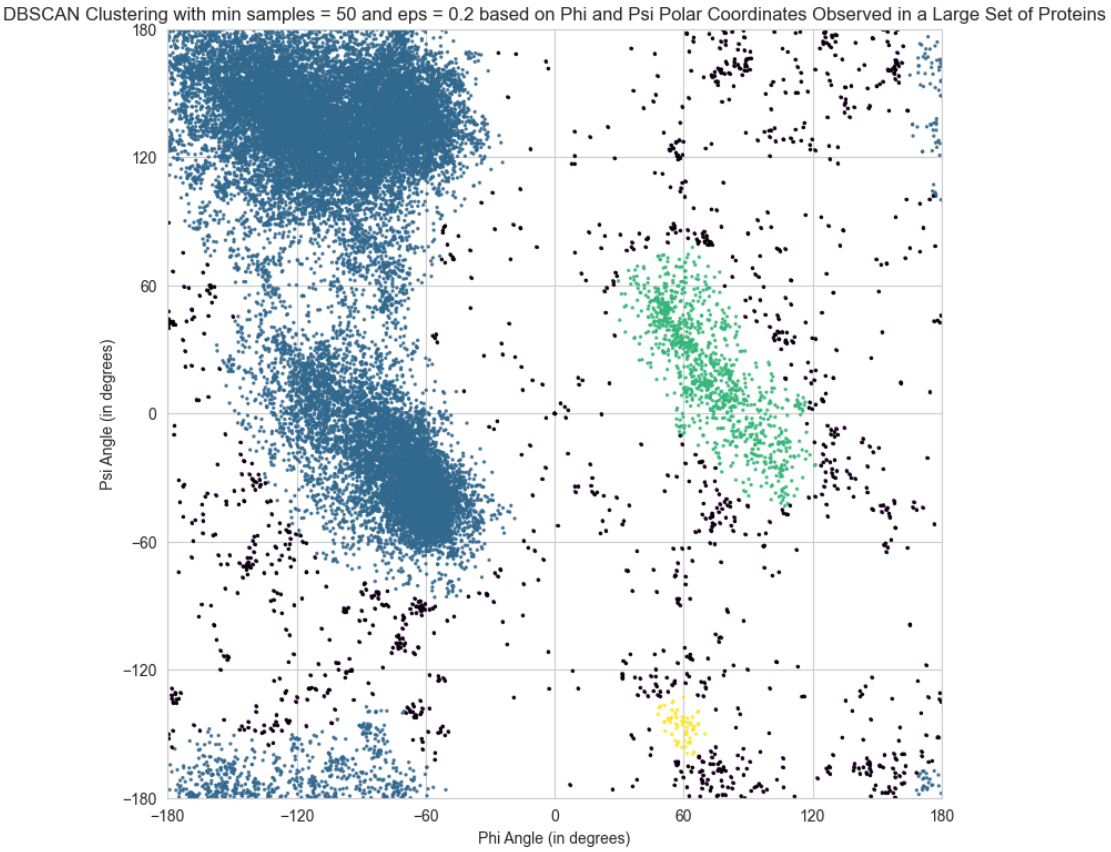

```
Number of clusters: 4
Number of outliers: 1037
```



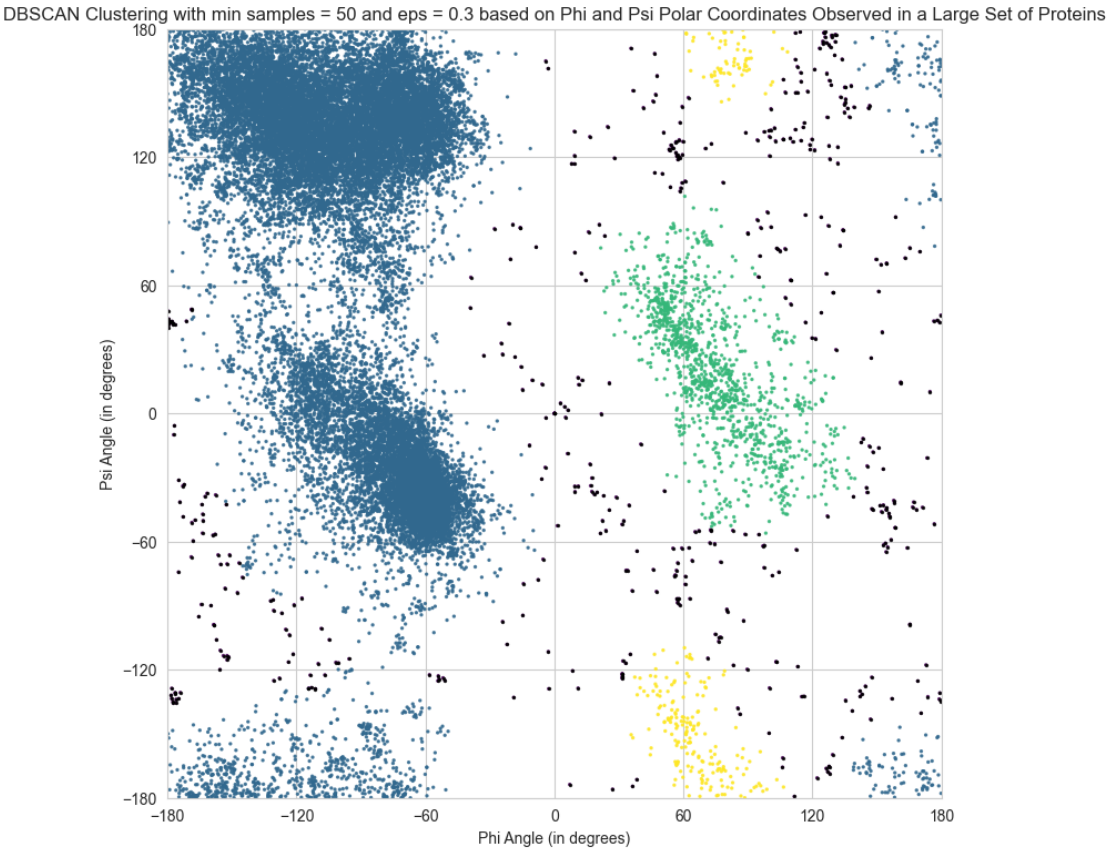

```
Number of clusters: 3
Number of outliers: 400
```



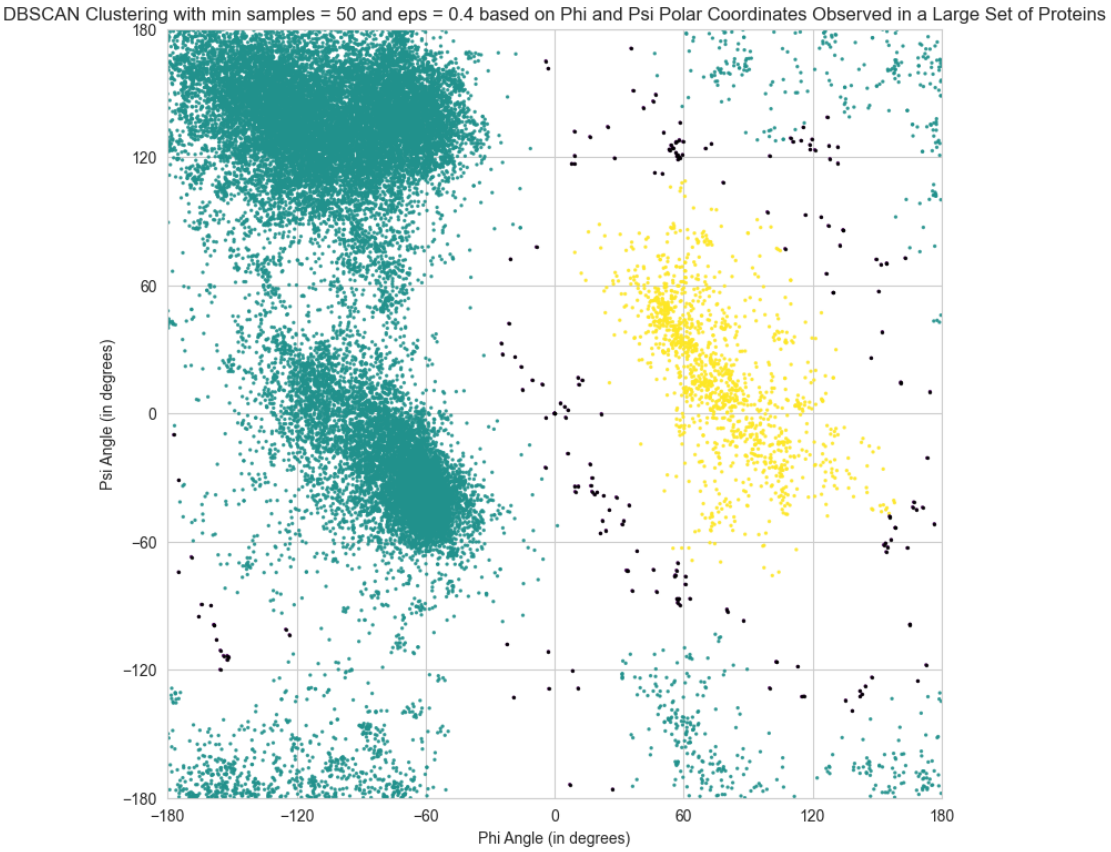

```
Number of clusters: 2
Number of outliers: 135
```




```
Number of clusters: 3
Number of outliers: 1295
```



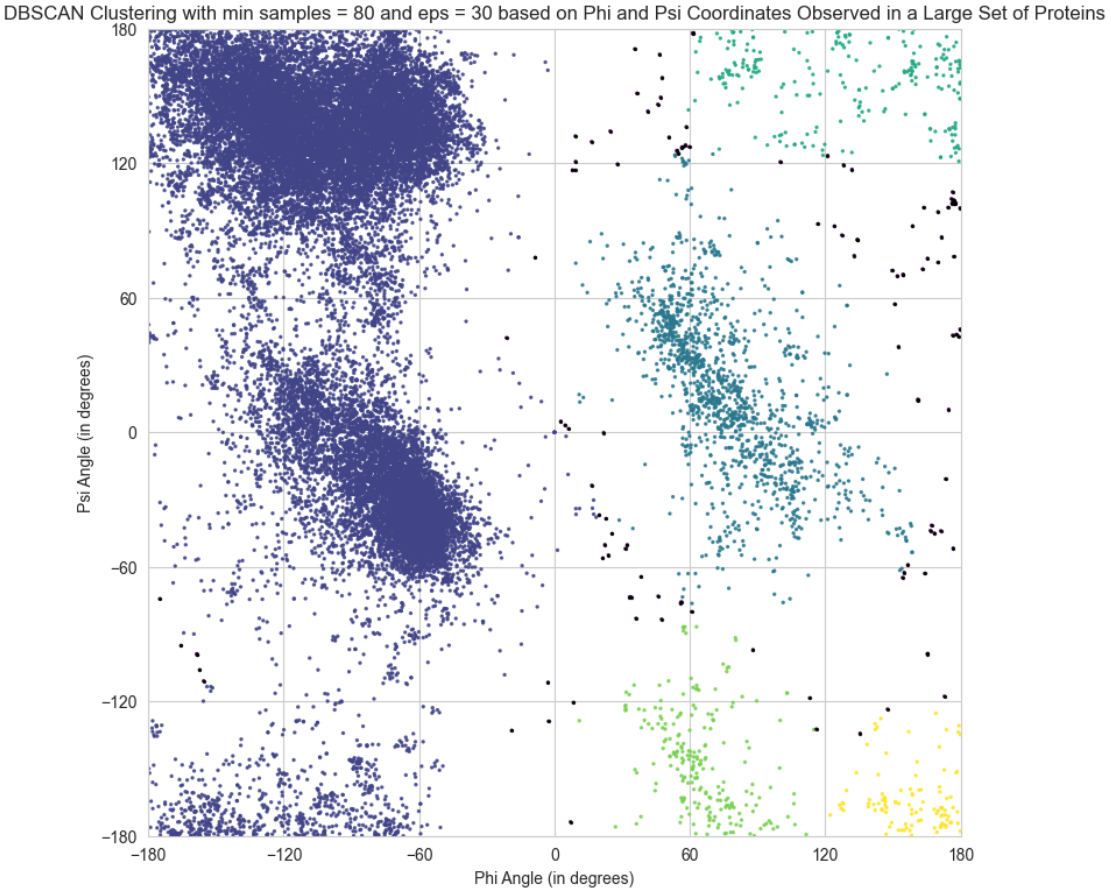

```
Number of clusters: 3
Number of outliers: 474
```




```
Number of clusters: 2
Number of outliers: 197
```

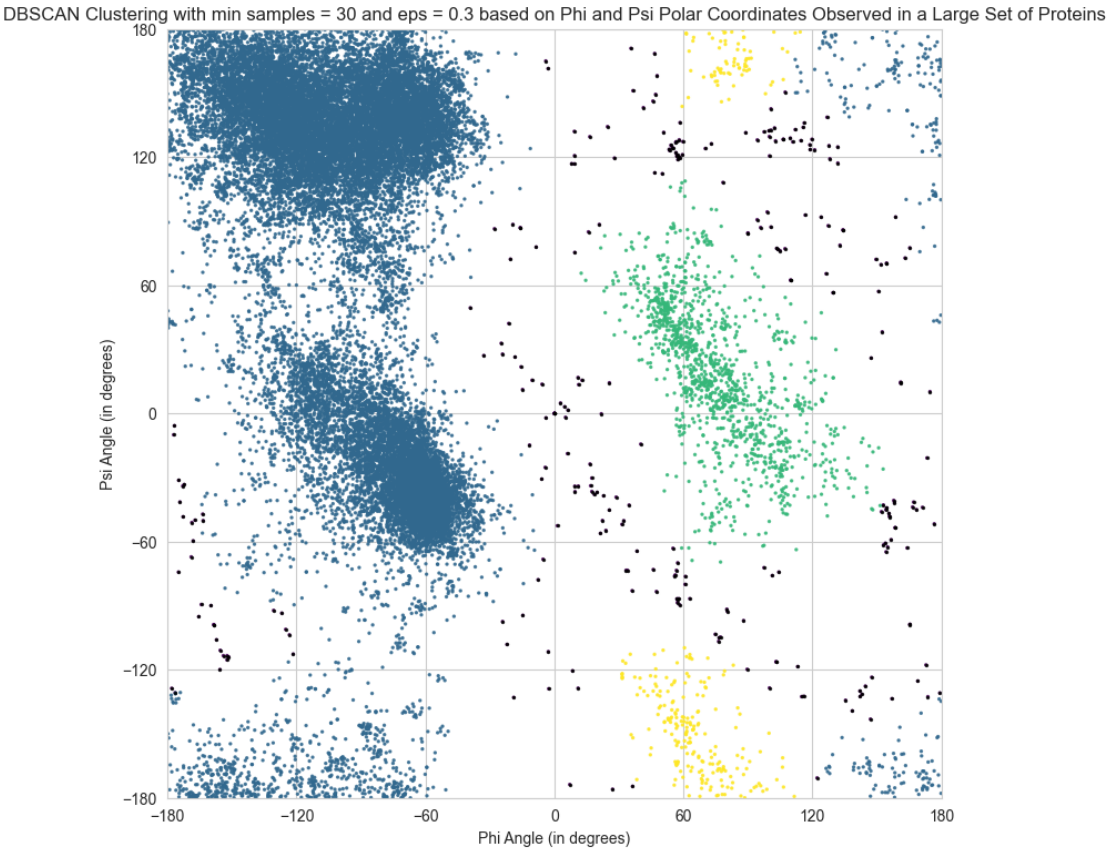
[18]:
```
# Performing DBSCAN on the original data
db = DBSCAN(eps=30, min_samples=80)
y_db = db.fit_predict(X)

core_samples_mask = np.zeros_like(db.labels_, dtype=bool)
core_samples_mask[db.core_sample_indices_] = True
labels = db.labels_

num_clusters = len(set(labels)) - (1 if -1 in labels else 0)
num_outliers = list(labels).count(-1)

plt.figure(figsize=(9, 9))
plt.scatter(X['phi'], X['psi'], c=y_db, cmap='viridis', s=2, alpha=0.8)

outliers_mask = labels == -1
plt.scatter(X['phi'][outliers_mask], X['psi'][outliers_mask], c='black', s=2,␣
↪alpha=0.8)
```

```
plt.xlim(-180, 180)
plt.ylim(-180, 180)
plt.xticks(range(-180, 181, 60))
plt.yticks(range(-180, 181, 60))
plt.xlabel('Phi Angle (in degrees)')
plt.ylabel('Psi Angle (in degrees)')

plt.title(f'DBSCAN Clustering with min samples = 80 and eps = 30 based on Phi␣
 ↪and Psi Coordinates Observed in a Large Set of Proteins')
plt.show()

print(f'Number of clusters: {num_clusters}')
print(f'Number of outliers: {num_outliers}')
```




```
Number of clusters: 5
Number of outliers: 119
```

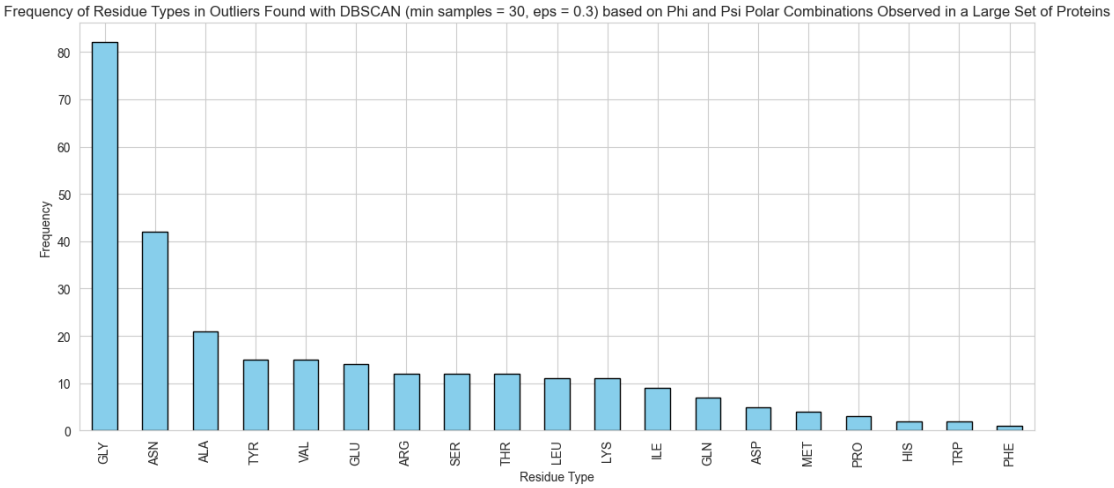
[19]:
```
# Chosen plot for (c)
db = DBSCAN(eps=0.3, min_samples=30)
y_db = db.fit_predict(X_polar)

core_samples_mask = np.zeros_like(db.labels_, dtype=bool)
core_samples_mask[db.core_sample_indices_] = True
labels = db.labels_

num_clusters = len(set(labels)) - (1 if -1 in labels else 0)
num_outliers = list(labels).count(-1)

plt.figure(figsize=(9, 9))
plt.scatter(X['phi'], X['psi'], c=y_db, cmap='viridis', s=2, alpha=0.8)

outliers_mask = labels == -1
plt.scatter(X['phi'][outliers_mask], X['psi'][outliers_mask], c='black', s=2,␣
 ↪alpha=0.8)

plt.xlim(-180, 180)
plt.ylim(-180, 180)
plt.xticks(range(-180, 181, 60))
plt.yticks(range(-180, 181, 60))
plt.xlabel('Phi Angle (in degrees)')
plt.ylabel('Psi Angle (in degrees)')

plt.title(f'DBSCAN Clustering with min samples = 30 and eps = 0.3 based on Phi␣
 ↪and Psi Polar Coordinates Observed in a Large Set of Proteins')
plt.show()

print(f'Number of clusters: {num_clusters}')
print(f'Number of outliers: {num_outliers}')
```




```
Number of clusters: 3
Number of outliers: 280
```

[20]:
```
X_residue = df[['residue name', 'phi', 'psi']].copy()
X_residue['label'] = y_db
outliers = X_residue[X_residue['label'] == -1]
```

[21]:
```
residue_counts = outliers['residue name'].value_counts()

plt.figure(figsize=(14, 6))
residue_counts.plot(kind='bar', color='skyblue', edgecolor='black')
plt.title('Frequency of Residue Types in Outliers Found with DBSCAN (min␣
 ↪samples = 30, eps = 0.3) based on Phi and Psi Polar Combinations Observed in␣
 ↪a Large Set of Proteins')
plt.xlabel('Residue Type')
plt.ylabel('Frequency')
plt.show()
```



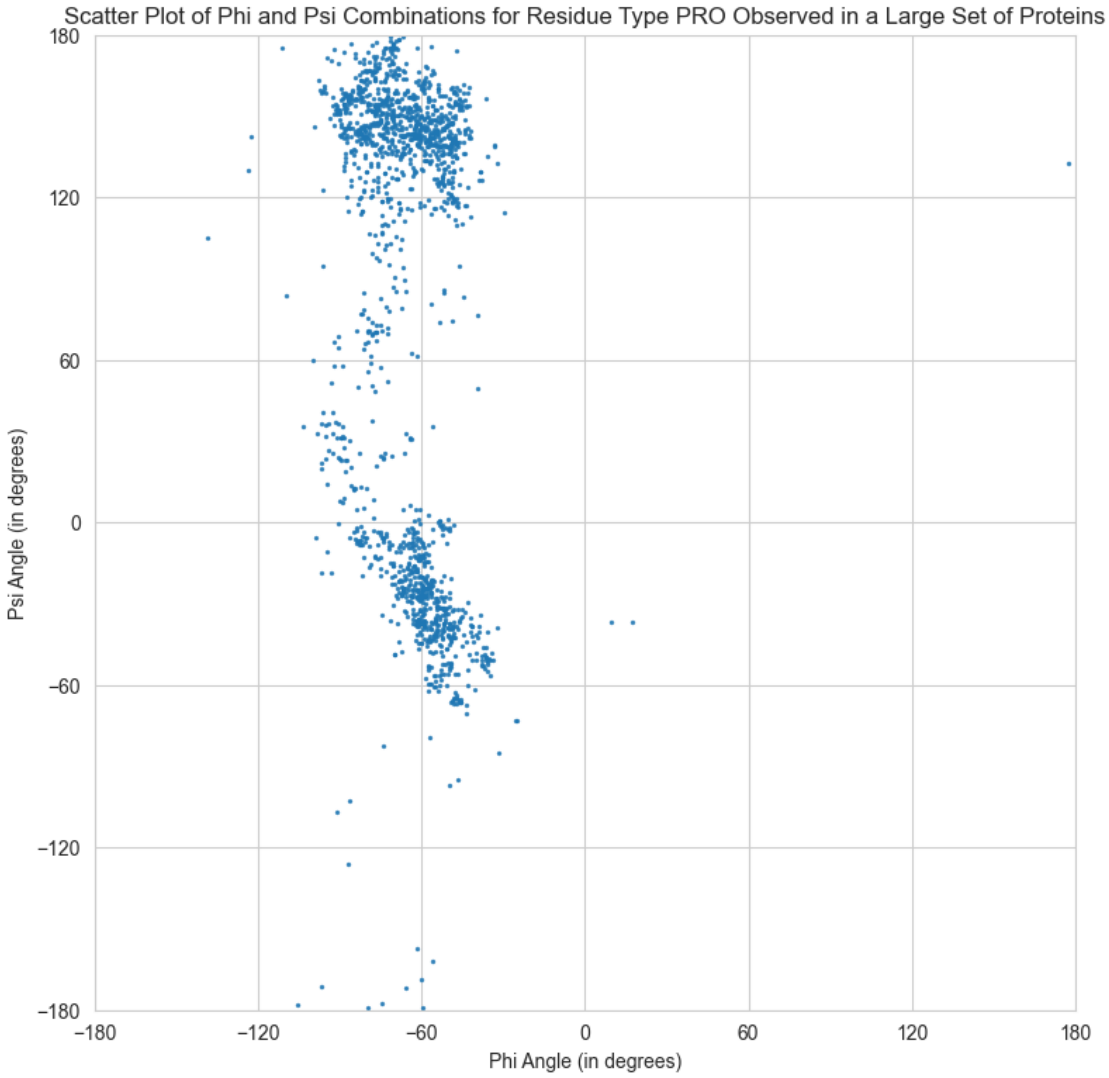
4 Task 4: The data file can be stratified by amino acid residue type. Use DBSCAN to cluster the data that have residue type PRO. Investigate how the clusters found for amino acid residues of type PRO differ from the general clusters.

[22]:
```
X_residue_pro = df[['residue name', 'phi', 'psi']].copy()
X_residue_pro = X_residue_pro[X_residue_pro['residue name'] == 'PRO']
```

[23]:
```
print(f'The number of rows with residue type PRO is: {len(X_residue_pro)}')
```

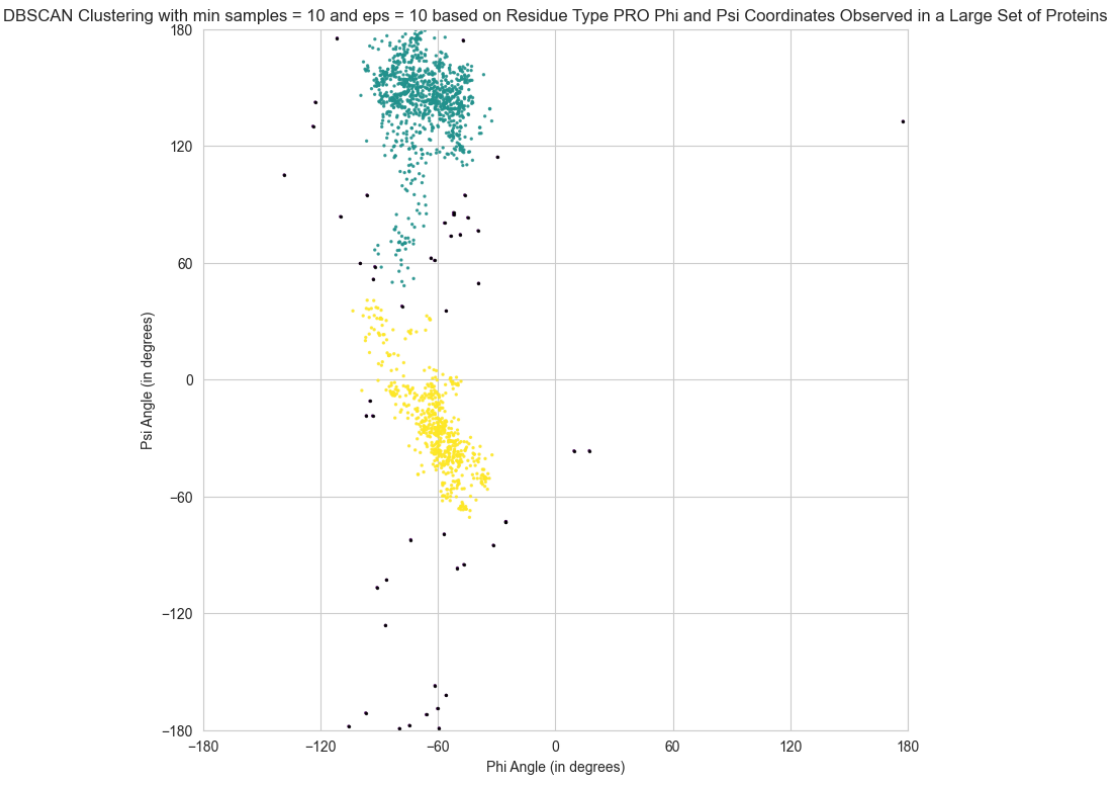
```
The number of rows with residue type PRO is: 1596
```

[24]:
```
# Draw scatter plot of the data
plt.figure(figsize=(9, 9))
plt.scatter(X_residue_pro['phi'], X_residue_pro['psi'], s=2, alpha=0.8)
plt.xlim(-180, 180)
plt.ylim(-180, 180)
plt.xticks(range(-180, 181, 60))
plt.yticks(range(-180, 181, 60))
plt.xlabel('Phi Angle (in degrees)')
plt.ylabel('Psi Angle (in degrees)')

plt.title('Scatter Plot of Phi and Psi Combinations for Residue Type PRO␣
 ↪Observed in a Large Set of Proteins')
plt.show()
```



[25]:
```
X_residue_pro_coordinates = X_residue_pro[['phi', 'psi']].copy()
db_residue = DBSCAN(eps=10, min_samples=10)
y_db_pro = db_residue.fit_predict(X_residue_pro_coordinates)

core_samples_mask = np.zeros_like(db_residue.labels_, dtype=bool)
core_samples_mask[db_residue.core_sample_indices_] = True
labels = db_residue.labels_

num_clusters = len(set(labels)) - (1 if -1 in labels else 0)
num_outliers = list(labels).count(-1)

plt.figure(figsize=(9, 9))
```

```
plt.scatter(X_residue_pro['phi'], X_residue_pro['psi'], c=y_db_pro,␣
 ↪cmap='viridis', s=2, alpha=0.8)

outliers_mask = labels == -1
plt.scatter(X_residue_pro['phi'][outliers_mask],␣
 ↪X_residue_pro['psi'][outliers_mask], c='black', s=2, alpha=0.8)

plt.xlim(-180, 180)
plt.ylim(-180, 180)
plt.xticks(range(-180, 181, 60))
plt.yticks(range(-180, 181, 60))
plt.xlabel('Phi Angle (in degrees)')
plt.ylabel('Psi Angle (in degrees)')

plt.title(f'DBSCAN Clustering with min samples = 10 and eps = 10 based on␣
 ↪Residue Type PRO Phi and Psi Coordinates Observed in a Large Set of␣
 ↪Proteins')
plt.show()

print(f'Number of clusters: {num_clusters}')
print(f'Number of outliers: {num_outliers}')
```



```
Number of clusters: 2
Number of outliers: 49
```