ProDy

Protein Dynamics & Sequence Analysis

Interactions Analysis

Release

Mikulska-Ruminska, Karolina

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CONTENTS

CHAPTER

ONE

INTRODUCTION

This tutorial shows how to predict and display the interactions within protein structure using the coordinates (single PDB) or ensemble of conformations (multi-model PDB or dcd file gerenarted by **NAMD_** program).

This module can be successfully used to study the distribution of different types of interactions (`hydrogen bonds`, `salt bridges`, `repulsive ionic binding`, `pi-cation`, `pi-stacking`, `hydrophobic interactions`, and `disulfide bonds`) within protein structure. It may help to distinguish the difference between wild type protein and its mutant, indentify regions or simply residues which are privileged to create a larger number of potential interactions in single PDB, ensemble PDB (NMR data) or during the molecular dynamics simulation.

1.1 Required Programs

Latest version of **ProDy_** is required.

1.2 Recommended Programs

Besides **ProDy_**, the **Matplotlib_** library and **VMD_** program are required for some steps in the tutorial. **IPython_** is highly recommended for interactive usage.

To take full advantage of InSty's capabilities in predicting hydrophobic interactions, we should download an additional component written in C++ and Fortran. The additional component (hpb.so file) is available in the ProDy repository (prody/proteins/hpbmodule folder) and should be chosen and selected according to the version of Python that is being used by user. This file should be copied to the ProDy folder (prody/proteins/) or to the local directory.

Moreover, in the case of the lack of hydrogen atoms in protein structure, additional package such as Openbabel[1] or PDBfixer[2] are required for predicting hydrogen bonds.

1.3 Getting Started

To follow this tutorial, you will need the following files:

```
1.5M Feb 29 20:20 5kqm_all_sci.pdb
222K Feb 29 20:20 addH_5kqm.pdb
3.3M Feb 29 20:20 addH_7laf.pdb
4.5M Feb 29 20:20 NAMD_D2_co100.dcd
```

We recommend that you will follow this tutorial by typing commands in an IPython session, e.g.:

[1] https://github.com/openbabel
[2] https://github.com/openmm/pdbfixer

```
$ ipython
```

or with pylab environment:

```
$ ipython --pylab
```

First, we will make necessary imports from ProDy and **Matplotlib_** packages.

```
In [1]: from prody import *

In [2]: from pylab import *

In [3]: import matplotlib

In [4]: ion()
```

We have included these imports in every part of the tutorial, so that code copied from the online pages is complete. You do not need to repeat imports in the same Python session.

CHAPTER

TWO

INTERACTIONS/STABILITY EVALUATION

This example shows how to perform Interactions/Stability Evaluation (**InSty**) analysis for a small protein (<200 residues) called tyrosine phosphatase LMW-PTP (PDB: **5KQM**) and visualize the results using **Matplotlib_** library and **VMD_** program. In the tutorial, we will use an already prepared structure for simulation (with hydrogens added). The same structure will be later analyzed with the trajectory file to show how the analysis of interactions in the course of the simulation can change. The file is available in tutorial files.

The tutorial will also include an example of a PDB structure directly downloaded from Protein Data Bank (PDB) which requires adding the missing hydrogen atoms to the protein and ligand structure.

2.1 Analysis of interactions for a single PDB structure

We start by parsing PDB file with LMW-PTP `5kqm_all_sci.pdb` which is avalable in the tutorial files. The PDB file contains protein structure with water and counter ions prepared using **VMD_** program.

Before that import everything from the ProDy packages.

```
In [1]: from prody import *

In [2]: from pylab import *

In [3]: import matplotlib
```

```
In [4]: PDBfile = '5kqm_all_sci.pdb'

In [5]: coords = parsePDB(PDBfile)

In [6]: coords
```

```
@> 19321 atoms and 1 coordinate set(s) were parsed in 0.23s.
```

For the analysis we will use only protein coordinates (`atoms`):

```
In [7]: atoms = coords.select('protein')

In [8]: atoms
```

```
@> 19321 atoms and 1 coordinate set(s) were parsed in 0.21s.
```

2.2 Compute all types of interactions

In the next step, we instantiate an `Interactions` instance:

```
In [9]: interactions = Interactions()
```

Now we can compute all available types of interactions (seven types: hydrogen bonds, salt bridges, repulsive ionic bonding, Pi-cation, Pi-stacking, hydrophobic interactions, and disulfide bonds) for protein structure by passing selected atoms (`atoms`) to `Interactions.calcProteinInteractions()` method:

```
In [10]: all_interactions = interactions.calcProteinInteractions(atoms)
```

```
@> Calculating interations.
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     ARG101    P      NH1_1516  <--->      ASP98    P      OD1_1463     2.0    33.1
@>      HSE72    P      NE2_1042  <--->      ASN15    P       OD1_165     2.6    34.8
@>     GLN143    P      NE2_2192  <--->     GLU139    P      OE2_2126     2.7     9.2
@>      HSE66    P       NE2_957  <--->     GLU139    P      OE1_2125     2.7     6.4
@>      ARG40    P         N_561  <--->       LYS6    P          O_37     2.7    17.1
@>      ARG58    P         N_813  <--->      ASP56    P       OD1_788     2.7    30.0
@>      ALA45    P         N_634  <--->      ARG75    P        O_1097     2.8    35.1
@>      ASN53    P       ND2_747  <--->      GLU50    P       OE1_708     2.8    18.2
@>      ALA74    P        N_1064  <--->      ASN53    P         O_751     2.8    21.3
@>      ASP56    P         N_780  <--->      ILE16    P         O_189     2.8    27.0
@>     LYS110    P       NZ_1667  <--->      THR84    P        O_1240     2.8    38.2
@>     LEU116    P        N_1758  <--->      CYS90    P        O_1342     2.8    15.0
@>     SER103    P        N_1546  <--->      LEU99    P        O_1485     2.8    29.1
@>     ASN134    P        N_2045  <--->     ASP137    P      OD2_2091     2.8    22.6
@>     PHE152    P        N_2321  <--->     CYS148    P        O_2275     2.8     8.3
@>      ASN95    P        N_1398  <--->      ASP92    P      OD1_1368     2.8    12.6
@>       LYS6    P          N_16  <--->      ASN38    P         O_536     2.8    25.0
@>      ILE77    P        N_1115  <--->      ALA45    P         O_643     2.8    12.2
@>      ARG58    P       NH2_832  <--->      ASP56    P       OD2_789     2.8    27.7
@>      LEU99    P        N_1467  <--->      ASN95    P        O_1411     2.8    15.5
@>     CYS149    P        N_2276  <--->     CYS145    P        O_2224     2.8     9.6
@>      GLY52    P         N_731  <--->      ALA74    P        O_1073     2.8     6.6
@>      ASP32    P         N_435  <--->      LYS28    P         O_385     2.8     8.8
@>      ILE88    P        N_1294  <--->     LYS112    P        O_1704     2.8    17.7
@>     GLN143    P        N_2180  <--->     GLU139    P        O_2128     2.8    21.7
@>      ARG27    P         N_340  <--->      GLU23    P         O_293     2.8    15.4
@>     TYR142    P        N_2159  <--->     PHE138    P        O_2113     2.9    14.2
@>     GLY133    P        N_2038  <--->     PRO130    P        O_1995     2.9    25.4
@>      PHE26    P         N_320  <--->      ALA22    P         O_278     2.9     4.9
@>      ASN15    P       ND2_166  <--->      SER19    P        OG_232     2.9    32.1
@>      ARG75    P      NH1_1090  <--->      ASP81    P      OD2_1194     2.9    19.7
@>      ARG75    P      NH2_1093  <--->      ASP42    P       OD2_610     2.9    23.5
@>      ARG97    P        N_1431  <--->      GLU93    P        O_1386     2.9    22.2
@>      ARG65    P       NH2_941  <--->     GLU139    P      OE1_2125     2.9    32.3
@>      VAL25    P         N_304  <--->      ILE21    P         O_268     2.9     8.2
@>     LEU153    P        N_2341  <--->     CYS149    P        O_2286     2.9    12.5
@>       SER7    P          N_38  <--->      ASP86    P      OD2_1270     2.9    39.9
@>      ASP86    P        N_1261  <--->       SER7    P         OG_45     2.9    34.7
@>      ARG58    P       NH2_832  <--->     TYR131    P        O_2016     2.9    33.1
@>      THR46    P         N_644  <--->      CYS12    P         O_130     2.9    36.1
@>     GLN144    P        N_2197  <--->     THR140    P        O_2142     2.9    23.3
@>      THR78    P        N_1134  <--->      ASP81    P      OD2_1194     2.9    12.4
@>      LEU89    P        N_1313  <--->       LEU9    P          O_83     2.9    29.5
@>      THR31    P         N_421  <--->      ARG27    P         O_363     2.9    24.1
@>      CYS90    P        N_1332  <--->     GLU114    P        O_1738     2.9    24.6
..
..
```

```
@> Number of detected hydrogen bonds: 124.
@> Calculating salt bridges.
@>      HSE66    P         NE2_957  <--->     GLU139    P   OE1_2125_2126     2.8
@>      ASP81    P   OD1_1193_1194  <--->      ARG75    P   NH1_1090_1093     2.9
@>      ASP32    P     OD1_443_444  <--->      LYS28    P          NZ_380     3.0
@>     ARG101    P   NH1_1516_1519  <--->      ASP98    P   OD1_1463_1464     3.1
@>      ARG27    P     NH1_356_359  <--->      GLU23    P     OE1_290_291     3.7
@>     GLU139    P   OE1_2125_2126  <--->      ARG65    P     NH1_938_941     3.8
@>     LYS102    P         NZ_1540  <--->      ASP98    P   OD1_1463_1464     3.9
@>      ARG58    P     NH1_829_832  <--->      ASP56    P     OD1_788_789     3.9
@>      ARG18    P     NH1_217_220  <--->      ASP92    P   OD1_1368_1369     4.1
@>     GLU114    P   OE1_1735_1736  <--->     LYS112    P         NZ_1699     4.1
@>     ASP120    P   OD1_1824_1825  <--->     ARG147    P   NH1_2257_2260     4.2
@>     LYS110    P         NZ_1667  <--->      ASP86    P   OD1_1269_1270     4.2
@>     GLU114    P   OE1_1735_1736  <--->     HSE157    P        NE2_2418     4.4
@>      ARG18    P     NH1_217_220  <--->     ASP129    P   OD1_1978_1979     4.6
@>      ARG75    P   NH1_1090_1093  <--->      ASP42    P     OD1_609_610     4.6
@>      GLU23    P     OE1_290_291  <--->      HSE72    P        NE2_1042     5.0
@> Number of detected salt bridges: 16.
@> Calculating repulsive ionic bonding.
@>     ARG101    P   NH1_1516_1519  <--->     LYS102    P         NZ_1540     4.3
@> Number of detected Repulsive Ionic Bonding interactions: 1.
@> Calculating Pi stacking interactions.
@>      HSE66       P             953_954_955_957_959  <--->     TYR142       P   2166_2167_2169_2171
@>     HSE157       P 2414_2415_2416_2418_2420_2423_2424  <--->     TYR119       P   1802_1803_1805_1
@>      TRP39       P         549_550_551_553_555_557  <--->      PHE26       P         327_328_330_3
@>     TYR131       P   2003_2004_2006_2008_2011_2013  <--->     TYR132       P   2024_2025_2027_2029
@> Number of detected Pi stacking interactions: 4.
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_5
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                    NH1_938_9
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                          NZ_
@> Number of detected cation-pi interactions: 3.
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      TYR87    P    OH_128614s  <--->     ALA156    P    CB_2401     3.0    22.0
@>      MET63    P     CE_89414s  <--->      ALA24    P     CB_298     3.3     5.2
@>      ILE68    P    CG2_97614s  <--->      MET63    P     CE_894     3.3    52.4
@>     TYR142    P    CZ_217114s  <--->     VAL146    P   CG2_2235     3.5    49.7
@>      PHE10    P     CD1_9214s  <--->      ALA22    P     CB_273     3.5    31.2
@>       LYS6    P      CD_2614s  <--->      TRP39    P    CZ2_555     3.5    68.7
@>      VAL30    P    CG1_41114s  <--->      PHE26    P    CE2_336     3.6    21.1
@>     ALA111    P    CB_167714s  <--->      ILE88    P    CD_1307     3.6    21.2
@>      VAL11    P    CG2_11414s  <--->      ILE88    P   CG2_1300     3.6     9.3
@>      VAL41    P    CG2_59514s  <--->      PHE26    P    CD2_334     3.6    16.6
@>     PHE152    P   CE1_233114s  <--->     ALA156    P    CB_2401     3.7    17.5
@>     VAL106    P   CG2_159814s  <--->      LYS79    P    CG_1155     3.7    25.1
@>      ILE77    P    CD_112814s  <--->      LEU99    P   CD2_1480     3.7    12.0
@>      PHE82    P   CD1_120514s  <--->      ILE88    P    CD_1307     3.7    17.6
@>     LEU116    P   CD2_177114s  <--->     ILE127    P    CD_1949     3.7    17.4
@>       VAL8    P     CG1_5514s  <--->      PHE26    P    CE2_336     3.7    12.1
@>      LEU96    P   CD1_142114s  <--->     ILE113    P   CG2_1711     3.7    17.0
@>       LEU9    P     CD2_7814s  <--->      ILE77    P    CD_1128     3.7    15.4
@>      LEU89    P   CD1_132214s  <--->       VAL8    P     CG2_59     3.8    15.9
@>     ILE126    P    CD_193014s  <--->     LEU125    P   CD1_1907     3.8    54.2
@>     VAL141    P   CG1_214914s  <--->     ILE127    P   CG2_1942     3.9    11.5
..
..
```

```
@> Number of detected hydrophobic interactions: 39.
@> Calculating disulfide bonds.
@> Number of detected disulfide bonds: 0.
```

All types of interactions will be displayed on the screen with all types of information such as distance or angle (if applied).

Moreover, we will have access to the details of each interaction type using the following methods:

`Interactions.getHydrogenBonds()` - hydrogen bonds:

```
In [11]: interactions.getHydrogenBonds()
```

```
[['ARG101', 'NH1_1516', 'P', 'ASP98', 'OD1_1463', 'P', 1.998, 33.1238],
 ['HSE72', 'NE2_1042', 'P', 'ASN15', 'OD1_165', 'P', 2.5997, 34.752],
 ['GLN143', 'NE2_2192', 'P', 'GLU139', 'OE2_2126', 'P', 2.7287, 9.1823],
 ['HSE66', 'NE2_957', 'P', 'GLU139', 'OE1_2125', 'P', 2.7314, 6.3592],
 ['ARG40', 'N_561', 'P', 'LYS6', 'O_37', 'P', 2.7479, 17.1499],
 ['ARG58', 'N_813', 'P', 'ASP56', 'OD1_788', 'P', 2.7499, 29.9737],
 ['ALA45', 'N_634', 'P', 'ARG75', 'O_1097', 'P', 2.7609, 35.0983],
 ['ASN53', 'ND2_747', 'P', 'GLU50', 'OE1_708', 'P', 2.7702, 18.2336],
 ['ALA74', 'N_1064', 'P', 'ASN53', 'O_751', 'P', 2.7782, 21.3375],
 ['ASP56', 'N_780', 'P', 'ILE16', 'O_189', 'P', 2.7793, 27.0481],
 ['LYS110', 'NZ_1667', 'P', 'THR84', 'O_1240', 'P', 2.7977, 38.2213],
 ['LEU116', 'N_1758', 'P', 'CYS90', 'O_1342', 'P', 2.8072, 15.0239],
 ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 2.8075, 29.107],
 ['ASN134', 'N_2045', 'P', 'ASP137', 'OD2_2091', 'P', 2.8132, 22.562],
 ['PHE152', 'N_2321', 'P', 'CYS148', 'O_2275', 'P', 2.8141, 8.2562],
 ['ASN95', 'N_1398', 'P', 'ASP92', 'OD1_1368', 'P', 2.8148, 12.5701],
 ['LYS6', 'N_16', 'P', 'ASN38', 'O_536', 'P', 2.8178, 25.0305],
 ['ILE77', 'N_1115', 'P', 'ALA45', 'O_643', 'P', 2.8179, 12.1855],
 ..
 ..
```

`Interactions.getSaltBridges()` - salt bridges (residues with oposite charges):

```
In [12]: interactions.getSaltBridges()
```

```
[['HSE66', 'NE2_957', 'P', 'GLU139', 'OE1_2125_2126', 'P', 2.8359],
 ['ASP81', 'OD1_1193_1194', 'P', 'ARG75', 'NH1_1090_1093', 'P', 2.9163],
 ['ASP32', 'OD1_443_444', 'P', 'LYS28', 'NZ_380', 'P', 3.037],
 ['ARG101', 'NH1_1516_1519', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.0699],
 ['ARG27', 'NH1_356_359', 'P', 'GLU23', 'OE1_290_291', 'P', 3.7148],
 ['GLU139', 'OE1_2125_2126', 'P', 'ARG65', 'NH1_938_941', 'P', 3.7799],
 ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.9359],
 ['ARG58', 'NH1_829_832', 'P', 'ASP56', 'OD1_788_789', 'P', 3.9486],
 ['ARG18', 'NH1_217_220', 'P', 'ASP92', 'OD1_1368_1369', 'P', 4.0693],
 ['GLU114', 'OE1_1735_1736', 'P', 'LYS112', 'NZ_1699', 'P', 4.0787],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 4.1543],
 ['LYS110', 'NZ_1667', 'P', 'ASP86', 'OD1_1269_1270', 'P', 4.1879],
 ['GLU114', 'OE1_1735_1736', 'P', 'HSE157', 'NE2_2418', 'P', 4.3835],
 ['ARG18', 'NH1_217_220', 'P', 'ASP129', 'OD1_1978_1979', 'P', 4.5608],
 ['ARG75', 'NH1_1090_1093', 'P', 'ASP42', 'OD1_609_610', 'P', 4.5612],
 ['GLU23', 'OE1_290_291', 'P', 'HSE72', 'NE2_1042', 'P', 4.99]]
```

`Interactions.getRepulsiveIonicBonding()` - repulsive ionic bonding (between residues with the same charges):

```
In [13]: interactions.getRepulsiveIonicBonding()
```

```
[['ARG101', 'NH1_1516_1519', 'P', 'LYS102', 'NZ_1540', 'P', 4.2655]]
```

`Interactions.getPiStacking()` - Pi-stacking interactions (HSE is a histidine (HIS) type in the CHARMM force field):

```
In [14]: interactions.getPiStacking()
```

```
[['HSE66',
  '953_954_955_957_959',
  'P',
  'TYR142',
  '2166_2167_2169_2171_2174_2176',
  'P',
  3.8882,
  162.1245],
 ['HSE157',
  '2414_2415_2416_2418_2420_2423_2424',
  'P',
  'TYR119',
  '1802_1803_1805_1807_1810_1812',
  'P',
  4.3605,
  3.0062],
 ['TRP39',
  '549_550_551_553_555_557',
  'P',
  'PHE26',
  '327_328_330_332_334_336',
  'P',
  4.8394,
  75.4588],
 ['TYR131',
  '2003_2004_2006_2008_2011_2013',
  'P',
  'TYR132',
  '2024_2025_2027_2029_2032_2034',
  'P',
  4.8732,
  91.4358]]
```

`Interactions.getPiCation()` - Pi-cation:

```
In [15]: interactions.getPiCation()
```

```
[['PHE85',
  '1248_1249_1251_1253_1255_1257',
  'P',
  'ARG40',
  'NH1_577_580',
  'P',
  3.6523],
 ['HSE66', '953_954_955_957_959', 'P', 'ARG65', 'NH1_938_941', 'P', 4.5323],
 ['HSE157',
  '2414_2415_2416_2418_2420_2423_2424',
  'P',
  'LYS112',
  'NZ_1699',
  'P',
  4.828]]
```

`Interactions.getHydrophohic()` - hydrophobic interactions:

```
In [16]: interactions.getHydrophohic()
```

```
[['TYR87', 'OH_1286', 'P', 'ALA156', 'CB_2401', 'P', 3.0459],
 ['MET63', 'CE_894', 'P', 'ALA24', 'CB_298', 'P', 3.3105],
 ['ILE68', 'CG2_976', 'P', 'MET63', 'CE_894', 'P', 3.3306],
 ['TYR142', 'CZ_2171', 'P', 'VAL146', 'CG2_2235', 'P', 3.4815],
 ['PHE10', 'CD1_92', 'P', 'ALA22', 'CB_273', 'P', 3.5334],
 ['LYS6', 'CD_26', 'P', 'TRP39', 'CZ2_555', 'P', 3.5427],
 ['VAL30', 'CG1_411', 'P', 'PHE26', 'CE2_336', 'P', 3.5603],
 ['ALA111', 'CB_1677', 'P', 'ILE88', 'CD_1307', 'P', 3.5627],
 ['VAL11', 'CG2_114', 'P', 'ILE88', 'CG2_1300', 'P', 3.6386],
 ['VAL41', 'CG2_595', 'P', 'PHE26', 'CD2_334', 'P', 3.6448],
 ['PHE152', 'CE1_2331', 'P', 'ALA156', 'CB_2401', 'P', 3.6594],
 ['VAL106', 'CG2_1598', 'P', 'LYS79', 'CG_1155', 'P', 3.6828],
 ['ILE77', 'CD_1128', 'P', 'LEU99', 'CD2_1480', 'P', 3.6917],
 ['PHE82', 'CD1_1205', 'P', 'ILE88', 'CD_1307', 'P', 3.692],
 ['LEU116', 'CD2_1771', 'P', 'ILE127', 'CD_1949', 'P', 3.7057],
 ['VAL8', 'CG1_55', 'P', 'PHE26', 'CE2_336', 'P', 3.7106],
 ..
 ..
```

`Interactions.getDisulfideBonds()` - disulfide bonds (none in the structure):

```
In [17]: interactions.getDisulfideBonds()
```

```
[]
```

To display residues with the biggest number of potential interactions and their types, we can use `Interactions.getFrequentInteractions()` method:

```
In [18]: frequent_interactions = interactions.getFrequentInteractions(contacts_min=3)

In [19]: frequent_interactions
```

```
@> The most frequent interactions between:
@> LEU9P  <--->  hp:ALA44P  hp:PHE85P  hb:LEU89P
@> CYS12P  <--->  hb:ASN15P  hb:SER19P  hb:THR46P
@> ILE16P  <--->  hb:ASP56P  hp:ALA74P  hp:TYR131P
@> PHE26P  <--->  hp:VAL8P  hp:VAL30P  ps:TRP39P  hp:VAL41P
@> TRP39P  <--->  hp:LYS6P  hp:ILE35P  hp:LEU153P
@> MET63P  <--->  hp:ILE21P  hp:ILE68P  hp:MET70P
@> ASP81P  <--->  hb:ARG75P  hb:THR78P  hb:PHE85P
@> THR84P  <--->  hb:SER7P  hb:ARG40P  hb:LYS110P
@> ASP86P  <--->  hb:SER7P  sb:LYS110P  hb:LYS112P
@> ILE88P  <--->  hp:VAL11P  hp:PHE82P  hp:ALA111P  hb:GLU114P
@> ASP92P  <--->  sb:ARG18P  hb:ASN95P  hb:LEU96P
@> LYS112P  <--->  hb:ILE88P  sb:GLU114P  pc:HSE157P
@> ILE127P  <--->  hb:ARG18P  hp:MET91P  hp:LEU116P  hp:VAL141P
@> Legend: hb-hydrogen bond, sb-salt bridge, rb-repulsive ionic bond, ps-Pi stacking interaction,pc-C
@> The biggest number of interactions: 4
```

The value of `contacts_min` can be modified to display residues with smaller or bigger number of interactions.

2.3 Visualize interactions in VMD

We can generate tcl files for visualizing each type of interaction with VMD_ using the `showProteinInteractions_VMD()` function in the following way:

```
In [20]: showProteinInteractions_VMD(atoms, interactions.getHydrogenBonds(),
   ....:                                     color='blue', filename='HBs.tcl')
   ....:

In [21]: showProteinInteractions_VMD(atoms, interactions.getSaltBridges(),
   ....:                                     color='yellow',filename='SBs.tcl')
   ....:

In [22]: showProteinInteractions_VMD(atoms, interactions.getRepulsiveIonicBonding(),
   ....:                                     color='red',filename='RIB.tcl')
   ....:

In [23]: showProteinInteractions_VMD(atoms, interactions.getPiStacking(),
   ....:                                     color='green',filename='PiStacking.tcl')
   ....:

In [24]: showProteinInteractions_VMD(atoms, interactions.getPiCation(),
   ....:                                     color='orange',filename='PiCation.tcl')
   ....:

In [25]: showProteinInteractions_VMD(atoms, interactions.getHydrophobic(),
   ....:                                     color='silver',filename='HPh.tcl')
   ....:

In [26]: showProteinInteractions_VMD(atoms, interactions.getDisulfideBonds(),
   ....:                                     color='black',filename='DiBs.tcl')
   ....:
```

```
@> TCL file saved
@> TCL file saved
@> TCL file saved
@> TCL file saved
@> TCL file saved
@> TCL file saved
@> Lack of results
@> TCL file saved
```

A `TCL file` will be saved and can be used in **VMD_** after uploading the PDB file with protein structure `5kqm_all_sci.pdb` and by running the following command line instruction in the **VMD_** *TK Console* (via *VMD Main*) for Linux, Windows and Mac users:

```
play HBs.tcl
```

The tcl file contains a method for drawing lines between selected pairs of residues. Those residues are also displayed. Now, we uploaded hydrogen bonds which are displayed in blue as we defined in `showProteinInteractions_VMD()` function.

Salt bridges in yellow (**VMD_** *TK Console*):

```
play SBs.tcl
```

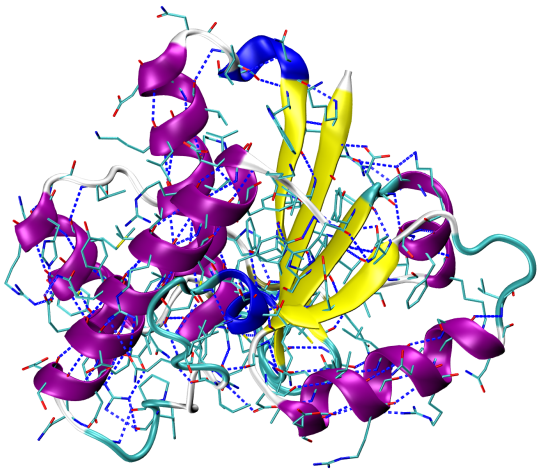
Repulsive ionic bonding in red (**VMD_** *TK Console*):

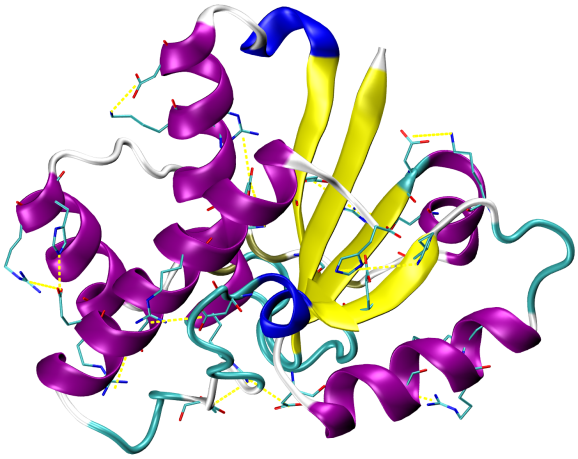
```
play RIB.tcl
```

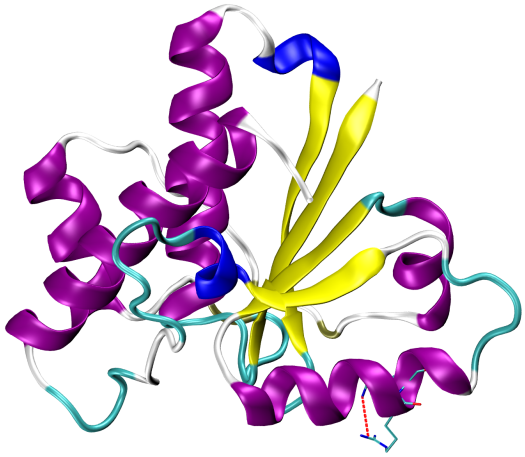
Pi-Pi stacking interactions in green (**VMD_** *TK Console*):

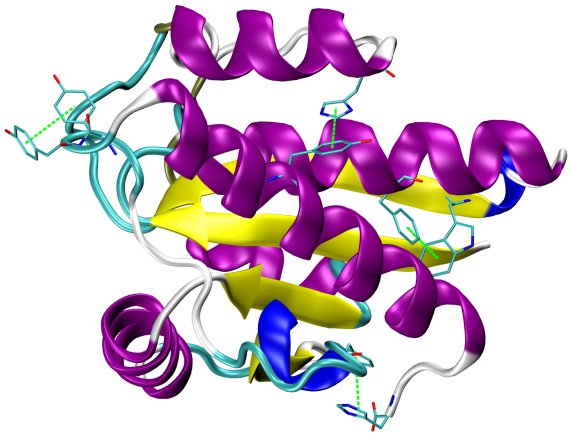
```
play PiStacking.tcl
```

Pi-cation interactions in orange (**VMD_** *TK Console*):

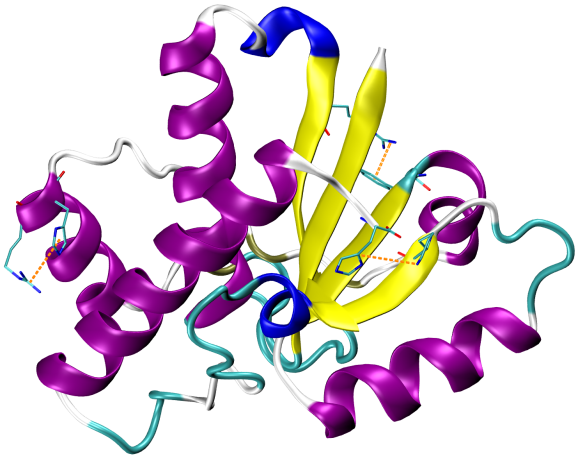








```
play PiCation.tcl
```



and hydrophobic interactions in grey (**VMD_** *TK Console*):

```
play HPh.tcl
```

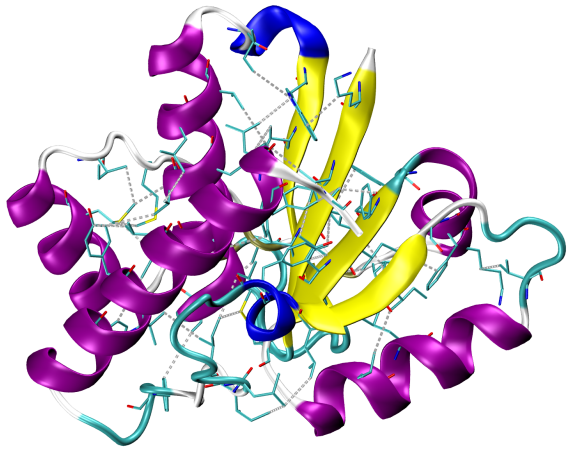
2.4 Additional selections

From the predicted interactions, we can select only interactions assigned to certain regions, chains, or between different chains (binding interface between two chains in protein complex).

We can compute them by adding additional parameters to the selected function. See examples below:

```
In [27]: interactions.getSaltBridges(selection='chain P')
```

```
[['HSE66', 'NE2_957', 'P', 'GLU139', 'OE1_2125_2126', 'P', 2.8359],
 ['ASP81', 'OD1_1193_1194', 'P', 'ARG75', 'NH1_1090_1093', 'P', 2.9163],
 ['ASP32', 'OD1_443_444', 'P', 'LYS28', 'NZ_380', 'P', 3.037],
 ['ARG101', 'NH1_1516_1519', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.0699],
 ['ARG27', 'NH1_356_359', 'P', 'GLU23', 'OE1_290_291', 'P', 3.7148],
 ['GLU139', 'OE1_2125_2126', 'P', 'ARG65', 'NH1_938_941', 'P', 3.7799],
 ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.9359],
```



```
 ['ARG58', 'NH1_829_832', 'P', 'ASP56', 'OD1_788_789', 'P', 3.9486],
 ['ARG18', 'NH1_217_220', 'P', 'ASP92', 'OD1_1368_1369', 'P', 4.0693],
 ['GLU114', 'OE1_1735_1736', 'P', 'LYS112', 'NZ_1699', 'P', 4.0787],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 4.1543],
 ['LYS110', 'NZ_1667', 'P', 'ASP86', 'OD1_1269_1270', 'P', 4.1879],
 ['GLU114', 'OE1_1735_1736', 'P', 'HSE157', 'NE2_2418', 'P', 4.3835],
 ['ARG18', 'NH1_217_220', 'P', 'ASP129', 'OD1_1978_1979', 'P', 4.5608],
 ['ARG75', 'NH1_1090_1093', 'P', 'ASP42', 'OD1_609_610', 'P', 4.5612],
 ['GLU23', 'OE1_290_291', 'P', 'HSE72', 'NE2_1042', 'P', 4.99]]
```

```
In [28]: interactions.getRepulsiveIonicBonding(selection='resid 102')
```

```
[['ARG101', 'NH1_1516_1519', 'P', 'LYS102', 'NZ_1540', 'P', 4.2655]]
```

```
In [29]: interactions.getPiStacking(selection='chain P and resid 26')
```

```
 [['TRP39',
'549_550_551_553_555_557',
'P',
'PHE26',
'327_328_330_332_334_336',
'P',
4.8394,
75.4588]]
```

It can be done for all kinds of interactions is a similar way. The function will return a list of interactions with following order:

1. Hydrogen bonds
2. Salt Bridges
3. RepulsiveIonicBonding
4. Pi stacking interactions
5. Pi-cation interactions
6. Hydrophobic interactions
7. Disulfide bonds

```
In [30]: allRes_20to50 = interactions.getInteractions(selection='resid 20 to 50')

In [31]: allRes_20to50
```

```
[[['ARG40', 'N_561', 'P', 'LYS6', 'O_37', 'P', 2.7479, 17.1499],
  ['ALA45', 'N_634', 'P', 'ARG75', 'O_1097', 'P', 2.7609, 35.0983],
  ['ASN53', 'ND2_747', 'P', 'GLU50', 'OE1_708', 'P', 2.7702, 18.2336],
  ['LYS6', 'N_16', 'P', 'ASN38', 'O_536', 'P', 2.8178, 25.0305],
  ['ILE77', 'N_1115', 'P', 'ALA45', 'O_643', 'P', 2.8179, 12.1855],
  ['ASP32', 'N_435', 'P', 'LYS28', 'O_385', 'P', 2.8357, 8.8318],
  ['ARG27', 'N_340', 'P', 'GLU23', 'O_293', 'P', 2.8446, 15.4167],
  ['PHE26', 'N_320', 'P', 'ALA22', 'O_278', 'P', 2.8541, 4.8732],
  ['ARG75', 'NH2_1093', 'P', 'ASP42', 'OD2_610', 'P', 2.8649, 23.5083],
  ['VAL25', 'N_304', 'P', 'ILE21', 'O_268', 'P', 2.8666, 8.2255],
  ['THR46', 'N_644', 'P', 'CYS12', 'O_130', 'P', 2.883, 36.1279],
  ['THR31', 'N_421', 'P', 'ARG27', 'O_363', 'P', 2.896, 24.1287],
  ['GLU23', 'N_279', 'P', 'SER19', 'O_235', 'P', 2.8979, 15.4146],
  ['PHE10', 'N_84', 'P', 'ASP42', 'O_612', 'P', 2.9026, 22.751],
  ['ARG27', 'NH2_359', 'P', 'GLU23', 'OE2_291', 'P', 2.9199, 31.5487],
  ['ASN38', 'N_523', 'P', 'ILE35', 'O_496', 'P', 2.9255, 29.091],
  ['GLN76', 'NE2_1110', 'P', 'THR46', 'O_657', 'P', 2.9381, 31.3836],
  ['ARG40', 'NH1_577', 'P', 'THR84', 'OG1_1233', 'P', 2.9482, 8.3748],
  ['ALA44', 'N_624', 'P', 'PHE10', 'O_103', 'P', 2.9499, 33.1772],
  ['VAL8', 'N_49', 'P', 'ARG40', 'O_584', 'P', 2.9631, 25.0079],
  ['ILE35', 'N_478', 'P', 'VAL30', 'O_420', 'P', 2.9811, 23.5092],
  ['ASN53', 'N_738', 'P', 'GLU50', 'O_711', 'P', 2.995, 28.587],
  ['ASN34', 'N_464', 'P', 'THR31', 'O_434', 'P', 3.0041, 18.2465],
  ['ASN15', 'ND2_166', 'P', 'SER43', 'OG_620', 'P', 3.0129, 25.6996],
  ['ARG27', 'NH1_356', 'P', 'GLU23', 'OE2_291', 'P', 3.0175, 36.9343],
  ['LEU29', 'N_386', 'P', 'VAL25', 'O_319', 'P', 3.0299, 19.109],
  ['SER47', 'N_658', 'P', 'LEU13', 'O_149', 'P', 3.0386, 28.8029],
  ['VAL30', 'N_405', 'P', 'PHE26', 'O_339', 'P', 3.0394, 17.6883],
  ['ALA24', 'N_294', 'P', 'PRO20', 'O_249', 'P', 3.0751, 29.9487],
  ['LYS28', 'N_364', 'P', 'ALA24', 'O_303', 'P', 3.0783, 19.9504],
  ['ALA22', 'N_269', 'P', 'ARG18', 'O_224', 'P', 3.088, 21.873],
  ['ASP42', 'N_601', 'P', 'VAL8', 'O_64', 'P', 3.1331, 35.5671],
  ['TRP39', 'N_537', 'P', 'SER36', 'O_507', 'P', 3.1343, 15.1776],
  ['CYS12', 'N_120', 'P', 'ALA44', 'O_633', 'P', 3.3349, 36.1006]],
 [['ASP32', 'OD1_443_444', 'P', 'LYS28', 'NZ_380', 'P', 3.037],
  ['ARG27', 'NH1_356_359', 'P', 'GLU23', 'OE1_290_291', 'P', 3.7148],
  ['ARG75', 'NH1_1090_1093', 'P', 'ASP42', 'OD1_609_610', 'P', 4.5612],
  ['GLU23', 'OE1_290_291', 'P', 'HSE72', 'NE2_1042', 'P', 4.99]],
 [],
 [['TRP39',
   '549_550_551_553_555_557',
   'P',
   'PHE26',
   '327_328_330_332_334_336',
   'P',
   4.8394,
   75.4588]],
 [['PHE85',
   '1248_1249_1251_1253_1255_1257',
   'P',
   'ARG40',
   'NH1_577_580',
   'P',
   3.6523]],
```

```
 [['MET63', 'CE_894', 'P', 'ALA24', 'CB_298', 'P', 3.3105],
  ['PHE10', 'CD1_92', 'P', 'ALA22', 'CB_273', 'P', 3.5334],
  ['LYS6', 'CD_26', 'P', 'TRP39', 'CZ2_555', 'P', 3.5427],
  ['VAL30', 'CG1_411', 'P', 'PHE26', 'CE2_336', 'P', 3.5603],
  ['VAL41', 'CG2_595', 'P', 'PHE26', 'CD2_334', 'P', 3.6448],
  ['VAL8', 'CG1_55', 'P', 'PHE26', 'CE2_336', 'P', 3.7106],
  ['ALA44', 'CB_628', 'P', 'LEU9', 'CD1_74', 'P', 3.8992],
  ['VAL25', 'CG2_314', 'P', 'TYR142', 'CE1_2169', 'P', 3.92],
  ['ILE21', 'CG2_256', 'P', 'MET63', 'SD_893', 'P', 3.9614],
  ['LEU153', 'CD1_2350', 'P', 'TRP39', 'NE1_547', 'P', 3.967],
  ['ILE35', 'CD_491', 'P', 'TRP39', 'NE1_547', 'P', 4.0172],
  ['LEU29', 'CD1_395', 'P', 'VAL25', 'CG1_310', 'P', 4.0642],
  ['ARG75', 'CG_1081', 'P', 'ALA44', 'CB_628', 'P', 4.0853],
  ['ARG40', 'CG_568', 'P', 'PHE85', 'CE2_1257', 'P', 4.2669],
  ['LYS28', 'CG_371', 'P', 'ILE68', 'CD_983', 'P', 4.2707],
  ['PHE138', 'CD2_2108', 'P', 'ILE21', 'CD_263', 'P', 4.3082]],
 []]
```

The list of hydrogen bonds, salt bridges and other types of interactions can be displayed as follows:

Hydrogen bonds:

```
In [32]: allRes_20to50[0]
```

```
[['ARG40', 'N_561', 'P', 'LYS6', 'O_37', 'P', 2.7479, 17.1499],
 ['ALA45', 'N_634', 'P', 'ARG75', 'O_1097', 'P', 2.7609, 35.0983],
 ['ASN53', 'ND2_747', 'P', 'GLU50', 'OE1_708', 'P', 2.7702, 18.2336],
 ['LYS6', 'N_16', 'P', 'ASN38', 'O_536', 'P', 2.8178, 25.0305],
 ['ILE77', 'N_1115', 'P', 'ALA45', 'O_643', 'P', 2.8179, 12.1855],
 ['ASP32', 'N_435', 'P', 'LYS28', 'O_385', 'P', 2.8357, 8.8318],
 ['ARG27', 'N_340', 'P', 'GLU23', 'O_293', 'P', 2.8446, 15.4167],
 ['PHE26', 'N_320', 'P', 'ALA22', 'O_278', 'P', 2.8541, 4.8732],
 ['ARG75', 'NH2_1093', 'P', 'ASP42', 'OD2_610', 'P', 2.8649, 23.5083],
 ['VAL25', 'N_304', 'P', 'ILE21', 'O_268', 'P', 2.8666, 8.2255],
 ['THR46', 'N_644', 'P', 'CYS12', 'O_130', 'P', 2.883, 36.1279],
 ['THR31', 'N_421', 'P', 'ARG27', 'O_363', 'P', 2.896, 24.1287],
 ['GLU23', 'N_279', 'P', 'SER19', 'O_235', 'P', 2.8979, 15.4146],
 ['PHE10', 'N_84', 'P', 'ASP42', 'O_612', 'P', 2.9026, 22.751],
 ['ARG27', 'NH2_359', 'P', 'GLU23', 'OE2_291', 'P', 2.9199, 31.5487],
 ['ASN38', 'N_523', 'P', 'ILE35', 'O_496', 'P', 2.9255, 29.091],
 ['GLN76', 'NE2_1110', 'P', 'THR46', 'O_657', 'P', 2.9381, 31.3836],
 ['ARG40', 'NH1_577', 'P', 'THR84', 'OG1_1233', 'P', 2.9482, 8.3748],
 ['ALA44', 'N_624', 'P', 'PHE10', 'O_103', 'P', 2.9499, 33.1772],
 ['VAL8', 'N_49', 'P', 'ARG40', 'O_584', 'P', 2.9631, 25.0079],
 ['ILE35', 'N_478', 'P', 'VAL30', 'O_420', 'P', 2.9811, 23.5092],
 ['ASN53', 'N_738', 'P', 'GLU50', 'O_711', 'P', 2.995, 28.587],
 ['ASN34', 'N_464', 'P', 'THR31', 'O_434', 'P', 3.0041, 18.2465],
 ['ASN15', 'ND2_166', 'P', 'SER43', 'OG_620', 'P', 3.0129, 25.6996],
 ['ARG27', 'NH1_356', 'P', 'GLU23', 'OE2_291', 'P', 3.0175, 36.9343],
 ['LEU29', 'N_386', 'P', 'VAL25', 'O_319', 'P', 3.0299, 19.109],
 ['SER47', 'N_658', 'P', 'LEU13', 'O_149', 'P', 3.0386, 28.8029],
 ['VAL30', 'N_405', 'P', 'PHE26', 'O_339', 'P', 3.0394, 17.6883],
 ['ALA24', 'N_294', 'P', 'PRO20', 'O_249', 'P', 3.0751, 29.9487],
 ['LYS28', 'N_364', 'P', 'ALA24', 'O_303', 'P', 3.0783, 19.9504],
 ['ALA22', 'N_269', 'P', 'ARG18', 'O_224', 'P', 3.088, 21.873],
 ['ASP42', 'N_601', 'P', 'VAL8', 'O_64', 'P', 3.1331, 35.5671],
 ['TRP39', 'N_537', 'P', 'SER36', 'O_507', 'P', 3.1343, 15.1776],
 ['CYS12', 'N_120', 'P', 'ALA44', 'O_633', 'P', 3.3349, 36.1006]]
```

Salt Bridges:

```
In [33]: allRes_20to50[1]
```

```
[['ASP32', 'OD1_443_444', 'P', 'LYS28', 'NZ_380', 'P', 3.037],
 ['ARG27', 'NH1_356_359', 'P', 'GLU23', 'OE1_290_291', 'P', 3.7148],
 ['ARG75', 'NH1_1090_1093', 'P', 'ASP42', 'OD1_609_610', 'P', 4.5612],
 ['GLU23', 'OE1_290_291', 'P', 'HSE72', 'NE2_1042', 'P', 4.99]]
```

We can also select one particular residue or a region of our interest:

```
In [34]: interactions.getPiCation(selection='resid 85')
```

```
[['PHE85',
  '1248_1249_1251_1253_1255_1257',
  'P',
  'ARG40',
  'NH1_577_580',
  'P',
  3.6523]]
```

```
In [35]: interactions.getHydrophobic(selection='resid 26 to 100')
```

```
[['TYR87', 'OH_1286', 'P', 'ALA156', 'CB_2401', 'P', 3.0459],
 ['MET63', 'CE_894', 'P', 'ALA24', 'CB_298', 'P', 3.3105],
 ['ILE68', 'CG2_976', 'P', 'MET63', 'CE_894', 'P', 3.3306],
 ['LYS6', 'CD_26', 'P', 'TRP39', 'CZ2_555', 'P', 3.5427],
 ['VAL30', 'CG1_411', 'P', 'PHE26', 'CE2_336', 'P', 3.5603],
 ['ALA111', 'CB_1677', 'P', 'ILE88', 'CD_1307', 'P', 3.5627],
 ['VAL11', 'CG2_114', 'P', 'ILE88', 'CG2_1300', 'P', 3.6386],
 ['VAL41', 'CG2_595', 'P', 'PHE26', 'CD2_334', 'P', 3.6448],
 ['VAL106', 'CG2_1598', 'P', 'LYS79', 'CG_1155', 'P', 3.6828],
 ['ILE77', 'CD_1128', 'P', 'LEU99', 'CD2_1480', 'P', 3.6917],
 ['PHE82', 'CD1_1205', 'P', 'ILE88', 'CD_1307', 'P', 3.692],
 ['VAL8', 'CG1_55', 'P', 'PHE26', 'CE2_336', 'P', 3.7106],
 ['MET70', 'CE_1014', 'P', 'MET63', 'CG_890', 'P', 3.7262],
 ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.7263],
 ['LEU9', 'CD2_78', 'P', 'ILE77', 'CD_1128', 'P', 3.745],
 ['LEU89', 'CD1_1322', 'P', 'VAL8', 'CG2_59', 'P', 3.7672],
 ['MET91', 'SD_1353', 'P', 'ILE127', 'CD_1949', 'P', 3.8864],
 ['ALA44', 'CB_628', 'P', 'LEU9', 'CD1_74', 'P', 3.8992],
 ['ILE21', 'CG2_256', 'P', 'MET63', 'SD_893', 'P', 3.9614],
 ['LEU153', 'CD1_2350', 'P', 'TRP39', 'NE1_547', 'P', 3.967],
 ['PHE85', 'CZ_1253', 'P', 'LEU9', 'CD1_74', 'P', 4.0119],
 ['ILE35', 'CD_491', 'P', 'TRP39', 'NE1_547', 'P', 4.0172],
 ['LEU29', 'CD1_395', 'P', 'VAL25', 'CG1_310', 'P', 4.0642],
 ['ALA74', 'CB_1068', 'P', 'ILE16', 'CG2_177', 'P', 4.0772],
 ['ARG75', 'CG_1081', 'P', 'ALA44', 'CB_628', 'P', 4.0853],
 ['LYS102', 'CD_1534', 'P', 'ILE77', 'CG2_1121', 'P', 4.1048],
 ['TYR119', 'CE1_1805', 'P', 'LEU89', 'CD2_1326', 'P', 4.1435],
 ['ARG40', 'CG_568', 'P', 'PHE85', 'CE2_1257', 'P', 4.2669],
 ['LYS28', 'CG_371', 'P', 'ILE68', 'CD_983', 'P', 4.2707],
 ['LYS112', 'CG_1690', 'P', 'TYR87', 'CE1_1283', 'P', 4.3083],
 ['ARG58', 'CG_820', 'P', 'PHE138', 'CE1_2104', 'P', 4.4781]]
```

2.5 Change selection criteria for interaction type

The `Interactions.buildInteractionMatrix()` method computes interactions using default parameters for interactions. However, it can be changed according to our needs. To do that, we need to recalculate the selected type of interactions using the preferable parameters.

We can do it using the following functions: `calcHydrogenBonds()`, `calcHydrogenBonds()`, `calcSaltBridges()`, `calcRepulsiveIonicBonding()`, `calcPiStacking()`, `calcPiCation()`, `calcHydrophohic()`, `calcDisulfideBonds()`, and use `Interactions.setNewHydrogenBonds()`, `Interactions.setNewSaltBridges()`, `Interactions.setNewRepulsiveIonicBonding()`, `Interactions.setNewPiStacking()`, `Interactions.setNewPiCation()`, `Interactions.setNewHydrophohic()`, `Interactions.setNewDisulfideBonds()` method to replace it in the main Instance.

For example: If we want to replace hydrogen bonds:

```
In [36]: newHydrogenBonds2 = calcHydrogenBonds(atoms, distA=2.8,
   ....:                                       angle=30, cutoff_dist=15)
   ....:

In [37]: interactions.setNewHydrogenBonds(newHydrogenBonds2)
```

```
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)    <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     GLN143    P      NE2_2192  <--->     GLU139    P      OE2_2126     2.7     9.2
@>      HSE66    P       NE2_957  <--->     GLU139    P      OE1_2125     2.7     6.4
@>      ARG40    P         N_561  <--->       LYS6    P          O_37     2.7    17.1
@>      ARG58    P         N_813  <--->      ASP56    P       OD1_788     2.7    30.0
@>      ASN53    P       ND2_747  <--->      GLU50    P       OE1_708     2.8    18.2
@>      ALA74    P        N_1064  <--->      ASN53    P         O_751     2.8    21.3
@>      ASP56    P         N_780  <--->      ILE16    P         O_189     2.8    27.0
@> Number of detected hydrogen bonds: 7.
@> Hydrogen Bonds are replaced
```

```
In [38]: interactions.getHydrogenBonds()
```

```
[['GLN143', 'NE2_2192', 'P', 'GLU139', 'OE2_2126', 'P', 2.7287, 9.1823],
 ['HSE66', 'NE2_957', 'P', 'GLU139', 'OE1_2125', 'P', 2.7314, 6.3592],
 ['ARG40', 'N_561', 'P', 'LYS6', 'O_37', 'P', 2.7479, 17.1499],
 ['ARG58', 'N_813', 'P', 'ASP56', 'OD1_788', 'P', 2.7499, 29.9737],
 ['ASN53', 'ND2_747', 'P', 'GLU50', 'OE1_708', 'P', 2.7702, 18.2336],
 ['ALA74', 'N_1064', 'P', 'ASN53', 'O_751', 'P', 2.7782, 21.3375],
 ['ASP56', 'N_780', 'P', 'ILE16', 'O_189', 'P', 2.7793, 27.0481]]
```

If we want to replace salt bridges, repulsive ionic bonding, or Pi-cation interactions:

```
In [39]: sb2 = calcSaltBridges(atoms, distA=6)

In [40]: interactions.setNewSaltBridges(sb2)

In [41]: rib2 = calcRepulsiveIonicBonding(atoms, distA=9)

In [42]: interactions.setNewRepulsiveIonicBonding(rib2)

In [43]: picat2 = calcPiCation(atoms, distA=7)

In [44]: interactions.setNewPiCation(picat2)
```

```
@> Calculating salt bridges.
@>      HSE66    P         NE2_957  <--->     GLU139    P   OE1_2125_2126     2.8
@>      ASP81    P   OD1_1193_1194  <--->      ARG75    P   NH1_1090_1093     2.9
@>      ASP32    P     OD1_443_444  <--->      LYS28    P          NZ_380     3.0
@>     ARG101    P   NH1_1516_1519  <--->      ASP98    P   OD1_1463_1464     3.1
@>      ARG27    P     NH1_356_359  <--->      GLU23    P     OE1_290_291     3.7
@>     GLU139    P   OE1_2125_2126  <--->      ARG65    P     NH1_938_941     3.8
@>     LYS102    P         NZ_1540  <--->      ASP98    P   OD1_1463_1464     3.9
@>      ARG58    P     NH1_829_832  <--->      ASP56    P     OD1_788_789     3.9
@>      ARG18    P     NH1_217_220  <--->      ASP92    P   OD1_1368_1369     4.1
@>     GLU114    P   OE1_1735_1736  <--->     LYS112    P         NZ_1699     4.1
@>     ASP120    P   OD1_1824_1825  <--->     ARG147    P   NH1_2257_2260     4.2
@>     LYS110    P         NZ_1667  <--->      ASP86    P   OD1_1269_1270     4.2
@>     GLU114    P   OE1_1735_1736  <--->     HSE157    P        NE2_2418     4.4
@>      ARG18    P     NH1_217_220  <--->     ASP129    P   OD1_1978_1979     4.6
@>      ARG75    P   NH1_1090_1093  <--->      ASP42    P     OD1_609_610     4.6
@>      GLU23    P     OE1_290_291  <--->      HSE72    P        NE2_1042     5.0
@>      ASP42    P     OD1_609_610  <--->      HSE72    P        NE2_1042     5.4
@>      ASP81    P   OD1_1193_1194  <--->      ARG40    P     NH1_577_580     5.8
@> Number of detected salt bridges: 18.
@> Salt Bridges are replaced
@> Calculating repulsive ionic bonding.
@>      ASP42    P     OD1_609_610  <--->      ASP81    P   OD1_1193_1194     6.7
@>      GLU80    P   OE1_1181_1182  <--->      ASP81    P   OD1_1193_1194     7.0
@>      ASP92    P   OD1_1368_1369  <--->     ASP129    P   OD1_1978_1979     7.6
@>     LYS110    P         NZ_1667  <--->      ARG40    P     NH1_577_580     7.8
@>      ASP92    P   OD1_1368_1369  <--->      GLU93    P   OE1_1383_1384     8.6
@>     GLU128    P   OE1_1966_1967  <--->     ASP137    P   OD1_2090_2091     8.9
@> Number of detected Repulsive Ionic Bonding interactions: 6.
@> Repulsive Ionic Bonding are replaced
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_5
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                    NH1_938_9
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                          NZ_
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                    NH1_829_8
@>     TYR131   P   2003_2004_2006_2008_2011_2013  <--->      ARG58   P                    NH1_829_8
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG75   P                  NH1_1090_10
@>      TRP39   P         549_550_551_553_555_557  <--->       LYS6   P                          NZ_
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->     LYS112   P                        NZ_16
@> Number of detected cation-pi interactions: 8.
@> Pi-Cation interactions are replaced
```

2.6 Assess the functional significance of a residue

For assessing the functional significance of each residue in protein structure, we counted the number of possible contacts based on:

1. Hydrogen bonds (`HBs`)
2. Salt Bridges (`SBs`)
3. Repulsive Ionic Bonding (`RIB`)
4. Pi stacking interactions (`PiStack`)
5. Pi-cation interactions (`PiCat`)
6. Hydrophobic interactions (`HPh`)

7. Disulfide Bonds (`DiBs`)

To compute the weighted interactions use the `Interactions.buildInteractionMatrix()` method:

```
In [45]: matrix = interactions.buildInteractionMatrix()
```

```
@> Calculating interactions
```

The results can be displayed in the following way:

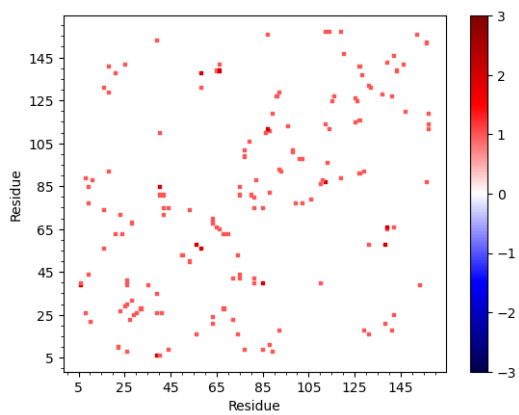
```
In [46]: import matplotlib.pylab as plt

In [47]: showAtomicMatrix(matrix, atoms=atoms.ca, cmap='seismic', markersize=8)

In [48]: plt.xlabel('Residue')

In [49]: plt.ylabel('Residue')

In [50]: plt.clim([-3,3])
```



The total number of interaction for each residue can be displayed on the plot using `showCumulativeInteractionTypes()` function.

```
In [51]: interactions.showCumulativeInteractionTypes()
```

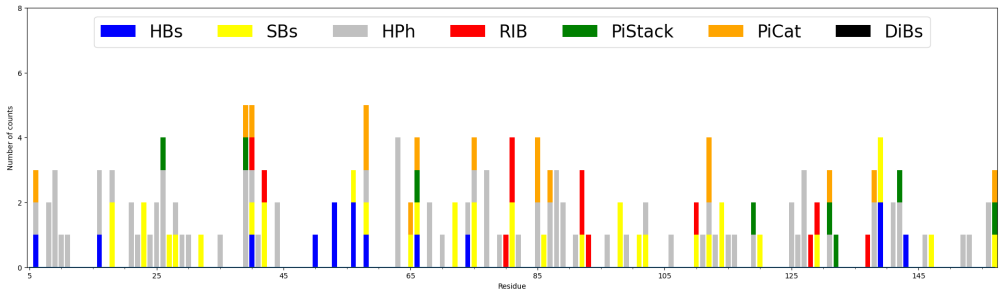
```
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
```

The results with the higest number of possible contacts can be saved in PDB file. They will be restored in `Occupancy` column and display in **VMD_**.

```
In [52]: interactions.saveInteractionsPDB(filename='5kqm_meanMatrix.pdb')
```

2.7 Visualize number of interactions onto 3D structure

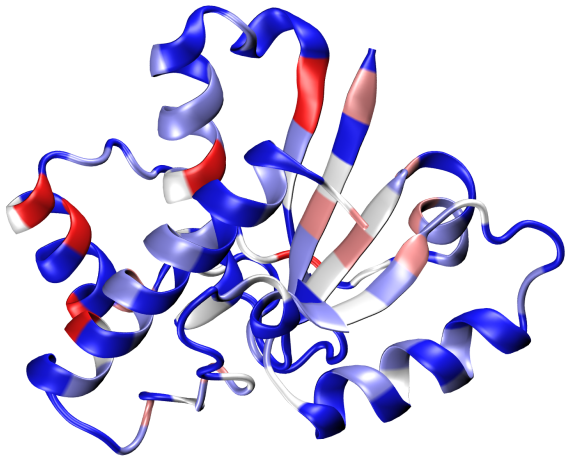
The number of the interaction can be saved to a PDB file in the *Occupancy* column by using `Interactions.saveInteractionsPDB()` method. Then the score would be displayed in color in any available graphical program, for example, in **VMD_**.




```
In [53]: interactions.saveInteractionsPDB(filename='5kqm_meanMatrix.pdb')
```

```
@> PDB file saved.
```

A file `5kqm_meanMatrix.pdb` will be saved and can be used in **VMD_** by uploading PDB structure and displaying it with *Coloring Method Occupancy*. By default blue colors correspond to the highest values but we can change it in *VMD Main -> Graphics -> Color Controls -> Color Scale -> Method to BWR*.



2.8 Exclude some interaction types from calculations

For analysis we can exclude some of the interaction types by assigning zero to the type of interactions (`HBs` - hydrogen bonds, `SBs` - salt bridges, `RIB` - repulsive ionic bonding, `PiCat` - Pi-Cation, `PiStack` - Pi-Stacking, `HPh` - hydrophobic interactions and finally DiBs - disulfide bonds).

```
In [54]: matrix = interactions.buildInteractionMatrix(RIB=0, HBs=0, HPh=0, DiBs=0)
```

```
@> Calculating interactions
```

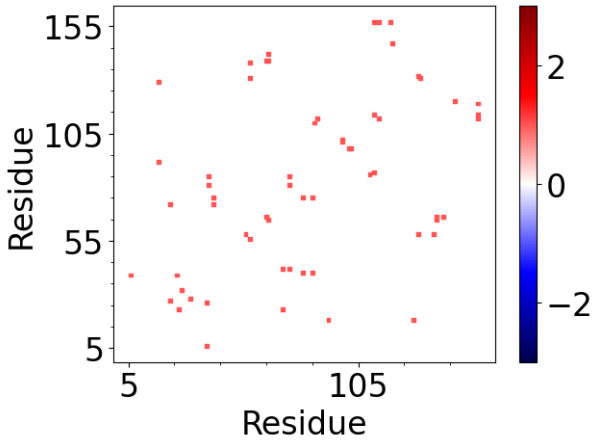
The results can be displayed in a similar way:

```
In [55]: showAtomicMatrix(matrix, atoms=atoms.ca, cmap='seismic', markersize=8)

In [56]: plt.xlabel('Residue')

In [57]: plt.ylabel('Residue')

In [58]: plt.clim([-3,3])
```


155
105
55
5
Residue
5
105
Residue
2
0
−2

CHAPTER

THREE

PDB STRUCTURE WITHOUT HYDROGENS

Very often, PDB structures downloaded directly from the PDB database will not have determined hydrogen atoms that are required, for example, for predicting hydrogen bonds. In such a case, we can use the `addHydrogens()` function. It will allow us to use one of two available methods (`openbabel` or `pdbfixer`) to predict the position of hydrogen atoms in protein structure.

To use one of those functions, we need to install additional Python package(s). For Anaconda[3] users, the installation will be the following:

Installation of Openbabel[4]:

```
conda install -c conda-forge openbabel
```

Installation of PDBfixer[5]:

```
conda install -c conda-forge pdbfixer
```

3.1 Add missing hydrogen atoms to the structure

We start by fetching the PDB file with **5KQM** code (`5kqm.pdb`). Openbabel[6] requires having the PDB file in the same folder. Therefore, it needs to be downloaded and saved to successfully perform the operation with adding missing hydrogens. A new file will be saved with the same name with the additional prefix '**addH_**'.

```
In [1]: from prody import *

In [2]: from pylab import *

In [3]: import matplotlib

In [4]: ion()    # turn interactive mode on
```

Openbabel[7] or PDBfixer[8] require PDB file saved in the direcory. Therefore first it needs to be downloaded.

```
In [5]: fetchPDB('5kqm', compressed=False)
```

```
'5kqm.pdb'
```

[3] https://www.anaconda.com/download
[4] https://github.com/openbabel
[5] https://github.com/openmm/pdbfixer
[6] https://github.com/openbabel
[7] https://github.com/openbabel
[8] https://github.com/openmm/pdbfixer

When PDB file is already in the local directory, we can choose between Openbabel[9] and PDBfixer[10] to add missing hydrogen bonds to the protein structure:

Openbabel:

```
In [6]: PDBname = '5kqm.pdb'

In [7]: addMissingAtoms(PDBname, method='openbabel')
```

```
@> Hydrogens were added to the structure. Structure addH_5kqm.pdb is saved in the local directry.
```

PDBfixer:

```
In [8]: addMissingAtoms(PDBname, method='pdbfixer')
```

```
@> Hydrogens were added to the structure. New structure is saved as addH_5kqm.pdb.
```

Next, we can parse the saved structure with hydrogen atoms to ProDy and analyze it in the same way as in the previous paragraph.

```
In [9]: atoms = parsePDB('addH_'+str(PDBname)).select('protein')
```

```
@> 2800 atoms and 1 coordinate set(s) were parsed in 0.03s.
```

[9] https://github.com/openbabel
[10] https://github.com/openmm/pdbfixer

CHAPTER

FOUR

PDB STRUCTURE WITH MULTIPLE CHAINS

This time we will use protein with two chains, lipoxygenase (PDB: **7LAF**) which contain chain A and chain B. First, we will add missing hydrogens to the protein structures and then we will perform analysis of interactions between two chains.

4.1 Add missing hydrogen atoms to the structure

We start by fetching the PDB file and adding missing hydrogens using Openbabel[11].

```
In [1]: fetchPDB('7laf', compressed=False)

In [2]: addMissingAtoms('7laf.pdb', method='openbabel')

In [3]: atoms = parsePDB('addH_7laf.pdb').select('protein')
```

```
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> 7laf downloaded (7laf.pdb)
@> PDB download via FTP completed (1 downloaded, 0 failed).
@> Hydrogens were added to the structure. Structure addH_7laf.pdb is saved in the local directry.
@> 21970 atoms and 1 coordinate set(s) were parsed in 0.24s.
```

```
In [4]: interactions = Interactions('7laf')
```

To compute all interactions:

```
In [5]: all_interactions = interactions.calcProteinInteractions(atoms)
```

```
@> Calculating interations.
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)    <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     ASP505    A      OD2_3935  <--->     TYR496    A       OH_3867     2.2    29.5
@>     ASP666    B     OD1_10390  <--->     SER648    B      OG_10241     2.3    17.8
@>     HIS394    A        N_3026  <--->     GLU141    A      OE2_1006     2.4    35.5
@>     ARG390    B      NH1_8204  <--->     TYR149    B        O_6273     2.4    35.6
@>     GLN641    A      NE2_4984  <--->     GLY621    A        O_4815     2.4     8.5
@>     ARG649    B     NH1_10251  <--->     GLU653    B     OE1_10281     2.4     4.9
@>     ARG463    B      NH1_8796  <--->     ASP459    B      OD1_8759     2.4    30.6
@>     TYR318    B        N_7621  <--->     LEU327    B        O_7687     2.4     4.3
@>     ASN301    A      ND2_2299  <--->     ASP428    A        O_3307     2.4    29.3
@>     ARG474    A      NH1_3686  <--->     ILE468    A        O_3625     2.5    37.5
@>     ARG474    B      NH1_8890  <--->     VAL465    B        O_8805     2.5    21.1
@>     SER517    B       OG_9247  <--->     ASN522    B      ND2_9287     2.5    26.7
@>     ASN522    B      ND2_9287  <--->     SER517    B       OG_9247     2.5    33.0
```

[11] https://github.com/openbabel

```
@>     TRP481    B        N_8937  <--->     GLY477    B        O_8911     2.5     7.9
@>      LEU36    A         N_274  <--->      VAL24    A         O_194     2.5    21.5
@>     SER526    A       OG_4113  <--->     GLN523    A        O_4087     2.5    24.9
@>     ARG138    B      NH2_6183  <--->     GLU507    B      OE1_9158     2.5    28.0
@>     TRP109    A         N_743  <--->     ASN173    A      OD1_1279     2.5     7.1
@>     THR431    B      OG1_8538  <--->     VAL427    B        O_8504     2.5    24.5
@>     SER501    B       OG_9107  <--->     SER498    B        O_9082     2.5    35.7
@>     GLN143    B        N_6219  <--->     GLN139    B        O_6187     2.5    11.9
@>     LEU329    A        N_2495  <--->     LEU316    A        O_2404     2.5    21.1
@>     LEU110    A         N_757  <--->      TRP87    A         O_551     2.6    33.6
@>     HIS373    A        N_2854  <--->     HIS368    A        O_2818     2.6    19.3
@>     ASN413    B      ND2_8402  <--->     GLU382    B      OE1_8140     2.6    20.3
@>     ARG535    B      NH1_9382  <--->     TYR496    B        O_9063     2.6    29.4
@>     ARG649    A      NH1_5047  <--->     GLU653    A      OE2_5078     2.6    19.6
@>     TRP109    B        N_5947  <--->     ASN173    B      OD1_6483     2.6    37.3
@>     ARG429    B        N_8516  <--->     GLN425    B        O_8488     2.6    23.9
@>     GLN575    B      NE2_9683  <--->     LEU594    B        O_9812     2.6    14.9
@>      ARG68    A         N_482  <--->      SER25    A         O_201     2.6    14.5
@>      HIS70    A         N_500  <--->      SER23    A         O_188     2.6    12.3
@>     ARG215    A      NH2_1620  <--->     GLU168    B      OE1_6442     2.6    24.8
@>     THR462    A        N_3576  <--->     GLU458    A        O_3543     2.6    22.5
@>     ARG463    B      NH2_8797  <--->     TYR471    B       OH_8856     2.6    19.7
@>     HIS405    A      ND1_3124  <--->     ASN672    A        O_5230     2.6    25.8
@>     GLN335    A      NE2_2547  <--->     ALA312    A        O_2377     2.6    10.5
@>     LEU110    B        N_5961  <--->      TRP87    B        O_5770     2.6    37.7
@>     TYR495    B       OH_9059  <--->     GLU630    B     OE1_10098     2.6    12.0
@>     ARG463    A      NH2_3593  <--->     ILE251    A        O_1918     2.6    39.3
@>     GLN319    B      NE2_7641  <--->     GLY324    B        O_7668     2.6    28.2
@>     HIS373    B        N_8058  <--->     HIS368    B        O_8022     2.6    20.9
@>     GLU364    B        N_7982  <--->     VAL360    B        O_7954     2.6    28.1
@>      TRP87    A         N_548  <--->     LEU110    A         O_760     2.6     8.9
@>     TYR408    A       OH_3157  <--->     ASP616    A      OD1_4775     2.6    37.7
@>     GLY493    B        N_9036  <--->     SER489    B        O_9008     2.6    32.4
@>     LEU354    B        N_7900  <--->     LYS350    B        O_7858     2.6    22.3
@>     LEU142    A        N_1007  <--->     ARG138    A         O_972     2.6     5.8
@>     VAL488    A        N_3794  <--->     VAL484    A        O_3759     2.6    11.4
@>     ASN655    A      ND2_5097  <--->     TYR662    A        O_5144     2.6    17.4
@>      THR95    A         N_632  <--->       ARG5    A          O_52     2.6    12.4
@>     ARG208    A        N_1551  <--->     GLU212    A      OE1_1591     2.6    21.7
@>     ARG463    A      NH2_3593  <--->     TYR471    A       OH_3652     2.6    35.2
@>     ARG208    B        N_6755  <--->     GLU212    B      OE1_6795     2.6    34.4
@>     SER550    B       OG_9500  <--->     ILE546    B        O_9466     2.6    22.5
@>     GLN119    B      NE2_6029  <--->     GLN137    B      OE1_6171     2.6    28.1
@>     LEU327    B        N_7684  <--->     TYR318    B        O_7624     2.6     6.3
@>     LEU420    A        N_3247  <--->     ALA416    A        O_3217     2.6    34.5
@>     CYS106    A         N_716  <--->      ARG90    A         O_582     2.7    36.5
@>     LEU607    B        N_9900  <--->     VAL603    B        O_9875     2.7    12.6
@>     VAL488    B        N_8998  <--->     VAL484    B        O_8963     2.7     4.8
@>     GLY583    B        N_9735  <--->     ASP352    B      OD2_7885     2.7    15.8
@>      SER25    A         N_198  <--->      ARG68    A         O_485     2.7    38.0
@>     ASN301    A      ND2_2299  <--->     THR431    A        O_3332     2.7    28.3
@>     ARG407    A      NH2_3145  <--->     ASP616    A        O_4772     2.7    29.7
@>     GLN509    B      NE2_9176  <--->     LEU532    B        O_9352     2.7    37.1
@>     ARG407    A      NH1_3144  <--->     ASP616    A      OD2_4776     2.7    11.0
@>     SER489    A        N_3801  <--->     GLU485    A        O_3766     2.7    24.6
@>     ARG215    A      NH1_1619  <--->     GLU168    B      OE2_6443     2.7    28.7
@>     ARG253    A        N_1934  <--->     ARG463    A        O_3586     2.7    10.7
@>     PHE288    B        N_7398  <--->     LEU317    B        O_7616     2.7    18.1
```

```
@>     GLN509    A      NE2_3972  <--->     LEU532    A        O_4148     2.7    27.8
@>     THR409    A      OG1_3163  <--->     VAL674    A        O_5244     2.7    37.9
@>     PHE309    B        N_7556  <--->     MET574    B        O_9670     2.7    12.8
@>     ASN445    B        N_8639  <--->     LEU441    B        O_8606     2.7    23.6
@>     GLY583    A        N_4531  <--->     ASP352    A      OD2_2681     2.7    14.6
@>     TYR451    B        N_8689  <--->     SER526    B        O_9315     2.7    38.7
@>       ARG5    A          N_49  <--->      THR95    A         O_635     2.7    15.9
@>     CYS106    B        N_5920  <--->      ARG90    B        O_5801     2.7    32.5
@>     TYR149    A        N_1066  <--->     ARG145    A        O_1032     2.7     8.1
@>     GLN575    A        N_4471  <--->     THR593    A        O_4601     2.7    15.0
@>     HIS160    A        N_1167  <--->     LYS518    A        O_4047     2.7    35.5
@>     PHE547    B        N_9471  <--->     THR543    B        O_9444     2.7    33.0
@>     ARG253    B        N_7138  <--->     ARG463    B        O_8790     2.7    16.2
@>     ASN655    A        N_5090  <--->     ILE651    A        O_5056     2.7    28.0
@>     LEU345    B        N_7817  <--->     ASP348    B      OD2_7846     2.7    14.0
@>     ASP504    A        N_3920  <--->     GLU500    A        O_3892     2.7    37.2
@>     ARG203    A      NH1_1514  <--->     GLU212    A      OE2_1592     2.7    38.1
@>     ASN569    A      ND2_4434  <--->     SER563    A        O_4384     2.7     2.5
@>     TRP481    A        N_3733  <--->     GLY477    A        O_3707     2.7     5.8
@>     ASN362    A        N_2765  <--->     THR358    A        O_2729     2.7    34.3
@>     MET314    A        N_2386  <--->     GLN332    A        O_2519     2.7    23.3
@>     SER430    B        N_8527  <--->     VAL426    B        O_8497     2.7    13.0
@>      TRP87    B        N_5767  <--->     LEU110    B        O_5964     2.7    31.2
@>     HIS368    B        N_8019  <--->     GLU364    B        O_7985     2.7    24.6
@>     ILE492    B        N_9028  <--->     VAL488    B        O_9001     2.7     2.1
@>     ASN413    A      ND2_3198  <--->     HIS378    A        O_2899     2.7    35.7
@>     ARG390    A      NH1_3000  <--->     TYR149    A        O_1069     2.7    18.4
@>     ARG407    B      NH2_8349  <--->     ASP616    B        O_9976     2.7    31.8
@>     SER430    A        N_3323  <--->     VAL426    A        O_3293     2.7    37.6
@>     ARG654    A        N_5079  <--->     GLY650    A        O_5052     2.7    22.2
@>     ASN445    A        N_3435  <--->     LEU441    A        O_3402     2.7     9.8
@>     HIS376    B        N_8084  <--->     LEU371    B        O_8046     2.7    15.5
@>     LYS518    B        N_9248  <--->     GLU514    B        O_9217     2.7    30.5
@>     ARG444    B      NH2_8638  <--->     SER296    B        O_7465     2.7    14.5
@>     GLU440    A        N_3390  <--->     GLU436    A        O_3363     2.7    23.1
@>     LEU607    A        N_4696  <--->     VAL603    A        O_4671     2.7     6.3
@>     GLN641    A        N_4976  <--->     ILE637    A        O_4948     2.7    35.5
@>     ARG444    B        N_8628  <--->     GLU440    B        O_8597     2.7    20.9
@>     ASP202    A      OD2_1504  <--->     GLU418    B      OE2_8442     2.7    31.6
@>     ILE403    B        N_8307  <--->     PHE399    B        O_8274     2.7    13.4
@>     LEU278    A        N_2119  <--->     ASP265    A      OD1_2043     2.7    32.7
@>     GLN575    B        N_9675  <--->     THR593    B        O_9805     2.7    22.3
@>     GLN136    A       NE2_959  <--->     GLU140    A       OE2_997     2.7    16.6
@>     TYR496    B        N_9060  <--->     ILE492    B        O_9031     2.7    35.5
@>     GLU364    A        N_2778  <--->     VAL360    A        O_2750     2.8    29.9
@>     ALA188    A        N_1398  <--->     PHE184    A        O_1361     2.8    22.9
@>     ASN672    B       N_10431  <--->     ARG618    B        O_9993     3.3    14.1
@>     ARG461    A        N_3565  <--->     PRO457    A        O_3536     3.3    31.9
@>     SER636    A        N_4939  <--->     ALA632    A        O_4908     3.3    26.8
@>     GLN136    B      NE2_6163  <--->     GLU140    B      OE2_6201     3.3    15.4
@>     ALA370    A        N_2834  <--->     SER366    A        O_2801     3.3    16.7
@>     VAL360    A        N_2747  <--->     ALA356    A        O_2715     3.3    23.8
@>     PHE229    A        N_1729  <--->     ALA225    A        O_1703     3.3    33.3
@>     ASN362    A      ND2_2772  <--->     PRO571    A        O_4446     3.3    10.2
@>     CYS161    A        N_1177  <--->     LYS152    A        O_1104     3.3     8.3
@>     ALA370    B        N_8038  <--->     SER366    B        O_8005     3.3    30.9
@>     ASN413    B        N_8395  <--->     THR409    B        O_8365     3.3    36.3
@>     THR372    A        N_2847  <--->     PHE367    A        O_2807     3.3    18.6
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@>     ARG215    B      NH1_6823  <--->     GLU212    B      OE2_6796     3.3    34.9
@>     ASN598    B      ND2_9845  <--->     ASN304    B      OD1_7525     3.3     7.3
@>     GLY424    B        N_8481  <--->     ASP428    B      OD2_8515     3.3    25.2
@>     ILE515    B        N_9223  <--->     TRP511    B        O_9185     3.3    19.4
@>     ARG361    A      NH1_2763  <--->     ASN569    A        O_4430     3.3    27.9
@>     CYS161    B        N_6381  <--->     LYS152    B        O_6308     3.3    19.0
@>      THR95    B      OG1_5856  <--->       ARG5    B        O_5309     3.3    14.8
@>     SER517    B       OG_9247  <--->     ASN522    B      OD1_9286     3.3    36.6
@>     ARG474    B      NH1_8890  <--->     ILE468    B        N_8826     3.3    28.8
@>     VAL268    A        N_2058  <--->     THR264    A        O_2033     3.3    27.6
@>     SER377    B        N_8094  <--->     THR372    B        O_8054     3.3    31.9
@>     ARG535    A        N_4169  <--->     ASP499    A      OD1_3887     3.3     1.1
@>     ARG634    B     NH2_10131  <--->     GLU626    B     OE1_10061     3.3    31.2
@>     ILE421    B        N_8459  <--->     ALA416    B        O_8421     3.3    24.8
@>      THR10    A          N_91  <--->      ALA49    A         O_335     3.3    21.1
@>     TYR473    B        N_8869  <--->     ASN244    B      OD1_7075     3.3    39.9
@>     GLN241    A      NE2_1845  <--->     ASN569    A      OD1_4433     3.3    38.6
@>     TYR495    A        N_3844  <--->     ILE491    A        O_3819     3.3    30.8
@>     ILE421    A        N_3255  <--->     ALA416    A        O_3217     3.3    34.5
@>       ARG5    B        N_5306  <--->      THR95    B        O_5854     3.3    34.8
@>     GLN139    A         N_980  <--->     GLN135    A         O_945     3.4    11.3
@>     GLN479    A        N_3716  <--->     ASP475    A        O_3691     3.4    33.6
@>     SER286    B        N_7384  <--->     GLU281    B        O_7348     3.4    16.8
@>     MET195    B        N_6647  <--->     ALA191    B        O_6620     3.4    27.9
@>     ARG618    A      NH1_4795  <--->     ASP625    A      OD2_4849     3.4     9.3
@>     VAL502    B        N_9108  <--->     SER498    B        O_9082     3.4    32.3
@>     ILE515    A        N_4019  <--->     TRP511    A        O_3981     3.4    28.7
@>     ARG407    B      NH2_8349  <--->     GLU671    B     OE2_10430     3.4    26.5
@>     ASN672    A        N_5227  <--->     ARG618    A        O_4789     3.4    31.4
@>     VAL167    B        N_6428  <--->     GLU418    B      OE1_8441     3.4    23.0
@>     SER320    B        N_7642  <--->     PRO325    B        O_7672     3.4    32.0
@>     HIS394    B        N_8230  <--->     GLU141    B      OE1_6209     3.4     4.5
@>     ARG203    A      NH1_1514  <--->     GLU212    A      OE1_1591     3.4    24.9
       ..
       ..
@> Number of detected hydrogen bonds: 669.
@> Calculating salt bridges.
@>     LYS196    A         NZ_1459  <--->     ASP202    A   OD1_1503_1504     2.4
@>     GLU168    B   OE1_6442_6443  <--->     ARG215    A   NH1_1619_1620     2.6
@>     ASP202    B   OD1_6707_6708  <--->     LYS196    B         NZ_6663     2.7
@>     ARG654    A   NH1_5088_5089  <--->     ASP476    A   OD1_3702_3703     2.8
@>     ASP505    B   OD1_9138_9139  <--->     HIS396    B        NE2_8255     2.9
@>     ARG203    A   NH1_1514_1515  <--->     GLU212    A   OE1_1591_1592     3.0
@>     GLU281    B   OE1_7352_7353  <--->     LYS284    B         NZ_7379     3.0
@>     ASP616    A   OD1_4775_4776  <--->     ARG407    A   NH1_3144_3145     3.0
@>     ASP505    A   OD1_3934_3935  <--->     HIS396    A        NE2_3051     3.0
@>     LYS582    B         NZ_9734  <--->     ASP348    B   OD1_7845_7846     3.1
@>     ARG635    A   NH1_4937_4938  <--->     GLU631    A   OE1_4903_4904     3.2
@>      GLU32    B   OE1_5509_5510  <--->      ARG68    B   NH1_5729_5730     3.3
@>     GLU212    B   OE1_6795_6796  <--->     ARG203    B   NH1_6718_6719     3.3
@>     ASP625    B OD1_10052_10053  <--->     ARG618    B  NH1_9999_10000     3.3
@>     ASP616    B   OD1_9979_9980  <--->     ARG407    B   NH1_8348_8349     3.3
@>     HIS292    A        NE2_2237  <--->     GLU364    A   OE1_2785_2786     3.4
@>     ARG618    A   NH1_4795_4796  <--->     ASP625    A   OD1_4848_4849     3.4
@>     ASP476    B   OD1_8906_8907  <--->     ARG654    B NH1_10292_10293     3.5
@>     ARG138    B   NH1_6182_6183  <--->     GLU507    B   OE1_9158_9159     3.5
@>     ARG649    B NH1_10251_10252  <--->     GLU653    B OE1_10281_10282     3.6
@>     ARG649    A   NH1_5047_5048  <--->     GLU653    A   OE1_5077_5078     3.6
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@>     ARG634    B NH1_10130_10131  <--->     GLU626    B OE1_10061_10062     3.7
@>     GLU364    B   OE1_7989_7990  <--->     HIS292    B        NE2_7441     3.7
@>     ARG220    B   NH1_6872_6873  <--->     GLU194    B   OE1_6645_6646     3.8
@>     GLU507    A   OE1_3954_3955  <--->     ARG138    A     NH1_978_979     3.8
@>     ASP602    A   OD1_4666_4667  <--->     ARG429    A   NH1_3321_3322     3.9
@>     GLU626    A   OE1_4857_4858  <--->     ARG634    A   NH1_4926_4927     3.9
@>     ARG220    A   NH1_1668_1669  <--->     GLU194    A   OE1_1441_1442     3.9
@>     LYS357    B         NZ_7929  <--->     ASP235    B   OD1_7001_7002     3.9
@>     LYS175    A         NZ_1297  <--->     GLU168    A   OE1_1238_1239     4.0
@>     ASP235    A   OD1_1797_1798  <--->     LYS357    A         NZ_2725     4.0
@>     GLU141    B   OE1_6209_6210  <--->     ARG145    B   NH1_6242_6243     4.0
@>     ARG429    B   NH1_8525_8526  <--->     ASP602    B   OD1_9870_9871     4.0
@>     GLU613    A   OE1_4756_4757  <--->     LYS180    A         NZ_1336     4.0
@>       ARG7    A       NH1_76_77  <--->      ASP52    A     OD1_361_362     4.1
@>     ARG463    B   NH1_8796_8797  <--->     ASP459    B   OD1_8759_8760     4.1
@>     GLU382    A   OE1_2936_2937  <--->     ARG417    A   NH1_3228_3229     4.1
@>     ASP348    A   OD1_2641_2642  <--->     LYS582    A         NZ_4530     4.2
@>      ASP20    B   OD1_5424_5425  <--->      LYS71    B         NZ_5756     4.2
@>     GLU194    A   OE1_1441_1442  <--->     LYS198    A         NZ_1476     4.2
@>      GLU32    A     OE1_252_253  <--->      ARG68    A     NH1_491_492     4.3
@>     ARG463    A   NH1_3592_3593  <--->     ASP459    A   OD1_3555_3556     4.3
@>     ARG208    A   NH1_1560_1561  <--->     GLU111    B   OE1_5976_5977     4.3
@>     GLU141    A   OE1_1005_1006  <--->     ARG145    A   NH1_1038_1039     4.4
@>     ASP475    A   OD1_3694_3695  <--->     ARG474    A   NH1_3686_3687     4.4
@>     ASP616    A   OD1_4775_4776  <--->     LYS180    A         NZ_1336     4.5
@>     ARG390    A   NH1_3000_3001  <--->     GLU514    A   OE1_4017_4018     4.6
@>      ARG63    B   NH1_5687_5688  <--->     ASP129    B   OD1_6102_6103     4.6
@>     ARG461    B   NH1_8778_8779  <--->     GLU458    B   OE1_8751_8752     4.6
@>     ARG444    A   NH1_3433_3434  <--->     GLU440    A   OE1_3397_3398     4.6
@>     GLU369    A   OE1_2832_2833  <--->     HIS368    A        NE2_2824     4.6
@>     HIS231    B        NE2_6962  <--->     GLU234    B   OE1_6993_6994     4.6
@>     LYS165    A         NZ_1216  <--->     ASP163    A   OD1_1197_1198     4.6
@>     LYS612    B         NZ_9952  <--->     ASP562    B   OD1_9583_9584     4.7
@>      ASP20    A     OD1_167_168  <--->      LYS71    A          NZ_518     4.7
@>     GLU212    B   OE1_6795_6796  <--->     ARG208    B   NH1_6764_6765     4.7
@>     GLU369    B   OE1_8036_8037  <--->     HIS368    B        NE2_8028     4.8
@>     HIS231    A        NE2_1758  <--->     GLU234    A   OE1_1789_1790     4.8
@>     GLU168    B   OE1_6442_6443  <--->     LYS175    B         NZ_6501     4.8
@>     ARG417    B   NH1_8432_8433  <--->     GLU382    B   OE1_8140_8141     4.9
@>     ARG474    B   NH1_8890_8891  <--->     ASP475    B   OD1_8898_8899     4.9
@>     ARG215    A   NH1_1619_1620  <--->     GLU212    A   OE1_1591_1592     4.9
@>      GLU12    B   OE1_5366_5367  <--->      ARG90    B   NH1_5807_5808     4.9
@>     LYS198    B         NZ_6680  <--->     GLU194    B   OE1_6645_6646     5.0
@> Number of detected salt bridges: 64.
@> Calculating repulsive ionic bonding.
@>     ASP352    A   OD1_2680_2681  <--->     ASP349    A   OD1_2649_2650     3.3
@>     LYS165    A         NZ_1216  <--->     LYS152    A         NZ_1109     3.8
@>     ARG203    B   NH1_6718_6719  <--->     ARG208    B   NH1_6764_6765     4.3
@> Number of detected Repulsive Ionic Bonding interactions: 3.
@> Calculating Pi stacking interactions.
@>     HIS227       B        6923_6924_6925_6926_6927  <--->     HIS231       B        6958_6959_696
@>     HIS227       A        1719_1720_1721_1722_1723  <--->     HIS231       A        1754_1755_175
@>     PHE640       A   4970_4971_4972_4973_4974_4975  <--->     PHE487       A   3788_3789_3790_379
@>     HIS411       B        8382_8383_8384_8385_8386  <--->     TYR176       B   6507_6508_6509_651
@>     TRP566       B   9609_9611_9612_9613_9614_9615  <--->     PHE229       B   6938_6939_6940_694
@>     PHE640       B10174_10175_10176_10177_10178_10179  <--->     PHE487       B   8992_8993_8994_
@>     HIS373       B        8063_8064_8065_8066_8067  <--->     HIS378       B        8105_8106_810
@>     PHE229       A   1734_1735_1736_1737_1738_1739  <--->     TRP566       A   4405_4407_4408_440
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@>     TYR176       A   1303_1304_1305_1306_1307_1308  <--->     HIS411       A        3178_3179_3180
@>     TYR256       B   7170_7171_7172_7173_7174_7175  <--->     HIS255       B        7160_7161_7162
@>     HIS553       B        9520_9521_9522_9523_9524  <--->     HIS378       B        8105_8106_8107
@>     HIS255       A        1956_1957_1958_1959_1960  <--->     TYR256       A   1966_1967_1968_1969
@>     PHE399       A   3072_3073_3074_3075_3076_3077  <--->     HIS394       A        3031_3032_3033
@>     TRP109       B   5954_5956_5957_5958_5959_5960  <--->      PHE88       B   5786_5787_5788_5789
@>     HIS553       A        4316_4317_4318_4319_4320  <--->     HIS378       A        2901_2902_2903
@>     HIS373       A        2859_2860_2861_2862_2863  <--->     HIS378       A        2901_2902_2903
@> Number of detected Pi stacking interactions: 16.
@> Calculating cation-Pi interactions.
@>     PHE399   B   8276_8277_8278_8279_8280_8281  <--->     ARG145   B            NH1_6242_6243
@>     PHE229   B   6938_6939_6940_6941_6942_6943  <--->     LYS214   B                 NZ_6813
@>     PHE219   B   6857_6858_6859_6860_6861_6862  <--->     ARG220   B            NH1_6872_6873
@>     HIS376   A        2885_2886_2887_2888_2889  <--->     LYS552   A                 NZ_4310
@>     PHE219   A   1653_1654_1655_1656_1657_1658  <--->     ARG220   A            NH1_1668_1669
@>     TYR408   B   8355_8356_8357_8358_8359_8360  <--->     ARG407   B            NH1_8348_8349
@>     PHE399   A   3072_3073_3074_3075_3076_3077  <--->     ARG145   A            NH1_1038_1039
@>     TYR408   A   3151_3152_3153_3154_3155_3156  <--->     ARG407   A            NH1_3144_3145
@>     TYR154   B   6324_6325_6326_6327_6328_6329  <--->     LYS152   B                 NZ_6313
@>     PHE344   A   2607_2608_2609_2610_2611_2612  <--->     LYS582   A                 NZ_4530
@>     TYR408   B   8355_8356_8357_8358_8359_8360  <--->     LYS180   B                 NZ_6540
@>     TYR472   B   8862_8863_8864_8865_8866_8867  <--->     ARG654   B          NH1_10292_10293
@>     HIS160   B        6376_6377_6378_6379_6380  <--->     LYS518   B                 NZ_9256
@>     TYR107   A         727_728_729_730_731_732  <--->      ARG90   A              NH1_588_589
@>     TYR472   A   3658_3659_3660_3661_3662_3663  <--->     ARG654   A            NH1_5088_5089
@> Number of detected cation-pi interactions: 15.
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>     ILE433    B   CD1_855114s  <--->     PHE438    B   CD1_8583     2.2    42.8
@>     MET446    A    SD_344914s  <--->     LEU449    A   CD1_3475     2.8    43.8
@>     ALA179    B    CB_653114s  <--->      PHE14    B   CE2_5382     2.9    48.5
@>     ILE421    A   CD1_326214s  <--->     TYR154    A    OH_1126     2.9    21.4
@>      PHE92    A    CE2_61314s  <--->      VAL69    A    CG2_499     3.0    33.3
@>     PHE438    A   CD1_337914s  <--->     ILE433    A   CG2_3346     3.0    43.4
@>     MET478    A    SD_371414s  <--->     ILE460    A   CD1_3564     3.0    30.7
@>     ILE460    B   CG2_876714s  <--->     VAL465    B   CG2_8808     3.0    42.3
@>       VAL6    B   CG2_532314s  <--->      LEU94    B   CD2_5850     3.1    23.4
@>     ARG474    B    CG_888614s  <--->     ILE460    B   CD1_8768     3.1    37.5
@>     LEU210    B   CD1_677814s  <--->     ILE591    B   CG1_9794     3.1    33.1
@>     TRP207    B   NE1_674914s  <--->     MET567    B    CE_9623     3.1    22.5
@>      VAL55    B   CG1_562614s  <--->      LEU36    B   CD1_5537     3.1    20.4
@>     ILE515    A   CG2_402514s  <--->     TYR541    A    OH_4229     3.2    29.9
@>     TYR472    B    OH_886814s  <--->     LEU658    B  CD2_10322     3.2    31.2
@>     ALA123    B    CB_605414s  <--->     TYR495    B   CE1_9056     3.2    30.9
@>     ARG220    B    CG_686814s  <--->     PHE219    B   CE2_6861     3.2    81.3
@>     LEU594    A   CD1_461114s  <--->     MET213    A    CE_1600     3.2    14.0
@>     ILE515    B   CG2_922914s  <--->     TYR541    B    OH_9433     3.2    29.6
@>     TRP158    B   CH2_636314s  <--->     ILE442    B   CD1_8618     3.2    45.7
@>     PHE367    A   CE2_281314s  <--->     ILE294    A   CG2_2248     3.2    17.1
@>       VAL8    A     CG2_8414s  <--->      PHE92    A    CD1_610     3.2    28.0
@>     PHE184    B   CD2_656914s  <--->     ILE197    A   CD1_1467     3.3    29.5
@>     TYR664    A   CD1_516614s  <--->     ALA558    A    CB_4348     3.3    38.4
@>     TRP608    B   NE1_991614s  <--->     ARG220    B    CG_6868     3.3    46.3
@>     LEU605    B   CD1_989314s  <--->     ALA191    B    CB_6621     3.3    16.4
@>     TYR472    A    OH_366414s  <--->     LEU658    A   CD2_5118     3.3    33.0
@>     LEU594    B   CD1_981514s  <--->     MET213    B    CE_6804     3.3    16.0
@>     ALA188    B    CB_660614s  <--->     LEU609    B   CD1_9928     3.3    30.9
@>     ALA370    A    CB_283814s  <--->     PHE438    A   CD2_3380     3.3    42.4
```

```
@>     LEU521    A   CD1_407414s  <--->     MET446    A    CE_3450     3.3    11.8
@>     LEU538    A   CD2_420114s  <--->     ILE492    A   CD1_3831     3.3    25.6
@>     LEU401    B   CD1_829714s  <--->     PHE487    B   CE2_8996     3.3    21.3
@>     TYR495    A   CE1_385214s  <--->     ALA123    A     CB_850     3.3    28.2
@>      VAL24    B   CG1_545314s  <--->      LEU67    B   CD1_5718     3.3    11.0
@>     PHE104    A    CE1_70614s  <--->      LEU94    A    CD1_630     3.3    16.3
@>     ILE468    A   CG2_362814s  <--->     TYR471    A   CD2_3648     3.3    15.5
@>     TRP359    B   CZ3_794914s  <--->     MET574    B    CG_9672     3.3    43.2
@>     LEU201    B   CD1_669914s  <--->     PHE192    B   CE1_6630     3.3    31.1
@>      PHE92    B   CE2_583214s  <--->       VAL8    B   CG2_5341     3.3    31.8
@>     TYR318    A   CD1_242314s  <--->     LEU272    A   CD2_2090     3.4    34.9
@>     LEU250    B   CD2_711814s  <--->     PHE367    B    CZ_8018     3.4    47.0
@>     LEU317    A   CD1_241514s  <--->     ILE251    A   CD1_1922     3.4    14.3
@>      ARG90    A     CG_58414s  <--->      PHE88    A    CE2_571     3.4    31.2
@>       PHE4    A     CD2_4514s  <--->      LEU57    A    CD1_403     3.4    14.5
@>     LEU441    A   CD1_340514s  <--->     ILE433    A   CD1_3347     3.4    15.4
@>     VAL290    A   CG2_221914s  <--->     LEU317    A   CD1_2415     3.4     9.6
@>     PHE547    A   CE1_427514s  <--->     ALA551    A    CB_4301     3.4    31.0
@>     PHE219    A   CE2_165714s  <--->     ARG220    A    CG_1664     3.4    91.6
@>      PHE45    A     CZ_31514s  <--->      LEU38    A    CD1_295     3.4    14.4
@>     MET148    A    CG_106314s  <--->     TYR149    A   CE2_1075     3.4    68.6
@>     LEU110    A    CD2_76414s  <--->      TRP87    A    CZ3_560     3.4    54.2
@>     PHE192    A    CZ_142814s  <--->     LYS196    A    CG_1456     3.4    36.2
@>     TYR473    A   CE2_367414s  <--->     ALA555    A    CB_4330     3.4    13.4
@>     PHE384    B   CD2_815614s  <--->     VAL545    B   CG1_9461     3.4    38.5
@>     TYR496    B   CD1_906614s  <--->     VAL502    B   CG2_9114     3.4    32.3
@>     ARG417    A    CG_322414s  <--->     ILE421    A   CD1_3262     3.4    19.2
@>     LEU210    A   CD2_157514s  <--->     MET213    A    CE_1600     3.4    42.7
@>     LEU456    B   CD1_873514s  <--->     ILE460    B   CD1_8768     3.4    39.6
@>     VAL263    A   CG2_202914s  <--->     PHE261    A    CZ_2015     3.4    35.6
@>     VAL597    A   CG2_463314s  <--->     TRP207    A   CD2_1544     3.4    51.7
@>     LEU355    B   CD1_791414s  <--->     TRP359    B   NE1_7945     3.4    38.6
@>     TRP511    A   CE3_398814s  <--->     LEU508    A   CD1_3962     3.4    36.6
@>     LEU605    A   CD1_468914s  <--->     ALA191    A    CB_1417     3.4    12.4
@>     LEU420    B   CD1_845714s  <--->     VAL426    B   CG1_8499     3.4    20.8
@>      VAL69    B   CG2_573714s  <--->      PHE92    B   CE1_5831     3.4    28.2
@>     LEU354    B   CD2_790714s  <--->     TRP232    B   CH2_6976     3.4    36.8
@>     VAL542    A   CG1_423514s  <--->     LEU401    A   CD2_3094     3.4     9.3
@>     VAL360    A   CG2_275314s  <--->     ILE331    A   CG2_2514     3.5    14.1
@>     VAL125    B   CG1_606914s  <--->     TRP127    B   CE2_6086     3.5    50.8
@>     LYS214    A    CD_160714s  <--->     PHE229    A    CZ_1739     3.5    36.1
@>     LEU329    B   CD2_770614s  <--->     VAL271    B   CG1_7285     3.5    17.7
@>     ILE294    B   CG2_745214s  <--->     LEU295    B   CD1_7460     3.5    41.1
@>     LEU419    B   CD1_844914s  <--->     LYS196    A    CD_1457     3.5    34.6
@>     LYS518    B    CG_925314s  <--->     TRP151    B   CE2_6300     3.5    61.9
@>     MET574    A    CG_446814s  <--->     TRP359    A   CZ3_2745     3.5    46.6
@>     PHE590    B   CE2_978714s  <--->     LEU594    B   CD1_9815     3.5    37.1
@>     ILE343    B   CG2_780414s  <--->     ALA330    B    CB_7711     3.5     3.4
@>     PHE547    B   CE2_948014s  <--->     ALA551    B    CB_9505     3.5    25.8
       ..
       ..

@> Number of detected hydrophobic interactions: 324.
@> Calculating disulfide bonds.
@> Number of detected disulfide bonds: 0.
```

To extract the interactions between protein's complex, specify *selection* and *selection2* and interaction type:

For hydrogen bonds:

```
In [6]: interactions.getHydrogenBonds(selection='chain A', selection2='chain B')
```

```
[['ARG215', 'NH2_1620', 'A', 'GLU168', 'OE1_6442', 'B', 2.5802, 24.8343],
 ['ARG215', 'NH1_1619', 'A', 'GLU168', 'OE2_6443', 'B', 2.6778, 28.6548],
 ['ASP202', 'OD2_1504', 'A', 'GLU418', 'OE2_8442', 'B', 2.744, 31.6383]]
```

For salt bridges:

```
In [7]: interactions.getSaltBridges(selection='chain A', selection2='chain B')
```

```
[['GLU168', 'OE1_6442_6443', 'B', 'ARG215', 'NH1_1619_1620', 'A', 2.6066],
 ['ARG208', 'NH1_1560_1561', 'A', 'GLU111', 'OE1_5976_5977', 'B', 4.3468]]
```

For hydrophobic interactions:

```
In [8]: interactions.getHydrophobic(selection='chain A', selection2='chain B')
```

```
[['PHE184', 'CD2_6569', 'B', 'ILE197', 'CD1_1467', 'A', 3.2502, 29.5284],
 ['LEU419', 'CD1_8449', 'B', 'LYS196', 'CD_1457', 'A', 3.4645, 34.5683],
 ['ALA182', 'CB_1349', 'A', 'ILE197', 'CD1_6671', 'B', 3.7348, 34.1782],
 ['ALA193', 'CB_6637', 'B', 'LEU186', 'CD1_1387', 'A', 4.2965, 20.2503]]
```

For Pi-stacking interaction:

```
In [9]: interactions.getPiStacking(selection='chain A', selection2='chain B')
```

```
[]
```

For Pi-cation interactions:

```
In [10]: interactions.getPiCation(selection='chain A', selection2='chain B')
```

```
[]
```

For repulsive ionic bonding interactions:

```
In [11]: interactions.getRepulsiveIonicBonding(selection='chain A', selection2='chain B')
```

```
[]
```

Non-zero interactions could be futher saved and used in **VMD_** program to display them:

```
In [12]: showProteinInteractions_VMD(atoms, interactions.getHydrogenBonds(),
   ....:                              color='blue', filename='HBs_7laf.tcl')
   ....:

In [13]: showProteinInteractions_VMD(atoms, interactions.getSaltBridges(),
   ....:                              color='yellow',filename='SBs_7laf.tcl')
   ....:

In [14]: showProteinInteractions_VMD(atoms, interactions.getHydrophobic(),
   ....:                              color='silver',filename='HPh_7laf.tcl')
   ....:
```

```
@> TCL file saved
@> TCL file saved
@> TCL file saved
```

CHAPTER

FIVE

ENSEMBLE PDB ANALYSIS

This example shows how to compute interactions for an Ensemble PDB (e.g. NMR data). The example is prepared for a NMR structure of ubiquitin (PDB: **2K39**) and visualize the results using **Matplotlib_** library and **VMD_** program.

5.1 Parse structure

We start by parsing PDB file which contain multiple conformations of ubiquitin structure.

```
In [1]: atoms = parsePDB('2k39')
```

```
@> Connecting wwPDB FTP server RCSB PDB (USA).
@> 2k39 downloaded (2k39.pdb.gz)
@> PDB download via FTP completed (1 downloaded, 0 failed).
@> 1231 atoms and 116 coordinate set(s) were parsed in 0.29s.
```

5.2 Compute interactions for an Ensemble PDB

To compute hydrogen bonds for each frame use `calcHydrogenBondsTrajectory()` function:

```
In [2]: calcHydrogenBondsTrajectory(atoms)
```

```
@> Model: 0
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      GLN49    A       NE2_784  <--->      GLU51    A       OE2_820     2.6    16.2
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE1_547     2.6     7.0
@>      GLY10    A         N_160  <--->       THR7    A         O_116     2.7    19.8
@>      ARG72    A        N_1149  <--->      GLN40    A         O_624     2.7    21.1
@>      ARG72    A      NH1_1158  <--->      GLN40    A       OE1_628     2.7     7.5
@>       LYS6    A          N_91  <--->      LEU67    A        O_1062     2.7     2.6
@>      GLU34    A         N_540  <--->      ILE30    A         O_473     2.8    28.2
@>      THR55    A         N_870  <--->      ASP58    A       OD2_921     2.8    19.7
@>      ILE44    A         N_698  <--->      HIS68    A        O_1081     2.9    20.2
@>      THR55    A       OG1_875  <--->      ASP58    A       OD2_921     2.9    13.2
@>      LYS29    A         N_448  <--->      ASN25    A         O_389     2.9    13.6
@>      LEU73    A        N_1173  <--->      LEU71    A        O_1133     2.9    27.8
@>      HIS68    A        N_1078  <--->      ILE44    A         O_701     2.9    21.8
@>      THR14    A       OG1_227  <--->       ILE3    A          O_39     2.9    13.1
@>      GLU51    A         N_812  <--->      TYR59    A        OH_937     3.0    23.4
@>      GLU64    A        N_1019  <--->       GLN2    A          O_22     3.0    23.2
@>      LEU50    A         N_793  <--->      LEU43    A         O_682     3.0    15.3
@>      GLN62    A         N_980  <--->      SER65    A       OG_1039     3.0    23.4
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     3.0    12.8
```

```
@>      SER65    A        N_1034  <--->      GLN62    A         O_983     3.0    18.3
@>      VAL17    A         N_270  <--->       MET1    A           O_3     3.0     8.8
@>      ASN60    A         N_947  <--->      SER57    A         O_906     3.1    28.5
@>      LYS33    A         N_518  <--->      LYS29    A         O_451     3.1    33.1
@>      VAL70    A        N_1114  <--->      ARG42    A         O_658     3.1    17.9
@>      ASP32    A         N_506  <--->      ALA28    A         O_441     3.1    10.6
@>      LEU67    A        N_1059  <--->       PHE4    A          O_58     3.1    32.7
@>       THR7    A         N_113  <--->      LYS11    A         O_170     3.1    10.9
@>      LEU15    A         N_236  <--->       ILE3    A          O_39     3.1    18.3
@>      GLU18    A         N_286  <--->      ASP21    A       OD2_333     3.1    29.0
@>      ILE61    A         N_961  <--->      LEU56    A         O_887     3.1    32.1
@>      GLN41    A       NE2_646  <--->      LYS27    A         O_419     3.1    30.7
@>       PHE4    A          N_55  <--->      SER65    A        O_1037     3.2    15.4
@>       ILE3    A          N_36  <--->      LEU15    A         O_239     3.2    33.3
@>      LYS48    A         N_754  <--->      PHE45    A         O_720     3.2    18.9
@>      ARG42    A         N_655  <--->      VAL70    A        O_1117     3.2    24.8
@>      SER57    A         N_903  <--->      PRO19    A         O_304     3.3    29.1
@>      PHE45    A         N_717  <--->      LYS48    A         O_757     3.3    15.6
@>       GLN2    A        NE2_27  <--->      THR14    A       OG1_227     3.3    19.4
@>      GLN41    A         N_638  <--->      PRO38    A         O_598     3.4    33.7
@>      THR66    A      OG1_1050  <--->      GLU64    A        O_1022     3.4    28.3
@>      LEU56    A         N_884  <--->      ASP21    A         O_329     3.4    23.8
@>      ALA28    A         N_438  <--->      GLU24    A         O_374     3.5    18.5
@>      GLN41    A       NE2_646  <--->      PRO37    A         O_584     3.5    26.0
@> Number of detected hydrogen bonds: 43.
@> Model: 1
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.5    28.9
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE1_547     2.5     7.3
@>      LYS33    A        NZ_526  <--->      GLU16    A       OE2_263     2.6    12.7
@>      SER65    A       OG_1039  <--->      GLN62    A         O_983     2.6    15.7
@>      LYS27    A        NZ_424  <--->      ASP52    A       OD2_834     2.6    29.5
@>      GLN62    A       NE2_988  <--->      ASN60    A       OD1_953     2.6    18.2
@>      ARG74    A      NH2_1202  <--->      GLY76    A      OXT_1227     2.6    19.4
@>      SER57    A        OG_908  <--->      THR55    A       OG1_875     2.6    24.1
@>      ARG74    A       NE_1199  <--->      GLY76    A        O_1226     2.7    22.0
@>      LYS29    A         N_448  <--->      ASN25    A         O_389     2.7    16.0
@>      LYS29    A        NZ_456  <--->      GLU16    A       OE1_262     2.7    23.7
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     2.7    14.9
@>      GLY35    A         N_555  <--->      GLN31    A         O_492     2.7    32.0
@>      THR55    A       OG1_875  <--->      ASP58    A       OD2_921     2.7    19.9
@>      LEU69    A        N_1095  <--->       LYS6    A          O_94     2.7    26.5
@>      GLU51    A         N_812  <--->      TYR59    A        OH_937     2.7    21.7
@>      GLU64    A        N_1019  <--->       GLN2    A          O_22     2.7     5.2
@>      VAL70    A        N_1114  <--->      ARG42    A         O_658     2.7    22.0
@>      THR55    A         N_870  <--->      ASP58    A       OD2_921     2.7    18.5
@>       THR7    A       OG1_118  <--->      LYS11    A         O_170     2.7    23.8
@>      ARG42    A         N_655  <--->      VAL70    A        O_1117     2.7    32.6
@>      GLU34    A         N_540  <--->      ILE30    A         O_473     2.8    22.0
@>      LEU15    A         N_236  <--->       ILE3    A          O_39     2.8    13.0
@>      LEU67    A        N_1059  <--->       PHE4    A          O_58     2.8     9.7
@>      LYS33    A        NZ_526  <--->      THR14    A         O_225     2.9    37.2
@>       VAL5    A          N_75  <--->      ILE13    A         O_206     2.9    17.0
@>       LYS6    A          N_91  <--->      LEU67    A        O_1062     2.9    14.9
@>      VAL17    A         N_270  <--->       MET1    A           O_3     2.9     9.5
@>      GLN41    A       NE2_646  <--->      ILE36    A         O_565     2.9    31.4
@>      GLN41    A       NE2_646  <--->      LYS27    A         O_419     2.9    10.1
```

```
@>      SER57    A         N_903  <--->      PRO19    A         O_304     2.9    33.8
@>      ALA28    A         N_438  <--->      GLU24    A         O_374     2.9    26.2
@>       THR7    A         N_113  <--->      LYS11    A         O_170     2.9    35.2
@>      ILE61    A         N_961  <--->      LEU56    A         O_887     3.0    18.2
@>       PHE4    A          N_55  <--->      SER65    A        O_1037     3.0     6.5
@>      ARG72    A      NH2_1159  <--->      ASP39    A       OD2_616     3.0    25.5
@>      GLU18    A         N_286  <--->      ASP21    A       OD2_333     3.0     1.5
@>      HIS68    A        N_1078  <--->      ILE44    A         O_701     3.0    27.8
@>      ILE30    A         N_470  <--->      VAL26    A         O_403     3.0    32.5
@>      ILE44    A         N_698  <--->      HIS68    A        O_1081     3.0    19.2
@>      ASN25    A         N_386  <--->      THR22    A       OG1_343     3.1    38.5
@>      ASP21    A         N_326  <--->      GLU18    A         O_289     3.1    21.6
@>      ARG72    A        N_1149  <--->      GLN40    A         O_624     3.1    13.3
@>      GLN40    A         N_621  <--->      PRO37    A         O_584     3.1    21.1
@>      LYS27    A         N_416  <--->      ILE23    A         O_355     3.1    36.2
@>      LYS33    A         N_518  <--->      LYS29    A         O_451     3.2    22.9
@>      TYR59    A         N_926  <--->      THR55    A         O_873     3.3    20.9
@>      ARG54    A         N_846  <--->      GLU51    A         O_815     3.3    24.1
@>      VAL26    A         N_400  <--->      THR22    A         O_341     3.4    23.5
@>      GLN41    A         N_638  <--->      PRO38    A         O_598     3.4    34.4
@>      ILE23    A         N_352  <--->      ARG54    A         O_849     3.5    23.1
@>      ASN60    A         N_947  <--->      SER57    A         O_906     3.5    25.0
@> Number of detected hydrogen bonds: 52.
@> Model: 2
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE2_548     2.5    27.6
@>       MET1    A           N_0  <--->      GLU16    A       OE2_263     2.6    11.9
@>       PHE4    A          N_55  <--->      SER65    A        O_1037     2.6    19.5
@>      GLN41    A       NE2_646  <--->      LYS27    A         O_419     2.6    39.4
@>      THR55    A       OG1_875  <--->      ASP58    A       OD2_921     2.6    26.1
@>      VAL17    A         N_270  <--->       MET1    A           O_3     2.7    14.9
@>      GLU18    A         N_286  <--->      ASP21    A       OD2_333     2.7     5.0
@>      GLU34    A         N_540  <--->      ILE30    A         O_473     2.7     7.6
@>      ILE44    A         N_698  <--->      HIS68    A        O_1081     2.7    13.8
@>      THR22    A         N_338  <--->      ASN25    A       OD1_392     2.7    20.3
@>      SER20    A        OG_320  <--->      GLU18    A       OE1_293     2.7    21.5
@>      GLU51    A         N_812  <--->      TYR59    A        OH_937     2.7    23.9
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.7    18.4
@>      GLN41    A       NE2_646  <--->      ILE36    A         O_565     2.8    31.7
@>       LYS6    A          N_91  <--->      LEU67    A        O_1062     2.8    14.6
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     2.8     7.4
@>      LYS11    A         N_167  <--->       THR7    A       OG1_118     2.8    30.1
@>      VAL70    A        N_1114  <--->      ARG42    A         O_658     2.8    28.1
@>      THR22    A       OG1_343  <--->      ASN25    A       OD1_392     2.8    16.5
@>      LEU56    A         N_884  <--->      ASP21    A         O_329     2.8    25.9
@>      HIS68    A        N_1078  <--->      ILE44    A         O_701     2.8     4.3
@>       THR7    A       OG1_118  <--->      LYS11    A         O_170     2.8    11.4
@>       VAL5    A          N_75  <--->      ILE13    A         O_206     2.8    37.9
@>      LYS63    A       NZ_1005  <--->       GLN2    A        OE1_26     2.8    13.5
@>      ARG54    A       NH1_855  <--->      ASP52    A         O_830     2.8     5.2
@>       THR7    A         N_113  <--->      LYS11    A         O_170     2.9    19.8
@>      ALA28    A         N_438  <--->      GLU24    A         O_374     2.9    26.5
@>      GLU64    A        N_1019  <--->       GLN2    A          O_22     2.9     6.5
@>      ILE61    A         N_961  <--->      LEU56    A         O_887     2.9     3.4
@>      LEU69    A        N_1095  <--->       LYS6    A          O_94     2.9    12.0
@>      GLN31    A         N_489  <--->      LYS27    A         O_419     2.9    26.1
@>      GLN40    A       NE2_629  <--->      GLY76    A        O_1226     2.9     3.8
```

```
@>      ASN25    A         N_386  <--->      THR22    A         O_341     2.9    29.4
@>      LEU67    A        N_1059  <--->       PHE4    A          O_58     3.0    23.6
@>       LYS6    A         NZ_99  <--->      THR12    A       OG1_194     3.0    11.7
@>      ILE30    A         N_470  <--->      VAL26    A         O_403     3.0    29.3
@>      ARG42    A         N_655  <--->      VAL70    A        O_1117     3.1     6.2
@>      ARG72    A      NH2_1159  <--->      ASP39    A         O_612     3.1    16.4
@>      GLN40    A       NE2_629  <--->      ARG72    A        O_1152     3.1    26.5
@>      SER57    A         N_903  <--->      PRO19    A         O_304     3.1     6.5
@>      ASP21    A         N_326  <--->      GLU18    A         O_289     3.1    31.9
@>      SER65    A        N_1034  <--->      GLN62    A         O_983     3.1    21.5
@>      ARG72    A        N_1149  <--->      GLN40    A         O_624     3.1    38.2
@>       ILE3    A          N_36  <--->      LEU15    A         O_239     3.1    17.0
@>      ASP32    A         N_506  <--->      ALA28    A         O_441     3.1    19.2
@>      GLN62    A         N_980  <--->      SER65    A       OG_1039     3.2    26.8
@>      GLN40    A         N_621  <--->      PRO37    A         O_584     3.2    36.5
@>      TYR59    A         N_926  <--->      THR55    A         O_873     3.2     9.2
@>      LYS48    A         N_754  <--->      PHE45    A         O_720     3.2    25.0
@>      PHE45    A         N_717  <--->      LYS48    A         O_757     3.3     3.9
@>      LYS29    A         N_448  <--->      ASN25    A         O_389     3.3    33.9
@>      LEU15    A         N_236  <--->       ILE3    A          O_39     3.3    36.1
@>      LYS27    A         N_416  <--->      ILE23    A         O_355     3.4     7.1
@> Number of detected hydrogen bonds: 53.
..
..
@> Model: 114
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      LYS27    A        NZ_424  <--->      ASP52    A       OD2_834     2.5     8.2
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE2_548     2.5    29.1
@>      LYS29    A        NZ_456  <--->      ASP21    A       OD2_333     2.6     6.4
@>       MET1    A           N_0  <--->      GLU16    A       OE2_263     2.6    10.9
@>      LEU69    A        N_1095  <--->       LYS6    A          O_94     2.7    16.8
@>      THR55    A       OG1_875  <--->      ASP58    A       OD2_921     2.7     2.4
@>      ASN25    A       ND2_393  <--->      ASP21    A       OD2_333     2.7    31.6
@>      HIS68    A        N_1078  <--->      ILE44    A         O_701     2.7    11.6
@>      SER57    A        OG_908  <--->      THR55    A       OG1_875     2.7    32.8
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.7    19.3
@>      THR55    A         N_870  <--->      ASP58    A       OD2_921     2.8    18.3
@>      ILE44    A         N_698  <--->      HIS68    A        O_1081     2.8     7.9
@>      GLU34    A         N_540  <--->      ILE30    A         O_473     2.8    14.8
@>       LYS6    A          N_91  <--->      LEU67    A        O_1062     2.8    19.2
@>       VAL5    A          N_75  <--->      ILE13    A         O_206     2.8    16.6
@>      GLU64    A        N_1019  <--->       GLN2    A          O_22     2.8    32.4
@>      ARG54    A        NE_853  <--->      GLU51    A       OE1_819     2.8     3.2
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     2.9    22.7
@>       THR7    A       OG1_118  <--->      LYS11    A         O_170     2.9    11.0
@>      ARG74    A      NH1_1201  <--->      GLY76    A        O_1226     2.9    34.6
@>      LEU50    A         N_793  <--->      LEU43    A         O_682     2.9    31.5
@>      LEU15    A         N_236  <--->       ILE3    A          O_39     2.9    18.9
@>      SER65    A       OG_1039  <--->      GLN62    A         O_983     2.9    33.9
@>      ALA28    A         N_438  <--->      GLU24    A         O_374     2.9    19.9
@>      VAL70    A        N_1114  <--->      ARG42    A         O_658     3.0     9.9
@>      SER57    A         N_903  <--->      PRO19    A         O_304     3.0    12.8
@>      GLU51    A         N_812  <--->      TYR59    A        OH_937     3.0    21.3
@>      LYS27    A         N_416  <--->      ILE23    A         O_355     3.0    16.1
@>      GLN31    A         N_489  <--->      LYS27    A         O_419     3.0    29.6
@>      LYS29    A         N_448  <--->      VAL26    A         O_403     3.0    38.6
@>      LYS48    A         N_754  <--->      PHE45    A         O_720     3.0    20.6
```

```
@>      ILE61    A         N_961  <--->      LEU56    A         O_887     3.1    13.3
@>       ILE3    A          N_36  <--->      LEU15    A         O_239     3.1     8.4
@>      ILE23    A         N_352  <--->      ARG54    A         O_849     3.1    21.3
@>      ILE30    A         N_470  <--->      VAL26    A         O_403     3.2     6.6
@>      ARG42    A         N_655  <--->      VAL70    A        O_1117     3.2    29.2
@>      VAL17    A         N_270  <--->       MET1    A           O_3     3.2    21.9
@>      PHE45    A         N_717  <--->      LYS48    A         O_757     3.2    19.4
@>      ASP21    A         N_326  <--->      GLU18    A         O_289     3.2    26.5
@>      ARG54    A         N_846  <--->      GLU51    A         O_815     3.3    31.0
@>       PHE4    A          N_55  <--->      SER65    A        O_1037     3.3    29.3
@>      GLN41    A       NE2_646  <--->      PRO37    A         O_584     3.4     9.0
@>      VAL26    A         N_400  <--->      ILE23    A         O_355     3.4    37.5
@> Number of detected hydrogen bonds: 43.
```

Similarly, it can be done with other interaction types. Salt bridges with `calcSaltBridgesTrajectory()`:

```
In [3]: calcSaltBridgesTrajectory(atoms)
```

```
@> Model: 0
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.7
@>      ASP32    A     OD1_512_513  <--->      LYS33    A          NZ_526     3.6
@>      LYS29    A          NZ_456  <--->      ASP21    A     OD1_332_333     4.5
@> Number of detected salt bridges: 3.
@> Model: 1
@> Calculating salt bridges.
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     2.5
@>      GLU16    A     OE1_262_263  <--->      LYS33    A          NZ_526     2.8
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.9
@>      LYS29    A          NZ_456  <--->      GLU16    A     OE1_262_263     3.3
@>      LYS63    A         NZ_1005  <--->      GLU64    A   OE1_1026_1027     3.7
@>      ASP39    A     OD1_615_616  <--->      ARG72    A   NH1_1158_1159     4.6
@> Number of detected salt bridges: 6.
@> Model: 2
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     3.1
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     4.8
@> Number of detected salt bridges: 2.
@> Model: 3
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.7
@>      ASP39    A     OD1_615_616  <--->      ARG72    A   NH1_1158_1159     2.8
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     3.1
@>      GLU51    A     OE1_819_820  <--->      ARG54    A     NH1_855_856     3.9
@> Number of detected salt bridges: 4.
@> Model: 4
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.8
@>      LYS63    A         NZ_1005  <--->      GLU64    A   OE1_1026_1027     3.3
@>      GLU51    A     OE1_819_820  <--->      ARG54    A     NH1_855_856     4.1
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     4.5
@>      GLU16    A     OE1_262_263  <--->      LYS33    A          NZ_526     4.9
@> Number of detected salt bridges: 5.
@> Model: 5
@> Calculating salt bridges.
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     2.5
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.5
@>      GLU16    A     OE1_262_263  <--->      LYS33    A          NZ_526     2.7
```

```
@>      LYS29    A          NZ_456  <--->      ASP21    A     OD1_332_333     3.1
@>      ASP58    A     OD1_920_921  <--->      ARG54    A     NH1_855_856     4.5
@>      GLU51    A     OE1_819_820  <--->      ARG54    A     NH1_855_856     4.9
@> Number of detected salt bridges: 6.
@> Model: 6
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.6
@>      LYS29    A          NZ_456  <--->      ASP21    A     OD1_332_333     3.0
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     3.4
@>      ASP58    A     OD1_920_921  <--->      ARG54    A     NH1_855_856     4.3
@> Number of detected salt bridges: 4.
@> Model: 7
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.7
@>      ASP58    A     OD1_920_921  <--->      ARG54    A     NH1_855_856     4.2
@> Number of detected salt bridges: 2.
@> Model: 8
@> Calculating salt bridges.
@>      GLU16    A     OE1_262_263  <--->      LYS33    A          NZ_526     2.5
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     3.2
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     3.4
@>      GLU51    A     OE1_819_820  <--->      ARG54    A     NH1_855_856     3.6
@>      LYS29    A          NZ_456  <--->      GLU16    A     OE1_262_263     4.6
@> Number of detected salt bridges: 5.
@> Model: 9
@> Calculating salt bridges.
@>      ASP39    A     OD1_615_616  <--->      ARG72    A   NH1_1158_1159     2.7
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     2.8
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     3.1
@>      GLU51    A     OE1_819_820  <--->      ARG54    A     NH1_855_856     3.7
@> Number of detected salt bridges: 4.
@> Model: 10
@> Calculating salt bridges.
@>      LYS63    A         NZ_1005  <--->      GLU64    A   OE1_1026_1027     2.6
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     2.6
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.9
@>      LYS29    A          NZ_456  <--->      ASP21    A     OD1_332_333     2.9
@>      ASP32    A     OD1_512_513  <--->      LYS33    A          NZ_526     3.7
@> Number of detected salt bridges: 5.
@> Model: 11
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.6
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     3.1
@>      LYS29    A          NZ_456  <--->      ASP21    A     OD1_332_333     3.2
@> Number of detected salt bridges: 3.
@> Model: 12
@> Calculating salt bridges.
@>      LYS27    A          NZ_424  <--->      GLU24    A     OE1_378_379     2.8
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.9
@>      LYS63    A         NZ_1005  <--->      GLU64    A   OE1_1026_1027     2.9
@>      LYS29    A          NZ_456  <--->      ASP21    A     OD1_332_333     3.0
@>      ASP32    A     OD1_512_513  <--->      LYS33    A          NZ_526     3.7
@>      ARG74    A   NH1_1201_1202  <--->      ASP39    A     OD1_615_616     4.3
@> Number of detected salt bridges: 6.
@> Model: 13
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.9
@>      LYS63    A         NZ_1005  <--->      GLU64    A   OE1_1026_1027     2.9
```

```
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     3.1
@>      GLU51    A     OE1_819_820  <--->      ARG54    A     NH1_855_856     3.9
@> Number of detected salt bridges: 4.
@> Model: 14
@> Calculating salt bridges.
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     2.6
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     3.0
@>      LYS29    A          NZ_456  <--->      ASP21    A     OD1_332_333     3.5
@> Number of detected salt bridges: 3.
@> Model: 15
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.5
@>      LYS29    A          NZ_456  <--->      ASP21    A     OD1_332_333     2.6
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     2.9
@>      ASP32    A     OD1_512_513  <--->      LYS33    A          NZ_526     3.4
@>      LYS63    A         NZ_1005  <--->      GLU64    A   OE1_1026_1027     3.5
@> Number of detected salt bridges: 5.
@> Model: 16
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.6
@>      LYS29    A          NZ_456  <--->      ASP21    A     OD1_332_333     3.3
@>      GLU51    A     OE1_819_820  <--->      ARG54    A     NH1_855_856     4.5
@> Number of detected salt bridges: 3.
..
..
@> Model: 112
@> Calculating salt bridges.
@>      LYS29    A          NZ_456  <--->      ASP21    A     OD1_332_333     2.6
@>      LYS63    A         NZ_1005  <--->      GLU64    A   OE1_1026_1027     3.5
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     4.0
@>      ASP58    A     OD1_920_921  <--->      ARG54    A     NH1_855_856     4.3
@>      LYS29    A          NZ_456  <--->      GLU18    A     OE1_293_294     4.7
@> Number of detected salt bridges: 5.
@> Model: 113
@> Calculating salt bridges.
@>      GLU16    A     OE1_262_263  <--->      LYS33    A          NZ_526     3.2
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     3.3
@>      LYS63    A         NZ_1005  <--->      GLU64    A   OE1_1026_1027     3.4
@>      LYS29    A          NZ_456  <--->      ASP21    A     OD1_332_333     3.4
@>      LYS27    A          NZ_424  <--->      GLU24    A     OE1_378_379     3.4
@>      ASP58    A     OD1_920_921  <--->      ARG54    A     NH1_855_856     4.5
@> Number of detected salt bridges: 6.
@> Model: 114
@> Calculating salt bridges.
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     2.9
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     3.1

@>      LYS29    A          NZ_456  <--->      ASP21    A     OD1_332_333     3.4
@>      ASP32    A     OD1_512_513  <--->      LYS33    A          NZ_526     3.7
@>      GLU51    A     OE1_819_820  <--->      ARG54    A     NH1_855_856     4.3
@> Number of detected salt bridges: 5.
```

Repulsive Ionic Bonding using `calcRepulsiveIonicBondingTrajectory()` for residues with the same charges:

```
In [4]: calcRepulsiveIonicBondingTrajectory(atoms)
```

```
@> Model: 0
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Model: 1
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
..
..
@> Model: 90
@> Calculating repulsive ionic bonding.
@>      ARG72    A   NH1_1158_1159  <--->      ARG42    A     NH1_664_665     4.4
..
..
@> Model: 111
@> Calculating repulsive ionic bonding.
@>      ARG72    A   NH1_1158_1159  <--->      ARG42    A     NH1_664_665     4.3
@> Number of detected Repulsive Ionic Bonding interactions: 1.
@> Model: 112
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Model: 113
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Model: 114
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
```

Pi-Stacking interactions using `calcPiStackingTrajectory()`:

```
In [5]: calcPiStackingTrajectory(atoms)
```

```
@> Model: 0
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
@> Model: 1
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
@> Model: 2
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
@> Model: 3
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
..
..
@> Calculating Pi stacking interactions.
@>      PHE45       A         722_723_724_725_726_727  <--->      TYR59       A         931_932_933_9
@> Number of detected Pi stacking interactions: 1.
..
..
@> Model: 113
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
@> Model: 114
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
```

Pi-Cation interactions using `calcPiCationTrajectory()`:

```
In [6]: calcPiCationTrajectory(atoms)
```

```
@> Model: 0
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
@> Model: 1
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
..
..
@> Model: 10
@> Calculating cation-Pi interactions.
@>      TYR59   A         931_932_933_934_935_936  <--->      ARG54   A                    NH1_855_8
@> Number of detected cation-pi interactions: 1.
@> Model: 11
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
@> Model: 12
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
@> Model: 13
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
@> Model: 14
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
@> Model: 15
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
@> Model: 16
@> Calculating cation-Pi interactions.
@>      TYR59   A         931_932_933_934_935_936  <--->      ARG54   A                    NH1_855_8
@> Number of detected cation-pi interactions: 1.
@> Model: 17
@> Calculating cation-Pi interactions.
@>      TYR59   A         931_932_933_934_935_936  <--->      ARG54   A                    NH1_855_8
@> Number of detected cation-pi interactions: 1.
..
..
@> Model: 114
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
```

Hydrophobic interactions using `calcHydrophohicTrajectory()`:

```
In [7]: calcHydrophobicTrajectory(atoms)
```

```
@> Model: 0
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      PHE45    A    CD1_72314s  <--->      LEU67    A   CD1_1065     3.6    25.2
@>      VAL17    A    CG2_27614s  <--->       ILE3    A     CG1_41     3.6    17.8
@>      ILE23    A    CD1_35914s  <--->      LEU56    A    CD2_891     3.6    22.8
@>      LEU43    A    CD1_68514s  <--->      ILE23    A    CG2_358     3.7    10.1
@>      LYS27    A     CG_42114s  <--->      LEU43    A    CD1_685     3.7    13.4
@>      ILE61    A    CD1_96814s  <--->      LEU56    A    CD2_891     3.8    40.6
@>      TYR59    A    CD2_93314s  <--->      ILE23    A    CD1_359     3.8    24.0
@>      LEU69    A   CD1_110114s  <--->      ILE30    A    CD1_477     3.8    10.5
```

```
@>       MET1    A       CE_714s  <--->       ILE3    A     CG2_42     3.8    28.7
@>       VAL5    A     CG1_8014s  <--->      LEU69    A   CD1_1101     3.9    14.6
@>      ILE13    A    CG2_20914s  <--->      LEU15    A    CD1_242     3.9    19.8
@>      ARG42    A     CG_66014s  <--->      VAL70    A   CG2_1120     4.0    42.9
@>      ILE44    A    CD1_70514s  <--->      VAL70    A   CG1_1119     4.0    17.7
@>      ALA46    A     CB_74114s  <--->      PHE45    A    CD2_724     4.1    50.7
@>      LYS11    A     CG_17214s  <--->      ILE13    A    CG1_208     4.1    30.5
@>       LEU8    A    CD1_13314s  <--->      VAL70    A   CG1_1119     4.5     8.8
@> Number of detected hydrophobic interactions: 16.
@> Model: 1
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      LEU15    A    CD1_24214s  <--->      LYS29    A     CD_454     3.5    18.8
@>       MET1    A       CE_714s  <--->      LEU56    A    CD2_891     3.5    12.0
@>      LEU43    A    CD1_68514s  <--->      LYS27    A     CG_421     3.5    17.3
@>      LEU67    A   CD1_106514s  <--->       ILE3    A     CD1_43     3.5    16.4
@>      VAL17    A    CG2_27614s  <--->      LEU56    A    CD2_891     3.6    12.5
@>      TYR59    A    CE2_93514s  <--->      ILE23    A    CD1_359     3.6    17.3
@>       VAL5    A     CG2_8114s  <--->      LEU15    A    CD2_243     3.7    24.5
@>      ILE30    A    CD1_47714s  <--->      LEU43    A    CD2_686     3.7    13.8
@>      PHE45    A    CD1_72314s  <--->      LEU67    A   CD2_1066     3.7    13.2
@>      LEU50    A    CD2_80014s  <--->      TYR59    A    CE1_934     3.7    41.8
@>      ILE13    A    CG2_20914s  <--->      LEU15    A    CD2_243     3.7    21.7
@>      ILE36    A    CG2_56814s  <--->      LEU73    A   CD2_1180     3.8    26.2
@>      LEU69    A   CD2_110214s  <--->      ILE36    A    CD1_569     3.9     7.9
@>      LYS11    A     CD_17314s  <--->      ILE13    A    CD1_210     3.9    29.1
@>      LYS33    A     CD_52414s  <--->      ILE13    A    CG2_209     3.9    11.1
@>      ARG42    A     CG_66014s  <--->      ILE44    A    CG2_704     4.0    15.7
@>      VAL26    A    CG1_40514s  <--->      LEU15    A     CG_241     4.1    15.5
@>      VAL70    A   CG2_112014s  <--->       LEU8    A    CD1_133     4.3    14.7
@>      ARG74    A    CG_119714s  <--->      LEU71    A   CD1_1136     4.5    17.2
@> Number of detected hydrophobic interactions: 19.
..
..
```

And disulfide bonds using `calcDisulfideBondsTrajectory()`:

```
In [8]: calcDisulfideBondsTrajectory(atoms)
```

```
@> Model: 0
@> Lack of cysteines in the structure.
@> Number of detected disulfide bonds: 0.
@> Model: 1
@> Lack of cysteines in the structure.
@> Number of detected disulfide bonds: 0.
@> Model: 2
@> Lack of cysteines in the structure.
@> Number of detected disulfide bonds: 0.
..
..
```

5.3 Select particular frames or change the default parameters of the interactions

The default parameters which are assigned to the interaction types could be changed as follows:

```
In [9]: calcHydrogenBondsTrajectory(atoms, distA=2.7, angle=35, cutoff_dist=10)
```

```
@> Model: 0
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      GLN49    A       NE2_784  <--->      GLU51    A       OE2_820     2.6    16.2
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE1_547     2.6     7.0
@>      GLY10    A         N_160  <--->       THR7    A         O_116     2.7    19.8
@>      ARG72    A        N_1149  <--->      GLN40    A         O_624     2.7    21.1
@> Number of detected hydrogen bonds: 4.
@> Model: 1
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.5    28.9
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE1_547     2.5     7.3
@>      LYS33    A        NZ_526  <--->      GLU16    A       OE2_263     2.6    12.7
@>      SER65    A       OG_1039  <--->      GLN62    A         O_983     2.6    15.7
@>      LYS27    A        NZ_424  <--->      ASP52    A       OD2_834     2.6    29.5
@>      GLN62    A       NE2_988  <--->      ASN60    A       OD1_953     2.6    18.2
@>      ARG74    A      NH2_1202  <--->      GLY76    A      OXT_1227     2.6    19.4
@>      SER57    A        OG_908  <--->      THR55    A       OG1_875     2.6    24.1
@>      ARG74    A       NE_1199  <--->      GLY76    A        O_1226     2.7    22.0
@>      LYS29    A         N_448  <--->      ASN25    A         O_389     2.7    16.0
@>      LYS29    A        NZ_456  <--->      GLU16    A       OE1_262     2.7    23.7
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     2.7    14.9
@>      GLY35    A         N_555  <--->      GLN31    A         O_492     2.7    32.0
@>      THR55    A       OG1_875  <--->      ASP58    A       OD2_921     2.7    19.9
@>      LEU69    A        N_1095  <--->       LYS6    A          O_94     2.7    26.5
@> Number of detected hydrogen bonds: 15.
@> Model: 2
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE2_548     2.5    27.6
@>       MET1    A           N_0  <--->      GLU16    A       OE2_263     2.6    11.9
@>       PHE4    A          N_55  <--->      SER65    A        O_1037     2.6    19.5
@>      THR55    A       OG1_875  <--->      ASP58    A       OD2_921     2.6    26.1
@>      VAL17    A         N_270  <--->       MET1    A           O_3     2.7    14.9
@>      GLU18    A         N_286  <--->      ASP21    A       OD2_333     2.7     5.0
@>      GLU34    A         N_540  <--->      ILE30    A         O_473     2.7     7.6
@>      ILE44    A         N_698  <--->      HIS68    A        O_1081     2.7    13.8
@> Number of detected hydrogen bonds: 8.
@> Model: 3
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      LYS29    A        NZ_456  <--->      GLU16    A         O_258     2.5    26.1
@>      ARG54    A       NH1_855  <--->      GLU51    A       OE1_819     2.5    15.4
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE2_548     2.6    24.7
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     2.6    17.0
@>       GLN2    A        NE2_27  <--->      GLU16    A       OE1_262     2.6     7.7
@>      LYS27    A        NZ_424  <--->      ASP52    A       OD1_833     2.6    12.0
@>      ARG72    A      NH1_1158  <--->      ASP39    A       OD1_615     2.7    21.2
@> Number of detected hydrogen bonds: 7.
@> Model: 4
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      ARG54    A        NE_853  <--->      GLU51    A       OE1_819     2.5    16.1
@>      ARG74    A      NH2_1202  <--->      GLN49    A       OE1_783     2.6    20.2
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE2_548     2.7    29.8
```

```
@> Number of detected hydrogen bonds: 3.
@> Model: 5
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      ARG54    A        NE_853  <--->      GLU51    A       OE1_819     2.5     8.7
@>      LYS27    A        NZ_424  <--->      ASP52    A       OD2_834     2.6    19.9
@>      LYS33    A        NZ_526  <--->      GLU16    A       OE1_262     2.6     9.0
@>      ARG74    A       NE_1199  <--->      GLY76    A        O_1226     2.6    19.2
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE1_547     2.6    18.4
@>      ARG72    A        N_1149  <--->      GLN40    A         O_624     2.6    15.8
@>      ARG74    A      NH2_1202  <--->      GLY76    A      OXT_1227     2.7    25.2
@>      GLU64    A        N_1019  <--->       GLN2    A          O_22     2.7    32.4
@> Number of detected hydrogen bonds: 8.
@> Model: 6
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE2_548     2.6    10.2
@>      LYS27    A        NZ_424  <--->      ASP52    A       OD2_834     2.6    31.7
@>      LYS29    A        NZ_456  <--->      ASP21    A       OD2_333     2.6    21.1
@>      ASN25    A       ND2_393  <--->      ASP21    A       OD2_333     2.7    10.1
@> Number of detected hydrogen bonds: 4.
@> Model: 7
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      THR55    A       OG1_875  <--->      ASP58    A       OD2_921     2.5    10.2
@>       GLN2    A        NE2_27  <--->      GLU16    A       OE2_263     2.6    14.9
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.7    23.3
@>      ALA28    A         N_438  <--->      GLU24    A         O_374     2.7    24.8
@>      ARG72    A        N_1149  <--->      GLN40    A         O_624     2.7    10.0
@> Number of detected hydrogen bonds: 5.
@> Model: 8
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE1_547     2.6    19.1
@>      ARG54    A        NE_853  <--->      GLU51    A       OE1_819     2.6    25.8
@>      ARG54    A       NH2_856  <--->      GLU51    A       OE2_820     2.6    28.0
@>       THR7    A       OG1_118  <--->      LYS11    A         O_170     2.6    24.5
@> Number of detected hydrogen bonds: 4.
@> Model: 9
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      ARG54    A       NH1_855  <--->      GLU51    A       OE1_819     2.5    11.5
@>      ARG72    A      NH1_1158  <--->      ASP39    A       OD1_615     2.5     7.0
@>      GLN41    A       NE2_646  <--->      LYS27    A         O_419     2.7     3.7
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE1_547     2.7    11.1
@> Number of detected hydrogen bonds: 4.
..
..
@> Model: 111
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      ARG54    A       NH2_856  <--->      GLU51    A       OE1_819     2.5    28.6
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.6    17.0
@>      LEU69    A        N_1095  <--->       LYS6    A          O_94     2.6    24.5
@>      LYS27    A        NZ_424  <--->      ASP52    A       OD1_833     2.6    10.8
@>      SER65    A       OG_1039  <--->      GLN62    A         O_983     2.6    24.6
@>      ARG74    A       NE_1199  <--->      GLY76    A        O_1226     2.7     8.4
@>       ILE3    A          N_36  <--->      LEU15    A         O_239     2.7    24.6
```

```
@>      GLN62    A       NE2_988  <--->      SER57    A        OG_908     2.7    11.5
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     2.7    17.3
@> Number of detected hydrogen bonds: 9.
@> Model: 112
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.6    32.7
@>      LEU69    A        N_1095  <--->       LYS6    A          O_94     2.6    21.2
@>      LYS29    A        NZ_456  <--->      ASP21    A       OD2_333     2.7    10.0
@> Number of detected hydrogen bonds: 3.
@> Model: 113
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.5    23.5
@>      ARG54    A       NH1_855  <--->      ASP58    A       OD2_921     2.6    16.3
@>      GLU34    A         N_540  <--->      ILE30    A         O_473     2.7    13.4
@>      LYS33    A        NZ_526  <--->      THR14    A         O_225     2.7    21.4
@>      LYS27    A        NZ_424  <--->      GLU24    A       OE1_378     2.7     7.7
@>      LYS33    A        NZ_526  <--->      GLU16    A       OE1_262     2.7    16.4
@> Number of detected hydrogen bonds: 6.
@> Model: 114
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      LYS27    A        NZ_424  <--->      ASP52    A       OD2_834     2.5     8.2
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE2_548     2.5    29.1
@>      LYS29    A        NZ_456  <--->      ASP21    A       OD2_333     2.6     6.4
@>       MET1    A           N_0  <--->      GLU16    A       OE2_263     2.6    10.9
@>      LEU69    A        N_1095  <--->       LYS6    A          O_94     2.7    16.8
@>      THR55    A       OG1_875  <--->      ASP58    A       OD2_921     2.7     2.4
@>      ASN25    A       ND2_393  <--->      ASP21    A       OD2_333     2.7    31.6
@> Number of detected hydrogen bonds: 7.
```

Similarly, for other interactions type. Moreover, we can also select frames that we would like to analyze as well as the selection with the protein structure. Below you will find such examples:

```
In [10]: calcPiCationTrajectory(atoms, distA=7, start_frame=15, stop_frame=20)
```

```
@> Model: 15
@> Calculating cation-Pi interactions.
@>      HIS68   A        1083_1084_1085_1086_1087  <--->       LYS6   A                        NZ_
@>      TYR59   A         931_932_933_934_935_936  <--->      LYS48   A                       NZ_
@> Number of detected cation-pi interactions: 2.
@> Model: 16
@> Calculating cation-Pi interactions.
@>      TYR59   A         931_932_933_934_935_936  <--->      ARG54   A                   NH1_855_
@> Number of detected cation-pi interactions: 1.
@> Model: 17
@> Calculating cation-Pi interactions.
@>      TYR59   A         931_932_933_934_935_936  <--->      ARG54   A                   NH1_855_
@> Number of detected cation-pi interactions: 1.
@> Model: 18
@> Calculating cation-Pi interactions.
@>      HIS68   A        1083_1084_1085_1086_1087  <--->       LYS6   A                        NZ_
@> Number of detected cation-pi interactions: 1.
@> Model: 19
@> Calculating cation-Pi interactions.
@>      TYR59   A         931_932_933_934_935_936  <--->      ARG54   A                   NH1_855_
@> Number of detected cation-pi interactions: 1.
```

```
In [11]: calcHydrophobicTrajectory(atoms, start_frame=10, stop_frame=13,
   ....:                                   selection='resid 50 to 60')
   ....:
```

```
@> Model: 10
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      ILE61    A       CD1_96814s  <--->      LEU56    A       CD2_891     3.4    37.9
@>      TYR59    A        CG_93114s  <--->      LEU50    A       CD2_800     3.5    47.9
@>      VAL17    A       CG2_27614s  <--->      LEU56    A       CD1_890     3.5    19.4
@> Number of detected hydrophobic interactions: 3.
@> Model: 11
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      VAL17    A       CG2_27614s  <--->      LEU56    A       CD1_890     3.5    18.9
@>      ILE23    A       CD1_35914s  <--->      LEU50    A       CD1_799     3.8    30.1
@> Number of detected hydrophobic interactions: 2.
@> Model: 12
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      TYR59    A       CE2_93514s  <--->      ILE23    A       CD1_359     3.4    24.5
@>      ILE61    A       CD1_96814s  <--->      LEU56    A       CD2_891     3.4    39.2
@>      LEU50    A       CD2_80014s  <--->      TYR59    A       CE1_934     3.6    44.7
@>      VAL17    A       CG2_27614s  <--->      LEU56    A       CD1_890     3.8    11.6
@> Number of detected hydrophobic interactions: 4.
```

5.4 Compute all types of interactions at once

Next, we instantiate an `InteractionsTrajectory` instance, which stores all the information about interactions in protein structures for multiple frames. With `InteractionsTrajectory.calcProteinInteractionsTrajectory()`, we can compute all types of interactions such as hydrogen bonds, salt bridges, repulsive ionic bonding, Pi-cation, Pi-stacking, hydrophobic and disulfide bonds) at once. Be aware that those computations may take a while, depending on the size of the system and the number of frames that are stored by the Ensemble PDB file. Therefore, we recommend saving the results as an `output` file. The `output` file, `calcProteinInteractionsEnseblePDB.pkl` can be reloaded and used with all available functions and methods.

```
In [12]: interactionsTrajectoryNMR = InteractionsTrajectory('ensambleNMR')

In [13]: interactionsTrajectoryNMR.calcProteinInteractionsTrajectory(atoms,
   ....: filename='calcProteinInteractionsEnseblePDB.pkl')
   ....:
```

```
@> Model: 0
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      GLN49    A       NE2_784  <--->      GLU51    A       OE2_820     2.6    16.2
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE1_547     2.6     7.0
@>      GLY10    A         N_160  <--->       THR7    A         O_116     2.7    19.8
@>      ARG72    A        N_1149  <--->      GLN40    A         O_624     2.7    21.1
@>      ARG72    A      NH1_1158  <--->      GLN40    A       OE1_628     2.7     7.5
@>       LYS6    A          N_91  <--->      LEU67    A        O_1062     2.7     2.6
@>      GLU34    A         N_540  <--->      ILE30    A         O_473     2.8    28.2
@>      THR55    A         N_870  <--->      ASP58    A       OD2_921     2.8    19.7
@>      ILE44    A         N_698  <--->      HIS68    A        O_1081     2.9    20.2
@>      THR55    A       OG1_875  <--->      ASP58    A       OD2_921     2.9    13.2
@>      LYS29    A         N_448  <--->      ASN25    A         O_389     2.9    13.6
```

```
@>      LEU73    A        N_1173  <--->      LEU71    A        O_1133     2.9    27.8
@>      HIS68    A        N_1078  <--->      ILE44    A         O_701     2.9    21.8
@>      THR14    A       OG1_227  <--->       ILE3    A          O_39     2.9    13.1
@>      GLU51    A         N_812  <--->      TYR59    A        OH_937     3.0    23.4
@>      GLU64    A        N_1019  <--->       GLN2    A          O_22     3.0    23.2
@>      LEU50    A         N_793  <--->      LEU43    A         O_682     3.0    15.3
@>      GLN62    A         N_980  <--->      SER65    A       OG_1039     3.0    23.4
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     3.0    12.8
@>      SER65    A        N_1034  <--->      GLN62    A         O_983     3.0    18.3
@>      VAL17    A         N_270  <--->       MET1    A           O_3     3.0     8.8
@>      ASN60    A         N_947  <--->      SER57    A         O_906     3.1    28.5
@>      LYS33    A         N_518  <--->      LYS29    A         O_451     3.1    33.1
@>      VAL70    A        N_1114  <--->      ARG42    A         O_658     3.1    17.9
@>      ASP32    A         N_506  <--->      ALA28    A         O_441     3.1    10.6
@>      LEU67    A        N_1059  <--->       PHE4    A          O_58     3.1    32.7
@>       THR7    A         N_113  <--->      LYS11    A         O_170     3.1    10.9
@>      LEU15    A         N_236  <--->       ILE3    A          O_39     3.1    18.3
@>      GLU18    A         N_286  <--->      ASP21    A       OD2_333     3.1    29.0
@>      ILE61    A         N_961  <--->      LEU56    A         O_887     3.1    32.1
@>      GLN41    A       NE2_646  <--->      LYS27    A         O_419     3.1    30.7
@>       PHE4    A          N_55  <--->      SER65    A        O_1037     3.2    15.4
@>       ILE3    A          N_36  <--->      LEU15    A         O_239     3.2    33.3
@>      LYS48    A         N_754  <--->      PHE45    A         O_720     3.2    18.9
@>      ARG42    A         N_655  <--->      VAL70    A        O_1117     3.2    24.8
@>      SER57    A         N_903  <--->      PRO19    A         O_304     3.3    29.1
@>      PHE45    A         N_717  <--->      LYS48    A         O_757     3.3    15.6
@>       GLN2    A        NE2_27  <--->      THR14    A       OG1_227     3.3    19.4
@>      GLN41    A         N_638  <--->      PRO38    A         O_598     3.4    33.7
@>      THR66    A      OG1_1050  <--->      GLU64    A        O_1022     3.4    28.3
@>      LEU56    A         N_884  <--->      ASP21    A         O_329     3.4    23.8
@>      ALA28    A         N_438  <--->      GLU24    A         O_374     3.5    18.5
@>      GLN41    A       NE2_646  <--->      PRO37    A         O_584     3.5    26.0
@> Number of detected hydrogen bonds: 43.
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.7
@>      ASP32    A     OD1_512_513  <--->      LYS33    A          NZ_526     3.6
@>      ASP21    A     OD1_332_333  <--->      LYS29    A          NZ_456     4.5
@> Number of detected salt bridges: 3.
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      PHE45    A    CD1_72314s  <--->      LEU67    A   CD1_1065     3.6    25.2
@>      VAL17    A    CG2_27614s  <--->       ILE3    A     CG1_41     3.6    17.8
@>      ILE23    A    CD1_35914s  <--->      LEU56    A    CD2_891     3.6    22.8
@>      LEU43    A    CD1_68514s  <--->      ILE23    A    CG2_358     3.7    10.1
@>      LYS27    A     CG_42114s  <--->      LEU43    A    CD1_685     3.7    13.4
@>      ILE61    A    CD1_96814s  <--->      LEU56    A    CD2_891     3.8    40.6
@>      TYR59    A    CD2_93314s  <--->      ILE23    A    CD1_359     3.8    24.0
@>      LEU69    A   CD1_110114s  <--->      ILE30    A    CD1_477     3.8    10.5
@>       MET1    A       CE_714s  <--->       ILE3    A     CG2_42     3.8    28.7
@>       VAL5    A     CG1_8014s  <--->      LEU69    A   CD1_1101     3.9    14.6
@>      ILE13    A    CG2_20914s  <--->      LEU15    A    CD1_242     3.9    19.8
@>      ARG42    A     CG_66014s  <--->      VAL70    A   CG2_1120     4.0    42.9
```

```
@>      ILE44    A    CD1_70514s  <--->      VAL70    A   CG1_1119     4.0    17.7
@>      ALA46    A     CB_74114s  <--->      PHE45    A    CD2_724     4.1    50.7
@>      LYS11    A     CG_17214s  <--->      ILE13    A    CG1_208     4.1    30.5
@>       LEU8    A    CD1_13314s  <--->      VAL70    A   CG1_1119     4.5     8.8
@> Number of detected hydrophobic interactions: 16.
@> Lack of cysteines in the structure.
@> Number of detected disulfide bonds: 0.
@> Model: 1
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.5    28.9
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE1_547     2.5     7.3
@>      LYS33    A        NZ_526  <--->      GLU16    A       OE2_263     2.6    12.7
@>      SER65    A       OG_1039  <--->      GLN62    A         O_983     2.6    15.7
@>      LYS27    A        NZ_424  <--->      ASP52    A       OD2_834     2.6    29.5
@>      GLN62    A       NE2_988  <--->      ASN60    A       OD1_953     2.6    18.2
@>      ARG74    A      NH2_1202  <--->      GLY76    A      OXT_1227     2.6    19.4
@>      SER57    A        OG_908  <--->      THR55    A       OG1_875     2.6    24.1
@>      ARG74    A       NE_1199  <--->      GLY76    A        O_1226     2.7    22.0
@>      LYS29    A         N_448  <--->      ASN25    A         O_389     2.7    16.0
@>      LYS29    A        NZ_456  <--->      GLU16    A       OE1_262     2.7    23.7
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     2.7    14.9
@>      GLY35    A         N_555  <--->      GLN31    A         O_492     2.7    32.0
@>      THR55    A       OG1_875  <--->      ASP58    A       OD2_921     2.7    19.9
@>      LEU69    A        N_1095  <--->       LYS6    A          O_94     2.7    26.5
@>      GLU51    A         N_812  <--->      TYR59    A        OH_937     2.7    21.7
@>      GLU64    A        N_1019  <--->       GLN2    A          O_22     2.7     5.2
@>      VAL70    A        N_1114  <--->      ARG42    A         O_658     2.7    22.0
@>      THR55    A         N_870  <--->      ASP58    A       OD2_921     2.7    18.5
@>       THR7    A       OG1_118  <--->      LYS11    A         O_170     2.7    23.8
@>      ARG42    A         N_655  <--->      VAL70    A        O_1117     2.7    32.6
@>      GLU34    A         N_540  <--->      ILE30    A         O_473     2.8    22.0
@>      LEU15    A         N_236  <--->       ILE3    A          O_39     2.8    13.0
@>      LEU67    A        N_1059  <--->       PHE4    A          O_58     2.8     9.7
@>      LYS33    A        NZ_526  <--->      THR14    A         O_225     2.9    37.2
@>       VAL5    A          N_75  <--->      ILE13    A         O_206     2.9    17.0
@>       LYS6    A          N_91  <--->      LEU67    A        O_1062     2.9    14.9
@>      VAL17    A         N_270  <--->       MET1    A           O_3     2.9     9.5
@>      GLN41    A       NE2_646  <--->      ILE36    A         O_565     2.9    31.4
@>      GLN41    A       NE2_646  <--->      LYS27    A         O_419     2.9    10.1
@>      SER57    A         N_903  <--->      PRO19    A         O_304     2.9    33.8
@>      ALA28    A         N_438  <--->      GLU24    A         O_374     2.9    26.2
@>       THR7    A         N_113  <--->      LYS11    A         O_170     2.9    35.2
@>      ILE61    A         N_961  <--->      LEU56    A         O_887     3.0    18.2
@>       PHE4    A          N_55  <--->      SER65    A        O_1037     3.0     6.5
@>      ARG72    A      NH2_1159  <--->      ASP39    A       OD2_616     3.0    25.5
@>      GLU18    A         N_286  <--->      ASP21    A       OD2_333     3.0     1.5
@>      HIS68    A        N_1078  <--->      ILE44    A         O_701     3.0    27.8
@>      ILE30    A         N_470  <--->      VAL26    A         O_403     3.0    32.5
@>      ILE44    A         N_698  <--->      HIS68    A        O_1081     3.0    19.2
@>      ASN25    A         N_386  <--->      THR22    A       OG1_343     3.1    38.5
@>      ASP21    A         N_326  <--->      GLU18    A         O_289     3.1    21.6
@>      ARG72    A        N_1149  <--->      GLN40    A         O_624     3.1    13.3
@>      GLN40    A         N_621  <--->      PRO37    A         O_584     3.1    21.1
@>      LYS27    A         N_416  <--->      ILE23    A         O_355     3.1    36.2
@>      LYS33    A         N_518  <--->      LYS29    A         O_451     3.2    22.9
@>      TYR59    A         N_926  <--->      THR55    A         O_873     3.3    20.9
@>      ARG54    A         N_846  <--->      GLU51    A         O_815     3.3    24.1
```

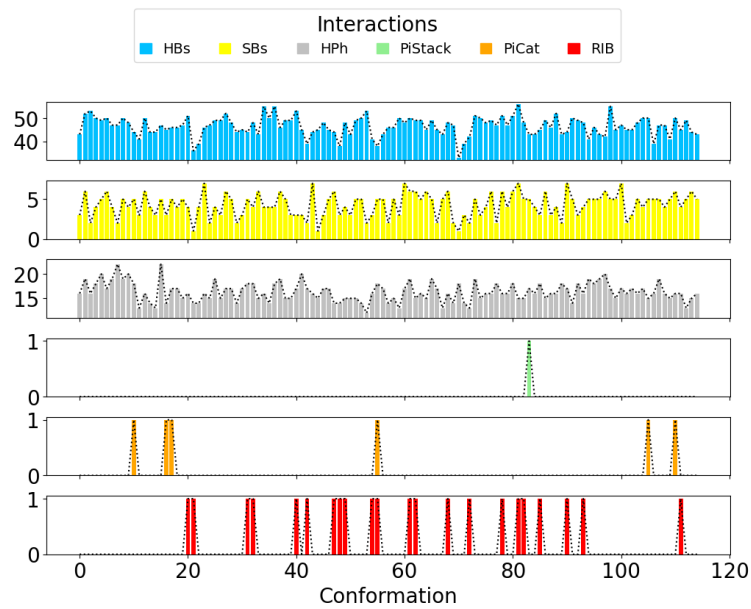
```
@>      VAL26    A         N_400  <--->      THR22    A         O_341     3.4    23.5
@>      GLN41    A         N_638  <--->      PRO38    A         O_598     3.4    34.4
@>      ILE23    A         N_352  <--->      ARG54    A         O_849     3.5    23.1
@>      ASN60    A         N_947  <--->      SER57    A         O_906     3.5    25.0
@> Number of detected hydrogen bonds: 52.
@> Calculating salt bridges.
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     2.5
@>      LYS33    A          NZ_526  <--->      GLU16    A     OE1_262_263     2.8
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.9
@>      LYS29    A          NZ_456  <--->      GLU16    A     OE1_262_263     3.3
@>      LYS63    A         NZ_1005  <--->      GLU64    A   OE1_1026_1027     3.7
@>      ASP39    A     OD1_615_616  <--->      ARG72    A   NH1_1158_1159     4.6
@> Number of detected salt bridges: 6.
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      LYS29    A     CD_45414s  <--->      LEU15    A    CD1_242     3.5    18.8
@>       MET1    A       CE_714s  <--->      LEU56    A    CD2_891     3.5    12.0
@>      LEU43    A    CD1_68514s  <--->      LYS27    A     CG_421     3.5    17.3
@>      LEU67    A   CD1_106514s  <--->       ILE3    A     CD1_43     3.5    16.4
@>      VAL17    A    CG2_27614s  <--->      LEU56    A    CD2_891     3.6    12.5
@>      TYR59    A    CE2_93514s  <--->      ILE23    A    CD1_359     3.6    17.3
@>       VAL5    A     CG2_8114s  <--->      LEU15    A    CD2_243     3.7    24.5
@>      ILE30    A    CD1_47714s  <--->      LEU43    A    CD2_686     3.7    13.8
@>      PHE45    A    CD1_72314s  <--->      LEU67    A   CD2_1066     3.7    13.2
@>      LEU50    A    CD2_80014s  <--->      TYR59    A    CE1_934     3.7    41.8
@>      ILE13    A    CG2_20914s  <--->      LEU15    A    CD2_243     3.7    21.7
@>      LEU73    A   CD2_118014s  <--->      ILE36    A    CG2_568     3.8    26.2
@>      LEU69    A   CD2_110214s  <--->      ILE36    A    CD1_569     3.9     7.9
@>      LYS11    A     CD_17314s  <--->      ILE13    A    CD1_210     3.9    29.1
@>      LYS33    A     CD_52414s  <--->      ILE13    A    CG2_209     3.9    11.1
@>      ARG42    A     CG_66014s  <--->      ILE44    A    CG2_704     4.0    15.7
@>      VAL26    A    CG1_40514s  <--->      LEU15    A     CG_241     4.1    15.5
@>      VAL70    A   CG2_112014s  <--->       LEU8    A    CD1_133     4.3    14.7
@>      ARG74    A    CG_119714s  <--->      LEU71    A   CD1_1136     4.5    17.2
@> Number of detected hydrophobic interactions: 19.
@> Lack of cysteines in the structure.
@> Number of detected disulfide bonds: 0.
@> Model: 2
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE2_548     2.5    27.6
@>       MET1    A           N_0  <--->      GLU16    A       OE2_263     2.6    11.9
@>       PHE4    A          N_55  <--->      SER65    A        O_1037     2.6    19.5
@>      GLN41    A       NE2_646  <--->      LYS27    A         O_419     2.6    39.4
@>      THR55    A       OG1_875  <--->      ASP58    A       OD2_921     2.6    26.1
@>      VAL17    A         N_270  <--->       MET1    A           O_3     2.7    14.9
@>      GLU18    A         N_286  <--->      ASP21    A       OD2_333     2.7     5.0
@>      GLU34    A         N_540  <--->      ILE30    A         O_473     2.7     7.6
@>      ILE44    A         N_698  <--->      HIS68    A        O_1081     2.7    13.8
@>      THR22    A         N_338  <--->      ASN25    A       OD1_392     2.7    20.3
@>      SER20    A        OG_320  <--->      GLU18    A       OE1_293     2.7    21.5
@>      GLU51    A         N_812  <--->      TYR59    A        OH_937     2.7    23.9
```

```
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.7    18.4
@>      GLN41    A       NE2_646  <--->      ILE36    A         O_565     2.8    31.7
@>       LYS6    A          N_91  <--->      LEU67    A        O_1062     2.8    14.6
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     2.8     7.4
@>      LYS11    A         N_167  <--->       THR7    A       OG1_118     2.8    30.1
@>      VAL70    A        N_1114  <--->      ARG42    A         O_658     2.8    28.1
@>      THR22    A       OG1_343  <--->      ASN25    A       OD1_392     2.8    16.5
@>      LEU56    A         N_884  <--->      ASP21    A         O_329     2.8    25.9
@>      HIS68    A        N_1078  <--->      ILE44    A         O_701     2.8     4.3
@>       THR7    A       OG1_118  <--->      LYS11    A         O_170     2.8    11.4
@>       VAL5    A          N_75  <--->      ILE13    A         O_206     2.8    37.9
@>      LYS63    A       NZ_1005  <--->       GLN2    A        OE1_26     2.8    13.5
@>      ARG54    A       NH1_855  <--->      ASP52    A         O_830     2.8     5.2
@>       THR7    A         N_113  <--->      LYS11    A         O_170     2.9    19.8
@>      ALA28    A         N_438  <--->      GLU24    A         O_374     2.9    26.5
@>      GLU64    A        N_1019  <--->       GLN2    A          O_22     2.9     6.5
@>      ILE61    A         N_961  <--->      LEU56    A         O_887     2.9     3.4
@>      LEU69    A        N_1095  <--->       LYS6    A          O_94     2.9    12.0
@>      GLN31    A         N_489  <--->      LYS27    A         O_419     2.9    26.1
@>      GLN40    A       NE2_629  <--->      GLY76    A        O_1226     2.9     3.8
@>      ASN25    A         N_386  <--->      THR22    A         O_341     2.9    29.4
@>      LEU67    A        N_1059  <--->       PHE4    A          O_58     3.0    23.6
@>       LYS6    A         NZ_99  <--->      THR12    A       OG1_194     3.0    11.7
@>      ILE30    A         N_470  <--->      VAL26    A         O_403     3.0    29.3
@>      ARG42    A         N_655  <--->      VAL70    A        O_1117     3.1     6.2
@>      ARG72    A      NH2_1159  <--->      ASP39    A         O_612     3.1    16.4
@>      GLN40    A       NE2_629  <--->      ARG72    A        O_1152     3.1    26.5
@>      SER57    A         N_903  <--->      PRO19    A         O_304     3.1     6.5
@>      ASP21    A         N_326  <--->      GLU18    A         O_289     3.1    31.9
@>      SER65    A        N_1034  <--->      GLN62    A         O_983     3.1    21.5
@>      ARG72    A        N_1149  <--->      GLN40    A         O_624     3.1    38.2
@>       ILE3    A          N_36  <--->      LEU15    A         O_239     3.1    17.0
@>      ASP32    A         N_506  <--->      ALA28    A         O_441     3.1    19.2
@>      GLN62    A         N_980  <--->      SER65    A       OG_1039     3.2    26.8
@>      GLN40    A         N_621  <--->      PRO37    A         O_584     3.2    36.5
@>      TYR59    A         N_926  <--->      THR55    A         O_873     3.2     9.2
@>      LYS48    A         N_754  <--->      PHE45    A         O_720     3.2    25.0
@>      PHE45    A         N_717  <--->      LYS48    A         O_757     3.3     3.9
@>      LYS29    A         N_448  <--->      ASN25    A         O_389     3.3    33.9
@>      LEU15    A         N_236  <--->       ILE3    A          O_39     3.3    36.1
@>      LYS27    A         N_416  <--->      ILE23    A         O_355     3.4     7.1
@> Number of detected hydrogen bonds: 53.
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     3.1
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     4.8
@> Number of detected salt bridges: 2.
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      ILE30    A    CG2_47614s  <--->      LEU69    A   CD2_1102     3.4    20.7
@>      ILE61    A    CG1_96614s  <--->      PHE45    A    CE1_725     3.5    28.7
@>      VAL17    A    CG1_27514s  <--->       ILE3    A     CD1_43     3.6    23.2
@>      LEU56    A    CD1_89014s  <--->      VAL17    A    CG2_276     3.6    20.2
```

```
@>      LEU71    A   CD2_113714s  <--->      ILE36    A    CG2_568     3.7    21.0
@>       MET1    A       CE_714s  <--->      VAL17    A    CG2_276     3.7    46.7
@>      TYR59    A    CE1_93414s  <--->      LEU50    A    CD2_800     3.7    43.5
@>      ILE23    A    CD1_35914s  <--->      TYR59    A    CD2_933     3.8    15.1
@>      LYS33    A     CD_52414s  <--->      ILE13    A    CG2_209     3.9    15.8
@>      LEU15    A    CD1_24214s  <--->       VAL5    A     CG2_81     3.9     8.0
@>      VAL70    A   CG1_111914s  <--->       LEU8    A    CD2_134     3.9    11.7
@>      VAL26    A    CG1_40514s  <--->      LEU43    A    CD2_686     4.0    10.8
@>      ARG42    A     CG_66014s  <--->      ILE44    A    CD1_705     4.1    21.0
@>      ALA46    A     CB_74114s  <--->      PHE45    A    CD2_724     4.1    46.2
@>      LYS27    A     CG_42114s  <--->      LEU43    A    CD2_686     4.1    13.4
@>      LYS29    A     CD_45414s  <--->      LEU15    A    CD2_243     4.4    11.2
@> Number of detected hydrophobic interactions: 16.
@> Lack of cysteines in the structure.
@> Number of detected disulfide bonds: 0.
..
..
```

The results can be displayed using `getTimeInteractions()`, where all the interactions are displayed and can be tracked per each conformation (frame in the Ensemble PDB file).

```
In [14]: number_of_counts = interactionsTrajectoryNMR.getTimeInteractions()
```



Each interaction type could be further counted with some additional quantitative analysis using `calcStatisticsInteractions()`:

```
In [15]: statistics = calcStatisticsInteractions(interactionsTrajectoryNMR.getHydrogenBonds())
```

```
@> Statistics for LYS11A-GLU34A:
@>   Average [Ang.]: 2.720873
@>   Standard deviation [Ang.]: 0.179343
@>   Weight: 0.8
@> Statistics for GLY10A-THR7A:
@>   Average [Ang.]: 3.037245
@>   Standard deviation [Ang.]: 0.1988
@>   Weight: 0.669565
```

```
@> Statistics for ARG72A-GLN40A:
@>   Average [Ang.]: 2.874946
@>   Standard deviation [Ang.]: 0.18885
@>   Weight: 0.782609
@> Statistics for LYS6A-LEU67A:
@>   Average [Ang.]: 2.920333
@>   Standard deviation [Ang.]: 0.157525
@>   Weight: 0.947826
@> Statistics for GLU34A-ILE30A:
@>   Average [Ang.]: 2.896524
@>   Standard deviation [Ang.]: 0.171493
@>   Weight: 0.878261
@> Statistics for THR55A-ASP58A:
@>   Average [Ang.]: 2.777835
@>   Standard deviation [Ang.]: 0.158068
@>   Weight: 1.504348
@> Statistics for ILE44A-HIS68A:
@>   Average [Ang.]: 2.941125
@>   Standard deviation [Ang.]: 0.177848
@>   Weight: 0.834783
@> Statistics for LYS29A-ASN25A:
@>   Average [Ang.]: 3.050209
@>   Standard deviation [Ang.]: 0.211243
@>   Weight: 0.582609
@> Statistics for HIS68A-ILE44A:
@>   Average [Ang.]: 2.951679
@>   Standard deviation [Ang.]: 0.195428
@>   Weight: 0.826087
@> Statistics for GLU51A-TYR59A:
@>   Average [Ang.]: 2.967038
@>   Standard deviation [Ang.]: 0.18416
@>   Weight: 0.834783
@> Statistics for GLU64A-GLN2A:
@>   Average [Ang.]: 2.860456
@>   Standard deviation [Ang.]: 0.142289
@>   Weight: 0.895652
@> Statistics for LEU50A-LEU43A:
@>   Average [Ang.]: 3.028411
@>   Standard deviation [Ang.]: 0.19173
@>   Weight: 0.773913
@> Statistics for ILE13A-VAL5A:
@>   Average [Ang.]: 2.900624
@>   Standard deviation [Ang.]: 0.149592
@>   Weight: 0.930435
@> Statistics for SER65A-GLN62A:
@>   Average [Ang.]: 2.989405
@>   Standard deviation [Ang.]: 0.276179
@>   Weight: 0.678261
@> Statistics for VAL17A-MET1A:
@>   Average [Ang.]: 2.917662
@>   Standard deviation [Ang.]: 0.146237
@>   Weight: 0.93913
@> Statistics for ASN60A-SER57A:
@>   Average [Ang.]: 3.176033
@>   Standard deviation [Ang.]: 0.176174
@>   Weight: 0.626087
@> Statistics for LYS33A-LYS29A:
@>   Average [Ang.]: 3.124632
```

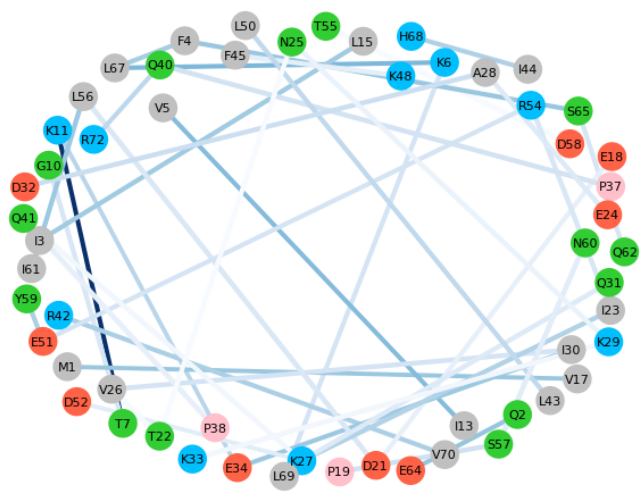
```
@>   Standard deviation [Ang.]: 0.203019
@>   Weight: 0.547826
@> Statistics for VAL70A-ARG42A:
@>   Average [Ang.]: 2.990983
@>   Standard deviation [Ang.]: 0.202089
@>   Weight: 0.921739
@> Statistics for ASP32A-ALA28A:
@>   Average [Ang.]: 3.06256
@>   Standard deviation [Ang.]: 0.189158
@>   Weight: 0.730435
@> Statistics for LEU67A-PHE4A:
@>   Average [Ang.]: 2.967632
@>   Standard deviation [Ang.]: 0.178013
@>   Weight: 0.852174
@> Statistics for THR7A-LYS11A:
@>   Average [Ang.]: 2.907541
@>   Standard deviation [Ang.]: 0.188693
@>   Weight: 1.46087
@> Statistics for LEU15A-ILE3A:
@>   Average [Ang.]: 3.006021
@>   Standard deviation [Ang.]: 0.198347
@>   Weight: 0.913043
@> Statistics for GLU18A-ASP21A:
@>   Average [Ang.]: 2.909238
@>   Standard deviation [Ang.]: 0.185235
@>   Weight: 0.6
@> Statistics for ILE61A-LEU56A:
@>   Average [Ang.]: 3.054711
@>   Standard deviation [Ang.]: 0.198213
@>   Weight: 0.878261
@> Statistics for GLN41A-LYS27A:
@>   Average [Ang.]: 2.989313
@>   Standard deviation [Ang.]: 0.183486
@>   Weight: 0.547826
@> Statistics for PHE4A-SER65A:
@>   Average [Ang.]: 2.992881
@>   Standard deviation [Ang.]: 0.18513
@>   Weight: 0.886957
@> Statistics for ILE3A-LEU15A:
@>   Average [Ang.]: 3.023158
@>   Standard deviation [Ang.]: 0.185656
@>   Weight: 0.869565
@> Statistics for LYS48A-PHE45A:
@>   Average [Ang.]: 3.081561
@>   Standard deviation [Ang.]: 0.189569
@>   Weight: 0.608696
@> Statistics for ARG42A-VAL70A:
@>   Average [Ang.]: 2.971445
@>   Standard deviation [Ang.]: 0.212987
@>   Weight: 0.834783
@> Statistics for SER57A-PRO19A:
@>   Average [Ang.]: 3.036466
@>   Standard deviation [Ang.]: 0.200139
@>   Weight: 0.713043
@> Statistics for PHE45A-LYS48A:
@>   Average [Ang.]: 3.03853
@>   Standard deviation [Ang.]: 0.184267
@>   Weight: 0.86087
```

```
..
..
```

To provide a better way for visualization of those results, another function, `showInteractionsGraph()`, could be used, which provides a graph with residue-residue pairs of interactions. The intensity of the color of the lines connecting two residues corresponds to the number of counts. Darker lines are assigned to the most frequent appearance of interaction. The distance between pairs corresponds to the average distance across all the frames. Moreover, ovals with residue names are color-coded: acidic residues: *red*, basic: *blue*, polar: *green*, non-polar: *silver*, and proline: *pink*.

Below is an example with additional parameters: `1-letter` code of residues, which can be used instead of 3-letter code, `cutoff` = 0.5 for the number of counts for residue interaction, `font_size` for the residue names displayed on the graph, and `seed`, which is a random number that can help to organize the graph in a nicer way.

```
In [16]: showInteractionsGraph(statistics, code='1-letter', cutoff=0.5,
    ....:                                                font_size=8, seed=42)
    ....:
```



We can also obtain a distribution of distance or angle for each residue by using `calcDistribution()`:

```
In [17]: statistics_2 = interactionsTrajectoryNMR.getHydrogenBonds()

In [18]: calcDistribution(statistics_2, 'THR55','ASP58')
```

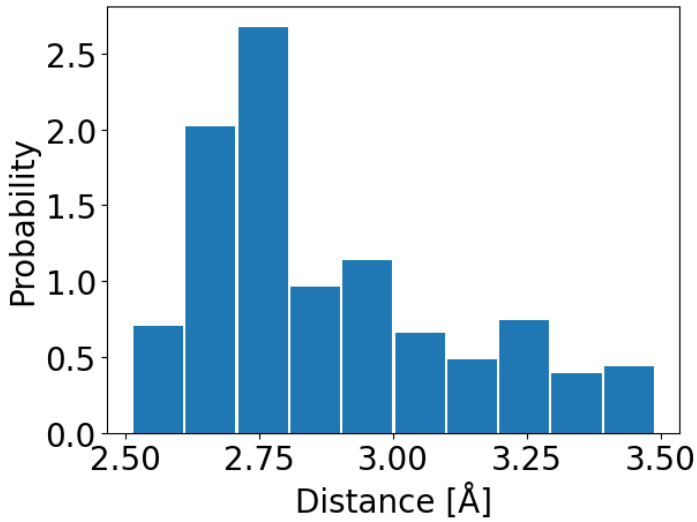
```
@> Additional contacts for THR55:
@> TYR59
@> SER57
```

We will obtain a histogram with distances for *LYS11* residue and information about other contact residues for this particular residue.

We can also give residue name and number and `calcDistribution()` will display contact residues for which we can display a histogram.

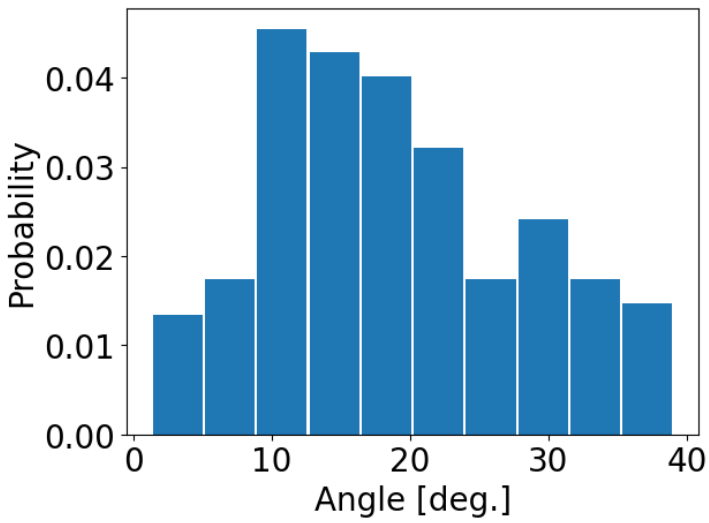
```
In [19]: calcDistribution(statistics_2, 'LYS11')
```

```
@> Possible contacts for LYS11:
@> GLY76
@> THR7
```




```
@> GLU34
@> LEU73
```

```
In [20]: calcDistribution(statistics_2, 'LYS11', 'THR7', metrics='angle')
```

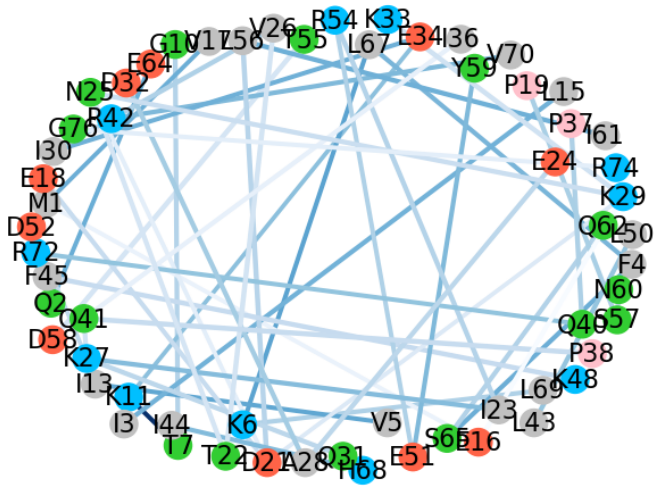



```
@> Additional contacts for LYS11:
@> GLY76
@> GLU34
@> LEU73
```

5.5 Selection of protein regions and conformations

Selection of the residue pairs can be made as needed by choosing pairs with a higher number of counts or by changing the selection to a certain region:

```
In [21]: showInteractionsGraph(statistics, code='1-letter', cutoff=50, font_size=16,
    ....: node_distance=3, seed=1)
    ....:
```

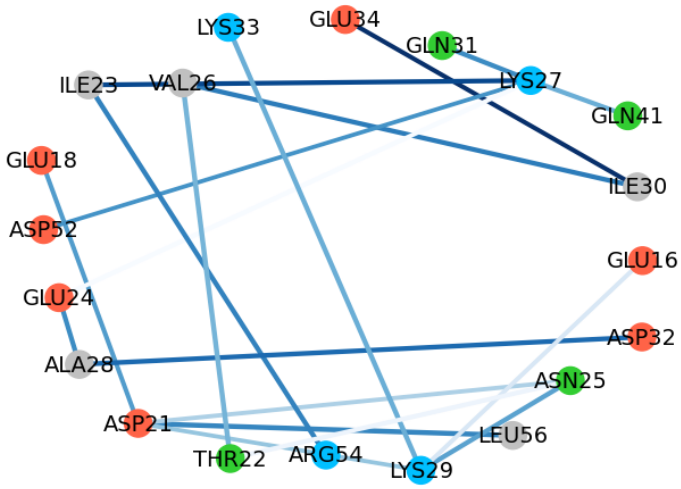



```
In [22]: hbs_20to30 = interactionsTrajectoryNMR.getHydrogenBonds(selection='resid 20 to 30')

In [23]: statistics2 = calcStatisticsInteractions(hbs_20to30)

In [24]: showInteractionsGraph(statistics2)
```

```
@> Statistics for GLU34A-ILE30A:
@>   Average [Ang.]: 2.896524
@>   Standard deviation [Ang.]: 0.171493
@>   Weight: 0.878261
@> Statistics for LYS29A-ASN25A:
@>   Average [Ang.]: 3.050209
@>   Standard deviation [Ang.]: 0.211243
@>   Weight: 0.582609
@> Statistics for LYS33A-LYS29A:
@>   Average [Ang.]: 3.124632
@>   Standard deviation [Ang.]: 0.203019
@>   Weight: 0.547826
@> Statistics for ASP32A-ALA28A:
@>   Average [Ang.]: 3.06256
@>   Standard deviation [Ang.]: 0.189158
@>   Weight: 0.730435
@> Statistics for GLU18A-ASP21A:
@>   Average [Ang.]: 2.909238
@>   Standard deviation [Ang.]: 0.185235
@>   Weight: 0.6
@> Statistics for GLN41A-LYS27A:
@>   Average [Ang.]: 2.989313
@>   Standard deviation [Ang.]: 0.183486
@>   Weight: 0.547826
@> Statistics for LEU56A-ASP21A:
@>   Average [Ang.]: 3.200349
@>   Standard deviation [Ang.]: 0.171184
@>   Weight: 0.66087
@> Statistics for ALA28A-GLU24A:
@>   Average [Ang.]: 3.044323
@>   Standard deviation [Ang.]: 0.201314
```

```
@>   Weight: 0.643478
@> Statistics for LYS27A-ASP52A:
@>   Average [Ang.]: 2.683467
@>   Standard deviation [Ang.]: 0.112508
@>   Weight: 0.626087
@> Statistics for LYS29A-GLU16A:
@>   Average [Ang.]: 2.768368
@>   Standard deviation [Ang.]: 0.147545
@>   Weight: 0.321739
@> Statistics for ILE30A-VAL26A:
@>   Average [Ang.]: 3.0535
@>   Standard deviation [Ang.]: 0.185896
@>   Weight: 0.686957
@> Statistics for ASN25A-THR22A:
@>   Average [Ang.]: 3.052567
@>   Standard deviation [Ang.]: 0.229106
@>   Weight: 0.521739
@> Statistics for ASP21A-GLU18A:
@>   Average [Ang.]: 3.115035
@>   Standard deviation [Ang.]: 0.196551
@>   Weight: 0.86087
@> Statistics for LYS27A-ILE23A:
@>   Average [Ang.]: 3.030938
@>   Standard deviation [Ang.]: 0.201816
@>   Weight: 0.817391
@> Statistics for VAL26A-THR22A:
@>   Average [Ang.]: 3.169813
@>   Standard deviation [Ang.]: 0.174811
@>   Weight: 0.530435
@> Statistics for ILE23A-ARG54A:
@>   Average [Ang.]: 3.098573
@>   Standard deviation [Ang.]: 0.202762
@>   Weight: 0.669565
@> Statistics for THR22A-ASN25A:
@>   Average [Ang.]: 2.897331
@>   Standard deviation [Ang.]: 0.186672
@>   Weight: 0.252174
@> Statistics for GLN31A-LYS27A:
@>   Average [Ang.]: 3.034919
@>   Standard deviation [Ang.]: 0.190252
@>   Weight: 0.643478
@> Statistics for LYS29A-ASP21A:
@>   Average [Ang.]: 2.658942
@>   Standard deviation [Ang.]: 0.149072
@>   Weight: 0.478261
@> Statistics for ASN25A-ASP21A:
@>   Average [Ang.]: 2.746326
@>   Standard deviation [Ang.]: 0.174366
@>   Weight: 0.434783
@> Statistics for LYS27A-GLU24A:
@>   Average [Ang.]: 2.817776
@>   Standard deviation [Ang.]: 0.244667
@>   Weight: 0.217391
```

The selection can be made at different stages of analysis. The example below shows how to analyze only certain frames (from 5th to 10th frame) for residues numbers between 10 and 30.




```
In [25]: interactionsTrajectoryNMR.calcProteinInteractionsTrajectory(atoms,
   ....:                 start_frame=5, stop_frame=10, selection='resid 10 to 30')
   ....:
```

```
@> Model: 5
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)    <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      LYS27    A        NZ_424  <--->      ASP52    A       OD2_834     2.6    19.9
@>      LYS33    A        NZ_526  <--->      GLU16    A       OE1_262     2.6     9.0
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE1_547     2.6    18.4
@>      LYS27    A        NZ_424  <--->      PRO38    A         O_598     2.7    19.3
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.7    29.3
@>       VAL5    A          N_75  <--->      ILE13    A         O_206     2.7    10.6
@>      LEU15    A         N_236  <--->       ILE3    A          O_39     2.8     9.8
@>      ILE23    A         N_352  <--->      ARG54    A         O_849     2.8    21.8
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     2.8     7.6
@>      GLU18    A         N_286  <--->      ASP21    A       OD2_333     2.8     8.8
@>      LYS33    A        NZ_526  <--->      THR14    A         O_225     2.9    18.2
@>      GLN31    A         N_489  <--->      LYS27    A         O_419     2.9    37.8
@>       ILE3    A          N_36  <--->      LEU15    A         O_239     2.9    14.8
@>      VAL17    A         N_270  <--->       MET1    A           O_3     3.0    15.3
@>      ILE30    A         N_470  <--->      VAL26    A         O_403     3.0    16.9
@>      THR22    A       OG1_343  <--->      ASN25    A       OD1_392     3.0    21.3
@>       THR7    A       OG1_118  <--->      LYS11    A         O_170     3.0    22.2
@>      VAL26    A         N_400  <--->      THR22    A         O_341     3.0    37.8
@>      GLU34    A         N_540  <--->      ILE30    A         O_473     3.1    21.2
@>      GLN41    A       NE2_646  <--->      LYS27    A         O_419     3.1    22.1
@>      GLN31    A       NE2_497  <--->      ALA28    A         O_441     3.2     5.3
@>      LYS33    A         N_518  <--->      LYS29    A         O_451     3.2    31.7
@>      ASP21    A         N_326  <--->      GLU18    A         O_289     3.3    23.7
@>      GLU24    A         N_371  <--->      THR22    A       OG1_343     3.4    19.1
@>      GLY10    A         N_160  <--->       THR7    A         O_116     3.4    17.1
@>      THR22    A         N_338  <--->      ASN25    A       OD1_392     3.5    28.4
@> Number of detected hydrogen bonds: 26.
@> Calculating salt bridges.
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     2.5
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.5
```

```
@>      LYS33    A          NZ_526  <--->      GLU16    A     OE1_262_263     2.7
@>      ASP21    A     OD1_332_333  <--->      LYS29    A          NZ_456     3.1
@> Number of detected salt bridges: 4.
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      VAL26    A    CG1_40514s  <--->      ILE30    A    CD1_477     3.6    25.5
@>      VAL17    A    CG2_27614s  <--->      LEU56    A    CD1_890     3.8    18.6
@>      LEU15    A    CD2_24314s  <--->      ILE30    A    CG1_475     3.8    13.1
@>       ILE3    A     CG1_4114s  <--->      VAL17    A    CG2_276     3.8    15.6
@>       VAL5    A     CG2_8114s  <--->      LEU15    A    CD2_243     3.8    20.4
@>      LYS33    A     CD_52414s  <--->      ILE13    A    CG2_209     3.9    14.6
@>      LYS11    A     CG_17214s  <--->      ILE13    A    CD1_210     4.1    25.6
@>      ILE23    A    CD1_35914s  <--->      LEU56    A    CD2_891     4.2    18.8
@>      LYS27    A     CG_42114s  <--->      LEU43    A    CD1_685     4.2    10.1
@> Number of detected hydrophobic interactions: 9.
@> Lack of cysteines in the structure.
@> Number of detected disulfide bonds: 0.
@> Model: 6
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE2_548     2.6    10.2
@>      LYS27    A        NZ_424  <--->      ASP52    A       OD2_834     2.6    31.7
@>      LYS29    A        NZ_456  <--->      ASP21    A       OD2_333     2.6    21.1
@>      ASN25    A       ND2_393  <--->      ASP21    A       OD2_333     2.7    10.1
@>      LYS29    A        NZ_456  <--->      GLU16    A         O_258     2.8    17.1
@>       THR7    A         N_113  <--->      LYS11    A         O_170     2.8     7.6
@>      GLU24    A         N_371  <--->      ASP52    A         O_830     2.8    16.2
@>      LYS27    A         N_416  <--->      ILE23    A         O_355     2.8     9.6
@>      GLN31    A         N_489  <--->      LYS27    A         O_419     2.8    28.6
@>      LEU15    A         N_236  <--->       ILE3    A          O_39     2.9    28.1
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.9    11.6
@>      ASP21    A         N_326  <--->      GLU18    A         O_289     2.9    34.6
@>      SER57    A         N_903  <--->      PRO19    A         O_304     2.9    22.4
@>      LYS11    A         N_167  <--->       THR7    A       OG1_118     2.9    30.6
@>      GLU18    A         N_286  <--->      ASP21    A       OD1_332     2.9    34.3
@>      VAL17    A         N_270  <--->       MET1    A           O_3     3.0    13.5
@>      GLN41    A       NE2_646  <--->      LYS27    A         O_419     3.0    22.3
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     3.1    28.8
@>      ILE30    A         N_470  <--->      VAL26    A         O_403     3.1    14.2
@>      ASP32    A         N_506  <--->      ALA28    A         O_441     3.1    20.3
@>      VAL26    A         N_400  <--->      THR22    A         O_341     3.1    34.4
@>       ILE3    A          N_36  <--->      LEU15    A         O_239     3.2    13.9
@>      LYS29    A         N_448  <--->      ASN25    A         O_389     3.2    36.0
@>      GLU34    A         N_540  <--->      ILE30    A         O_473     3.2    11.1
@>       VAL5    A          N_75  <--->      ILE13    A         O_206     3.2    10.5
@>      GLY10    A         N_160  <--->       THR7    A         O_116     3.2    29.6
@>      ILE23    A         N_352  <--->      ARG54    A         O_849     3.3     9.1
@>      ALA28    A         N_438  <--->      GLU24    A         O_374     3.4    35.6
@> Number of detected hydrogen bonds: 28.
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.6
@>      ASP21    A     OD1_332_333  <--->      LYS29    A          NZ_456     3.0
```

```
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     3.4
@> Number of detected salt bridges: 3.
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      VAL17    A    CG2_27614s  <--->       ILE3    A     CG2_42     3.4    21.2
@>      ILE13    A    CG2_20914s  <--->      LEU15    A    CD1_242     3.5    32.6
@>      LYS11    A     CD_17314s  <--->      ILE13    A    CD1_210     3.6    32.3
@>      LEU43    A    CD2_68614s  <--->      LYS27    A     CG_421     3.6    13.1
@>      LYS33    A     CD_52414s  <--->      LEU15    A    CD1_242     3.6    20.8
@>      LEU56    A    CD1_89014s  <--->      VAL17    A    CG2_276     3.8    11.7
@>      ILE30    A    CG1_47514s  <--->      LEU15    A    CD2_243     3.9    11.2
@>      ILE23    A    CG2_35814s  <--->      LEU43    A    CD2_686     3.9    15.4
@>      LYS29    A     CD_45414s  <--->      LEU15    A    CD2_243     4.5    14.6
@> Number of detected hydrophobic interactions: 9.

@> Lack of cysteines in the structure.
@> Number of detected disulfide bonds: 0.
@> Model: 7
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>       GLN2    A        NE2_27  <--->      GLU16    A       OE2_263     2.6    14.9
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.7    23.3
@>      ALA28    A         N_438  <--->      GLU24    A         O_374     2.7    24.8
@>      GLU34    A         N_540  <--->      ILE30    A         O_473     2.7    35.2
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE2_548     2.7    23.8
@>       THR7    A       OG1_118  <--->      LYS11    A         O_170     2.7    12.2
@>      VAL17    A         N_270  <--->       MET1    A           O_3     2.8    15.8
@>      GLY10    A         N_160  <--->       THR7    A         O_116     2.8     6.1
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     2.8    30.9
@>      LEU15    A         N_236  <--->       ILE3    A          O_39     2.9    12.9
@>      GLU18    A         N_286  <--->      ASP21    A       OD2_333     2.9    14.2
@>      GLN41    A       NE2_646  <--->      LYS27    A         O_419     2.9    25.8
@>       ILE3    A          N_36  <--->      LEU15    A         O_239     3.0    28.8
@>      SER57    A        OG_908  <--->      PRO19    A         O_304     3.0    15.4
@>       THR7    A         N_113  <--->      LYS11    A         O_170     3.0    15.8
@>      ASP21    A         N_326  <--->      GLU18    A         O_289     3.0    27.1
@>      LYS27    A         N_416  <--->      ILE23    A         O_355     3.0    31.1
@>      ASN25    A         N_386  <--->      THR22    A       OG1_343     3.1    21.5
@>       VAL5    A          N_75  <--->      ILE13    A         O_206     3.1    10.1
@>      VAL26    A         N_400  <--->      THR22    A         O_341     3.2    25.3
@>      LEU56    A         N_884  <--->      ASP21    A         O_329     3.2    13.0
@>      LYS33    A         N_518  <--->      LYS29    A         O_451     3.3    15.4
@>      THR12    A       OG1_194  <--->      GLY10    A         O_163     3.4    32.7
@> Number of detected hydrogen bonds: 23.
@> Calculating salt bridges.
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     2.7
@> Number of detected salt bridges: 1.
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
@> Calculating cation-Pi interactions.
```

```
@> Number of detected cation-pi interactions: 0.
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      ILE23    A    CD1_35914s  <--->      LEU56    A    CD2_891     3.5    16.7
@>      LEU43    A    CD1_68514s  <--->      ILE23    A    CG2_358     3.5    23.4
@>      ILE13    A    CG2_20914s  <--->      LEU15    A    CD1_242     3.6    27.7
@>      LEU50    A    CD2_80014s  <--->      ILE23    A    CD1_359     3.6    16.1
@>      VAL26    A    CG2_40614s  <--->      LEU56    A    CD2_891     3.7    17.6
@>      LYS27    A     CD_42214s  <--->      ILE23    A    CG2_358     3.7    35.4
@>       VAL5    A     CG2_8114s  <--->      LEU15    A    CD2_243     3.7    11.1
@>      VAL17    A    CG2_27614s  <--->       MET1    A       CE_7     3.8    54.3
@>      LYS29    A     CD_45414s  <--->      LEU15    A     CG_241     3.8    26.2
@>       ILE3    A     CD1_4314s  <--->      VAL26    A    CG1_405     3.9    14.1
@>      LYS33    A     CG_52314s  <--->      ILE13    A    CG2_209     3.9    17.6
@>      TYR59    A    CD2_93314s  <--->      ILE23    A    CG1_357     3.9     7.8
@>      ILE30    A    CD1_47714s  <--->      LEU15    A    CD1_242     4.0    10.9
@>      LYS11    A     CD_17314s  <--->      ILE13    A    CD1_210     4.1    30.0
@> Number of detected hydrophobic interactions: 14.
@> Lack of cysteines in the structure.
@> Number of detected disulfide bonds: 0.
@> Model: 8
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE1_547     2.6    19.1
@>       THR7    A       OG1_118  <--->      LYS11    A         O_170     2.6    24.5
@>      LYS27    A        NZ_424  <--->      ASP52    A       OD1_833     2.7     8.6
@>      LYS33    A        NZ_526  <--->      GLU16    A       OE1_262     2.7    32.9
@>      LYS33    A        NZ_526  <--->      GLU16    A       OE2_263     2.7    39.9
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.8    22.1
@>       ILE3    A          N_36  <--->      LEU15    A         O_239     2.8    20.9
@>      GLU34    A         N_540  <--->      ILE30    A         O_473     2.8    12.7
@>       THR7    A         N_113  <--->      LYS11    A         O_170     2.9    12.8
@>      SER57    A         N_903  <--->      PRO19    A         O_304     2.9    18.6
@>      ILE30    A         N_470  <--->      VAL26    A         O_403     2.9     7.4
@>      LEU15    A         N_236  <--->       ILE3    A          O_39     2.9    29.2
@>       VAL5    A          N_75  <--->      ILE13    A         O_206     3.0    17.0
@>      LEU56    A         N_884  <--->      ASP21    A         O_329     3.1    24.2
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     3.1    16.0
@>      GLU18    A         N_286  <--->      ASP21    A       OD2_333     3.1    21.5
@>      VAL17    A         N_270  <--->       MET1    A           O_3     3.2     8.9
@>      ALA28    A         N_438  <--->      GLU24    A         O_374     3.2    26.3
@>      LYS29    A         N_448  <--->      ASN25    A         O_389     3.2    34.3
@>      GLU24    A         N_371  <--->      ASP52    A         O_830     3.2    33.4
@>      GLY10    A         N_160  <--->       THR7    A         O_116     3.2    19.9
@>      VAL26    A         N_400  <--->      THR22    A         O_341     3.3    28.4
@>      ASP32    A         N_506  <--->      ALA28    A         O_441     3.3    22.5
@>      ILE23    A         N_352  <--->      ARG54    A         O_849     3.4    30.3
@> Number of detected hydrogen bonds: 24.
@> Calculating salt bridges.
@>      LYS33    A          NZ_526  <--->      GLU16    A     OE1_262_263     2.5
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     3.2
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     3.4
@>      LYS29    A          NZ_456  <--->      GLU16    A     OE1_262_263     4.6
@> Number of detected salt bridges: 4.
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
```

```
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      TYR59    A    CE2_93514s  <--->      ILE23    A    CD1_359     3.3    18.2
@>      ILE30    A    CD1_47714s  <--->       VAL5    A     CG2_81     3.6    17.6
@>      VAL26    A    CG1_40514s  <--->      ILE30    A    CD1_477     3.6    21.8
@>      VAL17    A    CG2_27614s  <--->       MET1    A       CG_5     3.6    48.0
@>      LEU56    A    CD1_89014s  <--->      VAL17    A    CG2_276     3.7    18.4
@>      LEU15    A    CD1_24214s  <--->      VAL26    A    CG1_405     3.7    12.1
@>       ILE3    A     CD1_4314s  <--->      VAL17    A    CG1_275     3.8    16.1
@>      LYS27    A     CG_42114s  <--->      LEU43    A    CD1_685     3.9    11.4
@>      LYS33    A     CG_52314s  <--->      LEU15    A    CD2_243     4.3     9.4
@> Number of detected hydrophobic interactions: 9.
@> Lack of cysteines in the structure.
@> Number of detected disulfide bonds: 0.
@> Model: 9
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      GLN41    A       NE2_646  <--->      LYS27    A         O_419     2.7     3.7
@>      LYS11    A        NZ_175  <--->      GLU34    A       OE1_547     2.7    11.1
@>      LYS27    A        NZ_424  <--->      ASP52    A       OD1_833     2.8    18.1
@>      GLU18    A         N_286  <--->      ASP21    A       OD2_333     2.8     5.2
@>       VAL5    A          N_75  <--->      ILE13    A         O_206     2.8    18.5
@>      ILE13    A         N_203  <--->       VAL5    A          O_78     2.8    22.3
@>       MET1    A           N_0  <--->      VAL17    A         O_273     2.9    29.4
@>       THR7    A       OG1_118  <--->      LYS11    A         O_170     3.0    14.7
@>      ILE23    A         N_352  <--->      ARG54    A         O_849     3.0    11.6
@>       GLN2    A        NE2_27  <--->      GLU16    A       OE1_262     3.0    25.2
@>      LYS33    A         N_518  <--->      LYS29    A         O_451     3.0    22.3
@>      LYS11    A         N_167  <--->       THR7    A       OG1_118     3.0    33.6
@>      LEU15    A         N_236  <--->       ILE3    A          O_39     3.0    10.0
@>      LYS27    A         N_416  <--->      ILE23    A         O_355     3.1     2.4
@>       THR7    A         N_113  <--->      LYS11    A         O_170     3.1    28.2
@>       ILE3    A          N_36  <--->      LEU15    A         O_239     3.1     7.6
@>      ASP21    A         N_326  <--->      GLU18    A         O_289     3.2    22.9
@>      VAL26    A         N_400  <--->      THR22    A         O_341     3.2     4.1
@>      GLY10    A         N_160  <--->       THR7    A         O_116     3.2    12.6
@>      LEU56    A         N_884  <--->      ASP21    A         O_329     3.2    19.8
@>      ALA28    A         N_438  <--->      GLU24    A         O_374     3.3    10.7
@>      ILE30    A         N_470  <--->      LYS27    A         O_419     3.3    35.7
@> Number of detected hydrogen bonds: 22.
@> Calculating salt bridges.
@>      LYS27    A          NZ_424  <--->      ASP52    A     OD1_833_834     2.8
@>      GLU34    A     OE1_547_548  <--->      LYS11    A          NZ_175     3.1
@> Number of detected salt bridges: 2.
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Calculating Pi stacking interactions.
@> Number of detected Pi stacking interactions: 0.
@> Calculating cation-Pi interactions.
@> Number of detected cation-pi interactions: 0.
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      LEU43    A    CD2_68614s  <--->      ILE23    A    CG2_358     3.7    13.3
@>      TYR59    A    CE2_93514s  <--->      ILE23    A    CD1_359     3.7    16.6
@>      LEU15    A    CD2_24314s  <--->       VAL5    A     CG2_81     3.7    19.2
@>      VAL17    A    CG2_27614s  <--->       ILE3    A     CG1_41     3.7    21.4
```

```
@>      LEU56    A    CD1_89014s  <--->      VAL17    A    CG2_276     3.7    17.4
@>      ILE30    A    CG2_47614s  <--->      LEU69    A   CD1_1101     3.8    16.9
@>      ILE13    A    CG2_20914s  <--->      LEU15    A    CD1_242     3.8    29.7
@>      VAL26    A    CG1_40514s  <--->      LEU15    A    CD2_243     3.9    16.7
@>      LYS33    A     CG_52314s  <--->      ILE13    A    CG2_209     4.1    13.9
@>      LYS27    A     CD_42214s  <--->      ILE23    A    CG2_358     4.2    35.1
@>      LYS29    A     CD_45414s  <--->      LEU15    A     CG_241     4.4    16.5
@> Number of detected hydrophobic interactions: 11.
@> Lack of cysteines in the structure.
@> Number of detected disulfide bonds: 0.
```

5.6 Import previously saved file with interactions

We previously saved `pkl` file `interactions_data_5kqm.pkl` with interactions, and now we will import it for analysis. To do that we need to initiate a new instance and use `parseInteractions()` function to parse `pkl` file:

```
In [26]: interactionsTrajectory2 = InteractionsTrajectory('5kqm_import')

In [27]: interactionsTrajectory2.parseInteractions('calcProteinInteractionsEnsemblePDB.pkl')
```

```
[[[['GLN49', 'NE2_784', 'A', 'GLU51', 'OE2_820', 'A', 2.5853, 16.2407],
   ['LYS11', 'NZ_175', 'A', 'GLU34', 'OE1_547', 'A', 2.6141, 7.0039],
   ['GLY10', 'N_160', 'A', 'THR7', 'O_116', 'A', 2.6801, 19.8254],
   ['ARG72', 'N_1149', 'A', 'GLN40', 'O_624', 'A', 2.6883, 21.0779],
   ['ARG72', 'NH1_1158', 'A', 'GLN40', 'OE1_628', 'A', 2.7336, 7.4598],
   ['LYS6', 'N_91', 'A', 'LEU67', 'O_1062', 'A', 2.7367, 2.6222],
   ['GLU34', 'N_540', 'A', 'ILE30', 'O_473', 'A', 2.7587, 28.1769],
   ['THR55', 'N_870', 'A', 'ASP58', 'OD2_921', 'A', 2.7775, 19.6842],
   ['ILE44', 'N_698', 'A', 'HIS68', 'O_1081', 'A', 2.8708, 20.2386],
   ['THR55', 'OG1_875', 'A', 'ASP58', 'OD2_921', 'A', 2.8819, 13.1563],
   ['LYS29', 'N_448', 'A', 'ASN25', 'O_389', 'A', 2.8866, 13.6397],
   ['LEU73', 'N_1173', 'A', 'LEU71', 'O_1133', 'A', 2.9102, 27.7682],
   ['HIS68', 'N_1078', 'A', 'ILE44', 'O_701', 'A', 2.9174, 21.7682],
   ['THR14', 'OG1_227', 'A', 'ILE3', 'O_39', 'A', 2.919, 13.0791],
   ['GLU51', 'N_812', 'A', 'TYR59', 'OH_937', 'A', 2.9532, 23.4224],
   ['GLU64', 'N_1019', 'A', 'GLN2', 'O_22', 'A', 2.9586, 23.2217],
   ['LEU50', 'N_793', 'A', 'LEU43', 'O_682', 'A', 2.995, 15.3383],
   ['GLN62', 'N_980', 'A', 'SER65', 'OG_1039', 'A', 3.0046, 23.3912],
   ['ILE13', 'N_203', 'A', 'VAL5', 'O_78', 'A', 3.0123, 12.8492],
   ['SER65', 'N_1034', 'A', 'GLN62', 'O_983', 'A', 3.0171, 18.3009],
   ['VAL17', 'N_270', 'A', 'MET1', 'O_3', 'A', 3.0299, 8.8346],
   ['ASN60', 'N_947', 'A', 'SER57', 'O_906', 'A', 3.0544, 28.4747],
   ['LYS33', 'N_518', 'A', 'LYS29', 'O_451', 'A', 3.0814, 33.0882],
   ['VAL70', 'N_1114', 'A', 'ARG42', 'O_658', 'A', 3.1015, 17.9449],
   ['ASP32', 'N_506', 'A', 'ALA28', 'O_441', 'A', 3.1118, 10.5675],
   ..
   ..
```

After parsing the file we will have access to the same functions as before:

```
In [28]: calcStatisticsInteractions(interactionsTrajectory2.getHydrogenBonds())
```

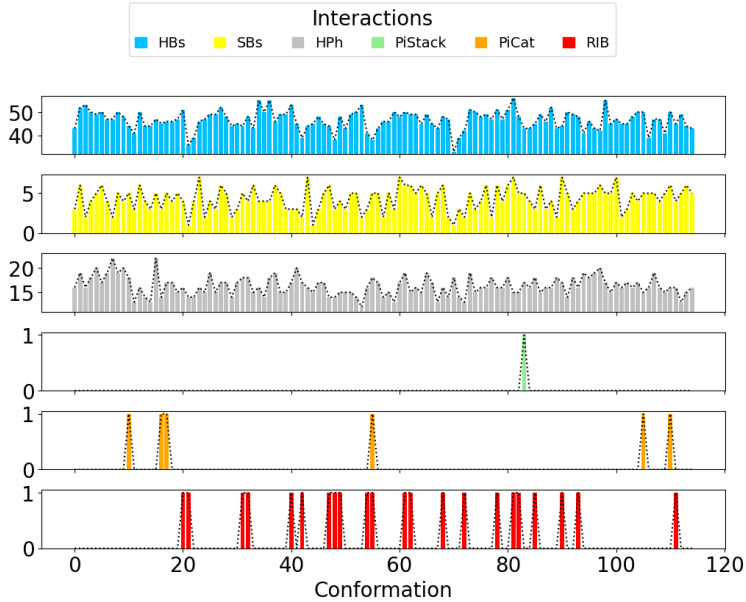
```
@> Statistics for LYS11A-GLU34A:
@>   Average [Ang.]: 2.720873
@>   Standard deviation [Ang.]: 0.179343
@>   Weight: 0.8
@> Statistics for GLY10A-THR7A:
```

```
@>   Average [Ang.]: 3.037245
@>   Standard deviation [Ang.]: 0.1988
@>   Weight: 0.669565
@> Statistics for ARG72A-GLN40A:
@>   Average [Ang.]: 2.874946
@>   Standard deviation [Ang.]: 0.18885
@>   Weight: 0.782609
@> Statistics for LYS6A-LEU67A:
@>   Average [Ang.]: 2.920333
@>   Standard deviation [Ang.]: 0.157525
@>   Weight: 0.947826
@> Statistics for GLU34A-ILE30A:
@>   Average [Ang.]: 2.896524
@>   Standard deviation [Ang.]: 0.171493
@>   Weight: 0.878261
@> Statistics for THR55A-ASP58A:
@>   Average [Ang.]: 2.777835
@>   Standard deviation [Ang.]: 0.158068
@>   Weight: 1.504348
@> Statistics for ILE44A-HIS68A:
@>   Average [Ang.]: 2.941125
@>   Standard deviation [Ang.]: 0.177848
@>   Weight: 0.834783
@> Statistics for LYS29A-ASN25A:
@>   Average [Ang.]: 3.050209
@>   Standard deviation [Ang.]: 0.211243
@>   Weight: 0.582609
@> Statistics for HIS68A-ILE44A:
@>   Average [Ang.]: 2.951679
@>   Standard deviation [Ang.]: 0.195428
@>   Weight: 0.826087
@> Statistics for GLU51A-TYR59A:
@>   Average [Ang.]: 2.967038
@>   Standard deviation [Ang.]: 0.18416
@>   Weight: 0.834783
@> Statistics for GLU64A-GLN2A:
@>   Average [Ang.]: 2.860456
@>   Standard deviation [Ang.]: 0.142289
@>   Weight: 0.895652
@> Statistics for LEU50A-LEU43A:
@>   Average [Ang.]: 3.028411
@>   Standard deviation [Ang.]: 0.19173
@>   Weight: 0.773913
@> Statistics for ILE13A-VAL5A:
@>   Average [Ang.]: 2.900624
@>   Standard deviation [Ang.]: 0.149592
@>   Weight: 0.930435
..
..
```

```
In [29]: time_interaction_import = interactionsTrajectory2.getTimeInteractions()
```

5.7 Change selection criteria for interaction type

The `calcProteinInteractionsTrajectory()` method computes interactions using default parameters for interactions. However, it can be changed according to our needs. To do that, we need to recalculate the selected type of interactions.



We can do it using the following functions: `calcHydrogenBonds()`, `calcHydrogenBonds()`, `calcSaltBridges()`, `calcRepulsiveIonicBonding()`, `calcPiStacking()`, `calcPiCation()`, `calcHydrophohic()`, `calcDisulfideBonds()`, and use `InteractionsTrajectory.setNewHydrogenBonds()`,`InteractionsTrajectory.setNewSaltBridges()`, `InteractionsTrajectory.setNewRepulsiveIonicBonding()`,`InteractionsTrajectory.setNewPiStackir` `InteractionsTrajectory.setNewPiCation()`,`InteractionsTrajectory.setNewHydrophohic()`, `InteractionsTrajectory.setNewDisulfideBonds()` method to replace it in the main Instance.

```
In [30]: picat2 = calcPiCation(atoms, distA=8)

In [31]: interactionsTrajectoryNMR.setNewPiCation(picat2).setNewPiCation(picat2)
```

```
@> Calculating cation-Pi interactions.
@>      TYR59   A         931_932_933_934_935_936  <--->      ARG54   A       NH1_855_856     5.7
@>       PHE4   A               60_61_62_63_64_65  <--->       LYS6   A             NZ_99     5.8
@>      TYR59   A         931_932_933_934_935_936  <--->      LYS48   A            NZ_762     6.4
@>      HIS68   A        1083_1084_1085_1086_1087  <--->       LYS6   A             NZ_99     7.2
@>      PHE45   A         722_723_724_725_726_727  <--->      LYS48   A            NZ_762     7.5
@> Number of detected cation-pi interactions: 5.
@> Pi-Cation interactions are replaced
```

Now, interactions are replaced:

```
In [32]: interactionsTrajectoryNMR.getPiCation()
```

```
[['TYR59',
  '931_932_933_934_935_936',
  'A',
  'ARG54',
  'NH1_855_856',
  'A',
  5.7097],
 ['PHE4', '60_61_62_63_64_65', 'A', 'LYS6', 'NZ_99', 'A', 5.8358],
 ['TYR59', '931_932_933_934_935_936', 'A', 'LYS48', 'NZ_762', 'A', 6.3869],
 ['HIS68', '1083_1084_1085_1086_1087', 'A', 'LYS6', 'NZ_99', 'A', 7.1937],
 ['PHE45', '722_723_724_725_726_727', 'A', 'LYS48', 'NZ_762', 'A', 7.5218]]
```

CHAPTER

SIX

TRAJECTORY ANALYSIS

This example shows how to compute interactions for a trajectory performed using NAMD[12] software for a small protein tyrosine phosphatase LMW-PTP in a complex with inhibitor *MES* (PDB: **5KQM**) and visualize the results using **Matplotlib_** library and **VMD_** program.

In the tutorial, we will use already prepared files for simulation (*PDB* and *DCD* file).

6.1 Parse trajectory

We start by parsing PDB and DCD files, which contain LMW-PTP protein structure (available as tutorial files). PDB file contains the coordinates of protein structure with water and counter ions. DCD file is a binary file that contains a short simulation computed in NAMD[13] package (20 frames). The commands shown below are explained in Trajectory Analysis tutorial[14].

```
In [1]: PDBfile = '5kqm_all_sci.pdb'

In [2]: DCDfile = 'NAMD_D2_co100.dcd'

In [3]: atoms = parsePDB(PDBfile)

In [4]: dcd = Trajectory(DCDfile)

In [5]: dcd.link(atoms)

In [6]: dcd.setCoords(atoms)
```

```
@> 19321 atoms and 1 coordinate set(s) were parsed in 0.17s.
```

To compute hydrogen bonds for each frame of the simulation use `calcHydrogenBondsTrajectory()` function:

```
In [7]: calcHydrogenBondsTrajectory(atoms, dcd)
```

```
@> Frame: 0
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)    <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     ARG101    P      NH1_1516  <--->      ASP98    P      OD1_1463     2.0    33.1
@>      HSE72    P      NE2_1042  <--->      ASN15    P       OD1_165     2.6    34.8
@>     GLN143    P      NE2_2192  <--->     GLU139    P      OE2_2126     2.7     9.2
@>      HSE66    P       NE2_957  <--->     GLU139    P      OE1_2125     2.7     6.4
@>      ARG40    P         N_561  <--->       LYS6    P          O_37     2.7    17.1
@>      ARG58    P         N_813  <--->      ASP56    P       OD1_788     2.7    30.0
```

[12] http://www.ks.uiuc.edu/Research/namd/
[13] http://www.ks.uiuc.edu/Research/namd/
[14] http://www.bahargroup.org/prody/tutorials/trajectory_analysis/

```
@>      ALA45    P         N_634  <--->      ARG75    P        O_1097     2.8    35.1
@>      ASN53    P       ND2_747  <--->      GLU50    P       OE1_708     2.8    18.2
@>      ALA74    P        N_1064  <--->      ASN53    P         O_751     2.8    21.3
@>      ASP56    P         N_780  <--->      ILE16    P         O_189     2.8    27.0
@>     LYS110    P       NZ_1667  <--->      THR84    P        O_1240     2.8    38.2
@>     LEU116    P        N_1758  <--->      CYS90    P        O_1342     2.8    15.0
@>     SER103    P        N_1546  <--->      LEU99    P        O_1485     2.8    29.1
@>     ASN134    P        N_2045  <--->     ASP137    P      OD2_2091     2.8    22.6
@>     PHE152    P        N_2321  <--->     CYS148    P        O_2275     2.8     8.3
@>      ASN95    P        N_1398  <--->      ASP92    P      OD1_1368     2.8    12.6
@>       LYS6    P          N_16  <--->      ASN38    P         O_536     2.8    25.0
@>      ILE77    P        N_1115  <--->      ALA45    P         O_643     2.8    12.2
@>      ARG58    P       NH2_832  <--->      ASP56    P       OD2_789     2.8    27.7
@>      LEU99    P        N_1467  <--->      ASN95    P        O_1411     2.8    15.5
@>     CYS149    P        N_2276  <--->     CYS145    P        O_2224     2.8     9.6
@>      GLY52    P         N_731  <--->      ALA74    P        O_1073     2.8     6.6
@>      ASP32    P         N_435  <--->      LYS28    P         O_385     2.8     8.8
@>      ILE88    P        N_1294  <--->     LYS112    P        O_1704     2.8    17.7
@>     GLN143    P        N_2180  <--->     GLU139    P        O_2128     2.8    21.7
@>      ARG27    P         N_340  <--->      GLU23    P         O_293     2.8    15.4
@>     TYR142    P        N_2159  <--->     PHE138    P        O_2113     2.9    14.2
@>     GLY133    P        N_2038  <--->     PRO130    P        O_1995     2.9    25.4
@>      PHE26    P         N_320  <--->      ALA22    P         O_278     2.9     4.9
@>      ASN15    P       ND2_166  <--->      SER19    P        OG_232     2.9    32.1
@>      ARG75    P      NH1_1090  <--->      ASP81    P      OD2_1194     2.9    19.7
@>      ARG75    P      NH2_1093  <--->      ASP42    P       OD2_610     2.9    23.5
@>      ARG97    P        N_1431  <--->      GLU93    P        O_1386     2.9    22.2
@>      ARG65    P       NH2_941  <--->     GLU139    P      OE1_2125     2.9    32.3
@>      VAL25    P         N_304  <--->      ILE21    P         O_268     2.9     8.2
@>     LEU153    P        N_2341  <--->     CYS149    P        O_2286     2.9    12.5
@>       SER7    P          N_38  <--->      ASP86    P      OD2_1270     2.9    39.9
@>      ASP86    P        N_1261  <--->       SER7    P         OG_45     2.9    34.7
@>      ARG58    P       NH2_832  <--->     TYR131    P        O_2016     2.9    33.1
@>      THR46    P         N_644  <--->      CYS12    P         O_130     2.9    36.1
@>     GLN144    P        N_2197  <--->     THR140    P        O_2142     2.9    23.3
@>      THR78    P        N_1134  <--->      ASP81    P      OD2_1194     2.9    12.4
@>      LEU89    P        N_1313  <--->       LEU9    P          O_83     2.9    29.5
@>      THR31    P         N_421  <--->      ARG27    P         O_363     2.9    24.1
@>      CYS90    P        N_1332  <--->     GLU114    P        O_1738     2.9    24.6
..
..
@>      ARG40    P       NH1_577  <--->      THR84    P      OG1_1233     2.9     8.4
@>      ALA44    P         N_624  <--->      PHE10    P         O_103     2.9    33.2
@>     GLU154    P        N_2360  <--->     ARG150    P        O_2310     3.0    22.6
@>       VAL8    P          N_49  <--->      ARG40    P         O_584     3.0    25.0
@>      SER19    P         N_225  <--->      CYS12    P        SG_127     3.3     8.0
@>      PHE82    P        N_1197  <--->      LYS79    P        O_1169     3.4    37.7
@>      ASP81    P        N_1185  <--->      THR78    P      OG1_1140     3.5    39.5
@>     LYS102    P       NZ_1540  <--->      ASP98    P      OD2_1464     3.5    26.1
@>     ARG147    P      NH2_2260  <--->     GLN124    P      OE1_1892     3.5    33.9
@>     VAL106    P        N_1588  <--->     SER103    P        O_1556     3.5    34.2
@> Number of detected hydrogen bonds: 124.

@> Frame: 1
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     LYS112    P       NZ_1699  <--->     GLU114    P      OE1_1735     2.5    20.8
@>      THR78    P        N_1134  <--->      ASP81    P      OD2_1194     2.5    15.6
```

```
@>      ARG27    P       NH2_359  <--->      GLU23    P       OE2_291     2.5    36.5
@>      THR78    P      OG1_1140  <--->      ASP81    P      OD2_1194     2.6    25.2
@>       SER7    P         OG_45  <--->      ASP86    P      OD2_1270     2.6    32.3
@>     LYS102    P       NZ_1540  <--->      ASP98    P      OD2_1464     2.6    18.6
@>     LYS112    P       NZ_1699  <--->     HSE157    P      OT1_2423     2.6    17.8
@>      ARG75    P      NH2_1093  <--->      ASP81    P      OD1_1193     2.6    17.6
@>     SER118    P       OG_1791  <--->     LEU115    P        O_1757     2.7    25.6
@>      ARG58    P        NE_826  <--->      ASP56    P       OD1_788     2.7     6.4
@>     GLN124    P        N_1881  <--->     ASP120    P      OD1_1824     2.7    17.2
@>     ARG147    P      NH1_2257  <--->     GLN124    P      OE1_1892     2.7    11.8
@>      ARG18    P       NH1_217  <--->      ASP92    P      OD2_1369     2.7    14.6
@>      ARG75    P      NH1_1090  <--->      ASP81    P      OD2_1194     2.7    23.9
@>      TYR87    P       OH_1286  <--->     HSE157    P      OT1_2423     2.7    11.6
@>      SER43    P        OG_620  <--->      GLU23    P       OE1_290     2.7    15.2
@>      LYS28    P        NZ_380  <--->      ASP32    P       OD1_443     2.7     3.6
@>     LYS110    P       NZ_1667  <--->      ASP86    P      OD1_1269     2.7    25.2
@>     THR140    P      OG1_2135  <--->     SER136    P        O_2081     2.7     5.2
@>     LEU116    P        N_1758  <--->      CYS90    P        O_1342     2.7    24.4
@>       THR5    P         OG1_8  <--->      ASN38    P         O_536     2.7    38.6
@>      LYS64    P         N_900  <--->      GLN60    P         O_860     2.7    26.8
@>     ARG147    P      NH1_2257  <--->     ASP120    P      OD2_1825     2.7    15.2
@>      ARG27    P         N_340  <--->      GLU23    P         O_293     2.7    21.9
@>     TYR119    P       OH_1808  <--->     GLU114    P      OE1_1735     2.7    15.9
@>      ARG18    P       NH1_217  <--->     ILE127    P        O_1954     2.8    16.0
@>     SER103    P        N_1546  <--->      LEU99    P        O_1485     2.8    13.6
@>     LYS102    P        N_1524  <--->      ASP98    P        O_1466     2.8    15.9
@>      ARG58    P       NH1_829  <--->     GLY133    P        O_2044     2.8    31.9
@>      ARG75    P      NH2_1093  <--->      ASP42    P       OD2_610     2.8    13.0
@>     LYS112    P        N_1683  <--->      ASP86    P        O_1272     2.8    13.2
..
..
@>     ILE127    P        N_1936  <--->      MET91    P        O_1359     3.3    29.4
@>     ASN104    P        N_1557  <--->     ASN100    P        O_1499     3.4    12.6
@>     GLN105    P        N_1571  <--->     ARG101    P        O_1523     3.4    38.7
@>     ARG147    P        N_2241  <--->     GLN143    P        O_2196     3.4    10.9
@>      ASP56    P         N_780  <--->      ILE16    P         O_189     3.4    25.5
@>      ASN95    P        N_1398  <--->      ASP92    P      OD1_1368     3.5    32.5
@>      HSE72    P      NE2_1042  <--->      ASN15    P       OD1_165     3.5     7.1
@>     VAL106    P        N_1588  <--->     LYS102    P        O_1545     3.5    29.8
@>      ILE21    P         N_250  <--->      CYS17    P         O_200     3.5    34.9
@>      LEU96    P        N_1412  <--->      ASP92    P        O_1371     3.5     8.7
@> Number of detected hydrogen bonds: 123.

@> Frame: 2
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      ARG18    P       NH1_217  <--->      ASP92    P      OD2_1369     2.5     4.9
@>      THR31    P       OG1_427  <--->      ARG27    P         O_363     2.5     5.5
@>      ARG58    P       NH2_832  <--->      ASP56    P       OD2_789     2.6     8.2
@>     LYS112    P       NZ_1699  <--->     HSE157    P      OT1_2423     2.6    19.0
@>      ARG75    P      NH2_1093  <--->      ASP42    P       OD2_610     2.6    25.0
@>     TYR119    P       OH_1808  <--->     GLU114    P      OE2_1736     2.6    10.3
@>     LYS102    P       NZ_1540  <--->      ASP98    P      OD2_1464     2.6     7.9
@>      TYR87    P       OH_1286  <--->     HSE157    P      OT1_2423     2.7    14.1
@>      LYS64    P         N_900  <--->      GLN60    P         O_860     2.7     4.9
@>      SER43    P        OG_620  <--->      GLU23    P       OE1_290     2.7     8.6
@>      THR78    P      OG1_1140  <--->      ASP81    P      OD2_1194     2.7     6.5
@>      ILE88    P        N_1294  <--->     LYS112    P        O_1704     2.7    25.0
```

```
@>     SER118    P       OG_1791  <--->     LEU115    P        O_1757     2.7    26.9
@>      LYS28    P        NZ_380  <--->      ASP32    P       OD2_444     2.7    13.9
@>      THR84    P      OG1_1233  <--->      GLU80    P        O_1184     2.7    13.4
@>      LEU89    P        N_1313  <--->       LEU9    P          O_83     2.8    11.8
@>     ARG147    P      NH1_2257  <--->     GLN124    P      OE1_1892     2.8    15.1
@>      ARG27    P       NH2_359  <--->      GLU23    P       OE2_291     2.8    18.0
@>      ILE35    P         N_478  <--->      VAL30    P         O_420     2.8    20.7
@>      PHE26    P         N_320  <--->      ALA22    P         O_278     2.8    21.8
@>      VAL11    P         N_104  <--->      LEU89    P        O_1331     2.8    10.3
@>      VAL25    P         N_304  <--->      ILE21    P         O_268     2.8     9.2
@>       SER7    P         OG_45  <--->      ASP86    P      OD2_1270     2.8    29.4
@>      HSE72    P      NE2_1042  <--->      ASN15    P       OD1_165     2.8    37.1
@>      ASN34    P         N_464  <--->      THR31    P         O_434     2.8    19.7
@>     LYS110    P        N_1651  <--->      PHE82    P        O_1216     2.8     9.2
@>     LYS110    P       NZ_1667  <--->      ASP86    P      OD1_1269     2.8    13.5
@>      ARG58    P        NE_826  <--->      ASP56    P       OD1_788     2.8     8.0
@>      ARG75    P      NH1_1090  <--->      ASP81    P      OD2_1194     2.8    14.9
@>       VAL8    P          N_49  <--->      ARG40    P         O_584     2.8    19.4
@>      ARG18    P       NH1_217  <--->     ILE127    P        O_1954     2.8     7.0
@>     LYS155    P        N_2375  <--->     ALA151    P        O_2320     2.8    15.1
@>      HSE66    P       NE2_957  <--->     GLU139    P      OE1_2125     2.8    28.9
@>     ARG147    P      NH1_2257  <--->     ASP120    P      OD2_1825     2.8    31.7
@>      ARG97    P        N_1431  <--->      GLU93    P        O_1386     2.8    15.2
@>     LYS123    P        N_1859  <--->     ASP120    P      OD1_1824     2.8    34.0
@>     LYS112    P        N_1683  <--->      ASP86    P        O_1272     2.8    10.3
@>      ASP86    P        N_1261  <--->       SER7    P         OG_45     2.8    22.0
@>      ARG65    P         N_922  <--->      SER61    P         O_871     2.8    24.4
@>     ILE127    P        N_1936  <--->      MET91    P        O_1359     2.8     4.1
@>     LYS112    P       NZ_1699  <--->     HSE157    P      ND1_2414     2.9    14.0
@>      GLY67    P         N_963  <--->      MET63    P         O_899     2.9    38.6
@>     SER103    P        N_1546  <--->      LEU99    P        O_1485     2.9    17.1
@>     LYS112    P       NZ_1699  <--->     GLU114    P      OE2_1736     2.9    18.1
@>      ARG75    P       NE_1087  <--->      ASP42    P       OD2_610     2.9    38.3
@>      ALA44    P         N_624  <--->      PHE10    P         O_103     2.9    30.1
@>      ILE68    P         N_970  <--->      MET63    P         O_899     2.9    12.9
@>      ARG58    P         N_813  <--->      ASP56    P       OD1_788     2.9    21.1
@>      THR78    P        N_1134  <--->      ASP81    P      OD2_1194     2.9    26.3
@>      ALA45    P         N_634  <--->      ARG75    P        O_1097     2.9    27.7
..
..
@>      HSE66    P         N_946  <--->      CYS62    P         O_882     2.9    17.6
@>      ASP32    P         N_435  <--->      LYS28    P         O_385     3.0    20.4
@>     VAL146    P        N_2225  <--->     TYR142    P        O_2179     3.0    20.7
@>     VAL106    P        N_1588  <--->     LYS102    P        O_1545     3.0    10.6
@>      ARG40    P         N_561  <--->       LYS6    P          O_37     3.4    33.1
@>     HSE157    P        N_2407  <--->     TYR119    P       OH_1808     3.4    27.6
@>      ARG65    P       NH1_938  <--->     GLU139    P      OE1_2125     3.4    32.0
@>     GLU114    P        N_1724  <--->      ILE88    P        O_1312     3.5    13.0
@>      ASP92    P        N_1360  <--->      ASN95    P      OD1_1406     3.5    35.4
@>      ASN15    P       ND2_166  <--->      SER43    P        OG_620     3.5    33.3
@> Number of detected hydrogen bonds: 113.
..
..
@> Frame: 20
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      ARG97    P       NE_1444  <--->      GLU93    P      OE1_1383     2.5    12.5
@>      SER19    P        OG_232  <--->      ASN15    P       OD1_165     2.6    31.5
```

```
@>      ARG27    P       NH1_356  <--->      GLU23    P       OE1_290     2.6    19.1
@>      THR78    P        N_1134  <--->      ASP81    P      OD2_1194     2.6    21.5
@>     GLN122    P      NE2_1854  <--->     ASP120    P      OD2_1825     2.6    39.7
@>     SER118    P       OG_1791  <--->     GLU114    P      OE2_1736     2.6    24.5
@>      ARG65    P       NH1_938  <--->     GLU139    P      OE1_2125     2.7     6.1
@>      ARG65    P       NH2_941  <--->     ASP135    P      OD1_2067     2.7    15.6
@>      SER43    P        OG_620  <--->      GLU23    P       OE2_291     2.7    13.9
@>      ARG75    P       NE_1087  <--->      ASP42    P       OD1_609     2.7    26.5
@>     ARG150    P       NE_2300  <--->     GLU154    P      OE2_2372     2.7     4.9
@>     VAL106    P        N_1588  <--->     LYS102    P        O_1545     2.7    16.2
@>      LYS28    P         N_364  <--->      ALA24    P         O_303     2.7    38.8
@>     HSE157    P      NE2_2418  <--->     PHE152    P        O_2340     2.7    28.5
@>      ARG58    P       NH2_832  <--->      ASP56    P       OD2_789     2.7    19.3
@>      ARG97    P      NH2_1450  <--->      GLU93    P      OE2_1384     2.7    15.8
@>      ARG75    P      NH2_1093  <--->      ASP42    P       OD1_609     2.7    30.5
@>      ALA45    P         N_634  <--->      ARG75    P        O_1097     2.7    22.3
@>      ARG75    P      NH2_1093  <--->      ASP81    P      OD1_1193     2.7    19.2
@>      THR31    P       OG1_427  <--->      ARG27    P         O_363     2.7    13.1
@>     ARG150    P      NH2_2306  <--->     GLU154    P      OE1_2371     2.7     8.5
@>      ARG75    P      NH1_1090  <--->      ASP81    P      OD2_1194     2.7    14.8
@>      GLY67    P         N_963  <--->      MET63    P         O_899     2.7    25.3
@>      LEU89    P        N_1313  <--->       LEU9    P          O_83     2.8    18.4
@>     ARG101    P      NH1_1516  <--->      ASP98    P      OD2_1464     2.8    11.5
@>      ILE77    P        N_1115  <--->      ALA45    P         O_643     2.8    39.9
@>     LYS110    P        N_1651  <--->      PHE82    P        O_1216     2.8    32.3
@>      LEU29    P         N_386  <--->      VAL25    P         O_319     2.8     5.4
@>     ASN100    P        N_1486  <--->      LEU96    P        O_1430     2.8     6.7
@>     LYS102    P        N_1524  <--->      ASP98    P        O_1466     2.8     4.9
@>      THR78    P      OG1_1140  <--->      ASP81    P      OD2_1194     2.8    10.5
@>       VAL8    P          N_49  <--->      ARG40    P         O_584     2.8    16.8
@>     GLU154    P        N_2360  <--->     ARG150    P        O_2310     2.8    15.1
@>     LYS110    P       NZ_1667  <--->      ASP86    P      OD2_1270     2.8    32.5
@>      ARG58    P        NE_826  <--->      ASP56    P       OD1_788     2.8     3.3
@>      ILE35    P         N_478  <--->      VAL30    P         O_420     2.8     7.9
@>      ARG58    P       NH1_829  <--->     GLY133    P        O_2044     2.8    34.3
@>     GLN105    P        N_1571  <--->     ARG101    P        O_1523     2.8    29.9
@>       SER7    P          N_38  <--->      ASP86    P      OD1_1269     2.8    10.5
@>     ARG101    P      NH2_1519  <--->      ASP98    P      OD1_1463     2.8    17.5
@>     GLN143    P        N_2180  <--->     GLU139    P        O_2128     2.8    20.5
@>     CYS149    P        N_2276  <--->     CYS145    P        O_2224     2.8    16.0
@>     SER103    P       OG_1553  <--->      LEU99    P        O_1485     2.9    21.4
@>      ARG18    P       NH1_217  <--->      ASP92    P      OD2_1369     2.9     6.7
@>      CYS90    P        N_1332  <--->     GLU114    P        O_1738     2.9     7.9
..
..
@>     ALA151    P        N_2311  <--->     ARG147    P        O_2264     3.3    28.5
@>      ILE88    P        N_1294  <--->     LYS112    P        O_1704     3.3     8.1
@>      CYS12    P         N_120  <--->      ALA44    P         O_633     3.4    24.0
@>     GLN124    P      NE2_1893  <--->     ILE126    P        O_1935     3.4     3.3
@>      ARG97    P        N_1431  <--->      GLU93    P        O_1386     3.4    28.8
@>      SER61    P         N_861  <--->      TYR57    P         O_812     3.4    29.6
@>     GLN122    P      NE2_1854  <--->     ASP120    P      OD1_1824     3.5    17.2
@> Number of detected hydrogen bonds: 114.
```

Similarly, it can be done with other interaction types. Salt bridges (residues with opposite changes) with `calcSaltBridgesTrajectory()`:

```
In [8]: calcSaltBridgesTrajectory(atoms, dcd)
```

```
@> Frame: 0
@> Calculating salt bridges.
@>     GLU139    P   OE1_2125_2126  <--->      HSE66    P         NE2_957     2.8
@>      ASP81    P   OD1_1193_1194  <--->      ARG75    P   NH1_1090_1093     2.9
@>      ASP32    P     OD1_443_444  <--->      LYS28    P          NZ_380     3.0
@>      ASP98    P   OD1_1463_1464  <--->     ARG101    P   NH1_1516_1519     3.1
@>      ARG27    P     NH1_356_359  <--->      GLU23    P     OE1_290_291     3.7
@>     GLU139    P   OE1_2125_2126  <--->      ARG65    P     NH1_938_941     3.8
@>     LYS102    P         NZ_1540  <--->      ASP98    P   OD1_1463_1464     3.9
@>      ARG58    P     NH1_829_832  <--->      ASP56    P     OD1_788_789     3.9
@>      ARG18    P     NH1_217_220  <--->      ASP92    P   OD1_1368_1369     4.1
@>     GLU114    P   OE1_1735_1736  <--->     LYS112    P         NZ_1699     4.1
@>     ASP120    P   OD1_1824_1825  <--->     ARG147    P   NH1_2257_2260     4.2
@>      ASP86    P   OD1_1269_1270  <--->     LYS110    P         NZ_1667     4.2
@>     HSE157    P        NE2_2418  <--->     GLU114    P   OE1_1735_1736     4.4
@>      ARG18    P     NH1_217_220  <--->     ASP129    P   OD1_1978_1979     4.6
@>      ARG75    P   NH1_1090_1093  <--->      ASP42    P     OD1_609_610     4.6
@>      GLU23    P     OE1_290_291  <--->      HSE72    P        NE2_1042     5.0
@> Number of detected salt bridges: 16.

@> Frame: 1
@> Calculating salt bridges.
@>      ASP32    P     OD1_443_444  <--->      LYS28    P          NZ_380     2.6
@>      ASP81    P   OD1_1193_1194  <--->      ARG75    P   NH1_1090_1093     2.6
@>      ASP98    P   OD1_1463_1464  <--->     ARG101    P   NH1_1516_1519     2.8
@>     GLU114    P   OE1_1735_1736  <--->     LYS112    P         NZ_1699     3.1
@>     HSE157    P        NE2_2418  <--->     GLU114    P   OE1_1735_1736     3.2
@>      ASP86    P   OD1_1269_1270  <--->     LYS110    P         NZ_1667     3.3
@>      ARG27    P     NH1_356_359  <--->      GLU23    P     OE1_290_291     3.4
@>     GLU139    P   OE1_2125_2126  <--->      ARG65    P     NH1_938_941     3.4
@>     LYS102    P         NZ_1540  <--->      ASP98    P   OD1_1463_1464     3.5
@>     ASP120    P   OD1_1824_1825  <--->     ARG147    P   NH1_2257_2260     3.8
@>      ARG58    P     NH1_829_832  <--->      ASP56    P     OD1_788_789     3.8
@>      ARG18    P     NH1_217_220  <--->      ASP92    P   OD1_1368_1369     3.8
@>     GLU139    P   OE1_2125_2126  <--->      HSE66    P         NE2_957     4.0
@>      ARG75    P   NH1_1090_1093  <--->      ASP42    P     OD1_609_610     4.5
@> Number of detected salt bridges: 14.

@> Frame: 2
@> Calculating salt bridges.
@>     GLU114    P   OE1_1735_1736  <--->     LYS112    P         NZ_1699     2.6
@>      ASP32    P     OD1_443_444  <--->      LYS28    P          NZ_380     2.6
@>     GLU139    P   OE1_2125_2126  <--->      ARG65    P     NH1_938_941     2.7
@>      ASP81    P   OD1_1193_1194  <--->      ARG75    P   NH1_1090_1093     2.9
@>     LYS102    P         NZ_1540  <--->      ASP98    P   OD1_1463_1464     3.1
@>      ARG58    P     NH1_829_832  <--->      ASP56    P     OD1_788_789     3.6
@>     GLU139    P   OE1_2125_2126  <--->      HSE66    P         NE2_957     3.6
@>      ARG18    P     NH1_217_220  <--->      ASP92    P   OD1_1368_1369     3.7
@>      ASP86    P   OD1_1269_1270  <--->     LYS110    P         NZ_1667     3.7
@>     ASP120    P   OD1_1824_1825  <--->     ARG147    P   NH1_2257_2260     3.8
@>      ARG27    P     NH1_356_359  <--->      GLU23    P     OE1_290_291     3.9
@>     HSE157    P        NE2_2418  <--->     GLU114    P   OE1_1735_1736     4.2
@>      ARG75    P   NH1_1090_1093  <--->      ASP42    P     OD1_609_610     4.3
@>      ARG18    P     NH1_217_220  <--->     ASP129    P   OD1_1978_1979     4.6
@>      ASP86    P   OD1_1269_1270  <--->       LYS6    P           NZ_32     5.0
@> Number of detected salt bridges: 15.
```

```
..
..

@> Frame: 18
@> Calculating salt bridges.
@>      ASP81    P   OD1_1193_1194  <--->      ARG75    P   NH1_1090_1093     2.6
@>      ASP32    P     OD1_443_444  <--->      LYS28    P          NZ_380     2.7
@>     ASP135    P   OD1_2067_2068  <--->      ARG65    P     NH1_938_941     2.8
@>     LYS102    P         NZ_1540  <--->      ASP98    P   OD1_1463_1464     3.0
@>      GLU23    P     OE1_290_291  <--->      HSE72    P        NE2_1042     3.4
@>      ARG27    P     NH1_356_359  <--->      GLU23    P     OE1_290_291     3.6
@>      ARG58    P     NH1_829_832  <--->      ASP56    P     OD1_788_789     3.6
@>      ASP98    P   OD1_1463_1464  <--->     ARG101    P   NH1_1516_1519     3.9
@>      ARG18    P     NH1_217_220  <--->      ASP92    P   OD1_1368_1369     4.2
@>      ARG97    P   NH1_1447_1450  <--->      GLU93    P   OE1_1383_1384     4.5
@>     ARG150    P   NH1_2303_2306  <--->     GLU154    P   OE1_2371_2372     4.5
@>      ARG75    P   NH1_1090_1093  <--->      ASP42    P     OD1_609_610     4.5
@>      ARG18    P     NH1_217_220  <--->     ASP129    P   OD1_1978_1979     4.7
@> Number of detected salt bridges: 13.

@> Frame: 19
@> Calculating salt bridges.
@>     ASP135    P   OD1_2067_2068  <--->      ARG65    P     NH1_938_941     2.7
@>      ASP81    P   OD1_1193_1194  <--->      ARG75    P   NH1_1090_1093     2.9
@>     LYS102    P         NZ_1540  <--->      ASP98    P   OD1_1463_1464     3.1
@>      ARG27    P     NH1_356_359  <--->      GLU23    P     OE1_290_291     3.3
@>      ASP98    P   OD1_1463_1464  <--->     ARG101    P   NH1_1516_1519     3.7
@>      ARG58    P     NH1_829_832  <--->      ASP56    P     OD1_788_789     3.7
@>      ARG97    P   NH1_1447_1450  <--->      GLU93    P   OE1_1383_1384     3.7
@>      ASP86    P   OD1_1269_1270  <--->     LYS110    P         NZ_1667     3.9
@>      ARG18    P     NH1_217_220  <--->      ASP92    P   OD1_1368_1369     3.9
@>      GLU23    P     OE1_290_291  <--->      HSE72    P        NE2_1042     4.0
@>     ARG150    P   NH1_2303_2306  <--->     GLU154    P   OE1_2371_2372     4.2
@>      ARG75    P   NH1_1090_1093  <--->      ASP42    P     OD1_609_610     4.6
@> Number of detected salt bridges: 12.

@> Frame: 20
@> Calculating salt bridges.
@>     ASP135    P   OD1_2067_2068  <--->      ARG65    P     NH1_938_941     2.5
@>      ASP81    P   OD1_1193_1194  <--->      ARG75    P   NH1_1090_1093     2.7
@>      ASP98    P   OD1_1463_1464  <--->     ARG101    P   NH1_1516_1519     2.8
@>      ASP86    P   OD1_1269_1270  <--->     LYS110    P         NZ_1667     3.4
@>      ARG97    P   NH1_1447_1450  <--->      GLU93    P   OE1_1383_1384     3.5
@>     ARG150    P   NH1_2303_2306  <--->     GLU154    P   OE1_2371_2372     3.7
@>      ARG58    P     NH1_829_832  <--->      ASP56    P     OD1_788_789     3.7
@>     GLU139    P   OE1_2125_2126  <--->      HSE66    P         NE2_957     3.9
@>      ARG18    P     NH1_217_220  <--->      ASP92    P   OD1_1368_1369     4.0
@>      ARG27    P     NH1_356_359  <--->      GLU23    P     OE1_290_291     4.0
@>      ARG75    P   NH1_1090_1093  <--->      ASP42    P     OD1_609_610     4.4
@>      GLU23    P     OE1_290_291  <--->      HSE72    P        NE2_1042     4.7
@>     GLU139    P   OE1_2125_2126  <--->      ARG65    P     NH1_938_941     4.8
@>      ARG18    P     NH1_217_220  <--->     ASP129    P   OD1_1978_1979     5.0
@> Number of detected salt bridges: 14.
```

Repulsive Ionic Bonding using `calcRepulsiveIonicBondingTrajectory()` for residues with the same charges:

```
In [9]: calcRepulsiveIonicBondingTrajectory(atoms, dcd, distA=7)
```

```
@> Frame: 0
@> Calculating repulsive ionic bonding.
@>     LYS102    P         NZ_1540  <--->     ARG101    P   NH1_1516_1519     4.3
@> Number of detected Repulsive Ionic Bonding interactions: 1.
@> Frame: 1
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Frame: 2
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Frame: 3
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Frame: 4
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Frame: 5
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Frame: 6
@> Calculating repulsive ionic bonding.
@>     LYS102    P         NZ_1540  <--->     ARG101    P   NH1_1516_1519     4.3
@> Number of detected Repulsive Ionic Bonding interactions: 1.
@> Frame: 7
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Frame: 8
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
@> Frame: 9
@> Calculating repulsive ionic bonding.
@>     LYS102    P         NZ_1540  <--->     ARG101    P   NH1_1516_1519     4.3
@> Number of detected Repulsive Ionic Bonding interactions: 1.
@> Frame: 10
@> Calculating repulsive ionic bonding.
@> Number of detected Repulsive Ionic Bonding interactions: 0.
..
..
@> Frame: 20
@> Calculating repulsive ionic bonding.
@>     ARG147    P   NH1_2257_2260  <--->     LYS123    P         NZ_1875     4.5
@> Number of detected Repulsive Ionic Bonding interactions: 1.
```

Pi-Stacking interactions using `calcPiStackingTrajectory()`:

```
In [10]: calcPiStackingTrajectory(atoms, dcd, distA=5)
```

```
@> Frame: 0
@> Calculating Pi stacking interactions.
@>      HSE66       P             953_954_955_957_959  <--->     TYR142       P   2166_2167_2169_2171
@>     HSE157       P2414_2415_2416_2418_2420_2423_2424  <--->     TYR119       P   1802_1803_1805_18
@>      PHE26       P         327_328_330_332_334_336  <--->      TRP39       P         549_550_551_5
@>     TYR132       P   2024_2025_2027_2029_2032_2034  <--->     TYR131       P   2003_2004_2006_2008
@> Number of detected Pi stacking interactions: 4.
@> Frame: 1
@> Calculating Pi stacking interactions.
```

```
@>      PHE26       P         327_328_330_332_334_336  <--->      TRP39       P         549_550_551_5
@>      HSE66       P             953_954_955_957_959  <--->     TYR142       P   2166_2167_2169_2171
@> Number of detected Pi stacking interactions: 2.
@> Frame: 2
@> Calculating Pi stacking interactions.
@>      HSE66       P             953_954_955_957_959  <--->     TYR142       P   2166_2167_2169_2171
@> Number of detected Pi stacking interactions: 1.
@> Frame: 3
@> Calculating Pi stacking interactions.
@>      HSE66       P             953_954_955_957_959  <--->     TYR142       P   2166_2167_2169_2171
@> Number of detected Pi stacking interactions: 1.
@> Frame: 4
@> Calculating Pi stacking interactions.
@>      HSE66       P             953_954_955_957_959  <--->     TYR142       P   2166_2167_2169_2171
@>      TYR87       P   1280_1281_1283_1285_1288_1290  <--->     PHE152       P   2328_2329_2331_2333
@> Number of detected Pi stacking interactions: 2.
..
..
@> Frame: 19
@> Calculating Pi stacking interactions.
@>     TYR132       P   2024_2025_2027_2029_2032_2034  <--->     TYR131       P   2003_2004_2006_2008
@>     TYR119       P   1802_1803_1805_1807_1810_1812  <--->     PHE152       P   2328_2329_2331_2333
@> Number of detected Pi stacking interactions: 2.
@> Frame: 20
@> Calculating Pi stacking interactions.
@>     TYR119       P   1802_1803_1805_1807_1810_1812  <--->     PHE152       P   2328_2329_2331_2333
@>      HSE66       P             953_954_955_957_959  <--->     TYR142       P   2166_2167_2169_2171
@>     TYR132       P   2024_2025_2027_2029_2032_2034  <--->     TYR131       P   2003_2004_2006_2008
@> Number of detected Pi stacking interactions: 3.
```

Pi-Cation interactions using `calcPiCationTrajectory()`:

```
In [11]: calcPiCationTrajectory(atoms, dcd)
```

```
@> Frame: 0
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_5
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                    NH1_938_9
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                          NZ_
@> Number of detected cation-pi interactions: 3.
@> Frame: 1
@> Calculating cation-Pi interactions.
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                          NZ_
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_5
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                    NH1_938_9
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->     LYS112   P                        NZ_16
@>     TYR131   P   2003_2004_2006_2008_2011_2013  <--->      ARG58   P                    NH1_829_8
@> Number of detected cation-pi interactions: 5.
@> Frame: 2
@> Calculating cation-Pi interactions.
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                          NZ_
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                    NH1_938_9
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_5
@> Number of detected cation-pi interactions: 3.
@> Frame: 3
@> Calculating cation-Pi interactions.
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                          NZ_
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_5
```

```
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                    NH1_938_
@> Number of detected cation-pi interactions: 3.
@> Frame: 4
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                    NH1_938_
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS155   P                          NZ_
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                          NZ_
@> Number of detected cation-pi interactions: 4.
..
..
@> Frame: 19
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_
@> Number of detected cation-pi interactions: 1.
@> Frame: 20
@> Calculating cation-Pi interactions.
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                    NH1_829_
@> Number of detected cation-pi interactions: 1.
```

Hydrophobic interactions using `calcHydrophohicTrajectory()`:

```
In [12]: calcHydrophohicTrajectory(atoms, dcd)
```

```
@> Frame: 0
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>     ALA156    P    CB_240114s  <--->      TYR87    P    OH_1286     3.0    22.0
@>      ALA24    P     CB_29814s  <--->      MET63    P     CE_894     3.3     5.2
@>      ILE68    P    CG2_97614s  <--->      MET63    P     CE_894     3.3    52.4
@>     TYR142    P    CZ_217114s  <--->     VAL146    P   CG2_2235     3.5    49.7
@>      PHE10    P     CD1_9214s  <--->      ALA22    P     CB_273     3.5    31.2
@>       LYS6    P      CD_2614s  <--->      TRP39    P    CZ2_555     3.5    68.7
@>      PHE26    P    CE2_33614s  <--->      VAL30    P    CG1_411     3.6    21.1
@>      ILE88    P    CD_130714s  <--->     ALA111    P    CB_1677     3.6    21.2
@>      VAL11    P    CG2_11414s  <--->      ILE88    P   CG2_1300     3.6     9.3
@>      VAL41    P    CG2_59514s  <--->      PHE26    P    CD2_334     3.6    16.6
@>     PHE152    P   CE1_233114s  <--->     ALA156    P    CB_2401     3.7    17.5
@>      LYS79    P    CG_115514s  <--->     VAL106    P   CG2_1598     3.7    25.1
@>      LEU99    P   CD2_148014s  <--->      ILE77    P    CD_1128     3.7    12.0
@>      PHE82    P   CD1_120514s  <--->      ILE88    P    CD_1307     3.7    17.6
@>     LEU116    P   CD2_177114s  <--->     ILE127    P    CD_1949     3.7    17.4
@>       VAL8    P     CG1_5514s  <--->      PHE26    P    CE2_336     3.7    12.1
@>      LEU96    P   CD1_142114s  <--->     ILE113    P   CG2_1711     3.7    17.0
@>       LEU9    P     CD2_7814s  <--->      ILE77    P    CD_1128     3.7    15.4
@>      LEU89    P   CD1_132214s  <--->       VAL8    P     CG2_59     3.8    15.9
@>     ILE126    P    CD_193014s  <--->     LEU125    P   CD1_1907     3.8    54.2
@>     VAL141    P   CG1_214914s  <--->     ILE127    P   CG2_1942     3.9    11.5
@>      MET91    P    SD_135314s  <--->     ILE127    P    CD_1949     3.9    35.9
@>      ALA44    P     CB_62814s  <--->       LEU9    P     CD1_74     3.9    15.1
@>      VAL25    P    CG2_31414s  <--->     TYR142    P   CE1_2169     3.9    12.0
@>      ILE21    P    CG2_25614s  <--->      MET63    P     SD_893     4.0    20.8
@>     LEU153    P   CD1_235014s  <--->      TRP39    P    NE1_547     4.0     9.4
@>      PHE85    P    CZ_125314s  <--->       LEU9    P     CD1_74     4.0    32.1
@>      ILE35    P     CD_49114s  <--->      TRP39    P    NE1_547     4.0    26.0
@>      LEU29    P    CD1_39514s  <--->      VAL25    P    CG1_310     4.1    19.7
@>      ALA74    P    CB_106814s  <--->      ILE16    P    CG2_177     4.1     6.7
@>      ARG75    P    CG_108114s  <--->      ALA44    P     CB_628     4.1    36.2
```

```
@>      ARG18    P     CG_20814s  <--->     VAL141    P   CG1_2149     4.1    20.3
@>     LYS102    P    CD_153414s  <--->      ILE77    P   CG2_1121     4.1    17.5
@>     TYR119    P   CE1_180514s  <--->      LEU89    P   CD2_1326     4.1    11.6
@>      ARG40    P     CG_56814s  <--->      PHE85    P   CE2_1257     4.3    60.9
@>      LYS28    P     CG_37114s  <--->      ILE68    P     CD_983     4.3    21.8
@>     PHE138    P   CD2_210814s  <--->      ILE21    P     CD_263     4.3     6.6
@>     TYR131    P   CE1_200614s  <--->      ILE16    P     CD_184     4.3     8.9
@>      ARG58    P     CG_82014s  <--->     PHE138    P   CE1_2104     4.5    59.4
@> Number of detected hydrophobic interactions: 39.
@> Frame: 1
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      MET63    P     SD_89314s  <--->     TYR142    P   CD1_2167     3.3    26.8
@>      ALA24    P     CB_29814s  <--->      MET63    P     CE_894     3.4     7.1
@>       VAL8    P     CG2_5914s  <--->      PHE10    P      CZ_96     3.4    27.8
@>      LEU96    P   CD1_142114s  <--->     ILE113    P   CG2_1711     3.4    13.3
@>     LEU116    P   CD1_176714s  <--->      PHE10    P     CE1_94     3.5    13.5
@>      PHE82    P    CZ_120914s  <--->      ILE77    P    CD_1128     3.6    20.4
@>      ILE68    P     CD_98314s  <--->     TYR142    P    OH_2172     3.6    27.4
@>      PHE26    P    CE2_33614s  <--->      VAL30    P    CG1_411     3.6    28.1
@>     ALA156    P    CB_240114s  <--->     PHE152    P   CD1_2329     3.6    24.5
@>      VAL11    P    CG2_11414s  <--->      ILE88    P   CG2_1300     3.6     8.6
@>     LYS102    P    CD_153414s  <--->      ILE77    P   CG2_1121     3.7    18.2
@>      LEU99    P   CD2_148014s  <--->      ILE77    P    CD_1128     3.7     8.0
@>     LEU153    P   CD1_235014s  <--->      VAL30    P    CG1_411     3.7    14.5
@>       LEU9    P     CD2_7814s  <--->      ILE77    P    CD_1128     3.7    16.0
@>      TRP39    P    CD1_54514s  <--->      VAL30    P    CG1_411     3.7    14.9
@>     PHE138    P   CD2_210814s  <--->      ILE21    P     CD_263     3.8    15.8
@>     TYR119    P    OH_180814s  <--->     ALA156    P    CB_2401     3.8    18.6
@>     VAL146    P   CG2_223514s  <--->     TYR142    P    CZ_2171     3.8    40.5
@>      VAL25    P    CG2_31414s  <--->     TYR142    P   CD1_2167     3.8    14.3
@>      MET91    P    CE_135414s  <--->     LEU116    P   CD2_1771     3.8    19.1
@>      ILE35    P     CD_49114s  <--->     LEU153    P   CD1_2350     3.9    17.2
@>      VAL41    P    CG2_59514s  <--->      PHE26    P    CD2_334     3.9    21.9
@>     ILE127    P    CD_194914s  <--->     LEU116    P   CD2_1771     3.9    11.7
@>      LEU29    P    CD1_39514s  <--->      VAL25    P    CG1_310     3.9    25.1
@>      ALA22    P     CB_27314s  <--->     LEU116    P   CD2_1771     4.0     7.3
@>     ALA111    P    CB_167714s  <--->      ILE88    P    CD_1307     4.0    14.9
@>      ARG75    P    CG_108114s  <--->      ALA44    P     CB_628     4.0    36.8
@>     ILE126    P    CD_193014s  <--->     LEU125    P    CG_1905     4.0    53.2
@>     VAL106    P   CG2_159814s  <--->      PHE82    P   CD2_1211     4.0    13.1
@>      PHE85    P    CZ_125314s  <--->       LEU9    P     CD1_74     4.1    28.5
@>      ARG40    P     CG_56814s  <--->      PHE85    P   CE2_1257     4.1    50.3
@>      TYR87    P   CD1_128114s  <--->      LEU89    P   CD2_1326     4.2    14.7
@>      LYS28    P     CG_37114s  <--->      ILE68    P    CG2_976     4.2    15.9
@>      LYS79    P    CG_115514s  <--->     VAL106    P   CG2_1598     4.2    20.4
@>      ARG18    P     CG_20814s  <--->     VAL141    P   CG1_2149     4.3    10.9
@>      ARG58    P     CG_82014s  <--->     PHE138    P   CD1_2102     4.3    48.8
@>      ALA74    P    CB_106814s  <--->      ILE16    P    CG2_177     4.4     4.3
@>     ARG150    P    CG_229414s  <--->      LEU29    P    CD2_399     4.5    22.3
@> Number of detected hydrophobic interactions: 38.
..
..
@> Frame: 20
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      LEU96    P   CD1_142114s  <--->     ILE113    P   CG2_1711     3.3    21.1
@>      ILE88    P    CD_130714s  <--->      PHE82    P   CD2_1211     3.4    25.2
```

```
@>      VAL11    P    CG2_11414s  <--->      LEU99    P   CD1_1476     3.4    11.5
@>      MET63    P     SD_89314s  <--->     TYR142    P   CE1_2169     3.4    37.7
@>      TRP39    P    NE1_54714s  <--->     LEU153    P   CD1_2350     3.4    19.2
@>     ALA111    P    CB_167714s  <--->      ILE88    P    CD_1307     3.5    23.0
@>      ILE35    P     CD_49114s  <--->     LEU153    P   CD1_2350     3.5    16.4
@>      VAL30    P    CG1_41114s  <--->     LEU153    P   CD2_2354     3.5     9.8
@>       LEU9    P     CD2_7814s  <--->      ILE77    P    CD_1128     3.5    17.0
@>      PHE10    P     CE1_9414s  <--->      LEU89    P   CD1_1322     3.5    25.4
@>     TYR119    P   CE1_180514s  <--->      LEU89    P   CD2_1326     3.6    18.5
@>      ALA24    P     CB_29814s  <--->      MET63    P     CE_894     3.6    13.8
@>      PHE26    P     CZ_33214s  <--->     LEU153    P   CD1_2350     3.6    27.1
@>       VAL8    P     CG2_5914s  <--->      LEU89    P   CD1_1322     3.6    13.0
@>      ALA22    P     CB_27314s  <--->      PHE10    P     CD1_92     3.6    29.5
@>      MET91    P    CE_135414s  <--->      ALA22    P     CB_273     3.7     9.1
@>      VAL41    P    CG2_59514s  <--->      PHE26    P    CD2_334     3.7    17.5
@>     LEU116    P   CD2_177114s  <--->      MET91    P    SD_1353     3.7    21.9
@>      ALA44    P     CB_62814s  <--->      VAL11    P    CG1_110     3.7    34.2
@>       LYS6    P      CD_2614s  <--->      TRP39    P    CH2_557     3.7    44.8
@>     VAL146    P   CG2_223514s  <--->     TYR142    P   CE2_2176     3.8    39.4
@>      PHE85    P   CE1_125114s  <--->       LEU9    P     CD1_74     3.8    31.6
@>      ILE21    P    CG2_25614s  <--->      VAL25    P    CG2_314     3.8    25.0
@>     VAL141    P   CG1_214914s  <--->      ILE21    P     CD_263     3.9    13.0
@>      ILE68    P    CG1_98014s  <--->      MET63    P     CE_894     3.9    37.2
@>     PHE152    P    CZ_233314s  <--->      LEU89    P   CD1_1322     3.9    18.0
@>      ARG18    P     CG_20814s  <--->     VAL141    P   CG1_2149     4.0    26.2
@>      ARG75    P    CG_108114s  <--->      ALA44    P     CB_628     4.2    27.4
@>     ILE127    P    CD_194914s  <--->     LEU116    P   CD2_1771     4.3     7.9
@>      LYS79    P    CG_115514s  <--->     VAL106    P   CG2_1598     4.3    15.6
@>      LEU29    P     CG_39314s  <--->      VAL25    P    CG1_310     4.3    21.7
@>     ILE126    P   CG1_192714s  <--->     LEU125    P    CG_1905     4.4    55.6
@> Number of detected hydrophobic interactions: 32.
```

In this particular example you will not have disulfide bonds, but you can compute it using `calcDisulfideBondsTrajectory()`:

```
In [13]: calcDisulfideBondsTrajectory(atoms, dcd)
```

```
@> Frame: 0
@> Calculating disulfide bonds.
@> Number of detected disulfide bonds: 0.
@> Frame: 1
@> Calculating disulfide bonds.
@> Number of detected disulfide bonds: 0.
@> Frame: 2
@> Calculating disulfide bonds.
@> Number of detected disulfide bonds: 0.
@> Frame: 3
@> Calculating disulfide bonds.
@> Number of detected disulfide bonds: 0.
@> Frame: 4
@> Calculating disulfide bonds.
@> Number of detected disulfide bonds: 0.
..
..
```

6.2 Compute all availabe types of interactions

First, we instantiate a `InteractionsTrajectory` instance, which stores all the information about interactions for protein structure for multiple frames. With `InteractionsTrajectory.calcProteinInteractionsTrajectory()`, we can compute all types of interactions such as hydrogen bonds, salt bridges, repulsive ionic bonding, Pi-cation, Pi-stacking, and hydrophobic) at once. Be aware that those computations may take a while, depending on the size of the system and the number of frames that are stored by the DCD file. Therefore, we recommend saving the results as a `filename` file. `filename` file, here `calcProteinInteractionsTrajectory.pkl`, can be reloaded and used with all available functions and methods.

```
In [14]: interactionsTrajectory = InteractionsTrajectory('trajectory')

In [15]: interactionsTrajectory.calcProteinInteractionsTrajectory(atoms, dcd,
   ....:     filename='calcProteinInteractionsTrajectory')
   ....:
```

```
@> Frame: 0
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)    <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     ARG101    P      NH1_1516  <--->      ASP98    P      OD1_1463     2.0    33.1
@>      HSE72    P      NE2_1042  <--->      ASN15    P       OD1_165     2.6    34.8
@>     GLN143    P      NE2_2192  <--->     GLU139    P      OE2_2126     2.7     9.2
@>      HSE66    P       NE2_957  <--->     GLU139    P      OE1_2125     2.7     6.4
@>      ARG40    P         N_561  <--->       LYS6    P          O_37     2.7    17.1
@>      ARG58    P         N_813  <--->      ASP56    P       OD1_788     2.7    30.0
@>      ALA45    P         N_634  <--->      ARG75    P        O_1097     2.8    35.1
@>      ASN53    P       ND2_747  <--->      GLU50    P       OE1_708     2.8    18.2
@>      ALA74    P        N_1064  <--->      ASN53    P         O_751     2.8    21.3
@>      ASP56    P         N_780  <--->      ILE16    P         O_189     2.8    27.0
@>     LYS110    P       NZ_1667  <--->      THR84    P        O_1240     2.8    38.2
@>     LEU116    P        N_1758  <--->      CYS90    P        O_1342     2.8    15.0
@>     SER103    P        N_1546  <--->      LEU99    P        O_1485     2.8    29.1
@>     ASN134    P        N_2045  <--->     ASP137    P      OD2_2091     2.8    22.6
@>     PHE152    P        N_2321  <--->     CYS148    P        O_2275     2.8     8.3
@>      ASN95    P        N_1398  <--->      ASP92    P      OD1_1368     2.8    12.6
@>       LYS6    P          N_16  <--->      ASN38    P         O_536     2.8    25.0
@>      ILE77    P        N_1115  <--->      ALA45    P         O_643     2.8    12.2
@>      ARG58    P       NH2_832  <--->      ASP56    P       OD2_789     2.8    27.7
@>      LEU99    P        N_1467  <--->      ASN95    P        O_1411     2.8    15.5
@>     CYS149    P        N_2276  <--->     CYS145    P        O_2224     2.8     9.6
@>      GLY52    P         N_731  <--->      ALA74    P        O_1073     2.8     6.6
@>      ASP32    P         N_435  <--->      LYS28    P         O_385     2.8     8.8
@>      ILE88    P        N_1294  <--->     LYS112    P        O_1704     2.8    17.7
@>     GLN143    P        N_2180  <--->     GLU139    P        O_2128     2.8    21.7
@>      ARG27    P         N_340  <--->      GLU23    P         O_293     2.8    15.4
@>     TYR142    P        N_2159  <--->     PHE138    P        O_2113     2.9    14.2
@>     GLY133    P        N_2038  <--->     PRO130    P        O_1995     2.9    25.4
@>      PHE26    P         N_320  <--->      ALA22    P         O_278     2.9     4.9
@>      ASN15    P       ND2_166  <--->      SER19    P        OG_232     2.9    32.1
@>      ARG75    P      NH1_1090  <--->      ASP81    P      OD2_1194     2.9    19.7
@>      ARG75    P      NH2_1093  <--->      ASP42    P       OD2_610     2.9    23.5
@>      ARG97    P        N_1431  <--->      GLU93    P        O_1386     2.9    22.2
@>      ARG65    P       NH2_941  <--->     GLU139    P      OE1_2125     2.9    32.3
@>      VAL25    P         N_304  <--->      ILE21    P         O_268     2.9     8.2
@>     LEU153    P        N_2341  <--->     CYS149    P        O_2286     2.9    12.5
@>       SER7    P          N_38  <--->      ASP86    P      OD2_1270     2.9    39.9
@>      ASP86    P        N_1261  <--->       SER7    P         OG_45     2.9    34.7
```

```
@>      ARG58    P       NH2_832  <--->     TYR131    P        O_2016     2.9    33.1
@>      THR46    P         N_644  <--->      CYS12    P         O_130     2.9    36.1
@>     GLN144    P        N_2197  <--->     THR140    P        O_2142     2.9    23.3
@>      THR78    P        N_1134  <--->      ASP81    P      OD2_1194     2.9    12.4
@>      LEU89    P        N_1313  <--->       LEU9    P          O_83     2.9    29.5
@>      THR31    P         N_421  <--->      ARG27    P         O_363     2.9    24.1
@>      CYS90    P        N_1332  <--->     GLU114    P        O_1738     2.9    24.6
@>     CYS148    P        N_2265  <--->     GLN144    P        O_2213     2.9     9.3
@>      GLU23    P         N_279  <--->      SER19    P         O_235     2.9    15.4
@>      ILE68    P         N_970  <--->      MET63    P         O_899     2.9    13.0
@>      PHE10    P          N_84  <--->      ASP42    P         O_612     2.9    22.8
@>     LYS112    P        N_1683  <--->      ASP86    P        O_1272     2.9    10.1
@>      SER61    P         N_861  <--->      TYR57    P         O_812     2.9    35.1
@>     CYS145    P        N_2214  <--->     VAL141    P        O_2158     2.9    15.9
@>      ARG27    P       NH2_359  <--->      GLU23    P       OE2_291     2.9    31.5
@>      LYS64    P         N_900  <--->      GLN60    P         O_860     2.9    22.9
@>       LEU9    P          N_65  <--->      TYR87    P        O_1293     2.9    16.4
@>      ASN38    P         N_523  <--->      ILE35    P         O_496     2.9    29.1
@>      VAL11    P         N_104  <--->      LEU89    P        O_1331     2.9    29.7
@>     ASN100    P        N_1486  <--->      LEU96    P        O_1430     2.9    10.3
..
..
@> Number of detected hydrogen bonds: 124.
@> Calculating salt bridges.
@>     GLU139    P   OE1_2125_2126  <--->      HSE66    P         NE2_957     2.8
@>      ASP81    P   OD1_1193_1194  <--->      ARG75    P   NH1_1090_1093     2.9
@>      ASP32    P     OD1_443_444  <--->      LYS28    P          NZ_380     3.0
@>      ASP98    P   OD1_1463_1464  <--->     ARG101    P   NH1_1516_1519     3.1
@>      ARG27    P     NH1_356_359  <--->      GLU23    P     OE1_290_291     3.7
@>     GLU139    P   OE1_2125_2126  <--->      ARG65    P     NH1_938_941     3.8
@>     LYS102    P         NZ_1540  <--->      ASP98    P   OD1_1463_1464     3.9
@>      ARG58    P     NH1_829_832  <--->      ASP56    P     OD1_788_789     3.9
@>      ARG18    P     NH1_217_220  <--->      ASP92    P   OD1_1368_1369     4.1
@>     GLU114    P   OE1_1735_1736  <--->     LYS112    P         NZ_1699     4.1
@>     ASP120    P   OD1_1824_1825  <--->     ARG147    P   NH1_2257_2260     4.2
@>      ASP86    P   OD1_1269_1270  <--->     LYS110    P         NZ_1667     4.2
@>     HSE157    P        NE2_2418  <--->     GLU114    P   OE1_1735_1736     4.4
@>      ARG18    P     NH1_217_220  <--->     ASP129    P   OD1_1978_1979     4.6
@>      ARG75    P   NH1_1090_1093  <--->      ASP42    P     OD1_609_610     4.6
@>      GLU23    P     OE1_290_291  <--->      HSE72    P        NE2_1042     5.0
@> Number of detected salt bridges: 16.
@> Calculating repulsive ionic bonding.
@>     LYS102    P         NZ_1540  <--->     ARG101    P   NH1_1516_1519     4.3
@> Number of detected Repulsive Ionic Bonding interactions: 1.
@> Calculating Pi stacking interactions.
@>      HSE66       P             953_954_955_957_959  <--->     TYR142       P   2166_2167_2169_2171
@>     HSE157       P2414_2415_2416_2418_2420_2423_2424  <--->     TYR119       P   1802_1803_1805_18
@>      PHE26       P         327_328_330_332_334_336  <--->      TRP39       P         549_550_551_5
@>     TYR132       P   2024_2025_2027_2029_2032_2034  <--->     TYR131       P   2003_2004_2006_2008
@> Number of detected Pi stacking interactions: 4.
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_5
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                    NH1_938_9
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                          NZ_
@> Number of detected cation-pi interactions: 3.
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>     ALA156    P    CB_240114s  <--->      TYR87    P    OH_1286     3.0    22.0
```

```
@>      ALA24    P     CB_29814s  <--->      MET63    P     CE_894     3.3     5.2
@>      ILE68    P    CG2_97614s  <--->      MET63    P     CE_894     3.3    52.4
@>     TYR142    P    CZ_217114s  <--->     VAL146    P   CG2_2235     3.5    49.7
@>      PHE10    P     CD1_9214s  <--->      ALA22    P     CB_273     3.5    31.2
@>       LYS6    P      CD_2614s  <--->      TRP39    P    CZ2_555     3.5    68.7
@>      PHE26    P    CE2_33614s  <--->      VAL30    P    CG1_411     3.6    21.1
@>      ILE88    P    CD_130714s  <--->     ALA111    P    CB_1677     3.6    21.2
@>      VAL11    P    CG2_11414s  <--->      ILE88    P   CG2_1300     3.6     9.3
@>      VAL41    P    CG2_59514s  <--->      PHE26    P    CD2_334     3.6    16.6
@>     PHE152    P   CE1_233114s  <--->     ALA156    P    CB_2401     3.7    17.5
@>      LYS79    P    CG_115514s  <--->     VAL106    P   CG2_1598     3.7    25.1
@>      LEU99    P   CD2_148014s  <--->      ILE77    P    CD_1128     3.7    12.0
@>      PHE82    P   CD1_120514s  <--->      ILE88    P    CD_1307     3.7    17.6
@>     LEU116    P   CD2_177114s  <--->     ILE127    P    CD_1949     3.7    17.4
@>       VAL8    P     CG1_5514s  <--->      PHE26    P    CE2_336     3.7    12.1
@>      LEU96    P   CD1_142114s  <--->     ILE113    P   CG2_1711     3.7    17.0
@>       LEU9    P     CD2_7814s  <--->      ILE77    P    CD_1128     3.7    15.4
@>      LEU89    P   CD1_132214s  <--->       VAL8    P     CG2_59     3.8    15.9
@>     ILE126    P    CD_193014s  <--->     LEU125    P   CD1_1907     3.8    54.2
@>     VAL141    P   CG1_214914s  <--->     ILE127    P   CG2_1942     3.9    11.5
@>      MET91    P    SD_135314s  <--->     ILE127    P    CD_1949     3.9    35.9
@>      ALA44    P     CB_62814s  <--->       LEU9    P     CD1_74     3.9    15.1
@>      VAL25    P    CG2_31414s  <--->     TYR142    P   CE1_2169     3.9    12.0
@>      ILE21    P    CG2_25614s  <--->      MET63    P     SD_893     4.0    20.8
@>     LEU153    P   CD1_235014s  <--->      TRP39    P    NE1_547     4.0     9.4
@>      PHE85    P    CZ_125314s  <--->       LEU9    P     CD1_74     4.0    32.1
@>      ILE35    P     CD_49114s  <--->      TRP39    P    NE1_547     4.0    26.0
@>      LEU29    P    CD1_39514s  <--->      VAL25    P    CG1_310     4.1    19.7
@>      ALA74    P    CB_106814s  <--->      ILE16    P    CG2_177     4.1     6.7
@>      ARG75    P    CG_108114s  <--->      ALA44    P     CB_628     4.1    36.2
@>      ARG18    P     CG_20814s  <--->     VAL141    P   CG1_2149     4.1    20.3
@>     LYS102    P    CD_153414s  <--->      ILE77    P   CG2_1121     4.1    17.5
@>     TYR119    P   CE1_180514s  <--->      LEU89    P   CD2_1326     4.1    11.6
@>      ARG40    P     CG_56814s  <--->      PHE85    P   CE2_1257     4.3    60.9
@>      LYS28    P     CG_37114s  <--->      ILE68    P     CD_983     4.3    21.8
@>     PHE138    P   CD2_210814s  <--->      ILE21    P     CD_263     4.3     6.6
@>     TYR131    P   CE1_200614s  <--->      ILE16    P     CD_184     4.3     8.9
@>      ARG58    P     CG_82014s  <--->     PHE138    P   CE1_2104     4.5    59.4
@> Number of detected hydrophobic interactions: 39.
@> Calculating disulfide bonds.
@> Number of detected disulfide bonds: 0.
..
..
@> Frame: 20
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      ARG97    P       NE_1444  <--->      GLU93    P      OE1_1383     2.5    12.5
@>      SER19    P        OG_232  <--->      ASN15    P       OD1_165     2.6    31.5
@>      ARG27    P       NH1_356  <--->      GLU23    P       OE1_290     2.6    19.1
@>      THR78    P        N_1134  <--->      ASP81    P      OD2_1194     2.6    21.5
@>     GLN122    P      NE2_1854  <--->     ASP120    P      OD2_1825     2.6    39.7
@>     SER118    P       OG_1791  <--->     GLU114    P      OE2_1736     2.6    24.5
@>      ARG65    P       NH1_938  <--->     GLU139    P      OE1_2125     2.7     6.1
@>      ARG65    P       NH2_941  <--->     ASP135    P      OD1_2067     2.7    15.6
@>      SER43    P        OG_620  <--->      GLU23    P       OE2_291     2.7    13.9
@>      ARG75    P       NE_1087  <--->      ASP42    P       OD1_609     2.7    26.5
@>     ARG150    P       NE_2300  <--->     GLU154    P      OE2_2372     2.7     4.9
@>     VAL106    P        N_1588  <--->     LYS102    P        O_1545     2.7    16.2
```

```
@>      LYS28    P         N_364  <--->      ALA24    P         O_303     2.7    38.8
@>     HSE157    P      NE2_2418  <--->     PHE152    P        O_2340     2.7    28.5
@>      ARG58    P       NH2_832  <--->      ASP56    P       OD2_789     2.7    19.3
@>      ARG97    P      NH2_1450  <--->      GLU93    P      OE2_1384     2.7    15.8
@>      ARG75    P      NH2_1093  <--->      ASP42    P       OD1_609     2.7    30.5
@>      ALA45    P         N_634  <--->      ARG75    P        O_1097     2.7    22.3
@>      ARG75    P      NH2_1093  <--->      ASP81    P      OD1_1193     2.7    19.2
@>      THR31    P       OG1_427  <--->      ARG27    P         O_363     2.7    13.1
@>     ARG150    P      NH2_2306  <--->     GLU154    P      OE1_2371     2.7     8.5
@>      ARG75    P      NH1_1090  <--->      ASP81    P      OD2_1194     2.7    14.8
@>      GLY67    P         N_963  <--->      MET63    P         O_899     2.7    25.3
@>      LEU89    P        N_1313  <--->       LEU9    P          O_83     2.8    18.4
@>     ARG101    P      NH1_1516  <--->      ASP98    P      OD2_1464     2.8    11.5
@>      ILE77    P        N_1115  <--->      ALA45    P         O_643     2.8    39.9
@>     LYS110    P        N_1651  <--->      PHE82    P        O_1216     2.8    32.3
@>      LEU29    P         N_386  <--->      VAL25    P         O_319     2.8     5.4
@>     ASN100    P        N_1486  <--->      LEU96    P        O_1430     2.8     6.7
@>     LYS102    P        N_1524  <--->      ASP98    P        O_1466     2.8     4.9
@>      THR78    P      OG1_1140  <--->      ASP81    P      OD2_1194     2.8    10.5
@>       VAL8    P          N_49  <--->      ARG40    P         O_584     2.8    16.8
@>     GLU154    P        N_2360  <--->     ARG150    P        O_2310     2.8    15.1
@>     LYS110    P       NZ_1667  <--->      ASP86    P      OD2_1270     2.8    32.5
@>      ARG58    P        NE_826  <--->      ASP56    P       OD1_788     2.8     3.3
@>      ILE35    P         N_478  <--->      VAL30    P         O_420     2.8     7.9
@>      ARG58    P       NH1_829  <--->     GLY133    P        O_2044     2.8    34.3
@>     GLN105    P        N_1571  <--->     ARG101    P        O_1523     2.8    29.9
@>       SER7    P          N_38  <--->      ASP86    P      OD1_1269     2.8    10.5
@>     ARG101    P      NH2_1519  <--->      ASP98    P      OD1_1463     2.8    17.5
@>     GLN143    P        N_2180  <--->     GLU139    P        O_2128     2.8    20.5
@>     CYS149    P        N_2276  <--->     CYS145    P        O_2224     2.8    16.0
@>     SER103    P       OG_1553  <--->      LEU99    P        O_1485     2.9    21.4
@>      ARG18    P       NH1_217  <--->      ASP92    P      OD2_1369     2.9     6.7
@>      CYS90    P        N_1332  <--->     GLU114    P        O_1738     2.9     7.9
@>      ARG18    P       NH1_217  <--->     ILE127    P        O_1954     2.9    13.0
@>     LYS155    P       NZ_2391  <--->     TYR119    P        O_1815     2.9    27.9
@>     ARG150    P        N_2287  <--->     VAL146    P        O_2240     2.9    39.3
@>      ARG65    P       NH1_938  <--->     ASP135    P      OD2_2068     2.9    39.2
@>      VAL30    P         N_405  <--->      PHE26    P         O_339     2.9     2.0
@>      VAL11    P         N_104  <--->      LEU89    P        O_1331     2.9    19.9
@>     GLN144    P        N_2197  <--->     THR140    P        O_2142     2.9    16.4
@>     LEU116    P        N_1758  <--->      CYS90    P        O_1342     2.9    22.2
@>     SER103    P        N_1546  <--->      LEU99    P        O_1485     2.9    35.6
@>      ASP56    P         N_780  <--->      ILE16    P         O_189     2.9     5.0
@>     GLU139    P        N_2114  <--->     ASP135    P        O_2070     2.9    33.1
@>      PHE10    P          N_84  <--->      ASP42    P         O_612     2.9    11.4
@>     LYS155    P        N_2375  <--->     ALA151    P        O_2320     2.9    39.0
@>      PHE26    P         N_320  <--->      ALA22    P         O_278     2.9    21.1
@>     THR140    P        N_2129  <--->     SER136    P        O_2081     3.0    36.4
@>      ALA74    P        N_1064  <--->      ASN53    P         O_751     3.0    20.8
@>       LYS6    P          N_16  <--->      ASN38    P         O_536     3.0    12.1
@>      ARG65    P         N_922  <--->      SER61    P         O_871     3.0    15.7
@>       LEU9    P          N_65  <--->      TYR87    P        O_1293     3.0     6.8
..
..
@> Number of detected hydrogen bonds: 114.
@> Calculating salt bridges.
@>     ASP135    P   OD1_2067_2068  <--->      ARG65    P     NH1_938_941     2.5
@>      ASP81    P   OD1_1193_1194  <--->      ARG75    P   NH1_1090_1093     2.7
```

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@>      ASP98    P   OD1_1463_1464  <--->     ARG101    P   NH1_1516_1519     2.8
@>      ASP86    P   OD1_1269_1270  <--->     LYS110    P         NZ_1667     3.4
@>      ARG97    P   NH1_1447_1450  <--->      GLU93    P   OE1_1383_1384     3.5
@>     ARG150    P   NH1_2303_2306  <--->     GLU154    P   OE1_2371_2372     3.7
@>      ARG58    P     NH1_829_832  <--->      ASP56    P     OD1_788_789     3.7
@>     GLU139    P   OE1_2125_2126  <--->      HSE66    P         NE2_957     3.9
@>      ARG18    P     NH1_217_220  <--->      ASP92    P   OD1_1368_1369     4.0
@>      ARG27    P     NH1_356_359  <--->      GLU23    P     OE1_290_291     4.0
@>      ARG75    P   NH1_1090_1093  <--->      ASP42    P     OD1_609_610     4.4
@>      GLU23    P     OE1_290_291  <--->      HSE72    P        NE2_1042     4.7
@>     GLU139    P   OE1_2125_2126  <--->      ARG65    P     NH1_938_941     4.8
@>      ARG18    P     NH1_217_220  <--->     ASP129    P   OD1_1978_1979     5.0
@> Number of detected salt bridges: 14.
@> Calculating repulsive ionic bonding.
@>     ARG147    P   NH1_2257_2260  <--->     LYS123    P         NZ_1875     4.5
@> Number of detected Repulsive Ionic Bonding interactions: 1.
@> Calculating Pi stacking interactions.
@>     TYR119       P   1802_1803_1805_1807_1810_1812  <--->     PHE152       P   2328_2329_2331_2333
@>      HSE66       P             953_954_955_957_959  <--->     TYR142       P   2166_2167_2169_2171
@>     TYR132       P   2024_2025_2027_2029_2032_2034  <--->     TYR131       P   2003_2004_2006_2008
@> Number of detected Pi stacking interactions: 3.
@> Calculating cation-Pi interactions.
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                    NH1_829_8
@> Number of detected cation-pi interactions: 1.
@> Hydrophobic Overlaping Areas are computed.
@> Calculating hydrophobic interactions.
@>      LEU96    P   CD1_142114s  <--->     ILE113    P   CG2_1711     3.3    21.1
@>      ILE88    P    CD_130714s  <--->      PHE82    P   CD2_1211     3.4    25.2
@>      VAL11    P    CG2_11414s  <--->      LEU99    P   CD1_1476     3.4    11.5
@>      MET63    P     SD_89314s  <--->     TYR142    P   CE1_2169     3.4    37.7
@>      TRP39    P    NE1_54714s  <--->     LEU153    P   CD1_2350     3.4    19.2
@>     ALA111    P    CB_167714s  <--->      ILE88    P    CD_1307     3.5    23.0
@>      ILE35    P     CD_49114s  <--->     LEU153    P   CD1_2350     3.5    16.4
@>      VAL30    P    CG1_41114s  <--->     LEU153    P   CD2_2354     3.5     9.8
@>       LEU9    P     CD2_7814s  <--->      ILE77    P    CD_1128     3.5    17.0
@>      PHE10    P     CE1_9414s  <--->      LEU89    P   CD1_1322     3.5    25.4
@>     TYR119    P   CE1_180514s  <--->      LEU89    P   CD2_1326     3.6    18.5
@>      ALA24    P     CB_29814s  <--->      MET63    P     CE_894     3.6    13.8
@>      PHE26    P     CZ_33214s  <--->     LEU153    P   CD1_2350     3.6    27.1
@>       VAL8    P     CG2_5914s  <--->      LEU89    P   CD1_1322     3.6    13.0
@>      ALA22    P     CB_27314s  <--->      PHE10    P     CD1_92     3.6    29.5
@>      MET91    P    CE_135414s  <--->      ALA22    P     CB_273     3.7     9.1
@>      VAL41    P    CG2_59514s  <--->      PHE26    P    CD2_334     3.7    17.5
@>     LEU116    P   CD2_177114s  <--->      MET91    P    SD_1353     3.7    21.9
@>      ALA44    P     CB_62814s  <--->      VAL11    P    CG1_110     3.7    34.2
@>       LYS6    P      CD_2614s  <--->      TRP39    P    CH2_557     3.7    44.8
@>     VAL146    P   CG2_223514s  <--->     TYR142    P   CE2_2176     3.8    39.4
@>      PHE85    P   CE1_125114s  <--->       LEU9    P     CD1_74     3.8    31.6
@>      ILE21    P    CG2_25614s  <--->      VAL25    P    CG2_314     3.8    25.0
@>     VAL141    P   CG1_214914s  <--->      ILE21    P     CD_263     3.9    13.0
@>      ILE68    P    CG1_98014s  <--->      MET63    P     CE_894     3.9    37.2
@>     PHE152    P    CZ_233314s  <--->      LEU89    P   CD1_1322     3.9    18.0
@>      ARG18    P     CG_20814s  <--->     VAL141    P   CG1_2149     4.0    26.2
@>      ARG75    P    CG_108114s  <--->      ALA44    P     CB_628     4.2    27.4
@>     ILE127    P    CD_194914s  <--->     LEU116    P   CD2_1771     4.3     7.9
@>      LYS79    P    CG_115514s  <--->     VAL106    P   CG2_1598     4.3    15.6
@>      LEU29    P     CG_39314s  <--->      VAL25    P    CG1_310     4.3    21.7
@>     ILE126    P   CG1_192714s  <--->     LEU125    P    CG_1905     4.4    55.6
```

```
@> Number of detected hydrophobic interactions: 32.
@> Calculating disulfide bonds.
@> Number of detected disulfide bonds: 0.
@> File with interactions saved.
```

The results are displayed on the screen and they can be fetch by using `InteractionsTrajectory.getInteractions()` method.

```
In [16]: interactionsTrajectory.getInteractions()
```

```
[[[['ARG101', 'NH1_1516', 'P', 'ASP98', 'OD1_1463', 'P', 1.998, 33.1238],
   ['HSE72', 'NE2_1042', 'P', 'ASN15', 'OD1_165', 'P', 2.5997, 34.752],
   ['GLN143', 'NE2_2192', 'P', 'GLU139', 'OE2_2126', 'P', 2.7287, 9.1822],
   ['HSE66', 'NE2_957', 'P', 'GLU139', 'OE1_2125', 'P', 2.7314, 6.3592],
   ['ARG40', 'N_561', 'P', 'LYS6', 'O_37', 'P', 2.7479, 17.1499],
   ['ARG58', 'N_813', 'P', 'ASP56', 'OD1_788', 'P', 2.7499, 29.9737],
   ['ALA45', 'N_634', 'P', 'ARG75', 'O_1097', 'P', 2.7609, 35.0983],
   ['ASN53', 'ND2_747', 'P', 'GLU50', 'OE1_708', 'P', 2.7702, 18.2336],
   ['ALA74', 'N_1064', 'P', 'ASN53', 'O_751', 'P', 2.7782, 21.3375],
   ['ASP56', 'N_780', 'P', 'ILE16', 'O_189', 'P', 2.7793, 27.0481],
   ['LYS110', 'NZ_1667', 'P', 'THR84', 'O_1240', 'P', 2.7977, 38.2213],
   ['LEU116', 'N_1758', 'P', 'CYS90', 'O_1342', 'P', 2.8072, 15.0239],
   ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 2.8075, 29.107],
   ['ASN134', 'N_2045', 'P', 'ASP137', 'OD2_2091', 'P', 2.8132, 22.562],
   ['PHE152', 'N_2321', 'P', 'CYS148', 'O_2275', 'P', 2.8141, 8.2562],
   ['ASN95', 'N_1398', 'P', 'ASP92', 'OD1_1368', 'P', 2.8148, 12.5701],
   ['LYS6', 'N_16', 'P', 'ASN38', 'O_536', 'P', 2.8178, 25.0306],
   ['ILE77', 'N_1115', 'P', 'ALA45', 'O_643', 'P', 2.8179, 12.1856],
   ['ARG58', 'NH2_832', 'P', 'ASP56', 'OD2_789', 'P', 2.8204, 27.6617],
   ['LEU99', 'N_1467', 'P', 'ASN95', 'O_1411', 'P', 2.8205, 15.4867],
   ['CYS149', 'N_2276', 'P', 'CYS145', 'O_2224', 'P', 2.8247, 9.5914],
   ['GLY52', 'N_731', 'P', 'ALA74', 'O_1073', 'P', 2.832, 6.6442],
   ['ASP32', 'N_435', 'P', 'LYS28', 'O_385', 'P', 2.8357, 8.8318],
   ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.8429, 17.7147],
   ['GLN143', 'N_2180', 'P', 'GLU139', 'O_2128', 'P', 2.8445, 21.6714],
   ['ARG27', 'N_340', 'P', 'GLU23', 'O_293', 'P', 2.8446, 15.4167],
   ['TYR142', 'N_2159', 'P', 'PHE138', 'O_2113', 'P', 2.8515, 14.2061],
   ['GLY133', 'N_2038', 'P', 'PRO130', 'O_1995', 'P', 2.854, 25.4301],
   ['PHE26', 'N_320', 'P', 'ALA22', 'O_278', 'P', 2.8541, 4.8732],
   ['ASN15', 'ND2_166', 'P', 'SER19', 'OG_232', 'P', 2.8592, 32.1244],
   ['ARG75', 'NH1_1090', 'P', 'ASP81', 'OD2_1194', 'P', 2.8632, 19.6664],
   ['ARG75', 'NH2_1093', 'P', 'ASP42', 'OD2_610', 'P', 2.8649, 23.5083],
   ['ARG97', 'N_1431', 'P', 'GLU93', 'O_1386', 'P', 2.8654, 22.24],
   ['ARG65', 'NH2_941', 'P', 'GLU139', 'OE1_2125', 'P', 2.8655, 32.3239],
   ['VAL25', 'N_304', 'P', 'ILE21', 'O_268', 'P', 2.8666, 8.2255],
   ['LEU153', 'N_2341', 'P', 'CYS149', 'O_2286', 'P', 2.8707, 12.4931],
   ['SER7', 'N_38', 'P', 'ASP86', 'OD2_1270', 'P', 2.8732, 39.8839],
   ['ASP86', 'N_1261', 'P', 'SER7', 'OG_45', 'P', 2.8753, 34.7426],
   ..
  [['LYS112', 'NZ_1699', 'P', 'GLU114', 'OE1_1735', 'P', 2.5487, 20.8176],
   ['THR78', 'N_1134', 'P', 'ASP81', 'OD2_1194', 'P', 2.5494, 15.6392],
   ['ARG27', 'NH2_359', 'P', 'GLU23', 'OE2_291', 'P', 2.5496, 36.5043],
   ['THR78', 'OG1_1140', 'P', 'ASP81', 'OD2_1194', 'P', 2.5756, 25.1514],
   ['SER7', 'OG_45', 'P', 'ASP86', 'OD2_1270', 'P', 2.5904, 32.2995],
   ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD2_1464', 'P', 2.5963, 18.6089],
   ['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT1_2423', 'P', 2.6334, 17.8203],
   ['ARG75', 'NH2_1093', 'P', 'ASP81', 'OD1_1193', 'P', 2.6367, 17.6426],
   ['SER118', 'OG_1791', 'P', 'LEU115', 'O_1757', 'P', 2.6547, 25.6442],
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  ['ARG58', 'NE_826', 'P', 'ASP56', 'OD1_788', 'P', 2.6611, 6.4459],
  ['GLN124', 'N_1881', 'P', 'ASP120', 'OD1_1824', 'P', 2.6666, 17.1571],
  ['ARG147', 'NH1_2257', 'P', 'GLN124', 'OE1_1892', 'P', 2.6875, 11.8479],
  ['ARG18', 'NH1_217', 'P', 'ASP92', 'OD2_1369', 'P', 2.6879, 14.5803],
  ['ARG75', 'NH1_1090', 'P', 'ASP81', 'OD2_1194', 'P', 2.6889, 23.9375],
  ['TYR87', 'OH_1286', 'P', 'HSE157', 'OT1_2423', 'P', 2.6945, 11.5603],
  ['SER43', 'OG_620', 'P', 'GLU23', 'OE1_290', 'P', 2.6978, 15.166],
  ['LYS28', 'NZ_380', 'P', 'ASP32', 'OD1_443', 'P', 2.7003, 3.632],
  ['LYS110', 'NZ_1667', 'P', 'ASP86', 'OD1_1269', 'P', 2.7025, 25.1511],
  ['THR140', 'OG1_2135', 'P', 'SER136', 'O_2081', 'P', 2.71, 5.2209],
  ['LEU116', 'N_1758', 'P', 'CYS90', 'O_1342', 'P', 2.7125, 24.3959],
  ['THR5', 'OG1_8', 'P', 'ASN38', 'O_536', 'P', 2.7162, 38.6072],
  ['LYS64', 'N_900', 'P', 'GLN60', 'O_860', 'P', 2.7222, 26.7806],
  ['ARG147', 'NH1_2257', 'P', 'ASP120', 'OD2_1825', 'P', 2.731, 15.2446],
  ['ARG27', 'N_340', 'P', 'GLU23', 'O_293', 'P', 2.7341, 21.9432],
  ['TYR119', 'OH_1808', 'P', 'GLU114', 'OE1_1735', 'P', 2.735, 15.8502],
  ['ARG18', 'NH1_217', 'P', 'ILE127', 'O_1954', 'P', 2.7501, 16.0113],
  ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 2.7535, 13.6202],
  ['LYS102', 'N_1524', 'P', 'ASP98', 'O_1466', 'P', 2.7626, 15.9446],
  ['ARG58', 'NH1_829', 'P', 'GLY133', 'O_2044', 'P', 2.7673, 31.8828],
  ['ARG75', 'NH2_1093', 'P', 'ASP42', 'OD2_610', 'P', 2.7744, 13.0389],
  ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.7935, 13.2257],
  ['GLU23', 'N_279', 'P', 'SER19', 'O_235', 'P', 2.8067, 10.8775],
  ['SER7', 'N_38', 'P', 'ASP86', 'OD2_1270', 'P', 2.813, 38.9132],
  ['VAL11', 'N_104', 'P', 'LEU89', 'O_1331', 'P', 2.8182, 13.801],
  ['PHE26', 'N_320', 'P', 'ALA22', 'O_278', 'P', 2.8212, 18.2267],
  ['LEU9', 'N_65', 'P', 'TYR87', 'O_1293', 'P', 2.8249, 34.2551],
  ['ARG65', 'NH2_941', 'P', 'GLU139', 'OE1_2125', 'P', 2.8308, 14.8745],
  ['ILE68', 'N_970', 'P', 'MET63', 'O_899', 'P', 2.8328, 9.2758],
  ..
 [['ARG18', 'NH1_217', 'P', 'ASP92', 'OD2_1369', 'P', 2.5097, 4.9218],
  ['THR31', 'OG1_427', 'P', 'ARG27', 'O_363', 'P', 2.5496, 5.4538],
  ['ARG58', 'NH2_832', 'P', 'ASP56', 'OD2_789', 'P', 2.5525, 8.1856],
  ['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT1_2423', 'P', 2.5902, 19.0335],
  ['ARG75', 'NH2_1093', 'P', 'ASP42', 'OD2_610', 'P', 2.6114, 24.975],
  ['TYR119', 'OH_1808', 'P', 'GLU114', 'OE2_1736', 'P', 2.6441, 10.2991],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD2_1464', 'P', 2.6466, 7.8982],
  ['TYR87', 'OH_1286', 'P', 'HSE157', 'OT1_2423', 'P', 2.6516, 14.0793],
  ['LYS64', 'N_900', 'P', 'GLN60', 'O_860', 'P', 2.6643, 4.9246],
  ['SER43', 'OG_620', 'P', 'GLU23', 'OE1_290', 'P', 2.7024, 8.6062],
  ['THR78', 'OG1_1140', 'P', 'ASP81', 'OD2_1194', 'P', 2.7158, 6.5273],
  ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.7184, 24.9984],
  ['SER118', 'OG_1791', 'P', 'LEU115', 'O_1757', 'P', 2.7238, 26.9156],
  ['LYS28', 'NZ_380', 'P', 'ASP32', 'OD2_444', 'P', 2.7274, 13.9298],
  ['THR84', 'OG1_1233', 'P', 'GLU80', 'O_1184', 'P', 2.7314, 13.4406],
  ['LEU89', 'N_1313', 'P', 'LEU9', 'O_83', 'P', 2.7581, 11.8493],
  ['ARG147', 'NH1_2257', 'P', 'GLN124', 'OE1_1892', 'P', 2.7633, 15.0984],
  ['ARG27', 'NH2_359', 'P', 'GLU23', 'OE2_291', 'P', 2.765, 17.97],
  ['ILE35', 'N_478', 'P', 'VAL30', 'O_420', 'P', 2.7659, 20.7163],
  ['PHE26', 'N_320', 'P', 'ALA22', 'O_278', 'P', 2.7663, 21.7712],
  ['VAL11', 'N_104', 'P', 'LEU89', 'O_1331', 'P', 2.767, 10.3325],
  ['VAL25', 'N_304', 'P', 'ILE21', 'O_268', 'P', 2.7679, 9.2024],
  ['SER7', 'OG_45', 'P', 'ASP86', 'OD2_1270', 'P', 2.7682, 29.4143],
  ['HSE72', 'NE2_1042', 'P', 'ASN15', 'OD1_165', 'P', 2.7756, 37.1399],
  ['ASN34', 'N_464', 'P', 'THR31', 'O_434', 'P', 2.7794, 19.6803],
  ['LYS110', 'N_1651', 'P', 'PHE82', 'O_1216', 'P', 2.7863, 9.1814],
  ['LYS110', 'NZ_1667', 'P', 'ASP86', 'OD1_1269', 'P', 2.7932, 13.508],
  ['ARG58', 'NE_826', 'P', 'ASP56', 'OD1_788', 'P', 2.8021, 8.0221],
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  ['ARG75', 'NH1_1090', 'P', 'ASP81', 'OD2_1194', 'P', 2.8066, 14.9419],
  ['VAL8', 'N_49', 'P', 'ARG40', 'O_584', 'P', 2.8114, 19.4027],
  ['ARG18', 'NH1_217', 'P', 'ILE127', 'O_1954', 'P', 2.8173, 6.9549],
  ['LYS155', 'N_2375', 'P', 'ALA151', 'O_2320', 'P', 2.8212, 15.1026],
  ['HSE66', 'NE2_957', 'P', 'GLU139', 'OE1_2125', 'P', 2.8239, 28.9105],
  ['ARG147', 'NH1_2257', 'P', 'ASP120', 'OD2_1825', 'P', 2.8257, 31.6579],
  ['ARG97', 'N_1431', 'P', 'GLU93', 'O_1386', 'P', 2.8291, 15.1587],
  ['LYS123', 'N_1859', 'P', 'ASP120', 'OD1_1824', 'P', 2.8292, 34.0011],
  ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.8381, 10.253],
  ['ASP86', 'N_1261', 'P', 'SER7', 'OG_45', 'P', 2.8406, 22.034],
  ['ARG65', 'N_922', 'P', 'SER61', 'O_871', 'P', 2.8423, 24.4142],
  ['ILE127', 'N_1936', 'P', 'MET91', 'O_1359', 'P', 2.8469, 4.126],
  ['LYS112', 'NZ_1699', 'P', 'HSE157', 'ND1_2414', 'P', 2.8616, 14.018],
  ['GLY67', 'N_963', 'P', 'MET63', 'O_899', 'P', 2.8626, 38.6183],
  ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 2.8761, 17.0562],
  ['LYS112', 'NZ_1699', 'P', 'GLU114', 'OE2_1736', 'P', 2.8761, 18.0626],
  ['ARG75', 'NE_1087', 'P', 'ASP42', 'OD2_610', 'P', 2.8795, 38.3078],
  ['ALA44', 'N_624', 'P', 'PHE10', 'O_103', 'P', 2.8798, 30.1431],
  ['ILE68', 'N_970', 'P', 'MET63', 'O_899', 'P', 2.8902, 12.9079],
  ['ARG58', 'N_813', 'P', 'ASP56', 'OD1_788', 'P', 2.903, 21.0711],
  ['THR78', 'N_1134', 'P', 'ASP81', 'OD2_1194', 'P', 2.9152, 26.3475],
  ['ALA45', 'N_634', 'P', 'ARG75', 'O_1097', 'P', 2.9235, 27.7222],
  ..
 [['SER118', 'OG_1791', 'P', 'GLU114', 'OE1_1735', 'P', 2.5321, 12.1754],
  ['SER7', 'OG_45', 'P', 'ASP86', 'OD2_1270', 'P', 2.5681, 8.2326],
  ['SER43', 'OG_620', 'P', 'GLU23', 'OE1_290', 'P', 2.5908, 6.4741],
  ['ARG101', 'NH2_1519', 'P', 'ASP98', 'OD1_1463', 'P', 2.5911, 17.069],
  ['ARG58', 'NH2_832', 'P', 'ASP56', 'OD2_789', 'P', 2.6234, 15.5609],
  ['THR78', 'OG1_1140', 'P', 'ASP81', 'OD2_1194', 'P', 2.6239, 11.6022],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD2_1464', 'P', 2.6274, 12.9418],
  ['ASP32', 'N_435', 'P', 'LYS28', 'O_385', 'P', 2.6388, 5.0129],
  ['CYS149', 'N_2276', 'P', 'CYS145', 'O_2224', 'P', 2.6571, 20.4048],
  ['TYR119', 'OH_1808', 'P', 'GLU114', 'OE2_1736', 'P', 2.6666, 5.0368],
  ['ARG65', 'NH2_941', 'P', 'GLU139', 'OE1_2125', 'P', 2.677, 21.8922],
  ['ARG18', 'NH2_220', 'P', 'ASP92', 'OD2_1369', 'P', 2.6813, 31.3689],
  ['LYS112', 'NZ_1699', 'P', 'GLU114', 'OE2_1736', 'P', 2.6844, 12.4337],
  ['SER103', 'OG_1553', 'P', 'LEU99', 'O_1485', 'P', 2.7018, 15.5273],
  ['LYS64', 'N_900', 'P', 'GLN60', 'O_860', 'P', 2.7094, 34.9749],
  ['HSE66', 'NE2_957', 'P', 'GLU139', 'OE1_2125', 'P', 2.7146, 21.3402],
  ['GLY52', 'N_731', 'P', 'ALA74', 'O_1073', 'P', 2.719, 23.3583],
  ['ARG27', 'NH2_359', 'P', 'GLU23', 'OE2_291', 'P', 2.7207, 8.4795],
  ['LEU116', 'N_1758', 'P', 'CYS90', 'O_1342', 'P', 2.7283, 14.8893],
  ['ARG18', 'NH1_217', 'P', 'ASP92', 'OD2_1369', 'P', 2.7353, 26.7201],
  ['THR31', 'OG1_427', 'P', 'ARG27', 'O_363', 'P', 2.7466, 22.4844],
  ['ARG18', 'NH1_217', 'P', 'ILE127', 'O_1954', 'P', 2.7489, 16.6396],
  ['ARG58', 'NH1_829', 'P', 'TYR132', 'O_2037', 'P', 2.7511, 23.6002],
  ['ARG147', 'NH1_2257', 'P', 'ASP120', 'OD1_1824', 'P', 2.7592, 19.3384],
  ['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT2_2424', 'P', 2.7625, 21.1367],
  ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.7703, 4.1752],
  ['ARG75', 'NH2_1093', 'P', 'ASP42', 'OD2_610', 'P', 2.7726, 18.0115],
  ['ARG65', 'NH1_938', 'P', 'GLU139', 'OE1_2125', 'P', 2.7749, 18.9952],
  ['GLY133', 'N_2038', 'P', 'ASP137', 'OD2_2091', 'P', 2.7764, 32.7458],
  ['ARG75', 'NH2_1093', 'P', 'ASP81', 'OD1_1193', 'P', 2.7783, 16.8911],
  ['TYR87', 'OH_1286', 'P', 'HSE157', 'OT2_2424', 'P', 2.7928, 9.9286],
  ['ILE35', 'N_478', 'P', 'VAL30', 'O_420', 'P', 2.7945, 6.0583],
  ['LYS28', 'NZ_380', 'P', 'ASP32', 'OD2_444', 'P', 2.7993, 35.4827],
  ['PHE152', 'N_2321', 'P', 'CYS148', 'O_2275', 'P', 2.8, 5.5477],
  ['LYS110', 'NZ_1667', 'P', 'ASP86', 'OD1_1269', 'P', 2.8021, 14.2767],
```

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   ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.813, 11.6498],
   ['GLN60', 'N_844', 'P', 'ASP56', 'O_791', 'P', 2.8156, 25.2584],
   ['ALA45', 'N_634', 'P', 'ARG75', 'O_1097', 'P', 2.8209, 30.082],
   ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.8375, 24.3092],
   ['ARG150', 'N_2287', 'P', 'VAL146', 'O_2240', 'P', 2.8394, 21.6561],
   ..
   ..
[['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.2931, 21.0747],
   ['ILE88', 'CD_1307', 'P', 'PHE82', 'CD2_1211', 'P', 3.3689, 25.2319],
   ['VAL11', 'CG2_114', 'P', 'LEU99', 'CD1_1476', 'P', 3.3771, 11.4804],
   ['MET63', 'SD_893', 'P', 'TYR142', 'CE1_2169', 'P', 3.3896, 37.7382],
   ['TRP39', 'NE1_547', 'P', 'LEU153', 'CD1_2350', 'P', 3.4345, 19.2142],
   ['ALA111', 'CB_1677', 'P', 'ILE88', 'CD_1307', 'P', 3.4669, 22.9943],
   ['ILE35', 'CD_491', 'P', 'LEU153', 'CD1_2350', 'P', 3.4868, 16.4472],
   ['VAL30', 'CG1_411', 'P', 'LEU153', 'CD2_2354', 'P', 3.4938, 9.7531],
   ['LEU9', 'CD2_78', 'P', 'ILE77', 'CD_1128', 'P', 3.5133, 16.9544],
   ['PHE10', 'CE1_94', 'P', 'LEU89', 'CD1_1322', 'P', 3.5468, 25.3848],
   ['TYR119', 'CE1_1805', 'P', 'LEU89', 'CD2_1326', 'P', 3.554, 18.5297],
   ['ALA24', 'CB_298', 'P', 'MET63', 'CE_894', 'P', 3.5859, 13.7697],
   ['PHE26', 'CZ_332', 'P', 'LEU153', 'CD1_2350', 'P', 3.6118, 27.1048],
   ['VAL8', 'CG2_59', 'P', 'LEU89', 'CD1_1322', 'P', 3.6199, 12.9537],
   ['ALA22', 'CB_273', 'P', 'PHE10', 'CD1_92', 'P', 3.6246, 29.4846],
   ['MET91', 'CE_1354', 'P', 'ALA22', 'CB_273', 'P', 3.6628, 9.0978],
   ['VAL41', 'CG2_595', 'P', 'PHE26', 'CD2_334', 'P', 3.6792, 17.4783],
   ['LEU116', 'CD2_1771', 'P', 'MET91', 'SD_1353', 'P', 3.6984, 21.9302],
   ['ALA44', 'CB_628', 'P', 'VAL11', 'CG1_110', 'P', 3.7022, 34.2417],
   ['LYS6', 'CD_26', 'P', 'TRP39', 'CH2_557', 'P', 3.7135, 44.8],
   ['VAL146', 'CG2_2235', 'P', 'TYR142', 'CE2_2176', 'P', 3.7622, 39.414],
   ['PHE85', 'CE1_1251', 'P', 'LEU9', 'CD1_74', 'P', 3.8118, 31.6126],
   ['ILE21', 'CG2_256', 'P', 'VAL25', 'CG2_314', 'P', 3.825, 25.047],
   ['VAL141', 'CG1_2149', 'P', 'ILE21', 'CD_263', 'P', 3.8615, 13.036],
   ['ILE68', 'CG1_980', 'P', 'MET63', 'CE_894', 'P', 3.8698, 37.1931],
   ['PHE152', 'CZ_2333', 'P', 'LEU89', 'CD1_1322', 'P', 3.9131, 17.9674],
   ['ARG18', 'CG_208', 'P', 'VAL141', 'CG1_2149', 'P', 3.9881, 26.173],
   ['ARG75', 'CG_1081', 'P', 'ALA44', 'CB_628', 'P', 4.1878, 27.3996],
   ['ILE127', 'CD_1949', 'P', 'LEU116', 'CD2_1771', 'P', 4.2643, 7.8575],
   ['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 4.2738, 15.6412],
   ['LEU29', 'CG_393', 'P', 'VAL25', 'CG1_310', 'P', 4.3325, 21.7286],
   ['ILE126', 'CG1_1927', 'P', 'LEU125', 'CG_1905', 'P', 4.4374, 55.6364]]],
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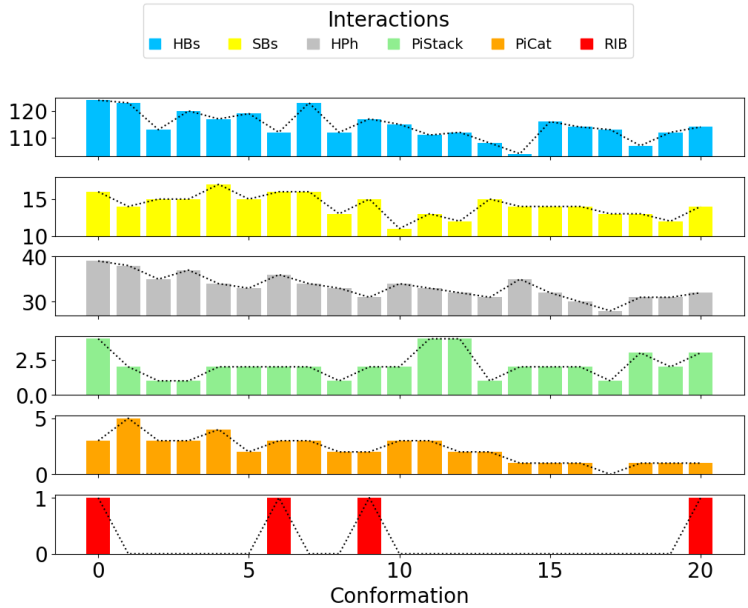
Moreover, we can display the evolution of each interaction type during the simulation. There are the following types of plots: hydrogen bonds (*blue*), salt bridges (*yellow*), hydrophobic interactions (*silver*), Pi-stacking (*green*), Pi-cation (*orange*), repulsive ionic bonding (*red*), disulfide bonds(*black*).

```
In [17]: interactionsTrajectory.getTimeInteractions()
```



If the structure is stable, we will not observe a lot of changes in protein structure.

Similar to the single PDB analysis, we have an access to each interaction type by using: `InteractionsTrajectory.getHydrogenBonds()` method, etc.

```
In [18]: interactionsTrajectory.getHydrogenBonds()
```

```
[[['ARG101', 'NH1_1516', 'P', 'ASP98', 'OD1_1463', 'P', 1.998, 33.1238],
  ['HSE72', 'NE2_1042', 'P', 'ASN15', 'OD1_165', 'P', 2.5997, 34.752],
  ['GLN143', 'NE2_2192', 'P', 'GLU139', 'OE2_2126', 'P', 2.7287, 9.1822],
  ['HSE66', 'NE2_957', 'P', 'GLU139', 'OE1_2125', 'P', 2.7314, 6.3592],
  ['ARG40', 'N_561', 'P', 'LYS6', 'O_37', 'P', 2.7479, 17.1499],
  ['ARG58', 'N_813', 'P', 'ASP56', 'OD1_788', 'P', 2.7499, 29.9737],
  ['ALA45', 'N_634', 'P', 'ARG75', 'O_1097', 'P', 2.7609, 35.0983],
  ['ASN53', 'ND2_747', 'P', 'GLU50', 'OE1_708', 'P', 2.7702, 18.2336],
  ['ALA74', 'N_1064', 'P', 'ASN53', 'O_751', 'P', 2.7782, 21.3375],
  ['ASP56', 'N_780', 'P', 'ILE16', 'O_189', 'P', 2.7793, 27.0481],
  ['LYS110', 'NZ_1667', 'P', 'THR84', 'O_1240', 'P', 2.7977, 38.2213],
  ['LEU116', 'N_1758', 'P', 'CYS90', 'O_1342', 'P', 2.8072, 15.0239],
  ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 2.8075, 29.107],
  ['ASN134', 'N_2045', 'P', 'ASP137', 'OD2_2091', 'P', 2.8132, 22.562],
  ['PHE152', 'N_2321', 'P', 'CYS148', 'O_2275', 'P', 2.8141, 8.2562],
  ['ASN95', 'N_1398', 'P', 'ASP92', 'OD1_1368', 'P', 2.8148, 12.5701],
  ['LYS6', 'N_16', 'P', 'ASN38', 'O_536', 'P', 2.8178, 25.0306],
  ['ILE77', 'N_1115', 'P', 'ALA45', 'O_643', 'P', 2.8179, 12.1856],
  ['ARG58', 'NH2_832', 'P', 'ASP56', 'OD2_789', 'P', 2.8204, 27.6617],
  ['LEU99', 'N_1467', 'P', 'ASN95', 'O_1411', 'P', 2.8205, 15.4867],
```

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['CYS149', 'N_2276', 'P', 'CYS145', 'O_2224', 'P', 2.8247, 9.5914],
['GLY52', 'N_731', 'P', 'ALA74', 'O_1073', 'P', 2.832, 6.6442],
['ASP32', 'N_435', 'P', 'LYS28', 'O_385', 'P', 2.8357, 8.8318],
['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.8429, 17.7147],
['GLN143', 'N_2180', 'P', 'GLU139', 'O_2128', 'P', 2.8445, 21.6714],
['ARG27', 'N_340', 'P', 'GLU23', 'O_293', 'P', 2.8446, 15.4167],
['TYR142', 'N_2159', 'P', 'PHE138', 'O_2113', 'P', 2.8515, 14.2061],
['GLY133', 'N_2038', 'P', 'PRO130', 'O_1995', 'P', 2.854, 25.4301],
['PHE26', 'N_320', 'P', 'ALA22', 'O_278', 'P', 2.8541, 4.8732],
['ASN15', 'ND2_166', 'P', 'SER19', 'OG_232', 'P', 2.8592, 32.1244],
['ARG75', 'NH1_1090', 'P', 'ASP81', 'OD2_1194', 'P', 2.8632, 19.6664],
['ARG75', 'NH2_1093', 'P', 'ASP42', 'OD2_610', 'P', 2.8649, 23.5083],
['ARG97', 'N_1431', 'P', 'GLU93', 'O_1386', 'P', 2.8654, 22.24],
['ARG65', 'NH2_941', 'P', 'GLU139', 'OE1_2125', 'P', 2.8655, 32.3239],
['VAL25', 'N_304', 'P', 'ILE21', 'O_268', 'P', 2.8666, 8.2255],
['LEU153', 'N_2341', 'P', 'CYS149', 'O_2286', 'P', 2.8707, 12.4931],
['SER7', 'N_38', 'P', 'ASP86', 'OD2_1270', 'P', 2.8732, 39.8839],
['ASP86', 'N_1261', 'P', 'SER7', 'OG_45', 'P', 2.8753, 34.7426],
['ARG58', 'NH2_832', 'P', 'TYR131', 'O_2016', 'P', 2.8815, 33.1098],
['THR46', 'N_644', 'P', 'CYS12', 'O_130', 'P', 2.883, 36.1279],
['GLN144', 'N_2197', 'P', 'THR140', 'O_2142', 'P', 2.8836, 23.2545],
['THR78', 'N_1134', 'P', 'ASP81', 'OD2_1194', 'P', 2.8869, 12.4465],
['LEU89', 'N_1313', 'P', 'LEU9', 'O_83', 'P', 2.8946, 29.5105],
['THR31', 'N_421', 'P', 'ARG27', 'O_363', 'P', 2.896, 24.1287],
['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.8975, 24.576],
['CYS148', 'N_2265', 'P', 'GLN144', 'O_2213', 'P', 2.8976, 9.3165],
['GLU23', 'N_279', 'P', 'SER19', 'O_235', 'P', 2.8979, 15.4146],
['ILE68', 'N_970', 'P', 'MET63', 'O_899', 'P', 2.8986, 12.9903],
['PHE10', 'N_84', 'P', 'ASP42', 'O_612', 'P', 2.9026, 22.751],
['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.912, 10.1158],
['SER61', 'N_861', 'P', 'TYR57', 'O_812', 'P', 2.9132, 35.1196],
['CYS145', 'N_2214', 'P', 'VAL141', 'O_2158', 'P', 2.9144, 15.8507],
['ARG27', 'NH2_359', 'P', 'GLU23', 'OE2_291', 'P', 2.9199, 31.5487],
['LYS64', 'N_900', 'P', 'GLN60', 'O_860', 'P', 2.9211, 22.8783],
['LEU9', 'N_65', 'P', 'TYR87', 'O_1293', 'P', 2.9229, 16.439],
['ASN38', 'N_523', 'P', 'ILE35', 'O_496', 'P', 2.9255, 29.091],
['VAL11', 'N_104', 'P', 'LEU89', 'O_1331', 'P', 2.9316, 29.7192],
['ASN100', 'N_1486', 'P', 'LEU96', 'O_1430', 'P', 2.933, 10.3321],
['GLN124', 'N_1881', 'P', 'ASP120', 'OD2_1825', 'P', 2.9333, 27.4547],
['LYS102', 'N_1524', 'P', 'ASP98', 'O_1466', 'P', 2.9361, 9.2855],
['GLN76', 'NE2_1110', 'P', 'THR46', 'O_657', 'P', 2.9381, 31.3836],
['ARG40', 'NH1_577', 'P', 'THR84', 'OG1_1233', 'P', 2.9482, 8.3748],
['ALA44', 'N_624', 'P', 'PHE10', 'O_103', 'P', 2.9499, 33.1771],
['GLU154', 'N_2360', 'P', 'ARG150', 'O_2310', 'P', 2.956, 22.5898],
['VAL8', 'N_49', 'P', 'ARG40', 'O_584', 'P', 2.9631, 25.0079],
['MET63', 'N_883', 'P', 'GLY59', 'O_843', 'P', 2.9733, 18.2731],
['GLN60', 'N_844', 'P', 'ASP56', 'O_791', 'P', 2.9795, 35.5229],
['ILE35', 'N_478', 'P', 'VAL30', 'O_420', 'P', 2.9811, 23.5092],
['VAL146', 'N_2225', 'P', 'TYR142', 'O_2179', 'P', 2.9914, 31.4798],
['ARG58', 'NH1_829', 'P', 'TYR131', 'O_2016', 'P', 2.9942, 38.0937],
['ASN53', 'N_738', 'P', 'GLU50', 'O_711', 'P', 2.995, 28.587],
['ARG101', 'N_1500', 'P', 'ARG97', 'O_1454', 'P', 2.9952, 32.2712],
['ARG18', 'NH1_217', 'P', 'ILE127', 'O_1954', 'P', 2.9957, 25.9507],
['ARG75', 'N_1074', 'P', 'ASN15', 'OD1_165', 'P', 3.0026, 25.0853],
['GLN144', 'NE2_2209', 'P', 'ILE126', 'O_1935', 'P', 3.0038, 18.2744],
['ASN34', 'N_464', 'P', 'THR31', 'O_434', 'P', 3.0041, 18.2465],
['ASN15', 'ND2_166', 'P', 'SER43', 'OG_620', 'P', 3.0129, 25.6996],
['ARG58', 'NE_826', 'P', 'ASP56', 'OD1_788', 'P', 3.017, 22.2284],
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  ['ARG27', 'NH1_356', 'P', 'GLU23', 'OE2_291', 'P', 3.0175, 36.9342],
  ['ILE127', 'N_1936', 'P', 'MET91', 'O_1359', 'P', 3.018, 17.5601],
  ['TYR119', 'OH_1808', 'P', 'HSE157', 'N_2407', 'P', 3.0224, 28.0923],
  ['HSE157', 'N_2407', 'P', 'TYR119', 'OH_1808', 'P', 3.0224, 19.1804],
  ['GLU139', 'N_2114', 'P', 'ASP135', 'O_2070', 'P', 3.0245, 27.9246],
  ['LEU29', 'N_386', 'P', 'VAL25', 'O_319', 'P', 3.0299, 19.1089],
  ['SER47', 'N_658', 'P', 'LEU13', 'O_149', 'P', 3.0386, 28.8029],
  ['VAL30', 'N_405', 'P', 'PHE26', 'O_339', 'P', 3.0394, 17.6883],
  ['GLN105', 'N_1571', 'P', 'LYS102', 'O_1545', 'P', 3.0464, 19.6807],
  ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.051, 21.4045],
  ['LYS155', 'N_2375', 'P', 'ALA151', 'O_2320', 'P', 3.0555, 21.3244],
  ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.059, 24.1606],
  ['ASP120', 'N_1816', 'P', 'GLY117', 'O_1783', 'P', 3.0623, 12.666],
  ['CYS62', 'N_872', 'P', 'ARG58', 'O_836', 'P', 3.0651, 20.443],
  ['ARG18', 'NH1_217', 'P', 'ASP92', 'OD2_1369', 'P', 3.0679, 4.2778],
  ['ALA24', 'N_294', 'P', 'PRO20', 'O_249', 'P', 3.0751, 29.9487],
  ['ARG150', 'N_2287', 'P', 'VAL146', 'O_2240', 'P', 3.078, 12.7022],
  ['LYS28', 'N_364', 'P', 'ALA24', 'O_303', 'P', 3.0783, 19.9504],
  ['VAL141', 'N_2143', 'P', 'ASP137', 'O_2093', 'P', 3.081, 18.4811],
  ['ASP98', 'N_1455', 'P', 'SER94', 'O_1397', 'P', 3.0844, 19.56],
  ['LEU96', 'N_1412', 'P', 'ASP92', 'O_1371', 'P', 3.085, 36.3254],
  ['ALA22', 'N_269', 'P', 'ARG18', 'O_224', 'P', 3.088, 21.873],
  ['ALA151', 'N_2311', 'P', 'ARG147', 'O_2264', 'P', 3.0991, 15.5713],
  ['GLY67', 'N_963', 'P', 'LYS64', 'O_921', 'P', 3.122, 22.7833],
  ['ASP42', 'N_601', 'P', 'VAL8', 'O_64', 'P', 3.1331, 35.5671],
  ['ARG65', 'N_922', 'P', 'SER61', 'O_871', 'P', 3.1339, 23.3682],
  ['TRP39', 'N_537', 'P', 'SER36', 'O_507', 'P', 3.1343, 15.1775],
  ['LYS123', 'N_1859', 'P', 'ASP120', 'O_1827', 'P', 3.1375, 18.6589],
  ['MET91', 'N_1343', 'P', 'ASN95', 'OD1_1406', 'P', 3.1581, 39.0427],
  ['THR140', 'N_2129', 'P', 'SER136', 'O_2081', 'P', 3.1742, 30.2937],
  ['PHE85', 'N_1241', 'P', 'ASP81', 'O_1196', 'P', 3.1845, 20.2243],
  ['ASN15', 'N_157', 'P', 'CYS12', 'SG_127', 'P', 3.2043, 37.4576],
  ['ALA111', 'N_1673', 'P', 'PHE82', 'O_1216', 'P', 3.2054, 20.58],
  ['ARG147', 'N_2241', 'P', 'GLN143', 'O_2196', 'P', 3.2416, 12.0678],
  ['ARG75', 'NH2_1093', 'P', 'ASP81', 'OD1_1193', 'P', 3.2447, 29.3403],
  ['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT2_2424', 'P', 3.2687, 28.6743],
  ['ARG147', 'NH1_2257', 'P', 'GLN124', 'OE1_1892', 'P', 3.3008, 29.853],
  ['PHE138', 'N_2094', 'P', 'ASN134', 'O_2058', 'P', 3.3062, 31.0247],
  ['SER7', 'OG_45', 'P', 'THR84', 'O_1240', 'P', 3.3227, 35.5231],
  ['CYS12', 'N_120', 'P', 'ALA44', 'O_633', 'P', 3.3349, 36.1006],
  ..
  ..
```

```
In [19]: interactionsTrajectory.getSaltBridges()
```

```
[[['GLU139', 'OE1_2125_2126', 'P', 'HSE66', 'NE2_957', 'P', 2.8359],
  ['ASP81', 'OD1_1193_1194', 'P', 'ARG75', 'NH1_1090_1093', 'P', 2.9163],
  ['ASP32', 'OD1_443_444', 'P', 'LYS28', 'NZ_380', 'P', 3.037],
  ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 3.0699],
  ['ARG27', 'NH1_356_359', 'P', 'GLU23', 'OE1_290_291', 'P', 3.7148],
  ['GLU139', 'OE1_2125_2126', 'P', 'ARG65', 'NH1_938_941', 'P', 3.7799],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.9359],
  ['ARG58', 'NH1_829_832', 'P', 'ASP56', 'OD1_788_789', 'P', 3.9486],
  ['ARG18', 'NH1_217_220', 'P', 'ASP92', 'OD1_1368_1369', 'P', 4.0693],
  ['GLU114', 'OE1_1735_1736', 'P', 'LYS112', 'NZ_1699', 'P', 4.0787],
  ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 4.1543],
  ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 4.1879],
  ['HSE157', 'NE2_2418', 'P', 'GLU114', 'OE1_1735_1736', 'P', 4.3835],
```

```
  ['ARG18', 'NH1_217_220', 'P', 'ASP129', 'OD1_1978_1979', 'P', 4.5608],
  ['ARG75', 'NH1_1090_1093', 'P', 'ASP42', 'OD1_609_610', 'P', 4.5612],
  ['GLU23', 'OE1_290_291', 'P', 'HSE72', 'NE2_1042', 'P', 4.99]],
 [['ASP32', 'OD1_443_444', 'P', 'LYS28', 'NZ_380', 'P', 2.5568],
  ['ASP81', 'OD1_1193_1194', 'P', 'ARG75', 'NH1_1090_1093', 'P', 2.6325],
  ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 2.8263],
  ['GLU114', 'OE1_1735_1736', 'P', 'LYS112', 'NZ_1699', 'P', 3.0552],
  ['HSE157', 'NE2_2418', 'P', 'GLU114', 'OE1_1735_1736', 'P', 3.2384],
  ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.3269],
  ['ARG27', 'NH1_356_359', 'P', 'GLU23', 'OE1_290_291', 'P', 3.4115],
  ['GLU139', 'OE1_2125_2126', 'P', 'ARG65', 'NH1_938_941', 'P', 3.4427],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.5063],
  ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 3.8015],
  ['ARG58', 'NH1_829_832', 'P', 'ASP56', 'OD1_788_789', 'P', 3.8017],
  ['ARG18', 'NH1_217_220', 'P', 'ASP92', 'OD1_1368_1369', 'P', 3.8368],
  ['GLU139', 'OE1_2125_2126', 'P', 'HSE66', 'NE2_957', 'P', 3.9677],
  ['ARG75', 'NH1_1090_1093', 'P', 'ASP42', 'OD1_609_610', 'P', 4.5207]],
 [['GLU114', 'OE1_1735_1736', 'P', 'LYS112', 'NZ_1699', 'P', 2.5925],
  ['ASP32', 'OD1_443_444', 'P', 'LYS28', 'NZ_380', 'P', 2.5955],
  ['GLU139', 'OE1_2125_2126', 'P', 'ARG65', 'NH1_938_941', 'P', 2.6677],
  ['ASP81', 'OD1_1193_1194', 'P', 'ARG75', 'NH1_1090_1093', 'P', 2.945],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.0796],
  ['ARG58', 'NH1_829_832', 'P', 'ASP56', 'OD1_788_789', 'P', 3.6],
  ['GLU139', 'OE1_2125_2126', 'P', 'HSE66', 'NE2_957', 'P', 3.6121],
  ['ARG18', 'NH1_217_220', 'P', 'ASP92', 'OD1_1368_1369', 'P', 3.6951],
  ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.7353],
  ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 3.8213],
  ['ARG27', 'NH1_356_359', 'P', 'GLU23', 'OE1_290_291', 'P', 3.897],
  ['HSE157', 'NE2_2418', 'P', 'GLU114', 'OE1_1735_1736', 'P', 4.2197],
  ['ARG75', 'NH1_1090_1093', 'P', 'ASP42', 'OD1_609_610', 'P', 4.3401],
  ['ARG18', 'NH1_217_220', 'P', 'ASP129', 'OD1_1978_1979', 'P', 4.6103],
  ['ASP86', 'OD1_1269_1270', 'P', 'LYS6', 'NZ_32', 'P', 4.9726]],
 [['ASP32', 'OD1_443_444', 'P', 'LYS28', 'NZ_380', 'P', 2.5045],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 2.8527],
  ['ASP81', 'OD1_1193_1194', 'P', 'ARG75', 'NH1_1090_1093', 'P', 2.8842],
  ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.2487],
  ..
  ..
```

```
In [20]: interactionsTrajectory.getHydrophobic()
```

```
[[['ALA156', 'CB_2401', 'P', 'TYR87', 'OH_1286', 'P', 3.0459, 21.959],
  ['ALA24', 'CB_298', 'P', 'MET63', 'CE_894', 'P', 3.3105, 5.1584],
  ['ILE68', 'CG2_976', 'P', 'MET63', 'CE_894', 'P', 3.3306, 52.4165],
  ['TYR142', 'CZ_2171', 'P', 'VAL146', 'CG2_2235', 'P', 3.4815, 49.7427],
  ['PHE10', 'CD1_92', 'P', 'ALA22', 'CB_273', 'P', 3.5334, 31.1973],
  ['LYS6', 'CD_26', 'P', 'TRP39', 'CZ2_555', 'P', 3.5427, 68.7284],
  ['PHE26', 'CE2_336', 'P', 'VAL30', 'CG1_411', 'P', 3.5603, 21.127],
  ['ILE88', 'CD_1307', 'P', 'ALA111', 'CB_1677', 'P', 3.5627, 21.2201],
  ['VAL11', 'CG2_114', 'P', 'ILE88', 'CG2_1300', 'P', 3.6386, 9.3289],
  ['VAL41', 'CG2_595', 'P', 'PHE26', 'CD2_334', 'P', 3.6448, 16.55],
  ['PHE152', 'CE1_2331', 'P', 'ALA156', 'CB_2401', 'P', 3.6594, 17.4765],
  ['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 3.6828, 25.1359],
  ['LEU99', 'CD2_1480', 'P', 'ILE77', 'CD_1128', 'P', 3.6917, 11.9735],
  ['PHE82', 'CD1_1205', 'P', 'ILE88', 'CD_1307', 'P', 3.692, 17.6138],
  ['LEU116', 'CD2_1771', 'P', 'ILE127', 'CD_1949', 'P', 3.7057, 17.4094],
  ['VAL8', 'CG1_55', 'P', 'PHE26', 'CE2_336', 'P', 3.7106, 12.1392],
  ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.7263, 16.9718],
```

```
  ['LEU9', 'CD2_78', 'P', 'ILE77', 'CD_1128', 'P', 3.745, 15.4175],
  ['LEU89', 'CD1_1322', 'P', 'VAL8', 'CG2_59', 'P', 3.7672, 15.9262],
  ['ILE126', 'CD_1930', 'P', 'LEU125', 'CD1_1907', 'P', 3.7885, 54.1512],
  ['VAL141', 'CG1_2149', 'P', 'ILE127', 'CG2_1942', 'P', 3.8659, 11.4623],
  ['MET91', 'SD_1353', 'P', 'ILE127', 'CD_1949', 'P', 3.8864, 35.855],
  ['ALA44', 'CB_628', 'P', 'LEU9', 'CD1_74', 'P', 3.8992, 15.0915],
  ['VAL25', 'CG2_314', 'P', 'TYR142', 'CE1_2169', 'P', 3.92, 12.0265],
  ['ILE21', 'CG2_256', 'P', 'MET63', 'SD_893', 'P', 3.9614, 20.7701],
  ['LEU153', 'CD1_2350', 'P', 'TRP39', 'NE1_547', 'P', 3.967, 9.4118],
  ['PHE85', 'CZ_1253', 'P', 'LEU9', 'CD1_74', 'P', 4.0119, 32.0573],
  ['ILE35', 'CD_491', 'P', 'TRP39', 'NE1_547', 'P', 4.0172, 25.9805],
  ['LEU29', 'CD1_395', 'P', 'VAL25', 'CG1_310', 'P', 4.0642, 19.7098],
  ['ALA74', 'CB_1068', 'P', 'ILE16', 'CG2_177', 'P', 4.0772, 6.6731],
  ['ARG75', 'CG_1081', 'P', 'ALA44', 'CB_628', 'P', 4.0853, 36.2109],
  ['ARG18', 'CG_208', 'P', 'VAL141', 'CG1_2149', 'P', 4.104, 20.3057],
  ['LYS102', 'CD_1534', 'P', 'ILE77', 'CG2_1121', 'P', 4.1048, 17.4819],
  ['TYR119', 'CE1_1805', 'P', 'LEU89', 'CD2_1326', 'P', 4.1435, 11.5628],
  ['ARG40', 'CG_568', 'P', 'PHE85', 'CE2_1257', 'P', 4.2669, 60.8933],
  ['LYS28', 'CG_371', 'P', 'ILE68', 'CD_983', 'P', 4.2707, 21.8011],
  ['PHE138', 'CD2_2108', 'P', 'ILE21', 'CD_263', 'P', 4.3082, 6.5618],
  ['TYR131', 'CE1_2006', 'P', 'ILE16', 'CD_184', 'P', 4.3352, 8.9118],
  ['ARG58', 'CG_820', 'P', 'PHE138', 'CE1_2104', 'P', 4.4781, 59.4126]],
 [['MET63', 'SD_893', 'P', 'TYR142', 'CD1_2167', 'P', 3.3036, 26.7569],
  ['ALA24', 'CB_298', 'P', 'MET63', 'CE_894', 'P', 3.3592, 7.0868],
  ['VAL8', 'CG2_59', 'P', 'PHE10', 'CZ_96', 'P', 3.3808, 27.8216],
  ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.429, 13.2977],
  ['LEU116', 'CD1_1767', 'P', 'PHE10', 'CE1_94', 'P', 3.549, 13.546],
  ['PHE82', 'CZ_1209', 'P', 'ILE77', 'CD_1128', 'P', 3.5608, 20.4262],
  ['ILE68', 'CD_983', 'P', 'TYR142', 'OH_2172', 'P', 3.5692, 27.4475],
  ['PHE26', 'CE2_336', 'P', 'VAL30', 'CG1_411', 'P', 3.5789, 28.1292],
  ['ALA156', 'CB_2401', 'P', 'PHE152', 'CD1_2329', 'P', 3.6255, 24.4807],
  ['VAL11', 'CG2_114', 'P', 'ILE88', 'CG2_1300', 'P', 3.6421, 8.6093],
  ..
  ..
```

```
In [21]: interactionsTrajectory.getPiCation()
```

```
[[['PHE85',
   '1248_1249_1251_1253_1255_1257',
   'P',
   'ARG40',
   'NH1_577_580',
   'P',
   3.6523],
  ['HSE66', '953_954_955_957_959', 'P', 'ARG65', 'NH1_938_941', 'P', 4.5323],
  ['HSE157',
   '2414_2415_2416_2418_2420_2423_2424',
   'P',
   'LYS112',
   'NZ_1699',
   'P',
   4.828]],
 [['HSE157',
   '2414_2415_2416_2418_2420_2423_2424',
   'P',
   'LYS112',
   'NZ_1699',
   'P',
```

```
  3.4611],
 ['PHE85',
  '1248_1249_1251_1253_1255_1257',
  'P',
  'ARG40',
  'NH1_577_580',
  'P',
  3.924],
 ['HSE66', '953_954_955_957_959', 'P', 'ARG65', 'NH1_938_941', 'P', 4.8561],
 ['TYR87',
  '1280_1281_1283_1285_1288_1290',
  'P',
  'LYS112',
  'NZ_1699',
  'P',
  4.9287],
 ['TYR131',
  '2003_2004_2006_2008_2011_2013',
  'P',
  'ARG58',
  'NH1_829_832',
  'P',
  4.9441]],
[['HSE157',
  '2414_2415_2416_2418_2420_2423_2424',
  'P',
  'LYS112',
  'NZ_1699',
  'P',
  2.693],
 ['HSE66', '953_954_955_957_959', 'P', 'ARG65', 'NH1_938_941', 'P', 4.0971],
 ['PHE85',
  '1248_1249_1251_1253_1255_1257',
  'P',
  'ARG40',
  'NH1_577_580',
  'P',
  4.4856]],
[['HSE157',
  '2414_2415_2416_2418_2420_2423_2424',
  'P',
  'LYS112',
  'NZ_1699',
  'P',
  2.5938],
 ['PHE85',
  '1248_1249_1251_1253_1255_1257',
  'P',
  'ARG40',
  'NH1_577_580',
  'P',
  3.5816],
 ['HSE66', '953_954_955_957_959', 'P', 'ARG65', 'NH1_938_941', 'P', 3.8296]],
[['PHE85',
  '1248_1249_1251_1253_1255_1257',
  'P',
  'ARG40',
  'NH1_577_580',
```

```
   'P',
   3.9363],
  ['HSE66', '953_954_955_957_959', 'P', 'ARG65', 'NH1_938_941', 'P', 4.7618],
  ['HSE157',
   '2414_2415_2416_2418_2420_2423_2424',
   'P',
   'LYS155',
   'NZ_2391',
   'P',
   4.8181],
  ['HSE157',
   '2414_2415_2416_2418_2420_2423_2424',
   'P',
   'LYS112',
   'NZ_1699',
   'P',
   4.8867]],
 [['HSE66', '953_954_955_957_959', 'P', 'ARG65', 'NH1_938_941', 'P', 4.2935],
  ['HSE157',
   '2414_2415_2416_2418_2420_2423_2424',
   'P',
   'LYS112',
   'NZ_1699',
   'P',
   4.3158]],
 [['PHE85',
   '1248_1249_1251_1253_1255_1257',
   'P',
   'ARG40',
   'NH1_577_580',
   'P',
   3.8709],
  ['HSE66', '953_954_955_957_959', 'P', 'ARG65', 'NH1_938_941', 'P', 4.4195],
  ['PHE138',
   '2101_2102_2104_2106_2108_2110',
   'P',
   'ARG58',
   'NH1_829_832',
   'P',
   4.9708]],
  ..
  ..
```

```
In [22]: interactionsTrajectory.getPiStacking()
```

```
[[['HSE66',
   '953_954_955_957_959',
   'P',
   'TYR142',
   '2166_2167_2169_2171_2174_2176',
   'P',
   3.8882,
   162.1245],
  ['HSE157',
   '2414_2415_2416_2418_2420_2423_2424',
   'P',
   'TYR119',
   '1802_1803_1805_1807_1810_1812',
```

```
   'P',
   4.3605,
   3.0063],
  ['PHE26',
   '327_328_330_332_334_336',
   'P',
   'TRP39',
   '549_550_551_553_555_557',
   'P',
   4.8394,
   75.4587],
  ['TYR132',
   '2024_2025_2027_2029_2032_2034',
   'P',
   'TYR131',
   '2003_2004_2006_2008_2011_2013',
   'P',
   4.8732,
   91.4358]],
 [['PHE26',
   '327_328_330_332_334_336',
   'P',
   'TRP39',
   '549_550_551_553_555_557',
   'P',
   4.8046,
   70.9506],
  ['HSE66',
   '953_954_955_957_959',
   'P',
   'TYR142',
   '2166_2167_2169_2171_2174_2176',
   'P',
   4.8351,
   138.8872]],
 [['HSE66',
   '953_954_955_957_959',
   'P',
   'TYR142',
   '2166_2167_2169_2171_2174_2176',
   'P',
   3.6419,
   174.2245]],
 [['HSE66',
   '953_954_955_957_959',
   'P',
   'TYR142',
   '2166_2167_2169_2171_2174_2176',
   'P',
   4.1376,
   143.3286]],
 [['HSE66',
   '953_954_955_957_959',
   'P',
   'TYR142',
   '2166_2167_2169_2171_2174_2176',
   'P',
   4.2999,
```

```
   137.4965],
  ['TYR87',
   '1280_1281_1283_1285_1288_1290',
   'P',
   'PHE152',
   '2328_2329_2331_2333_2335_2337',
   'P',
   4.9646,
   73.7093]],
 [['HSE66',
   '953_954_955_957_959',
   'P',
   'TYR142',
   '2166_2167_2169_2171_2174_2176',
   'P',
   4.2623,
   158.0688],
   ..
   ..
```

Once we compute interactions, we can also select two that are interesting for us by using `selection` or `selection` and `selection2` if we want to compare two chains of protein structure. Here, we can display all interactions with residues with numbers between 100 and 106.

```
In [23]: interactionsTrajectory.getInteractions(selection='resid 100 to 106')
```

```
[[['ARG101', 'NH1_1516', 'P', 'ASP98', 'OD1_1463', 'P', 1.998, 33.1238],
  ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 2.8075, 29.107],
  ['ASN100', 'N_1486', 'P', 'LEU96', 'O_1430', 'P', 2.933, 10.3321],
  ['LYS102', 'N_1524', 'P', 'ASP98', 'O_1466', 'P', 2.9361, 9.2855],
  ['ARG101', 'N_1500', 'P', 'ARG97', 'O_1454', 'P', 2.9952, 32.2712],
  ['GLN105', 'N_1571', 'P', 'LYS102', 'O_1545', 'P', 3.0464, 19.6807],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD2_1464', 'P', 3.4548, 26.1223],
  ['VAL106', 'N_1588', 'P', 'SER103', 'O_1556', 'P', 3.4974, 34.2367]],
 [['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD2_1464', 'P', 2.5963, 18.6089],
  ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 2.7535, 13.6202],
  ['LYS102', 'N_1524', 'P', 'ASP98', 'O_1466', 'P', 2.7626, 15.9446],
  ['ARG101', 'NH2_1519', 'P', 'ASP98', 'OD2_1464', 'P', 2.9067, 16.7879],
  ['ASN100', 'N_1486', 'P', 'LEU96', 'O_1430', 'P', 3.0125, 16.6445],
  ['ARG101', 'NH1_1516', 'P', 'ASP98', 'OD1_1463', 'P', 3.0551, 13.8509],
  ['SER103', 'OG_1553', 'P', 'LEU99', 'O_1485', 'P', 3.1649, 39.2608],
  ['ARG101', 'N_1500', 'P', 'ARG97', 'O_1454', 'P', 3.2195, 25.4359],
  ['ASN104', 'N_1557', 'P', 'ASN100', 'O_1499', 'P', 3.3521, 12.6376],
  ['GLN105', 'N_1571', 'P', 'ARG101', 'O_1523', 'P', 3.3904, 38.6896],
  ['VAL106', 'N_1588', 'P', 'LYS102', 'O_1545', 'P', 3.46, 29.7639]],
 [['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD2_1464', 'P', 2.6466, 7.8982],
  ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 2.8761, 17.0562],
  ['LYS102', 'N_1524', 'P', 'ASP98', 'O_1466', 'P', 2.9269, 16.8394],
  ['VAL106', 'N_1588', 'P', 'LYS102', 'O_1545', 'P', 2.984, 10.6183],
  ['ARG101', 'N_1500', 'P', 'ARG97', 'O_1454', 'P', 3.101, 38.8603],
  ['ASN100', 'N_1486', 'P', 'LEU96', 'O_1430', 'P', 3.2553, 38.5648]],
 [['ARG101', 'NH2_1519', 'P', 'ASP98', 'OD1_1463', 'P', 2.5911, 17.069],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD2_1464', 'P', 2.6274, 12.9418],
  ['SER103', 'OG_1553', 'P', 'LEU99', 'O_1485', 'P', 2.7018, 15.5273],
  ['LYS102', 'N_1524', 'P', 'ASP98', 'O_1466', 'P', 2.8801, 16.6129],
  ['ARG101', 'N_1500', 'P', 'ARG97', 'O_1454', 'P', 2.9348, 25.5713],
  ['GLN105', 'N_1571', 'P', 'LYS102', 'O_1545', 'P', 2.9562, 38.6882],
  ['ARG101', 'NE_1513', 'P', 'ASP98', 'OD1_1463', 'P', 3.1464, 36.9083],
```

```
 ['LYS102', 'NZ_1540', 'P', 'SER47', 'OG_665', 'P', 3.155, 33.2035],
 ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 3.2314, 26.449]],
[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD2_1464', 'P', 2.6718, 15.3661],
 ['ASN100', 'N_1486', 'P', 'LEU96', 'O_1430', 'P', 2.6858, 28.5654],
 ['ARG101', 'NH2_1519', 'P', 'ASP98', 'OD1_1463', 'P', 2.7479, 25.7898],
 ['LYS102', 'N_1524', 'P', 'ASP98', 'O_1466', 'P', 2.7584, 9.5766],
 ['SER103', 'OG_1553', 'P', 'LEU99', 'O_1485', 'P', 2.8029, 24.9678],
 ['ARG101', 'NE_1513', 'P', 'ASP98', 'OD1_1463', 'P', 2.9645, 18.3577],
 ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 3.0085, 24.3135],
 ['ARG101', 'N_1500', 'P', 'ARG97', 'O_1454', 'P', 3.2018, 39.9842],
 ['VAL106', 'N_1588', 'P', 'LYS102', 'O_1545', 'P', 3.2421, 26.211],
 ['ASN104', 'N_1557', 'P', 'ARG101', 'O_1523', 'P', 3.3623, 38.1443]],
[['SER103', 'OG_1553', 'P', 'LEU99', 'O_1485', 'P', 2.6595, 13.3173],
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  ['LYS102', 'CD_1534', 'P', 'ILE77', 'CG2_1121', 'P', 4.1048, 17.4819]],
 [['LYS102', 'CD_1534', 'P', 'ILE77', 'CG2_1121', 'P', 3.6601, 18.1513],
  ['VAL106', 'CG2_1598', 'P', 'PHE82', 'CD2_1211', 'P', 4.0401, 13.1367],
  ['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 4.2489, 20.4475]],
 [['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 3.9579, 24.0447],
  ['LYS102', 'CD_1534', 'P', 'ILE77', 'CG2_1121', 'P', 3.993, 10.9852]],
 [['LYS79', 'CG_1155', 'P', 'VAL106', 'CG1_1594', 'P', 3.7771, 25.8417],
  ['LYS102', 'CD_1534', 'P', 'ILE77', 'CG2_1121', 'P', 4.2695, 6.7328]],
 [['VAL106', 'CG2_1598', 'P', 'PHE82', 'CD2_1211', 'P', 3.7581, 24.2415],
  ['LYS102', 'CD_1534', 'P', 'LEU99', 'CD2_1480', 'P', 4.3995, 30.7521]],
 [['LYS79', 'CD_1158', 'P', 'VAL106', 'CG2_1598', 'P', 3.9758, 19.5257],
  ['LYS102', 'CD_1534', 'P', 'ILE77', 'CG2_1121', 'P', 4.2315, 11.0609]],
 [['VAL106', 'CG1_1594', 'P', 'PHE82', 'CG_1204', 'P', 3.8971, 17.973],
  ['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 4.0318, 20.1861]],
 [['VAL106', 'CG2_1598', 'P', 'PHE82', 'CD2_1211', 'P', 3.9504, 18.2026],
  ['LYS102', 'CD_1534', 'P', 'LEU99', 'CD2_1480', 'P', 4.0183, 24.7812],
  ['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 4.354, 18.5823]],
 [['LYS102', 'CD_1534', 'P', 'ILE77', 'CG2_1121', 'P', 4.1345, 9.1889],
  ['LYS79', 'CD_1158', 'P', 'VAL106', 'CG2_1598', 'P', 4.1488, 19.0544]],
 [['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 3.7492, 21.5977]],
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 [['VAL106', 'CG2_1598', 'P', 'PHE82', 'CD2_1211', 'P', 3.7532, 20.5214],
  ['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 4.1843, 21.2188]],
 [['LYS79', 'CD_1158', 'P', 'VAL106', 'CG2_1598', 'P', 4.1132, 33.2299],
  ['LYS102', 'CD_1534', 'P', 'LEU99', 'CD2_1480', 'P', 4.2545, 30.9532]],
 [['VAL106', 'CG1_1594', 'P', 'PHE82', 'CG_1204', 'P', 4.2115, 22.6531],
  ['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 4.4451, 30.8638]],
 [['LYS102', 'CD_1534', 'P', 'PHE82', 'CE2_1213', 'P', 4.1132, 21.6908],
  ['VAL106', 'CG2_1598', 'P', 'PHE82', 'CD2_1211', 'P', 4.301, 14.4692]],
 [['VAL106', 'CG1_1594', 'P', 'PHE82', 'CD1_1205', 'P', 3.769, 29.2683]],
 [['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 3.7591, 26.6179]],
 [['LYS79', 'CG_1155', 'P', 'VAL106', 'CG1_1594', 'P', 3.7466, 15.362],
  ['LYS102', 'CD_1534', 'P', 'PHE82', 'CZ_1209', 'P', 4.3692, 20.969]],
 [['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 3.7838, 20.4368],
  ['LYS102', 'CD_1534', 'P', 'ILE77', 'CG2_1121', 'P', 4.2006, 12.5337]],
 [['LYS102', 'CD_1534', 'P', 'PHE82', 'CZ_1209', 'P', 4.3001, 14.6918]],
 [['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 4.2078, 41.8606],
  ['LYS102', 'CD_1534', 'P', 'ILE77', 'CG2_1121', 'P', 4.3141, 10.5395]],
 [['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 4.2738, 15.6412]],
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We can apply the same selection to any type of interaction, for example:

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In [24]: interactionsTrajectory.getHydrophobic(selection='chain P and resid 90 to 100')
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[[['LEU99', 'CD2_1480', 'P', 'ILE77', 'CD_1128', 'P', 3.6917, 11.9735],
  ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.7263, 16.9718],
  ['MET91', 'SD_1353', 'P', 'ILE127', 'CD_1949', 'P', 3.8864, 35.855]],
 [['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.429, 13.2977],
  ['LEU99', 'CD2_1480', 'P', 'ILE77', 'CD_1128', 'P', 3.6871, 7.95],
  ['MET91', 'CE_1354', 'P', 'LEU116', 'CD2_1771', 'P', 3.8434, 19.1277]],
 [['ILE88', 'CG2_1300', 'P', 'LEU99', 'CD1_1476', 'P', 3.5436, 9.3247],
  ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.57, 23.3065],
  ['LEU116', 'CD2_1771', 'P', 'MET91', 'SD_1353', 'P', 3.6654, 17.4729]],
 [['LEU99', 'CD1_1476', 'P', 'ILE88', 'CG2_1300', 'P', 3.5506, 10.5506],
  ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.6132, 25.5246],
  ['LEU116', 'CD2_1771', 'P', 'MET91', 'CE_1354', 'P', 3.6989, 21.7296]],
 [['VAL11', 'CG2_114', 'P', 'LEU99', 'CD1_1476', 'P', 3.681, 13.3699],
  ['LEU116', 'CD2_1771', 'P', 'MET91', 'CE_1354', 'P', 3.7838, 19.4208],
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 ['ILE127', 'CD_1949', 'P', 'MET91', 'SD_1353', 'P', 3.8538, 35.0746],
 ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CD_1718', 'P', 3.993, 32.6427],
 ['LYS102', 'CD_1534', 'P', 'LEU99', 'CD2_1480', 'P', 4.3995, 30.7521]],
[['LEU99', 'CD2_1480', 'P', 'ILE77', 'CD_1128', 'P', 3.4473, 9.6836],
 ['ILE127', 'CD_1949', 'P', 'MET91', 'SD_1353', 'P', 3.7931, 33.4972],
 ['LEU116', 'CD2_1771', 'P', 'MET91', 'CE_1354', 'P', 3.8599, 15.7656],
 ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG1_1715', 'P', 4.0839, 25.8005]],
[['LEU99', 'CD2_1480', 'P', 'ILE77', 'CD_1128', 'P', 3.6656, 11.2061],
 ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CD_1718', 'P', 3.7465, 13.9407],
 ['MET91', 'CE_1354', 'P', 'ALA22', 'CB_273', 'P', 4.1873, 5.8643]],
[['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.577, 21.8565],
 ['LEU116', 'CD2_1771', 'P', 'MET91', 'CE_1354', 'P', 3.7311, 16.6688],
 ['LEU99', 'CD1_1476', 'P', 'ILE77', 'CD_1128', 'P', 3.7918, 13.9645],
 ['LYS102', 'CD_1534', 'P', 'LEU99', 'CD2_1480', 'P', 4.0183, 24.7812]],
[['LEU99', 'CD1_1476', 'P', 'ILE88', 'CG2_1300', 'P', 3.493, 12.0525],
 ['LEU116', 'CD2_1771', 'P', 'MET91', 'SD_1353', 'P', 3.8477, 17.8661],
 ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.9465, 13.0407],
 ['ARG18', 'CG_208', 'P', 'MET91', 'CG_1350', 'P', 4.4773, 45.2545]],
[['MET91', 'SD_1353', 'P', 'ILE127', 'CD_1949', 'P', 3.6073, 35.8986],
 ['LEU99', 'CD1_1476', 'P', 'VAL11', 'CG1_110', 'P', 3.8196, 19.5026],
 ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.8266, 8.1345]],
[['LEU116', 'CD2_1771', 'P', 'MET91', 'CE_1354', 'P', 3.688, 16.5389],
 ['LEU99', 'CD2_1480', 'P', 'ILE77', 'CD_1128', 'P', 3.8303, 12.8658],
 ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.9125, 20.3824],
 ['ARG18', 'CG_208', 'P', 'MET91', 'CG_1350', 'P', 4.3469, 47.3018]],
[['LEU116', 'CD2_1771', 'P', 'MET91', 'SD_1353', 'P', 3.4146, 25.9366],
 ['LEU99', 'CD2_1480', 'P', 'PHE82', 'CZ_1209', 'P', 3.6458, 17.5698],
 ['ILE113', 'CG2_1711', 'P', 'LEU99', 'CD1_1476', 'P', 3.7998, 30.7151],
 ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 4.0071, 18.0266],
 ['LYS102', 'CD_1534', 'P', 'LEU99', 'CD2_1480', 'P', 4.2545, 30.9532]],
[['LEU116', 'CD2_1771', 'P', 'MET91', 'SD_1353', 'P', 3.5757, 19.6775],
 ['LEU99', 'CD2_1480', 'P', 'ILE88', 'CG2_1300', 'P', 3.8102, 10.1337],
 ['ILE113', 'CG2_1711', 'P', 'LEU96', 'CG_1419', 'P', 3.8694, 28.8723]],
[['VAL11', 'CG2_114', 'P', 'LEU99', 'CD1_1476', 'P', 3.5696, 9.6273],
 ['LEU116', 'CD2_1771', 'P', 'MET91', 'SD_1353', 'P', 3.8426, 17.9602]],
[['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.511, 19.586],
 ['LEU99', 'CD1_1476', 'P', 'VAL11', 'CG2_114', 'P', 3.5732, 10.7329],
 ['MET91', 'CE_1354', 'P', 'LEU116', 'CD2_1771', 'P', 3.9678, 13.6217]],
[['VAL11', 'CG2_114', 'P', 'LEU99', 'CD1_1476', 'P', 3.6543, 13.7308],
 ['ILE113', 'CG2_1711', 'P', 'LEU96', 'CG_1419', 'P', 3.7456, 22.5419],
 ['LEU116', 'CD2_1771', 'P', 'MET91', 'SD_1353', 'P', 3.8152, 17.9895]],
[['VAL11', 'CG2_114', 'P', 'LEU99', 'CD1_1476', 'P', 3.4849, 12.5888],
 ['MET91', 'CE_1354', 'P', 'ALA22', 'CB_273', 'P', 3.5767, 9.5877],
 ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.7229, 15.3003],
 ['ILE127', 'CD_1949', 'P', 'MET91', 'SD_1353', 'P', 4.274, 35.6655]],
[['LEU116', 'CD2_1771', 'P', 'MET91', 'SD_1353', 'P', 3.6286, 22.7844],
 ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.6984, 12.3956],
 ['ALA22', 'CB_273', 'P', 'MET91', 'CE_1354', 'P', 3.7795, 8.4161],
 ['LEU99', 'CD2_1480', 'P', 'ILE88', 'CG2_1300', 'P', 3.7921, 7.4352]],
[['ILE127', 'CD_1949', 'P', 'MET91', 'SD_1353', 'P', 3.4598, 42.01],
 ['LEU99', 'CD1_1476', 'P', 'ILE113', 'CG2_1711', 'P', 3.6609, 33.0336],
 ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.7378, 17.5379],
 ['LEU116', 'CD2_1771', 'P', 'MET91', 'CE_1354', 'P', 3.7686, 14.0166]],
[['LEU99', 'CD1_1476', 'P', 'VAL11', 'CG2_114', 'P', 3.518, 18.8799],
 ['LEU116', 'CD2_1771', 'P', 'MET91', 'CE_1354', 'P', 3.5399, 12.2359],
 ['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.7165, 21.0434]],
[['LEU96', 'CD1_1421', 'P', 'ILE113', 'CG2_1711', 'P', 3.2931, 21.0747],
 ['VAL11', 'CG2_114', 'P', 'LEU99', 'CD1_1476', 'P', 3.3771, 11.4804],
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  ['MET91', 'CE_1354', 'P', 'ALA22', 'CB_273', 'P', 3.6628, 9.0978],
  ['LEU116', 'CD2_1771', 'P', 'MET91', 'SD_1353', 'P', 3.6984, 21.9302]]]
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In [25]: interactionsTrajectory.getHydrogenBonds(selection='chain P and resid 112 to 115')
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[[['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.8429, 17.7147],
  ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.8975, 24.576],
  ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.912, 10.1158],
  ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.051, 21.4045],
  ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.059, 24.1606],
  ['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT2_2424', 'P', 3.2687, 28.6743]],
 [['LYS112', 'NZ_1699', 'P', 'GLU114', 'OE1_1735', 'P', 2.5487, 20.8176],
  ['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT1_2423', 'P', 2.6334, 17.8203],
  ['SER118', 'OG_1791', 'P', 'LEU115', 'O_1757', 'P', 2.6547, 25.6442],
  ['TYR119', 'OH_1808', 'P', 'GLU114', 'OE1_1735', 'P', 2.735, 15.8502],
  ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.7935, 13.2257],
  ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.8946, 17.9316],
  ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.9523, 13.8795],
  ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.0323, 8.8409],
  ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.2094, 37.0837],
  ['CYS90', 'SG_1339', 'P', 'GLU114', 'O_1738', 'P', 3.2322, 23.7336],
  ['HSE157', 'NE2_2418', 'P', 'GLU114', 'OE2_1736', 'P', 3.253, 23.8402]],
 [['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT1_2423', 'P', 2.5902, 19.0335],
  ['TYR119', 'OH_1808', 'P', 'GLU114', 'OE2_1736', 'P', 2.6441, 10.2991],
  ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.7184, 24.9984],
  ['SER118', 'OG_1791', 'P', 'LEU115', 'O_1757', 'P', 2.7238, 26.9156],
  ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.8381, 10.253],
  ['LYS112', 'NZ_1699', 'P', 'HSE157', 'ND1_2414', 'P', 2.8616, 14.018],
  ['LYS112', 'NZ_1699', 'P', 'GLU114', 'OE2_1736', 'P', 2.8761, 18.0626],
  ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.0416, 27.2343],
  ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 3.195, 38.6534],
  ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.4603, 13.0317]],
 [['SER118', 'OG_1791', 'P', 'GLU114', 'OE1_1735', 'P', 2.5321, 12.1754],
  ['TYR119', 'OH_1808', 'P', 'GLU114', 'OE2_1736', 'P', 2.6666, 5.0368],
  ['LYS112', 'NZ_1699', 'P', 'GLU114', 'OE2_1736', 'P', 2.6844, 12.4337],
  ['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT2_2424', 'P', 2.7625, 21.1367],
  ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.7703, 4.1752],
  ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.813, 11.6498],
  ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.8375, 24.3092],
  ['LYS112', 'NZ_1699', 'P', 'HSE157', 'ND1_2414', 'P', 2.8399, 24.5852],
  ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 2.9985, 12.7544]],
 [['TYR119', 'OH_1808', 'P', 'GLU114', 'OE2_1736', 'P', 2.6438, 28.5062],
  ['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT2_2424', 'P', 2.7748, 6.971],
  ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.8324, 30.6076],
  ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.8567, 3.076],
  ['LYS112', 'NZ_1699', 'P', 'GLU114', 'OE2_1736', 'P', 2.8677, 22.3219],
  ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.9251, 9.0077],
  ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.0506, 7.4102],
  ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.4475, 19.9922]],
 [['TYR119', 'OH_1808', 'P', 'GLU114', 'OE1_1735', 'P', 2.6085, 18.3035],
  ['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT1_2423', 'P', 2.7054, 1.3697],
  ['LYS112', 'NZ_1699', 'P', 'GLU114', 'OE1_1735', 'P', 2.7093, 27.1289],
  ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.8128, 18.817],
  ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 3.0762, 12.1723],
  ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.1037, 10.0101],
  ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 3.1356, 19.0662],
  ['CYS90', 'SG_1339', 'P', 'GLU114', 'O_1738', 'P', 3.3017, 27.3282],
  ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.3047, 11.3911]],
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[['SER118', 'OG_1791', 'P', 'GLU114', 'OE2_1736', 'P', 2.652, 10.3503],
 ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.762, 14.1022],
 ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.7884, 21.6503],
 ['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT1_2423', 'P', 2.7994, 5.7305],
 ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.8628, 30.0771],
 ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 2.9474, 28.4869],
 ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.4304, 27.1097]],
[['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.7778, 28.0614],
 ['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT1_2423', 'P', 2.7868, 18.8919],
 ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.8504, 18.6098],
 ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 2.9351, 15.9934],
 ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.9391, 14.958]],
[['SER118', 'OG_1791', 'P', 'GLU114', 'OE2_1736', 'P', 2.6858, 23.9752],
 ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.8512, 7.2231],
 ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 2.9951, 23.9118],
 ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.0881, 6.5417],
 ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 3.1217, 14.0883],
 ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 3.2069, 19.3312],
 ['CYS90', 'SG_1339', 'P', 'GLU114', 'O_1738', 'P', 3.2331, 32.7145]],
[['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT1_2423', 'P', 2.6385, 22.7134],
 ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.6967, 1.035],
 ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.7267, 17.2895],
 ['SER118', 'OG_1791', 'P', 'GLU114', 'OE2_1736', 'P', 2.8598, 29.0811],
 ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.9766, 16.8905],
 ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.0616, 27.2229],
 ['CYS90', 'SG_1339', 'P', 'GLU114', 'O_1738', 'P', 3.4089, 25.9472]],
[['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT2_2424', 'P', 2.8001, 13.1653],
 ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.8336, 11.5184],
 ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.8683, 15.5308],
 ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.8949, 10.1824],
 ['SER118', 'OG_1791', 'P', 'GLU114', 'OE2_1736', 'P', 2.9677, 16.3497],
 ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.089, 17.9789]],
[['LYS112', 'NZ_1699', 'P', 'HSE157', 'OT2_2424', 'P', 2.7045, 11.8564],
 ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.8002, 5.9828],
 ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.8444, 31.549],
 ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.0718, 34.4381],
 ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 3.3002, 12.0528]],
[['SER118', 'OG_1791', 'P', 'GLU114', 'OE2_1736', 'P', 2.549, 18.6576],
 ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.7292, 11.3872],
 ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.7951, 19.2119],
 ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.861, 9.3445],
 ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 2.8723, 5.3509],
 ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.2056, 13.0868]],
[['SER118', 'OG_1791', 'P', 'GLU114', 'OE2_1736', 'P', 2.7432, 12.0576],
 ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.8455, 10.8341],
 ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.8979, 18.8959],
 ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.9513, 25.3055],
 ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.2646, 30.184]],
[['SER118', 'OG_1791', 'P', 'GLU114', 'OE2_1736', 'P', 2.7509, 33.4365],
 ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.7569, 15.9129],
 ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.8989, 5.3091],
 ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 3.0521, 14.9906],
 ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.2193, 17.7506]],
[['SER118', 'OG_1791', 'P', 'GLU114', 'OE1_1735', 'P', 2.9107, 11.3311],
 ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.9279, 24.4459],
 ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.9572, 22.8551],
 ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 3.0531, 39.2571],
 ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.2647, 19.7898]],
```

```
 [['SER118', 'OG_1791', 'P', 'GLU114', 'OE1_1735', 'P', 2.7301, 6.4912],
  ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 3.0067, 19.0131],
  ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 3.0515, 32.6929],
  ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 3.0654, 16.9354],
  ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.2584, 28.3632]],
 [['SER118', 'OG_1791', 'P', 'LEU115', 'O_1757', 'P', 2.7161, 4.3692],
  ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.7665, 15.6553],
  ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.833, 1.7101],
  ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.9604, 20.771],
  ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.1924, 36.5103],
  ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.3101, 22.7426]],
 [['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.7306, 1.388],
  ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 2.7477, 25.8134],
  ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.7669, 4.8657],
  ['SER118', 'OG_1791', 'P', 'GLU114', 'OE2_1736', 'P', 2.7852, 20.1148]],
 [['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.8181, 19.759],
  ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 2.8698, 4.299],
  ['LYS112', 'N_1683', 'P', 'ASP86', 'O_1272', 'P', 3.0671, 23.7084],
  ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.1112, 27.1195],
  ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.1262, 21.7619]],
 [['SER118', 'OG_1791', 'P', 'GLU114', 'OE2_1736', 'P', 2.6334, 24.4833],
  ['CYS90', 'N_1332', 'P', 'GLU114', 'O_1738', 'P', 2.8598, 7.853],
  ['SER118', 'N_1784', 'P', 'LEU115', 'O_1757', 'P', 3.0172, 19.6851],
  ['GLU114', 'N_1724', 'P', 'ILE88', 'O_1312', 'P', 3.2603, 11.1927],
  ['ILE88', 'N_1294', 'P', 'LYS112', 'O_1704', 'P', 3.3213, 8.0609]]]
```

```
In [26]: interactionsTrajectory.getSaltBridges(selection='chain P and resid 100 to 120')
```

```
[[['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 3.0699],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.9359],
  ['GLU114', 'OE1_1735_1736', 'P', 'LYS112', 'NZ_1699', 'P', 4.0787],
  ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 4.1543],
  ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 4.1879],
  ['HSE157', 'NE2_2418', 'P', 'GLU114', 'OE1_1735_1736', 'P', 4.3835]],
 [['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 2.8263],
  ['GLU114', 'OE1_1735_1736', 'P', 'LYS112', 'NZ_1699', 'P', 3.0552],
  ['HSE157', 'NE2_2418', 'P', 'GLU114', 'OE1_1735_1736', 'P', 3.2384],
  ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.3269],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.5063],
  ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 3.8015]],
 [['GLU114', 'OE1_1735_1736', 'P', 'LYS112', 'NZ_1699', 'P', 2.5925],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.0796],
  ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.7353],
  ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 3.8213],
  ['HSE157', 'NE2_2418', 'P', 'GLU114', 'OE1_1735_1736', 'P', 4.2197]],
 [['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 2.8527],
  ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.2487],
  ['GLU114', 'OE1_1735_1736', 'P', 'LYS112', 'NZ_1699', 'P', 3.281],
  ['HSE157', 'NE2_2418', 'P', 'GLU114', 'OE1_1735_1736', 'P', 3.4289],
  ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.5055],
  ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 4.7295]],
 [['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 2.5251],
  ['GLU114', 'OE1_1735_1736', 'P', 'LYS112', 'NZ_1699', 'P', 2.5476],
  ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 2.8031],
  ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 3.7693],
  ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.6639]],
 [['GLU114', 'OE1_1735_1736', 'P', 'LYS112', 'NZ_1699', 'P', 2.5445],
  ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 2.784],
```

```
 ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 2.9545],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 4.4269],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.7415]],
[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 2.7833],
 ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.7841],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 4.6393],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.6905],
 ['HSE157', 'NE2_2418', 'P', 'GLU114', 'OE1_1735_1736', 'P', 4.9985]],
[['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 2.7718],
 ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.118],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 3.7333],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 4.385]],
[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 2.9802],
 ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.1049],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.3115],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 4.4854]],
[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.1925],
 ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.3668],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.3314],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 4.6386]],
[['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 2.7461],
 ['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.1321],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.377]],
[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 2.5465],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG150', 'NH1_2303_2306', 'P', 3.7315],
 ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.886],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.1424]],
[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 2.8662],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.7765],
 ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 4.9921]],
[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.4575],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG150', 'NH1_2303_2306', 'P', 3.6085],
 ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.9194],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 4.3166],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.7844]],
[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 2.7106],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG150', 'NH1_2303_2306', 'P', 3.7026],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 3.794],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.2495]],
[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 2.9739],
 ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.397],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG150', 'NH1_2303_2306', 'P', 3.5529],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 3.9267],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.3131]],
[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.0533],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG147', 'NH1_2257_2260', 'P', 3.7951],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG150', 'NH1_2303_2306', 'P', 3.8215],
 ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.9526],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.8328]],
[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.2511],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 3.6196],
 ['ASP120', 'OD1_1824_1825', 'P', 'ARG150', 'NH1_2303_2306', 'P', 3.9186]],
[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 2.955],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 3.9277]],
[['LYS102', 'NZ_1540', 'P', 'ASP98', 'OD1_1463_1464', 'P', 3.1188],
 ['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 3.6654],
 ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.9234]],
[['ASP98', 'OD1_1463_1464', 'P', 'ARG101', 'NH1_1516_1519', 'P', 2.7506],
```

```
  ['ASP86', 'OD1_1269_1270', 'P', 'LYS110', 'NZ_1667', 'P', 3.4341]]]
```

```
In [27]: interactionsTrajectory.getRepulsiveIonicBonding(selection='chain P')
```

```
[[['LYS102', 'NZ_1540', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.2655]],
 [],
 [],
 [],
 [],
 [],
 [['LYS102', 'NZ_1540', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.2903]],
 [],
 [],
 [['LYS102', 'NZ_1540', 'P', 'ARG101', 'NH1_1516_1519', 'P', 4.3093]],
 [],
 [],
 [],
 [],
 [],
 [],
 [],
 [],
 [],
 [],
 [['ARG147', 'NH1_2257_2260', 'P', 'LYS123', 'NZ_1875', 'P', 4.4846]]]
```

6.3 Change selection criteria for interaction type

The `interactionsTrajectory.calcProteinInteractionsTrajectory()` method computes interactions using default parameters for interactions. However, it can be changed according to our needs. To do that, we need to recalculate the selected types of interactions.

We can do it using the following functions: `calcHydrogenBondsTrajectory()`, `calcHydrogenBondsTrajectory()`, `calcSaltBridgesTrajectory()`, `calcRepulsiveIonicBondingTrajectory()`, `calcPiStackingTrajectory()`, `calcPiCationTrajectory()`, `calcHydrophohicTrajectory()`, and use `InteractionsTrajectory.setNewHydrogenBondsTrajectory()`, `InteractionsTrajectory.setNewSaltBridgesTrajectory()`, `InteractionsTrajectory.setNewRepulsive`, `InteractionsTrajectory.setNewPiStackingTrajectory()`, `InteractionsTrajectory.setNewPiCationTr`, `InteractionsTrajectory.setNewHydrophohicTrajectory()` method to replace it in the main Instance.

For example:

Repulsive ionic bonding:

```
In [28]: newRIB = calcRepulsiveIonicBondingTrajectory(atoms, dcd, distA=8)

In [29]: interactionsTrajectory.setNewRepulsiveIonicBondingTrajectory(newRIB)
```

```
@> Frame: 0
@> Calculating repulsive ionic bonding.
@>      ARG75    P   NH1_1090_1093  <--->      ARG40    P     NH1_577_580     6.7
@>      ASP81    P   OD1_1193_1194  <--->      GLU80    P   OE1_1181_1182     7.0
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     7.6
@> Number of detected Repulsive Ionic Bonding interactions: 3.
@> Frame: 1
```

```
@> Calculating repulsive ionic bonding.
@>     ARG101    P   NH1_1516_1519  <--->     LYS102    P         NZ_1540     4.5
@>      ASP92    P   OD1_1368_1369  <--->      GLU93    P   OE1_1383_1384     7.9
@> Number of detected Repulsive Ionic Bonding interactions: 2.
@> Frame: 2
@> Calculating repulsive ionic bonding.
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     6.8
@>     ASP137    P   OD1_2090_2091  <--->     GLU128    P   OE1_1966_1967     7.7
@>      ASP81    P   OD1_1193_1194  <--->      GLU80    P   OE1_1181_1182     7.9
@> Number of detected Repulsive Ionic Bonding interactions: 3.
@> Frame: 3
@> Calculating repulsive ionic bonding.
@>      GLU80    P   OE1_1181_1182  <--->      ASP81    P   OD1_1193_1194     6.3
@>      ASP42    P     OD1_609_610  <--->      ASP81    P   OD1_1193_1194     6.8
@> Number of detected Repulsive Ionic Bonding interactions: 2.
@> Frame: 4
@> Calculating repulsive ionic bonding.
@>     ARG101    P   NH1_1516_1519  <--->     LYS102    P         NZ_1540     6.0
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     6.8
@>      ARG75    P   NH1_1090_1093  <--->      ARG40    P     NH1_577_580     7.0
@> Number of detected Repulsive Ionic Bonding interactions: 3.
@> Frame: 5
@> Calculating repulsive ionic bonding.
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     6.1
@>      ASP42    P     OD1_609_610  <--->      ASP81    P   OD1_1193_1194     6.6
@>      LYS79    P         NZ_1164  <--->     LYS102    P         NZ_1540     7.8
@> Number of detected Repulsive Ionic Bonding interactions: 3.
@> Frame: 6
@> Calculating repulsive ionic bonding.
@>      ASP42    P     OD1_609_610  <--->      ASP81    P   OD1_1193_1194     6.1
@>     LYS112    P         NZ_1699  <--->       LYS6    P           NZ_32     6.4
@>      LYS79    P         NZ_1164  <--->     LYS107    P         NZ_1620     7.1
@> Number of detected Repulsive Ionic Bonding interactions: 3.
@> Frame: 7
@> Calculating repulsive ionic bonding.
@>     ARG147    P   NH1_2257_2260  <--->     LYS123    P         NZ_1875     4.8
@>      ASP42    P     OD1_609_610  <--->      GLU23    P     OE1_290_291     5.9
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     6.4
@>      ARG75    P   NH1_1090_1093  <--->      ARG40    P     NH1_577_580     6.9
@> Number of detected Repulsive Ionic Bonding interactions: 4.
@> Frame: 8
@> Calculating repulsive ionic bonding.
@>     LYS123    P         NZ_1875  <--->     ARG147    P   NH1_2257_2260     5.1
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     7.0
@>      ASP81    P   OD1_1193_1194  <--->      GLU80    P   OE1_1181_1182     7.2
@> Number of detected Repulsive Ionic Bonding interactions: 3.
@> Frame: 9
@> Calculating repulsive ionic bonding.
@>     ARG101    P   NH1_1516_1519  <--->     LYS102    P         NZ_1540     4.3
@>      GLU93    P   OE1_1383_1384  <--->     GLU128    P   OE1_1966_1967     6.2
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     6.4
@> Number of detected Repulsive Ionic Bonding interactions: 3.
@> Frame: 10
@> Calculating repulsive ionic bonding.
@>     ARG101    P   NH1_1516_1519  <--->     LYS102    P         NZ_1540     4.6
@>     LYS123    P         NZ_1875  <--->     ARG147    P   NH1_2257_2260     4.7
@>      ASP92    P   OD1_1368_1369  <--->     GLU128    P   OE1_1966_1967     6.4
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     7.4
```

```
@> Number of detected Repulsive Ionic Bonding interactions: 4.
@> Frame: 11
@> Calculating repulsive ionic bonding.
@>     ARG101    P   NH1_1516_1519  <--->     LYS102    P         NZ_1540     5.3
@>      ASP42    P     OD1_609_610  <--->      ASP81    P   OD1_1193_1194     6.6
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     7.7
@> Number of detected Repulsive Ionic Bonding interactions: 3.
@> Frame: 12
@> Calculating repulsive ionic bonding.
@>     LYS123    P         NZ_1875  <--->     ARG147    P   NH1_2257_2260     5.9
@>      ARG75    P   NH1_1090_1093  <--->      ARG40    P     NH1_577_580     6.2
@>     ARG150    P   NH1_2303_2306  <--->     ARG147    P   NH1_2257_2260     7.2
@> Number of detected Repulsive Ionic Bonding interactions: 3.
@> Frame: 13
@> Calculating repulsive ionic bonding.
@>      ASP42    P     OD1_609_610  <--->      ASP81    P   OD1_1193_1194     6.6
@>     ASP129    P   OD1_1978_1979  <--->     GLU128    P   OE1_1966_1967     6.6
@>     ARG101    P   NH1_1516_1519  <--->     LYS102    P         NZ_1540     7.8
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     7.8
@> Number of detected Repulsive Ionic Bonding interactions: 4.
@> Frame: 14
@> Calculating repulsive ionic bonding.
@>     LYS123    P         NZ_1875  <--->     ARG147    P   NH1_2257_2260     7.0
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     7.1
@>      ASP81    P   OD1_1193_1194  <--->      GLU80    P   OE1_1181_1182     7.2
@>      ASP92    P   OD1_1368_1369  <--->     GLU128    P   OE1_1966_1967     8.0
@> Number of detected Repulsive Ionic Bonding interactions: 4.
@> Frame: 15
@> Calculating repulsive ionic bonding.
@>     LYS123    P         NZ_1875  <--->     ARG147    P   NH1_2257_2260     6.5
@>     GLU154    P   OE1_2371_2372  <--->     ASP120    P   OD1_1824_1825     6.5
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     6.6
@> Number of detected Repulsive Ionic Bonding interactions: 3.
@> Frame: 16
@> Calculating repulsive ionic bonding.
@>      ASP42    P     OD1_609_610  <--->      GLU23    P     OE1_290_291     5.6
@>     ARG101    P   NH1_1516_1519  <--->     LYS102    P         NZ_1540     7.1
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     7.2
@>     ASP129    P   OD1_1978_1979  <--->     GLU128    P   OE1_1966_1967     7.2
@> Number of detected Repulsive Ionic Bonding interactions: 4.
@> Frame: 17
@> Calculating repulsive ionic bonding.
@>     ARG101    P   NH1_1516_1519  <--->     LYS102    P         NZ_1540     4.9
@>      ASP42    P     OD1_609_610  <--->      ASP81    P   OD1_1193_1194     6.5
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     7.4
@>     GLU128    P   OE1_1966_1967  <--->     ASP129    P   OD1_1978_1979     8.0
@> Number of detected Repulsive Ionic Bonding interactions: 4.
@> Frame: 18
@> Calculating repulsive ionic bonding.
@>      ASP42    P     OD1_609_610  <--->      GLU23    P     OE1_290_291     5.7
@>     ASP135    P   OD1_2067_2068  <--->     GLU139    P   OE1_2125_2126     5.9
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     6.8
@>      ASP92    P   OD1_1368_1369  <--->     GLU128    P   OE1_1966_1967     6.8
@>      GLU93    P   OE1_1383_1384  <--->     GLU128    P   OE1_1966_1967     7.3
@> Number of detected Repulsive Ionic Bonding interactions: 5.
@> Frame: 19
@> Calculating repulsive ionic bonding.
@>     LYS123    P         NZ_1875  <--->     ARG147    P   NH1_2257_2260     5.3
```

```
@>     GLU139    P   OE1_2125_2126  <--->     ASP135    P   OD1_2067_2068     6.0
@>      LYS79    P         NZ_1164  <--->     LYS107    P         NZ_1620     6.1
@>      ASP81    P   OD1_1193_1194  <--->      GLU80    P   OE1_1181_1182     7.0
@> Number of detected Repulsive Ionic Bonding interactions: 4.
@> Frame: 20
@> Calculating repulsive ionic bonding.
@>     LYS123    P         NZ_1875  <--->     ARG147    P   NH1_2257_2260     4.5
@>     ASP135    P   OD1_2067_2068  <--->     GLU139    P   OE1_2125_2126     5.5
@>     ASP129    P   OD1_1978_1979  <--->      ASP92    P   OD1_1368_1369     7.1
@>      LYS79    P         NZ_1164  <--->     LYS102    P         NZ_1540     7.9
@> Number of detected Repulsive Ionic Bonding interactions: 4.

@> Repulsive Ionic Bonding are replaced
```

Pi-cation interactions:

```
In [30]: newPiCation = calcPiCationTrajectory(atoms, dcd, distA=6)

In [31]: interactionsTrajectory.setNewPiCationTrajectory(newPiCation)
```

```
@> Frame: 0
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_5
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                    NH1_938_9
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                          NZ_
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                    NH1_829_8
@>     TYR131   P   2003_2004_2006_2008_2011_2013  <--->      ARG58   P                    NH1_829_8
@> Number of detected cation-pi interactions: 5.
@> Frame: 1
@> Calculating cation-Pi interactions.
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                          NZ_
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_5
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                    NH1_938_9
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->     LYS112   P                        NZ_16
@>     TYR131   P   2003_2004_2006_2008_2011_2013  <--->      ARG58   P                    NH1_829_8
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                    NH1_829_8
@>      TRP39   P         549_550_551_553_555_557  <--->       LYS6   P                          NZ_
@> Number of detected cation-pi interactions: 7.
@> Frame: 2
@> Calculating cation-Pi interactions.
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                          NZ_
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                    NH1_938_9
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_5
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->     LYS112   P                        NZ_16
@> Number of detected cation-pi interactions: 4.
@> Frame: 3
@> Calculating cation-Pi interactions.
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                          NZ_
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_5
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                    NH1_938_9
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                    NH1_829_8
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->     LYS112   P                        NZ_16
@> Number of detected cation-pi interactions: 5.
@> Frame: 4
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                    NH1_577_5
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                    NH1_938_9
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS155   P                          NZ_
```

```
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                    NZ_
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->     LYS112   P                  NZ_16
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                NH1_829_8
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->       LYS6   P                    NZ_
@> Number of detected cation-pi interactions: 7.
@> Frame: 5
@> Calculating cation-Pi interactions.
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                NH1_938_9
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                    NZ_
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                NH1_577_5
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->     LYS112   P                  NZ_16
@> Number of detected cation-pi interactions: 4.
@> Frame: 6
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                NH1_577_5
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                NH1_938_9
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                NH1_829_8
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                    NZ_
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->       LYS6   P                    NZ_
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->     LYS112   P                  NZ_16
@> Number of detected cation-pi interactions: 6.
@> Frame: 7
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                NH1_577_5
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                NH1_938_9
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                    NZ_
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                NH1_829_8
@> Number of detected cation-pi interactions: 4.
@> Frame: 8
@> Calculating cation-Pi interactions.
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                NH1_938_9
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                NH1_577_5
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                    NZ_
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                NH1_829_8
@> Number of detected cation-pi interactions: 4.
@> Frame: 9
@> Calculating cation-Pi interactions.
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                NH1_938_9
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                NH1_577_5
@>      TRP39   P         549_550_551_553_555_557  <--->       LYS6   P                    NZ_
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->     LYS112   P                  NZ_16
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                NH1_829_8
@>     PHE152   P   2328_2329_2331_2333_2335_2337  <--->       LYS6   P                    NZ_
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG75   P              NH1_1090_10
@> Number of detected cation-pi interactions: 7.
@> Frame: 10
@> Calculating cation-Pi interactions.
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                NH1_938_9
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                NH1_829_8
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                NH1_577_5
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->     LYS112   P                  NZ_16
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG75   P              NH1_1090_10
@> Number of detected cation-pi interactions: 5.
@> Frame: 11
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                NH1_577_5
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS155   P                    NZ_
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                NH1_938_9
```

```
@>      TRP39   P         549_550_551_553_555_557  <--->       LYS6   P                    NZ_
       HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS112   P                  NZ_
@>
@> Number of detected cation-pi interactions: 5.
@> Frame: 12
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                  NH1_577_5
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                  NH1_938_9
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                  NH1_829_8
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->     LYS112   P                      NZ_16
@>      HSE72   P        1038_1039_1040_1042_1044  <--->      ARG27   P                  NH1_356_3
@> Number of detected cation-pi interactions: 5.
@> Frame: 13
@> Calculating cation-Pi interactions.
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                  NH1_938_9
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                  NH1_577_5
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                  NH1_829_8
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG75   P                NH1_1090_10
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->     LYS155   P                  NZ_
@>      TRP39   P         549_550_551_553_555_557  <--->       LYS6   P                    NZ_
@> Number of detected cation-pi interactions: 6.
@> Frame: 14
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                  NH1_577_5
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->       LYS6   P                     N
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                  NH1_829_8
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                  NH1_938_9
@> Number of detected cation-pi interactions: 4.
@> Frame: 15
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                  NH1_577_5
@>     HSE157   P2414_2415_2416_2418_2420_2423_2424  <--->       LYS6   P                     N
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                  NH1_829_8
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                  NH1_938_9
@> Number of detected cation-pi interactions: 4.
@> Frame: 16
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                  NH1_577_5
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->       LYS6   P                      NZ_
@> Number of detected cation-pi interactions: 2.
@> Frame: 17
@> Calculating cation-Pi interactions.
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                  NH1_829_8
@>      TRP39   P         549_550_551_553_555_557  <--->       LYS6   P                      NZ_
@> Number of detected cation-pi interactions: 2.
@> Frame: 18
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                  NH1_577_5
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                  NH1_829_8
@>      TRP39   P         549_550_551_553_555_557  <--->       LYS6   P                      NZ_
@>      TYR87   P   1280_1281_1283_1285_1288_1290  <--->     LYS112   P                      NZ_16
@>      HSE72   P        1038_1039_1040_1042_1044  <--->      ARG27   P                  NH1_356_3
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                  NH1_938_9
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG75   P                NH1_1090_10
@> Number of detected cation-pi interactions: 7.
@> Frame: 19
@> Calculating cation-Pi interactions.
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                  NH1_577_5
```

```
@>      TRP39   P         549_550_551_553_555_557  <--->       LYS6   P                    NZ_
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                NH1_829_8
@>      HSE66   P             953_954_955_957_959  <--->      ARG65   P                NH1_938_9
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG75   P               NH1_1090_10
@> Number of detected cation-pi interactions: 5.
@> Frame: 20
@> Calculating cation-Pi interactions.
@>     PHE138   P   2101_2102_2104_2106_2108_2110  <--->      ARG58   P                NH1_829_8
@>      TRP39   P         549_550_551_553_555_557  <--->       LYS6   P                    NZ_
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG40   P                NH1_577_5
@>      PHE85   P   1248_1249_1251_1253_1255_1257  <--->      ARG75   P               NH1_1090_10
@> Number of detected cation-pi interactions: 4.
   Pi-Cation interactions are replaced
```

We can check whether the interactions were replaced. The repulsive ionic bonding can be found by using `getInteractions()` and selecting *2* (0 - hydrogen bonds, 1 - salt bridges, 2 - repulsive ionic bonding, 3 - Pi-Stacking, 4 - Pi-Cation, 5 - hydrophobic, 6 - disulfide bonds).

```
In [32]: interactionsTrajectory.getInteractions()[2]
```

```
[[['ARG75', 'NH1_1090_1093', 'P', 'ARG40', 'NH1_577_580', 'P', 6.666],
  ['ASP81', 'OD1_1193_1194', 'P', 'GLU80', 'OE1_1181_1182', 'P', 6.9843],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 7.6316]],
 [['ARG101', 'NH1_1516_1519', 'P', 'LYS102', 'NZ_1540', 'P', 4.5002],
  ['ASP92', 'OD1_1368_1369', 'P', 'GLU93', 'OE1_1383_1384', 'P', 7.9458]],
 [['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 6.8023],
  ['ASP137', 'OD1_2090_2091', 'P', 'GLU128', 'OE1_1966_1967', 'P', 7.7429],
  ['ASP81', 'OD1_1193_1194', 'P', 'GLU80', 'OE1_1181_1182', 'P', 7.9228]],
 [['GLU80', 'OE1_1181_1182', 'P', 'ASP81', 'OD1_1193_1194', 'P', 6.2655],
  ['ASP42', 'OD1_609_610', 'P', 'ASP81', 'OD1_1193_1194', 'P', 6.8064]],
 [['ARG101', 'NH1_1516_1519', 'P', 'LYS102', 'NZ_1540', 'P', 6.0034],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 6.8451],
  ['ARG75', 'NH1_1090_1093', 'P', 'ARG40', 'NH1_577_580', 'P', 7.0306]],
 [['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 6.1332],
  ['ASP42', 'OD1_609_610', 'P', 'ASP81', 'OD1_1193_1194', 'P', 6.6231],
  ['LYS79', 'NZ_1164', 'P', 'LYS102', 'NZ_1540', 'P', 7.81]],
 [['ASP42', 'OD1_609_610', 'P', 'ASP81', 'OD1_1193_1194', 'P', 6.1141],
  ['LYS112', 'NZ_1699', 'P', 'LYS6', 'NZ_32', 'P', 6.4258],
  ['LYS79', 'NZ_1164', 'P', 'LYS107', 'NZ_1620', 'P', 7.0898]],
 [['ARG147', 'NH1_2257_2260', 'P', 'LYS123', 'NZ_1875', 'P', 4.8418],
  ['ASP42', 'OD1_609_610', 'P', 'GLU23', 'OE1_290_291', 'P', 5.8605],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 6.3776],
  ['ARG75', 'NH1_1090_1093', 'P', 'ARG40', 'NH1_577_580', 'P', 6.9162]],
 [['LYS123', 'NZ_1875', 'P', 'ARG147', 'NH1_2257_2260', 'P', 5.1095],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 6.9653],
  ['ASP81', 'OD1_1193_1194', 'P', 'GLU80', 'OE1_1181_1182', 'P', 7.1885]],
 [['ARG101', 'NH1_1516_1519', 'P', 'LYS102', 'NZ_1540', 'P', 4.3093],
  ['GLU93', 'OE1_1383_1384', 'P', 'GLU128', 'OE1_1966_1967', 'P', 6.2251],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 6.3655]],
 [['ARG101', 'NH1_1516_1519', 'P', 'LYS102', 'NZ_1540', 'P', 4.6267],
  ['LYS123', 'NZ_1875', 'P', 'ARG147', 'NH1_2257_2260', 'P', 4.6563],
  ['ASP92', 'OD1_1368_1369', 'P', 'GLU128', 'OE1_1966_1967', 'P', 6.4486],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 7.3554]],
 [['ARG101', 'NH1_1516_1519', 'P', 'LYS102', 'NZ_1540', 'P', 5.2803],
  ['ASP42', 'OD1_609_610', 'P', 'ASP81', 'OD1_1193_1194', 'P', 6.6125],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 7.7231]],
 [['LYS123', 'NZ_1875', 'P', 'ARG147', 'NH1_2257_2260', 'P', 5.903],
  ['ARG75', 'NH1_1090_1093', 'P', 'ARG40', 'NH1_577_580', 'P', 6.2264],
```

```
  ['ARG150', 'NH1_2303_2306', 'P', 'ARG147', 'NH1_2257_2260', 'P', 7.2115]],
 [['ASP42', 'OD1_609_610', 'P', 'ASP81', 'OD1_1193_1194', 'P', 6.5807],
  ['ASP129', 'OD1_1978_1979', 'P', 'GLU128', 'OE1_1966_1967', 'P', 6.6156],
  ['ARG101', 'NH1_1516_1519', 'P', 'LYS102', 'NZ_1540', 'P', 7.7691],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 7.8267]],
 [['LYS123', 'NZ_1875', 'P', 'ARG147', 'NH1_2257_2260', 'P', 6.9607],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 7.0793],
  ['ASP81', 'OD1_1193_1194', 'P', 'GLU80', 'OE1_1181_1182', 'P', 7.1994],
  ['ASP92', 'OD1_1368_1369', 'P', 'GLU128', 'OE1_1966_1967', 'P', 7.9662]],
 [['LYS123', 'NZ_1875', 'P', 'ARG147', 'NH1_2257_2260', 'P', 6.4558],
  ['GLU154', 'OE1_2371_2372', 'P', 'ASP120', 'OD1_1824_1825', 'P', 6.5391],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 6.6406]],
 [['ASP42', 'OD1_609_610', 'P', 'GLU23', 'OE1_290_291', 'P', 5.5599],
  ['ARG101', 'NH1_1516_1519', 'P', 'LYS102', 'NZ_1540', 'P', 7.1302],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 7.1991],
  ['ASP129', 'OD1_1978_1979', 'P', 'GLU128', 'OE1_1966_1967', 'P', 7.2499]],
 [['ARG101', 'NH1_1516_1519', 'P', 'LYS102', 'NZ_1540', 'P', 4.913],
  ['ASP42', 'OD1_609_610', 'P', 'ASP81', 'OD1_1193_1194', 'P', 6.4678],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 7.3594],
  ['GLU128', 'OE1_1966_1967', 'P', 'ASP129', 'OD1_1978_1979', 'P', 7.9788]],
 [['ASP42', 'OD1_609_610', 'P', 'GLU23', 'OE1_290_291', 'P', 5.6704],
  ['ASP135', 'OD1_2067_2068', 'P', 'GLU139', 'OE1_2125_2126', 'P', 5.9135],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 6.7566],
  ['ASP92', 'OD1_1368_1369', 'P', 'GLU128', 'OE1_1966_1967', 'P', 6.7899],
  ['GLU93', 'OE1_1383_1384', 'P', 'GLU128', 'OE1_1966_1967', 'P', 7.3464]],
 [['LYS123', 'NZ_1875', 'P', 'ARG147', 'NH1_2257_2260', 'P', 5.3159],
  ['GLU139', 'OE1_2125_2126', 'P', 'ASP135', 'OD1_2067_2068', 'P', 6.0087],
  ['LYS79', 'NZ_1164', 'P', 'LYS107', 'NZ_1620', 'P', 6.0679],
  ['ASP81', 'OD1_1193_1194', 'P', 'GLU80', 'OE1_1181_1182', 'P', 6.9706]],
 [['LYS123', 'NZ_1875', 'P', 'ARG147', 'NH1_2257_2260', 'P', 4.4846],
  ['ASP135', 'OD1_2067_2068', 'P', 'GLU139', 'OE1_2125_2126', 'P', 5.4686],
  ['ASP129', 'OD1_1978_1979', 'P', 'ASP92', 'OD1_1368_1369', 'P', 7.0978],
  ['LYS79', 'NZ_1164', 'P', 'LYS102', 'NZ_1540', 'P', 7.9242]]]
```

```
In [33]: interactionsTrajectory.getInteractions()[4]
```

```
[[['PHE85',
   '1248_1249_1251_1253_1255_1257',
   'P',
   'ARG40',
   'NH1_577_580',
   'P',
   3.6523],
  ['HSE66', '953_954_955_957_959', 'P', 'ARG65', 'NH1_938_941', 'P', 4.5323],
  ['HSE157',
   '2414_2415_2416_2418_2420_2423_2424',
   'P',
   'LYS112',
   'NZ_1699',
   'P',
   4.828],
  ['PHE138',
   '2101_2102_2104_2106_2108_2110',
   'P',
   'ARG58',
   'NH1_829_832',
   'P',
   5.0448],
```

```
 ['TYR131',
  '2003_2004_2006_2008_2011_2013',
  'P',
  'ARG58',
  'NH1_829_832',
  'P',
  5.0915]],
  ..
  ..
```

6.4 Statistics

Using `calcStatisticsInteractions()` function, we can compute the statistics of interaction in the trajectory, such as the average distance between residues (usually the center of the mass; details are described in the function which computes the specific type of interactions), standard deviation for the distance value and weight. Weight is the number of counts for the whole trajectory and is divided by the number of frames in the dcd file. Weight equal to 1 corresponds to the contact that was main the whole time of the simulation. Note that weight can be >1 when multiple contacts are present between the same residues.

For example:

```
In [34]: interactions = interactionsTrajectory.getPiCation()

In [35]: calcStatisticsInteractions(interactions)
```

```
@> Statistics for PHE85P-ARG40P:
@>   Average [Ang.]: 4.385379791259766
@>   Standard deviation [Ang.]: 0.5366479754447937
@>   Weight: 0.952381
@> Statistics for HSE66P-ARG65P:
@>   Average [Ang.]: 4.717772006988525
@>   Standard deviation [Ang.]: 0.6487299799919128
@>   Weight: 0.857143
@> Statistics for HSE157P-LYS112P:
@>   Average [Ang.]: 4.388020038604736
@>   Standard deviation [Ang.]: 1.0506110191345215
@>   Weight: 0.47619
@> Statistics for PHE138P-ARG58P:
@>   Average [Ang.]: 5.318399906158447
@>   Standard deviation [Ang.]: 0.24265700578689575
@>   Weight: 0.809524
@> Statistics for TYR87P-LYS112P:
@>   Average [Ang.]: 5.441559791564941
@>   Standard deviation [Ang.]: 0.25401198863983154
@>   Weight: 0.47619
@> Statistics for TRP39P-LYS6P:
@>   Average [Ang.]: 5.522061824798584
@>   Standard deviation [Ang.]: 0.31886300444602966
@>   Weight: 0.380952
@> Statistics for PHE85P-ARG75P:
@>   Average [Ang.]: 5.877999782562256
@>   Standard deviation [Ang.]: 0.06788399815559387
@>   Weight: 0.285714
```

```
In [36]: calcStatisticsInteractions(interactionsTrajectory.getHydrogenBonds())
```

```
@> Statistics for ARG101P-ASP98P:
@>   Average [Ang.]: 2.793931
@>   Standard deviation [Ang.]: 0.205527
@>   Weight: 1.52381
@> Statistics for HSE72P-ASN15P:
@>   Average [Ang.]: 2.989283
@>   Standard deviation [Ang.]: 0.270697
@>   Weight: 0.285714
@> Statistics for GLN143P-GLU139P:
@>   Average [Ang.]: 3.051633
@>   Standard deviation [Ang.]: 0.20753
@>   Weight: 1.285714
@> Statistics for HSE66P-GLU139P:
@>   Average [Ang.]: 2.900411
@>   Standard deviation [Ang.]: 0.169455
@>   Weight: 0.428571
@> Statistics for ARG40P-LYS6P:
@>   Average [Ang.]: 3.055475
@>   Standard deviation [Ang.]: 0.213814
@>   Weight: 0.380952
@> Statistics for ARG58P-ASP56P:
@>   Average [Ang.]: 2.827481
@>   Standard deviation [Ang.]: 0.171087
@>   Weight: 2.952381
@> Statistics for ALA45P-ARG75P:
@>   Average [Ang.]: 2.840721
@>   Standard deviation [Ang.]: 0.105565
@>   Weight: 0.904762
@> Statistics for ASN53P-GLU50P:
@>   Average [Ang.]: 2.980214
@>   Standard deviation [Ang.]: 0.147229
@>   Weight: 0.333333
@> Statistics for ALA74P-ASN53P:
@>   Average [Ang.]: 2.98522
@>   Standard deviation [Ang.]: 0.148331
@>   Weight: 0.952381
@> Statistics for ASP56P-ILE16P:
@>   Average [Ang.]: 3.085957
@>   Standard deviation [Ang.]: 0.21134
@>   Weight: 0.666667
@> Statistics for LYS110P-THR84P:
@>   Average [Ang.]: 2.774475
@>   Standard deviation [Ang.]: 0.080304
@>   Weight: 0.380952
@> Statistics for LEU116P-CYS90P:
@>   Average [Ang.]: 2.887425
@>   Standard deviation [Ang.]: 0.118768
@>   Weight: 0.952381
@> Statistics for SER103P-LEU99P:
@>   Average [Ang.]: 2.897324
@>   Standard deviation [Ang.]: 0.17182
@>   Weight: 1.380952
@> Statistics for ASN134P-ASP137P:
@>   Average [Ang.]: 2.917242
@>   Standard deviation [Ang.]: 0.160488
@>   Weight: 0.904762
@> Statistics for PHE152P-CYS148P:
@>   Average [Ang.]: 2.956784
```

```
@>   Standard deviation [Ang.]: 0.160039
@>   Weight: 0.904762
@> Statistics for ASN95P-ASP92P:
@>   Average [Ang.]: 3.061373
@>   Standard deviation [Ang.]: 0.215848
@>   Weight: 0.714286
@> Statistics for LYS6P-ASN38P:
@>   Average [Ang.]: 3.006786
@>   Standard deviation [Ang.]: 0.154497
@>   Weight: 0.333333
@> Statistics for ILE77P-ALA45P:
@>   Average [Ang.]: 2.819429
@>   Standard deviation [Ang.]: 0.092538
@>   Weight: 0.666667
@> Statistics for LEU99P-ASN95P:
@>   Average [Ang.]: 3.027242
@>   Standard deviation [Ang.]: 0.19744
@>   Weight: 0.904762
@> Statistics for CYS149P-CYS145P:
@>   Average [Ang.]: 2.928052
@>   Standard deviation [Ang.]: 0.146811
@>   Weight: 1.190476
@> Statistics for GLY52P-ALA74P:
@>   Average [Ang.]: 2.887583
@>   Standard deviation [Ang.]: 0.088417
@>   Weight: 0.285714
@> Statistics for ASP32P-LYS28P:
@>   Average [Ang.]: 2.86277
@>   Standard deviation [Ang.]: 0.119982
@>   Weight: 0.952381
@> Statistics for ILE88P-LYS112P:
@>   Average [Ang.]: 2.906433
@>   Standard deviation [Ang.]: 0.147086
@>   Weight: 1.0
@> Statistics for ARG27P-GLU23P:
@>   Average [Ang.]: 2.790357
@>   Standard deviation [Ang.]: 0.140396
@>   Weight: 2.0
@> Statistics for TYR142P-PHE138P:
@>   Average [Ang.]: 3.094219
@>   Standard deviation [Ang.]: 0.152889
@>   Weight: 1.0
@> Statistics for PHE26P-ALA22P:
@>   Average [Ang.]: 3.023619
@>   Standard deviation [Ang.]: 0.150087
@>   Weight: 1.0
@> Statistics for ASN15P-SER19P:
@>   Average [Ang.]: 2.96532
@>   Standard deviation [Ang.]: 0.213496
@>   Weight: 0.238095
@> Statistics for ARG75P-ASP81P:
@>   Average [Ang.]: 2.782441
@>   Standard deviation [Ang.]: 0.185369
@>   Weight: 2.095238
@> Statistics for ARG75P-ASP42P:
@>   Average [Ang.]: 2.760572
@>   Standard deviation [Ang.]: 0.134486
@>   Weight: 1.380952
```

```
@> Statistics for ARG97P-GLU93P:
@>   Average [Ang.]: 2.881173
@>   Standard deviation [Ang.]: 0.223159
@>   Weight: 1.952381
@> Statistics for ARG65P-GLU139P:
@>   Average [Ang.]: 2.826732
@>   Standard deviation [Ang.]: 0.198775
@>   Weight: 1.047619
@> Statistics for VAL25P-ILE21P:
@>   Average [Ang.]: 2.975267
@>   Standard deviation [Ang.]: 0.121046
@>   Weight: 1.0
@> Statistics for LEU153P-CYS149P:
@>   Average [Ang.]: 3.04695
@>   Standard deviation [Ang.]: 0.1793
@>   Weight: 0.952381
@> Statistics for SER7P-ASP86P:
@>   Average [Ang.]: 2.758983
@>   Standard deviation [Ang.]: 0.122097
@>   Weight: 1.142857
..
..
@> Statistics for ALA83P-LYS79P:
@>   Average [Ang.]: 3.225643
@>   Standard deviation [Ang.]: 0.148806
@>   Weight: 0.333333
@> Statistics for GLN60P-MET70P:
@>   Average [Ang.]: 2.902757
@>   Standard deviation [Ang.]: 0.162208
@>   Weight: 0.333333
@> Statistics for GLN124P-ILE126P:
@>   Average [Ang.]: 2.98456
@>   Standard deviation [Ang.]: 0.198396
@>   Weight: 0.238095
@> Statistics for SER19P-ASN15P:
@>   Average [Ang.]: 2.691612
@>   Standard deviation [Ang.]: 0.10843
@>   Weight: 0.380952
@> Statistics for ASN95P-THR46P:
@>   Average [Ang.]: 3.056129
@>   Standard deviation [Ang.]: 0.197107
@>   Weight: 0.333333
@> Statistics for ARG150P-ASP120P:
@>   Average [Ang.]: 2.752571
@>   Standard deviation [Ang.]: 0.112541
@>   Weight: 0.333333
@> Statistics for LYS155P-HSE157P:
@>   Average [Ang.]: 2.833843
@>   Standard deviation [Ang.]: 0.185712
@>   Weight: 0.333333
@> Statistics for ARG65P-ASP135P:
@>   Average [Ang.]: 2.86488
@>   Standard deviation [Ang.]: 0.213607
@>   Weight: 0.47619
```

For better visualization of the results, we can use `showInteractionsGraph()`, which displays results as a graph with residue-residue pairs of interactions. The intensity of the color of the lines connecting two residues corresponds to the number of counts. Darker lines are assigned to the most frequent appearance of interaction. The distance between

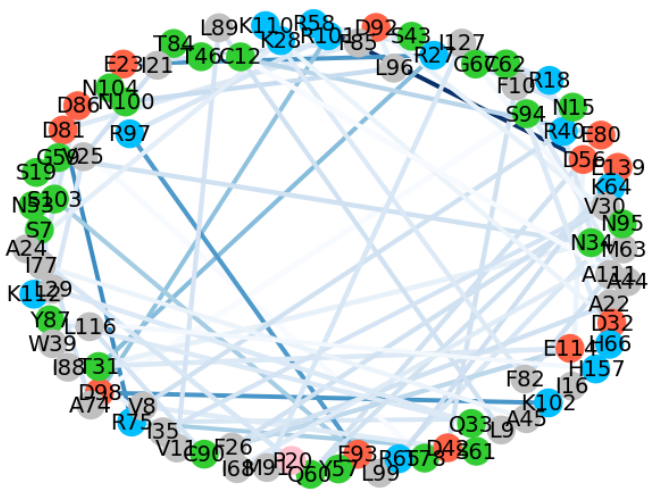
pairs corresponds to the average distance across all the frames. Moreover, ovals with residue names are color-coded: acidic residues: *red*, basic: *blue*, polar: *green*, non-polar: *silver*, and proline: *pink*. The same function can be applied to ensemble PDB (more examples can be found there). We will also change the region of protein structure, which we would like to analyze from residue 1 to 100.

```
In [37]: statistics = calcStatisticsInteractions(interactionsTrajectory.getHydrogenBonds(selection='

In [38]: showInteractionsGraph(statistics, code='1-letter', cutoff=0.5)
```

```
@> Statistics for ARG101P-ASP98P:
@>   Average [Ang.]: 2.793931
@>   Standard deviation [Ang.]: 0.205527
@>   Weight: 1.52381
@> Statistics for HSE72P-ASN15P:
@>   Average [Ang.]: 2.989283
@>   Standard deviation [Ang.]: 0.270697
@>   Weight: 0.285714
@> Statistics for HSE66P-GLU139P:
@>   Average [Ang.]: 2.900411
@>   Standard deviation [Ang.]: 0.169455
@>   Weight: 0.428571
@> Statistics for ARG40P-LYS6P:
@>   Average [Ang.]: 3.055475
@>   Standard deviation [Ang.]: 0.213814
@>   Weight: 0.380952
@> Statistics for ARG58P-ASP56P:
@>   Average [Ang.]: 2.827481
@>   Standard deviation [Ang.]: 0.171087
@>   Weight: 2.952381
@> Statistics for ALA45P-ARG75P:
@>   Average [Ang.]: 2.840721
@>   Standard deviation [Ang.]: 0.105565
@>   Weight: 0.904762
@> Statistics for ASN53P-GLU50P:
@>   Average [Ang.]: 2.980214
@>   Standard deviation [Ang.]: 0.147229
@>   Weight: 0.333333
@> Statistics for ALA74P-ASN53P:
@>   Average [Ang.]: 2.98522
@>   Standard deviation [Ang.]: 0.148331
@>   Weight: 0.952381
@> Statistics for ASP56P-ILE16P:
@>   Average [Ang.]: 3.085957
@>   Standard deviation [Ang.]: 0.21134
@>   Weight: 0.666667
@> Statistics for LYS110P-THR84P:
@>   Average [Ang.]: 2.774475
@>   Standard deviation [Ang.]: 0.080304
@>   Weight: 0.380952
@> Statistics for LEU116P-CYS90P:
@>   Average [Ang.]: 2.887425
@>   Standard deviation [Ang.]: 0.118768
@>   Weight: 0.952381
@> Statistics for SER103P-LEU99P:
@>   Average [Ang.]: 2.897324
@>   Standard deviation [Ang.]: 0.17182
@>   Weight: 1.380952
@> Statistics for ASN95P-ASP92P:
@>   Average [Ang.]: 3.061373
```

```
@>   Standard deviation [Ang.]: 0.215848
@>   Weight: 0.714286
@> Statistics for LYS6P-ASN38P:
@>   Average [Ang.]: 3.006786
@>   Standard deviation [Ang.]: 0.154497
@>   Weight: 0.333333
@> Statistics for ILE77P-ALA45P:
@>   Average [Ang.]: 2.819429
@>   Standard deviation [Ang.]: 0.092538
@>   Weight: 0.666667
@> Statistics for LEU99P-ASN95P:
@>   Average [Ang.]: 3.027242
@>   Standard deviation [Ang.]: 0.19744
@>   Weight: 0.904762
@> Statistics for GLY52P-ALA74P:
@>   Average [Ang.]: 2.887583
@>   Standard deviation [Ang.]: 0.088417
@>   Weight: 0.285714
..
..
```



6.5 Compare two independent frames

With this analysis, we can also compare interactions between frames. Below, we will compute hydrogen bonds for frame 0 and frame 18 and we will compare them using the `compareInteractions()` function. That function will be helpful in checking the difference between interactions. The results will be saved as `diff_fr0_vsfr18.dat` file.

Let's check the interactions for the initail frame in our trajectory:

```
In [39]: frame0 = dcd.getFrame(0)

In [40]: at0 = frame0.getAtoms()

In [41]: hb0 = calcHydrogenBonds(at0.select('protein'))
```

```
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)   <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>     ARG101    P      NH1_1516  <--->      ASP98    P      OD1_1463     2.0    33.1
@>      HSE72    P      NE2_1042  <--->      ASN15    P       OD1_165     2.6    34.8
@>     GLN143    P      NE2_2192  <--->     GLU139    P      OE2_2126     2.7     9.2
@>      HSE66    P       NE2_957  <--->     GLU139    P      OE1_2125     2.7     6.4
@>      ARG40    P         N_561  <--->       LYS6    P          O_37     2.7    17.1
@>      ARG58    P         N_813  <--->      ASP56    P       OD1_788     2.7    30.0
@>      ALA45    P         N_634  <--->      ARG75    P        O_1097     2.8    35.1
@>      ASN53    P       ND2_747  <--->      GLU50    P       OE1_708     2.8    18.2
@>      ALA74    P        N_1064  <--->      ASN53    P         O_751     2.8    21.3
@>      ASP56    P         N_780  <--->      ILE16    P         O_189     2.8    27.0
@>     LYS110    P       NZ_1667  <--->      THR84    P        O_1240     2.8    38.2
@>     LEU116    P        N_1758  <--->      CYS90    P        O_1342     2.8    15.0
@>     SER103    P        N_1546  <--->      LEU99    P        O_1485     2.8    29.1
@>     ASN134    P        N_2045  <--->     ASP137    P      OD2_2091     2.8    22.6
@>     PHE152    P        N_2321  <--->     CYS148    P        O_2275     2.8     8.3
@>      ASN95    P        N_1398  <--->      ASP92    P      OD1_1368     2.8    12.6
@>       LYS6    P          N_16  <--->      ASN38    P         O_536     2.8    25.0
@>      ILE77    P        N_1115  <--->      ALA45    P         O_643     2.8    12.2
@>      ARG58    P       NH2_832  <--->      ASP56    P       OD2_789     2.8    27.7
@>      LEU99    P        N_1467  <--->      ASN95    P        O_1411     2.8    15.5
@>     CYS149    P        N_2276  <--->     CYS145    P        O_2224     2.8     9.6
@>      GLY52    P         N_731  <--->      ALA74    P        O_1073     2.8     6.6
@>      ASP32    P         N_435  <--->      LYS28    P         O_385     2.8     8.8
@>      ILE88    P        N_1294  <--->     LYS112    P        O_1704     2.8    17.7
@>     GLN143    P        N_2180  <--->     GLU139    P        O_2128     2.8    21.7
@>      ARG27    P         N_340  <--->      GLU23    P         O_293     2.8    15.4
@>     TYR142    P        N_2159  <--->     PHE138    P        O_2113     2.9    14.2
@>     GLY133    P        N_2038  <--->     PRO130    P        O_1995     2.9    25.4
@>      PHE26    P         N_320  <--->      ALA22    P         O_278     2.9     4.9
@>      ASN15    P       ND2_166  <--->      SER19    P        OG_232     2.9    32.1
@>      ARG75    P      NH1_1090  <--->      ASP81    P      OD2_1194     2.9    19.7
@>      ARG75    P      NH2_1093  <--->      ASP42    P       OD2_610     2.9    23.5
@>      ARG97    P        N_1431  <--->      GLU93    P        O_1386     2.9    22.2
@>      ARG65    P       NH2_941  <--->     GLU139    P      OE1_2125     2.9    32.3
@>      VAL25    P         N_304  <--->      ILE21    P         O_268     2.9     8.2
@>     LEU153    P        N_2341  <--->     CYS149    P        O_2286     2.9    12.5
@>       SER7    P          N_38  <--->      ASP86    P      OD2_1270     2.9    39.9
@>      ASP86    P        N_1261  <--->       SER7    P         OG_45     2.9    34.7
@>      ARG58    P       NH2_832  <--->     TYR131    P        O_2016     2.9    33.1
@>      THR46    P         N_644  <--->      CYS12    P         O_130     2.9    36.1
@>     GLN144    P        N_2197  <--->     THR140    P        O_2142     2.9    23.3
@>      THR78    P        N_1134  <--->      ASP81    P      OD2_1194     2.9    12.4
@>      LEU89    P        N_1313  <--->       LEU9    P          O_83     2.9    29.5
@>      THR31    P         N_421  <--->      ARG27    P         O_363     2.9    24.1
@>      CYS90    P        N_1332  <--->     GLU114    P        O_1738     2.9    24.6
@>     CYS148    P        N_2265  <--->     GLN144    P        O_2213     2.9     9.3
@>      GLU23    P         N_279  <--->      SER19    P         O_235     2.9    15.4
@>      ILE68    P         N_970  <--->      MET63    P         O_899     2.9    13.0
@>      PHE10    P          N_84  <--->      ASP42    P         O_612     2.9    22.8
@>     LYS112    P        N_1683  <--->      ASP86    P        O_1272     2.9    10.1
@>      SER61    P         N_861  <--->      TYR57    P         O_812     2.9    35.1
@>     CYS145    P        N_2214  <--->     VAL141    P        O_2158     2.9    15.9
@>      ARG27    P       NH2_359  <--->      GLU23    P       OE2_291     2.9    31.5
@>      LYS64    P         N_900  <--->      GLN60    P         O_860     2.9    22.9
@>       LEU9    P          N_65  <--->      TYR87    P        O_1293     2.9    16.4
@>      ASN38    P         N_523  <--->      ILE35    P         O_496     2.9    29.1
```

```
@>      VAL11    P         N_104  <--->      LEU89    P        O_1331     2.9    29.7
@>     ASN100    P        N_1486  <--->      LEU96    P        O_1430     2.9    10.3
@>     GLN124    P        N_1881  <--->     ASP120    P      OD2_1825     2.9    27.5
@>     LYS102    P        N_1524  <--->      ASP98    P        O_1466     2.9     9.3
@>      GLN76    P      NE2_1110  <--->      THR46    P         O_657     2.9    31.4
@>      ARG40    P       NH1_577  <--->      THR84    P      OG1_1233     2.9     8.4
@>      ALA44    P         N_624  <--->      PHE10    P         O_103     2.9    33.2
@>     GLU154    P        N_2360  <--->     ARG150    P        O_2310     3.0    22.6
@>       VAL8    P          N_49  <--->      ARG40    P         O_584     3.0    25.0
@>      MET63    P         N_883  <--->      GLY59    P         O_843     3.0    18.3
@>      GLN60    P         N_844  <--->      ASP56    P         O_791     3.0    35.5
@>      ILE35    P         N_478  <--->      VAL30    P         O_420     3.0    23.5
@>     VAL146    P        N_2225  <--->     TYR142    P        O_2179     3.0    31.5
@>      ARG58    P       NH1_829  <--->     TYR131    P        O_2016     3.0    38.1
@>      ASN53    P         N_738  <--->      GLU50    P         O_711     3.0    28.6
@>     ARG101    P        N_1500  <--->      ARG97    P        O_1454     3.0    32.3
@>      ARG18    P       NH1_217  <--->     ILE127    P        O_1954     3.0    26.0
@>      ARG75    P        N_1074  <--->      ASN15    P       OD1_165     3.0    25.1
@>     GLN144    P      NE2_2209  <--->     ILE126    P        O_1935     3.0    18.3
@>      ASN34    P         N_464  <--->      THR31    P         O_434     3.0    18.2
@>      ASN15    P       ND2_166  <--->      SER43    P        OG_620     3.0    25.7
@>      ARG58    P        NE_826  <--->      ASP56    P       OD1_788     3.0    22.2
@>      ARG27    P       NH1_356  <--->      GLU23    P       OE2_291     3.0    36.9
@>     ILE127    P        N_1936  <--->      MET91    P        O_1359     3.0    17.6
@>     TYR119    P       OH_1808  <--->     HSE157    P        N_2407     3.0    28.1
@>     HSE157    P        N_2407  <--->     TYR119    P       OH_1808     3.0    19.2
@>     GLU139    P        N_2114  <--->     ASP135    P        O_2070     3.0    27.9
@>      LEU29    P         N_386  <--->      VAL25    P         O_319     3.0    19.1
@>      SER47    P         N_658  <--->      LEU13    P         O_149     3.0    28.8
@>      VAL30    P         N_405  <--->      PHE26    P         O_339     3.0    17.7
@>     GLN105    P        N_1571  <--->     LYS102    P        O_1545     3.0    19.7
@>     SER118    P        N_1784  <--->     LEU115    P        O_1757     3.1    21.4
@>     LYS155    P        N_2375  <--->     ALA151    P        O_2320     3.1    21.3
@>     GLU114    P        N_1724  <--->      ILE88    P        O_1312     3.1    24.2
@>     ASP120    P        N_1816  <--->     GLY117    P        O_1783     3.1    12.7
@>      CYS62    P         N_872  <--->      ARG58    P         O_836     3.1    20.4
@>      ARG18    P       NH1_217  <--->      ASP92    P      OD2_1369     3.1     4.3
@>      ALA24    P         N_294  <--->      PRO20    P         O_249     3.1    29.9
@>     ARG150    P        N_2287  <--->     VAL146    P        O_2240     3.1    12.7
@>      LYS28    P         N_364  <--->      ALA24    P         O_303     3.1    20.0
@>     VAL141    P        N_2143  <--->     ASP137    P        O_2093     3.1    18.5
@>      ASP98    P        N_1455  <--->      SER94    P        O_1397     3.1    19.6
@>      LEU96    P        N_1412  <--->      ASP92    P        O_1371     3.1    36.3
@>      ALA22    P         N_269  <--->      ARG18    P         O_224     3.1    21.9
@>     ALA151    P        N_2311  <--->     ARG147    P        O_2264     3.1    15.6
@>      GLY67    P         N_963  <--->      LYS64    P         O_921     3.1    22.8
@>      ASP42    P         N_601  <--->       VAL8    P          O_64     3.1    35.6
@>      ARG65    P         N_922  <--->      SER61    P         O_871     3.1    23.4
@>      TRP39    P         N_537  <--->      SER36    P         O_507     3.1    15.2
@>     LYS123    P        N_1859  <--->     ASP120    P        O_1827     3.1    18.7
@>      MET91    P        N_1343  <--->      ASN95    P      OD1_1406     3.2    39.0
@>     THR140    P        N_2129  <--->     SER136    P        O_2081     3.2    30.3
@>      PHE85    P        N_1241  <--->      ASP81    P        O_1196     3.2    20.2
@>      ASN15    P         N_157  <--->      CYS12    P        SG_127     3.2    37.5
@>     ALA111    P        N_1673  <--->      PHE82    P        O_1216     3.2    20.6
@>     ARG147    P        N_2241  <--->     GLN143    P        O_2196     3.2    12.1
@>      ARG75    P      NH2_1093  <--->      ASP81    P      OD1_1193     3.2    29.3
@>     LYS112    P       NZ_1699  <--->     HSE157    P      OT2_2424     3.3    28.7
```

```
@>     ARG147    P      NH1_2257  <--->     GLN124    P      OE1_1892     3.3    29.9
@>     PHE138    P        N_2094  <--->     ASN134    P        O_2058     3.3    31.0
@>       SER7    P         OG_45  <--->      THR84    P        O_1240     3.3    35.5
@>      CYS12    P         N_120  <--->      ALA44    P         O_633     3.3    36.1
@>      SER19    P         N_225  <--->      CYS12    P        SG_127     3.3     8.0
@>      PHE82    P        N_1197  <--->      LYS79    P        O_1169     3.4    37.7
@>      ASP81    P        N_1185  <--->      THR78    P      OG1_1140     3.5    39.5
@>     LYS102    P       NZ_1540  <--->      ASP98    P      OD2_1464     3.5    26.1
@>     ARG147    P      NH2_2260  <--->     GLN124    P      OE1_1892     3.5    33.9
@>     VAL106    P        N_1588  <--->     SER103    P        O_1556     3.5    34.2
@> Number of detected hydrogen bonds: 124.
```

Let's check the interactions for frame number 18 in our trajectory:

```
In [42]: frame18 = dcd.getFrame(18)

In [43]: at18 = frame18.getAtoms()

In [44]: hb18 = calcHydrogenBonds(at18.select('protein'))
```

```
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)    <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      ARG75    P      NH2_1093  <--->      ASP81    P      OD1_1193     2.6    18.5
@>      ARG58    P       NH2_832  <--->      ASP56    P       OD2_789     2.6    21.5
@>      ARG27    P       NH2_359  <--->      GLU23    P       OE2_291     2.7    18.4
@>      LYS28    P        NZ_380  <--->      ASP32    P       OD2_444     2.7    25.9
@>     ARG150    P       NE_2300  <--->     GLU154    P      OE1_2371     2.7    22.4
@>      ARG18    P       NH1_217  <--->      ASP92    P      OD2_1369     2.7    25.9
@>      ARG75    P       NE_1087  <--->      ASP42    P       OD1_609     2.7    16.1
@>      ARG58    P        NE_826  <--->      ASP56    P       OD1_788     2.7     2.1
@>      SER19    P        OG_232  <--->      ASN15    P       OD1_165     2.7     8.1
@>      ILE88    P        N_1294  <--->     LYS112    P        O_1704     2.7     1.4
@>       VAL8    P          N_49  <--->      ARG40    P         O_584     2.7    11.5
@>      THR78    P        N_1134  <--->      ASP81    P      OD2_1194     2.7    28.1
@>     ASN134    P        N_2045  <--->     ASP137    P      OD1_2090     2.7    12.5
@>     LYS155    P       NZ_2391  <--->     HSE157    P      OT2_2424     2.7    38.9
@>     LYS112    P        N_1683  <--->      ASP86    P        O_1272     2.7    25.8
@>     CYS145    P        N_2214  <--->     VAL141    P        O_2158     2.7    13.7
@>     LYS102    P       NZ_1540  <--->      ASP98    P      OD1_1463     2.8    29.5
@>     GLN143    P        N_2180  <--->     GLU139    P        O_2128     2.8    21.3
@>      LEU29    P         N_386  <--->      VAL25    P         O_319     2.8    16.9
@>      THR84    P      OG1_1233  <--->      GLU80    P        O_1184     2.8    10.5
@>      CYS90    P        N_1332  <--->     GLU114    P        O_1738     2.8     4.9
@>      THR31    P       OG1_427  <--->      ARG27    P         O_363     2.8    21.2
@>      ASP98    P        N_1455  <--->      SER94    P        O_1397     2.8     6.1
@>      SER43    P        OG_620  <--->      GLU23    P       OE1_290     2.8    13.9
@>     LYS110    P        N_1651  <--->      PHE82    P        O_1216     2.8    36.4
@>     SER118    P       OG_1791  <--->     GLU114    P      OE2_1736     2.8    20.1
@>      ARG65    P       NH1_938  <--->     ASP135    P      OD2_2068     2.8    12.3
@>      LYS64    P         N_900  <--->      GLN60    P         O_860     2.8     3.3
@>     ARG101    P      NH2_1519  <--->      ASP98    P      OD2_1464     2.8     8.9
@>      ARG75    P      NH1_1090  <--->      ASP81    P      OD2_1194     2.8    25.1
@>      ARG65    P         N_922  <--->      SER61    P         O_871     2.8    24.3
@>      ARG58    P       NH1_829  <--->     GLY133    P        O_2044     2.8    34.0
@>     ILE127    P        N_1936  <--->      MET91    P        O_1359     2.8    22.3
@>      THR78    P      OG1_1140  <--->      ASP81    P      OD2_1194     2.8    12.4
@>      THR84    P        N_1227  <--->      GLU80    P        O_1184     2.8    10.8
@>      GLN33    P         N_447  <--->      LEU29    P         O_404     2.8     6.2
```

```
@>       SER7    P          N_38  <--->      ASP86    P      OD1_1269     2.8    25.3
@>      ASP32    P         N_435  <--->      LYS28    P         O_385     2.8    16.9
@>      ASP86    P        N_1261  <--->       SER7    P          O_48     2.8    35.1
@>     LYS102    P        N_1524  <--->      ASP98    P        O_1466     2.8    29.0
@>      ASP42    P         N_601  <--->       VAL8    P          O_64     2.9    25.5
@>      SER61    P         N_861  <--->      TYR57    P         O_812     2.9    32.8
@>     CYS149    P        N_2276  <--->     CYS145    P        O_2224     2.9     2.6
@>     VAL146    P        N_2225  <--->     TYR142    P        O_2179     2.9     9.7
@>      GLN60    P         N_844  <--->      ASP56    P         O_791     2.9    25.1
@>     LYS155    P        N_2375  <--->     ARG150    P        O_2310     2.9    13.4
@>      ALA74    P        N_1064  <--->      ASN53    P         O_751     2.9    16.2
@>      TYR87    P        N_1273  <--->       SER7    P          O_48     2.9    18.2
@>     GLN144    P        N_2197  <--->     THR140    P        O_2142     2.9    16.3
@>      LEU89    P        N_1313  <--->       LEU9    P          O_83     2.9    28.6
@>     ARG101    P        N_1500  <--->      ARG97    P        O_1454     2.9     3.1
@>      CYS12    P        SG_127  <--->      SER19    P        OG_232     3.0    35.8
@>      ASN53    P       ND2_747  <--->      GLU50    P       OE2_709     3.0    21.4
@>      ALA45    P         N_634  <--->      ARG75    P        O_1097     3.0    11.5
@>      ASP56    P         N_780  <--->      ILE16    P         O_189     3.0    15.2
@>      ARG58    P         N_813  <--->      ASP56    P       OD1_788     3.0    14.2
@>      ILE77    P        N_1115  <--->      ALA45    P         O_643     3.0    12.8
@>      GLY67    P         N_963  <--->      MET63    P         O_899     3.0    16.3
@>      ARG18    P       NH1_217  <--->     ILE127    P        O_1954     3.0    33.1
@>      ARG75    P      NH1_1090  <--->      ASP81    P      OD1_1193     3.0    39.7
@>     THR140    P        N_2129  <--->     SER136    P        O_2081     3.0    18.5
@>     LEU153    P        N_2341  <--->     CYS149    P        O_2286     3.0    12.0
@>     ASN104    P        N_1557  <--->     ASN100    P        O_1499     3.0    38.4
@>      CYS62    P         N_872  <--->      ARG58    P         O_836     3.0    39.7
@>      VAL11    P         N_104  <--->      LEU89    P        O_1331     3.0    15.4
@>     VAL106    P        N_1588  <--->     LYS102    P        O_1545     3.0     2.4
@>     ALA151    P        N_2311  <--->     ARG147    P        O_2264     3.0    21.7
@>      ARG40    P         N_561  <--->       LYS6    P          O_37     3.0    33.0
@>       LEU9    P          N_65  <--->      TYR87    P        O_1293     3.0    39.7
@>      ARG27    P         N_340  <--->      GLU23    P         O_293     3.0    17.9
@>      ASN95    P      ND2_1407  <--->      THR46    P       OG1_650     3.0    38.8
@>      ARG27    P       NH2_359  <--->      VAL41    P         O_600     3.0    32.9
@>      LEU99    P        N_1467  <--->      ASN95    P        O_1411     3.0    21.7
@>     GLU154    P        N_2360  <--->     ARG150    P        O_2310     3.0    37.1
@>     ALA111    P        N_1673  <--->      PHE82    P        O_1216     3.0    18.4
@>     ARG150    P      NH2_2306  <--->     GLU154    P      OE1_2371     3.0    31.0
@>      VAL25    P         N_304  <--->      ILE21    P         O_268     3.0    10.3
@>      ASN15    P       ND2_166  <--->      SER43    P        OG_620     3.1    18.8
@>      MET63    P         N_883  <--->      GLY59    P         O_843     3.1    15.7
@>      VAL30    P         N_405  <--->      PHE26    P         O_339     3.1     6.2
@>     ARG150    P        N_2287  <--->     VAL146    P        O_2240     3.1    30.1
@>     PHE138    P        N_2094  <--->     ASN134    P        O_2058     3.1    10.8
@>     VAL141    P        N_2143  <--->     ASP137    P        O_2093     3.1    10.8
@>      PHE10    P          N_84  <--->      ASP42    P         O_612     3.1    17.6
@>     CYS148    P        N_2265  <--->     GLN144    P        O_2213     3.1    23.2
@>      PHE26    P         N_320  <--->      ALA22    P         O_278     3.1     9.0
@>      GLN76    P      NE2_1110  <--->      THR46    P         O_657     3.1    11.9
@>     LEU116    P        N_1758  <--->      CYS90    P        O_1342     3.2    18.5
@>      GLU23    P         N_279  <--->      SER19    P         O_235     3.2     2.4
@>      ALA44    P         N_624  <--->      PHE10    P         O_103     3.2    38.7
@>      ARG65    P       NH2_941  <--->     ASP135    P      OD1_2067     3.2    19.6
@>      ASN34    P         N_464  <--->      THR31    P         O_434     3.2    38.6
@>      ARG97    P        N_1431  <--->      GLU93    P        O_1386     3.2    17.8
@>      ALA22    P         N_269  <--->      ARG18    P         O_224     3.2    11.6
```

```
@>     GLN105    P        N_1571  <--->     ARG101    P        O_1523     3.2    28.1
@>       LYS6    P          N_16  <--->      ASN38    P         O_536     3.2    31.6
@>      ASN95    P        N_1398  <--->      ASP92    P      OD1_1368     3.2    11.6
@>     CYS145    P       SG_2221  <--->     VAL141    P        O_2158     3.3    30.4
@>      HSE66    P         N_946  <--->      CYS62    P         O_882     3.3    14.7
@>     ARG147    P        N_2241  <--->     GLN143    P        O_2196     3.3    26.0
@>     TYR142    P        N_2159  <--->     PHE138    P        O_2113     3.3    11.5
@>      TRP39    P         N_537  <--->      ILE35    P         O_496     3.4    35.3
@>     GLN124    P        N_1881  <--->     GLN144    P      OE1_2208     3.4    35.9
@>      CYS12    P         N_120  <--->      ALA44    P         O_633     3.4    35.7
@>     SER103    P       OG_1553  <--->      LEU99    P        O_1485     3.4    14.9
@>      PHE85    P        N_1241  <--->      ASP81    P        O_1196     3.4    24.1
@>      SER19    P         N_225  <--->      CYS12    P        SG_127     3.5     7.6
@> Number of detected hydrogen bonds: 107.
```

And compare them using `compareInteractions()`. We will obtain information on which interactions are newly maintained, which are stable, and which ones were lost.

```
In [45]: compareInteractions(hb0, hb18, filename='diff_fr0_vsfr18.dat')
```

```
@> Which interactions disappeared: 23
@> TYR87P <---> SER7P
@> SER43P <---> GLU23P
@> ASN104P <---> ASN100P
@> LYS155P <---> HSE157P
@> ARG150P <---> GLU154P
@> ASN95P <---> THR46P
@> LYS110P <---> PHE82P
@> SER19P <---> ASN15P
@> LYS155P <---> ARG150P
@> SER118P <---> GLU114P
@> GLY67P <---> MET63P
@> ARG65P <---> ASP135P
@> TRP39P <---> ILE35P
@> THR84P <---> GLU80P
@> HSE66P <---> CYS62P
@> GLN105P <---> ARG101P
@> CYS12P <---> SER19P
@> ARG58P <---> GLY133P
@> VAL106P <---> LYS102P
@> LYS28P <---> ASP32P
@> GLN124P <---> GLN144P
@> ARG27P <---> VAL41P
@> GLN33P <---> LEU29P

Which interactions appeared: 41
@> SER118P <---> LEU115P
@> GLY67P <---> LYS64P
@> GLU139P <---> ASP135P
@> ARG75P <---> ASN15P
@> PHE82P <---> LYS79P
@> ARG147P <---> GLN124P
@> GLY52P <---> ALA74P
@> ASP81P <---> THR78P
@> GLN144P <---> ILE126P
@> ASN38P <---> ILE35P
@> SER47P <---> LEU13P
@> ARG58P <---> TYR131P
```

```
@> LYS155P <---> ALA151P
@> MET91P <---> ASN95P
@> PHE152P <---> CYS148P
@> LYS28P <---> ALA24P
@> ASN100P <---> LEU96P
@> VAL106P <---> SER103P
@> SER7P <---> THR84P
@> ALA24P <---> PRO20P
@> HSE66P <---> GLU139P
@> GLU114P <---> ILE88P
@> LEU96P <---> ASP92P
@> GLN105P <---> LYS102P
@> LYS123P <---> ASP120P
@> GLY133P <---> PRO130P
@> TYR119P <---> HSE157P
@> ASN15P <---> SER19P
@> ILE35P <---> VAL30P
@> ARG65P <---> GLU139P
@> HSE157P <---> TYR119P
@> ASP120P <---> GLY117P
@> ARG40P <---> THR84P
@> ILE68P <---> MET63P
@> ASN15P <---> CYS12P
@> HSE72P <---> ASN15P
@> LYS110P <---> THR84P
@> GLN124P <---> ASP120P
@> TRP39P <---> SER36P
@> THR46P <---> CYS12P
@> LYS112P <---> HSE157P

@> Which interactions are the same: 73
@> GLN60P <---> ASP56P
@> ARG150P <---> VAL146P
@> ARG101P <---> ASP98P
@> ILE77P <---> ALA45P
@> VAL11P <---> LEU89P
@> SER61P <---> TYR57P
@> ARG18P <---> ASP92P
@> ALA22P <---> ARG18P
@> THR31P <---> ARG27P
@> ALA44P <---> PHE10P
@> LEU153P <---> CYS149P
@> ARG58P <---> ASP56P
@> ALA111P <---> PHE82P
@> CYS62P <---> ARG58P
@> VAL146P <---> TYR142P
@> GLU23P <---> SER19P
@> ARG27P <---> GLU23P
@> CYS149P <---> CYS145P
@> LYS64P <---> GLN60P
@> VAL8P <---> ARG40P
@> ARG40P <---> LYS6P
@> ARG65P <---> SER61P
@> ASP32P <---> LYS28P
@> ILE88P <---> LYS112P
@> ALA45P <---> ARG75P
@> PHE26P <---> ALA22P
@> ASN95P <---> ASP92P
```

```
@> VAL30P <---> PHE26P
@> THR140P <---> SER136P
@> LEU89P <---> LEU9P
@> SER103P <---> LEU99P
@> LEU116P <---> CYS90P
@> PHE10P <---> ASP42P
@> ASN15P <---> SER43P
@> TYR142P <---> PHE138P
@> ASN34P <---> THR31P
@> ASN134P <---> ASP137P
@> LEU99P <---> ASN95P
@> ASP98P <---> SER94P
@> GLN144P <---> THR140P
@> ARG97P <---> GLU93P
@> GLN76P <---> THR46P
@> LYS6P <---> ASN38P
@> ARG75P <---> ASP81P
@> ASN53P <---> GLU50P
@> THR78P <---> ASP81P
@> VAL141P <---> ASP137P
@> SER19P <---> CYS12P
@> GLN143P <---> GLU139P
@> LEU29P <---> VAL25P
@> ALA151P <---> ARG147P
@> GLU154P <---> ARG150P
@> ALA74P <---> ASN53P
@> CYS148P <---> GLN144P
@> SER7P <---> ASP86P
@> LYS102P <---> ASP98P
@> MET63P <---> GLY59P
@> ASP56P <---> ILE16P
@> PHE138P <---> ASN134P
@> CYS90P <---> GLU114P
@> ASP42P <---> VAL8P
@> CYS145P <---> VAL141P
@> ARG147P <---> GLN143P
@> PHE85P <---> ASP81P
@> VAL25P <---> ILE21P
@> LEU9P <---> TYR87P
@> ASP86P <---> SER7P
@> ARG101P <---> ARG97P
@> ILE127P <---> MET91P
@> LYS112P <---> ASP86P
@> CYS12P <---> ALA44P
@> ARG75P <---> ASP42P
@> ARG18P <---> ILE127P
```

We can also all the tools that are shown for single PDB analysis in this tutorial. For example, we can compute all interactions for `frame0` and `frame18` and display the interactions:

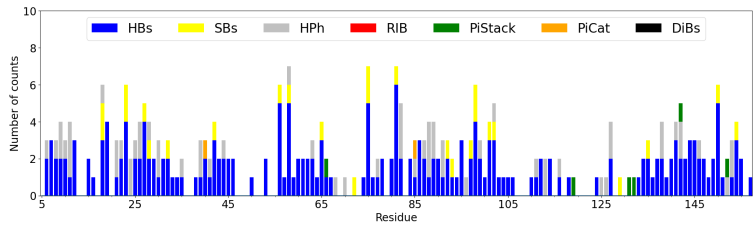
```
In [46]: interactions0 = Interactions()

In [47]: interactions0.calcProteinInteractions(at0)

In [48]: matrix0 = interactions0.buildInteractionMatrix()
```

```
In [49]: interactions0.showCumulativeInteractionTypes()
```

```
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
```




```
In [50]: interactions18 = Interactions()

In [51]: interactions18.calcProteinInteractions(at18)

In [52]: matrix18 = interactions18.buildInteractionMatrix()
```

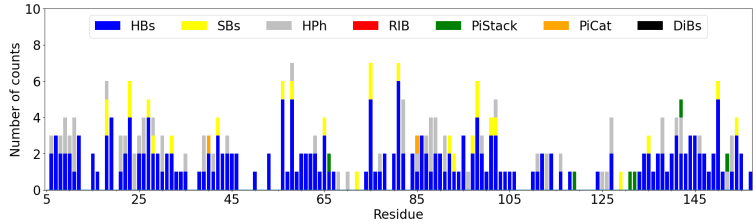
```
@> Calculating interations.
@> Calculating hydrogen bonds.
@>      DONOR (res chid atom)    <--->       ACCEPTOR (res chid atom)    Distance  Angle
@>      ARG75    P      NH2_1093  <--->      ASP81    P      OD1_1193     2.6    18.5
@>      ARG58    P       NH2_832  <--->      ASP56    P       OD2_789     2.6    21.5
@>      ARG27    P       NH2_359  <--->      GLU23    P       OE2_291     2.7    18.4
@>      LYS28    P        NZ_380  <--->      ASP32    P       OD2_444     2.7    25.9
@>     ARG150    P       NE_2300  <--->     GLU154    P      OE1_2371     2.7    22.4
@>      ARG18    P       NH1_217  <--->      ASP92    P      OD2_1369     2.7    25.9
@>      ARG75    P       NE_1087  <--->      ASP42    P       OD1_609     2.7    16.1
@>      ARG58    P        NE_826  <--->      ASP56    P       OD1_788     2.7     2.1
@>      SER19    P        OG_232  <--->      ASN15    P       OD1_165     2.7     8.1
@>      ILE88    P        N_1294  <--->     LYS112    P        O_1704     2.7     1.4
@>       VAL8    P          N_49  <--->      ARG40    P         O_584     2.7    11.5
@>      THR78    P        N_1134  <--->      ASP81    P      OD2_1194     2.7    28.1
@>     ASN134    P        N_2045  <--->     ASP137    P      OD1_2090     2.7    12.5
@>     LYS155    P       NZ_2391  <--->     HSE157    P      OT2_2424     2.7    38.9
@>     LYS112    P        N_1683  <--->      ASP86    P        O_1272     2.7    25.8
```

```
In [53]: interactions18.showCumulativeInteractionTypes()
```

```
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
@> Calculating interactions
```

6.6 Parse previously saved data

To upload and further use the interactions data use `InteractionsTrajectory.parseInteractions()` function:




```
In [54]: interactionsTrajectory2 = InteractionsTrajectory('5kqm_import')

In [55]: interactionsTrajectory2.parseInteractions('calcProteinInteractionsTrajectory.pkl')
```

```
[[[['ARG101', 'NH1_1516', 'P', 'ASP98', 'OD1_1463', 'P', 1.998, 33.1238],
   ['HSE72', 'NE2_1042', 'P', 'ASN15', 'OD1_165', 'P', 2.5997, 34.752],
   ['GLN143', 'NE2_2192', 'P', 'GLU139', 'OE2_2126', 'P', 2.7287, 9.1822],
   ['HSE66', 'NE2_957', 'P', 'GLU139', 'OE1_2125', 'P', 2.7314, 6.3592],
   ['ARG40', 'N_561', 'P', 'LYS6', 'O_37', 'P', 2.7479, 17.1499],
   ['ARG58', 'N_813', 'P', 'ASP56', 'OD1_788', 'P', 2.7499, 29.9737],
   ['ALA45', 'N_634', 'P', 'ARG75', 'O_1097', 'P', 2.7609, 35.0983],
   ['ASN53', 'ND2_747', 'P', 'GLU50', 'OE1_708', 'P', 2.7702, 18.2336],
   ['ALA74', 'N_1064', 'P', 'ASN53', 'O_751', 'P', 2.7782, 21.3375],
   ['ASP56', 'N_780', 'P', 'ILE16', 'O_189', 'P', 2.7793, 27.0481],
   ['LYS110', 'NZ_1667', 'P', 'THR84', 'O_1240', 'P', 2.7977, 38.2213],
   ['LEU116', 'N_1758', 'P', 'CYS90', 'O_1342', 'P', 2.8072, 15.0239],
   ['SER103', 'N_1546', 'P', 'LEU99', 'O_1485', 'P', 2.8075, 29.107],
   ['ASN134', 'N_2045', 'P', 'ASP137', 'OD2_2091', 'P', 2.8132, 22.562],
   ['PHE152', 'N_2321', 'P', 'CYS148', 'O_2275', 'P', 2.8141, 8.2562],
   ['ASN95', 'N_1398', 'P', 'ASP92', 'OD1_1368', 'P', 2.8148, 12.5701],
   ['LYS6', 'N_16', 'P', 'ASN38', 'O_536', 'P', 2.8178, 25.0306],
   ['ILE77', 'N_1115', 'P', 'ALA45', 'O_643', 'P', 2.8179, 12.1856],
   ['ARG58', 'NH2_832', 'P', 'ASP56', 'OD2_789', 'P', 2.8204, 27.6617],
   ['LEU99', 'N_1467', 'P', 'ASN95', 'O_1411', 'P', 2.8205, 15.4867],
   ['CYS149', 'N_2276', 'P', 'CYS145', 'O_2224', 'P', 2.8247, 9.5914],
   ['GLY52', 'N_731', 'P', 'ALA74', 'O_1073', 'P', 2.832, 6.6442],
   ['ASP32', 'N_435', 'P', 'LYS28', 'O_385', 'P', 2.8357, 8.8318],
   ..
   ..
```

After uploading, we have access to all data, for example:

```
In [56]: interactionsTrajectory2.getHydrophohic()
```

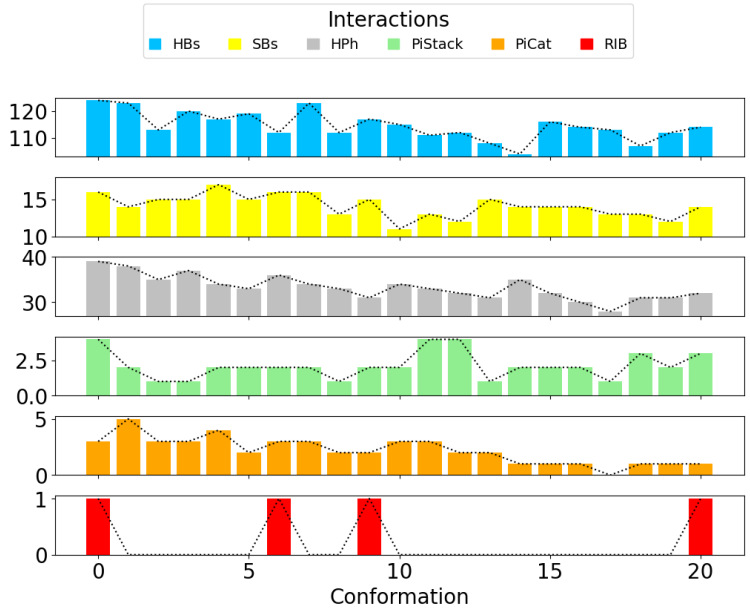
```
[[['ALA156', 'CB_2401', 'P', 'TYR87', 'OH_1286', 'P', 3.0459, 21.959],
  ['ALA24', 'CB_298', 'P', 'MET63', 'CE_894', 'P', 3.3105, 5.1584],
  ['ILE68', 'CG2_976', 'P', 'MET63', 'CE_894', 'P', 3.3306, 52.4165],
  ['TYR142', 'CZ_2171', 'P', 'VAL146', 'CG2_2235', 'P', 3.4815, 49.7427],
  ['PHE10', 'CD1_92', 'P', 'ALA22', 'CB_273', 'P', 3.5334, 31.1973],
  ['LYS6', 'CD_26', 'P', 'TRP39', 'CZ2_555', 'P', 3.5427, 68.7284],
  ['PHE26', 'CE2_336', 'P', 'VAL30', 'CG1_411', 'P', 3.5603, 21.127],
  ['ILE88', 'CD_1307', 'P', 'ALA111', 'CB_1677', 'P', 3.5627, 21.2201],
  ['VAL11', 'CG2_114', 'P', 'ILE88', 'CG2_1300', 'P', 3.6386, 9.3289],
  ['VAL41', 'CG2_595', 'P', 'PHE26', 'CD2_334', 'P', 3.6448, 16.55],
  ['PHE152', 'CE1_2331', 'P', 'ALA156', 'CB_2401', 'P', 3.6594, 17.4765],
  ['LYS79', 'CG_1155', 'P', 'VAL106', 'CG2_1598', 'P', 3.6828, 25.1359],
  ['LEU99', 'CD2_1480', 'P', 'ILE77', 'CD_1128', 'P', 3.6917, 11.9735],
  ['PHE82', 'CD1_1205', 'P', 'ILE88', 'CD_1307', 'P', 3.692, 17.6138],
  ['LEU116', 'CD2_1771', 'P', 'ILE127', 'CD_1949', 'P', 3.7057, 17.4094],
```

```
..
..
```

```
In [57]: calcStatisticsInteractions(interactionsTrajectory2.getHydrogenBonds())
```

```
@> Statistics for ARG101P-ASP98P:
@>   Average [Ang.]: 2.793931
@>   Standard deviation [Ang.]: 0.205527
@>   Weight: 1.52381
@> Statistics for HSE72P-ASN15P:
@>   Average [Ang.]: 2.989283
@>   Standard deviation [Ang.]: 0.270697
@>   Weight: 0.285714
@> Statistics for GLN143P-GLU139P:
@>   Average [Ang.]: 3.051633
@>   Standard deviation [Ang.]: 0.20753
@>   Weight: 1.285714
@> Statistics for HSE66P-GLU139P:
@>   Average [Ang.]: 2.900411
@>   Standard deviation [Ang.]: 0.169455
@>   Weight: 0.428571
@> Statistics for ARG40P-LYS6P:
@>   Average [Ang.]: 3.055475
@>   Standard deviation [Ang.]: 0.213814
@>   Weight: 0.380952
@> Statistics for ARG58P-ASP56P:
@>   Average [Ang.]: 2.827481
@>   Standard deviation [Ang.]: 0.171087
@>   Weight: 2.952381
..
..
```

```
In [58]: interactionsTrajectory2.getTimeInteractions()
```



Acknowledgments

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[15] http://www.nih.gov/
[16] http://mmbios.org/