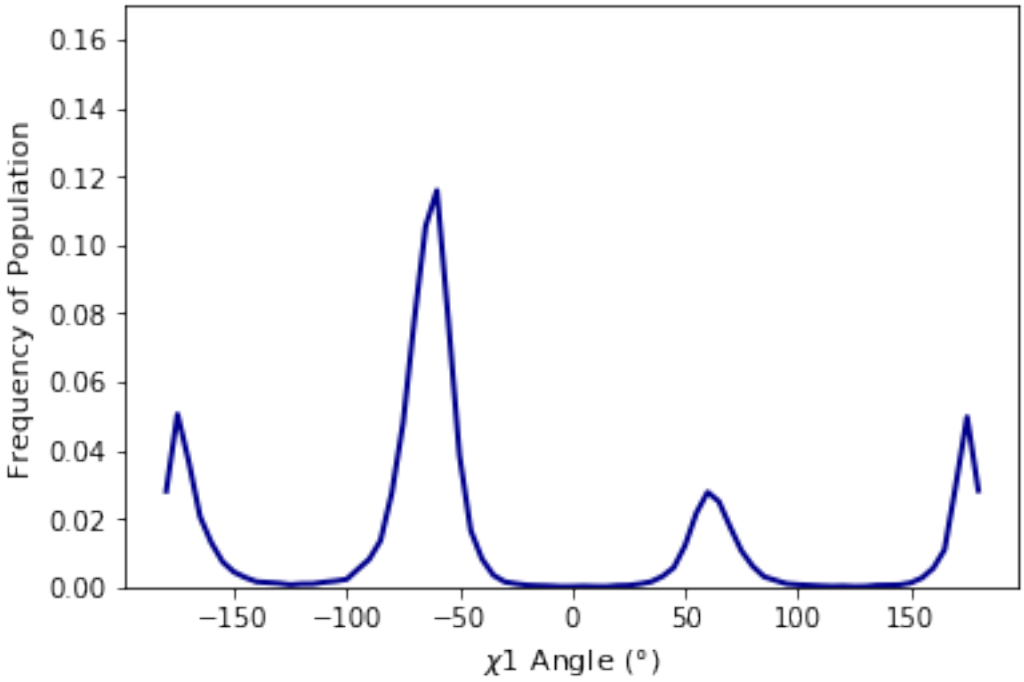
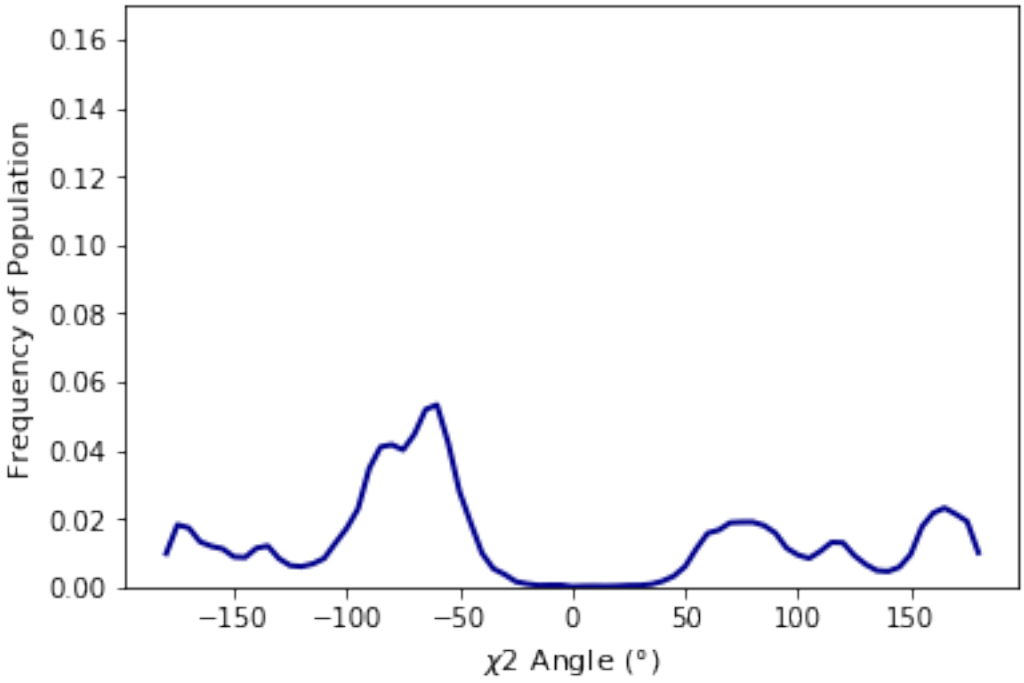
configuration_analysis

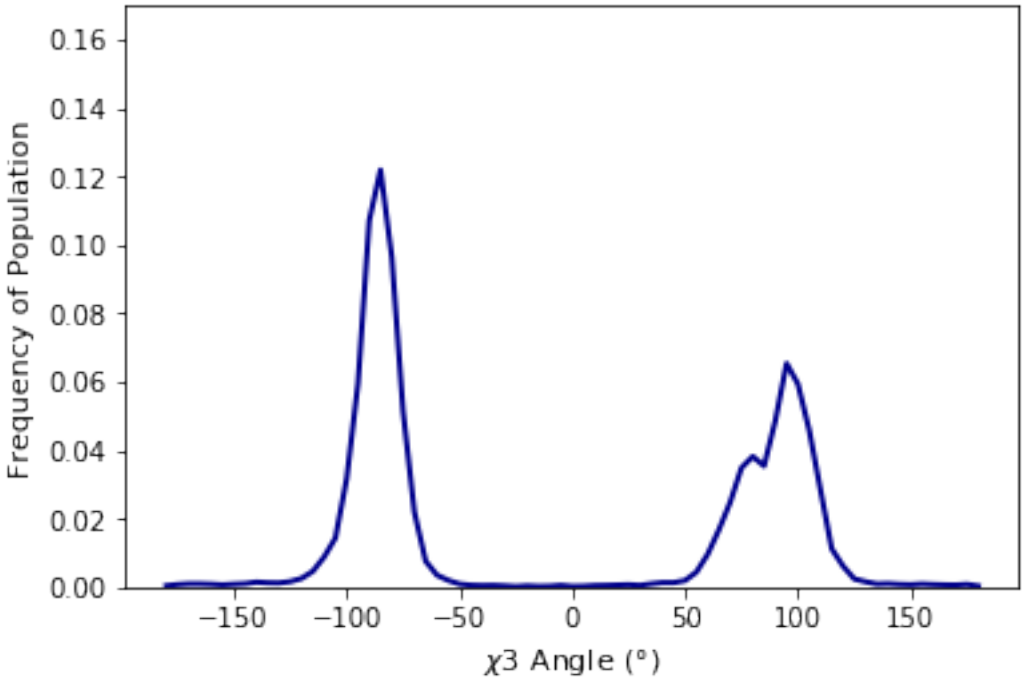
August 26, 2018

Analyse the distribution of side chain dihedral angles: Intro The resultant cystine residue from the formation of the covalent disulfide bond between the thiol groups of two cysteine side chains is comprised of five dihedral angles. Based on X-ray structures we look at the distribution of these angles (X1, X2 and X3) to define their different conformations.

```
/home/david/coding/lib/python2.7/site-packages/ipykernel_launcher.py:9: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: http://pandas.pydata.org/pandas-docs/stable/indexing.html#
  if __name__ == '__main__':
/home/david/coding/lib/python2.7/site-packages/ipykernel_launcher.py:10: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: http://pandas.pydata.org/pandas-docs/stable/indexing.html#
  # Remove the CWD from sys.path while we load stuff.
/home/david/coding/lib/python2.7/site-packages/ipykernel_launcher.py:11: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: http://pandas.pydata.org/pandas-docs/stable/indexing.html#
  # This is added back by InteractiveShellApp.init_path()
/home/david/coding/lib/python2.7/site-packages/ipykernel_launcher.py:12: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: http://pandas.pydata.org/pandas-docs/stable/indexing.html#
  if sys.path[0] == '':
/home/david/coding/lib/python2.7/site-packages/ipykernel_launcher.py:13: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: http://pandas.pydata.org/pandas-docs/stable/indexing.html#
  del sys.path[0]
```


Frequency of Population
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
−150
−100
−50
0
50
100
150
χ1 Angle (°)


Frequency of Population
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
−150
−100
−50
0
50
100
150
χ2 Angle (°)



Cystine dihedral distribution: Results In agreement with previous analysis, can see that X1 adopts the 'Gauche-, Gauche+ and Trans' conformations with a very narrow distribution. Therefore defined as: Gauche+ (+60) = +30 to +90 Gauche- (-60) = -90 to -30 Trans (180) = 150 to 210

X2 also adopts these conformations, however a greater distribution is observed. Therefore the following ranges were used for classificaiton Gauche+ (+60) = +30 to +120 Gauche- (-60) = -120 to -30 Trans (180) = 150 to 210

X3 angle distribution follows the previously identified 'Right Handed (+90)' or 'Left Handed (-90)' Right Handed (+90) = +60 to +120 Left Handed (-90) = -120 to -60

Frequency of Configurations: Intro Based on the definitions above, there is a possible 90 configurations a cystine can adopt when considering all five X angles (X1, X2, X3, X2, X1). Below calculates the frequency of those configurations If a disulfide had a dihedral angle ouf of the defined ranges above it was excluded from analysis

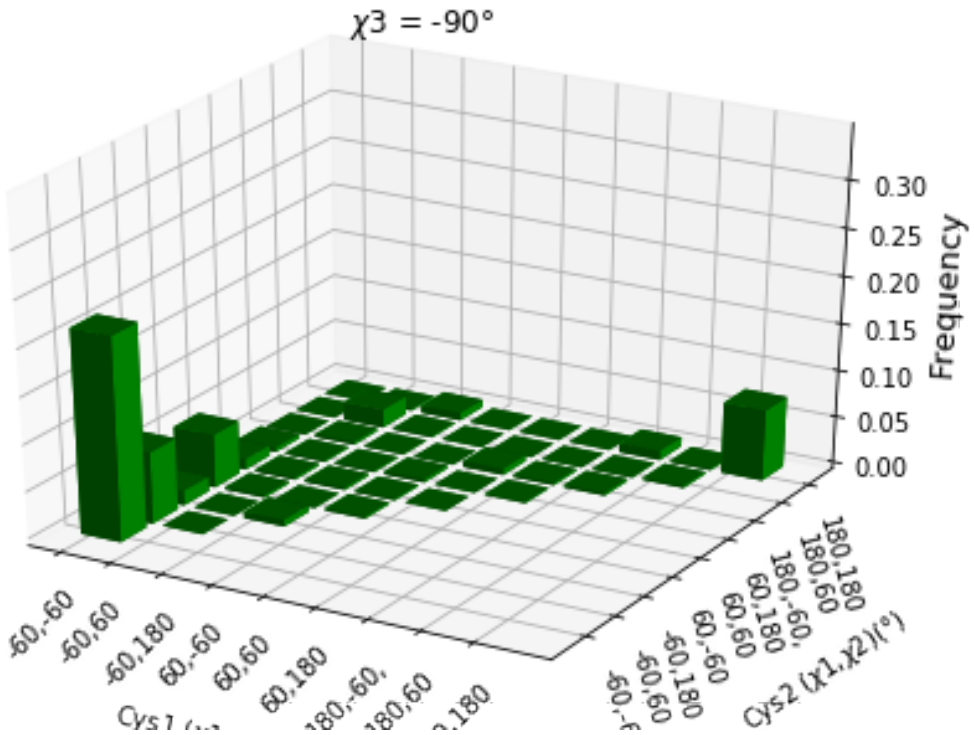
```
Total Number of Disulfides: 19605
Total Number of Disulfides in Defined Configurations for Structural Analysis: 15538
```

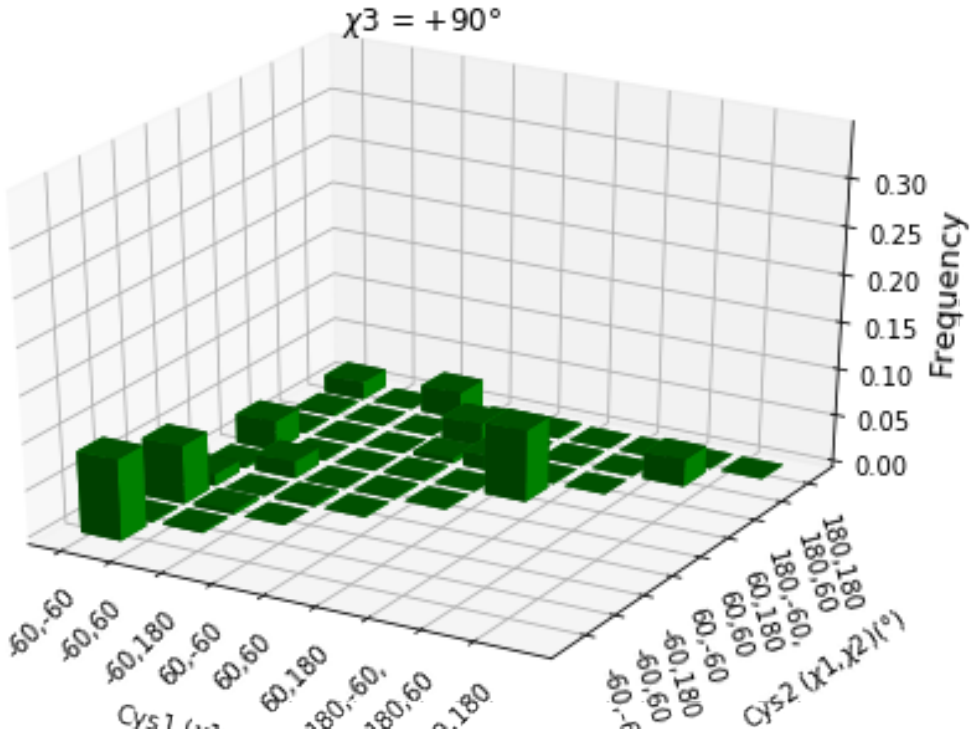
```
/home/david/coding/lib/python2.7/site-packages/ipykernel_launcher.py:192: SettingWithCopyWarning
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: http://pandas.pydata.org/pandas-docs/stable/indexing.html#
```

Generate Configuration Frequency Graphs Generate a 3D plot tha shows the frequency of population for each configuration

1 Generate configuration graphs for all cystines

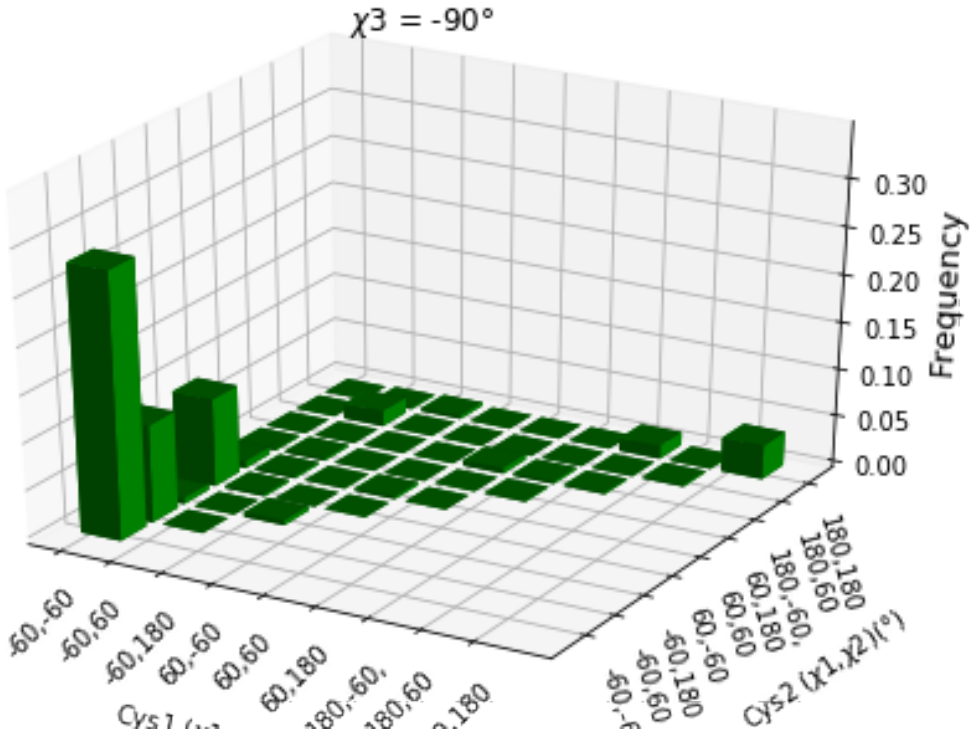
Out[5]: ()

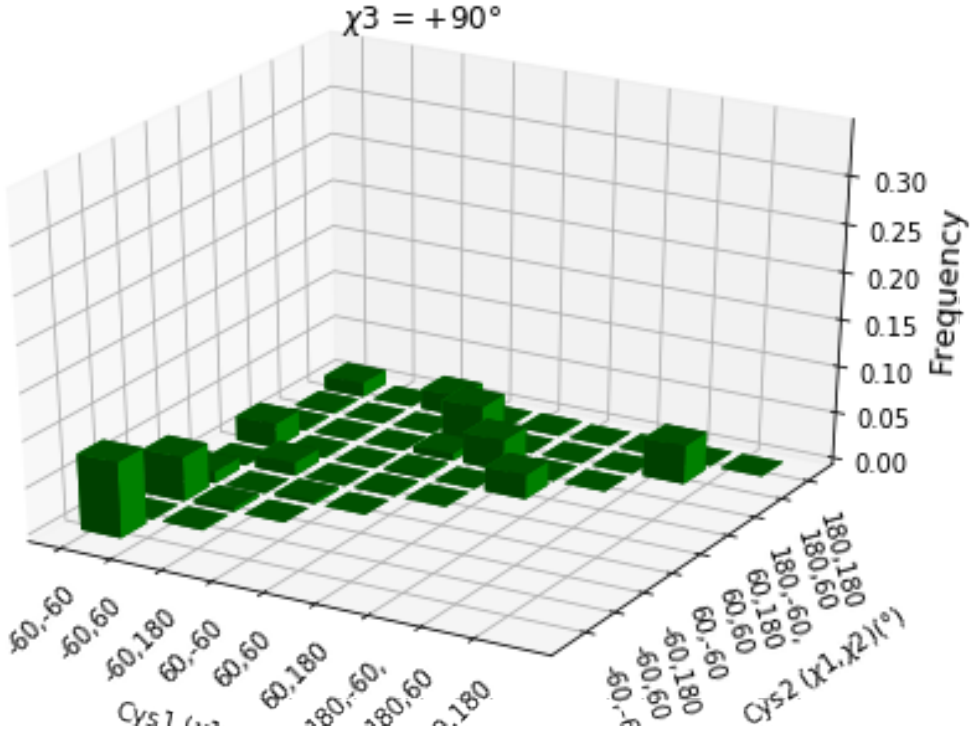




1.1 Generate configuration graphs for peptide cystines

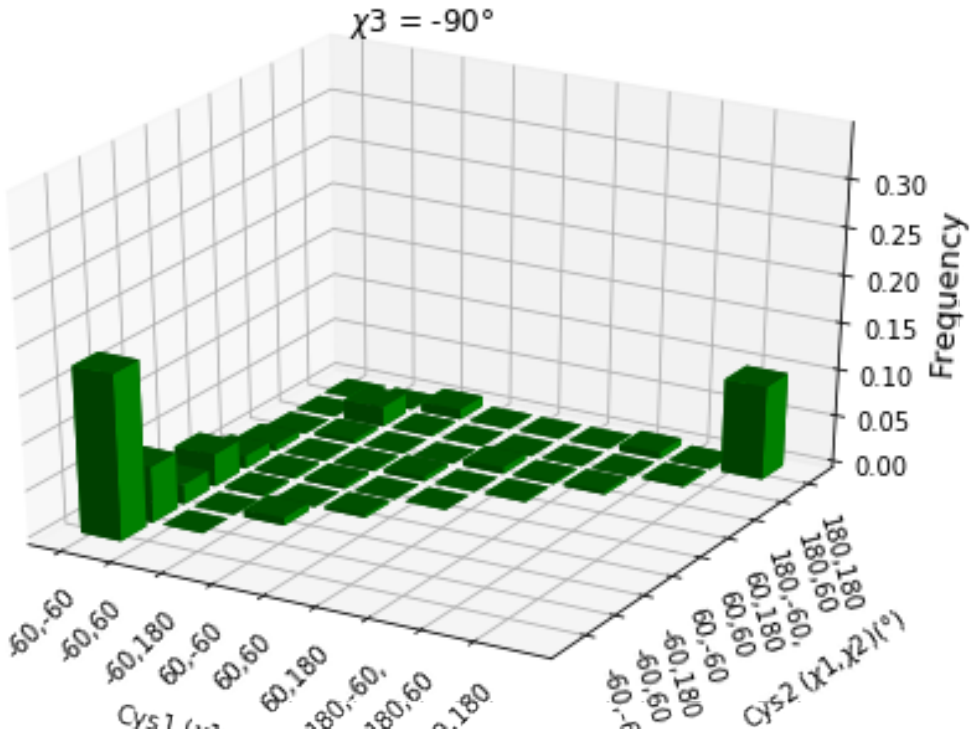
Out[6]: ()

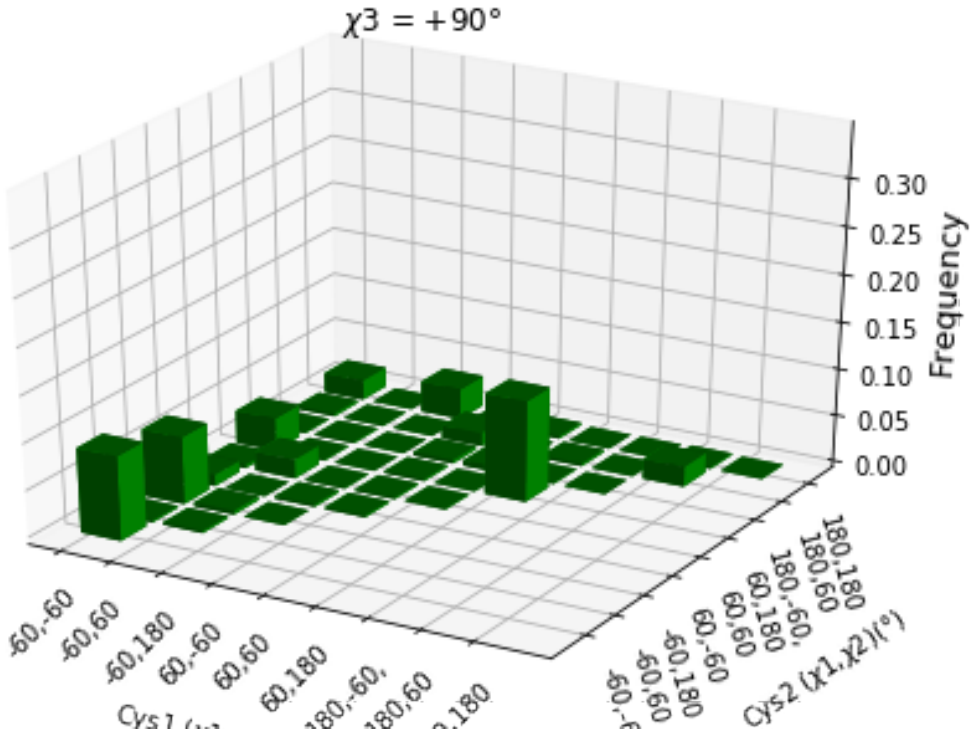

χ3 = -90°
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Frequency
-60,-60
-60,60
-60,180
60,-60
60,60
60,180
180,-60,
180,60
60,-60
60,60
60,180
180,-60,
180,60
180,180
Cys2 (χ1,χ2)(°)


χ3 = +90°
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Frequency
-60,-60
-60,60
-60,180
60,-60
60,60
60,180
180,-60,
180,60
60,-60
60,60
60,180
180,-60,
180,60
180,180
Cys2 (χ1,χ2)(°)

1.2 Generate configuration graphs for protein cystines

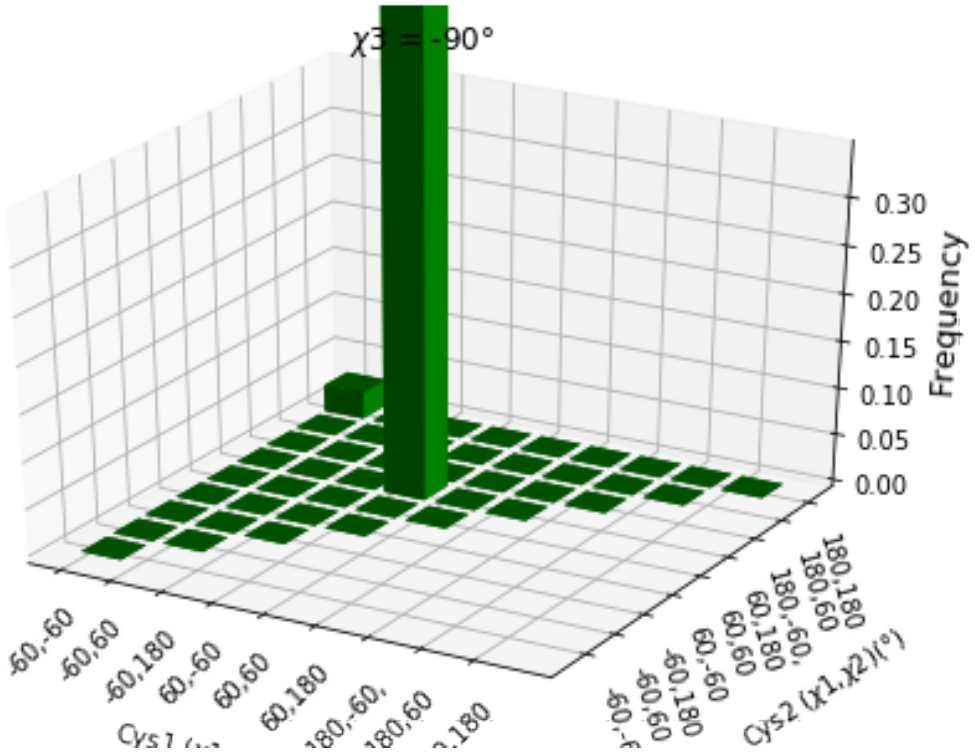
Out[7]: ()





1.3 For Vicinal Disulfides

Out[8]: ()


χ3 = -90°
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Frequency
-60,-60
-60,60
-60,180
60,-60
60,60
60,180
180,-60,
180,60
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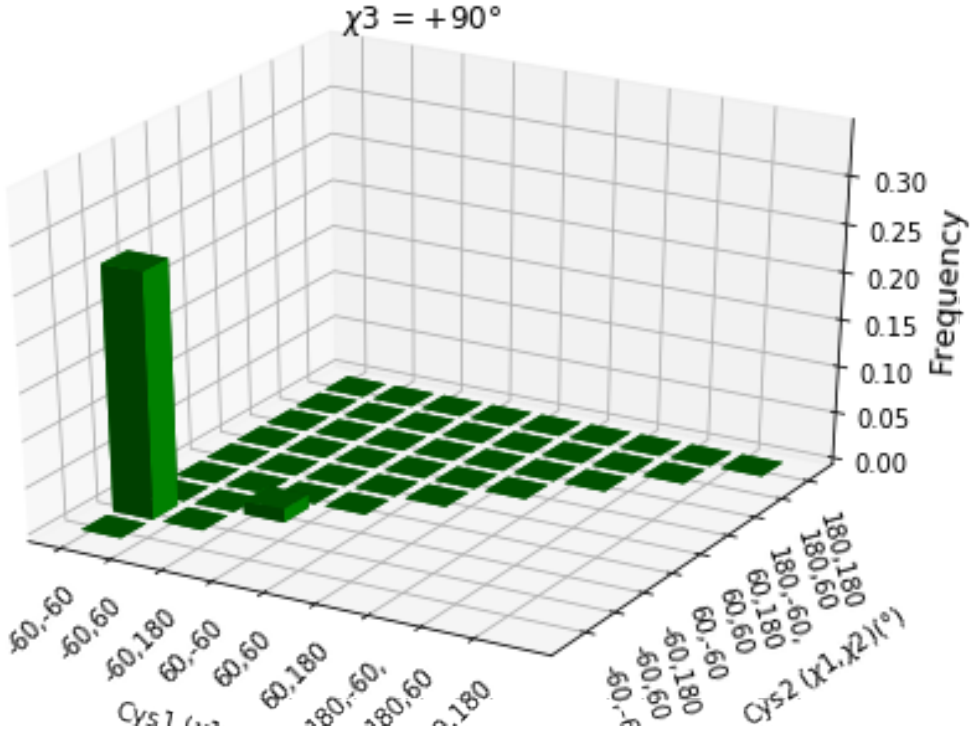
180,-60,
60,180
60,60
60,-60
-60,180
-60,60
Cys2 (χ1,χ2)(°)


χ3 = +90°
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Frequency
-60,-60
-60,60
-60,180
60,-60
60,60
60,180
180,-60,
180,60
180,180
180,-60,
60,180
60,60
60,-60
-60,180
-60,60
Cys2 (χ1,χ2)(°)

1.4 CONFIGURATION FUNCTION

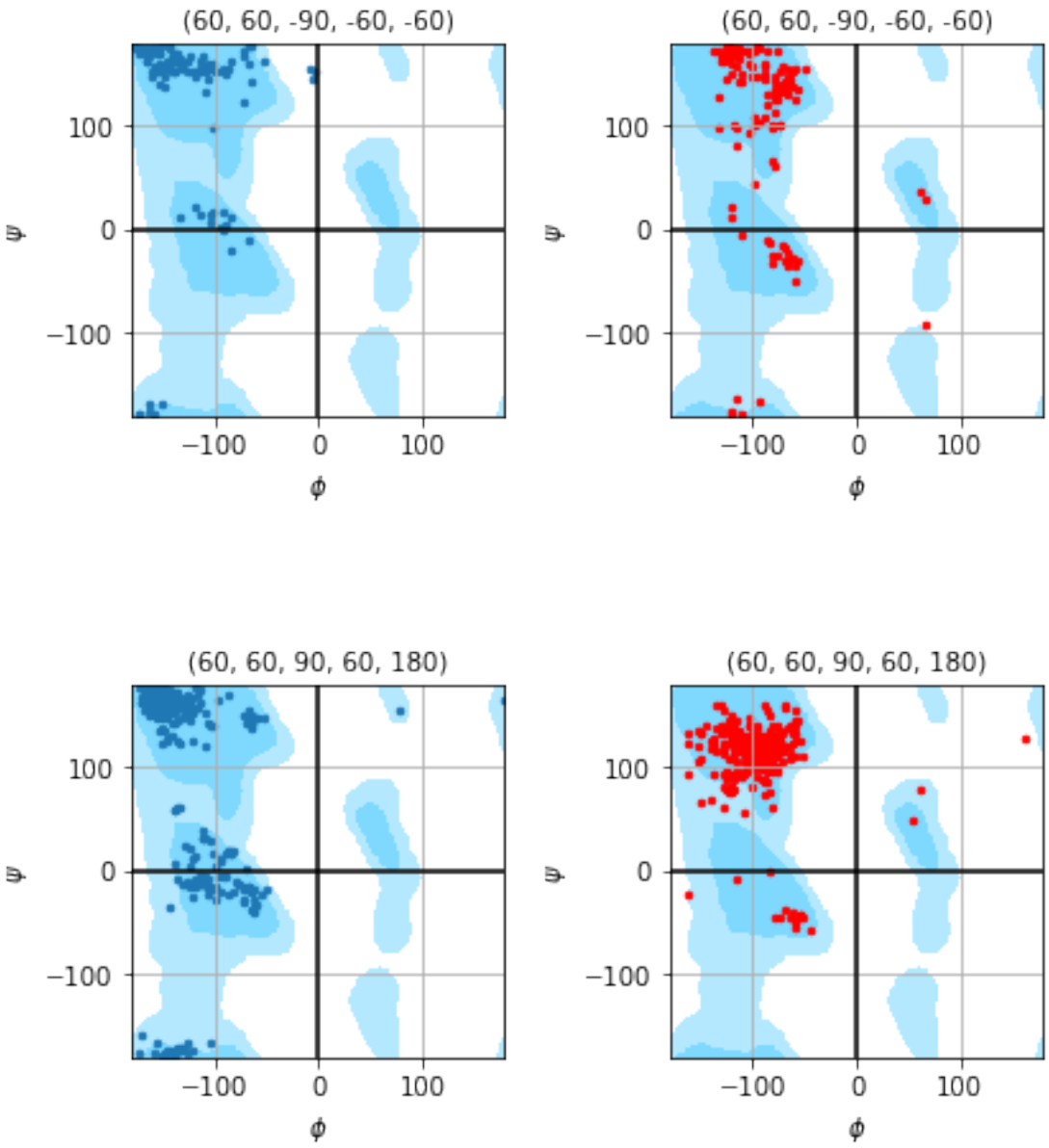
1.4.1 The below funciton returns individual dataframes for each configuration

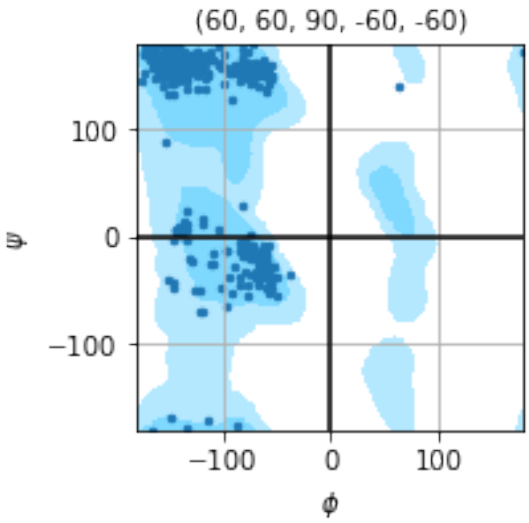
1.4.2 It will be called to generate figures that investigate structural features based on configuration

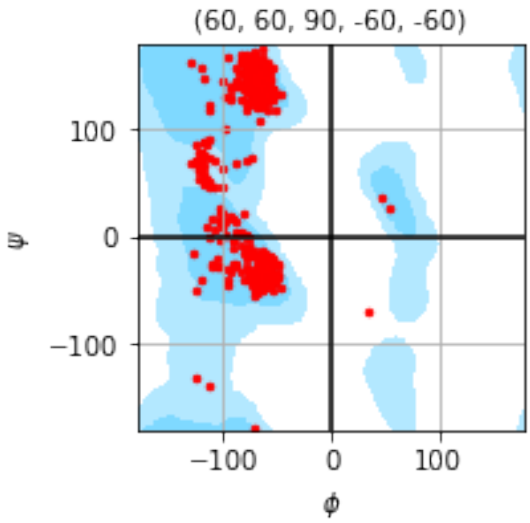
1.4.3 It re-writes the dataframe to ensure Cys1 - Cys2 == Cys2 - Cys1 based on configuration order

1.5 Function to generate Ramachandran Plots

1.6 Call each configuration and




(60, 60, 90, -60, -60)
100
0
−100
ψ
−100
0
100
ϕ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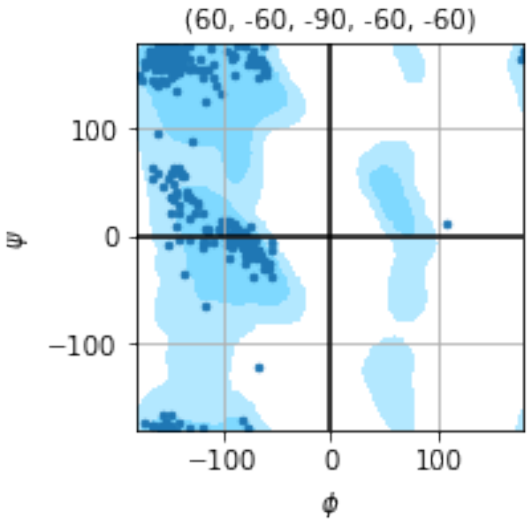
(60, -60, -90, -60, -60)
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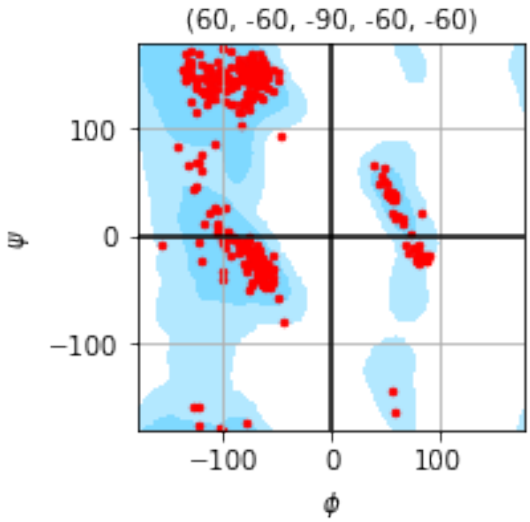
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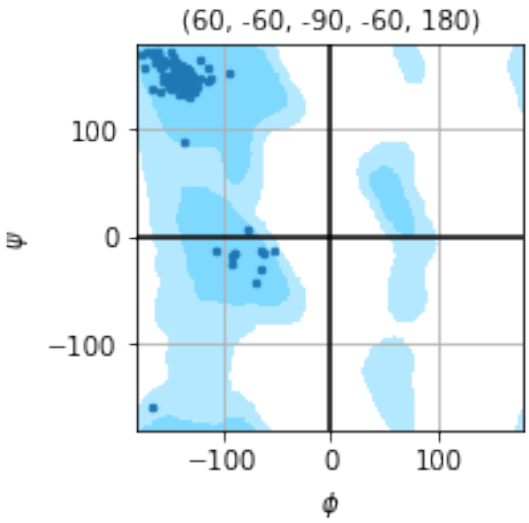
(60, -60, -90, -60, 180)
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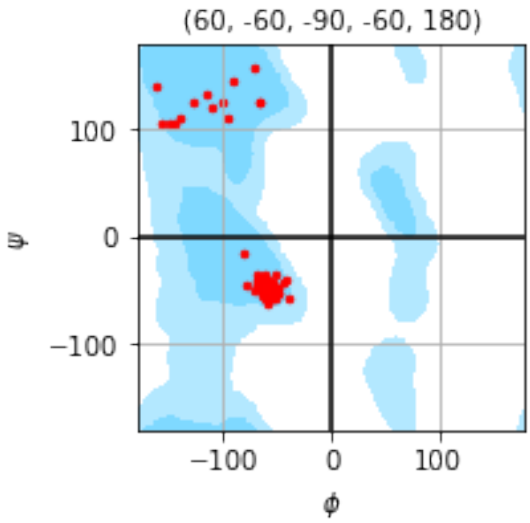
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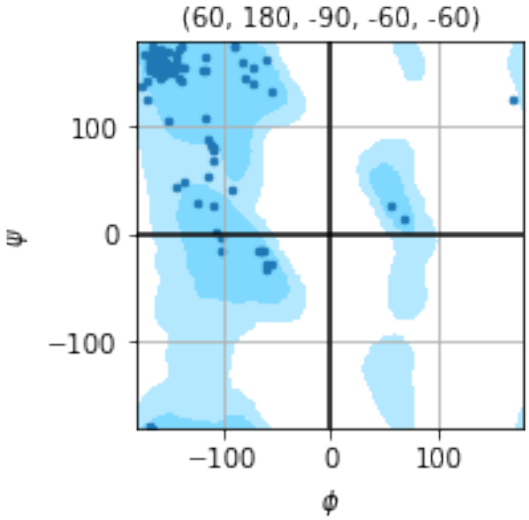
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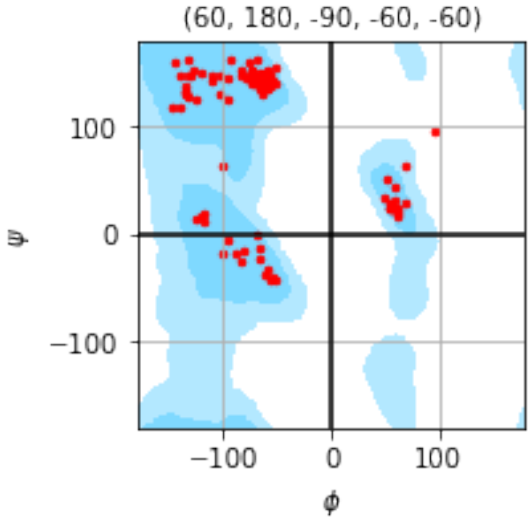
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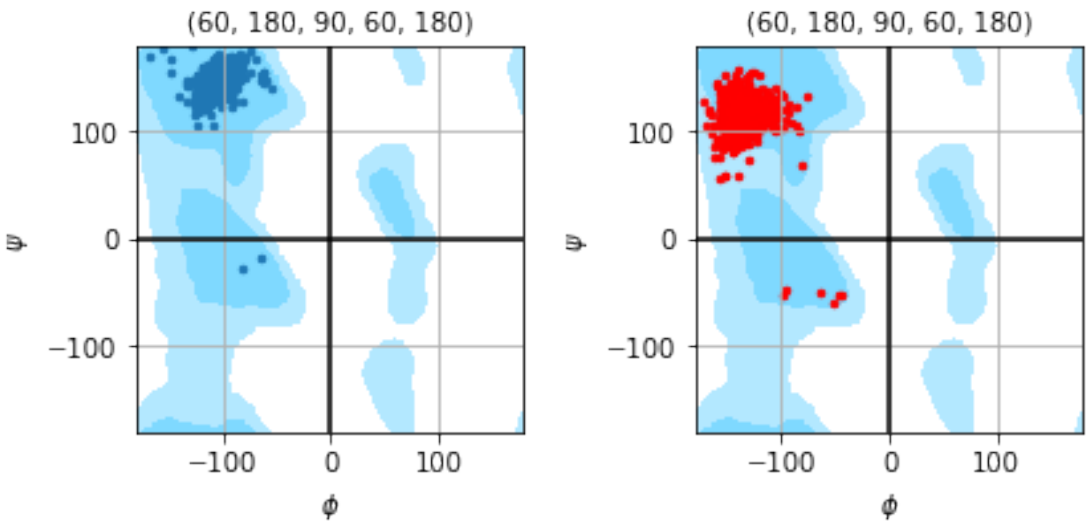
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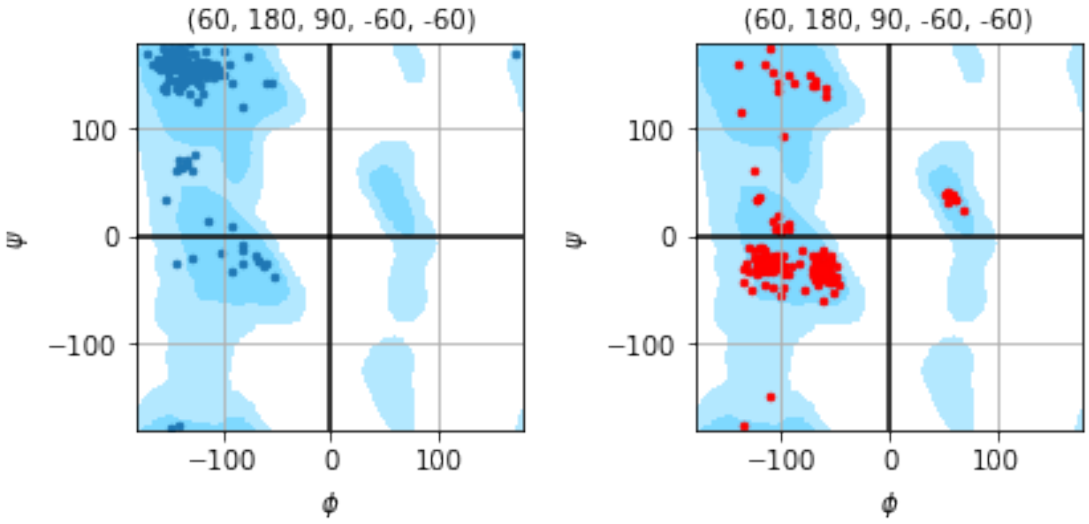
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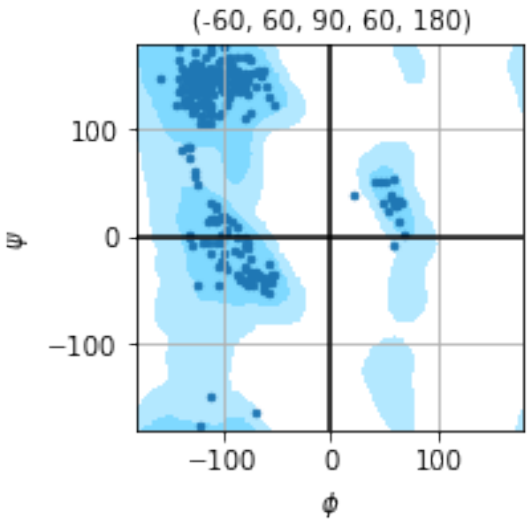
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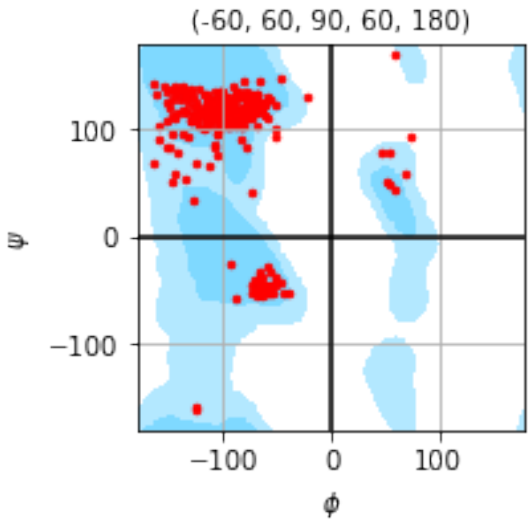
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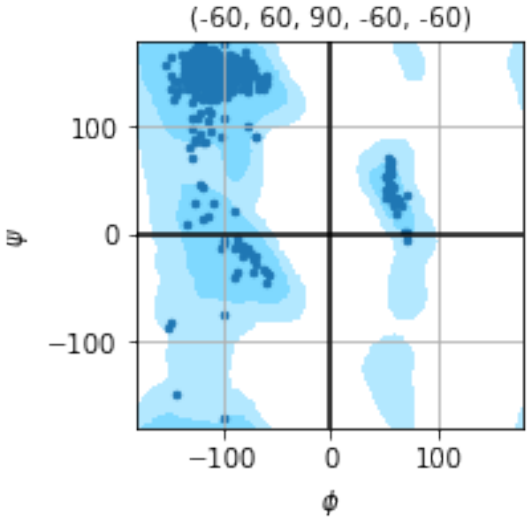
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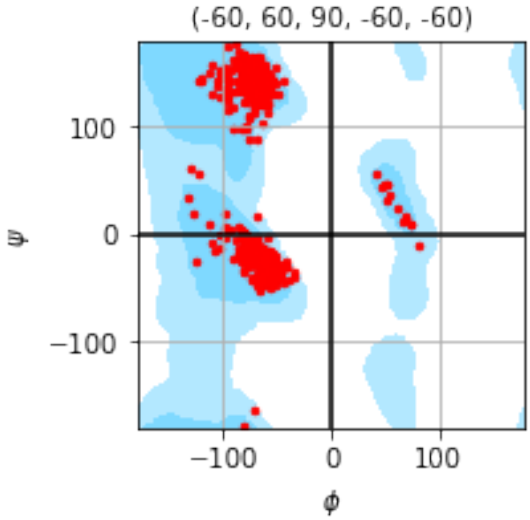
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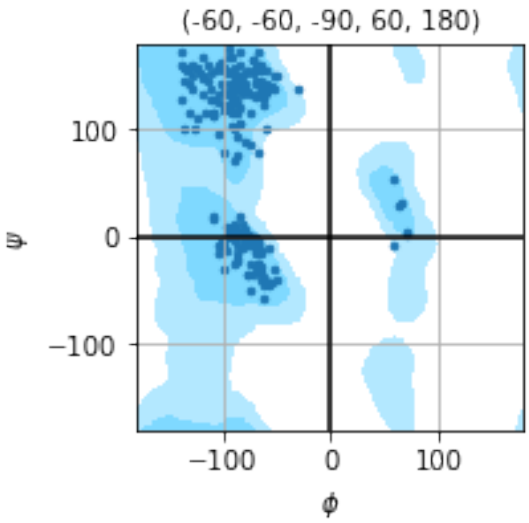
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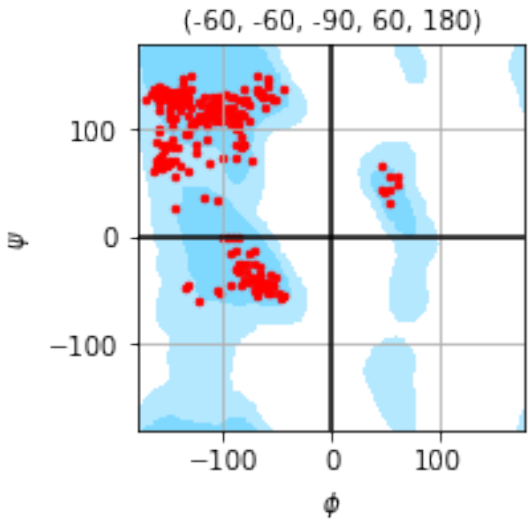
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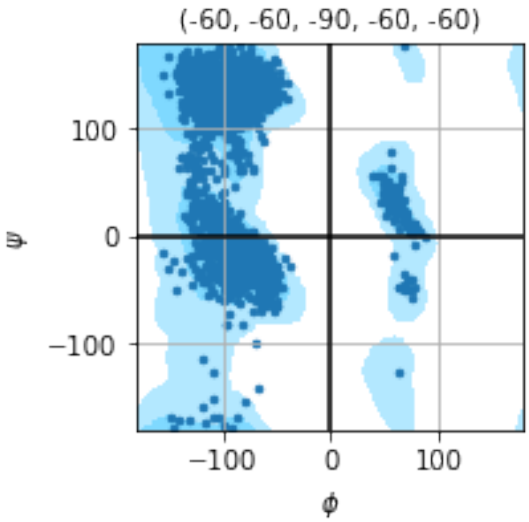
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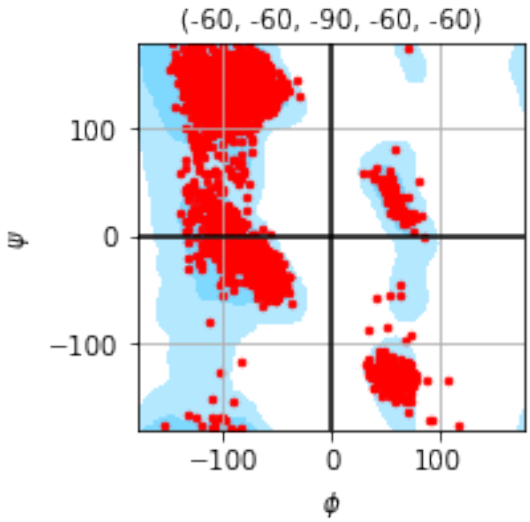
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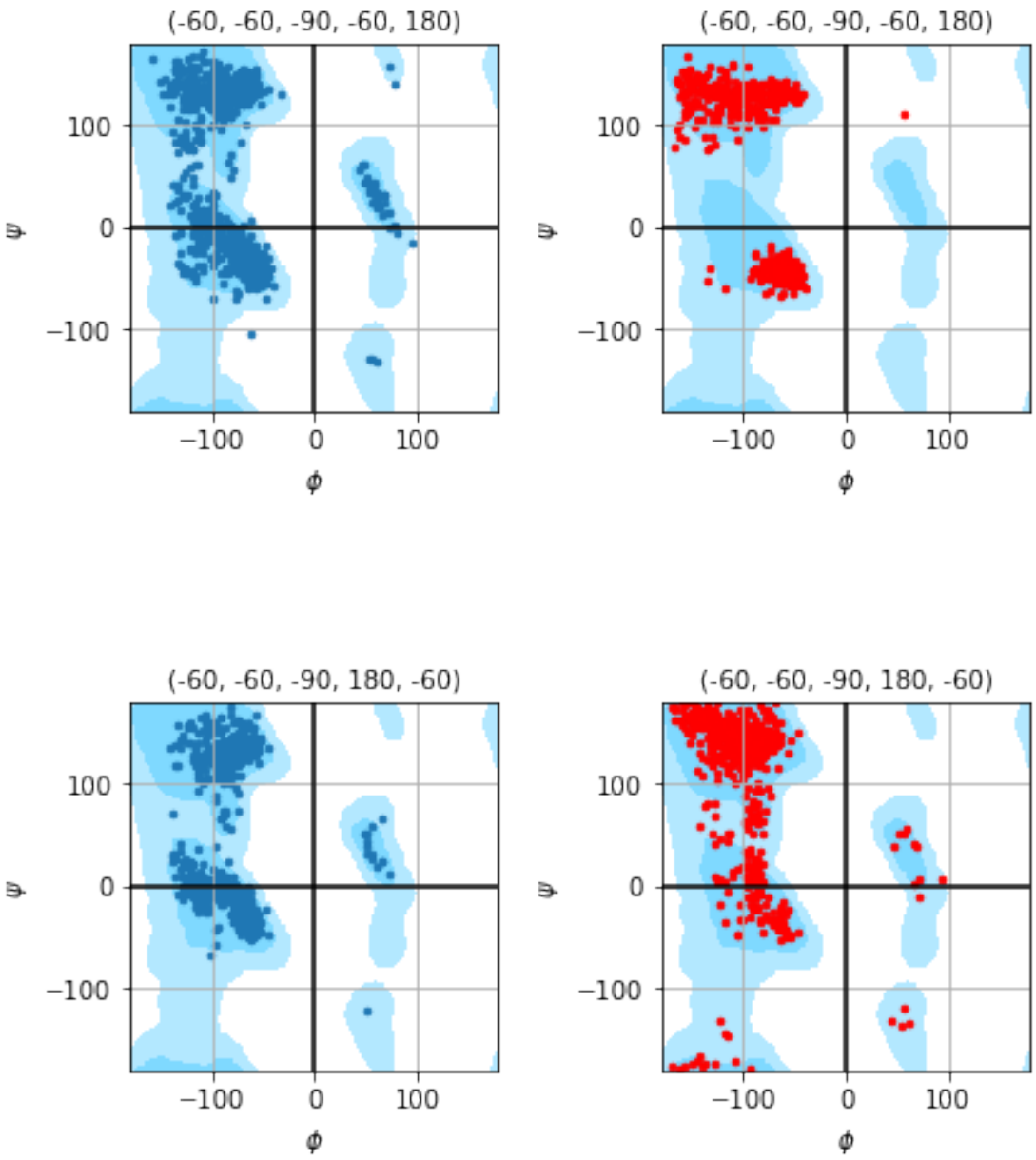
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ψ
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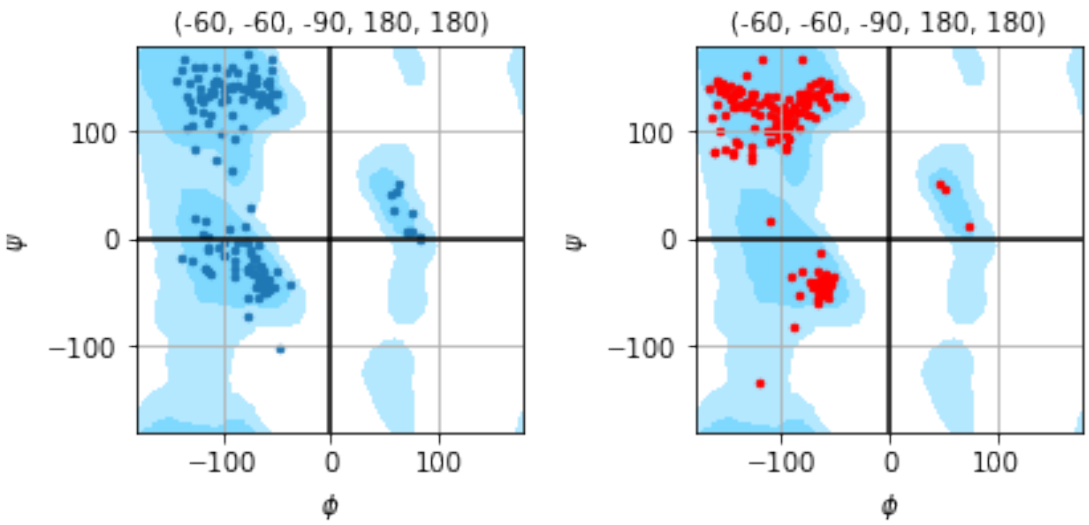
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100
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ψ
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100
ϕ

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ψ
−100
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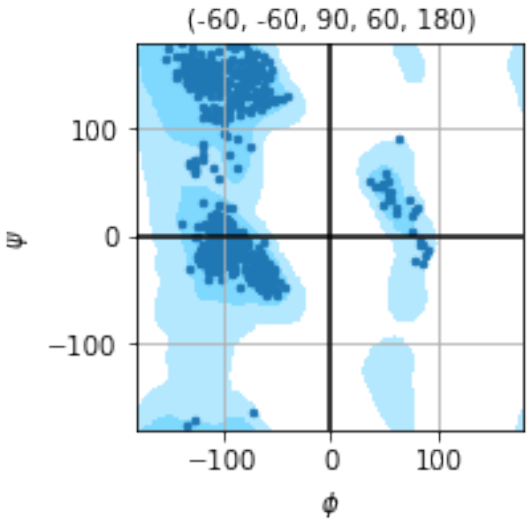
100
ϕ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100
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−100
ψ
−100
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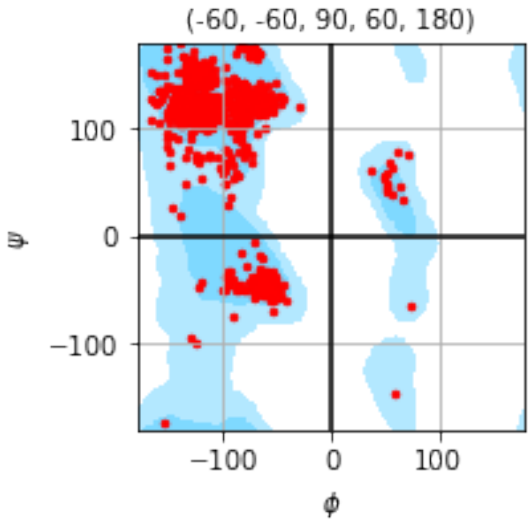
(-60, -60, 90, 60, 180)
100
0
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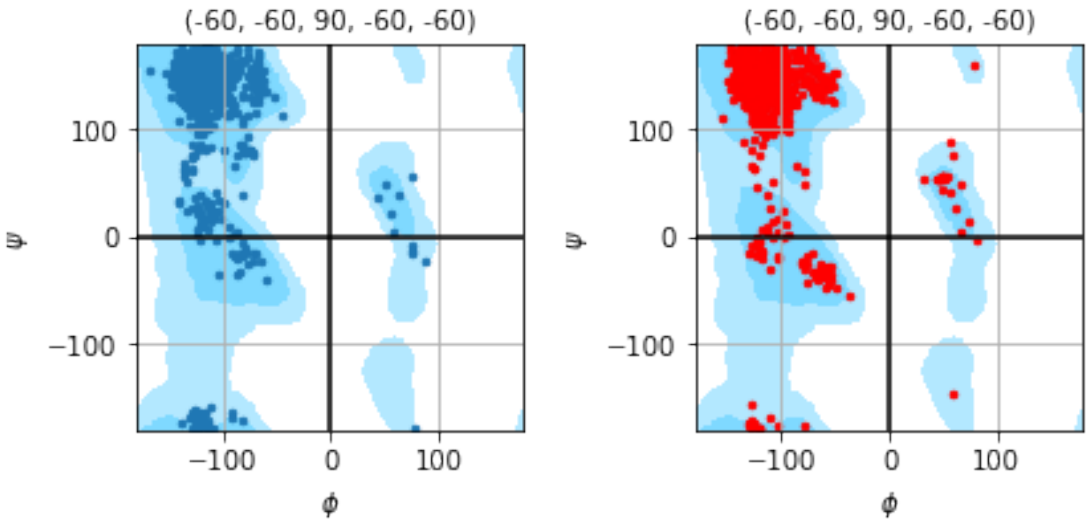
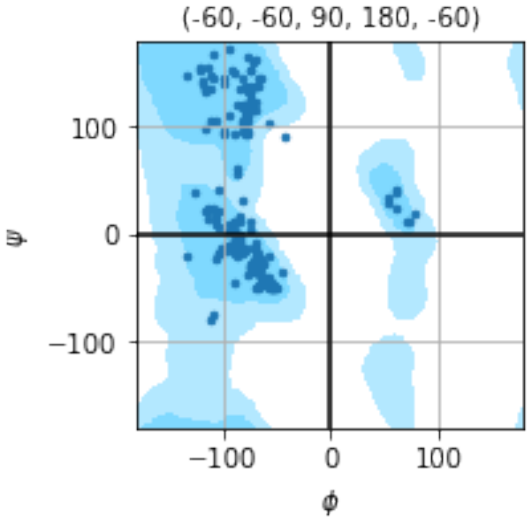

(-60, -60, 90, -60, -60)
100
0
−100
ψ
−100
0
100
ϕ

(-60, -60, 90, -60, -60)
100
0
−100
ψ
−100
0
100
ϕ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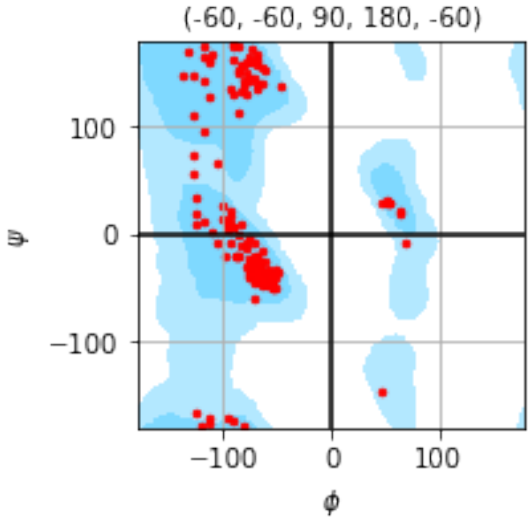
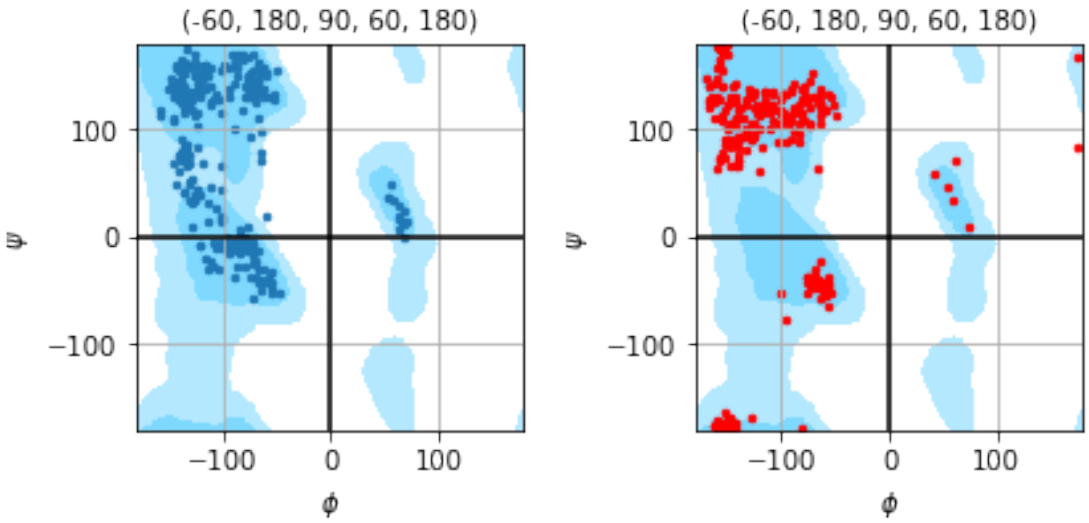
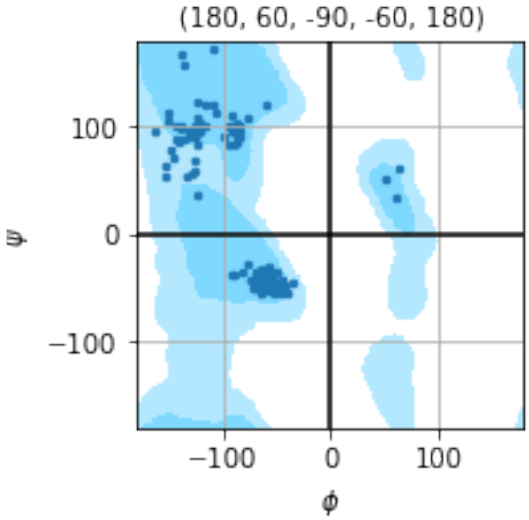
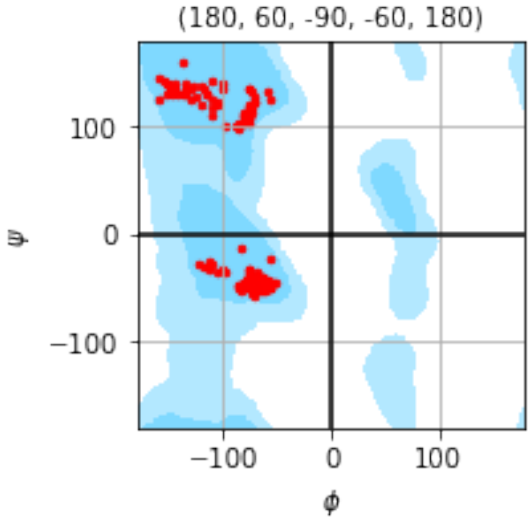
100
0
−100
ψ
−100
0
100
ϕ


(-60, -60, 90, 180, -60)
100
0
−100
ψ
−100
0
100
ϕ


(-60, 180, 90, 60, 180)
100
0
−100
ψ
−100
0
100
ϕ

(-60, 180, 90, 60, 180)
100
0
−100
ψ
−100
0
100
ϕ


(180, 60, -90, -60, 180)
100
0
−100
ψ
−100
0
100
ϕ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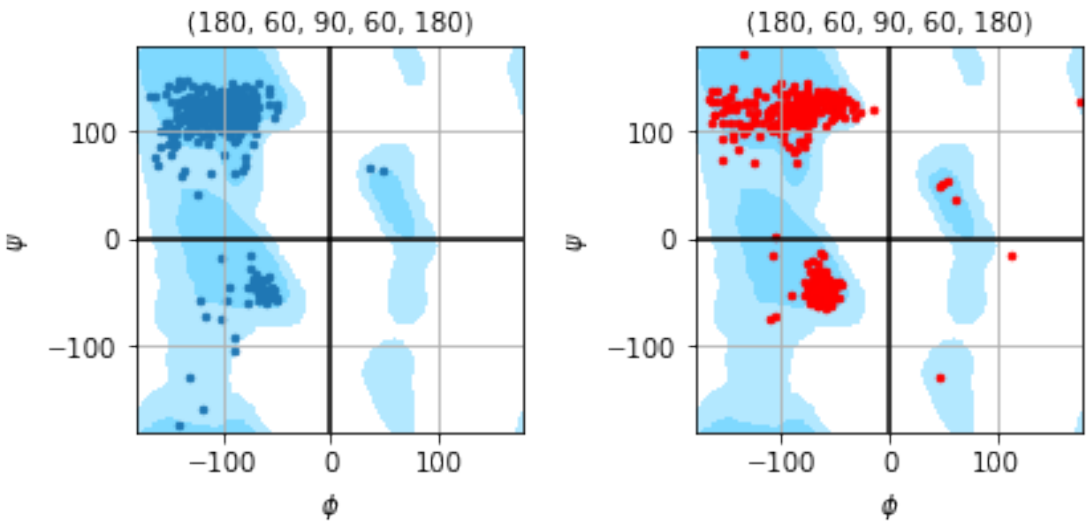
100
0
−100
ψ
−100
0
100
ϕ


(180, 60, 90, 60, 180)
100
0
−100
ψ
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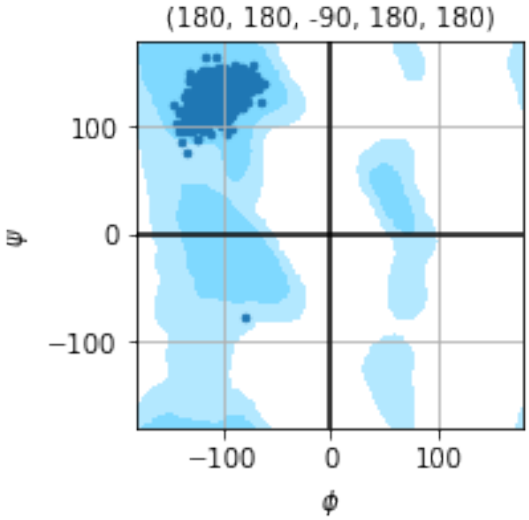
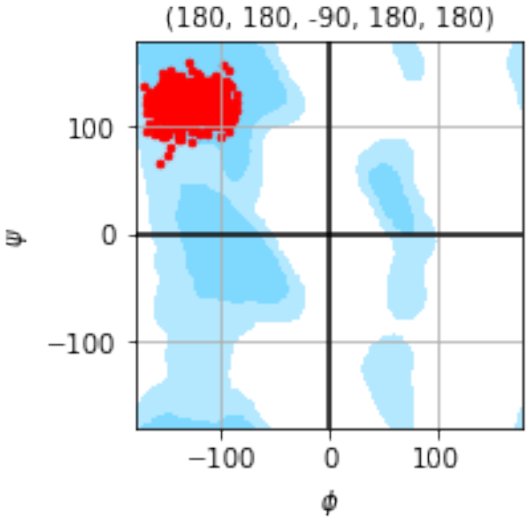
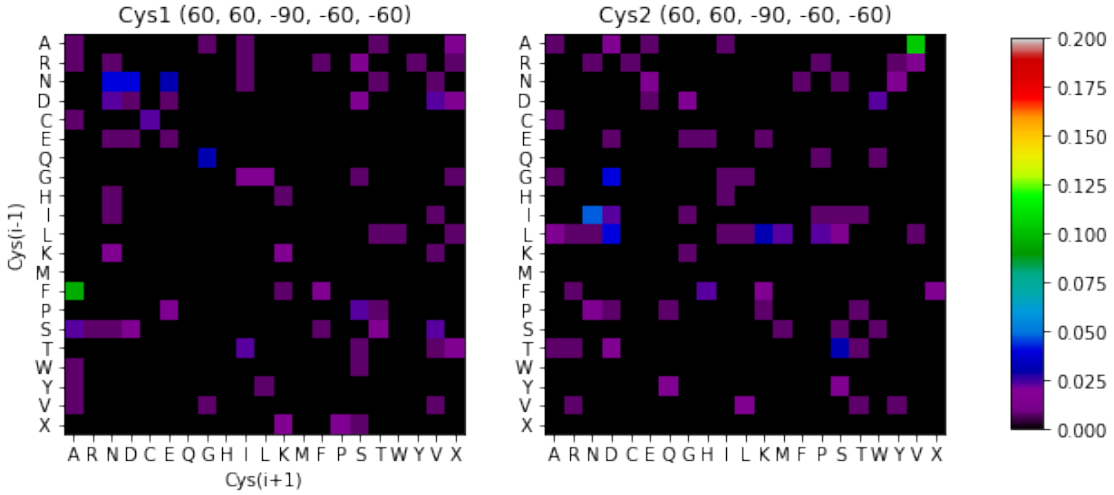
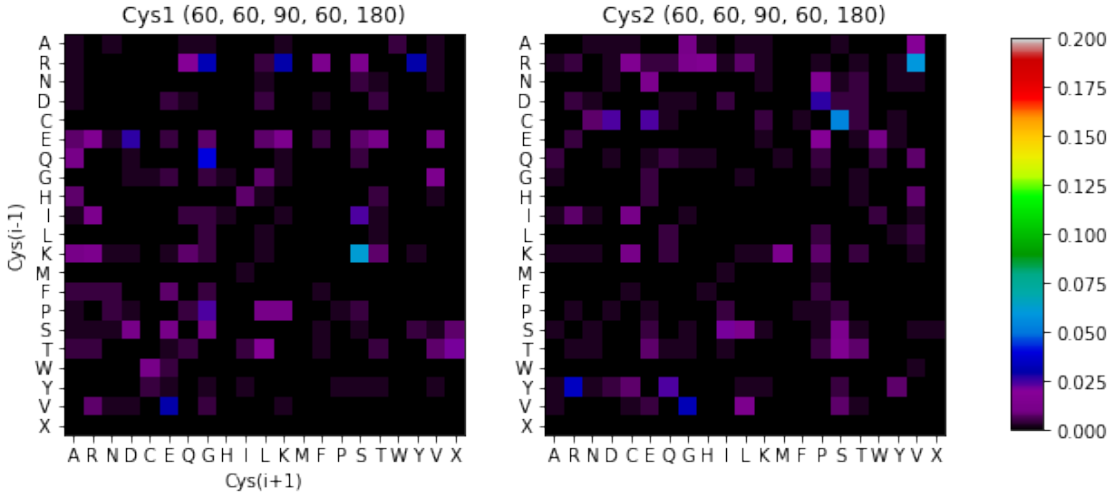
0
100
ϕ

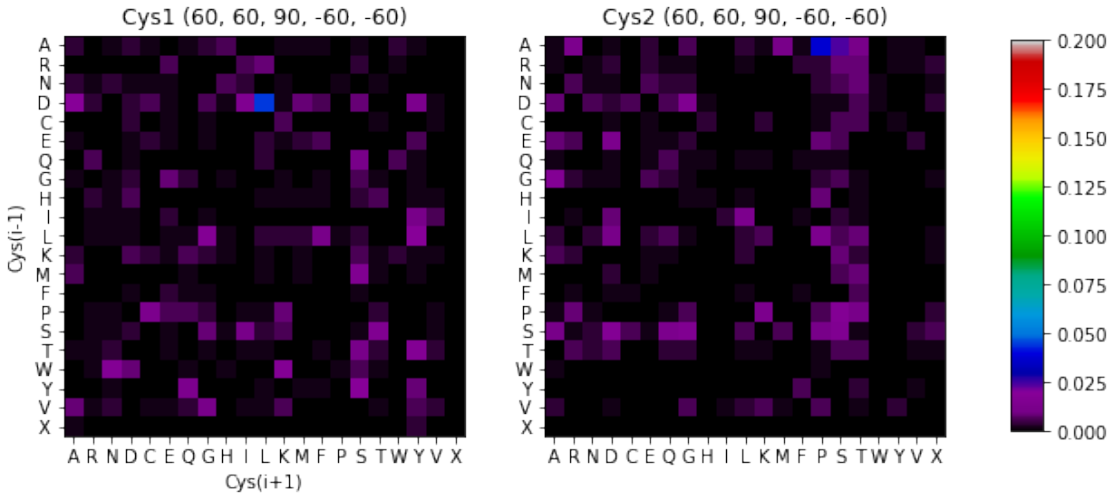
(180, 60, 90, 60, 180)
100
0
−100
ψ
−100
0
100
ϕ

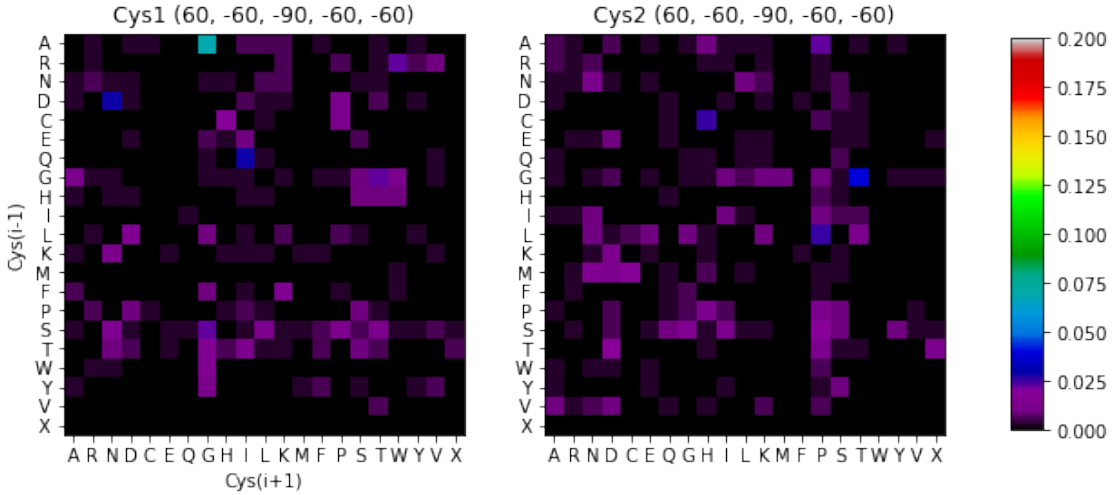

(180, 180, -90, 180, 180)
100
0
−100
ψ
−100
0
100
ϕ

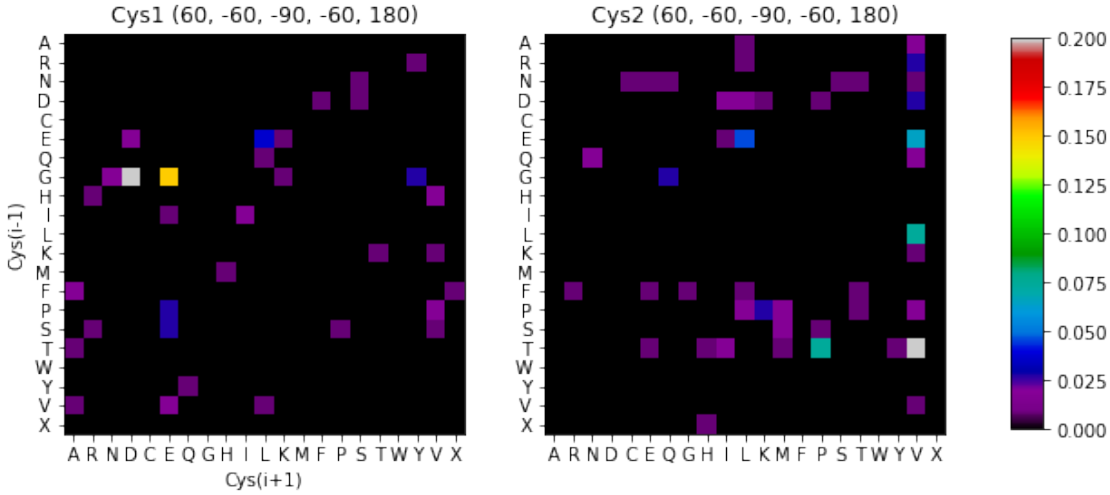

(180, 180, -90, 180, 180)
100
0
−100
ψ
−100
0
100
ϕ

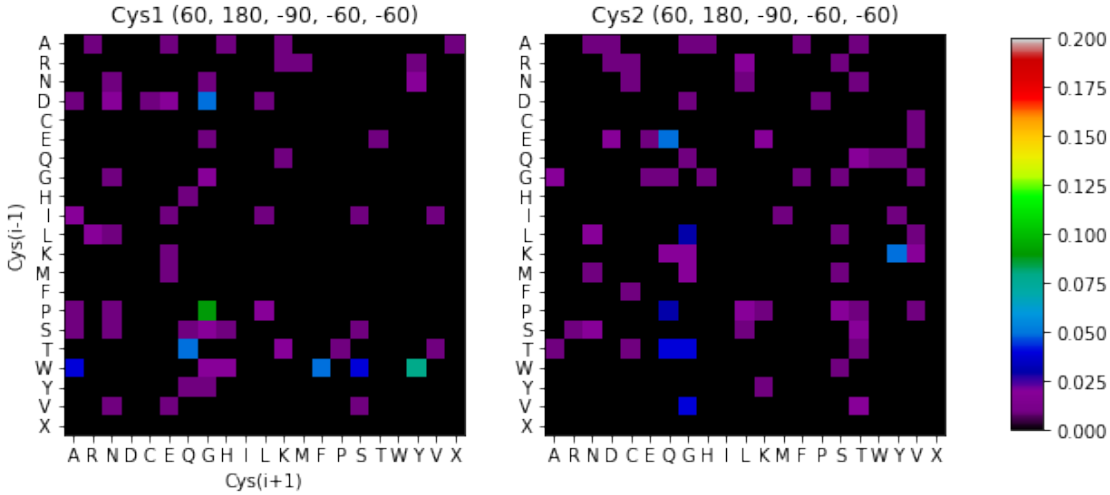

Cys1 (60, 60, -90, -60, -60)
Cys2 (60, 60, -90, -60, -60)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

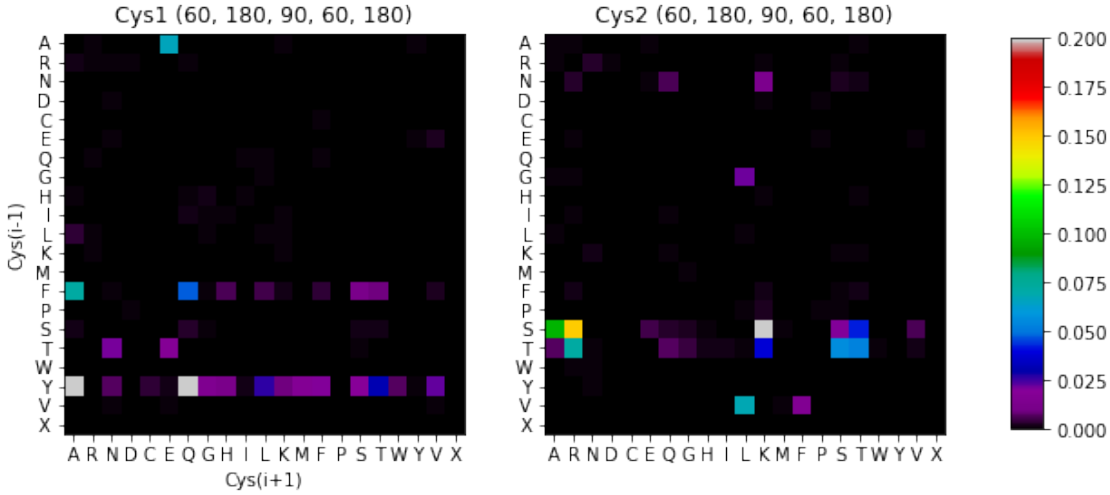

Cys1 (60, 60, 90, 60, 180)
Cys2 (60, 60, 90, 60, 180)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

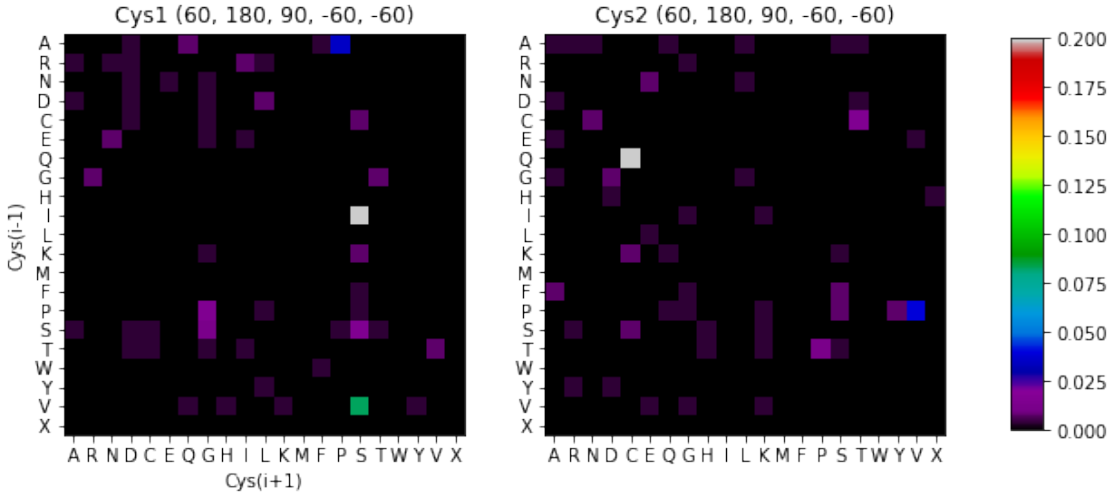

Cys1 (60, 60, 90, -60, -60)
Cys2 (60, 60, 90, -60, -60)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

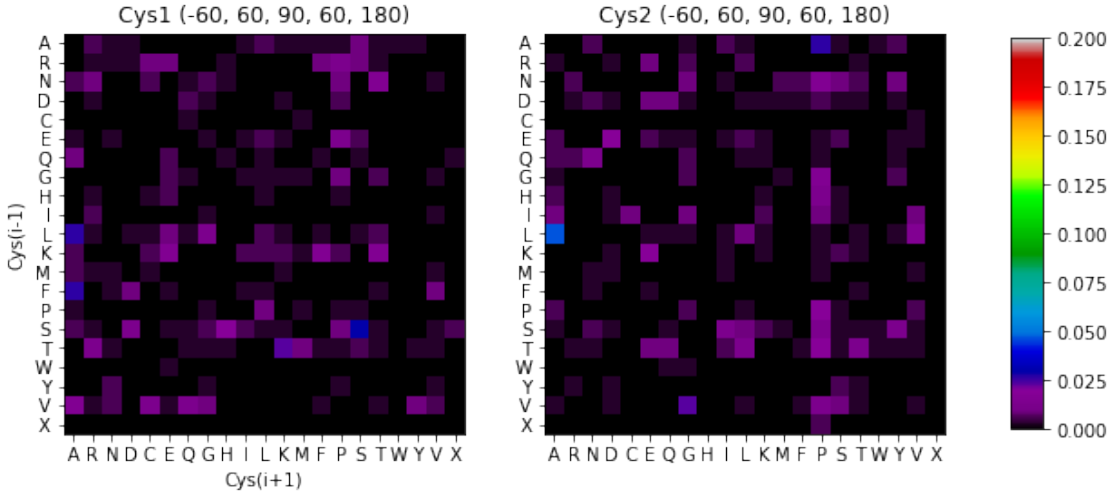

Cys1 (60, -60, -90, -60, -60)
Cys2 (60, -60, -90, -60, -60)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

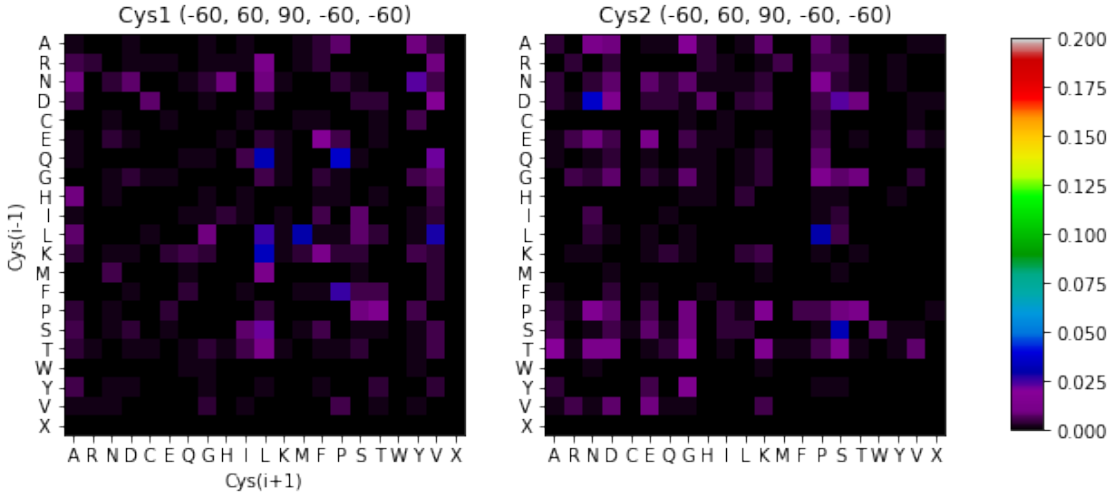

Cys1 (60, -60, -90, -60, 180)
Cys2 (60, -60, -90, -60, 180)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

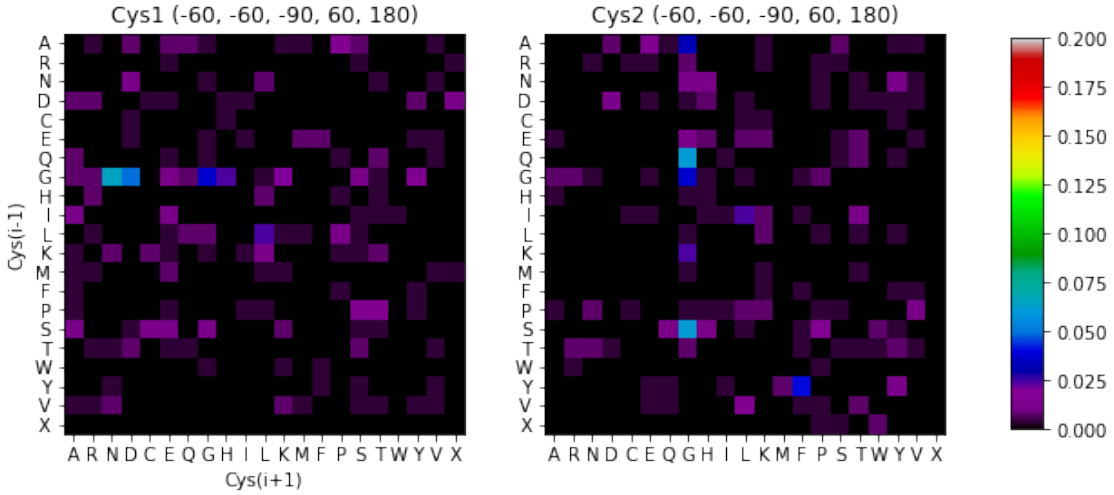

Cys1 (60, 180, -90, -60, -60)
Cys2 (60, 180, -90, -60, -60)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

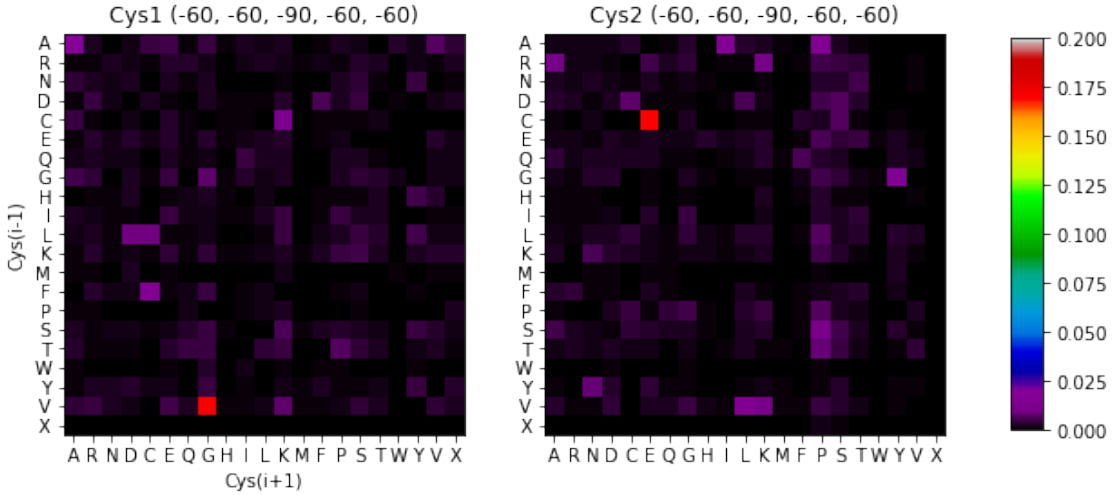

Cys1 (60, 180, 90, 60, 180)
Cys2 (60, 180, 90, 60, 180)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

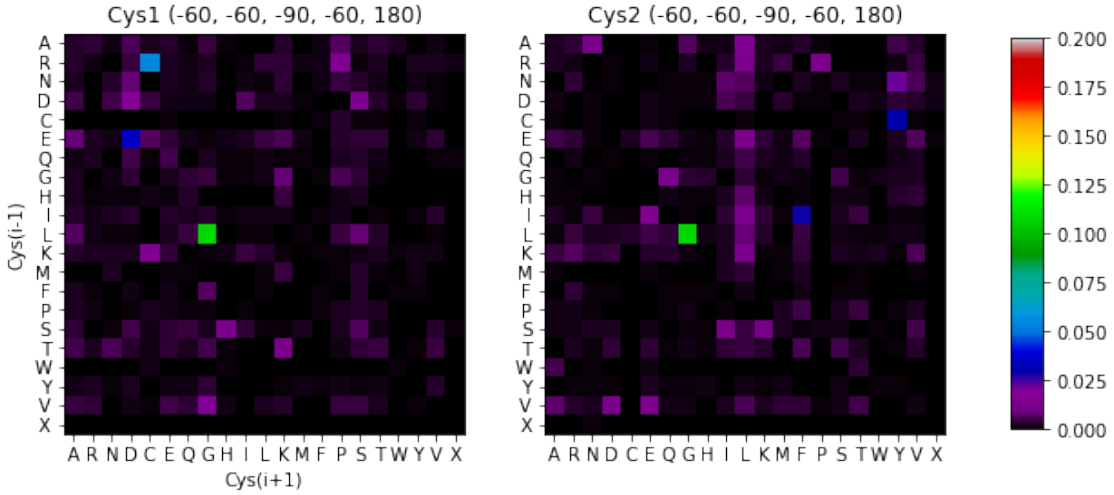

Cys1 (60, 180, 90, -60, -60)
Cys2 (60, 180, 90, -60, -60)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

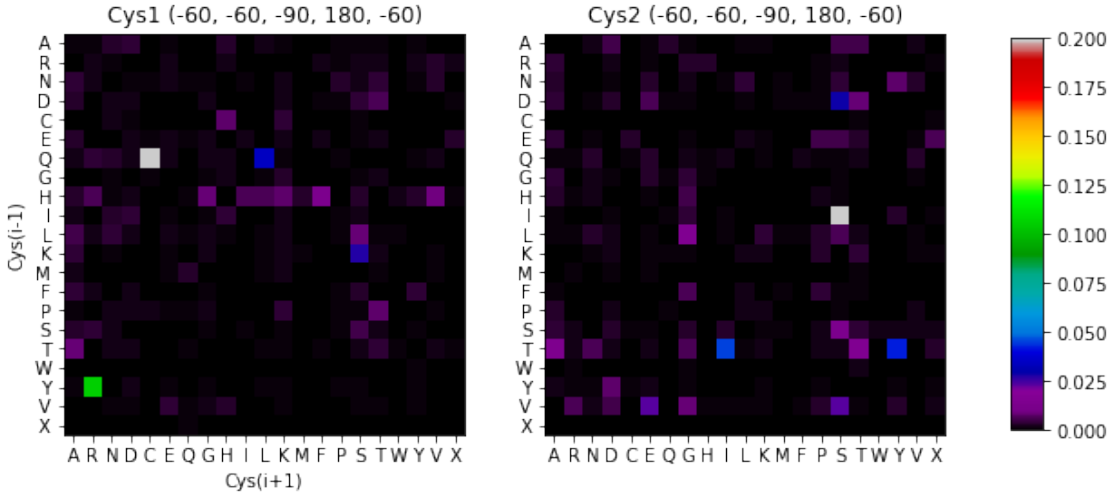

Cys1 (-60, 60, 90, 60, 180)
Cys2 (-60, 60, 90, 60, 180)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

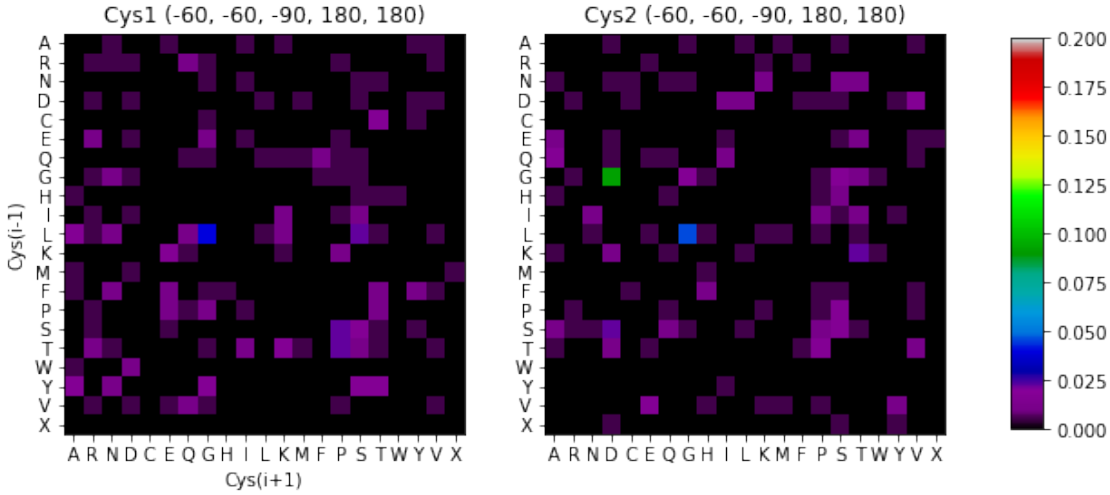

Cys1 (-60, 60, 90, -60, -60)
Cys2 (-60, 60, 90, -60, -60)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

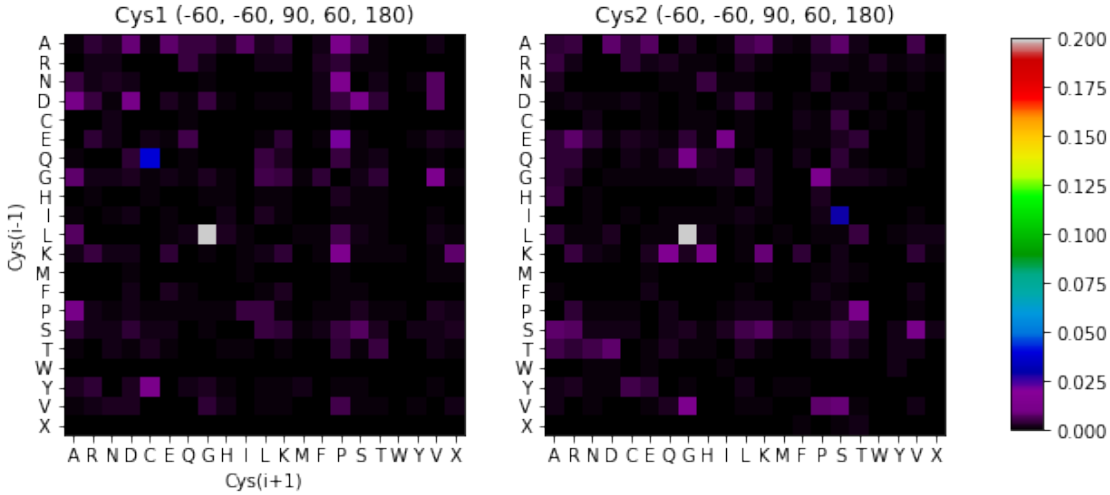

Cys1 (-60, -60, -90, 60, 180)
Cys2 (-60, -60, -90, 60, 180)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

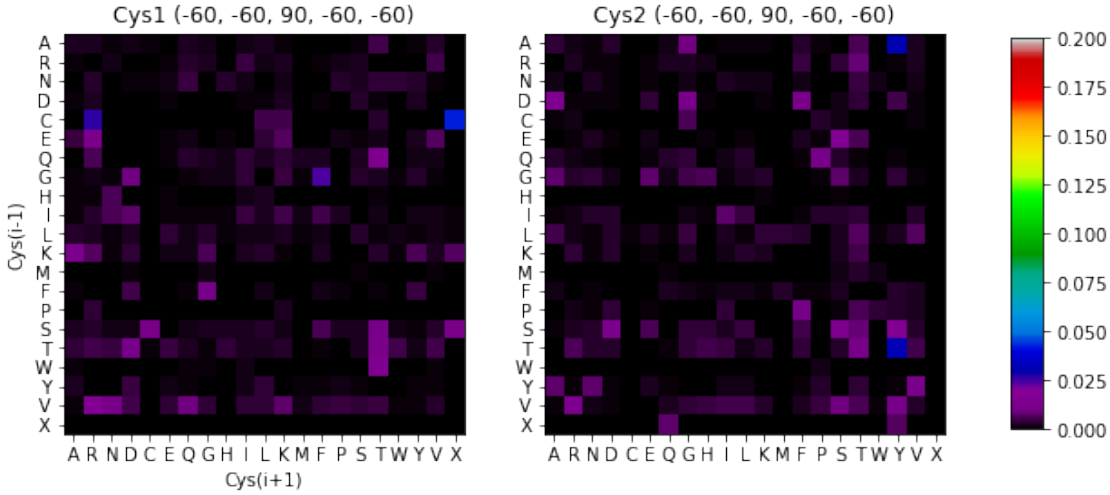

Cys1 (-60, -60, -90, -60, -60)
Cys2 (-60, -60, -90, -60, -60)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

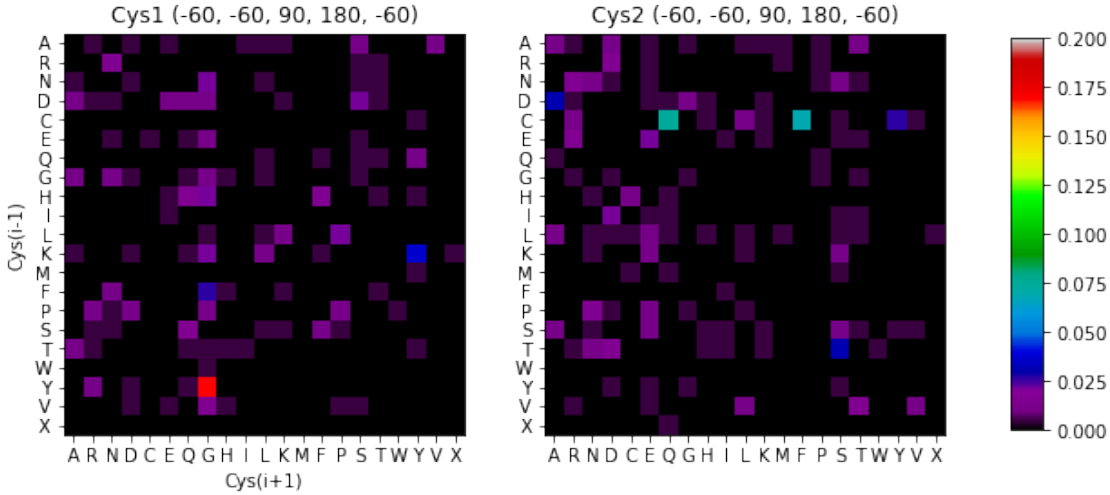

Cys1 (-60, -60, -90, -60, 180)
Cys2 (-60, -60, -90, -60, 180)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

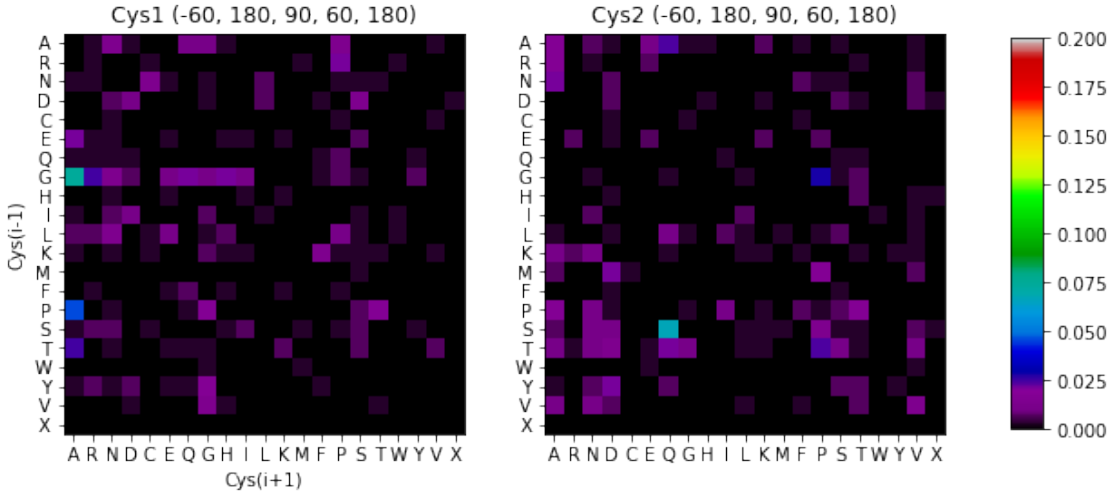

Cys1 (-60, -60, -90, 180, -60)
Cys2 (-60, -60, -90, 180, -60)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

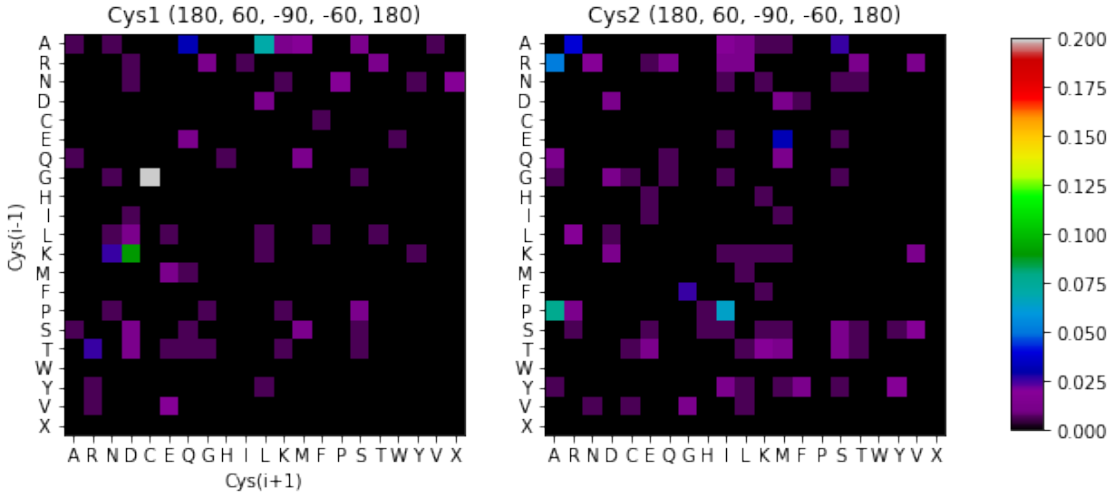

Cys1 (-60, -60, -90, 180, 180)
Cys2 (-60, -60, -90, 180, 180)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

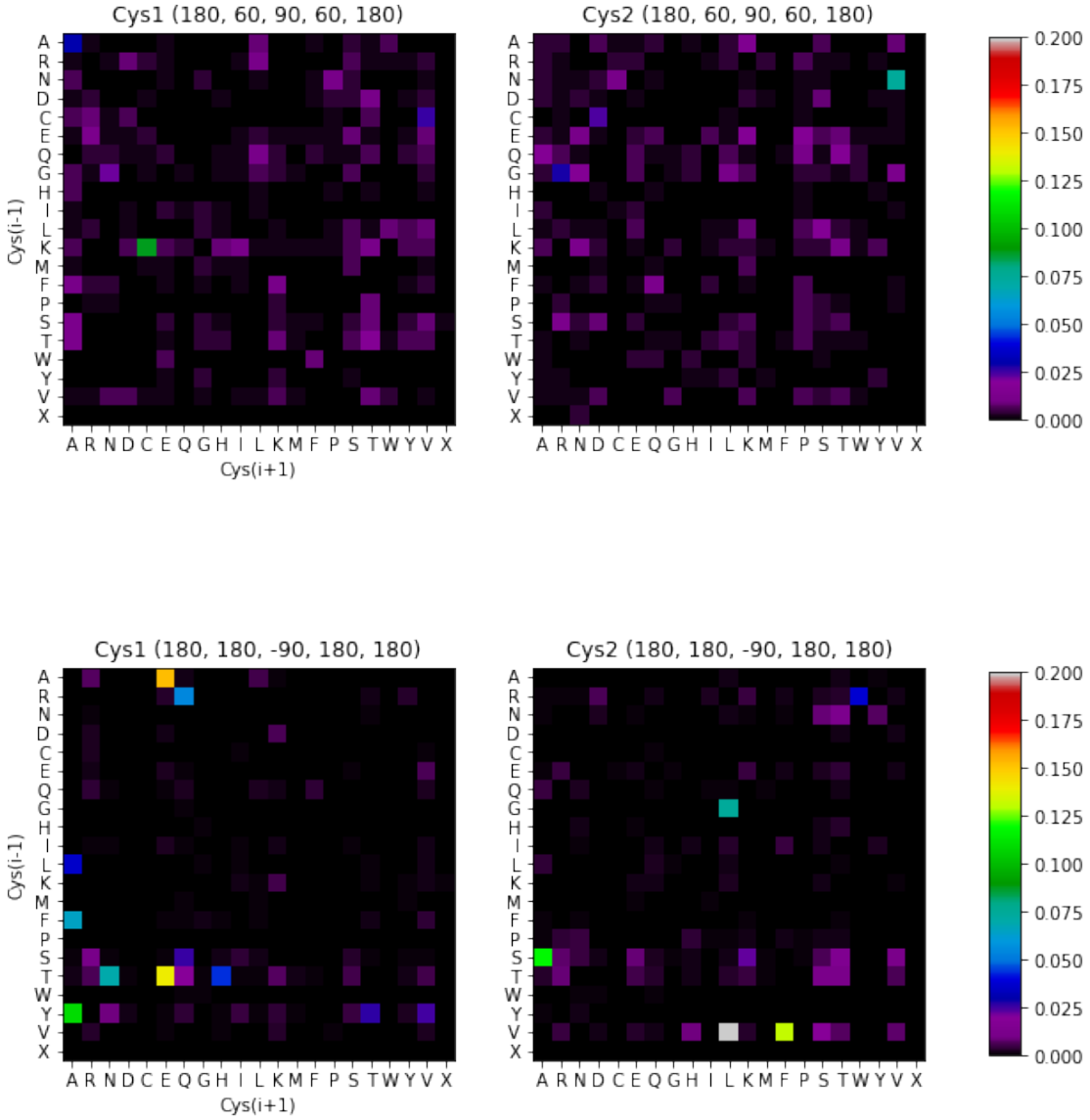

Cys1 (-60, -60, 90, 60, 180)
Cys2 (-60, -60, 90, 60, 180)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000


Cys1 (-60, -60, 90, -60, -60)
Cys2 (-60, -60, 90, -60, -60)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

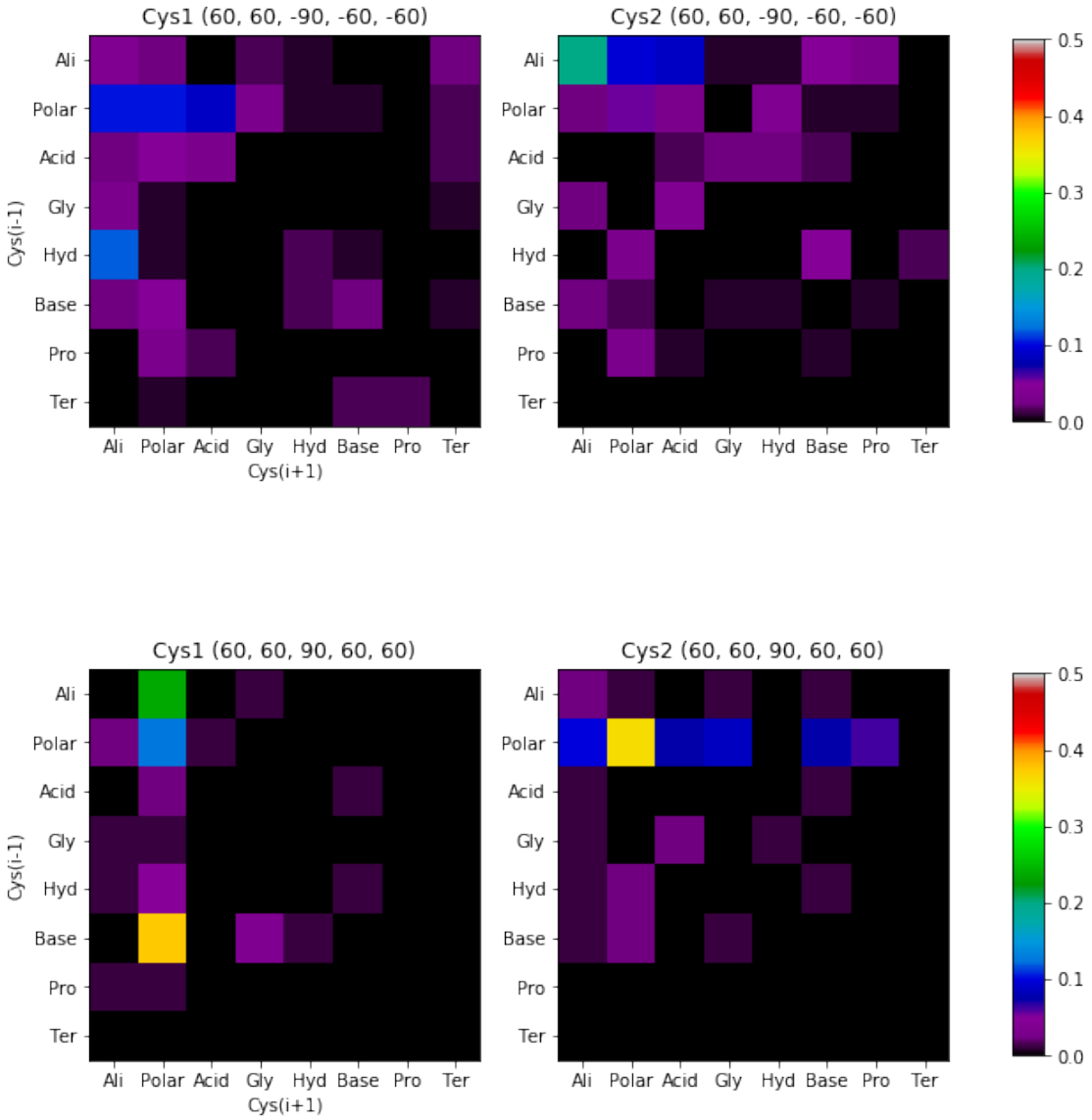

Cys1 (-60, -60, 90, 180, -60)
Cys2 (-60, -60, 90, 180, -60)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

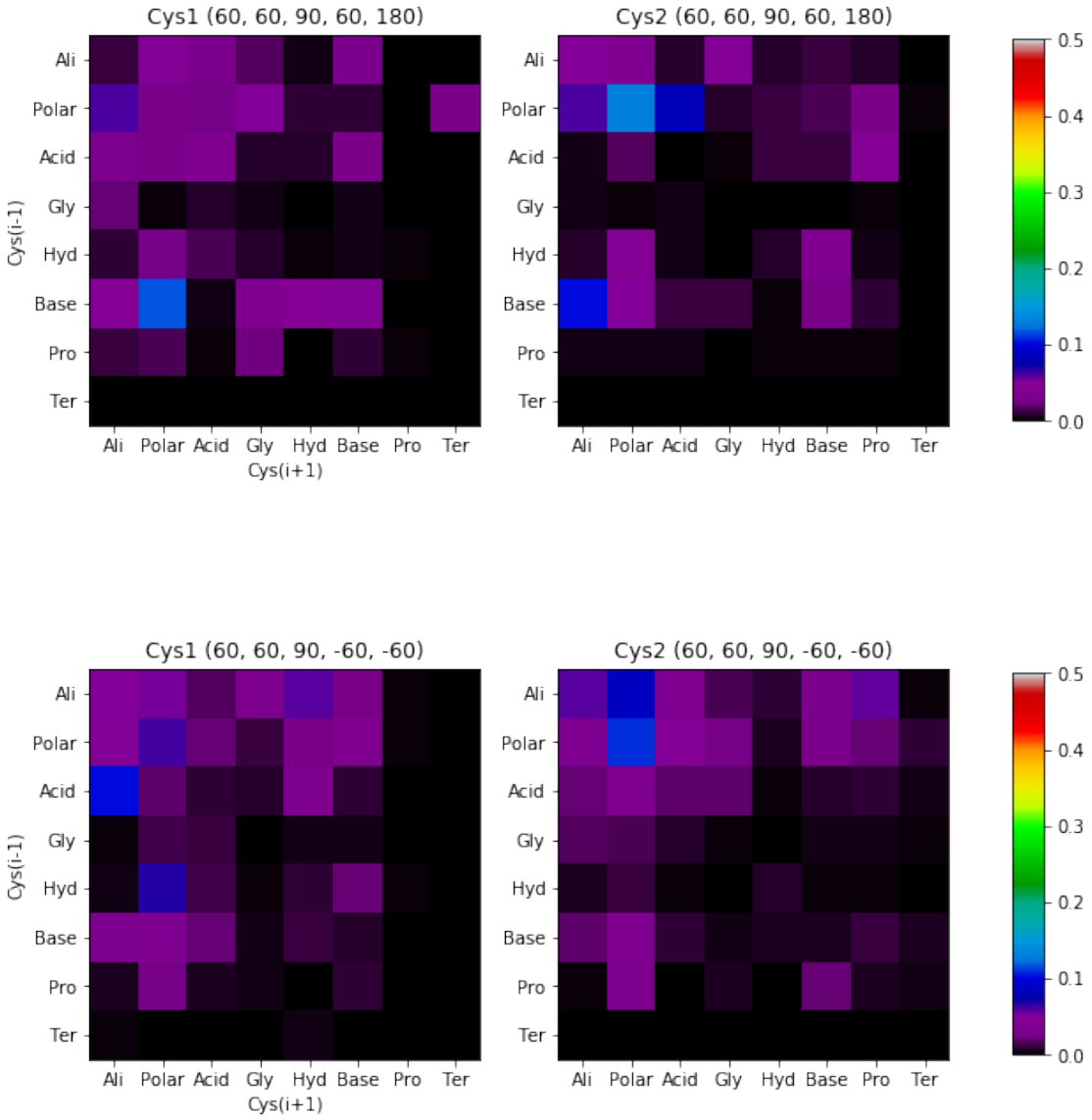

Cys1 (-60, 180, 90, 60, 180)
Cys2 (-60, 180, 90, 60, 180)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

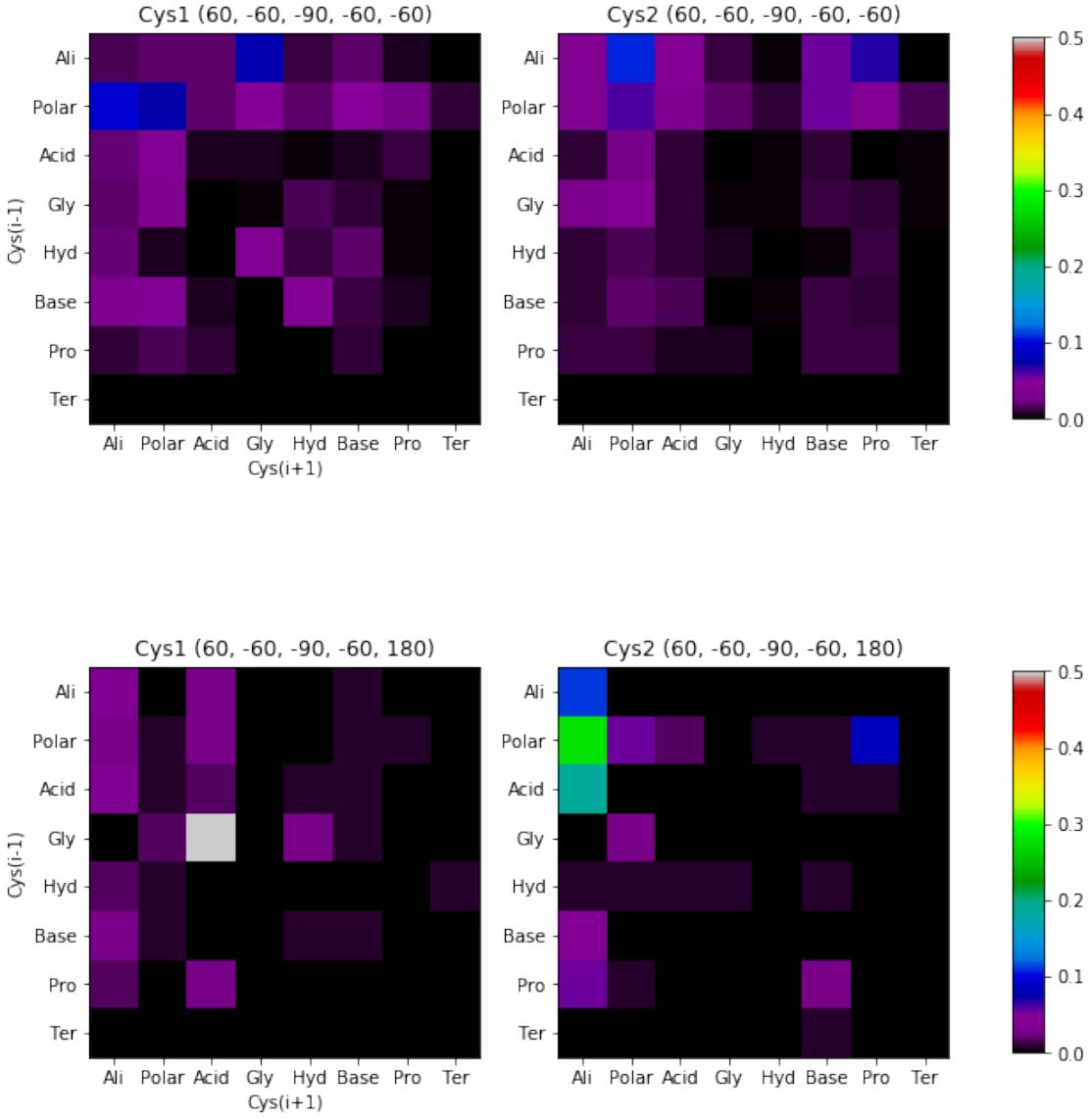

Cys1 (180, 60, -90, -60, 180)
Cys2 (180, 60, -90, -60, 180)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

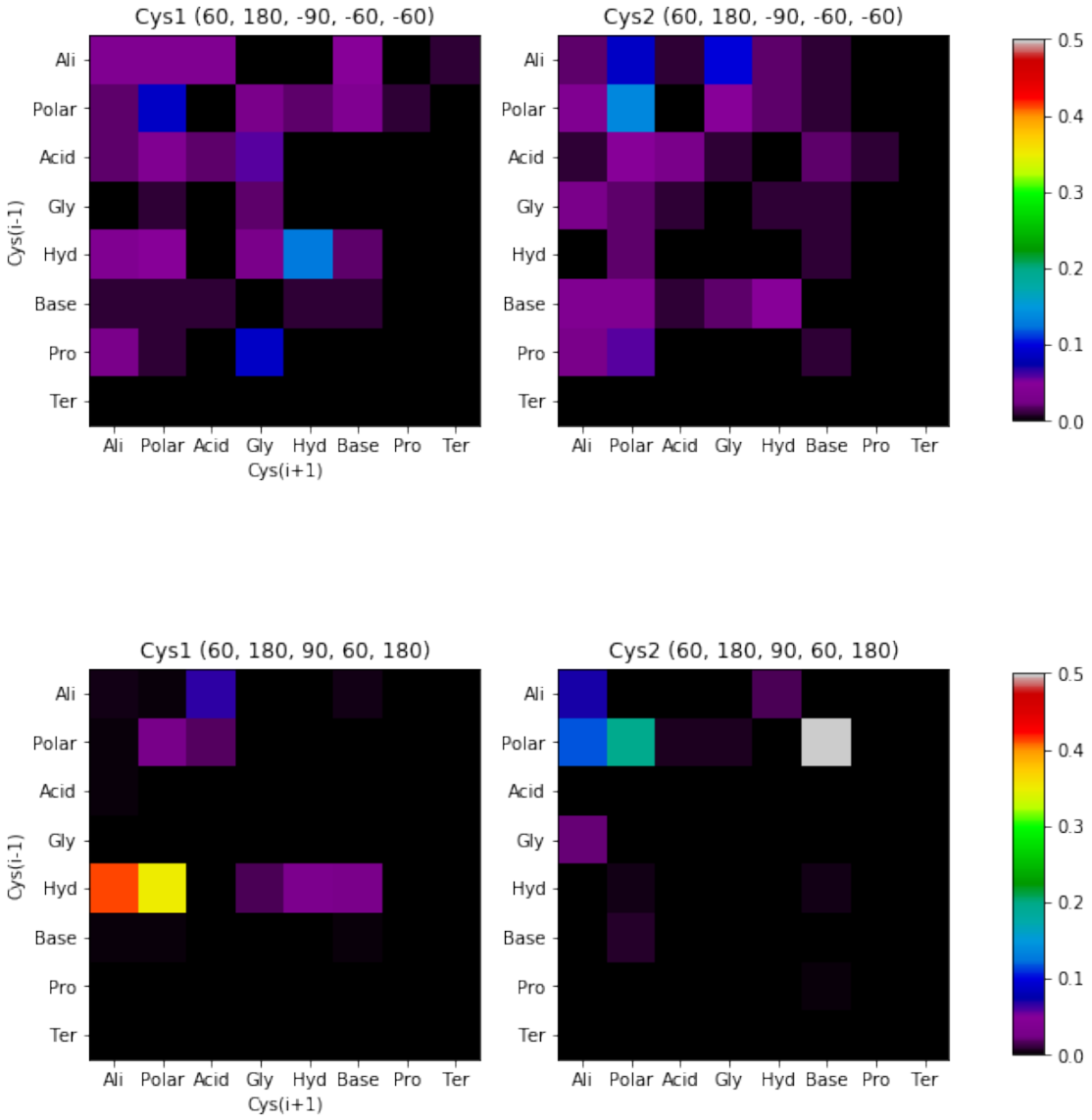

Cys1 (180, 60, 90, 60, 180)
Cys2 (180, 60, 90, 60, 180)
Cys1 (180, 180, -90, 180, 180)
Cys2 (180, 180, -90, 180, 180)
Cys(i-1)
Cys(i+1)
A R N D C E Q G H I L K M F P S T W Y V X
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000

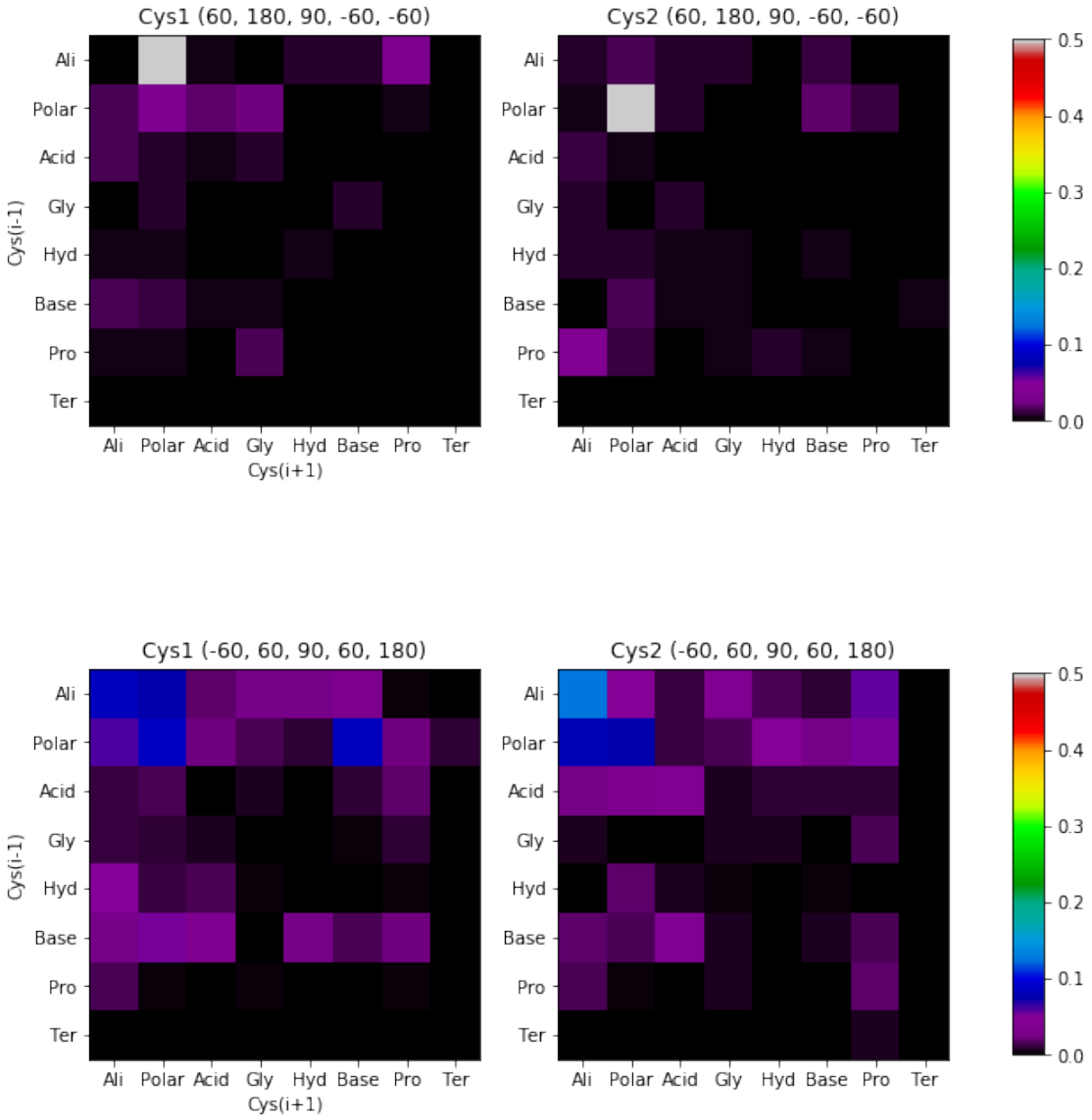
1.6.1 Frequency of Amino Acid by Biochemical Property

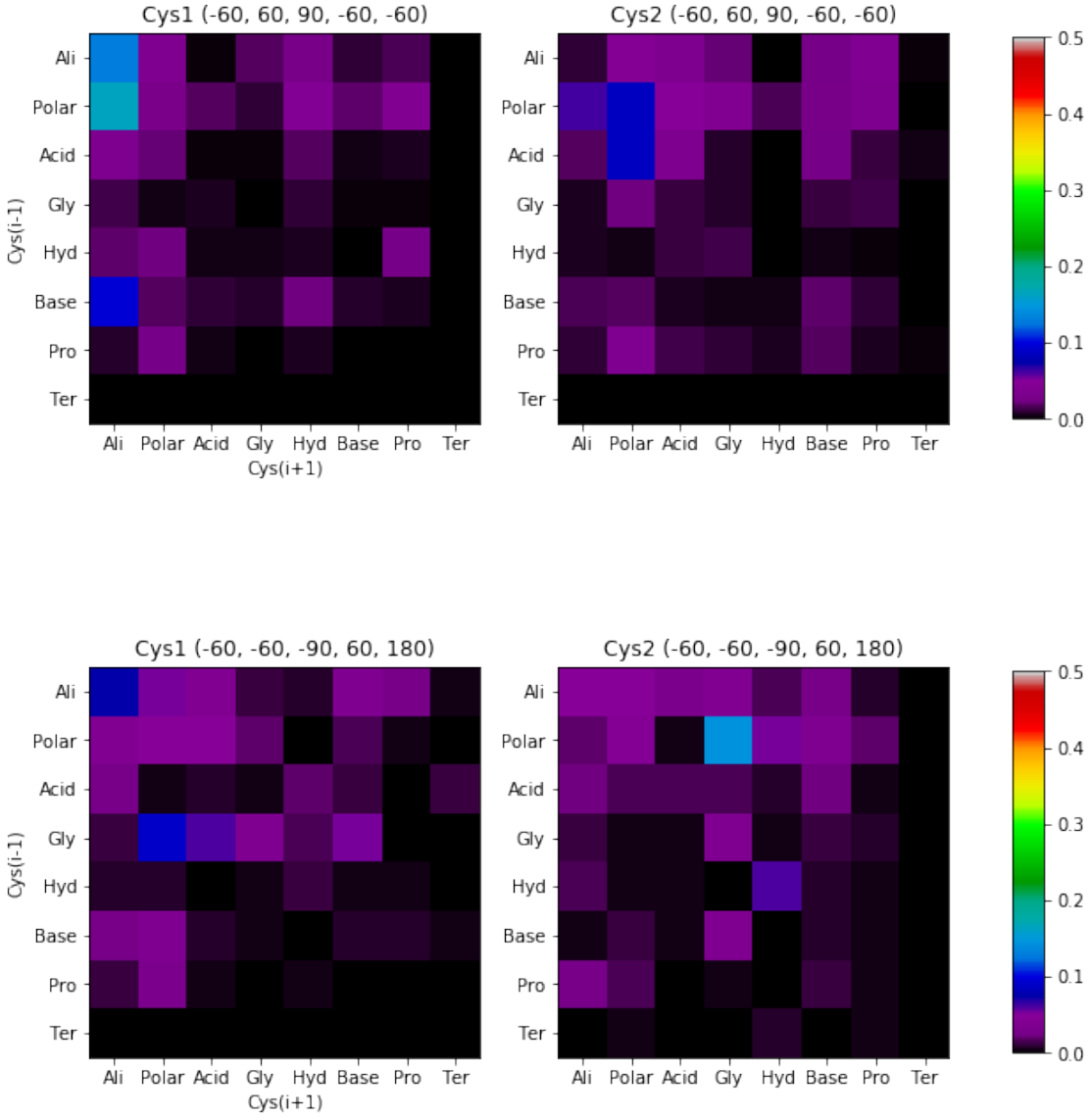


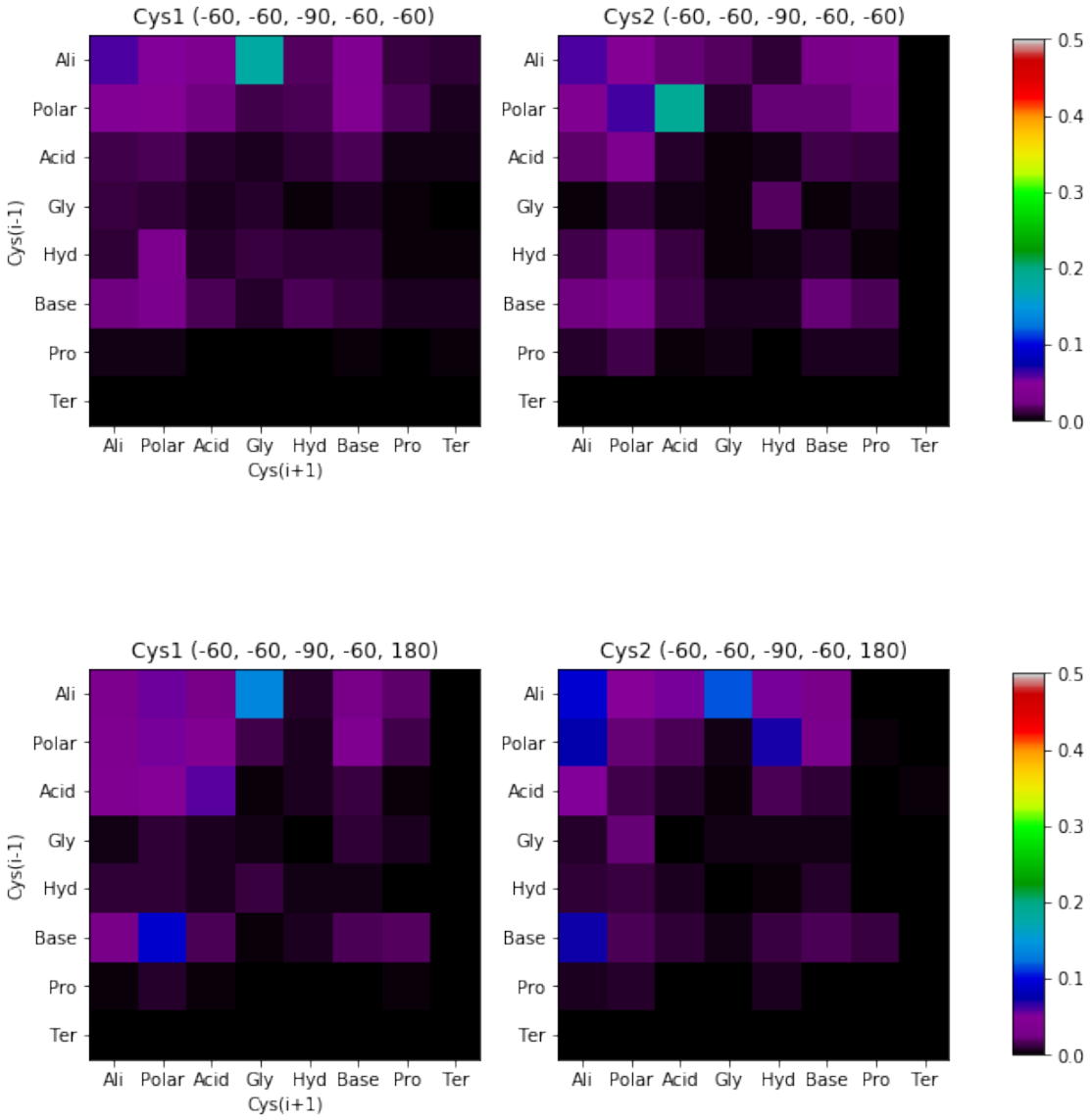

Cys1 (60, 60, 90, 60, 180)
Cys2 (60, 60, 90, 60, 180)
Cys1 (60, 60, 90, -60, -60)
Cys2 (60, 60, 90, -60, -60)
Ali
Polar
Acid
Gly
Hyd
Base
Pro
Ter
Cys(i-1)
Cys(i+1)
0.5
0.4
0.3
0.2
0.1
0.0

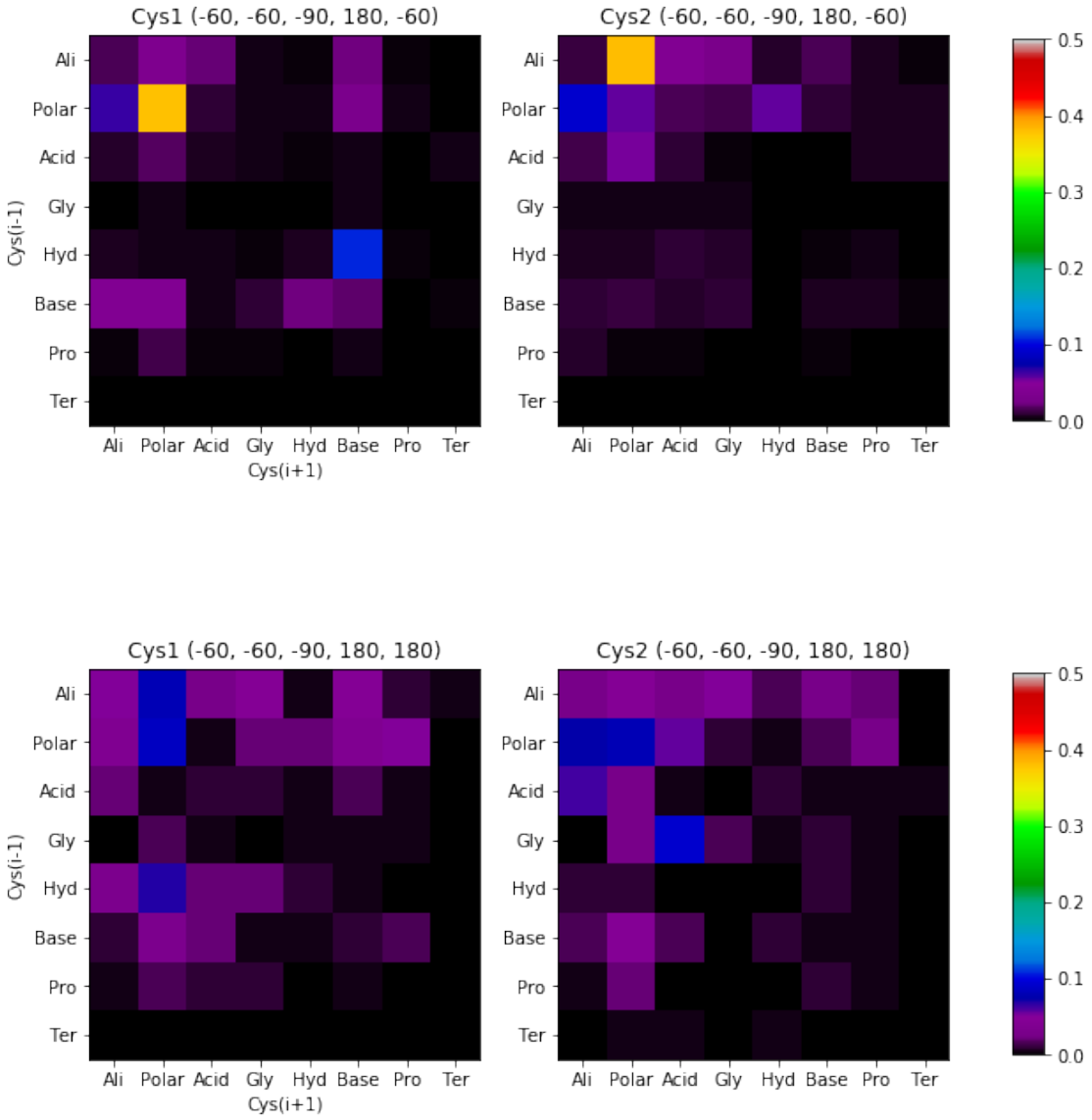

Cys1 (60, -60, -90, -60, -60)
Cys2 (60, -60, -90, -60, -60)
Cys1 (60, -60, -90, -60, 180)
Cys2 (60, -60, -90, -60, 180)
Ali
Polar
Acid
Gly
Hyd
Base
Pro
Ter
Cys(i-1)
Cys(i+1)
0.5
0.4
0.3
0.2
0.1
0.0

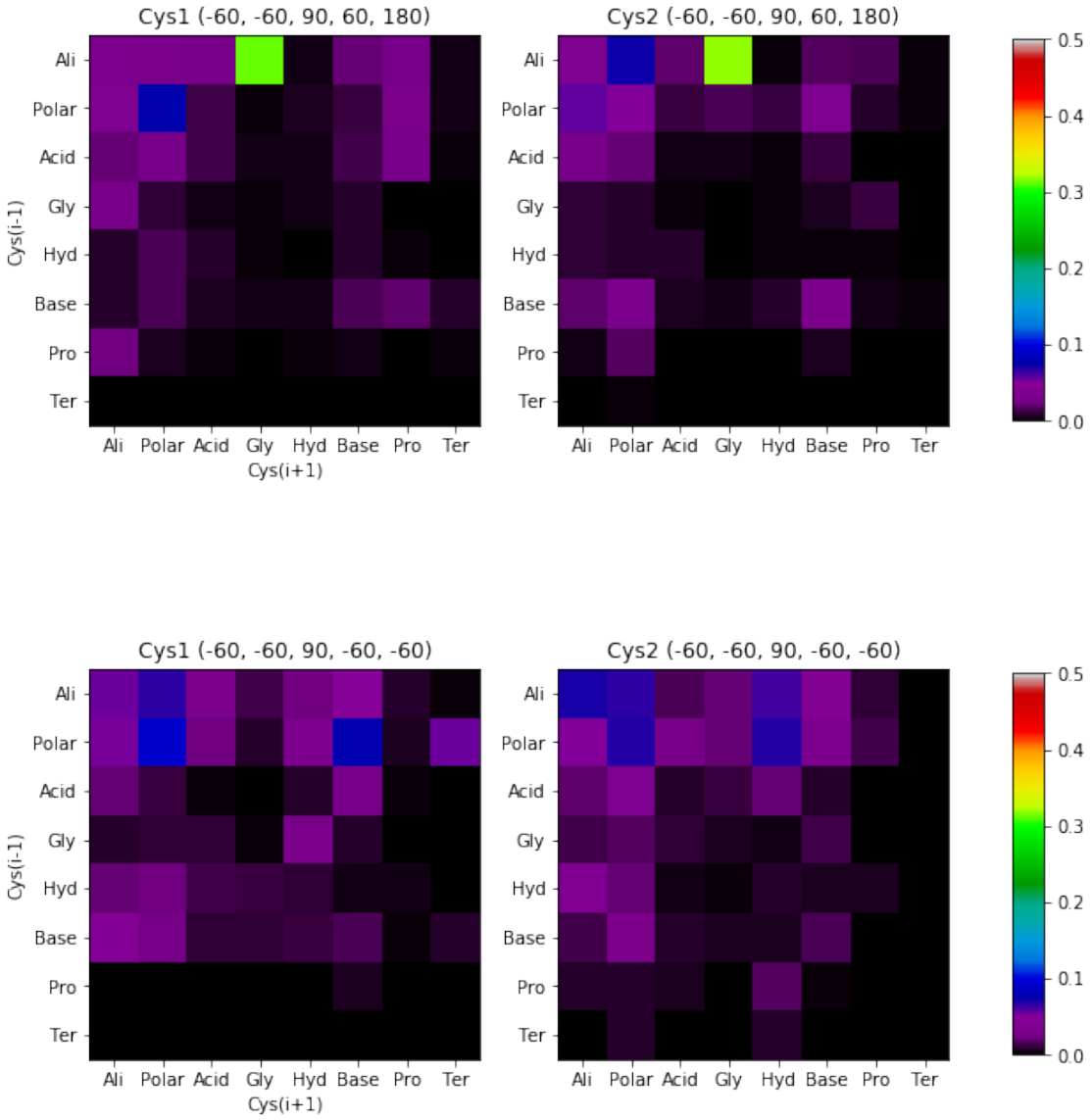

Cys1 (60, 180, -90, -60, -60)
Cys2 (60, 180, -90, -60, -60)
Cys1 (60, 180, 90, 60, 180)
Cys2 (60, 180, 90, 60, 180)
Ali
Polar
Acid
Gly
Hyd
Base
Pro
Ter
Cys(i-1)
Cys(i+1)
0.5
0.4
0.3
0.2
0.1
0.0

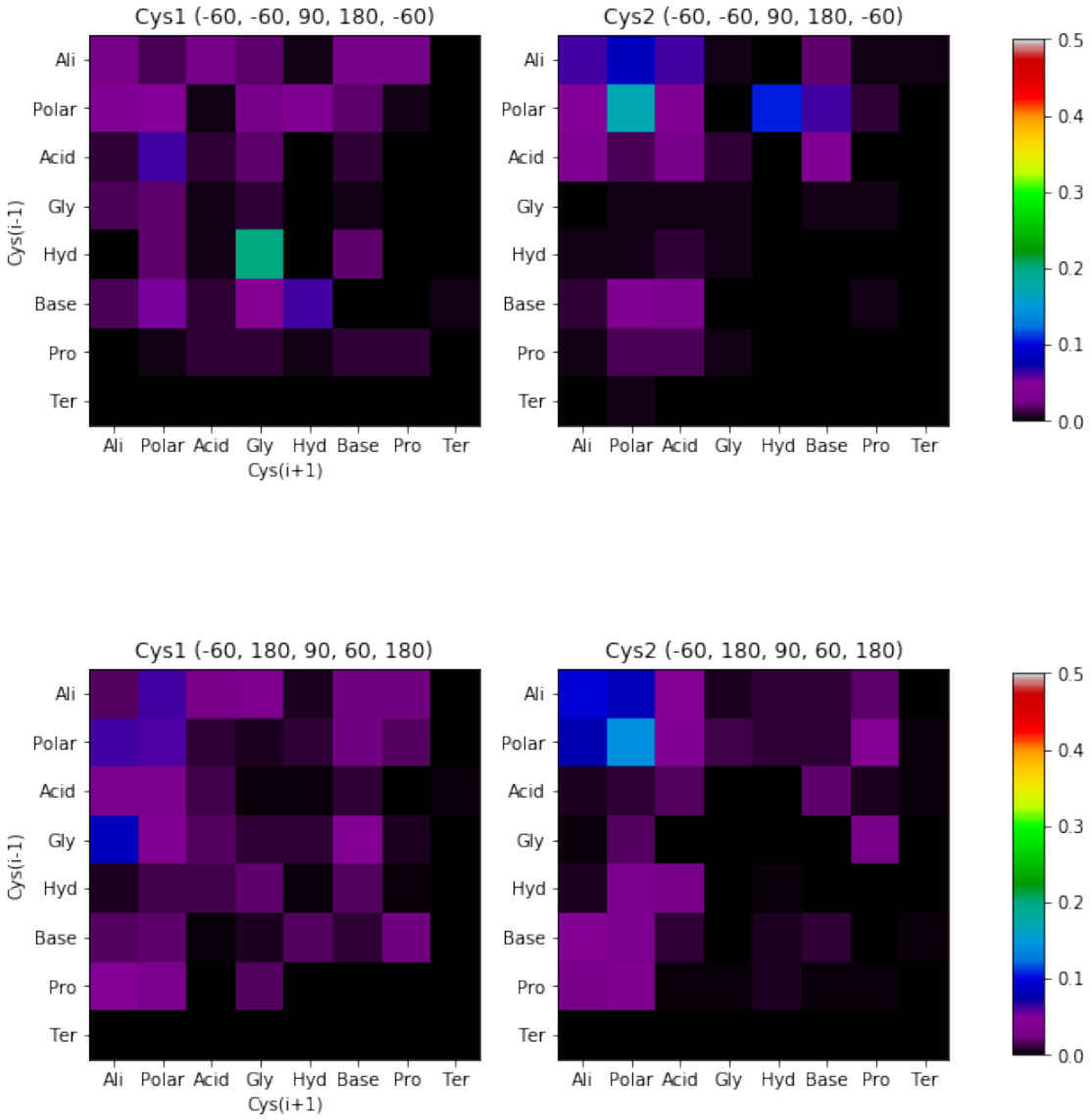

Cys1 (60, 180, 90, -60, -60)
Cys2 (60, 180, 90, -60, -60)
Cys1 (-60, 60, 90, 60, 180)
Cys2 (-60, 60, 90, 60, 180)
Cys(i-1)
Cys(i+1)
Ali
Polar
Acid
Gly
Hyd
Base
Pro
Ter
0.5
0.4
0.3
0.2
0.1
0.0

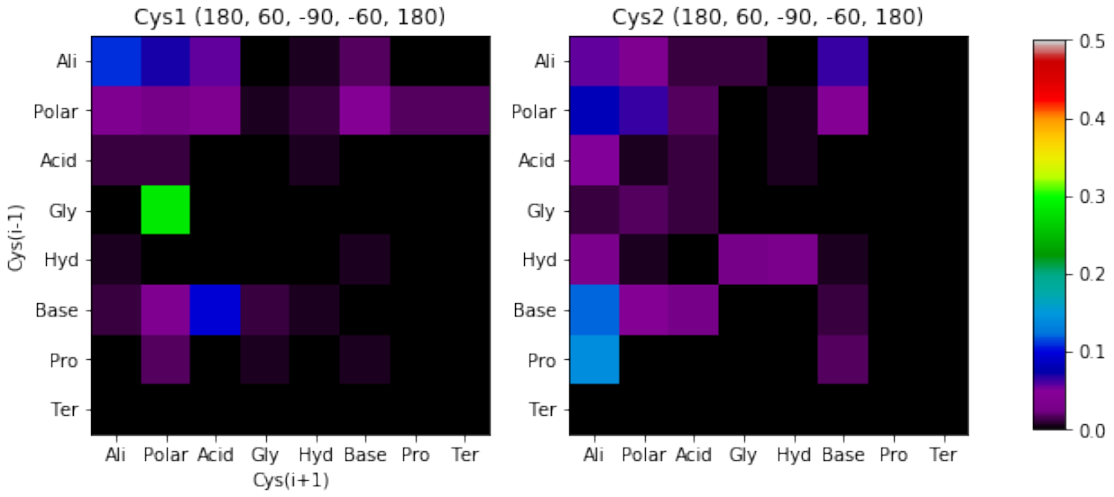

Cys1 (-60, 60, 90, -60, -60)
Cys2 (-60, 60, 90, -60, -60)
Cys1 (-60, -60, -90, 60, 180)
Cys2 (-60, -60, -90, 60, 180)
Cys(i-1)
Cys(i+1)
Ali
Polar
Acid
Gly
Hyd
Base
Pro
Ter
0.5
0.4
0.3
0.2
0.1
0.0

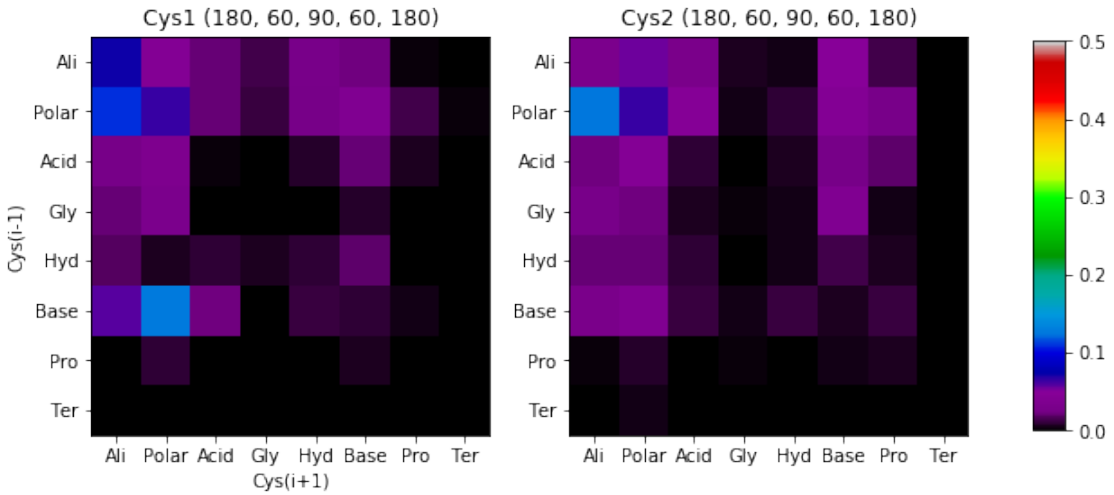

Cys1 (-60, -60, -90, -60, -60)
Cys2 (-60, -60, -90, -60, -60)
Cys1 (-60, -60, -90, -60, 180)
Cys2 (-60, -60, -90, -60, 180)
Ali
Polar
Acid
Gly
Hyd
Base
Pro
Ter
Cys(i-1)
Cys(i+1)
0.5
0.4
0.3
0.2
0.1
0.0

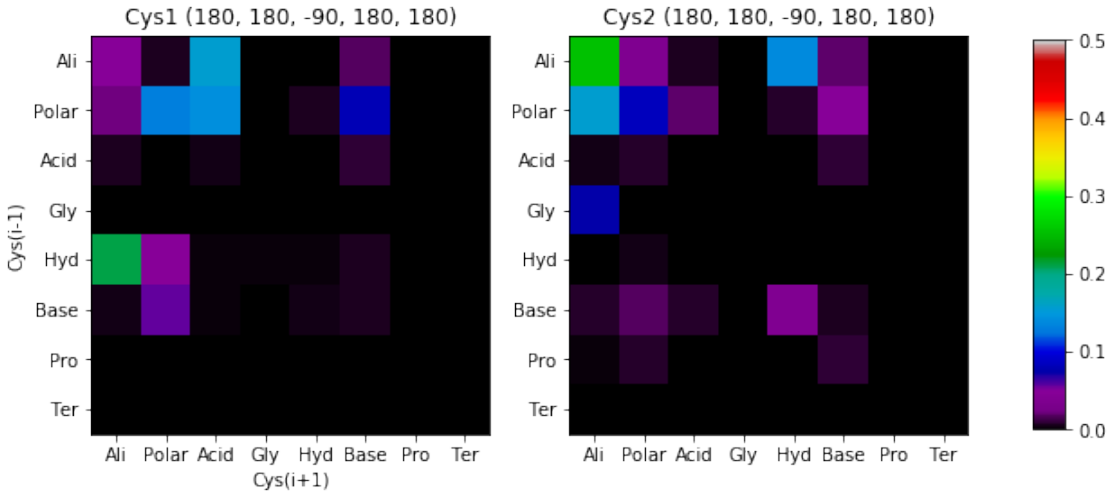

Cys1 (-60, -60, -90, 180, -60)
Cys2 (-60, -60, -90, 180, -60)
Cys1 (-60, -60, -90, 180, 180)
Cys2 (-60, -60, -90, 180, 180)
Cys(i-1)
Cys(i+1)
Ali
Polar
Acid
Gly
Hyd
Base
Pro
Ter
0.5
0.4
0.3
0.2
0.1
0.0


Cys1 (-60, -60, 90, 60, 180)
Cys2 (-60, -60, 90, 60, 180)
Cys1 (-60, -60, 90, -60, -60)
Cys2 (-60, -60, 90, -60, -60)
Cys(i-1)
Cys(i+1)
Ali
Polar
Acid
Gly
Hyd
Base
Pro
Ter
0.5
0.4
0.3
0.2
0.1
0.0

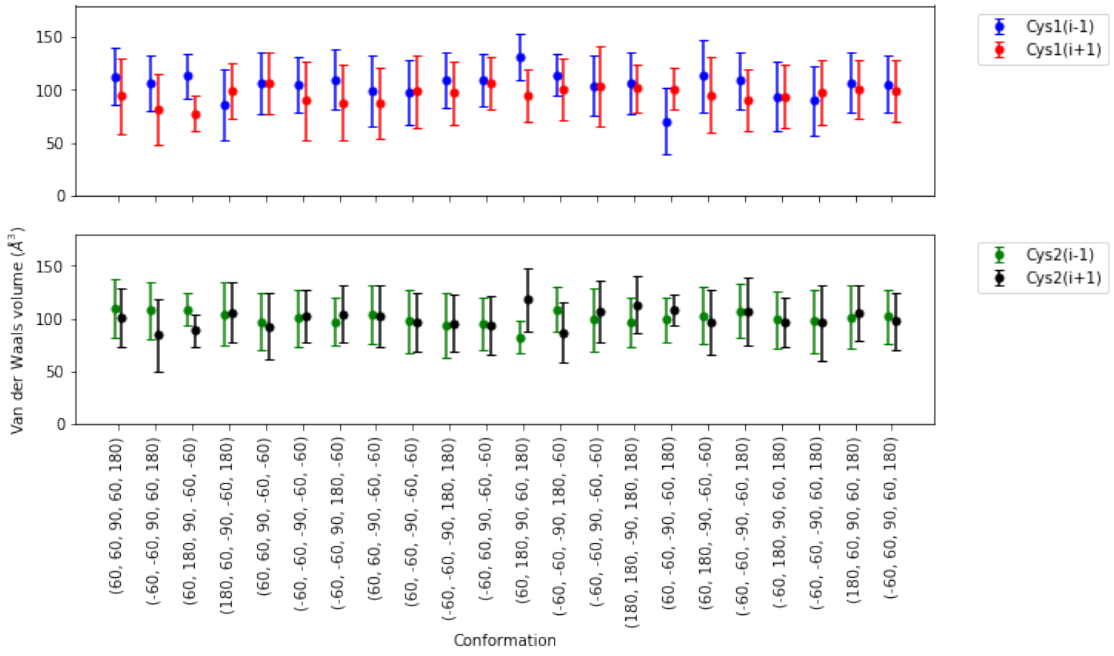

Cys1 (-60, -60, 90, 180, -60)
Cys2 (-60, -60, 90, 180, -60)
Cys1 (-60, 180, 90, 60, 180)
Cys2 (-60, 180, 90, 60, 180)
Ali
Polar
Acid
Gly
Hyd
Base
Pro
Ter
Cys(i-1)
Cys(i+1)
0.5
0.4
0.3
0.2
0.1
0.0


Cys1 (180, 60, -90, -60, 180)
Cys2 (180, 60, -90, -60, 180)
Ali
Polar
Acid
Gly
Hyd
Base
Pro
Ter
Cys(i-1)
Cys(i+1)
0.5
0.4
0.3
0.2
0.1
0.0


Cys1 (180, 60, 90, 60, 180)
Cys2 (180, 60, 90, 60, 180)
Ali
Polar
Acid
Gly
Hyd
Base
Pro
Ter
Cys(i-1)
Cys(i+1)
0.5
0.4
0.3
0.2
0.1
0.0



1.6.2 Frequency of Amino Acid by VDW Radi

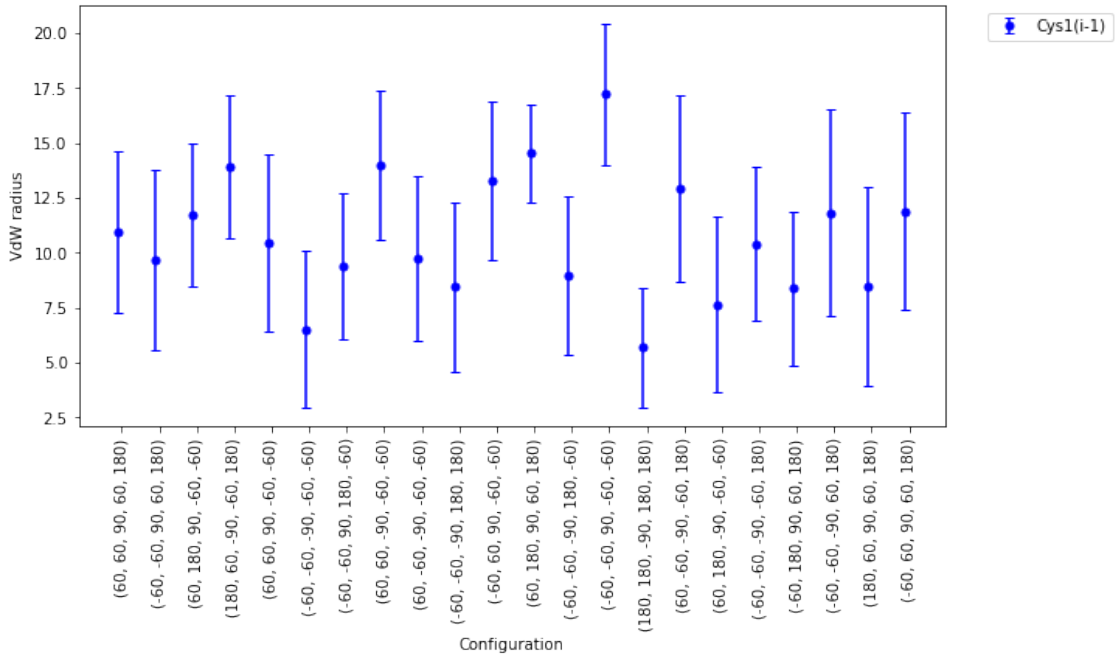


Out[14]: ()

```
(60, 60, -90, -60, -60) 14.020357311082645
(60, 60, 90, 60, 180) 10.94146046003315
(60, 60, 90, -60, -60) 10.43890017018778
(60, -60, -90, -60, -60) 9.729912143632106
```

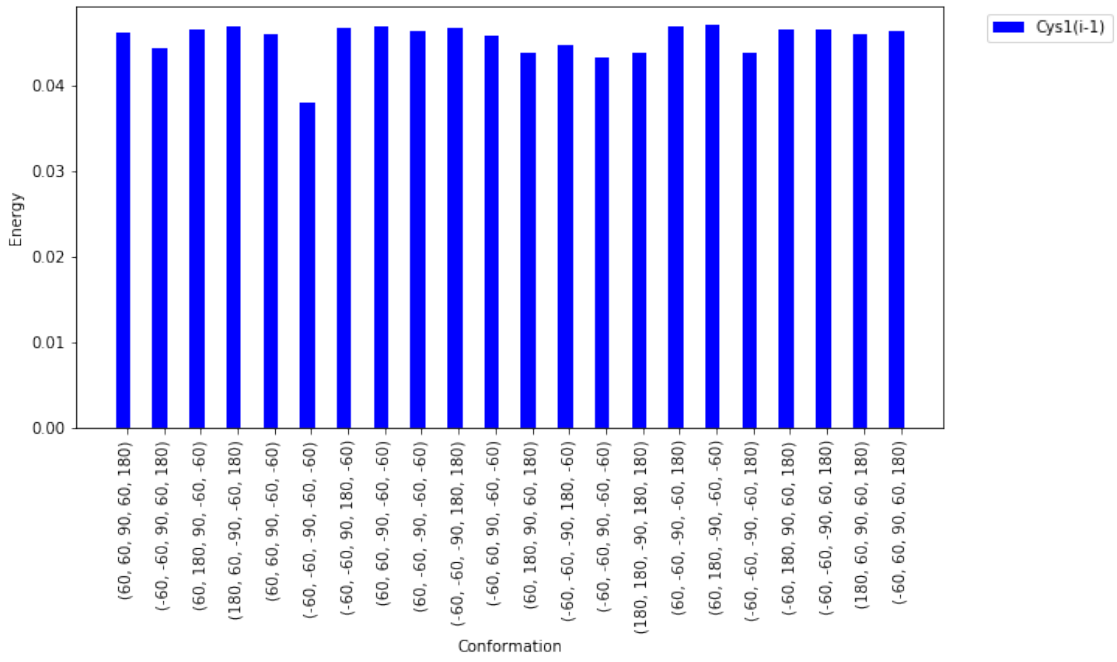
```
(60, -60, -90, -60, 180) 12.91536445628846
(60, 180, -90, -60, -60) 7.642602000650002
(60, 180, 90, 60, 180) 14.546032212688422
(60, 180, 90, -60, -60) 11.707496947589744
(-60, 60, 90, 60, 180) 11.888714858685315
(-60, 60, 90, -60, -60) 13.290180158957144
(-60, -60, -90, 60, 180) 11.819749037119658
(-60, -60, -90, -60, -60) 6.524539662137568
(-60, -60, -90, -60, 180) 10.409521748311489
(-60, -60, -90, 180, -60) 8.957282444078768
(-60, -60, -90, 180, 180) 8.447279527899408
(-60, -60, 90, 60, 180) 9.673237960921325
(-60, -60, 90, -60, -60) 17.22122359748012
(-60, -60, 90, 180, -60) 9.405272451410811
(-60, 180, 90, 60, 180) 8.379706433324529
(180, 60, -90, -60, 180) 13.951319572960529
(180, 60, 90, 60, 180) 8.473521595474157
(180, 180, -90, 180, 180) 5.687167499307144
```

Out[15]: ()




```
(60, 60, -90, -60, -60) 0.0469502309429
(60, 60, 90, 60, 180) 0.0462157352289
(60, 60, 90, -60, -60) 0.0459843158415
(60, -60, -90, -60, -60) 0.0464094741215
```

```
(60, -60, -90, -60, 180) 0.0470046519656
(60, 180, -90, -60, -60) 0.0470228063209
(60, 180, 90, 60, 180) 0.0438089678949
(60, 180, 90, -60, -60) 0.0465650498305
(-60, 60, 90, 60, 180) 0.0464363634417
(-60, 60, 90, -60, -60) 0.045839530003
(-60, -60, -90, 60, 180) 0.0465980268482
(-60, -60, -90, -60, -60) 0.038086471394
(-60, -60, -90, -60, 180) 0.0438315294846
(-60, -60, -90, 180, -60) 0.0446946581
(-60, -60, -90, 180, 180) 0.0468054160543
(-60, -60, 90, 60, 180) 0.0444422438124
(-60, -60, 90, -60, -60) 0.0433769137097
(-60, -60, 90, 180, -60) 0.0467602530691
(-60, 180, 90, 60, 180) 0.0464842051513
(180, 60, -90, -60, 180) 0.046859669219
(180, 60, 90, 60, 180) 0.0459665624221
(180, 180, -90, 180, 180) 0.043856925162
```

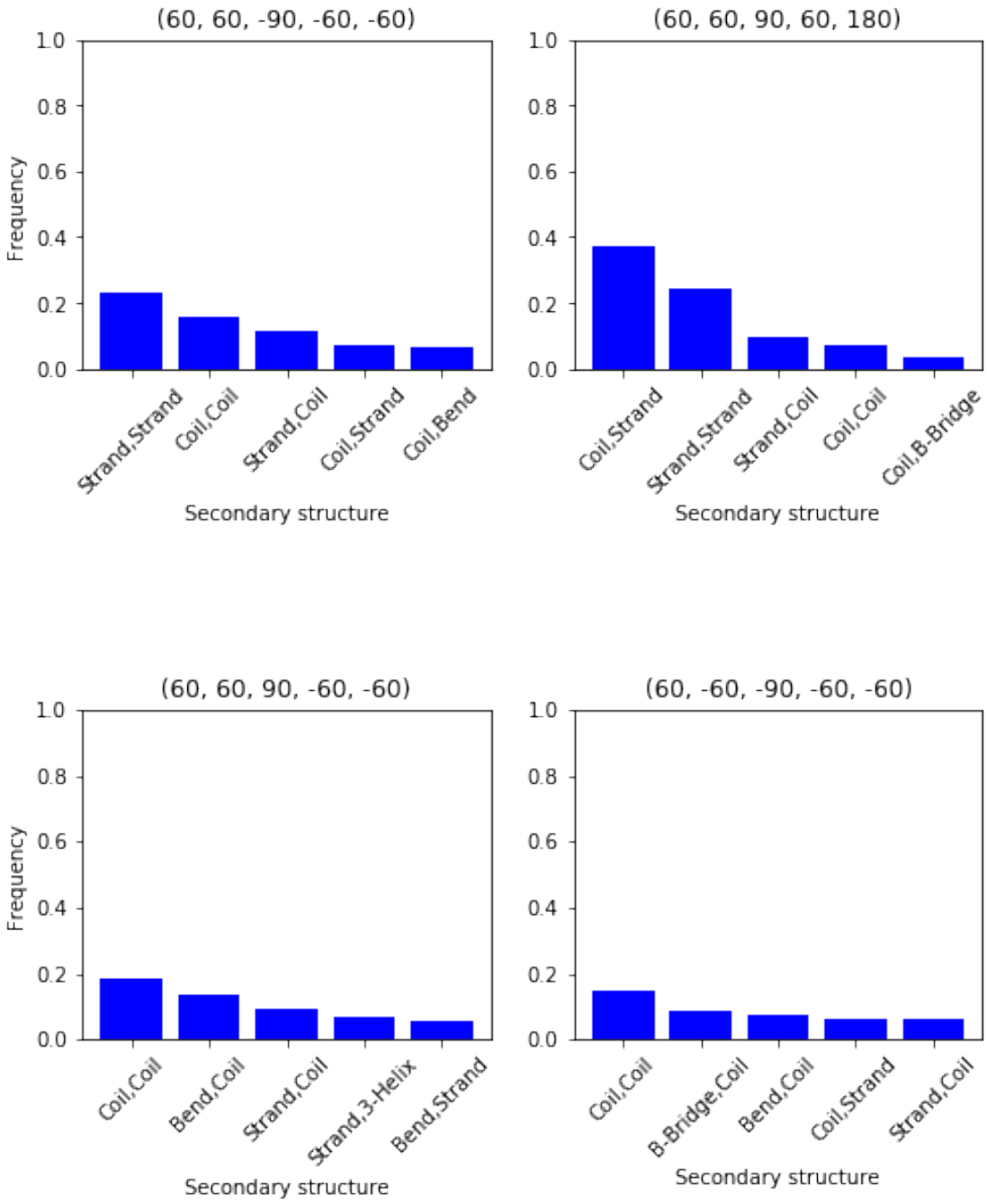


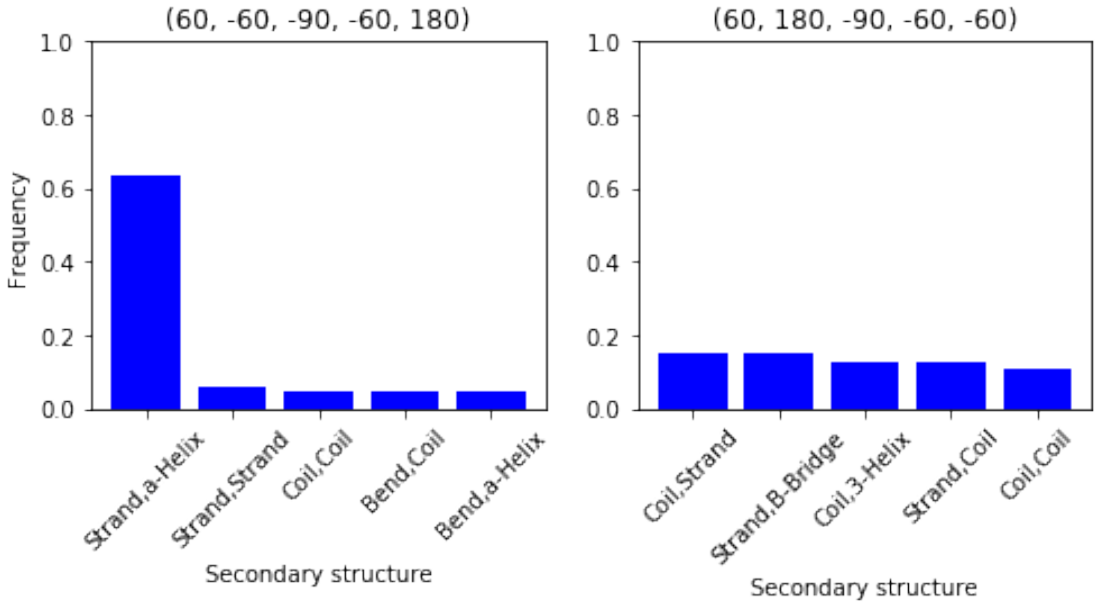
Out[16]: ()

1.7 Secondary Structure

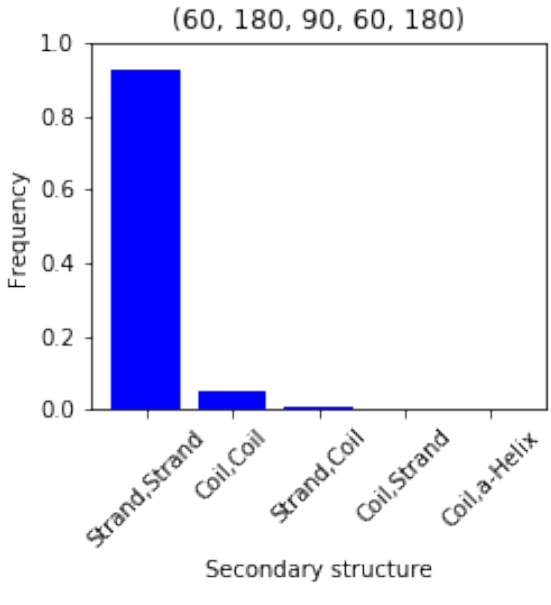
```
/home/david/coding/lib/python2.7/site-packages/ipykernel_launcher.py:90: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
```

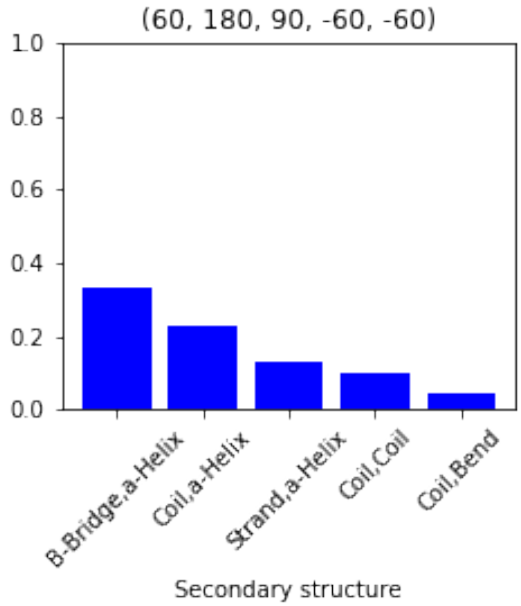
```
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: http://pandas.pydata.org/pandas-docs/stable/indexing.html#
```

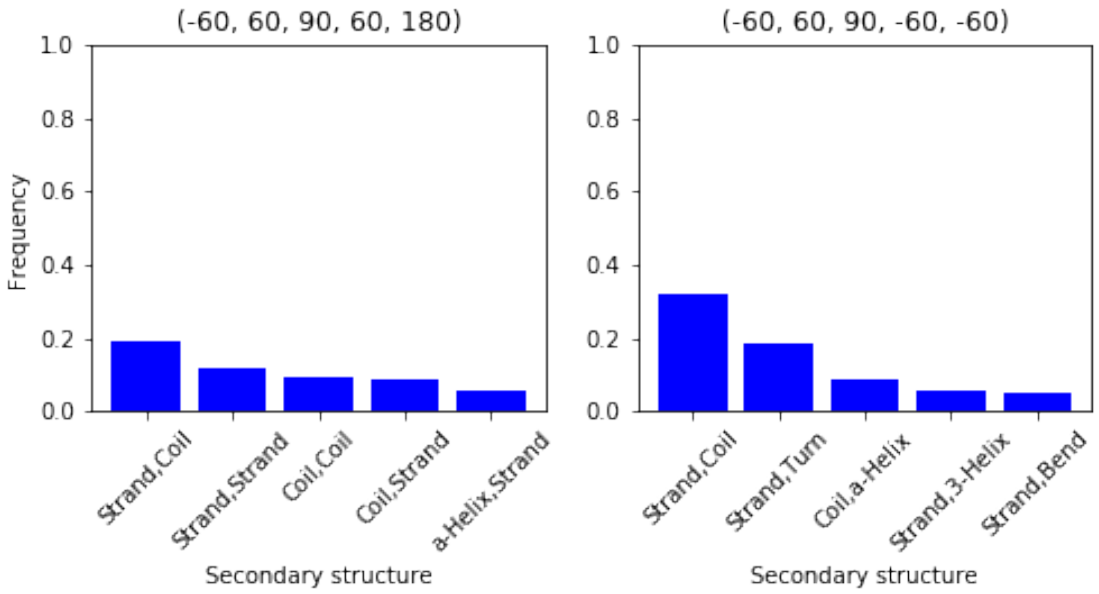



(60, -60, -90, -60, 180)
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
Strand,a-Helix
Strand,Strand
Coil,Coil
Bend,Coil
Bend,a-Helix
Secondary structure

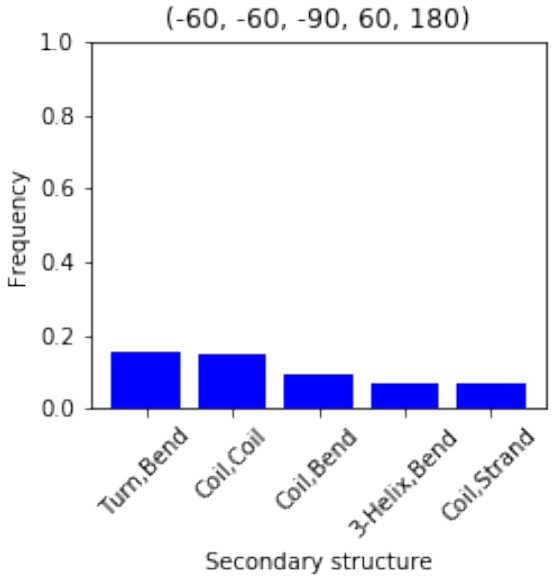
(60, 180, -90, -60, -60)
1.0
0.8
0.6
0.4
0.2
0.0
Coil,Strand
Strand,B-Bridge
Coil,3-Helix
Strand,Coil
Coil,Coil
Secondary structure

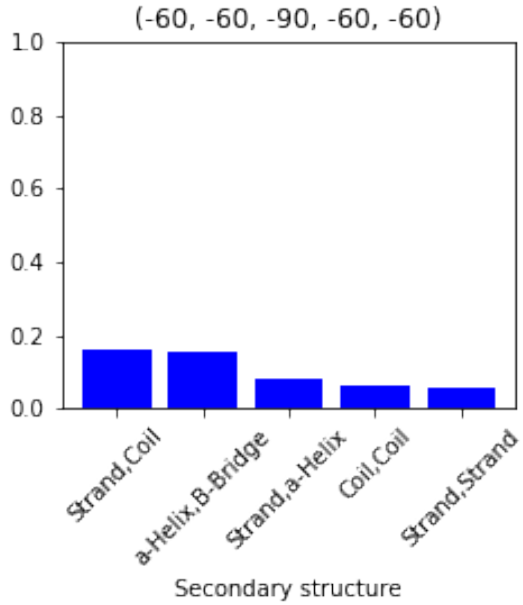

(60, 180, 90, 60, 180)
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
Strand,Strand
Coil,Coil
Strand,Coil
Coil,Strand
Coil,a-Helix
Secondary structure

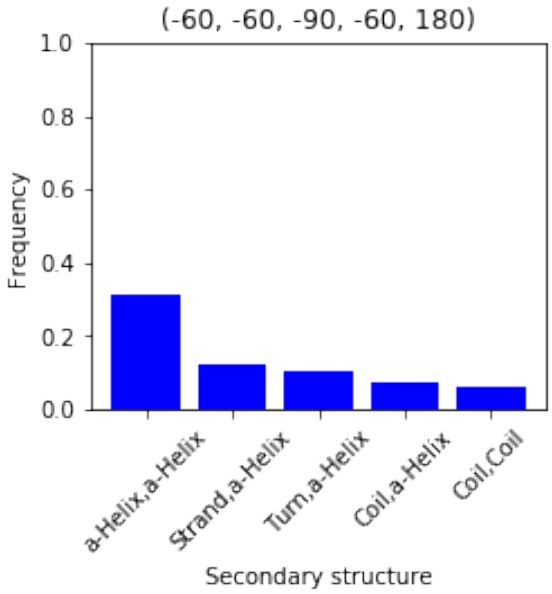

(60, 180, 90, -60, -60)
1.0
0.8
0.6
0.4
0.2
0.0
B-Bridge,a-Helix
Coil,a-Helix
Strand,a-Helix
Coil,Coil
Coil,Bend
Secondary structure

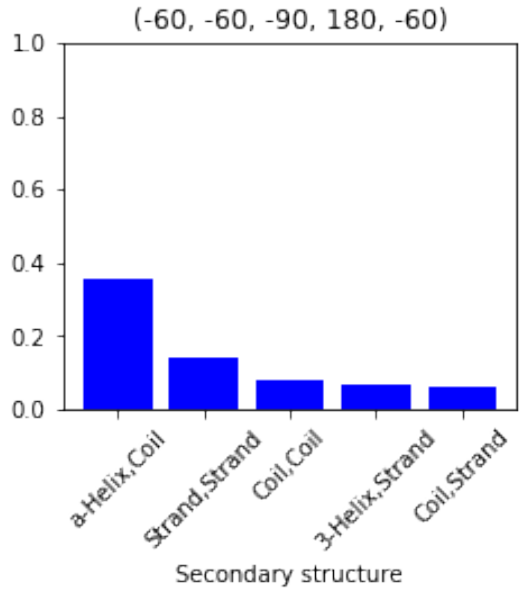

(-60, 60, 90, 60, 180)
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
Strand,Coil
Strand,Strand
Coil,Coil
Coil,Strand
a-Helix,Strand
Secondary structure

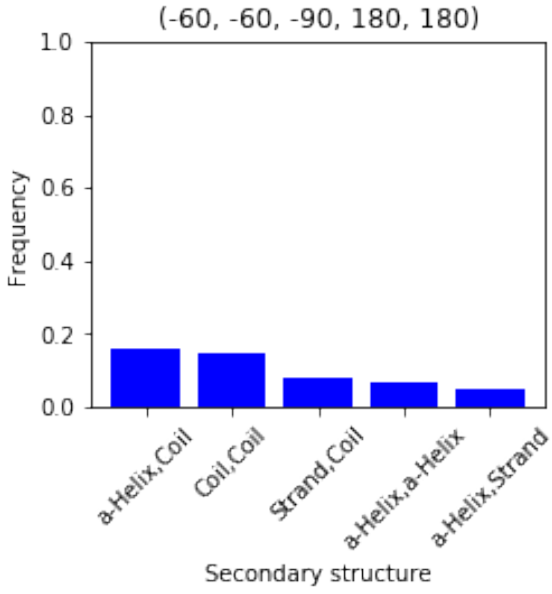
(-60, 60, 90, -60, -60)
1.0
0.8
0.6
0.4
0.2
0.0
Strand,Coil
Strand,Turn
Coil,a-Helix
Strand,3-Helix
Strand,Bend
Secondary structure

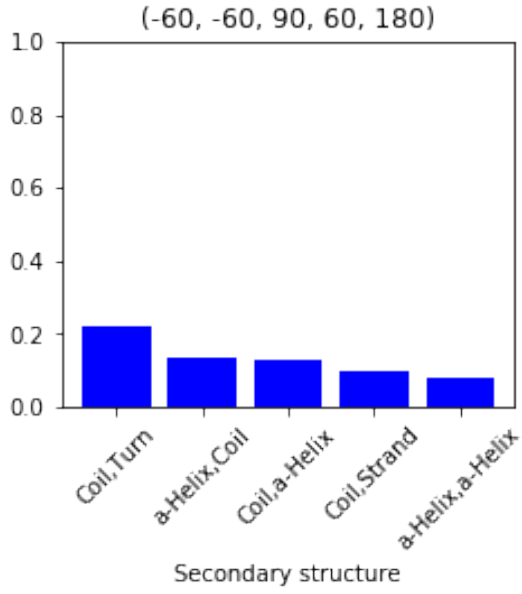

(-60, -60, -90, 60, 180)
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
Turn,Bend
Coil,Coil
Coil,Bend
3-Helix,Bend
Coil,Strand
Secondary structure

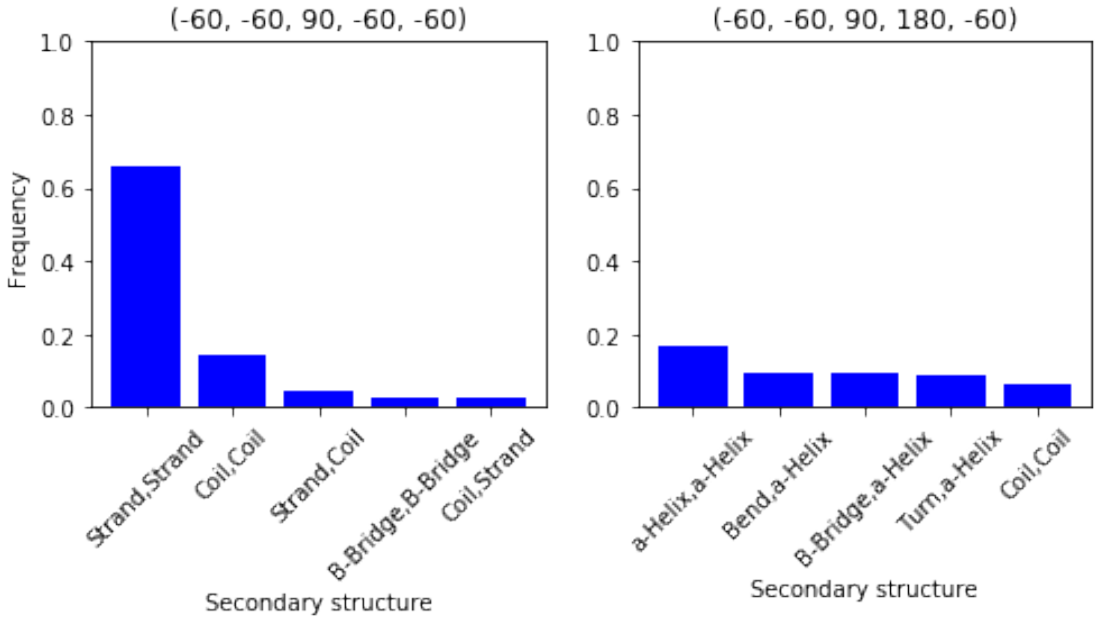

(-60, -60, -90, -60, -60)
1.0
0.8
0.6
0.4
0.2
0.0
Strand,Coil
a-Helix,B-Bridge
Strand,a-Helix
Coil,Coil
Strand,Strand
Secondary structure


(-60, -60, -90, -60, 180)
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
a-Helix,a-Helix
Strand,a-Helix
Turn,a-Helix
Coil,a-Helix
Coil,Coil
Secondary structure

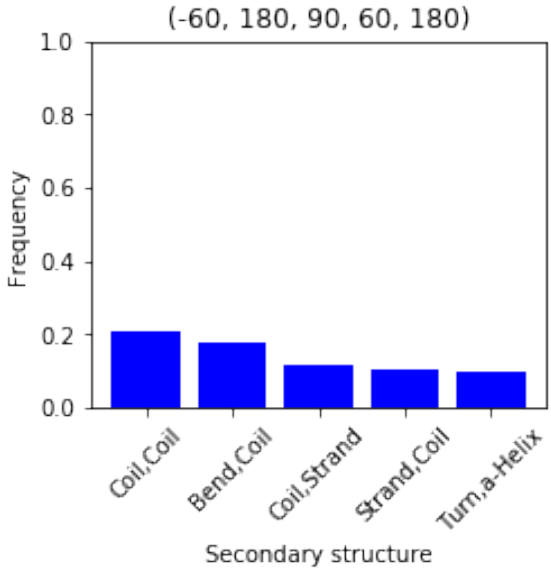

(-60, -60, -90, 180, -60)
1.0
0.8
0.6
0.4
0.2
0.0
a-Helix,Coil
Strand,Strand
Coil,Coil
3-Helix,Strand
Coil,Strand
Secondary structure

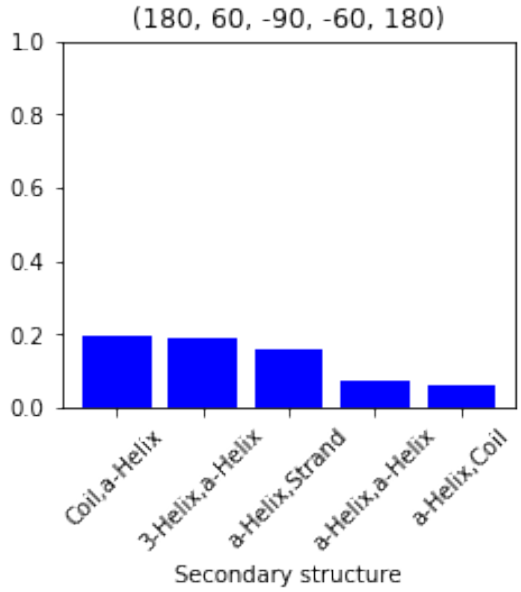

(-60, -60, -90, 180, 180)
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
a-Helix,Coil
Coil,Coil
Strand,Coil
a-Helix,a-Helix
a-Helix,Strand
Secondary structure

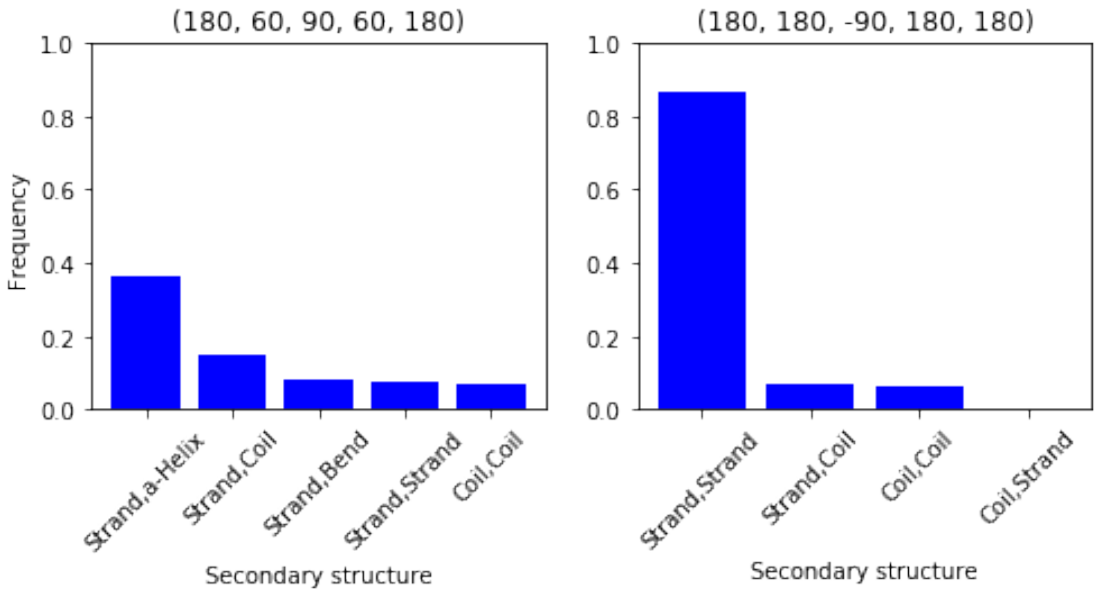

(-60, -60, 90, 60, 180)
1.0
0.8
0.6
0.4
0.2
0.0
Coil,Turn
a-Helix,Coil
Coil,a-Helix
Coil,Strand
a-Helix,a-Helix
Secondary structure

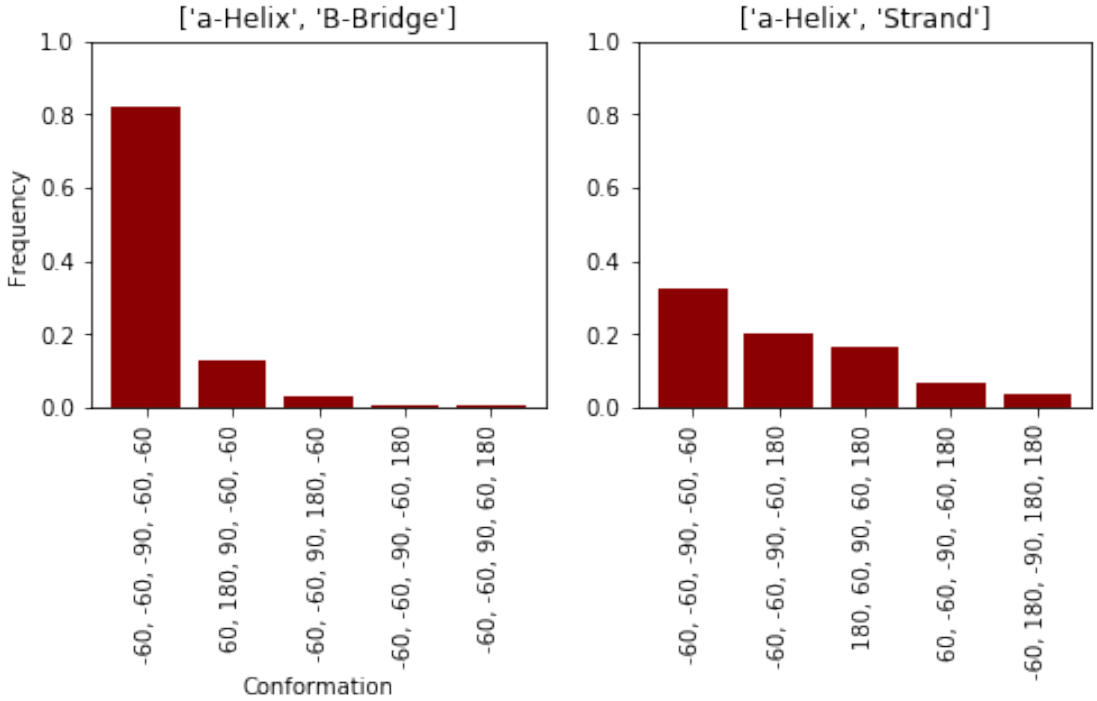

(-60, -60, 90, -60, -60)
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
Strand,Strand
Coil,Coil
Strand,Coil
B-Bridge,B-Bridge
Coil,Strand
Secondary structure

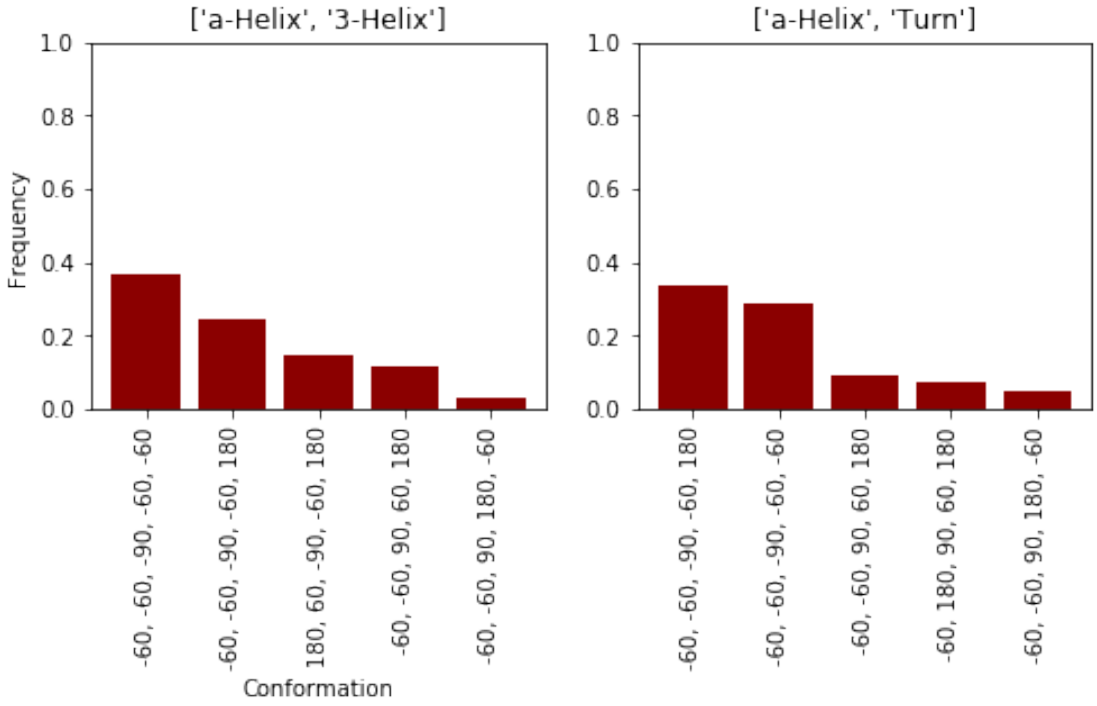
(-60, -60, 90, 180, -60)
1.0
0.8
0.6
0.4
0.2
0.0
a-Helix,a-Helix
Bend,a-Helix
B-Bridge,a-Helix
Turn,a-Helix
Coil,Coil
Secondary structure

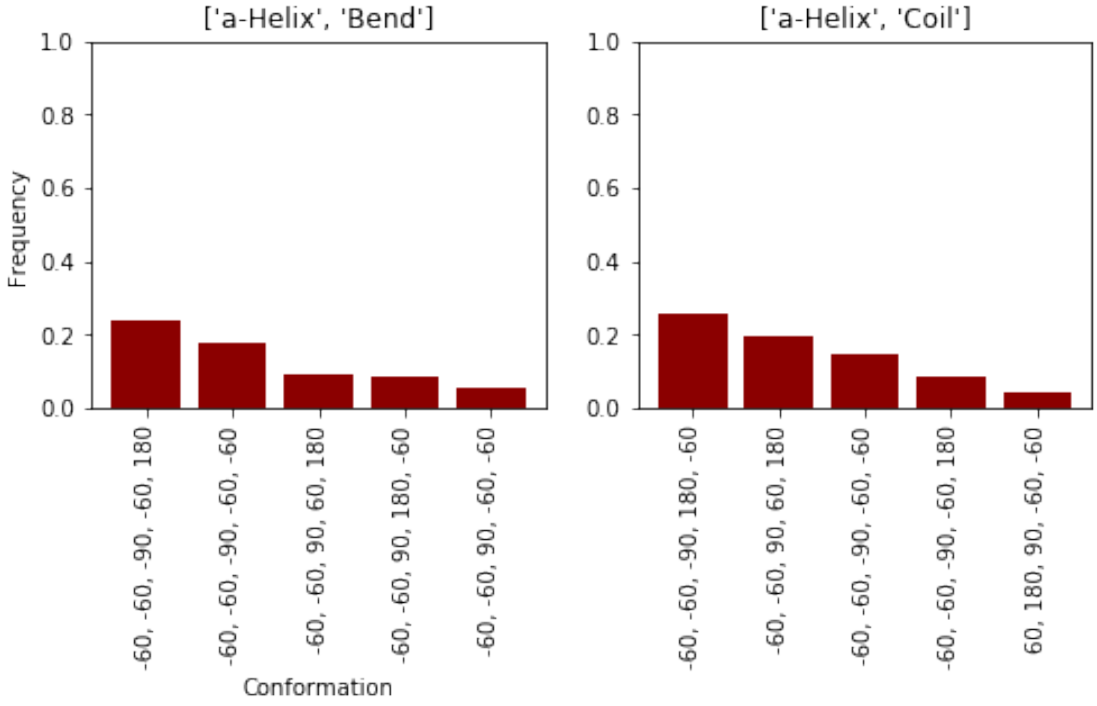

(-60, 180, 90, 60, 180)
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
Coil,Coil
Bend,Coil
Coil,Strand
Strand,Coil
Turn,a-Helix
Secondary structure

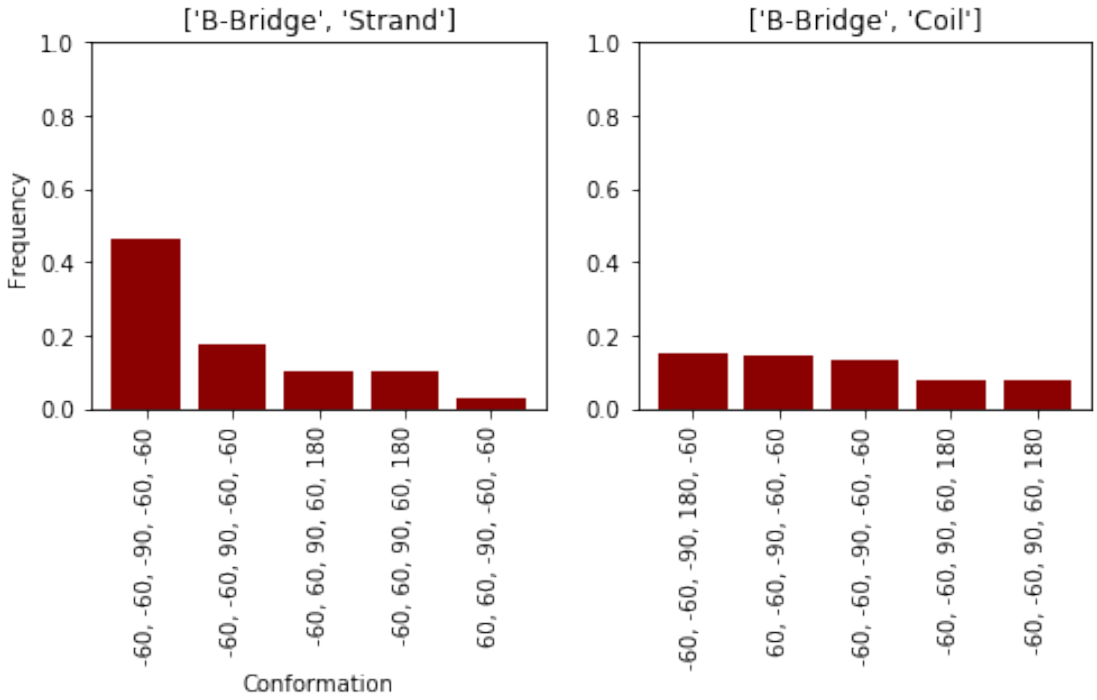

(180, 60, -90, -60, 180)
1.0
0.8
0.6
0.4
0.2
0.0
Coil,a-Helix
3-Helix,a-Helix
a-Helix,Strand
a-Helix,a-Helix
a-Helix,Coil
Secondary structure


(180, 60, 90, 60, 180)
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
Strand,a-Helix
Strand,Coil
Strand,Bend
Strand,Strand
Coil,Coil
Secondary structure
(180, 180, -90, 180, 180)
Strand,Strand
Strand,Coil
Coil,Coil
Coil,Strand
Secondary structure


['a-Helix', 'B-Bridge']
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
-60, -60, -90, -60, -60
60, 180, 90, -60, -60
-60, -60, 90, 180, -60
-60, -60, -90, -60, 180
-60, -60, 90, 60, 180
Conformation
['a-Helix', 'Strand']
-60, -60, -90, -60, -60
-60, -60, -90, -60, 180
180, 60, 90, 60, 180
60, -60, -90, -60, 180
-60, 180, -90, 180, 180


['a-Helix', '3-Helix']
['a-Helix', 'Turn']
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
-60, -60, -90, -60, -60
-60, -60, -90, -60, 180
180, 60, -90, -60, 180
-60, -60, 90, 60, 180
-60, -60, 90, 180, -60
-60, -60, -90, -60, 180
-60, -60, -90, -60, -60
-60, -60, 90, 60, 180
-60, 180, 90, 60, 180
-60, -60, 90, 180, -60
Conformation


['a-Helix', 'Bend']
['a-Helix', 'Coil']
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
-60, -60, -90, -60, 180
-60, -60, -90, -60, -60
-60, -60, 90, 60, 180
-60, -60, 90, 180, -60
-60, -60, 90, -60, -60
-60, -60, -90, 180, -60
-60, -60, 90, 60, 180
-60, -60, -90, -60, -60
-60, -60, -90, -60, 180
60, 180, 90, -60, -60
Conformation


['B-Bridge', 'Strand']
['B-Bridge', 'Coil']
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
-60, -60, -90, -60, -60
-60, -60, 90, -60, -60
-60, 60, 90, 60, 180
-60, 60, 90, 60, 180
60, 60, -90, -60, -60
-60, -60, -90, 180, -60
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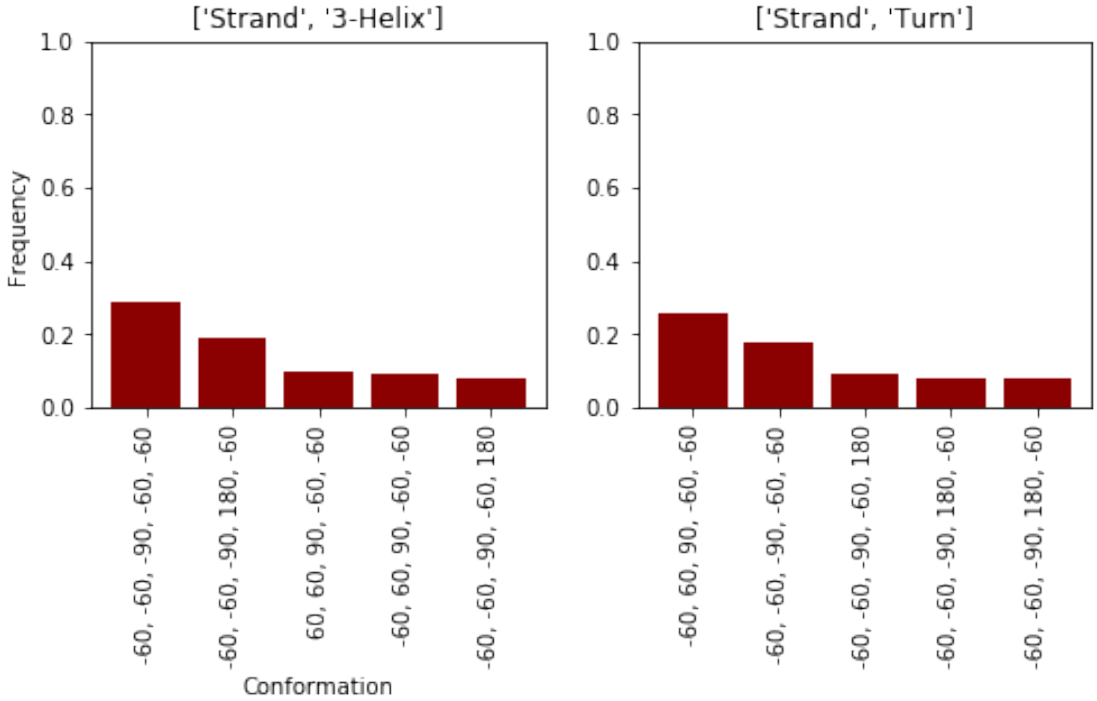
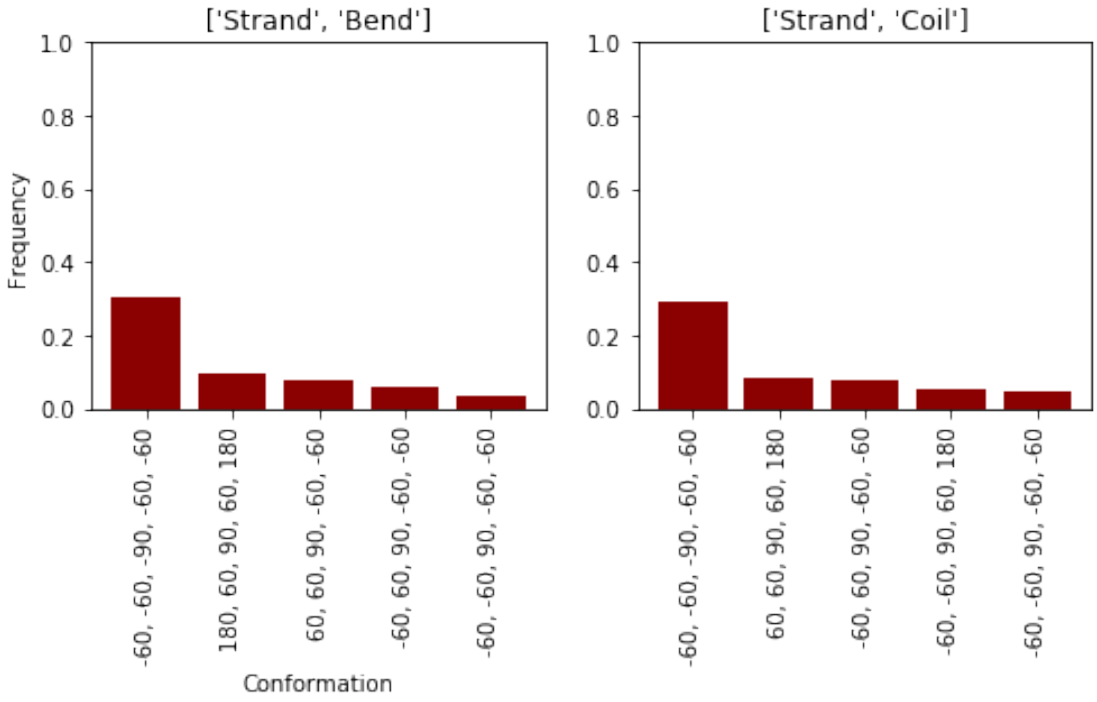
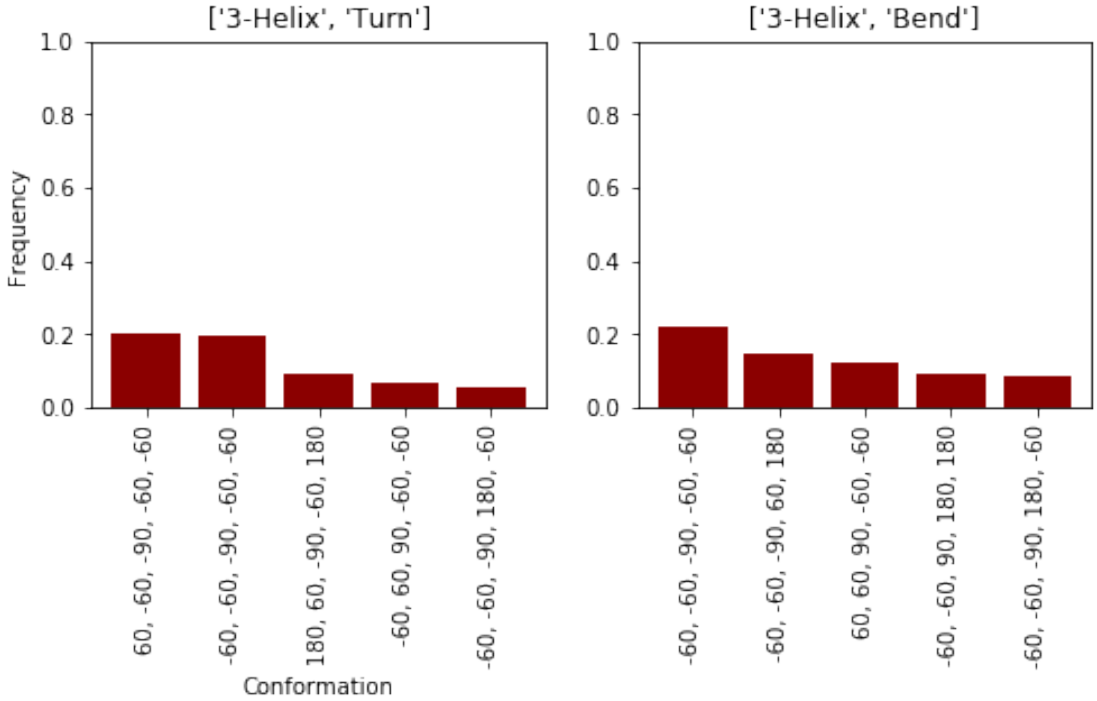
-60, -60, 90, 60, 180
Conformation

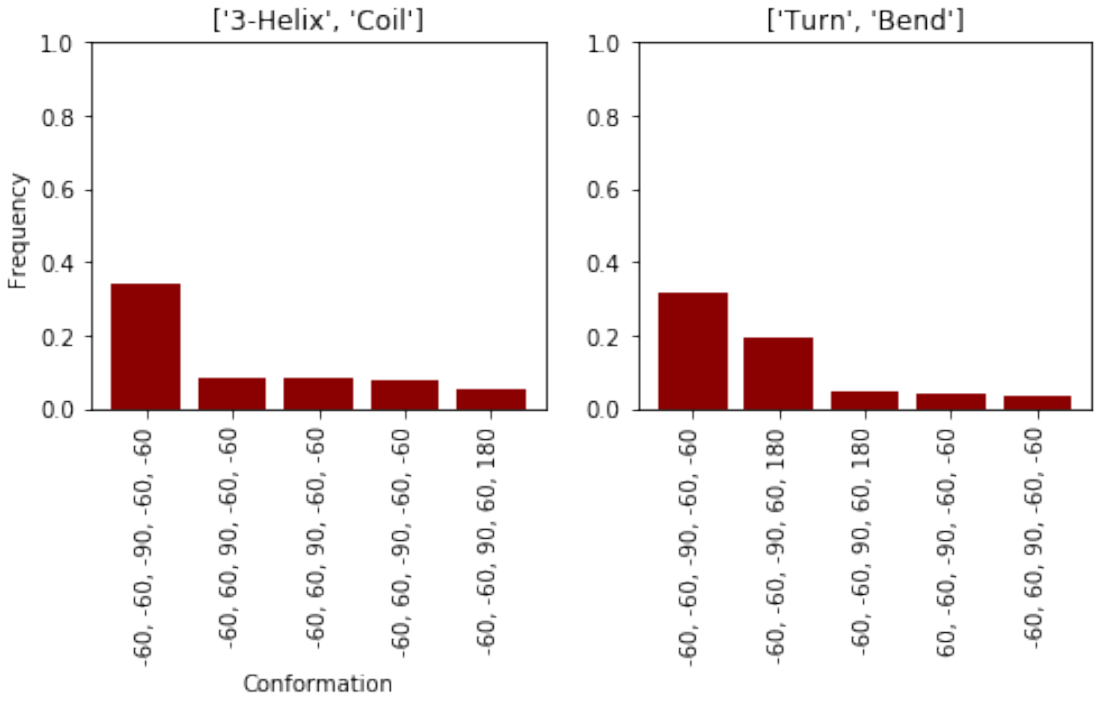

['Strand', '3-Helix']
['Strand', 'Turn']
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
-60, -60, -90, -60, -60
-60, -60, -90, 180, -60
60, 60, 90, -60, -60
-60, 60, 90, -60, -60
-60, -60, -90, -60, 180
-60, 60, 90, -60, -60
-60, -60, -90, -60, -60
-60, -60, -90, -60, 180
-60, -60, -90, 180, -60
-60, -60, -90, 180, -60
Conformation

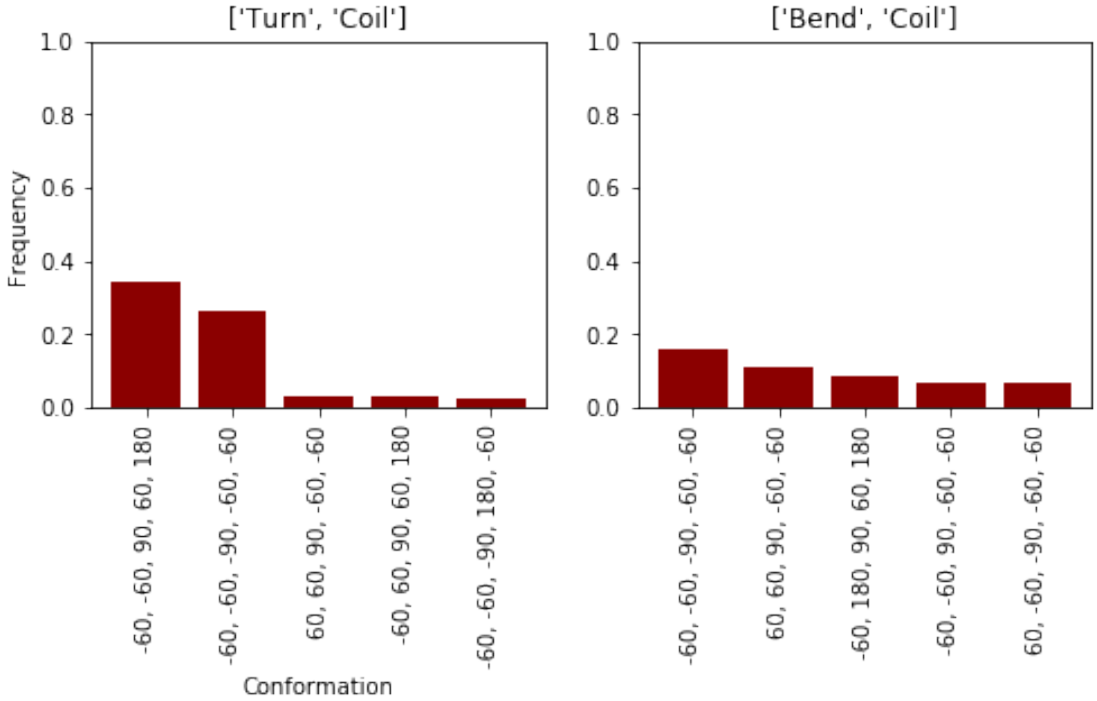

['Strand', 'Bend']
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
-60, -60, -90, -60, -60
180, 60, 90, 60, 180
60, 60, 90, -60, -60
-60, 60, 90, -60, -60
-60, -60, 90, -60, -60
Conformation

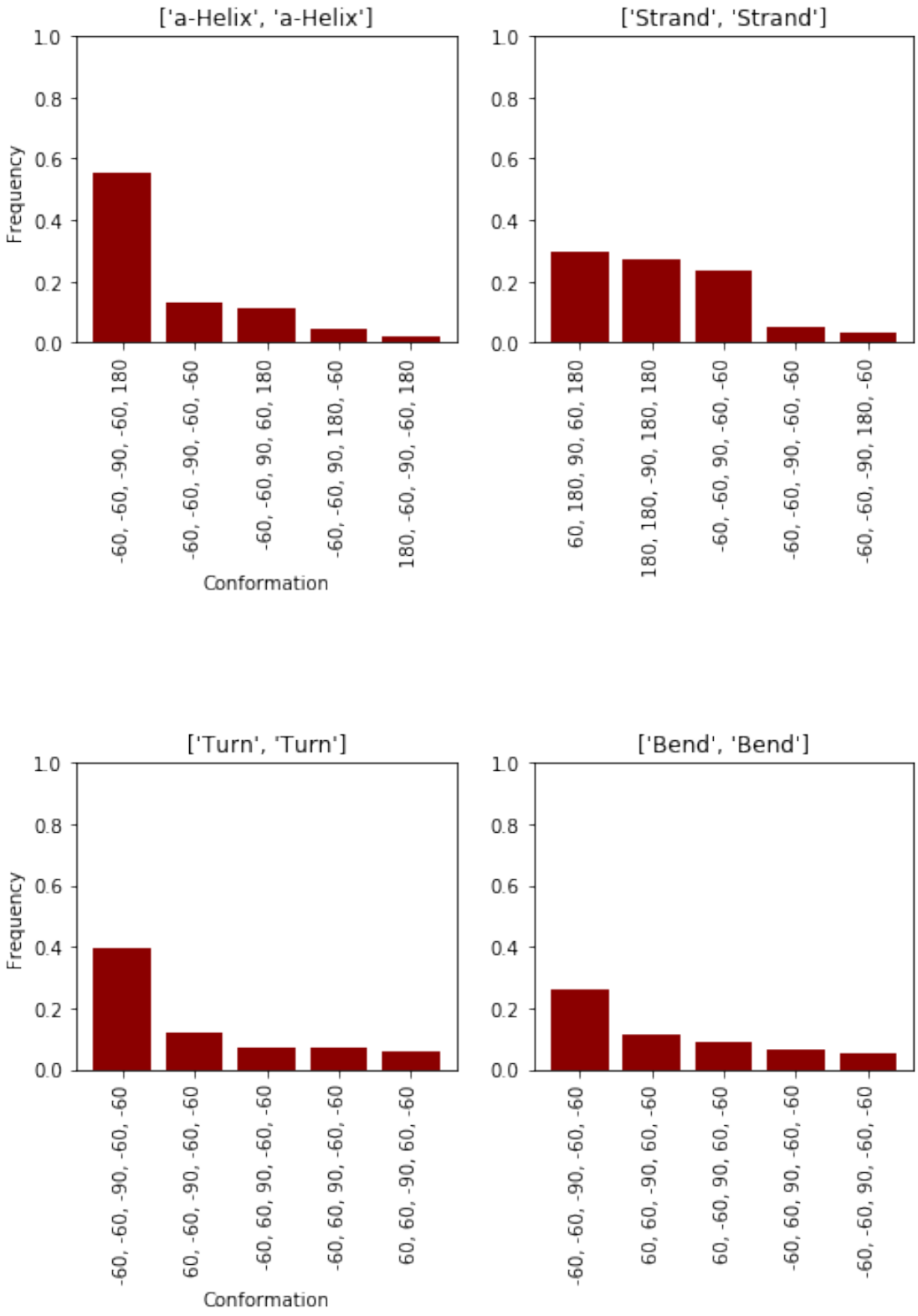
['Strand', 'Coil']
1.0
0.8
0.6
0.4
0.2
0.0
-60, -60, -90, -60, -60
60, 60, 90, 60, 180
-60, 60, 90, -60, -60
-60, -60, 90, 60, 180
-60, -60, 90, -60, -60


['3-Helix', 'Turn']
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
60, -60, -90, -60, -60
-60, -60, -90, -60, -60
180, 60, -90, -60, 180
-60, 60, 90, -60, -60
-60, -60, -90, 180, -60
Conformation

['3-Helix', 'Bend']
1.0
0.8
0.6
0.4
0.2
0.0
-60, -60, -90, -60, -60
-60, -60, -90, 60, 180
60, 60, 90, -60, -60
-60, -60, 90, 180, 180
-60, -60, -90, 180, -60


['3-Helix', 'Coil']
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
-60, -60, -90, -60, -60
-60, 60, 90, -60, -60
-60, 60, 90, -60, -60
-60, 60, -90, -60, -60
-60, -60, 90, 60, 180
Conformation
['Turn', 'Bend']
-60, -60, -90, -60, -60
-60, -60, -90, 60, 180
-60, -60, 90, 60, 180
60, -60, -90, -60, -60
-60, 60, 90, -60, -60


['Turn', 'Coil']
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
-60, -60, 90, 60, 180
-60, -60, -90, -60, -60
60, 60, 90, -60, -60
-60, 60, 90, 60, 180
-60, -60, -90, 180, -60
Conformation
['Bend', 'Coil']
-60, -60, -90, -60, -60
60, 60, 90, -60, -60
-60, 180, 90, 60, 180
-60, -60, 90, -60, -60
60, -60, -90, -60, -60


['a-Helix', 'a-Helix']
['Strand', 'Strand']
['Turn', 'Turn']
['Bend', 'Bend']
Frequency
Conformation
1.0
0.8
0.6
0.4
0.2
0.0
-60, -60, -90, -60, 180
-60, -60, -90, -60, -60
-60, -60, 90, 60, 180
-60, -60, 90, 180, -60
180, -60, -90, -60, 180
60, 180, 90, 60, 180
180, 180, -90, 180, 180
-60, -60, 90, -60, -60
-60, -60, -90, -60, -60
-60, -60, -90, 180, -60
-60, -60, -90, -60, -60
60, -60, -90, -60, -60
-60, -60, 90, -60, -60
-60, -60, 90, -60, -60
60, 60, -90, -60, -60
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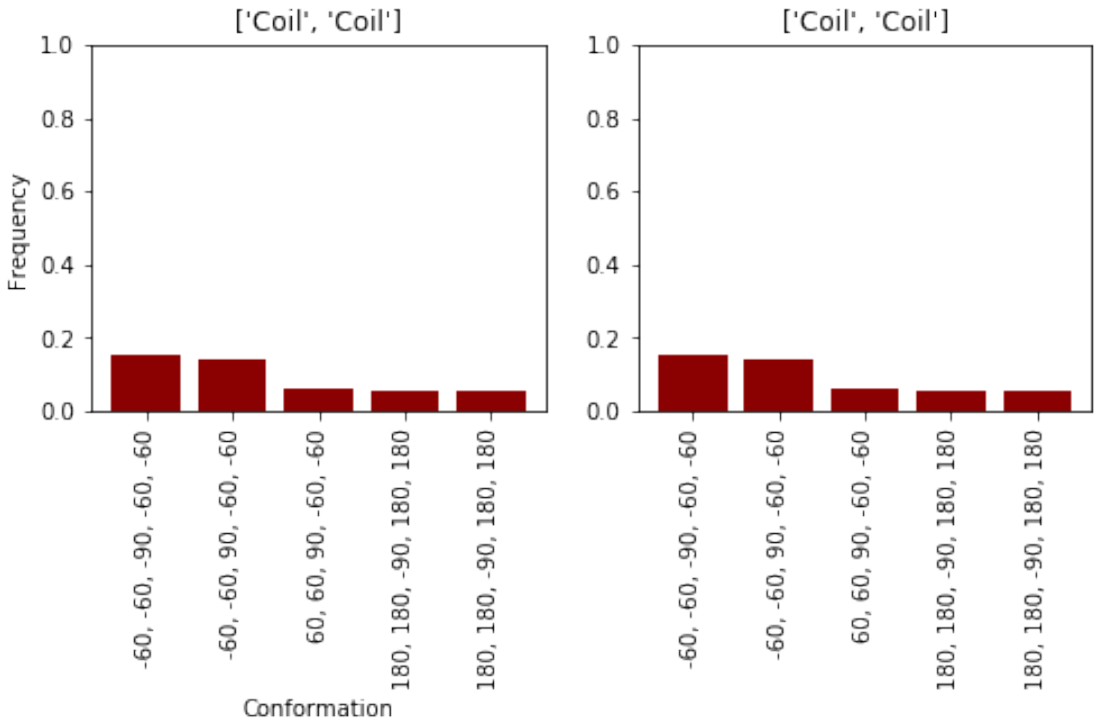
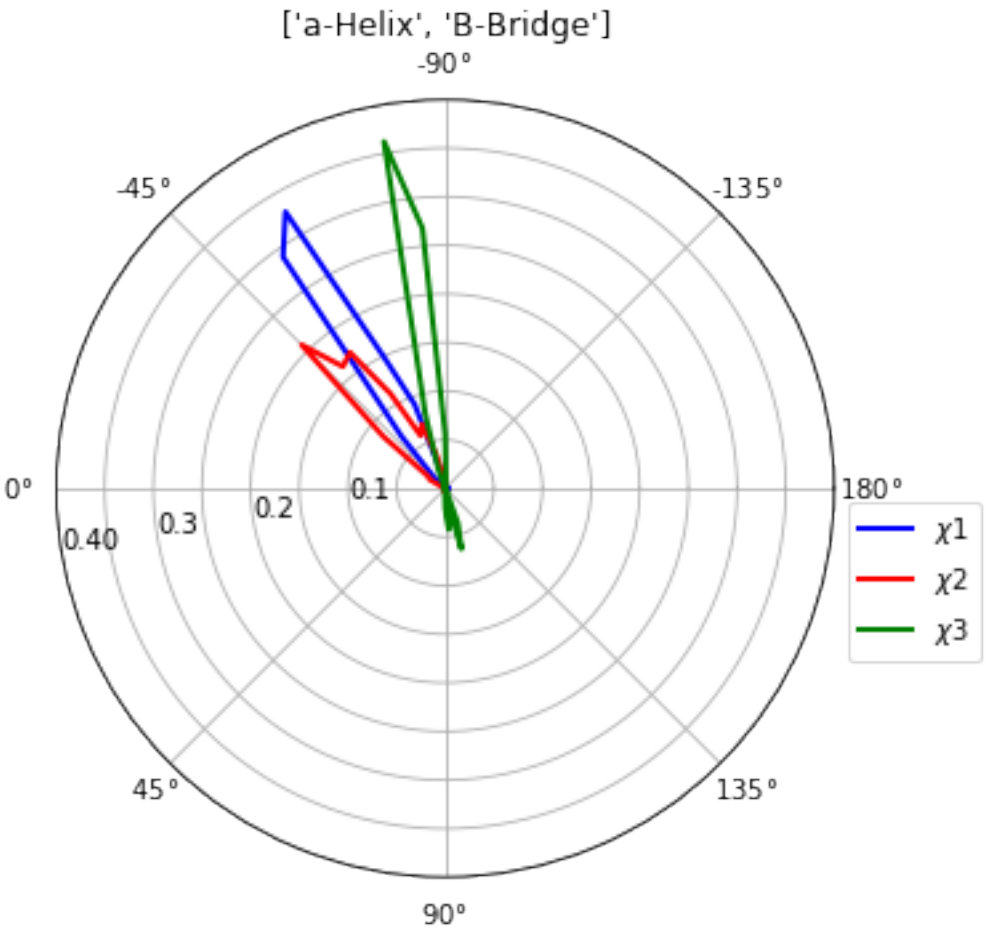
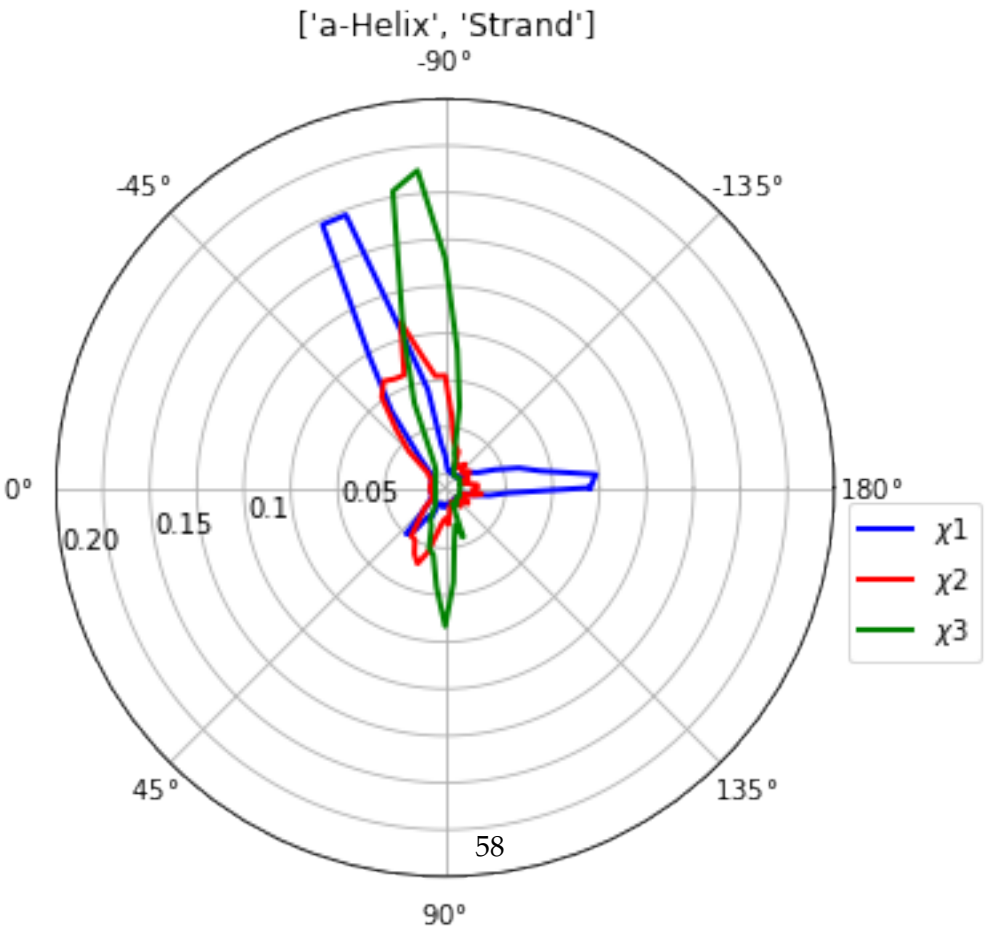
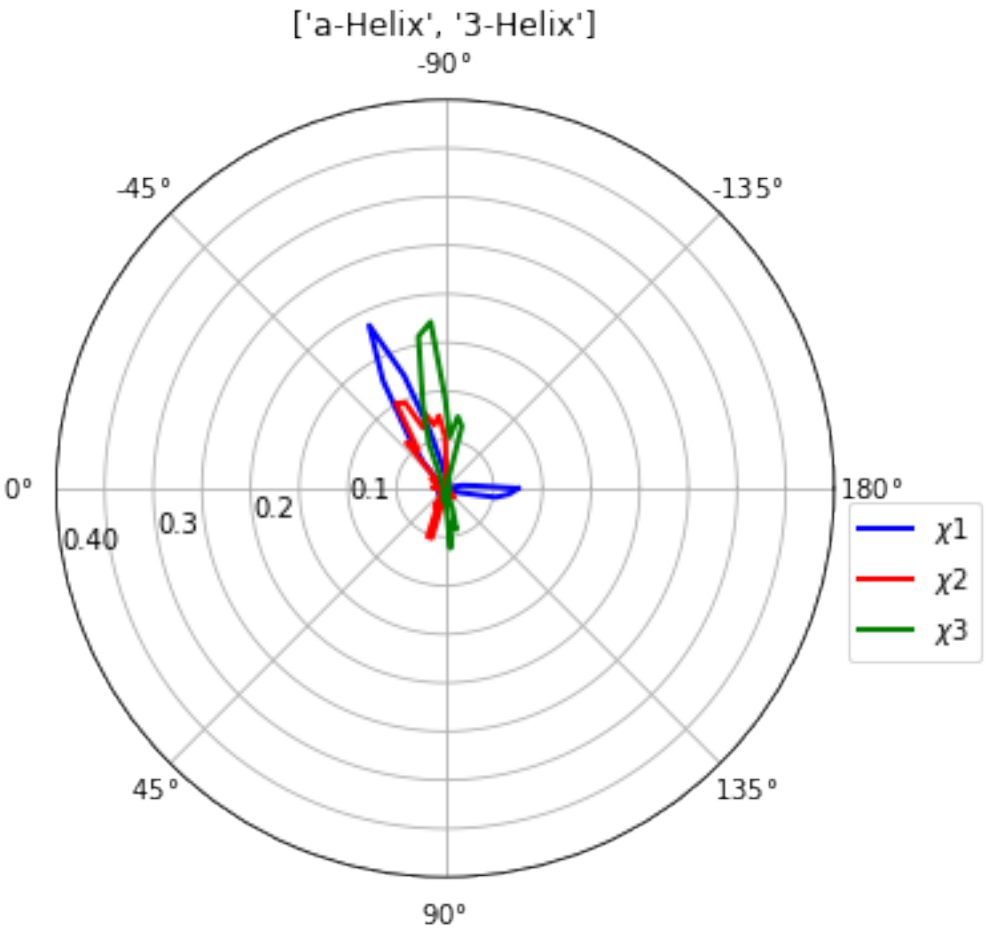
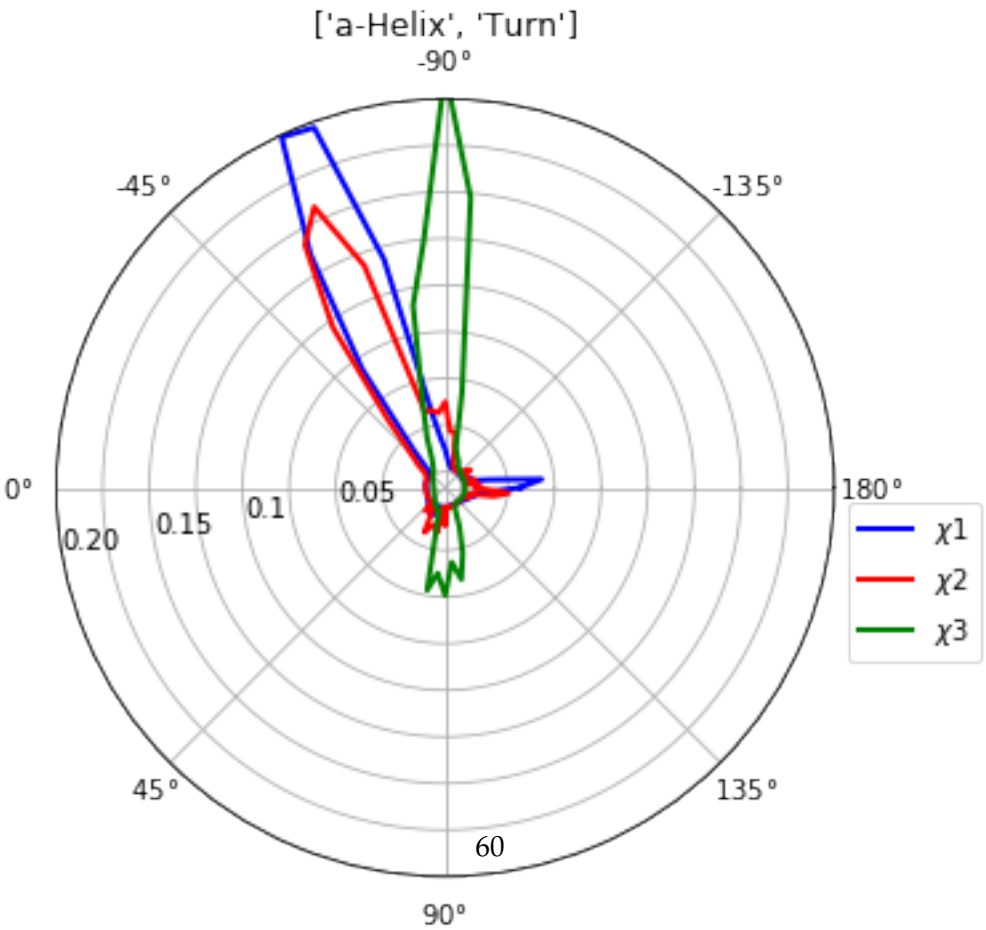
-60, 60, 90, -60, -60
-60, -60, 90, 60, -60

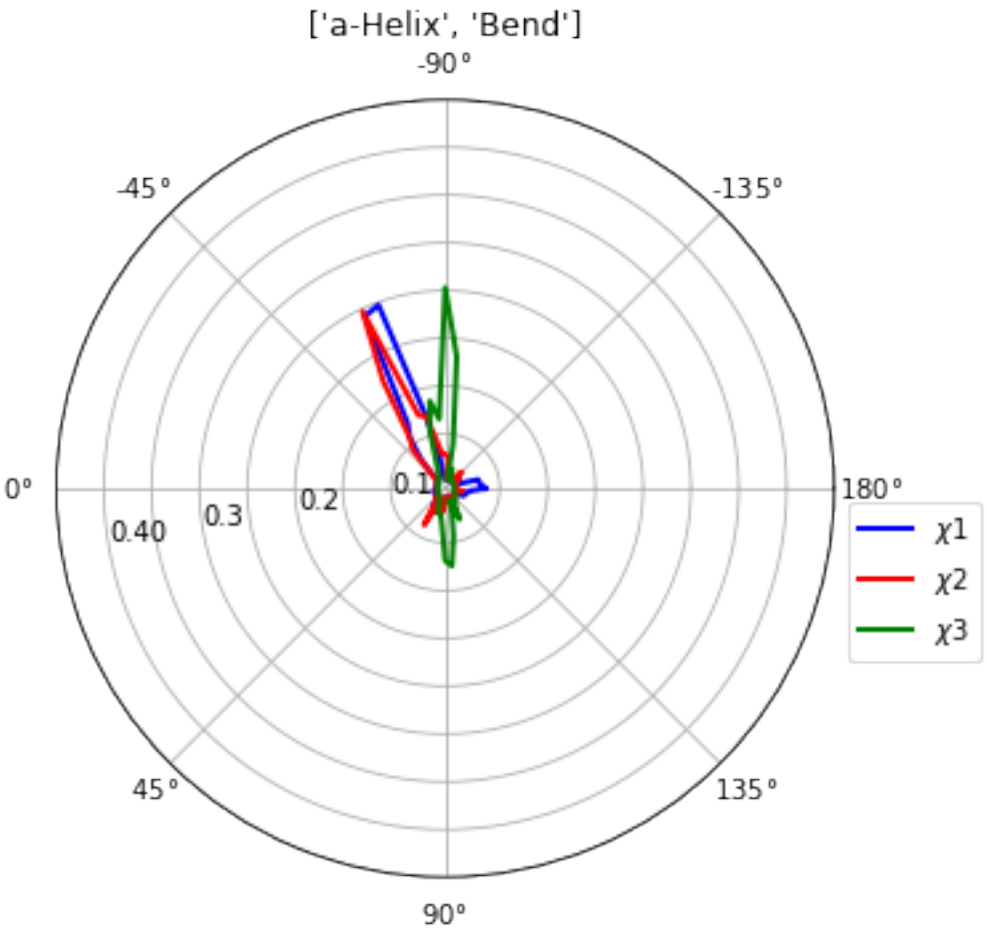

['Coil', 'Coil']
['Coil', 'Coil']
Frequency
1.0
0.8
0.6
0.4
0.2
0.0
-60, -60, -90, -60, -60
-60, -60, 90, -60, -60
60, 60, 90, -60, -60
180, 180, -90, 180, 180
180, 180, -90, 180, 180
Conformation

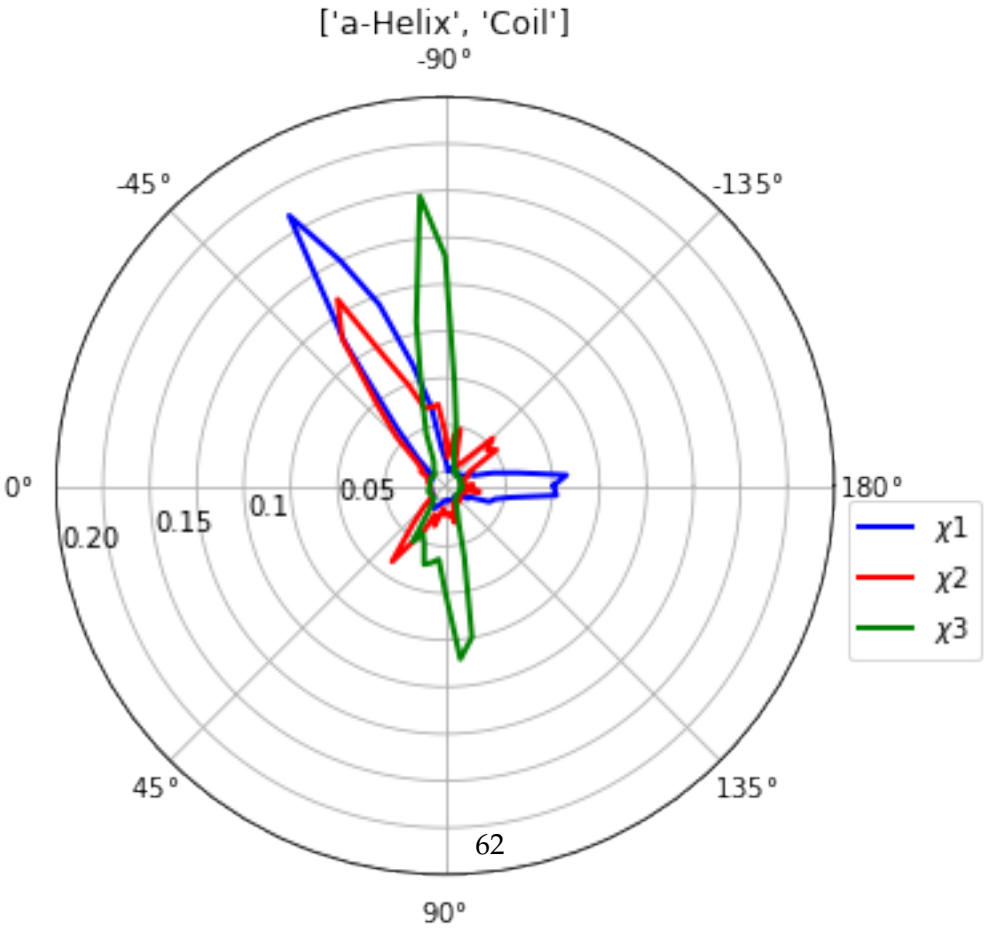

['a-Helix', 'B-Bridge']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.1
0.2
0.3
0.40
χ1
χ2
χ3

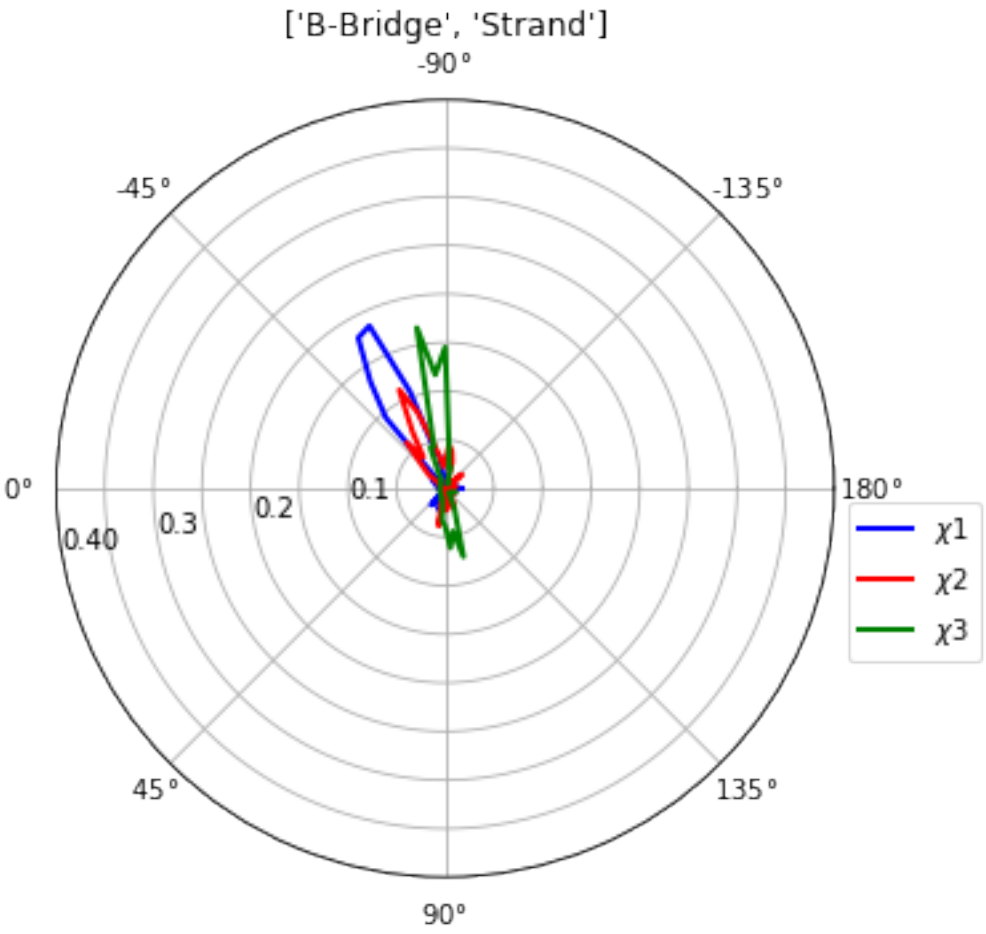

['a-Helix', 'Strand']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.05
0.1
0.15
0.20
χ1
χ2
χ3

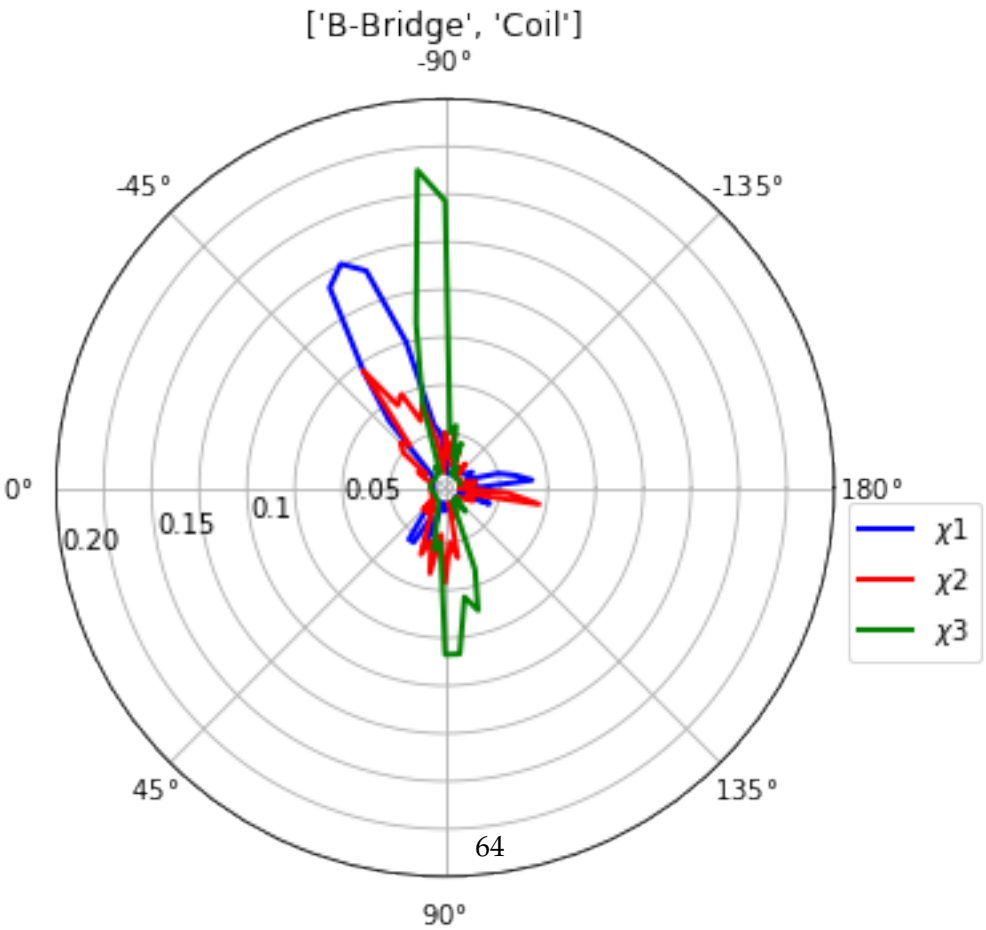

['a-Helix', '3-Helix']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.1
0.2
0.3
0.40
χ1
χ2
χ3

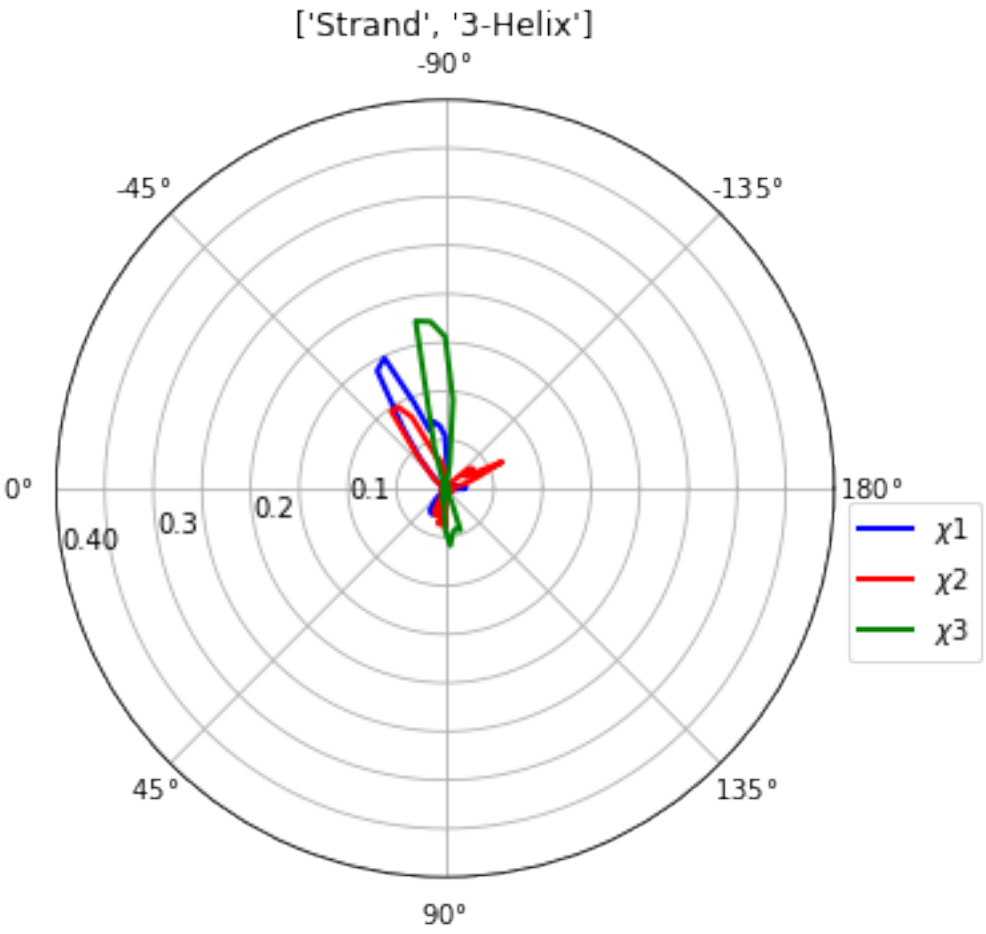

['a-Helix', 'Turn']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.05
0.1
0.15
0.20
χ1
χ2
χ3

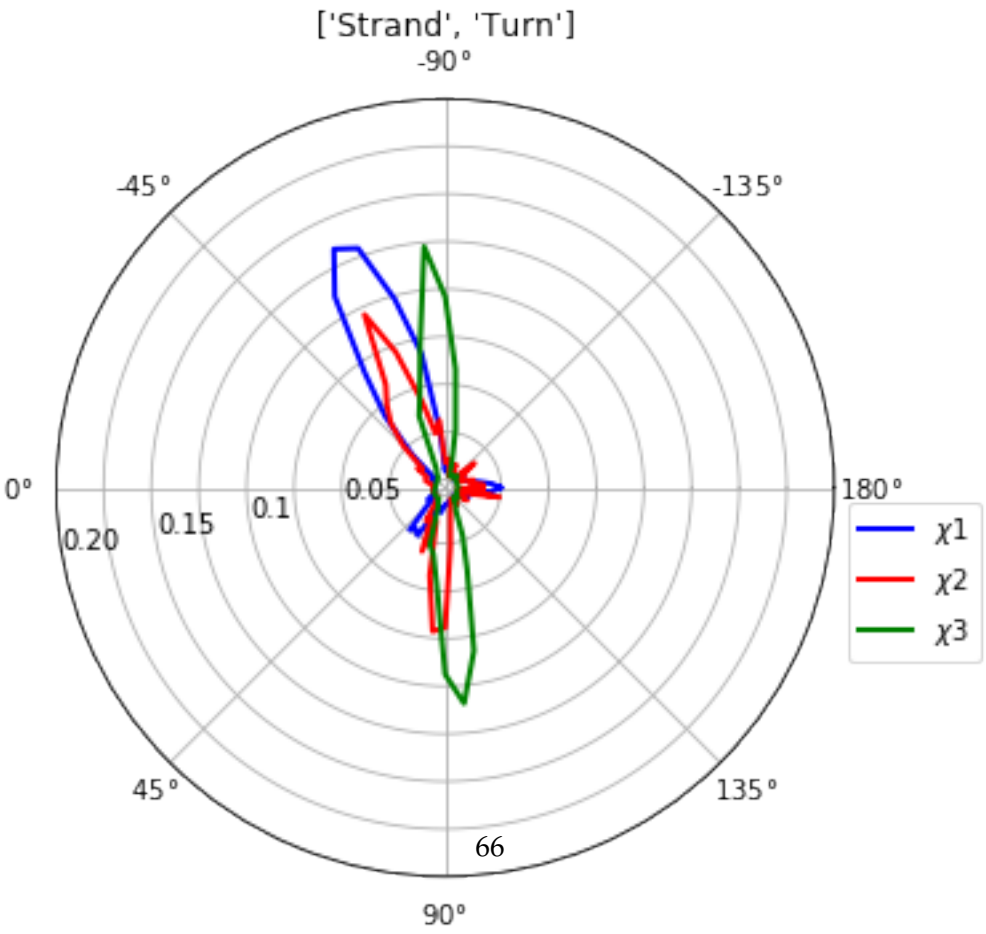

['a-Helix', 'Bend']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.1
0.2
0.3
0.40
χ1
χ2
χ3

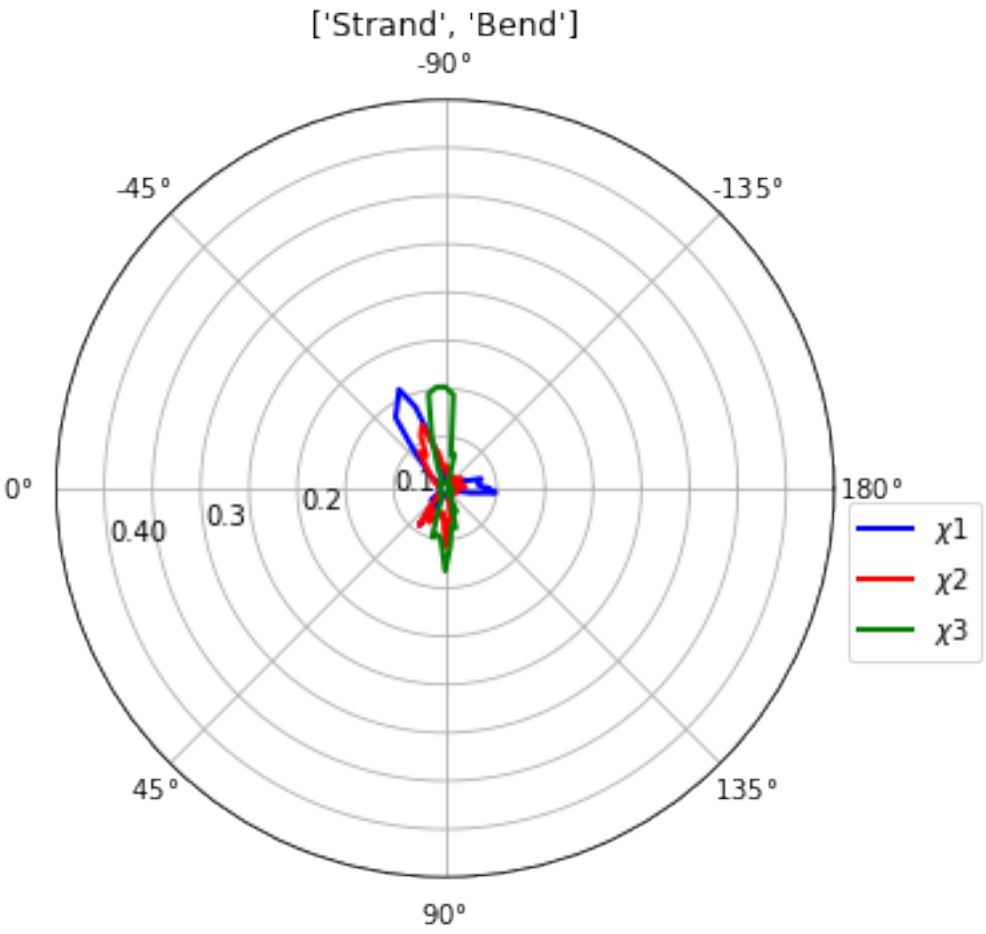

['a-Helix', 'Coil']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.05
0.1
0.15
0.20
χ1
χ2
χ3

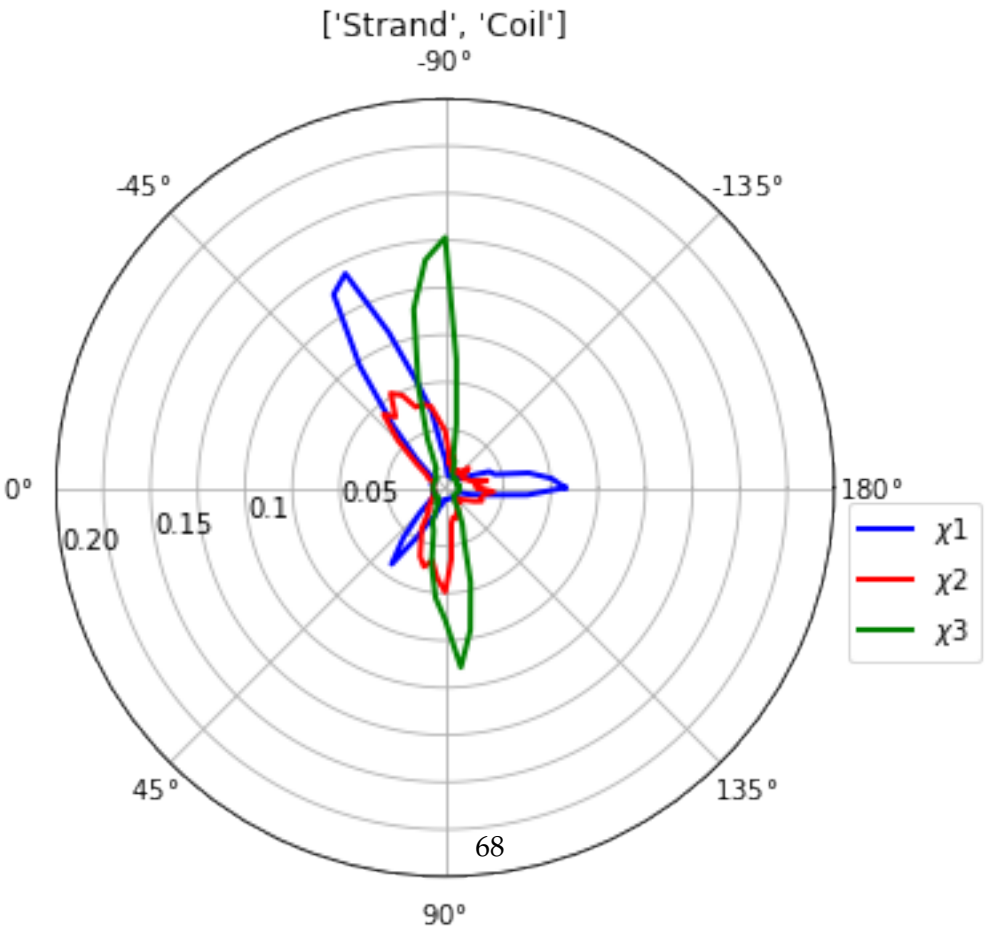

['B-Bridge', 'Strand']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.1
0.2
0.3
0.40
χ1
χ2
χ3

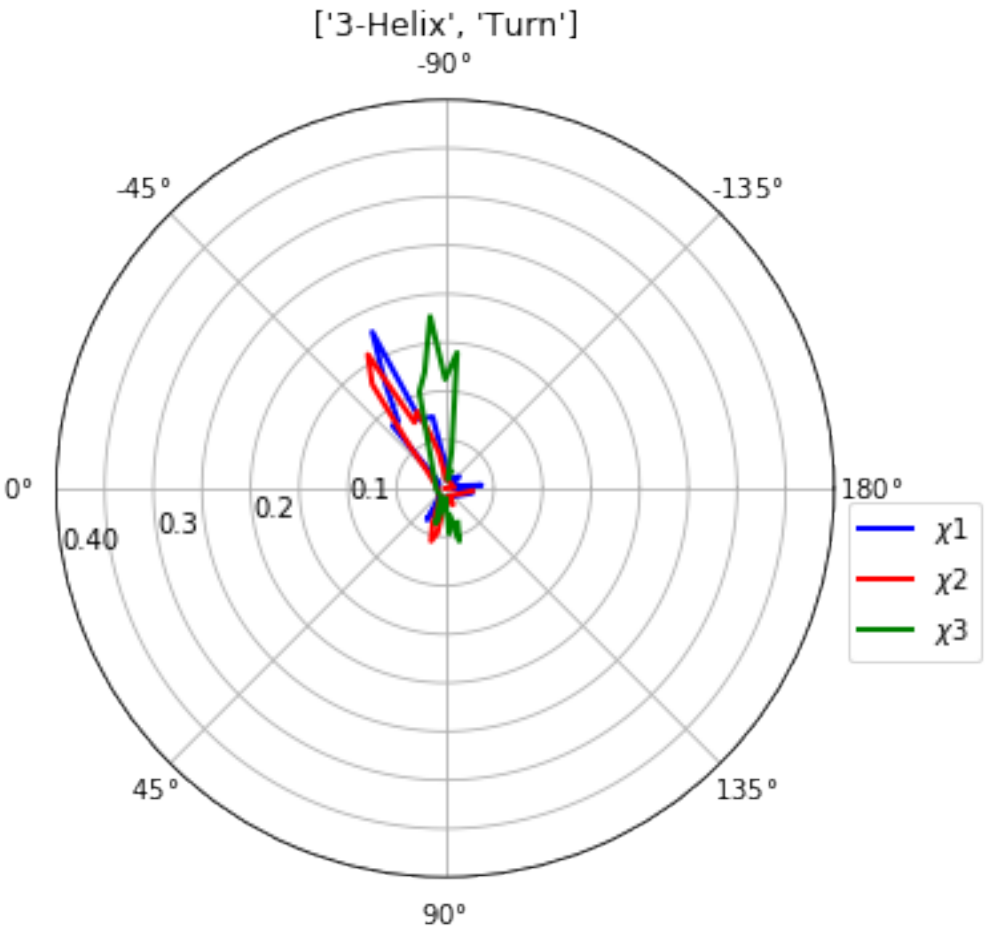

['B-Bridge', 'Coil']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.05
0.1
0.15
0.20
χ1
χ2
χ3

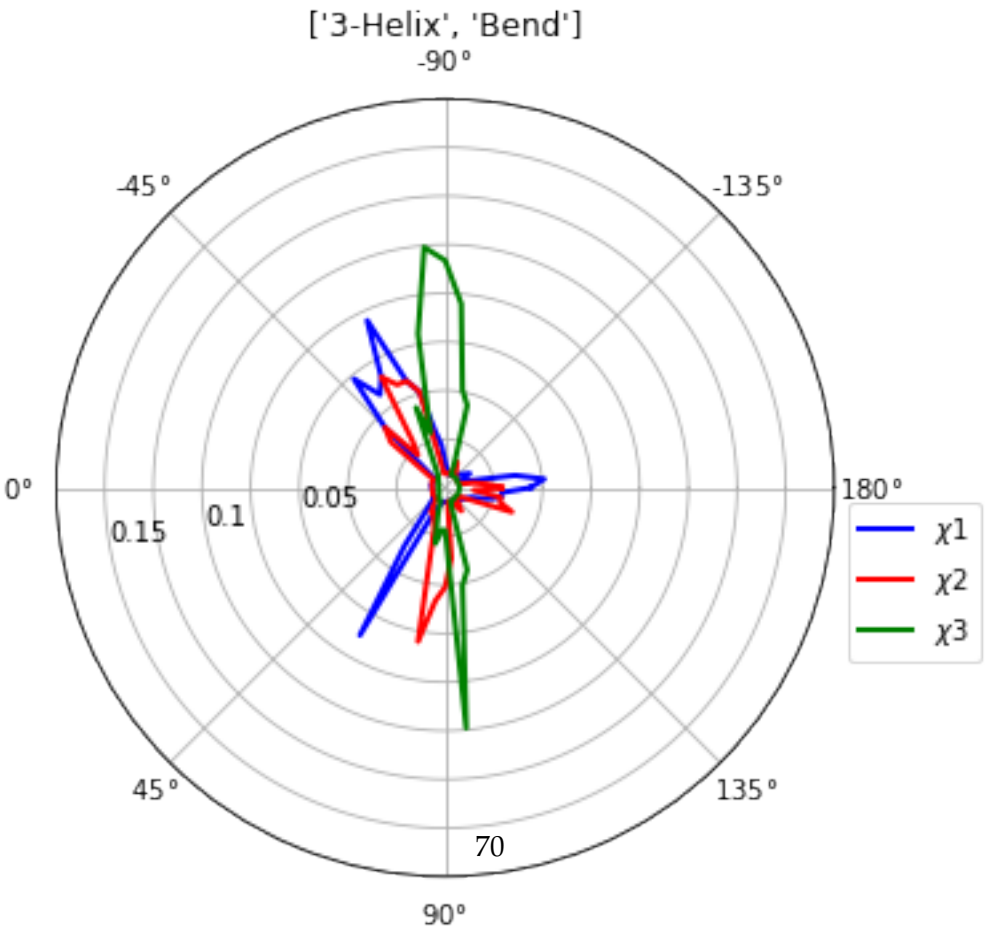

['Strand', '3-Helix']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.1
0.2
0.3
0.40
χ1
χ2
χ3

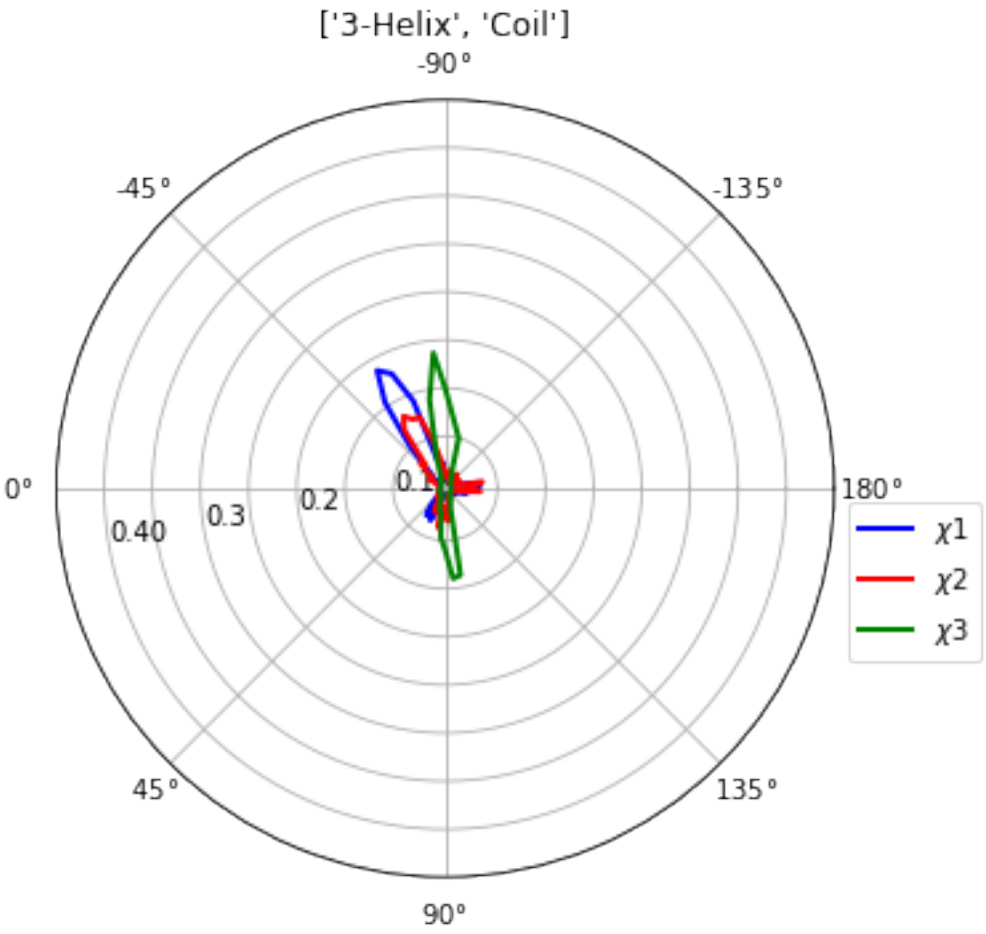

['Strand', 'Turn']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.05
0.1
0.15
0.20
χ1
χ2
χ3

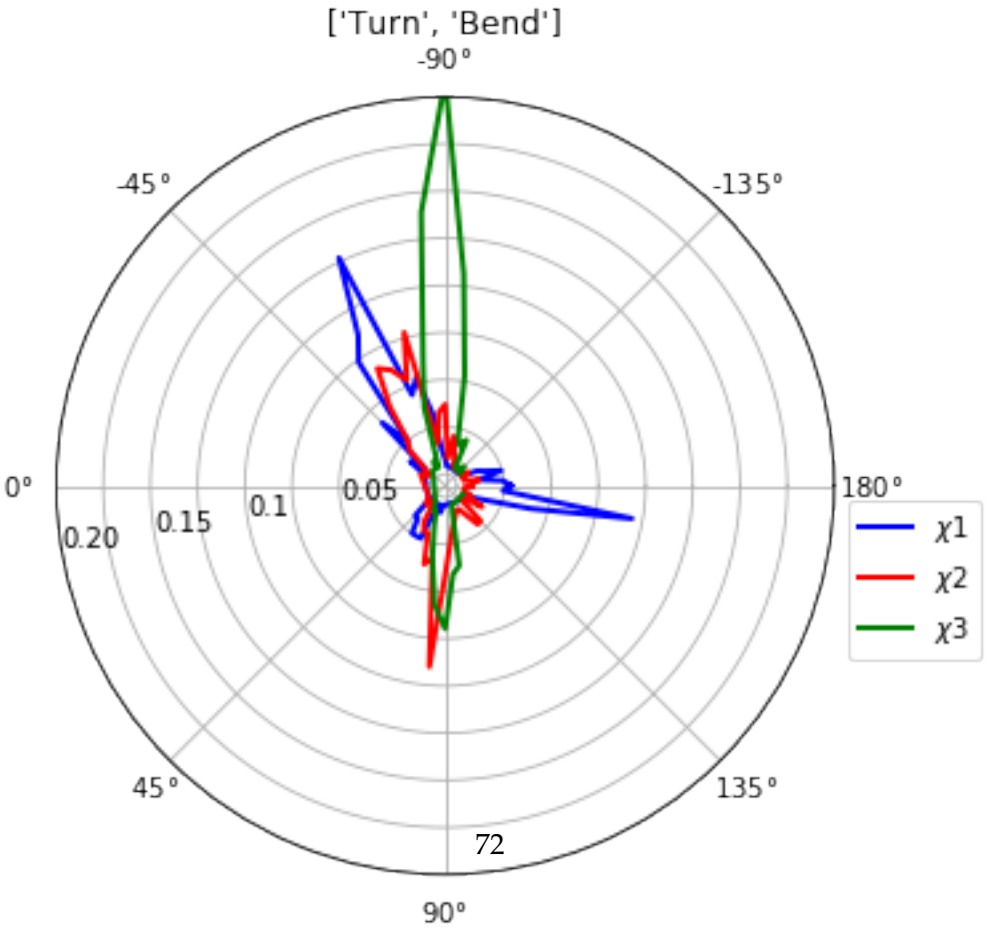

['Strand', 'Bend']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.1
0.2
0.3
0.40
χ1
χ2
χ3

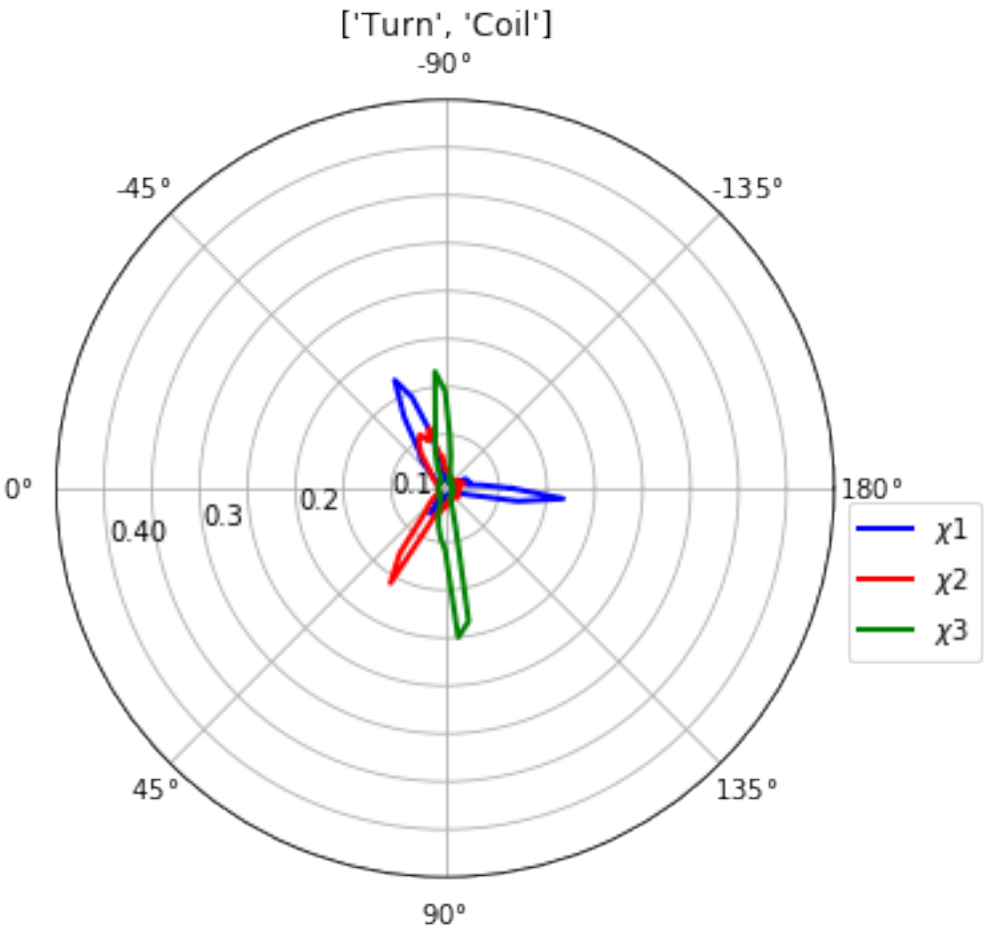

['Strand', 'Coil']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.05
0.1
0.15
0.20
χ1
χ2
χ3

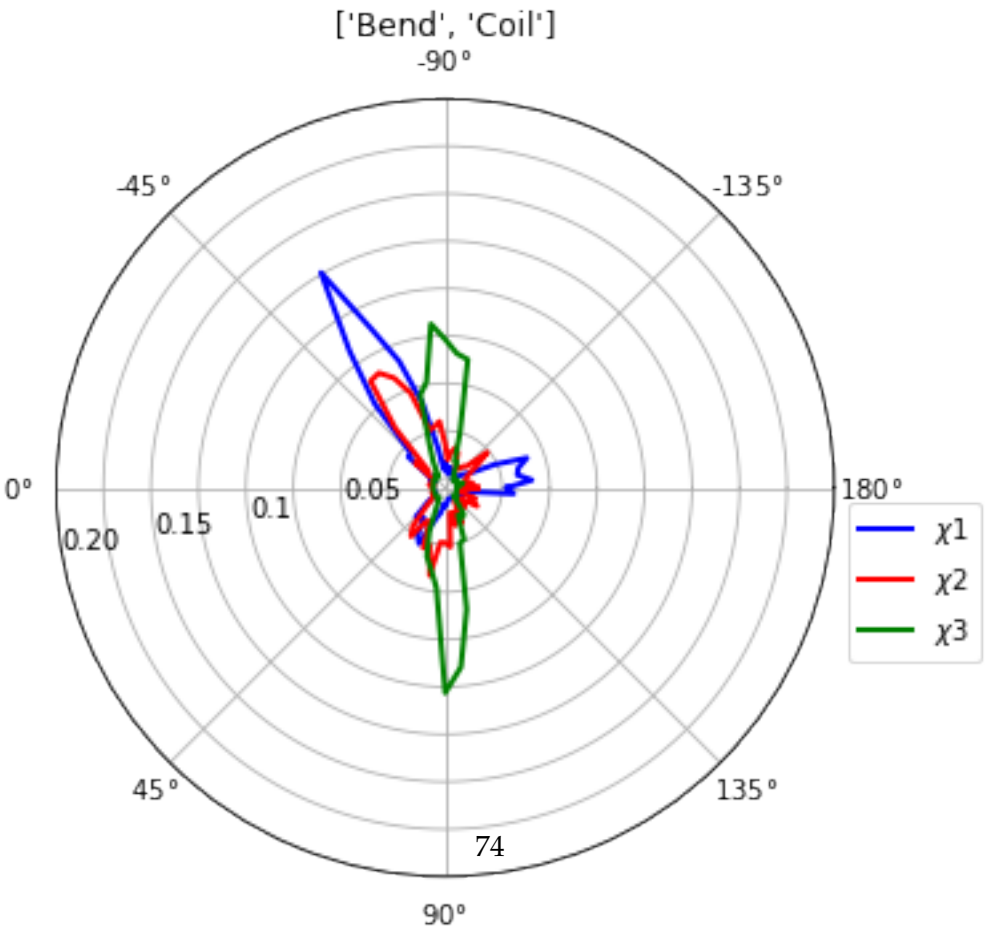

['3-Helix', 'Turn']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.1
0.2
0.3
0.40
χ1
χ2
χ3


['3-Helix', 'Bend']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.05
0.1
0.15
χ1
χ2
χ3


['3-Helix', 'Coil']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.1
0.2
0.3
0.40
χ1
χ2
χ3


['Turn', 'Bend']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.05
0.1
0.15
0.20
χ1
χ2
χ3


['Turn', 'Coil']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.1
0.2
0.3
0.40
χ1
χ2
χ3


['Bend', 'Coil']
-90°
-45°
-135°
0°
180°
45°
135°
90°
0.05
0.1
0.15
0.20
χ1
χ2
χ3

1.8 Dihedral configuraiton by Secondary Structure

1.9 Energy analysis